



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2023 – 04:41 pm BST

PDB ID : 8CCQ  
Title : Crystal structure of arsenite oxidase from *Pseudorhizobium banfieldiae* str. NT-26 (NT-26 Aio) bound to antimony trioxide  
Authors : Engrola, F.; Santos-Silva, T.; Romao, M.J.; Correia, M.A.S.  
Deposited on : 2023-01-27  
Resolution : 1.89 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

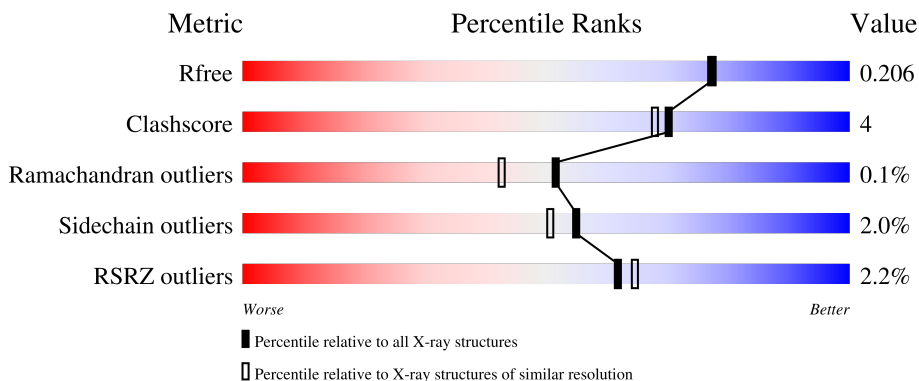
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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.



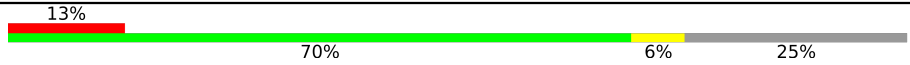

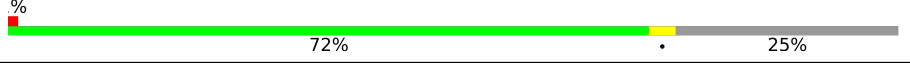
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	845	 90% 9% .
1	C	845	 92% 7% .
1	E	845	 91% 8% .
1	G	845	 90% 9% .
2	B	175	 73% 25% . 6%

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	D	175	 13% 70% 6% 25%
2	F	175	 14% 70% 6% 25%
2	H	175	 % 72% 6% 25%

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 34457 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 AroA.

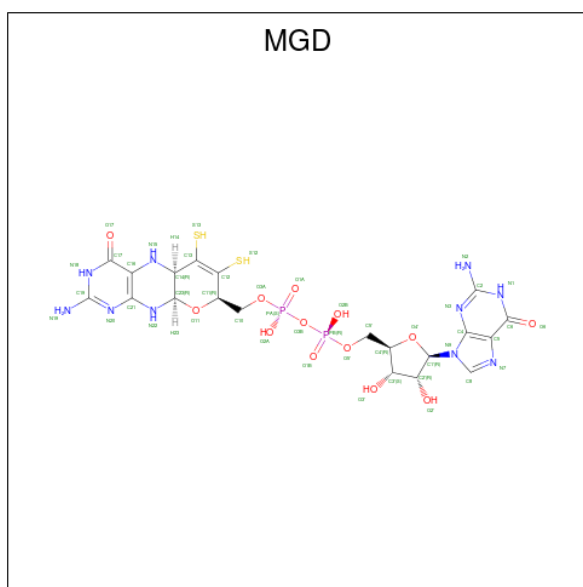
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	843	Total 6570	C 4104	N 1172	O 1257	S 37	0	4	0
1	C	843	Total 6564	C 4100	N 1171	O 1256	S 37	0	3	0
1	E	843	Total 6564	C 4100	N 1171	O 1256	S 37	0	3	0
1	G	843	Total 6559	C 4097	N 1171	O 1254	S 37	0	2	0

- Molecule 2 is a protein called AroB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	132	Total 995	C 629	N 166	O 198	S 2	0	0	0
2	D	132	Total 995	C 629	N 166	O 198	S 2	0	0	0
2	F	132	Total 995	C 629	N 166	O 198	S 2	0	0	0
2	H	132	Total 995	C 629	N 166	O 198	S 2	0	0	0

- Molecule 3 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
3	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	C	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	C	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	G	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
3	G	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 4 is OXYGEN ATOM (three-letter code: O) (formula: O) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total 2 2	0	0
4	C	2	Total 2 2	0	0
4	E	2	Total 2 2	0	0

*Continued on next page...*

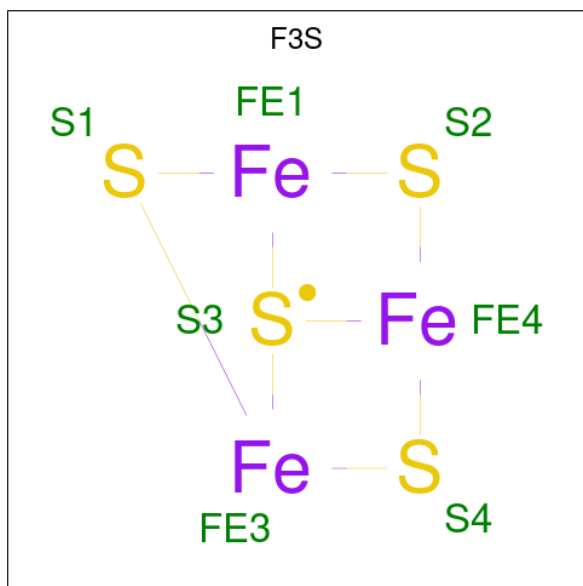
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	2	Total O 2 2	0	0

- Molecule 5 is MOLYBDENUM(IV) ION (three-letter code: 4MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mo 1 1	0	0
5	C	1	Total Mo 1 1	0	0
5	E	1	Total Mo 1 1	0	0
5	G	1	Total Mo 1 1	0	0

- Molecule 6 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



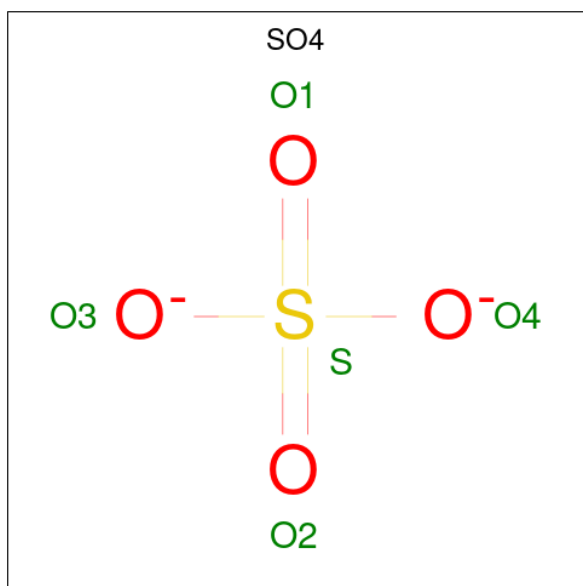
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Fe S 7 3 4	0	0
6	C	1	Total Fe S 7 3 4	0	0
6	E	1	Total Fe S 7 3 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
6	G	1	7	3	4	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



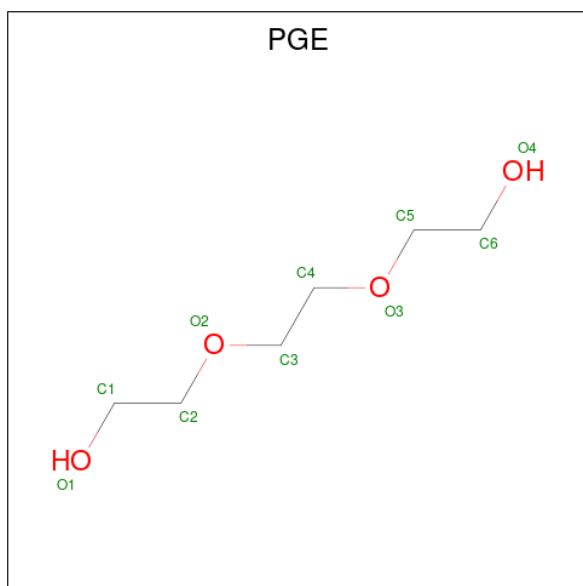
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	A	1	5	4	1	0	0
7	A	1	5	4	1	0	0
7	A	1	5	4	1	0	0
7	C	1	5	4	1	0	0
7	C	1	5	4	1	0	0
7	C	1	5	4	1	0	0
7	E	1	5	4	1	0	0
7	E	1	5	4	1	0	0
7	E	1	5	4	1	0	0
7	G	1	5	4	1	0	0

Continued on next page...

Continued from previous page...

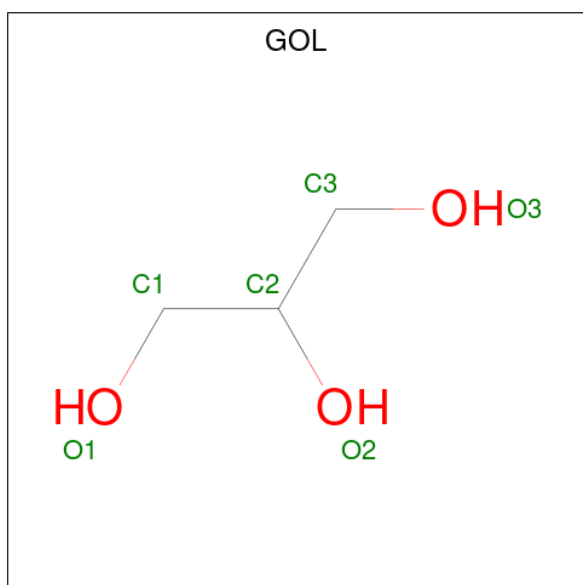
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



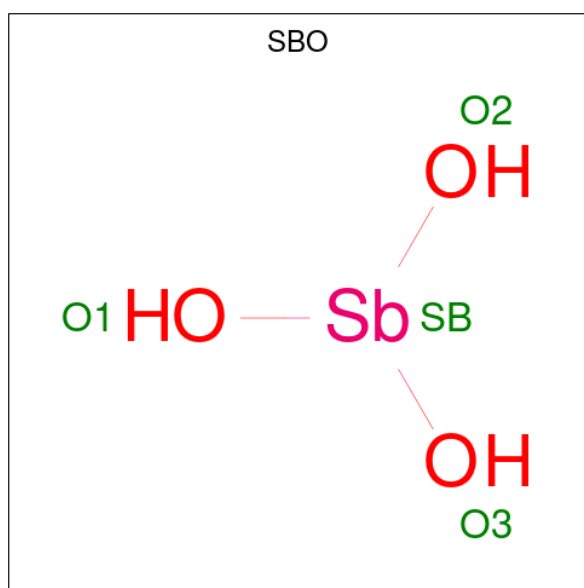
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



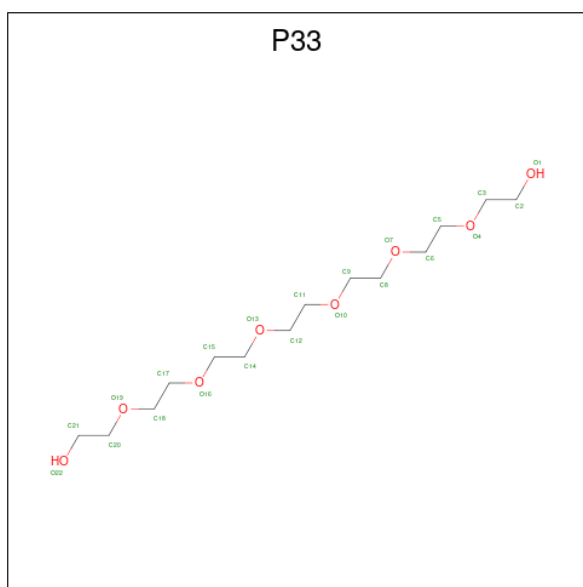
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	C	1	Total C O 6 3 3	0	0
9	E	1	Total C O 6 3 3	0	0
9	G	1	Total C O 6 3 3	0	0
9	G	1	Total C O 6 3 3	0	0

- Molecule 10 is TRIHYDROXYANTIMONITE(III) (three-letter code: SBO) (formula:  $\text{H}_3\text{O}_3\text{Sb}$ ) (labeled as "Ligand of Interest" by depositor).



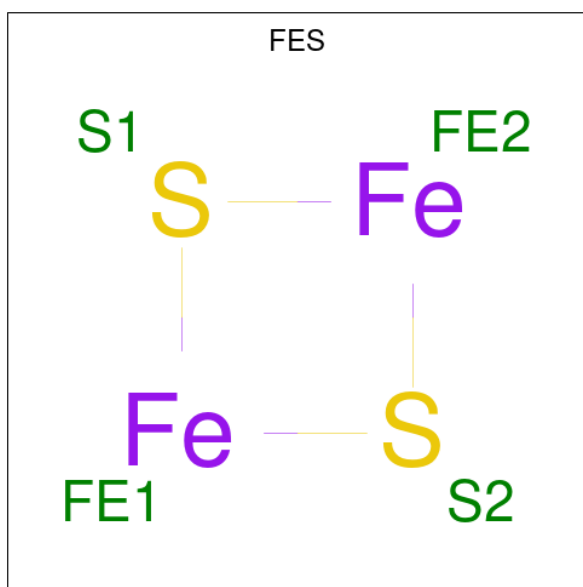
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O Sb 4 3 1	0	0
10	C	1	Total O Sb 4 3 1	0	0
10	E	1	Total O Sb 4 3 1	0	0
10	G	1	Total O Sb 4 3 1	0	0

- Molecule 11 is 3,6,9,12,15,18-HEXAOXAIICOSANE-1,20-DIOL (three-letter code: P33) (formula:  $\text{C}_{14}\text{H}_{30}\text{O}_8$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			22	14	8		
11	C	1	Total	C	O	0	0
			22	14	8		
11	E	1	Total	C	O	0	0
			22	14	8		
11	G	1	Total	C	O	0	0
			22	14	8		
11	G	1	Total	C	O	0	0
			22	14	8		

- Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	Fe	S	0	0
			4	2	2		
12	D	1	Total	Fe	S	0	0
			4	2	2		
12	F	1	Total	Fe	S	0	0
			4	2	2		
12	H	1	Total	Fe	S	0	0
			4	2	2		

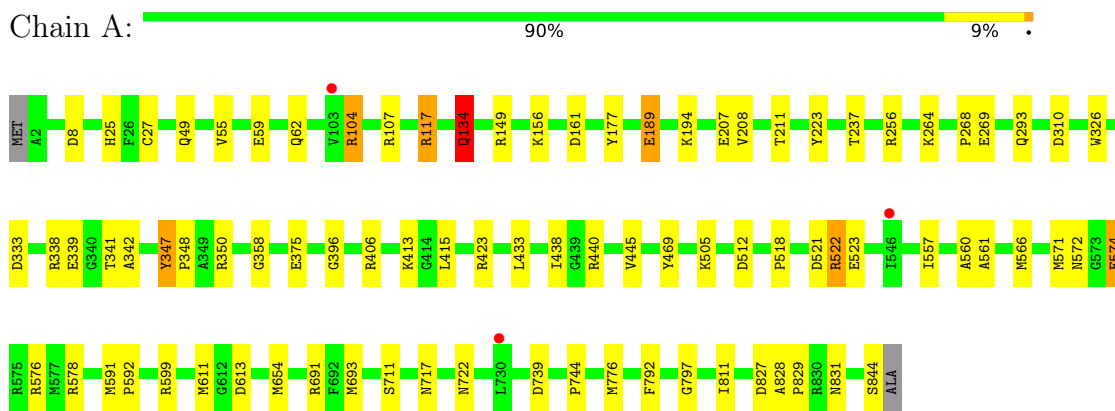
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	851	Total	O	0	0
			851	851		
13	B	111	Total	O	0	0
			111	111		
13	C	730	Total	O	0	0
			730	730		
13	D	94	Total	O	0	0
			94	94		
13	E	749	Total	O	0	0
			749	749		
13	F	86	Total	O	0	0
			86	86		
13	G	823	Total	O	0	0
			823	823		
13	H	123	Total	O	0	0
			123	123		

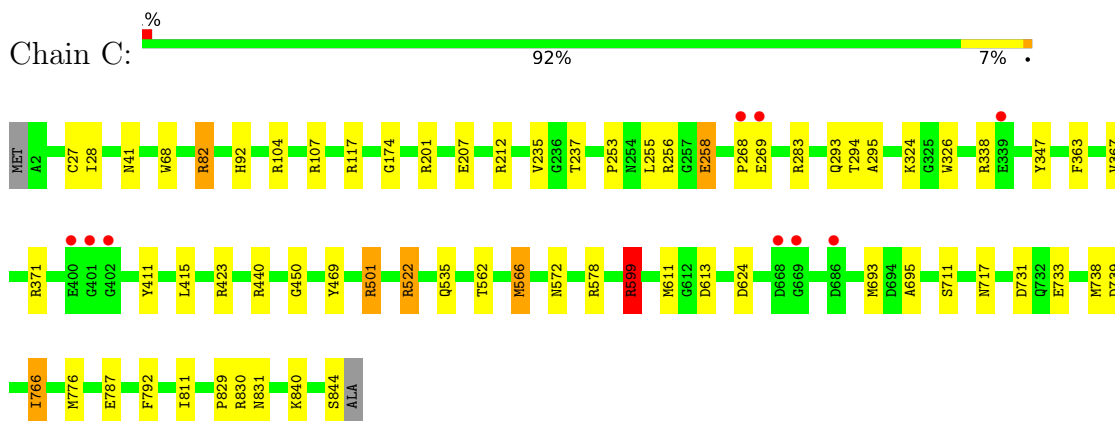
### 3 Residue-property plots [i](#)

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.

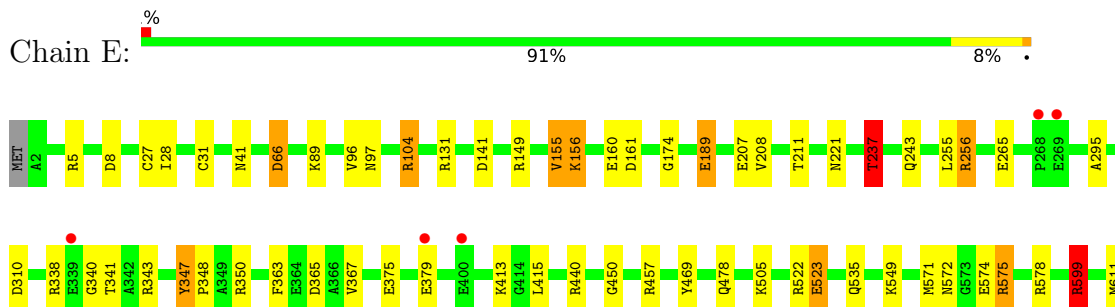
- Molecule 1: AroA



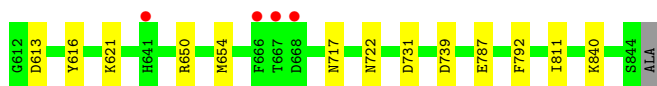
- Molecule 1: AroA



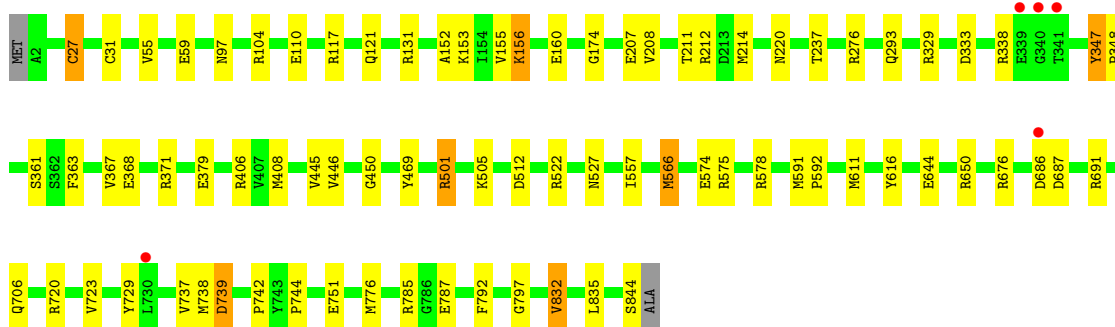
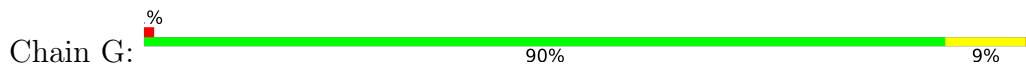
- Molecule 1: AroA



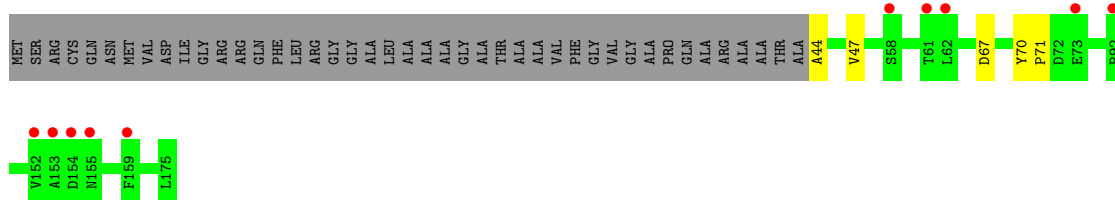
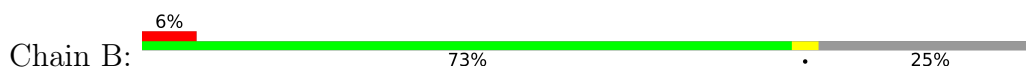




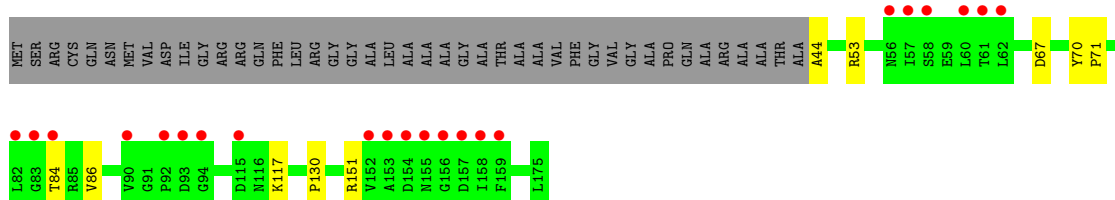
• Molecule 1: AroA



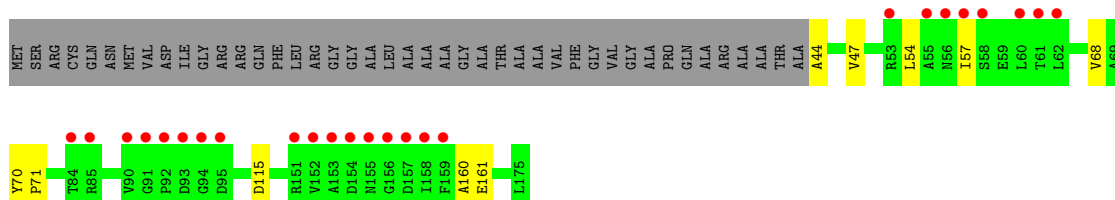
• Molecule 2: AroB




• Molecule 2: AroB

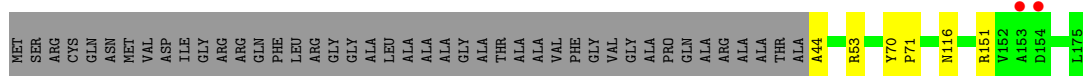


• Molecule 2: AroB



## ● Molecule 2: AroB

Chain H: 



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.53Å 148.40Å 232.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.53 – 1.89 50.01 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.8 (141.53-1.89) 99.8 (50.01-1.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.155 , 0.200 0.164 , 0.206	Depositor DCC
$R_{free}$ test set	19519 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.019 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	34457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: F3S, FES, O, P33, PGE, SBO, GOL, SO4, MGD, 4MO

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	0.97	9/6730 (0.1%)	1.02	33/9117 (0.4%)
1	C	0.94	7/6721 (0.1%)	1.05	26/9105 (0.3%)
1	E	0.95	7/6721 (0.1%)	1.02	31/9105 (0.3%)
1	G	0.95	5/6713 (0.1%)	0.98	24/9094 (0.3%)
2	B	0.85	0/1018	0.89	1/1387 (0.1%)
2	D	0.85	0/1018	0.88	3/1387 (0.2%)
2	F	0.84	0/1018	0.91	0/1387
2	H	0.81	0/1018	0.91	3/1387 (0.2%)
All	All	0.94	28/30957 (0.1%)	1.00	121/41969 (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	C	0	1

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	787	GLU	CD-OE1	10.05	1.36	1.25
1	G	787	GLU	CD-OE1	7.99	1.34	1.25
1	C	522	ARG	CZ-NH1	7.94	1.43	1.33
1	E	787	GLU	CD-OE1	7.88	1.34	1.25
1	A	739	ASP	CG-OD2	7.49	1.42	1.25

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	599	ARG	NE-CZ-NH2	-26.66	106.97	120.30
1	E	599	ARG	NE-CZ-NH2	-22.03	109.28	120.30
1	C	599	ARG	NE-CZ-NH1	19.86	130.23	120.30
1	G	104	ARG	NE-CZ-NH2	-15.90	112.35	120.30
1	A	104	ARG	NE-CZ-NH2	-15.72	112.44	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	599	ARG	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	6570	0	6329	62	0
1	C	6564	0	6321	46	0
1	E	6564	0	6321	43	0
1	G	6559	0	6317	39	1
2	B	995	0	947	5	0
2	D	995	0	947	6	0
2	F	995	0	947	9	0
2	H	995	0	947	3	0
3	A	94	0	44	2	0
3	C	94	0	44	3	0
3	E	94	0	44	4	0
3	G	94	0	44	3	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
4	G	2	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	A	7	0	0	0	0
6	C	7	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	7	0	0	0	0
6	G	7	0	0	0	0
7	A	15	0	0	0	0
7	C	15	0	0	0	0
7	E	15	0	0	0	0
7	G	10	0	0	0	0
8	A	10	0	14	1	0
9	A	6	0	8	0	0
9	C	6	0	8	0	0
9	E	6	0	8	0	0
9	G	12	0	16	1	0
10	A	4	0	0	1	0
10	C	4	0	0	1	0
10	E	4	0	0	1	0
10	G	4	0	0	1	0
11	A	22	0	30	2	0
11	C	22	0	30	3	0
11	E	22	0	30	1	0
11	G	44	0	60	3	0
12	B	4	0	0	0	0
12	D	4	0	0	0	0
12	F	4	0	0	0	0
12	H	4	0	0	0	0
13	A	851	0	0	29	0
13	B	111	0	0	3	0
13	C	730	0	0	20	1
13	D	94	0	0	3	0
13	E	749	0	0	19	0
13	F	86	0	0	6	0
13	G	823	0	0	15	2
13	H	123	0	0	2	0
All	All	34457	0	29456	216	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 216 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:C:693:MET:SD	13:C:2739:HOH:O	1.90	1.26
1:A:693:MET:SD	13:A:2828:HOH:O	1.98	1.17

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ILE:HG12	13:A:2693:HOH:O	1.46	1.14
1:C:738:MET:SD	13:C:2703:HOH:O	2.06	1.13
1:E:478:GLN:OE1	13:E:2101:HOH:O	1.83	0.94

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:2878:HOH:O	13:G:2878:HOH:O[2_545]	1.26	0.94
13:C:2353:HOH:O	13:C:2353:HOH:O[2_555]	1.39	0.81
13:G:2114:HOH:O	13:G:2114:HOH:O[2_545]	1.44	0.76
1:G:686:ASP:O	1:G:686:ASP:O[2_545]	2.18	0.02

## 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	845/845 (100%)	813 (96%)	31 (4%)	1 (0%)	51	42
1	C	844/845 (100%)	810 (96%)	33 (4%)	1 (0%)	51	42
1	E	844/845 (100%)	815 (97%)	28 (3%)	1 (0%)	51	42
1	G	843/845 (100%)	811 (96%)	32 (4%)	0	100	100
2	B	130/175 (74%)	123 (95%)	7 (5%)	0	100	100
2	D	130/175 (74%)	122 (94%)	8 (6%)	0	100	100
2	F	130/175 (74%)	120 (92%)	10 (8%)	0	100	100
2	H	130/175 (74%)	123 (95%)	7 (5%)	0	100	100
All	All	3896/4080 (96%)	3737 (96%)	156 (4%)	3 (0%)	51	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	811	ILE
1	C	811	ILE
1	A	811	ILE

### 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	681/678 (100%)	667 (98%)	14 (2%)	53	48
1	C	680/678 (100%)	669 (98%)	11 (2%)	62	60
1	E	680/678 (100%)	665 (98%)	15 (2%)	52	47
1	G	679/678 (100%)	661 (97%)	18 (3%)	44	38
2	B	105/130 (81%)	105 (100%)	0	100	100
2	D	105/130 (81%)	105 (100%)	0	100	100
2	F	105/130 (81%)	101 (96%)	4 (4%)	33	24
2	H	105/130 (81%)	105 (100%)	0	100	100
All	All	3140/3232 (97%)	3078 (98%)	62 (2%)	55	51

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	237	THR
1	G	644	GLU
1	E	505	LYS
1	G	616	TYR
1	G	792	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	E	478	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 54 ligands modelled in this entry, 12 are monoatomic - leaving 42 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
3	MGD	G	2002	5	41,52,52	1.57	6 (14%)	40,81,81	1.75	9 (22%)
7	SO4	E	2009	-	4,4,4	0.34	0	6,6,6	0.40	0
9	GOL	C	2010	-	5,5,5	1.35	0	5,5,5	0.89	0
3	MGD	G	2001	5	41,52,52	1.40	8 (19%)	40,81,81	1.63	8 (20%)
7	SO4	G	2007	-	4,4,4	0.59	0	6,6,6	0.92	0
11	P33	G	2010	-	21,21,21	0.67	0	20,20,20	1.16	2 (10%)
3	MGD	A	2002	5	41,52,52	1.51	5 (12%)	40,81,81	1.57	6 (15%)
9	GOL	G	2011	-	5,5,5	1.07	0	5,5,5	1.65	1 (20%)
7	SO4	C	2008	-	4,4,4	0.36	0	6,6,6	0.84	0
6	F3S	G	2006	1	0,9,9	-	-	-	-	-
3	MGD	E	2002	5	41,52,52	1.50	5 (12%)	40,81,81	1.64	6 (15%)
7	SO4	A	2009	-	4,4,4	0.77	0	6,6,6	0.92	0
10	SBO	G	2013	-	0,3,3	-	-	-	-	-
10	SBO	A	2012	-	0,3,3	-	-	-	-	-
10	SBO	C	2011	-	0,3,3	-	-	-	-	-
12	FES	B	201	2	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SO4	E	2007	-	4,4,4	0.39	0	6,6,6	0.61	0
7	SO4	A	2008	-	4,4,4	0.38	0	6,6,6	0.78	0
11	P33	G	2009	-	21,21,21	1.03	1 (4%)	20,20,20	1.69	6 (30%)
12	FES	D	201	2	0,4,4	-	-	-	-	-
6	F3S	E	2006	1	0,9,9	-	-	-	-	-
7	SO4	C	2009	-	4,4,4	0.45	0	6,6,6	0.53	0
8	PGE	A	2010	-	9,9,9	1.01	0	8,8,8	1.89	4 (50%)
11	P33	E	2012	-	21,21,21	0.76	0	20,20,20	1.14	1 (5%)
11	P33	C	2012	-	21,21,21	0.73	0	20,20,20	1.44	4 (20%)
7	SO4	G	2008	-	4,4,4	0.49	0	6,6,6	0.40	0
11	P33	A	2013	-	21,21,21	0.58	0	20,20,20	0.74	0
3	MGD	C	2002	5	41,52,52	1.76	9 (21%)	40,81,81	1.52	4 (10%)
3	MGD	C	2001	5	41,52,52	1.49	8 (19%)	40,81,81	1.78	9 (22%)
12	FES	F	201	2	0,4,4	-	-	-	-	-
7	SO4	A	2007	-	4,4,4	0.46	0	6,6,6	1.05	0
9	GOL	A	2011	-	5,5,5	0.71	0	5,5,5	1.47	0
3	MGD	E	2001	5	41,52,52	1.38	4 (9%)	40,81,81	1.54	7 (17%)
12	FES	H	201	2	0,4,4	-	-	-	-	-
6	F3S	A	2006	1	0,9,9	-	-	-	-	-
7	SO4	C	2007	-	4,4,4	0.73	0	6,6,6	0.93	0
10	SBO	E	2011	-	0,3,3	-	-	-	-	-
7	SO4	E	2008	-	4,4,4	0.75	0	6,6,6	1.25	1 (16%)
9	GOL	G	2012	-	5,5,5	1.33	0	5,5,5	2.46	3 (60%)
3	MGD	A	2001	5	41,52,52	1.58	4 (9%)	40,81,81	1.64	8 (20%)
9	GOL	E	2010	-	5,5,5	0.91	0	5,5,5	1.72	1 (20%)
6	F3S	C	2006	1	0,9,9	-	-	-	-	-

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
3	MGD	G	2002	5	-	4/18/66/66	0/6/6/6
9	GOL	C	2010	-	-	2/4/4/4	-
3	MGD	G	2001	5	-	4/18/66/66	0/6/6/6
11	P33	G	2010	-	-	10/19/19/19	-
3	MGD	A	2002	5	-	3/18/66/66	0/6/6/6
9	GOL	G	2011	-	-	2/4/4/4	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	F3S	G	2006	1	-	-	0/3/3/3
3	MGD	E	2002	5	-	4/18/66/66	0/6/6/6
12	FES	B	201	2	-	-	0/1/1/1
11	P33	G	2009	-	-	13/19/19/19	-
12	FES	D	201	2	-	-	0/1/1/1
6	F3S	E	2006	1	-	-	0/3/3/3
8	PGE	A	2010	-	-	5/7/7/7	-
11	P33	E	2012	-	-	10/19/19/19	-
11	P33	C	2012	-	-	11/19/19/19	-
11	P33	A	2013	-	-	5/19/19/19	-
3	MGD	C	2002	5	-	3/18/66/66	0/6/6/6
3	MGD	C	2001	5	-	5/18/66/66	0/6/6/6
12	FES	F	201	2	-	-	0/1/1/1
9	GOL	A	2011	-	-	2/4/4/4	-
3	MGD	E	2001	5	-	4/18/66/66	0/6/6/6
12	FES	H	201	2	-	-	0/1/1/1
6	F3S	A	2006	1	-	-	0/3/3/3
9	GOL	G	2012	-	-	2/4/4/4	-
3	MGD	A	2001	5	-	5/18/66/66	0/6/6/6
9	GOL	E	2010	-	-	4/4/4/4	-
6	F3S	C	2006	1	-	-	0/3/3/3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2002	MGD	C16-C21	6.46	1.49	1.38
3	G	2002	MGD	C16-C21	5.97	1.48	1.38
3	E	2001	MGD	C16-C21	5.92	1.48	1.38
3	A	2002	MGD	C16-C21	5.36	1.47	1.38
3	A	2001	MGD	C16-C21	5.32	1.47	1.38

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2002	MGD	O11-C23-N22	-6.05	102.35	108.57
3	G	2002	MGD	O11-C23-N22	-5.79	102.62	108.57
3	E	2002	MGD	O17-C17-C16	-4.65	116.58	127.24
3	G	2001	MGD	C19-N20-C21	4.55	121.64	113.43
3	C	2001	MGD	O17-C17-C16	-4.30	117.39	127.24

There are no chirality outliers.

5 of 98 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	MGD	C5'-O5'-PB-O3B
3	A	2002	MGD	C5'-O5'-PB-O3B
3	C	2001	MGD	PA-O3B-PB-O5'
3	C	2001	MGD	C5'-O5'-PB-O3B
3	C	2002	MGD	C5'-O5'-PB-O1B

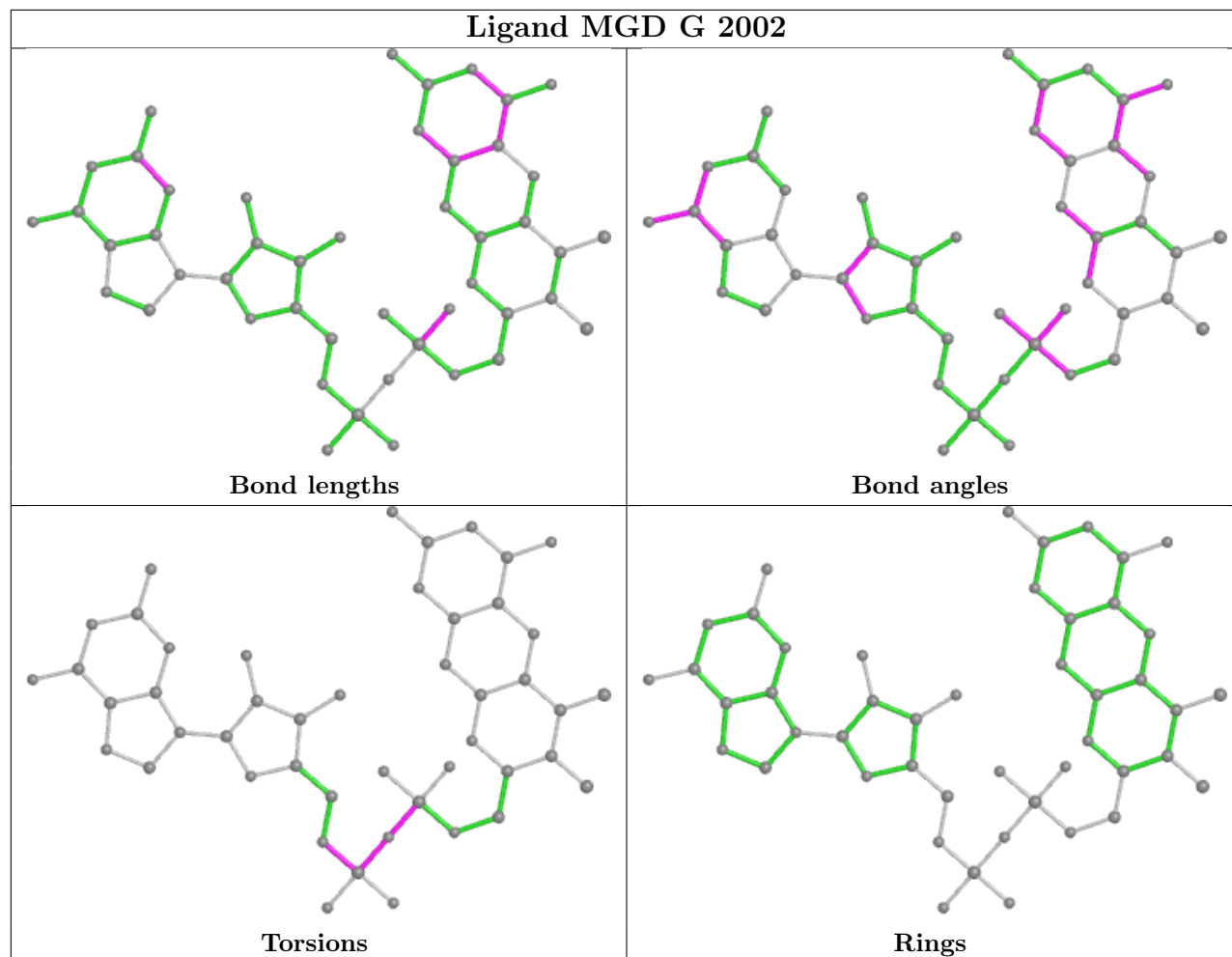
There are no ring outliers.

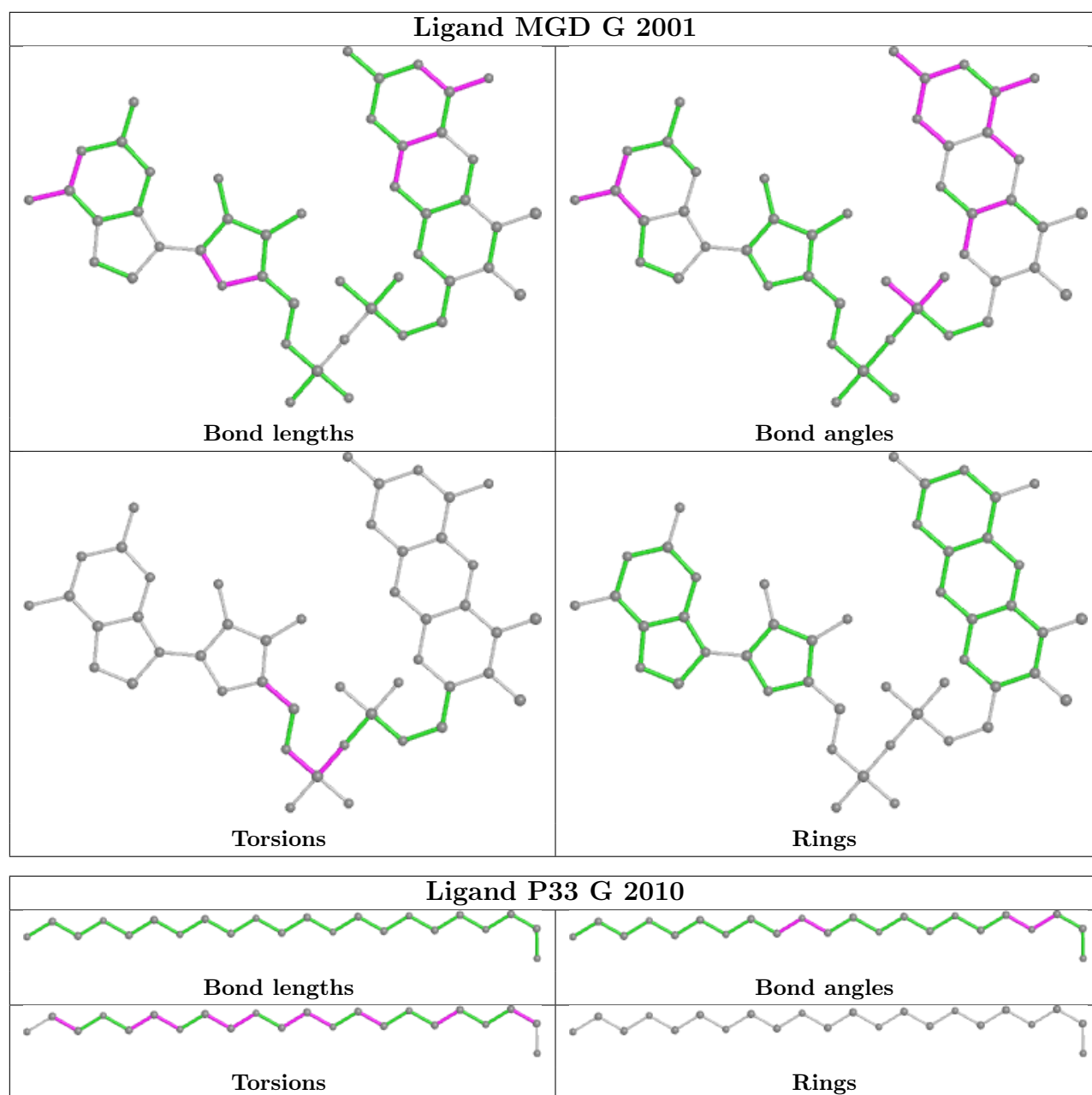
18 monomers are involved in 27 short contacts:

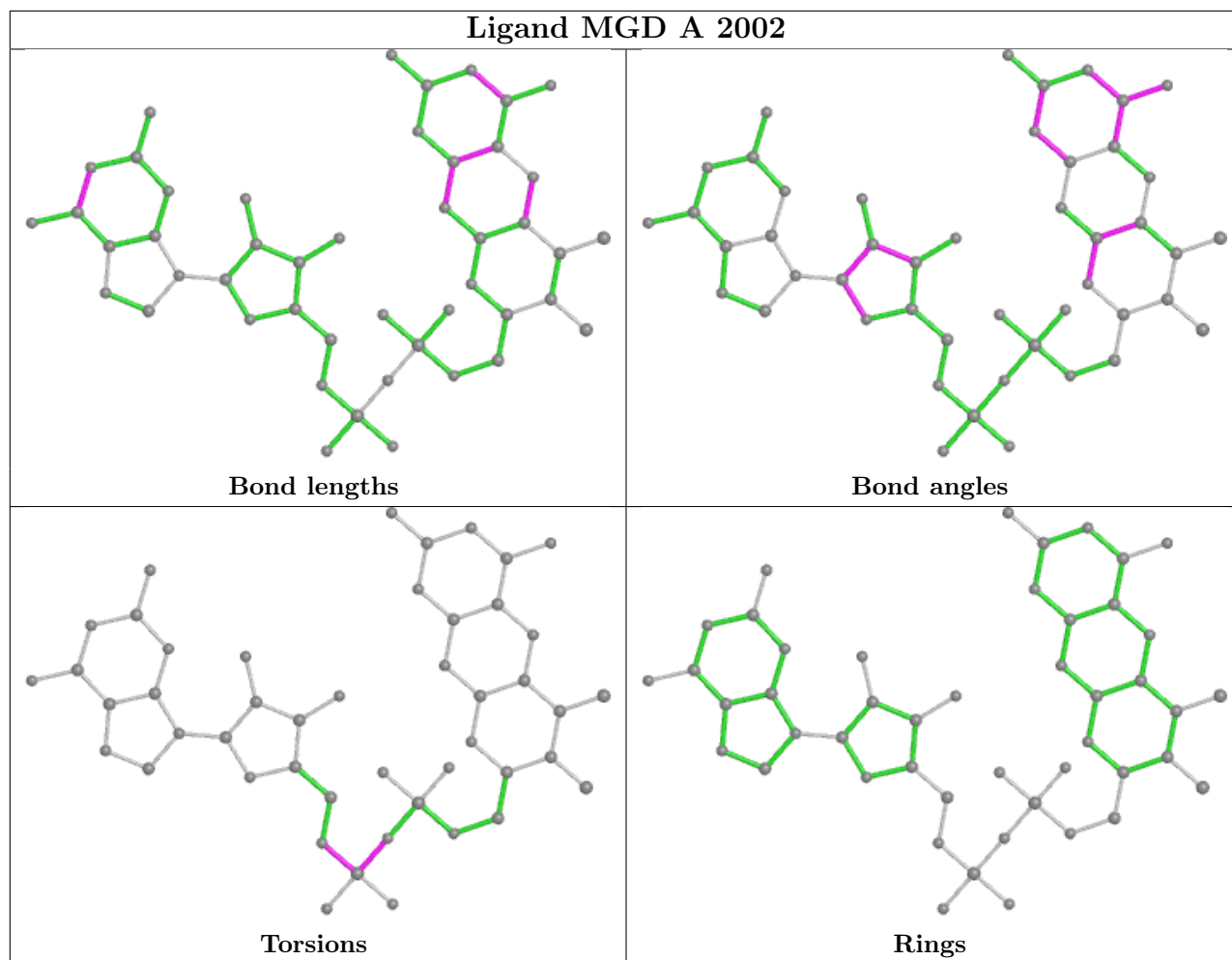
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2002	MGD	1	0
3	G	2001	MGD	2	0
3	A	2002	MGD	1	0
3	E	2002	MGD	2	0
10	G	2013	SBO	1	0
10	A	2012	SBO	1	0
10	C	2011	SBO	1	0
11	G	2009	P33	3	0
8	A	2010	PGE	1	0
11	E	2012	P33	1	0
11	C	2012	P33	3	0
11	A	2013	P33	2	0
3	C	2002	MGD	2	0
3	C	2001	MGD	1	0
3	E	2001	MGD	2	0
10	E	2011	SBO	1	0
9	G	2012	GOL	1	0
3	A	2001	MGD	1	0

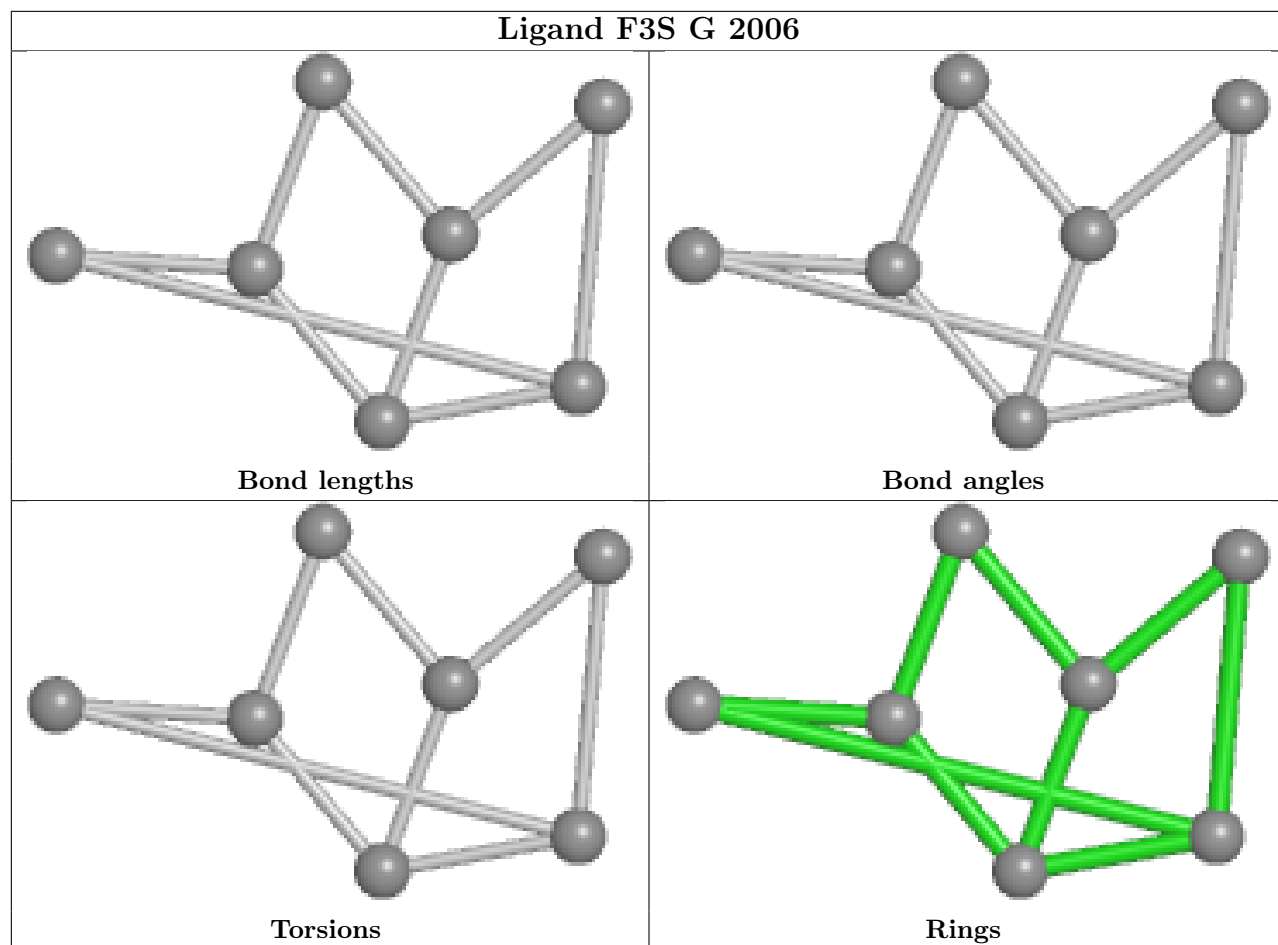
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

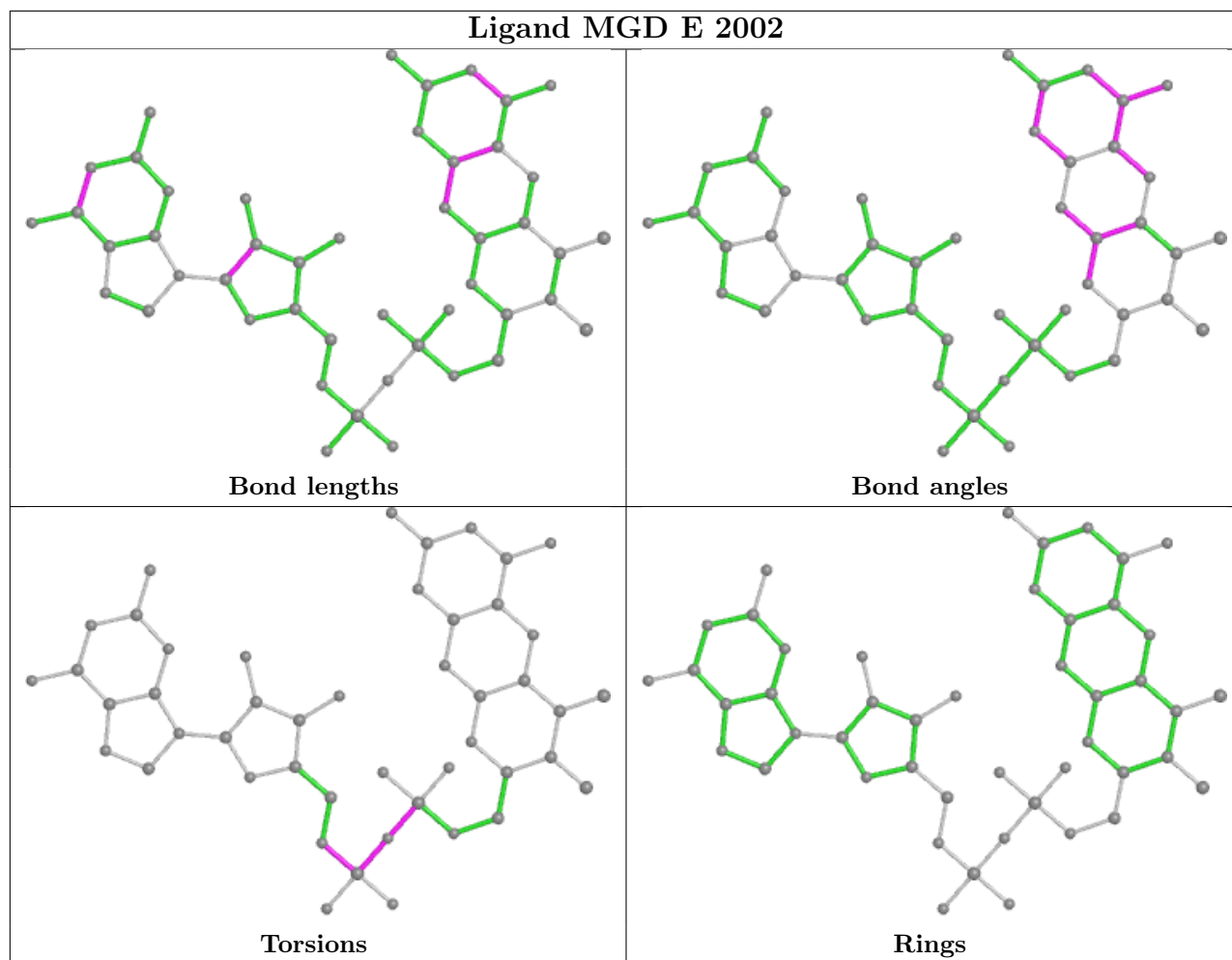


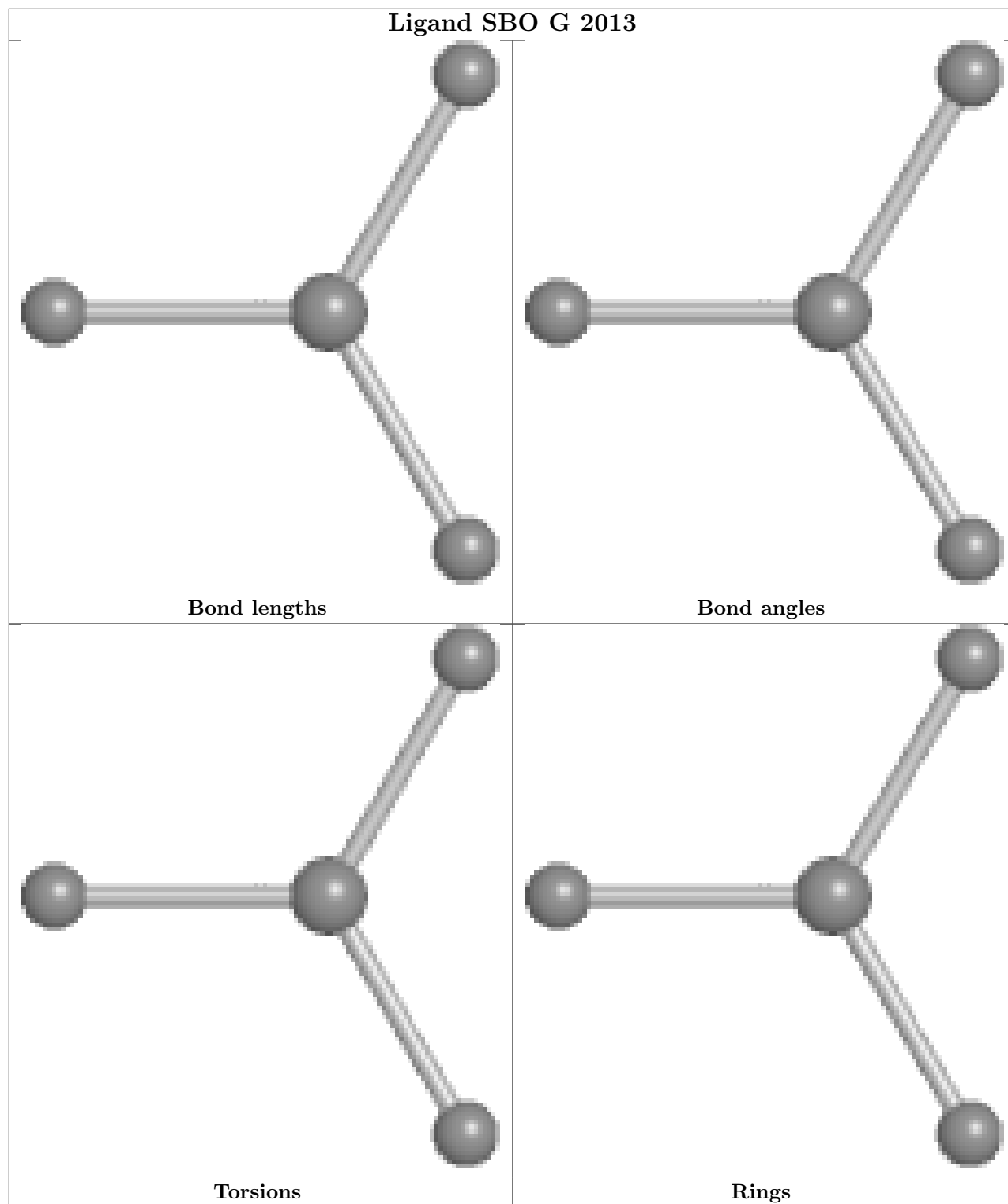


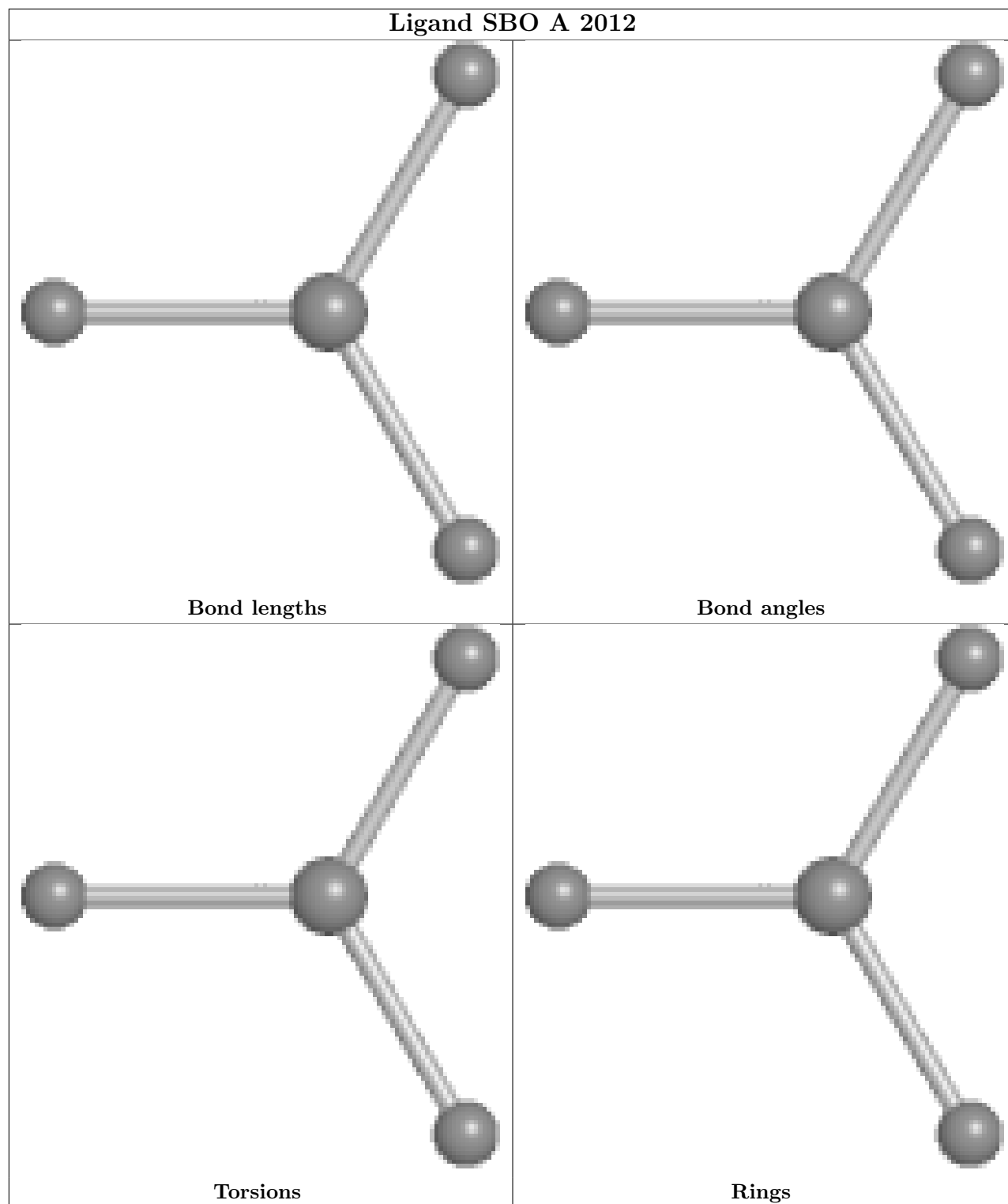


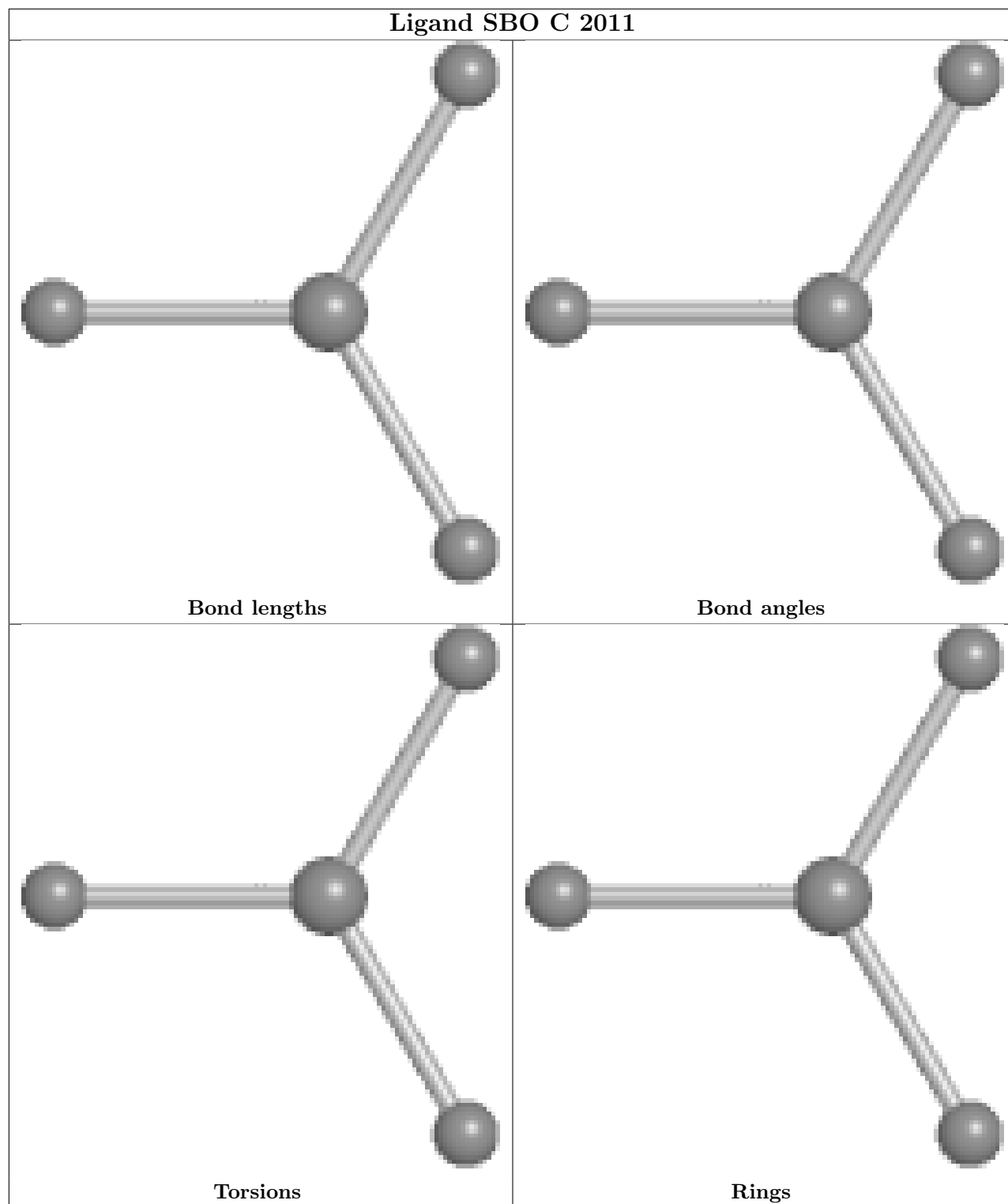


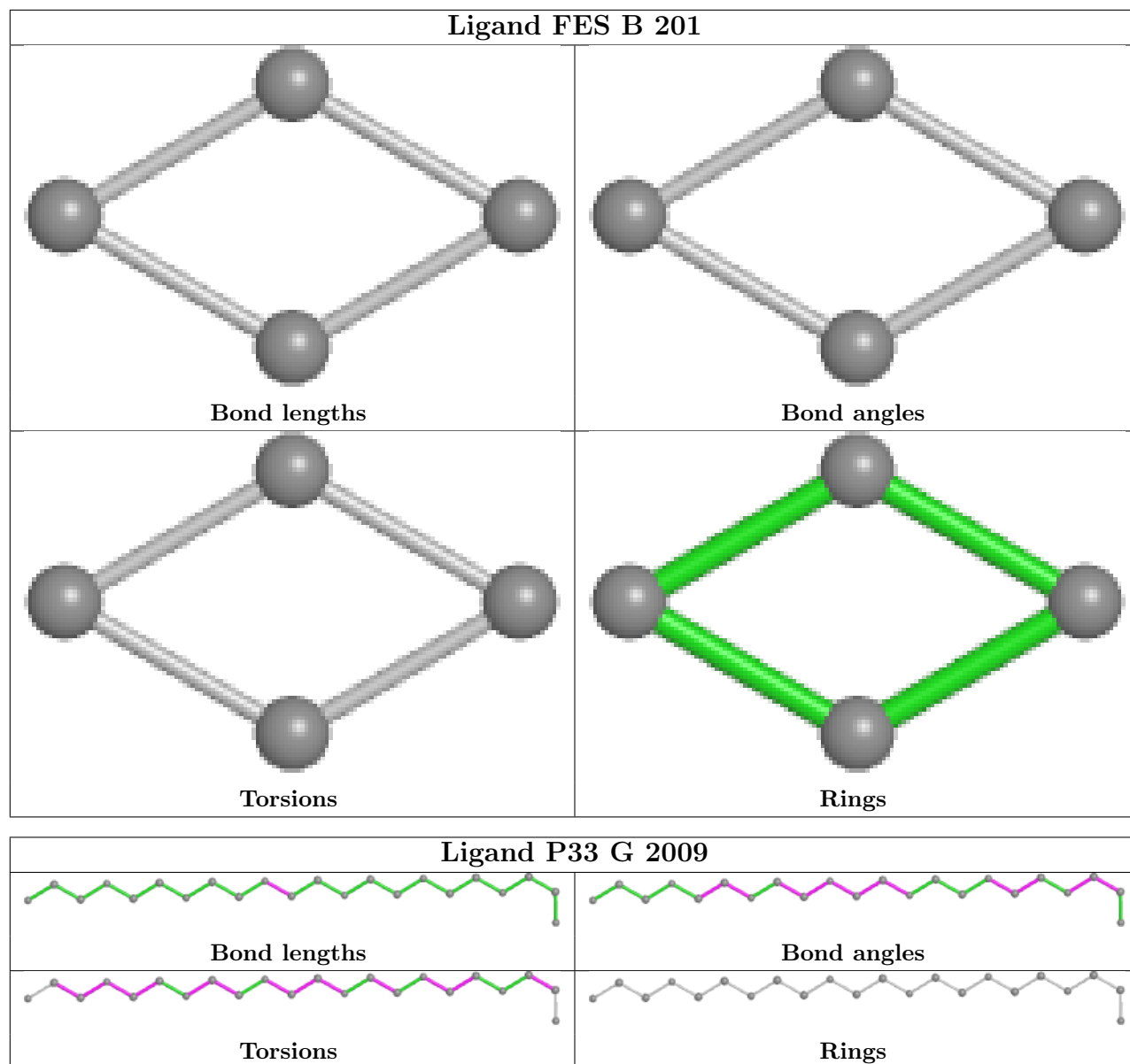


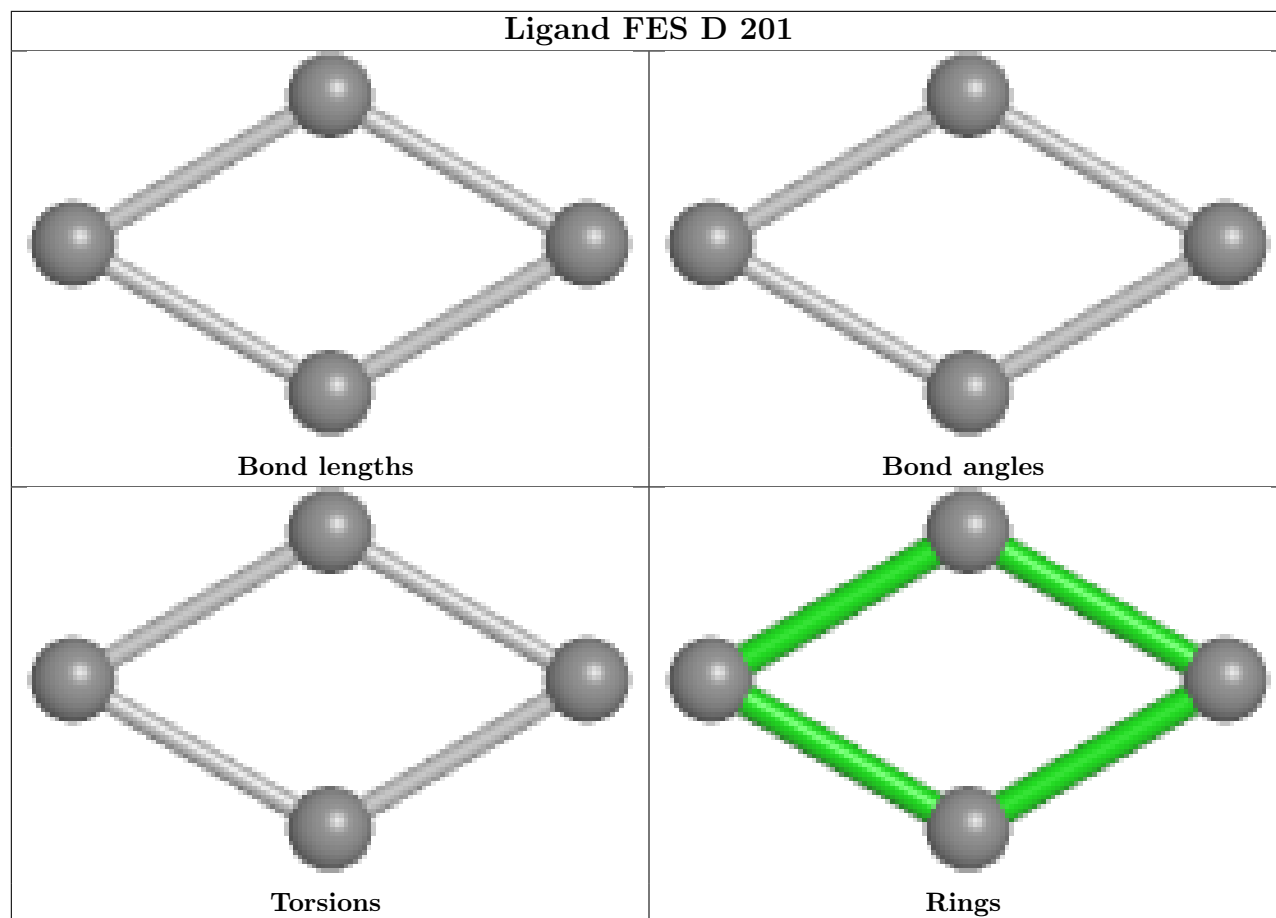


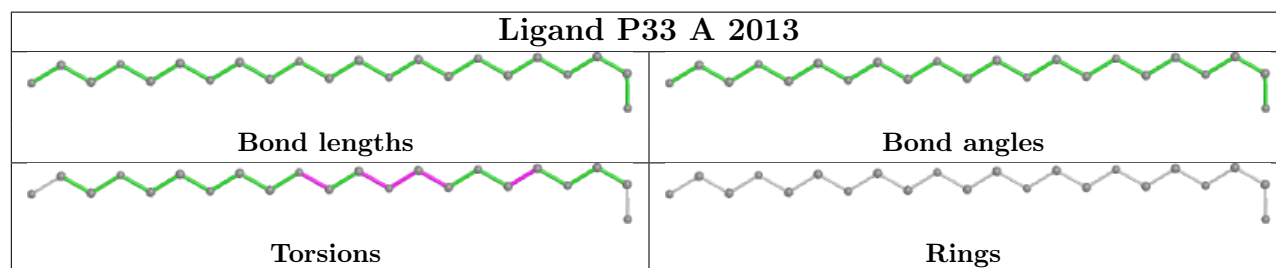
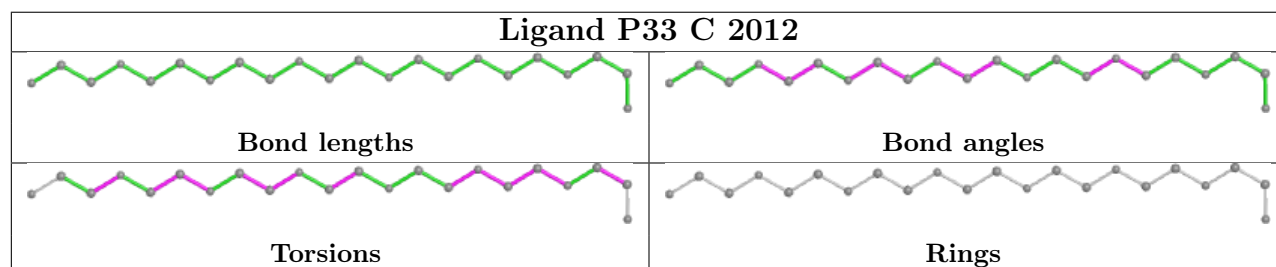
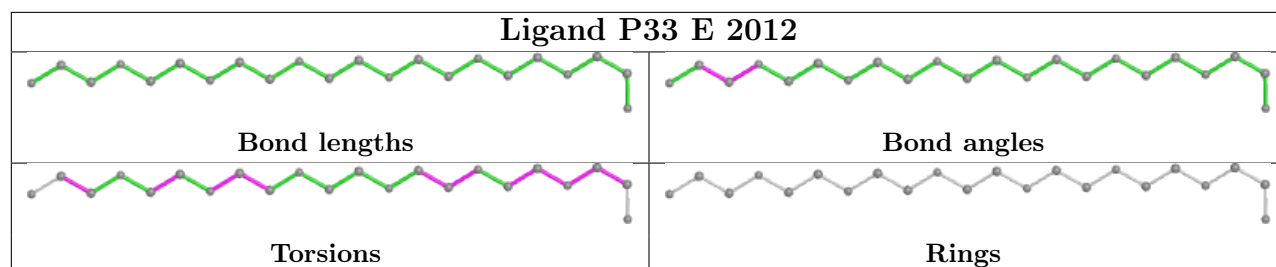
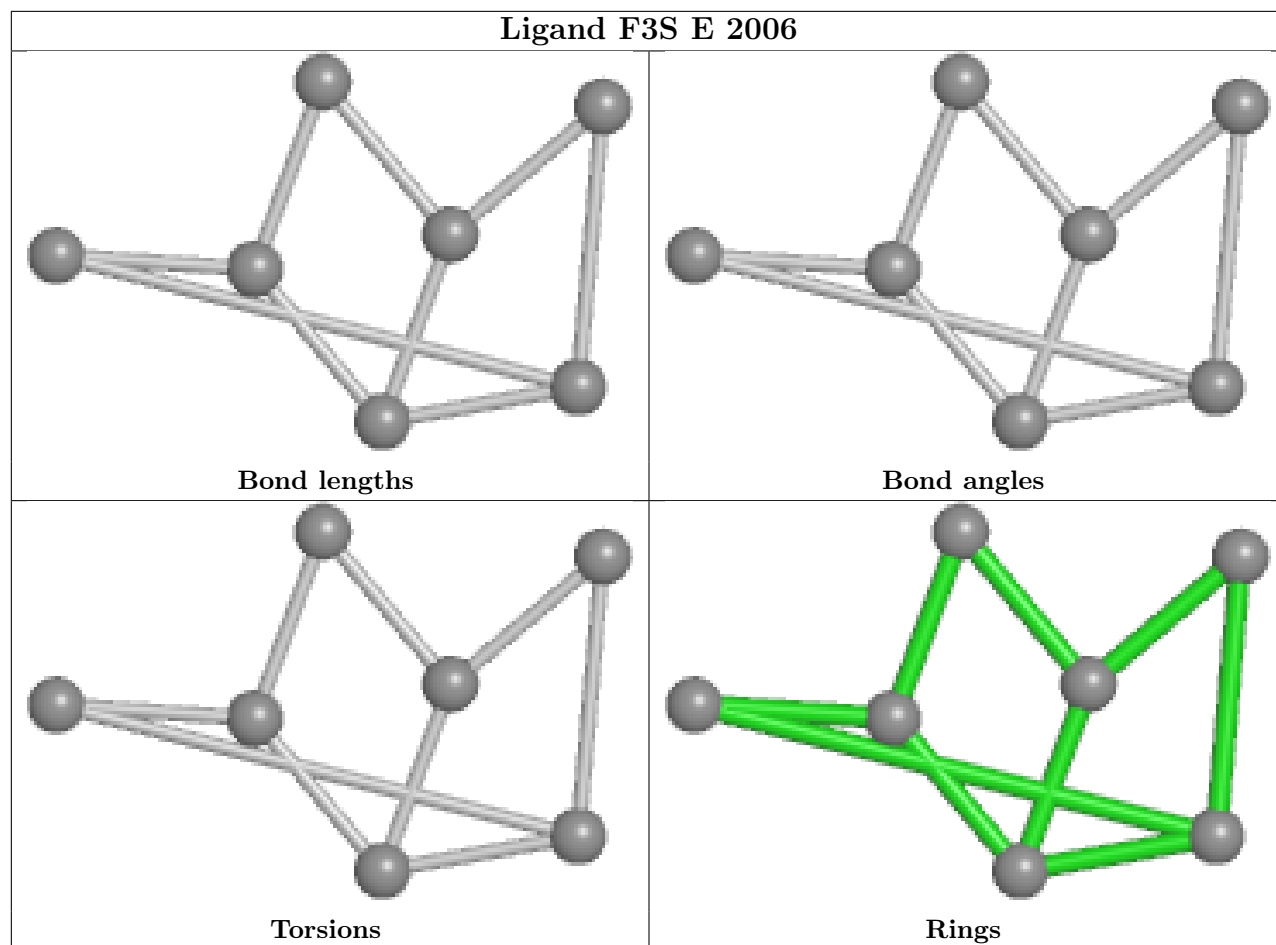


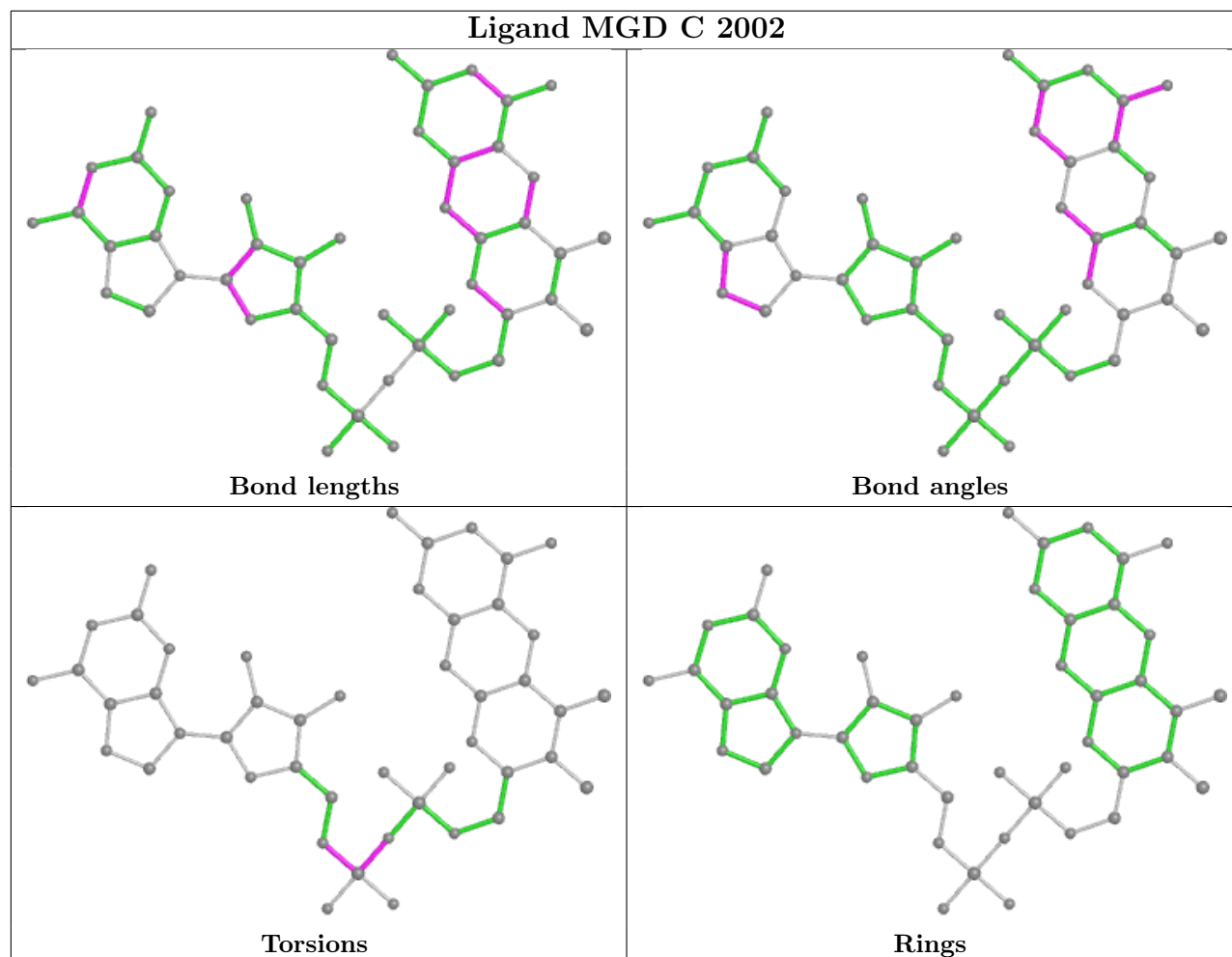




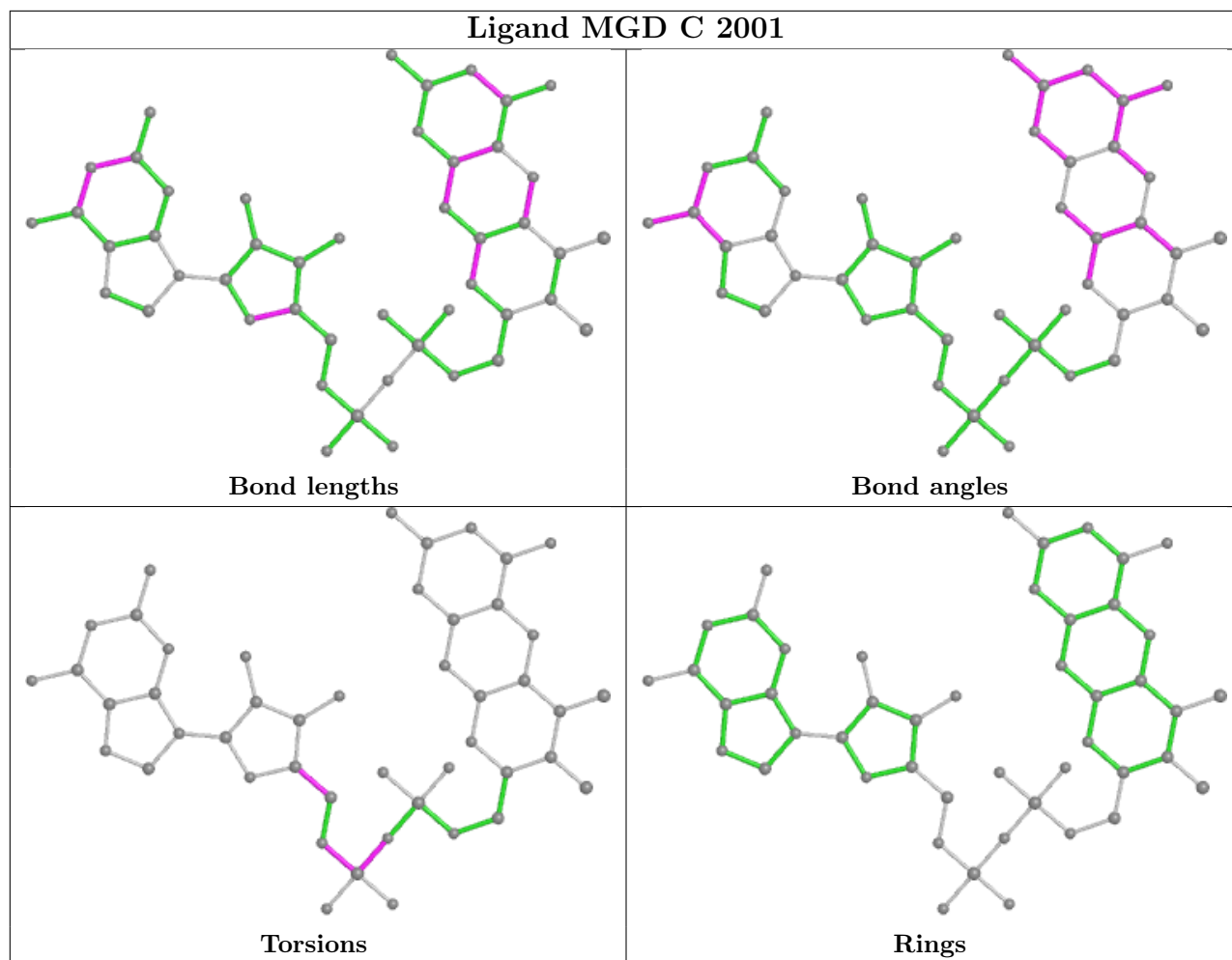


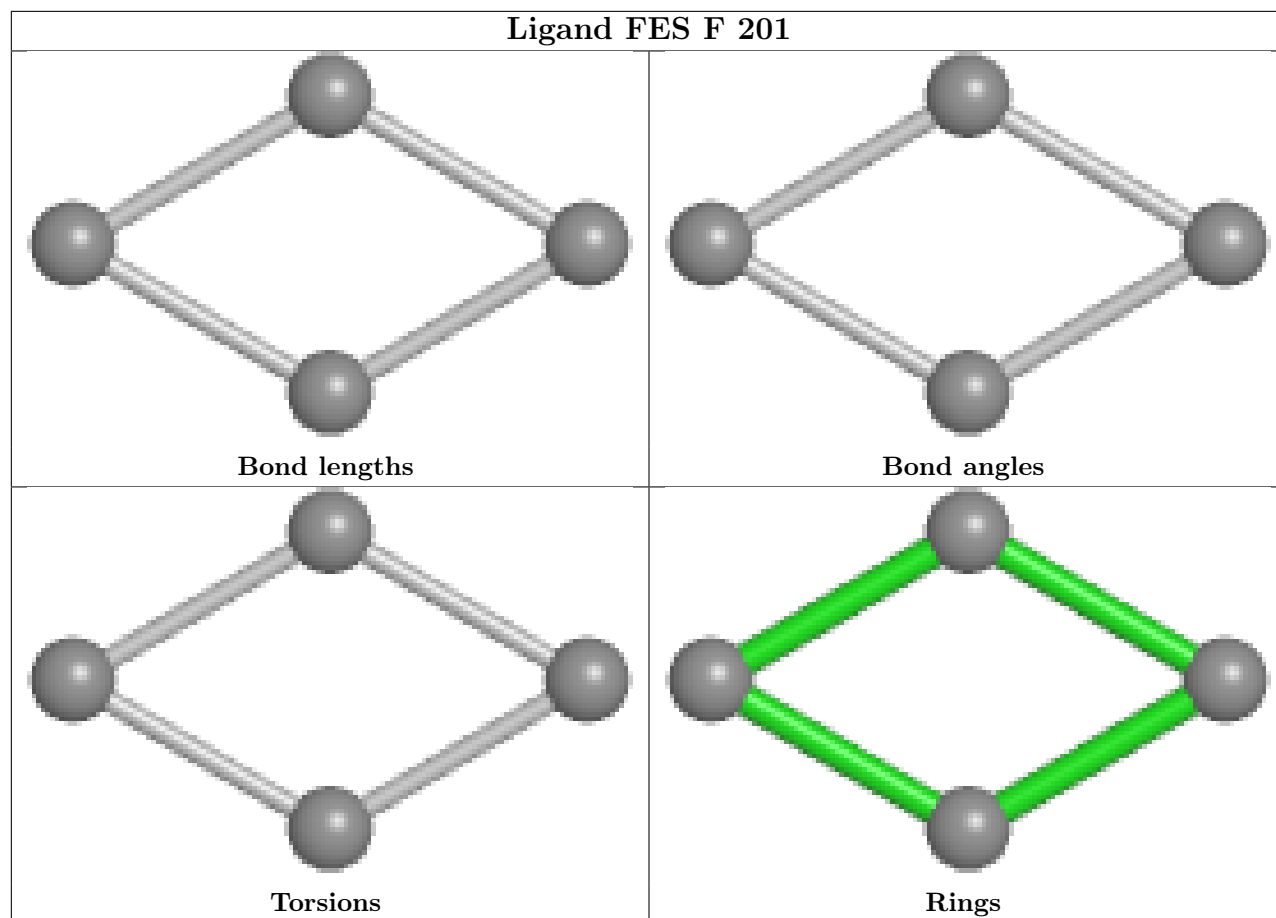


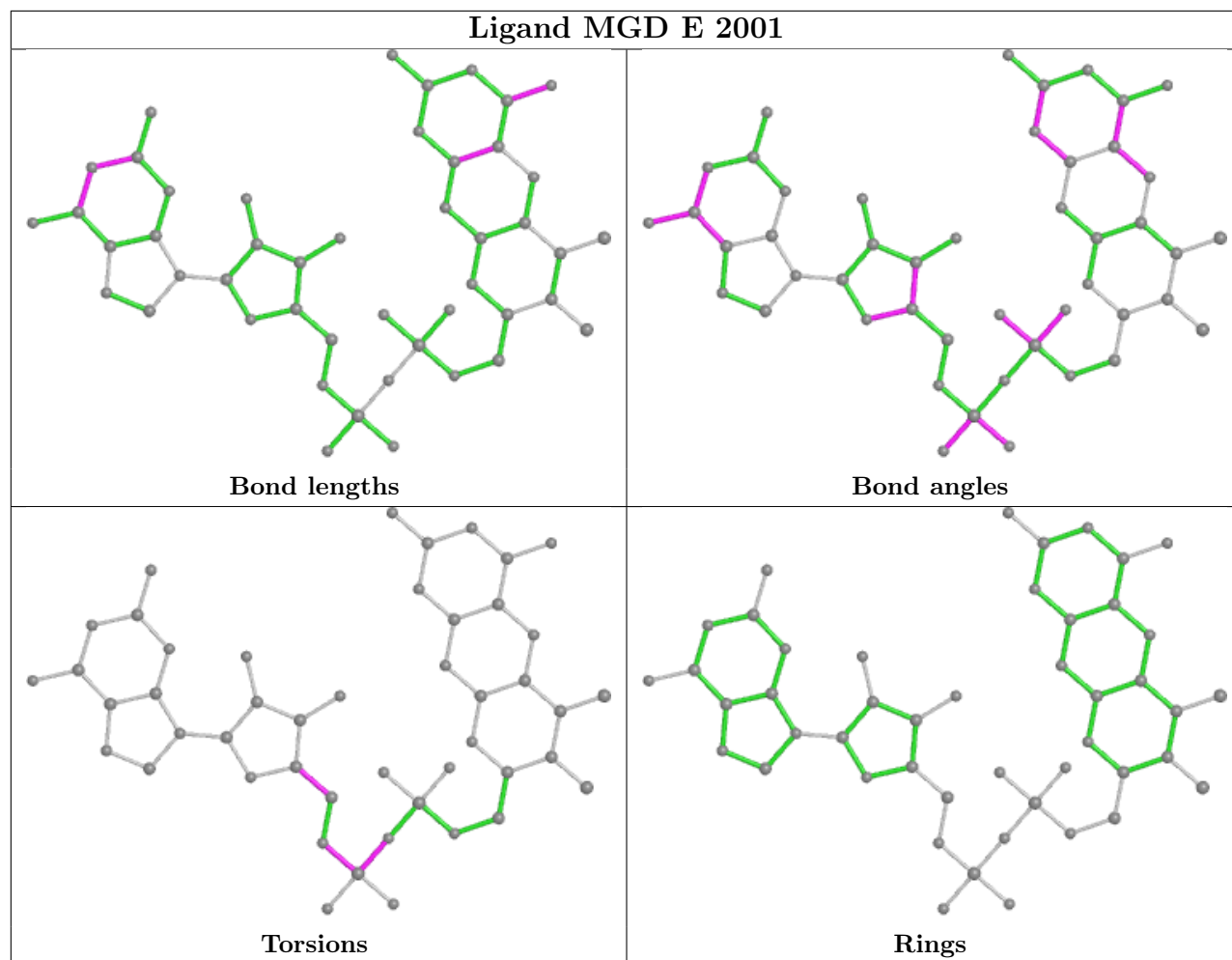


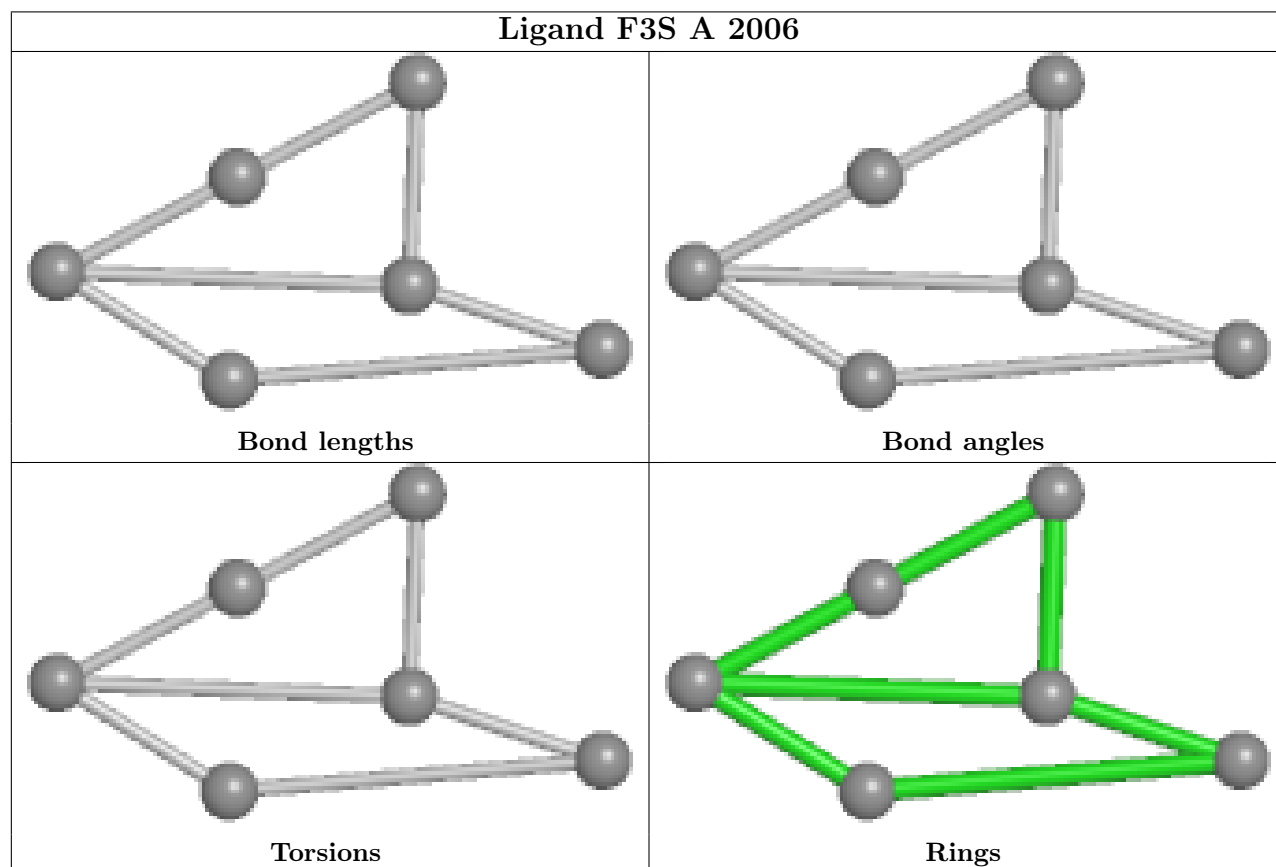
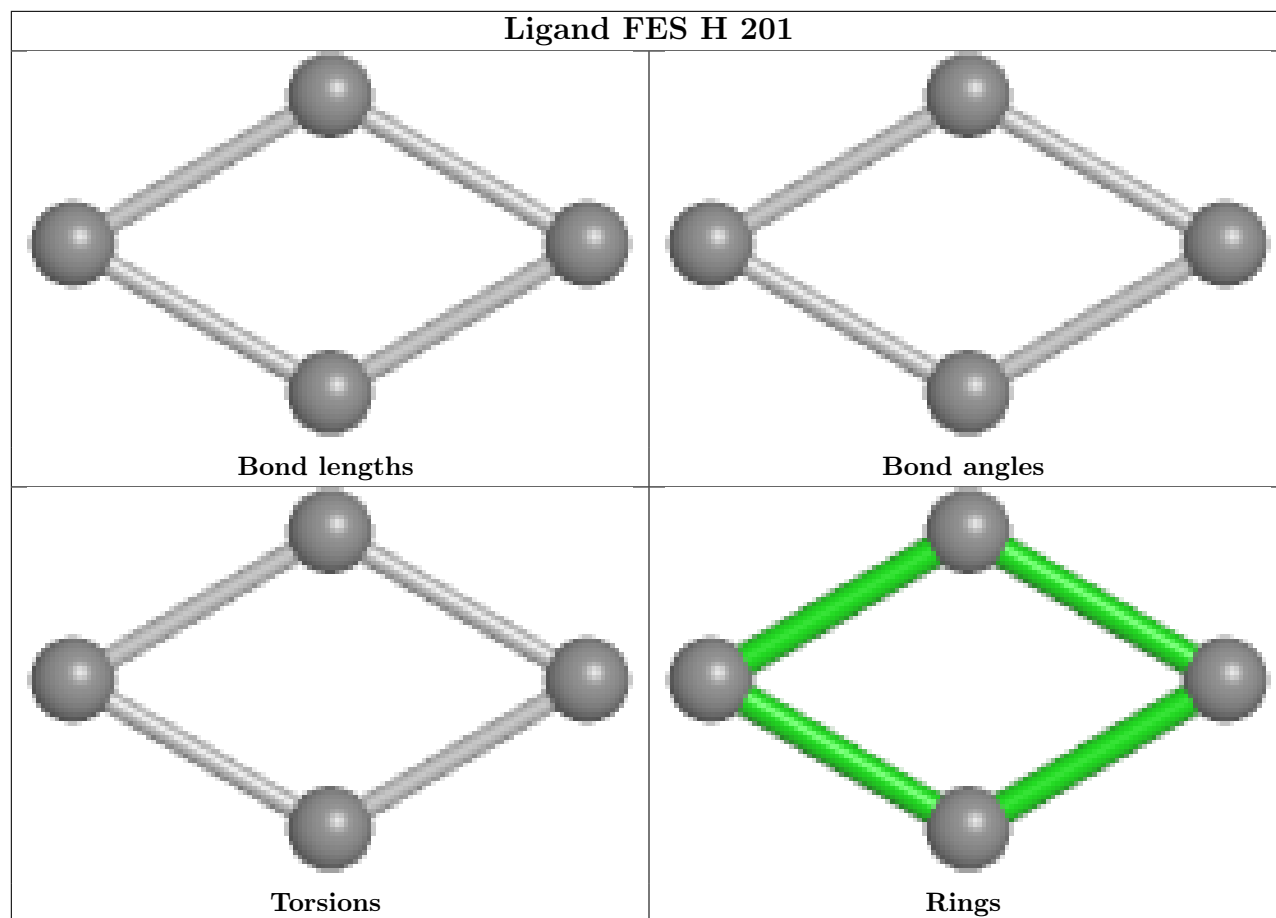


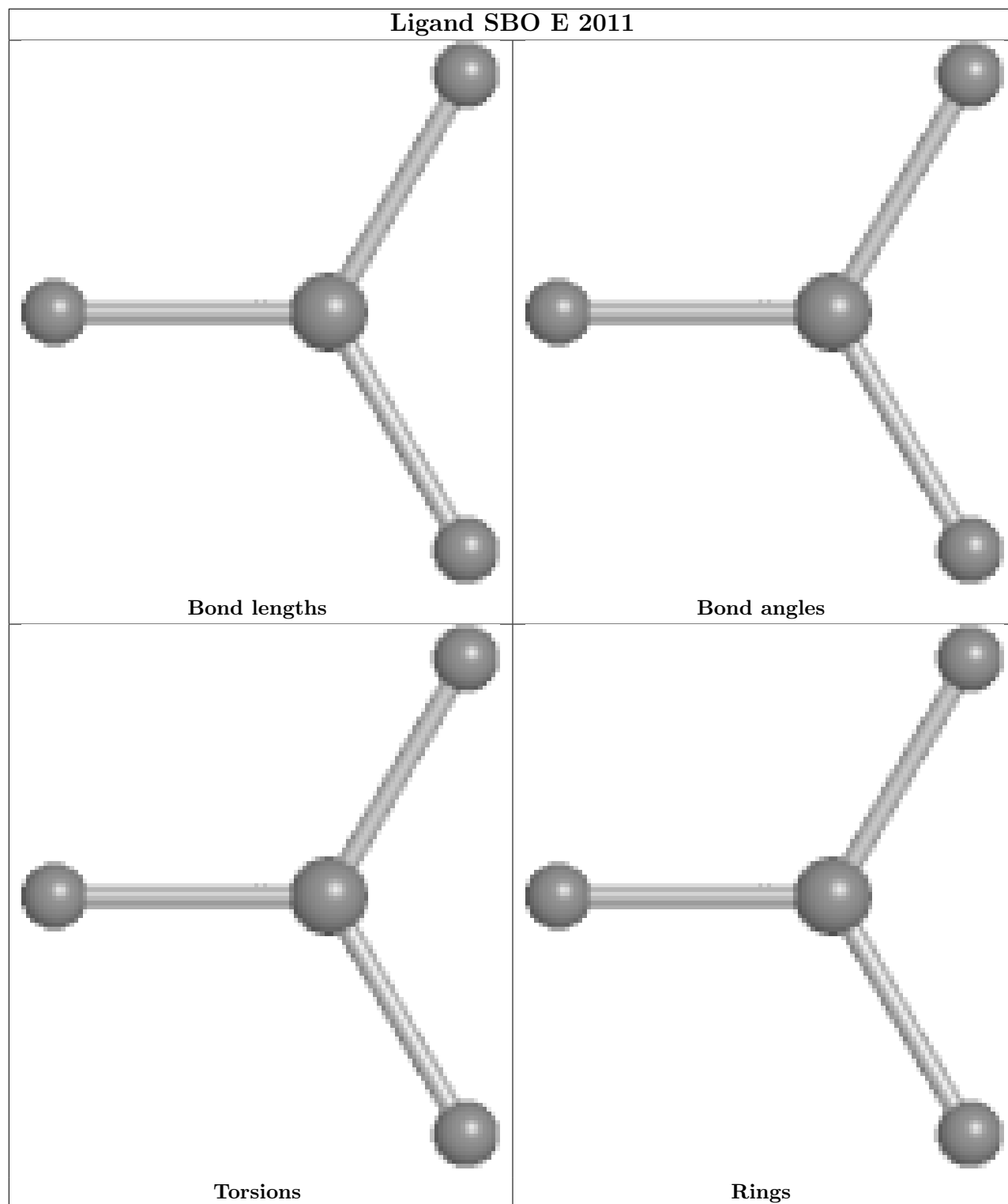


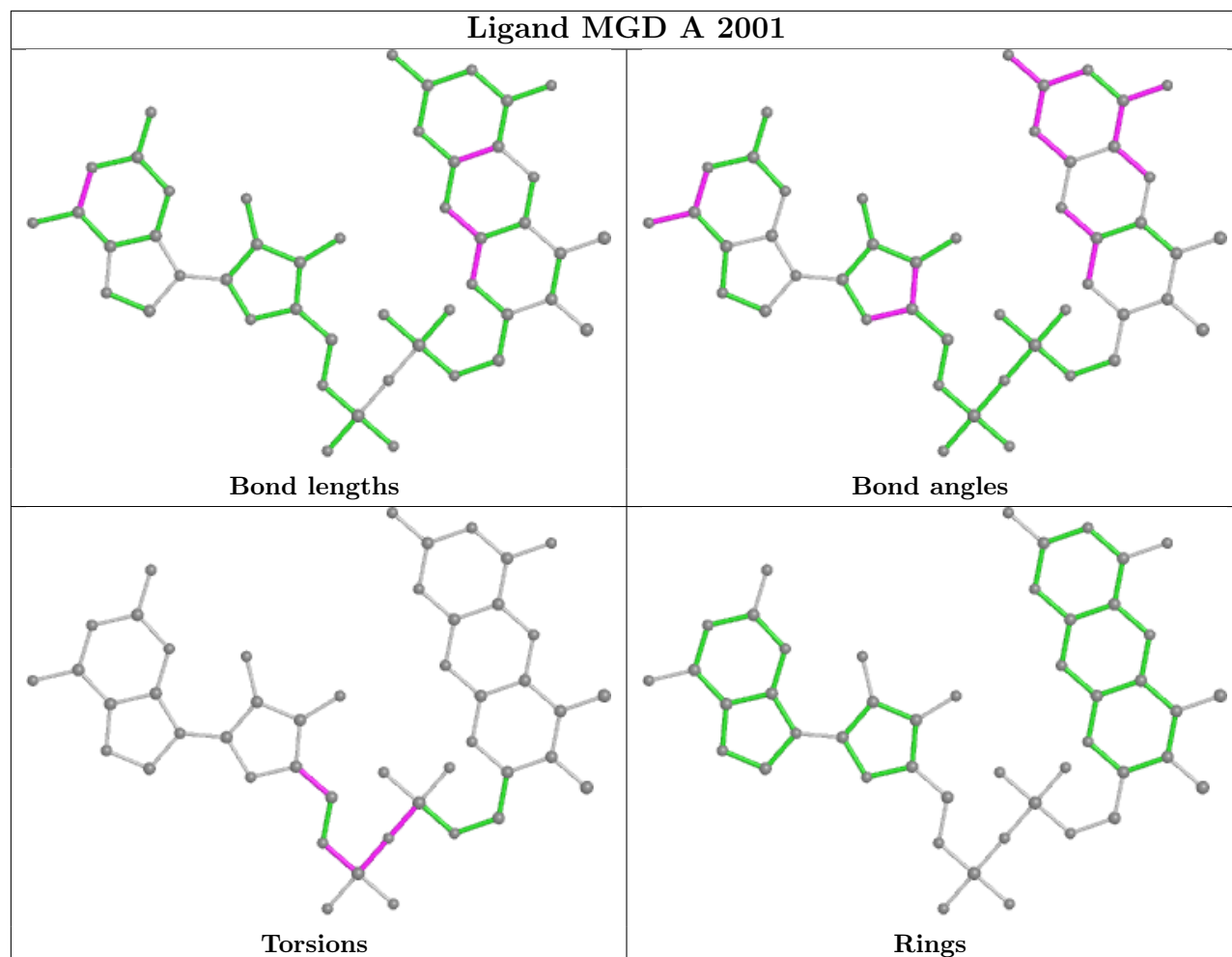


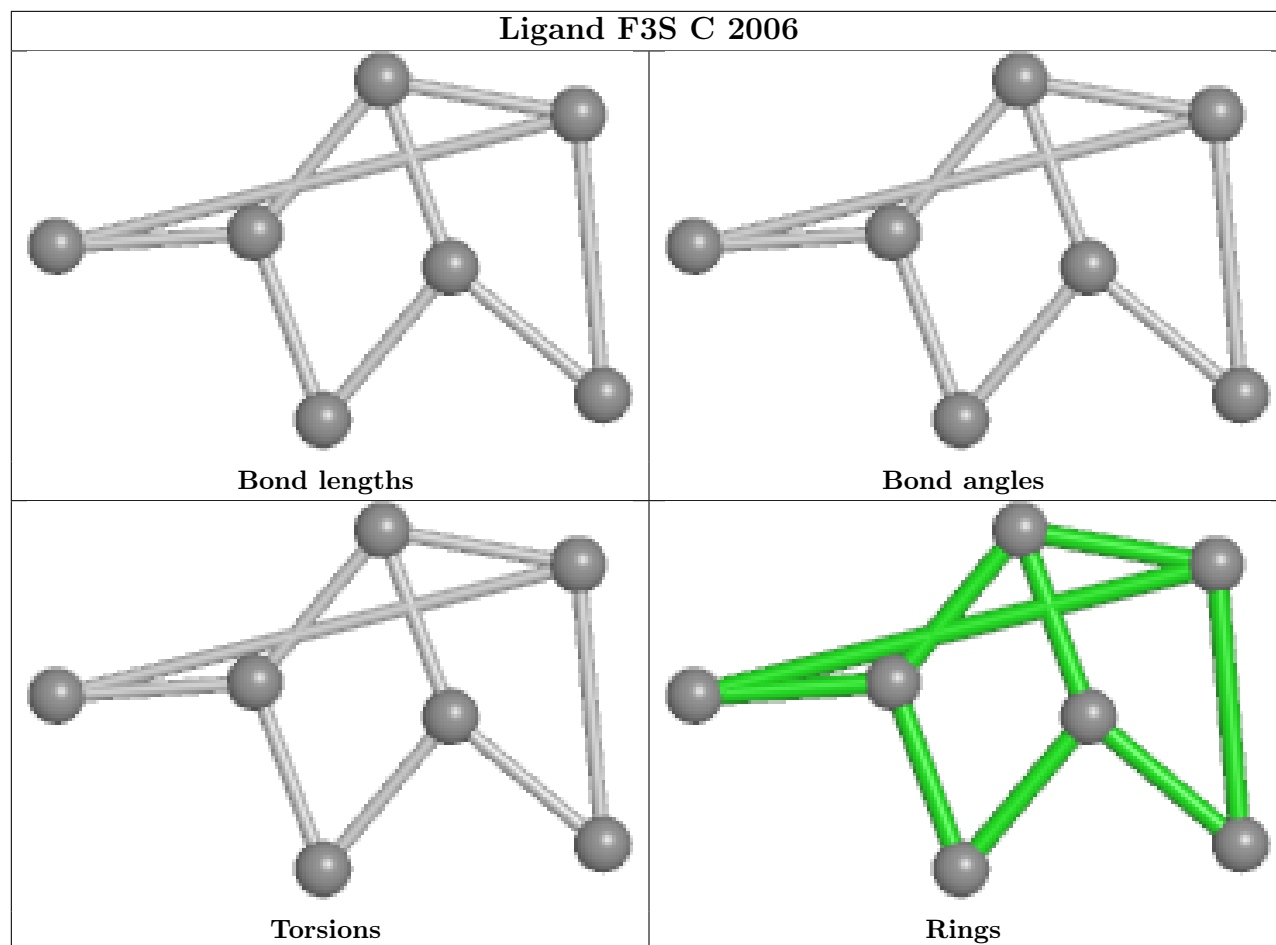












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	843/845 (99%)	-0.34	3 (0%) 92 93	14, 23, 41, 66	0
1	C	843/845 (99%)	-0.30	9 (1%) 80 82	17, 27, 45, 75	0
1	E	843/845 (99%)	-0.36	9 (1%) 80 82	16, 27, 46, 81	0
1	G	843/845 (99%)	-0.33	5 (0%) 89 90	16, 25, 42, 71	0
2	B	132/175 (75%)	0.04	10 (7%) 13 15	20, 33, 50, 67	0
2	D	132/175 (75%)	0.41	22 (16%) 1 1	23, 34, 56, 69	0
2	F	132/175 (75%)	0.56	25 (18%) 1 1	25, 38, 56, 69	0
2	H	132/175 (75%)	-0.15	2 (1%) 73 76	20, 30, 50, 65	0
All	All	3900/4080 (95%)	-0.26	85 (2%) 62 64	14, 26, 47, 81	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	57	ILE	5.7
2	F	57	ILE	5.2
1	G	340	GLY	4.8
2	D	154	ASP	4.7
2	F	154	ASP	4.7

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands i

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

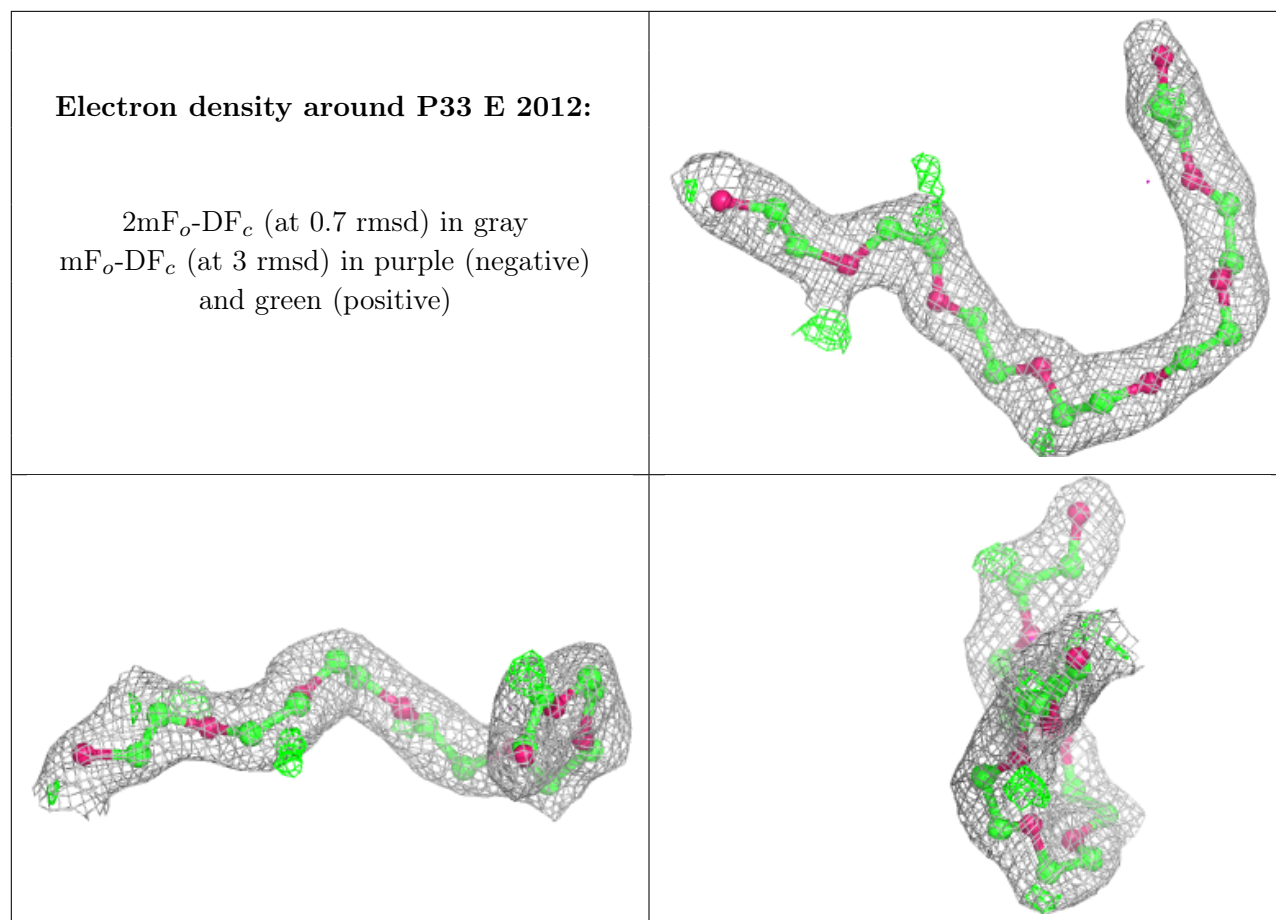
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	GOL	G	2012	6/6	0.84	0.16	34,44,48,51	0
9	GOL	C	2010	6/6	0.88	0.18	32,40,50,51	0
11	P33	E	2012	22/22	0.89	0.13	35,45,51,53	0
11	P33	A	2013	22/22	0.91	0.11	37,41,48,52	0
11	P33	C	2012	22/22	0.91	0.11	39,47,55,57	0
9	GOL	G	2011	6/6	0.91	0.21	32,42,45,48	0
11	P33	G	2009	22/22	0.91	0.16	26,37,42,47	0
7	SO4	E	2009	5/5	0.92	0.23	81,82,96,98	0
11	P33	G	2010	22/22	0.92	0.14	38,48,54,57	0
8	PGE	A	2010	10/10	0.93	0.20	32,39,43,43	0
7	SO4	C	2009	5/5	0.94	0.23	76,78,83,90	0
9	GOL	E	2010	6/6	0.94	0.19	34,43,46,59	0
9	GOL	A	2011	6/6	0.94	0.17	31,39,44,54	0
7	SO4	G	2008	5/5	0.95	0.26	70,75,83,98	0
7	SO4	C	2008	5/5	0.96	0.19	65,69,74,78	0
7	SO4	A	2007	5/5	0.96	0.12	58,59,74,74	0
7	SO4	E	2007	5/5	0.96	0.20	71,72,76,86	0
7	SO4	A	2008	5/5	0.96	0.20	57,66,74,85	0
3	MGD	G	2002	47/47	0.98	0.10	17,22,24,26	0
7	SO4	C	2007	5/5	0.98	0.07	27,29,37,43	0
7	SO4	E	2008	5/5	0.98	0.08	30,32,45,45	0
3	MGD	C	2002	47/47	0.98	0.10	19,22,26,27	0
4	O	C	2003	1/1	0.99	0.07	19,19,19,19	0
4	O	E	2004	1/1	0.99	0.08	26,26,26,26	0
7	SO4	G	2007	5/5	0.99	0.07	29,31,38,40	0
4	O	G	2004	1/1	0.99	0.08	33,33,33,33	0
6	F3S	A	2006	7/7	0.99	0.07	21,22,23,24	0
6	F3S	C	2006	7/7	0.99	0.06	23,25,26,26	0
6	F3S	E	2006	7/7	0.99	0.06	24,26,27,28	0
6	F3S	G	2006	7/7	0.99	0.07	22,23,26,26	0
3	MGD	C	2001	47/47	0.99	0.10	18,20,25,27	0
3	MGD	A	2001	47/47	0.99	0.11	14,17,21,23	0
7	SO4	A	2009	5/5	0.99	0.05	27,30,37,39	0
3	MGD	E	2001	47/47	0.99	0.08	15,20,23,29	0
3	MGD	E	2002	47/47	0.99	0.08	17,22,28,31	0
3	MGD	G	2001	47/47	0.99	0.10	17,20,25,26	0
3	MGD	A	2002	47/47	0.99	0.10	15,17,20,22	0

*Continued on next page...*

*Continued from previous page...*

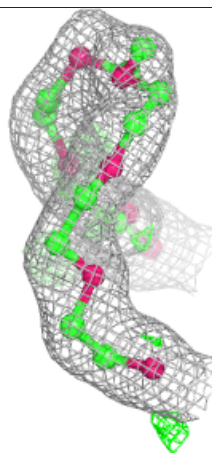
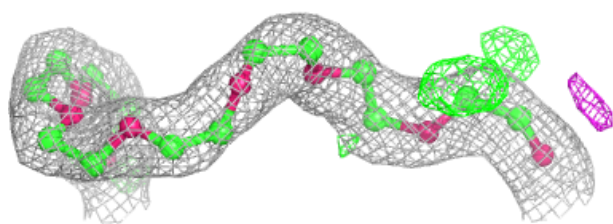
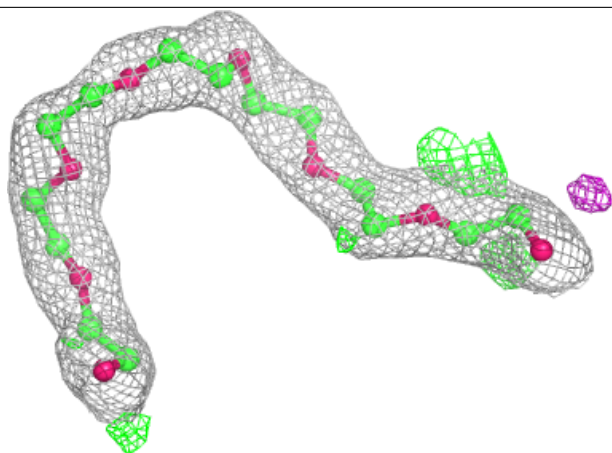
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	FES	B	201	4/4	0.99	0.05	23,24,25,25	0
12	FES	D	201	4/4	0.99	0.06	27,29,29,30	0
12	FES	F	201	4/4	0.99	0.05	28,29,30,30	0
4	O	A	2004	1/1	1.00	0.07	25,25,25,25	0
10	SBO	A	2012	4/4	1.00	0.10	22,22,24,30	4
10	SBO	C	2011	4/4	1.00	0.09	27,27,27,29	4
10	SBO	E	2011	4/4	1.00	0.08	26,26,27,29	4
10	SBO	G	2013	4/4	1.00	0.10	25,26,27,28	4
4	O	G	2003	1/1	1.00	0.10	27,27,27,27	0
4	O	A	2003	1/1	1.00	0.06	29,29,29,29	0
5	4MO	A	2005	1/1	1.00	0.05	21,21,21,21	0
5	4MO	C	2005	1/1	1.00	0.04	24,24,24,24	0
5	4MO	E	2005	1/1	1.00	0.04	25,25,25,25	0
5	4MO	G	2005	1/1	1.00	0.04	22,22,22,22	0
4	O	C	2004	1/1	1.00	0.05	25,25,25,25	0
4	O	E	2003	1/1	1.00	0.05	28,28,28,28	0
12	FES	H	201	4/4	1.00	0.05	24,25,26,27	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.

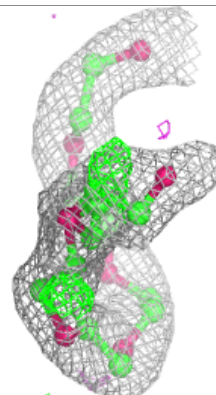
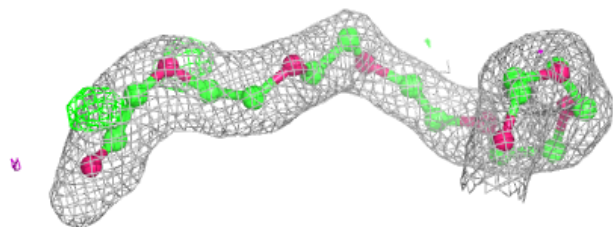
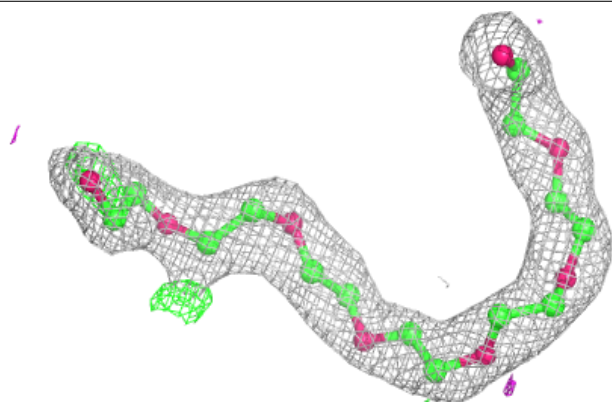


**Electron density around P33 A 2013:**

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

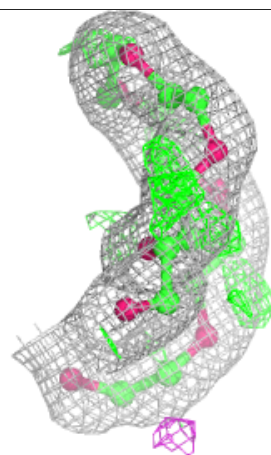
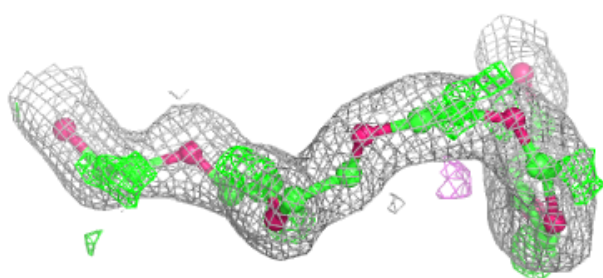
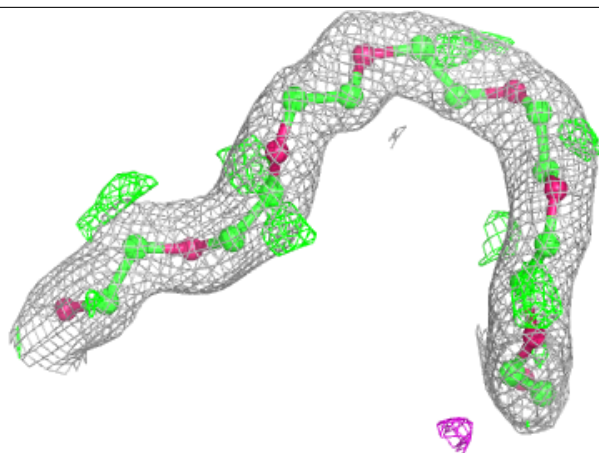
**Electron density around P33 C 2012:**

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

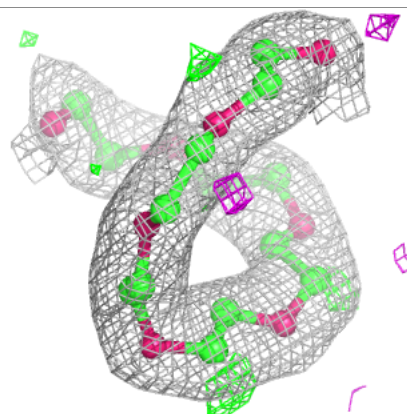
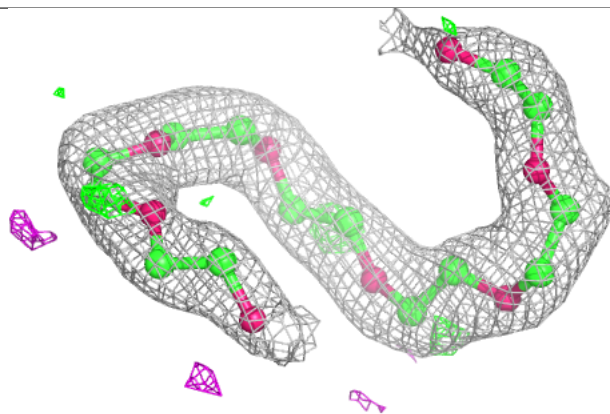
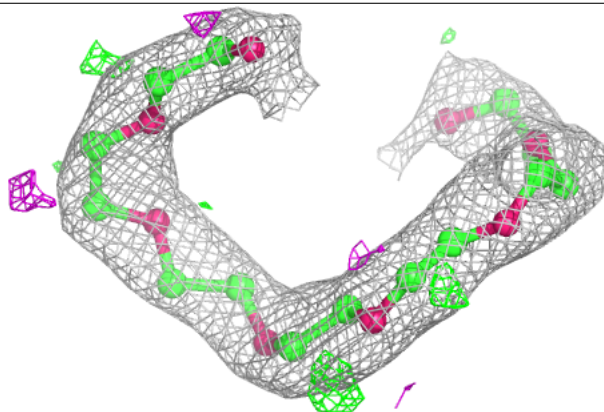


**Electron density around P33 G 2009:**

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

**Electron density around P33 G 2010:**

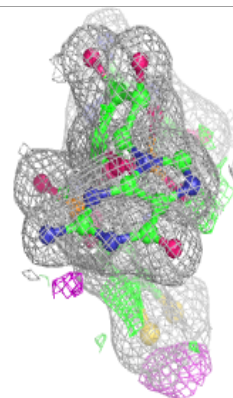
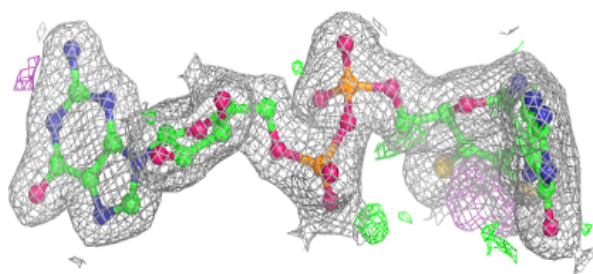
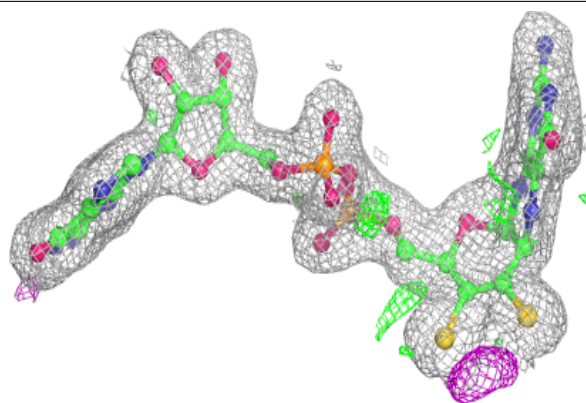
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



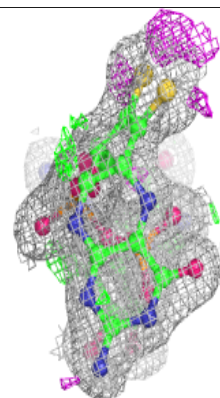
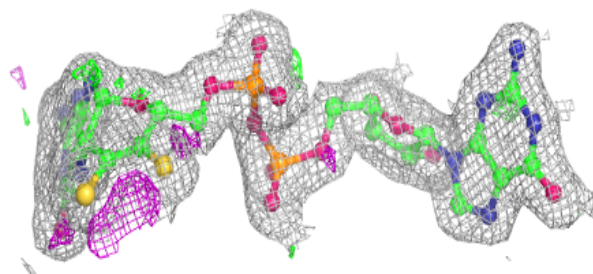
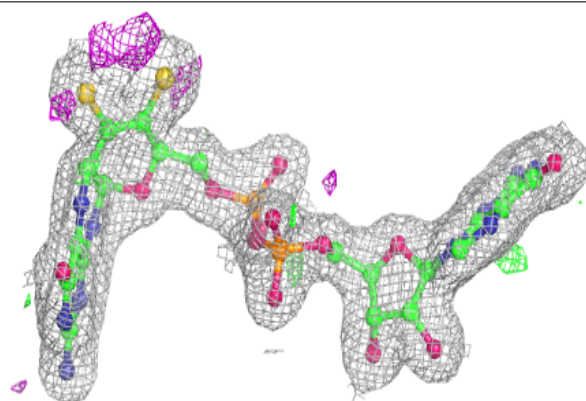


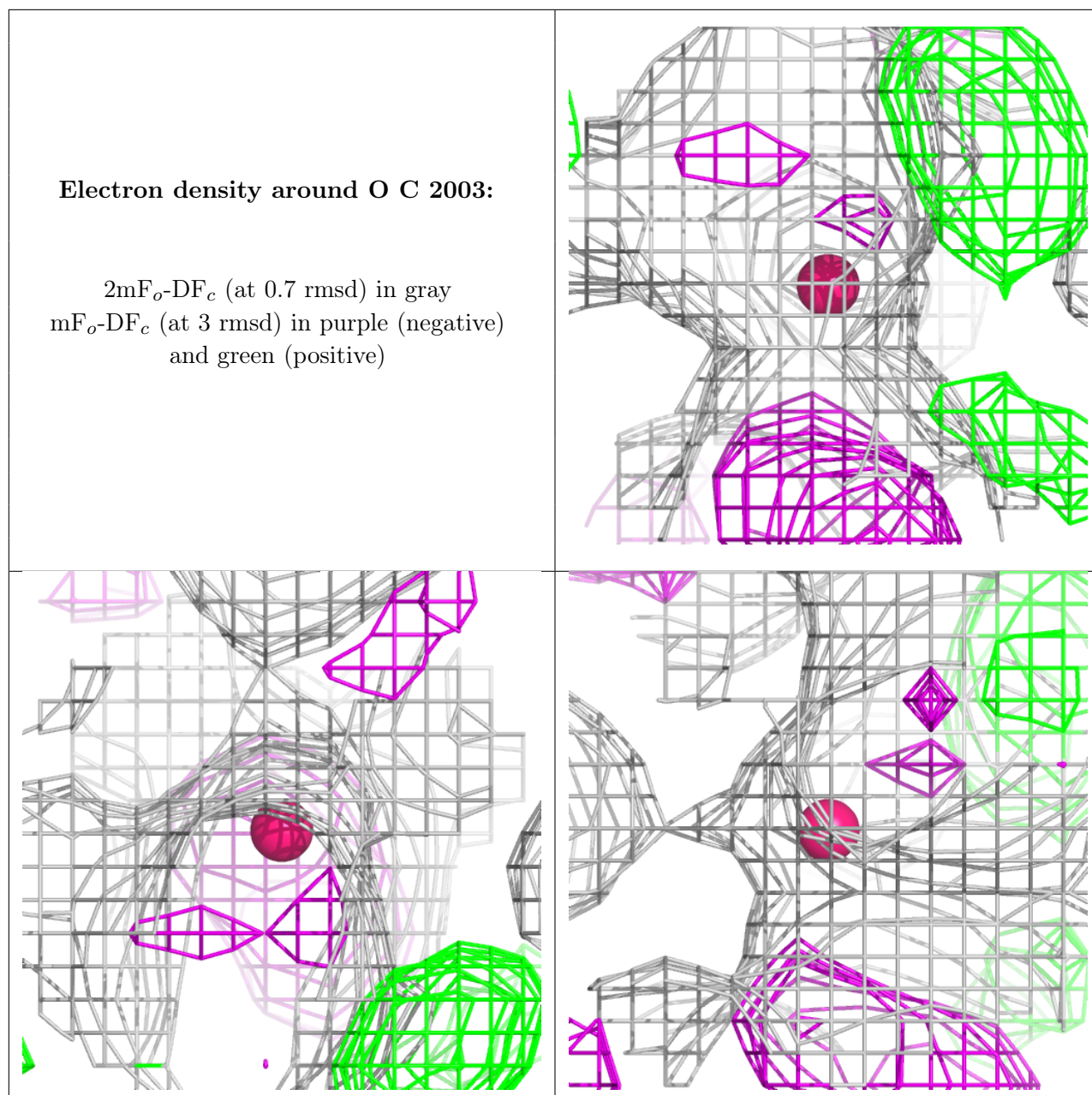
**Electron density around MGD G 2002:**

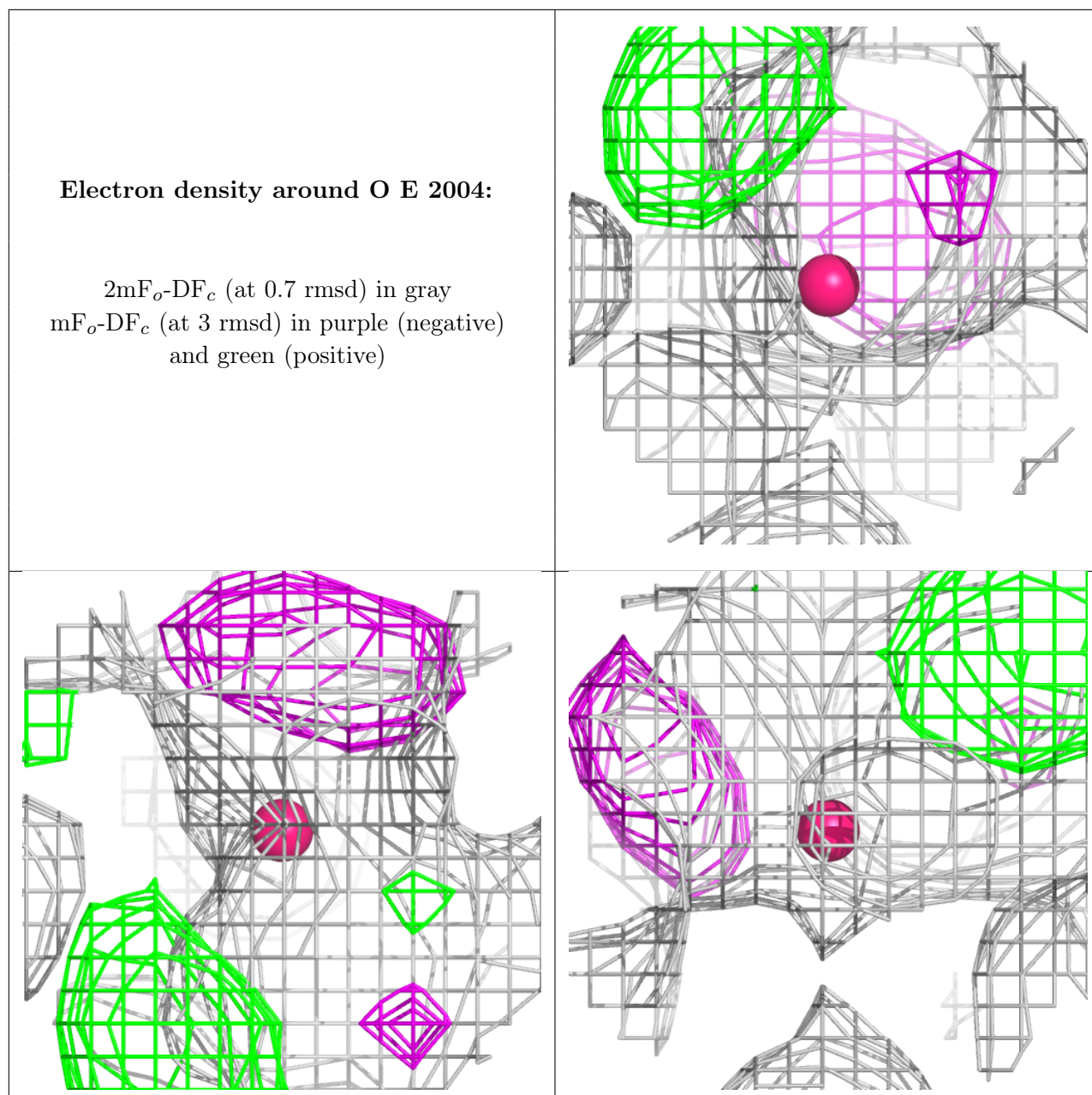
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around MGD C 2002:**

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



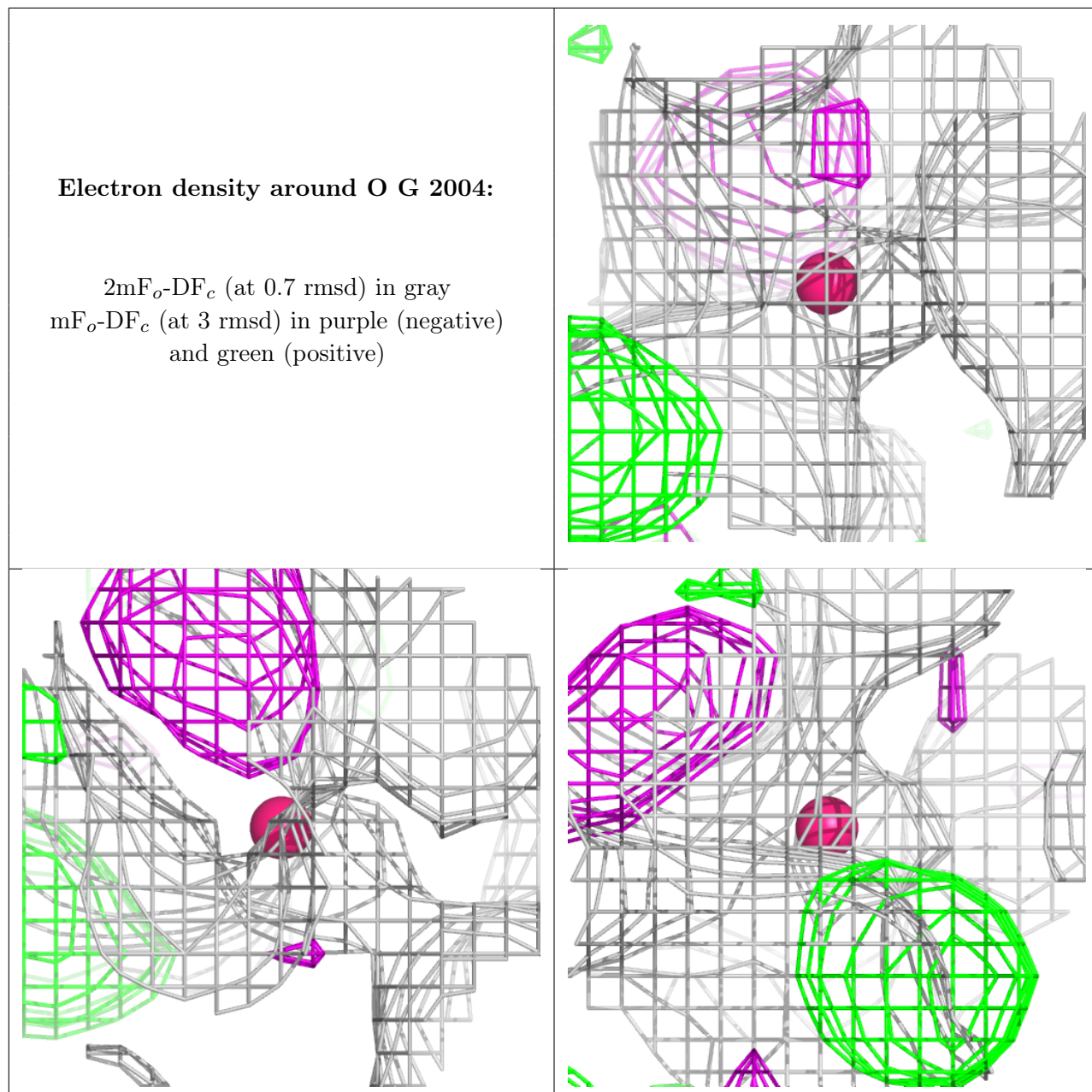






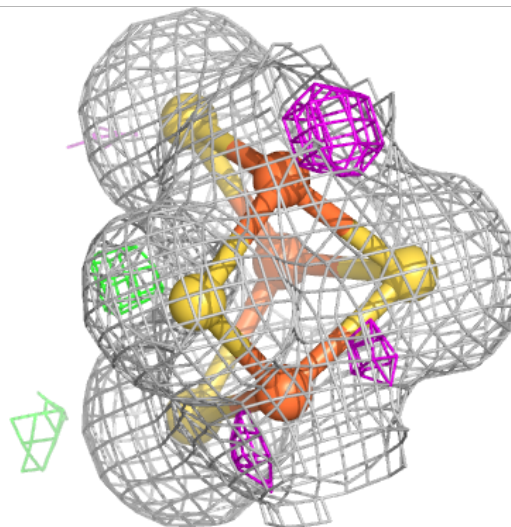
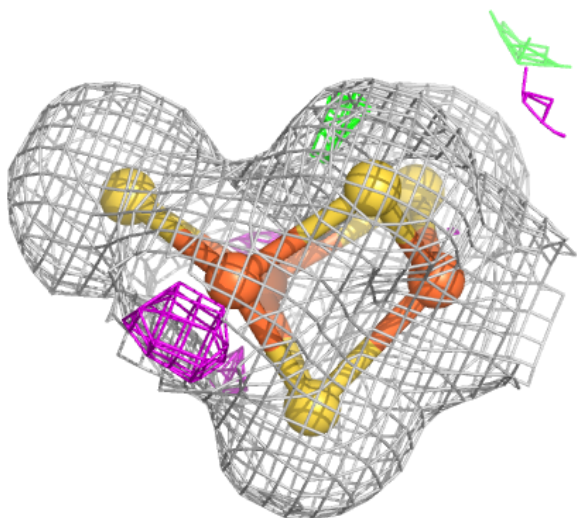
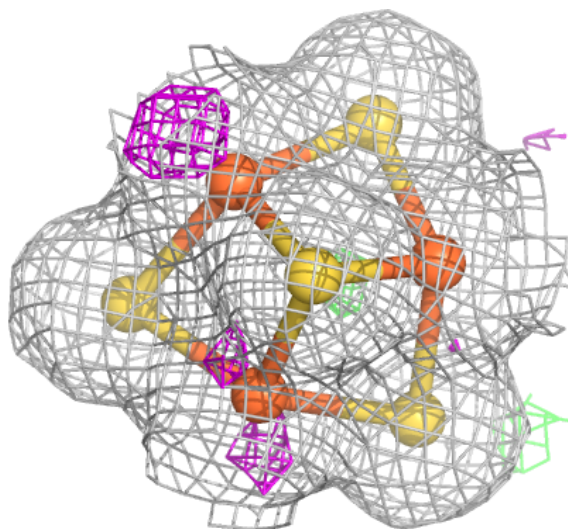
**Electron density around O G 2004:**

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



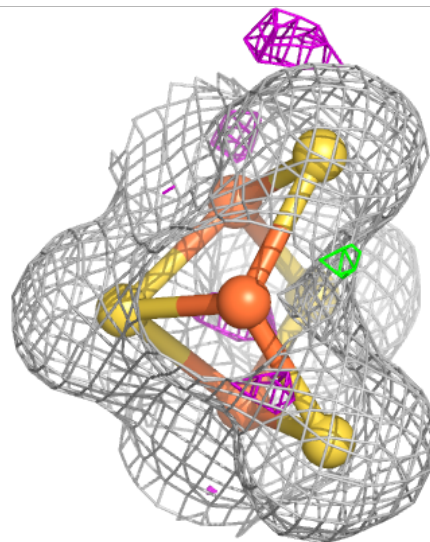
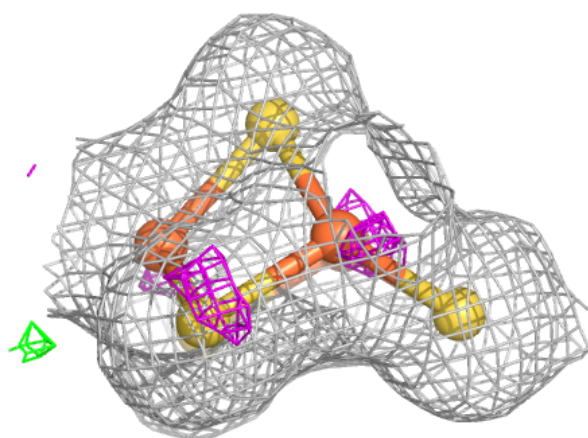
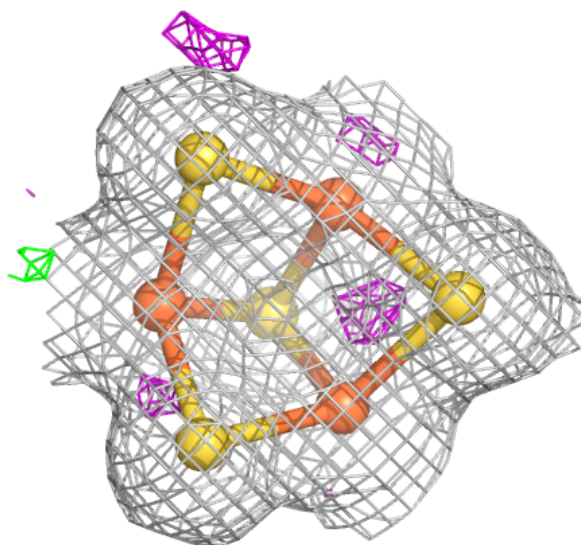
**Electron density around F3S A 2006:**

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



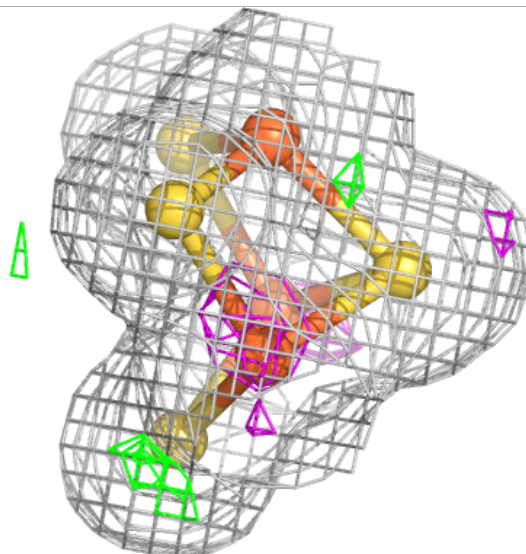
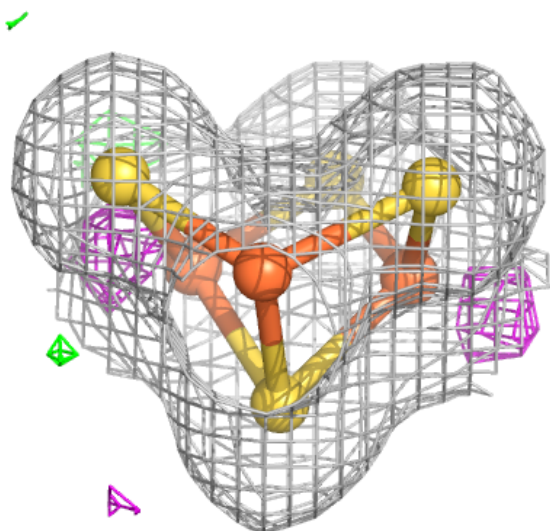
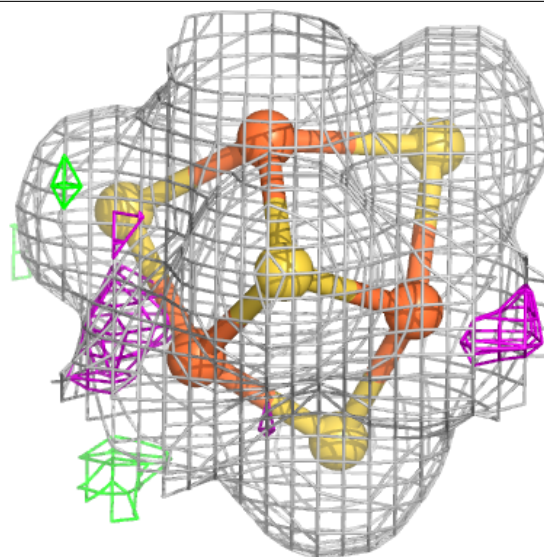
**Electron density around F3S C 2006:**

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



**Electron density around F3S E 2006:**

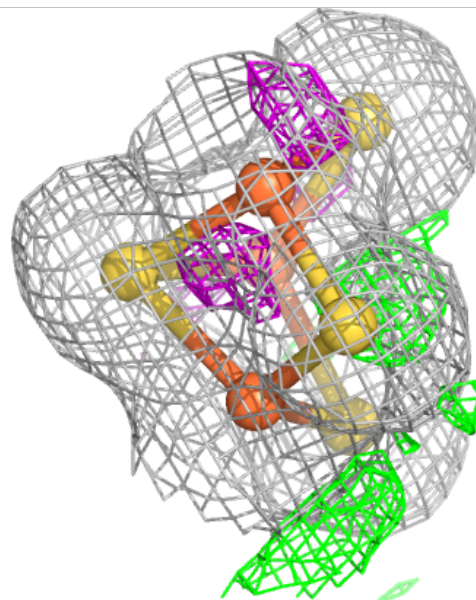
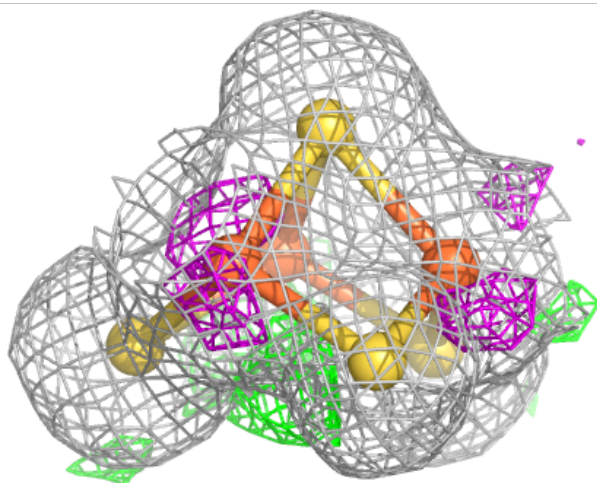
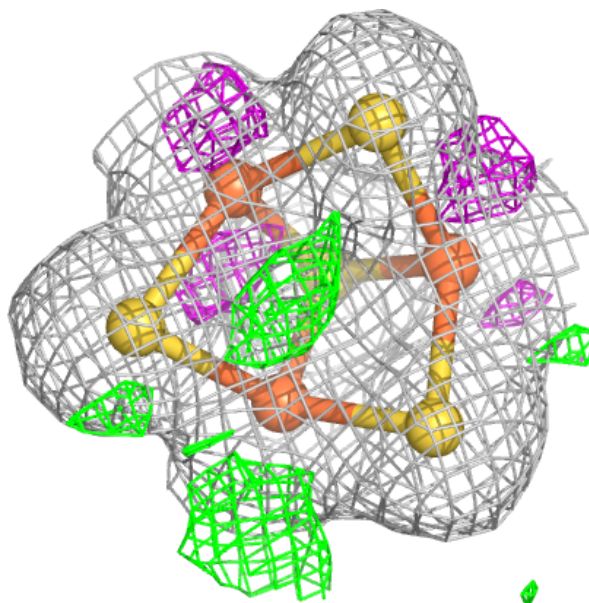
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





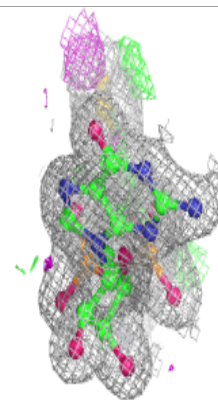
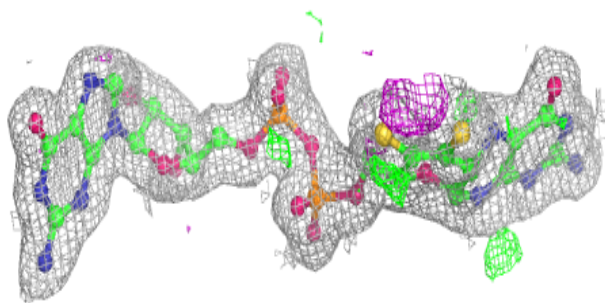
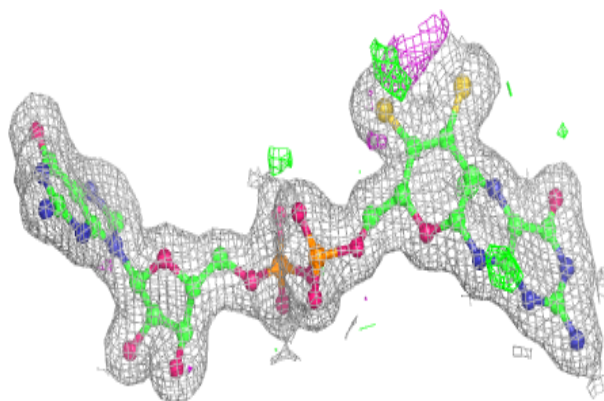
**Electron density around F3S G 2006:**

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

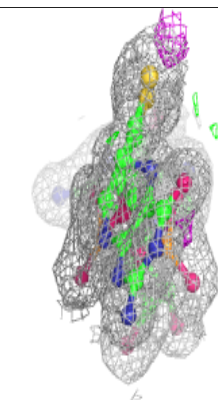
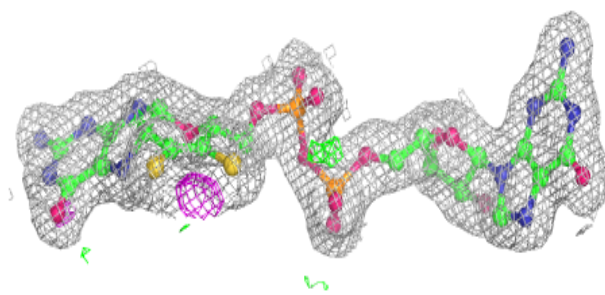
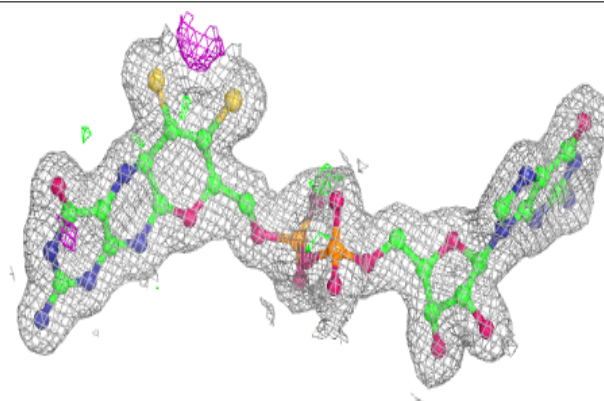


**Electron density around MGD C 2001:**

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

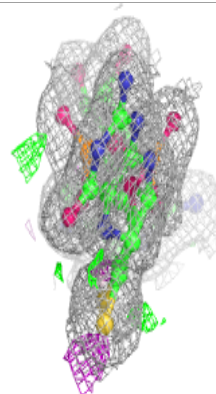
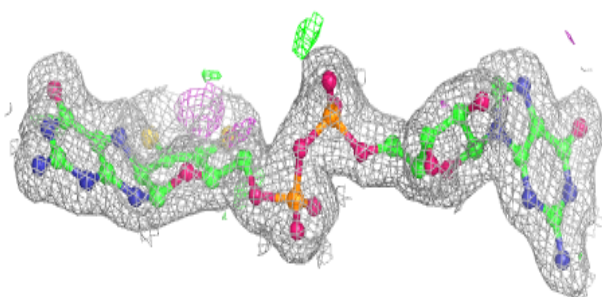
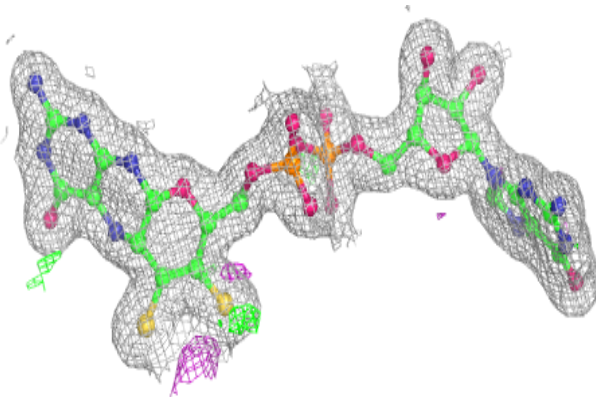
**Electron density around MGD A 2001:**

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

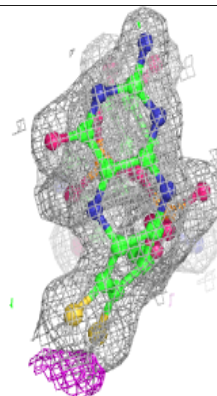
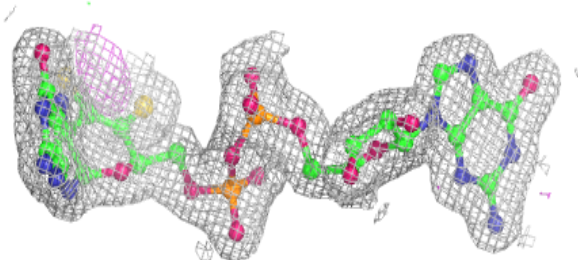
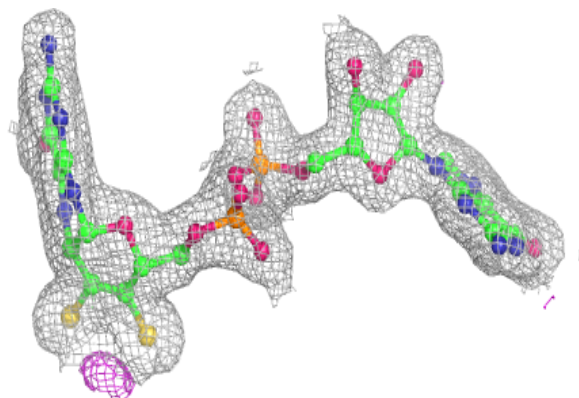


**Electron density around MGD E 2001:**

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

**Electron density around MGD E 2002:**

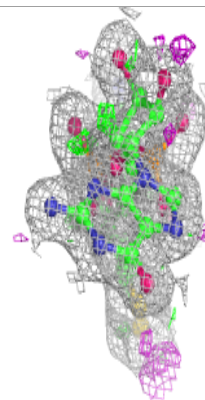
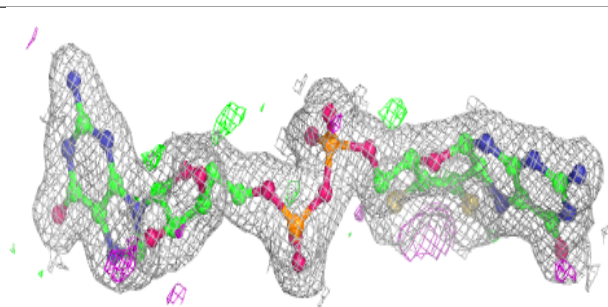
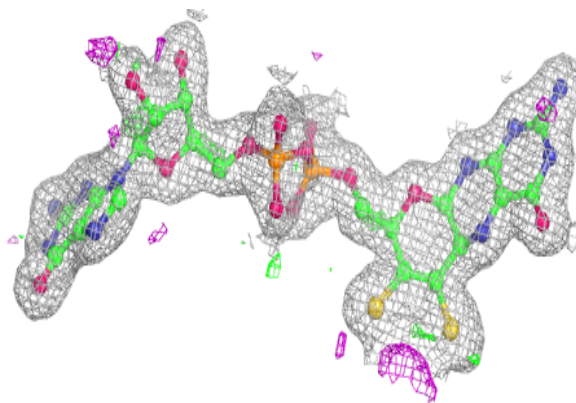
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



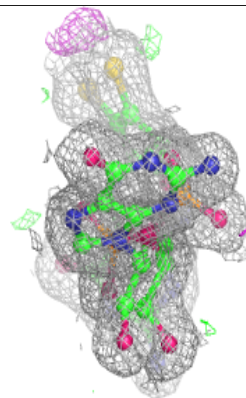
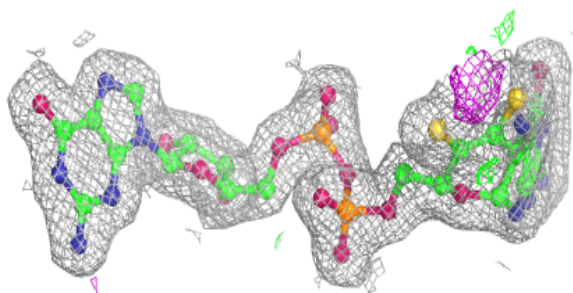
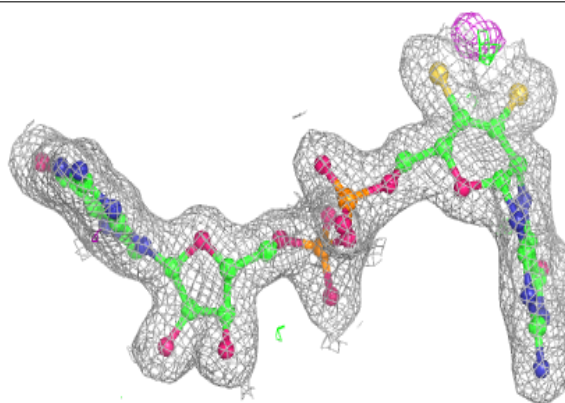


**Electron density around MGD G 2001:**

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

**Electron density around MGD A 2002:**

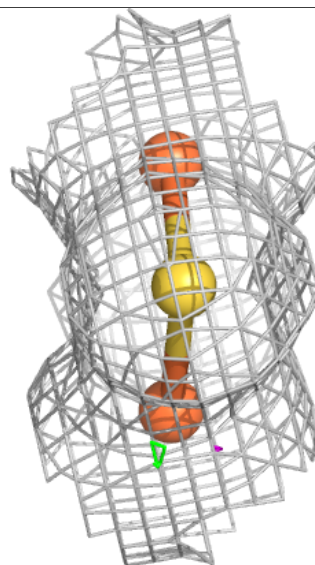
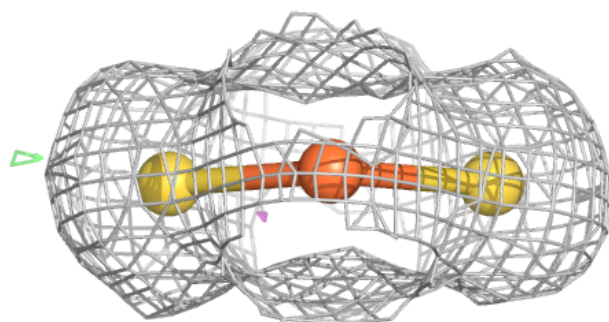
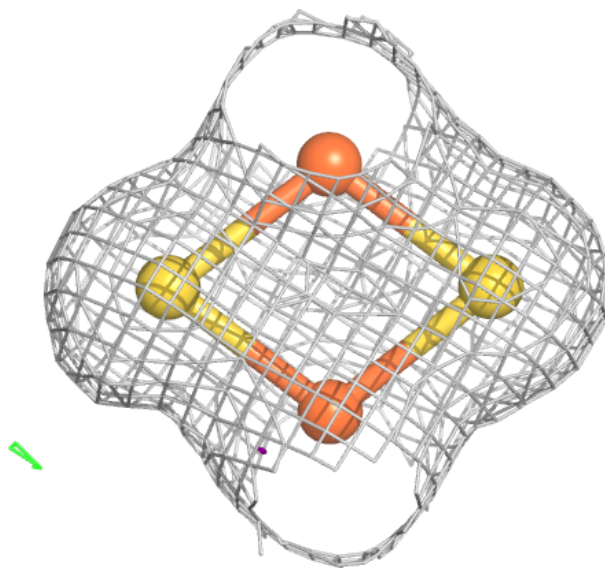
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





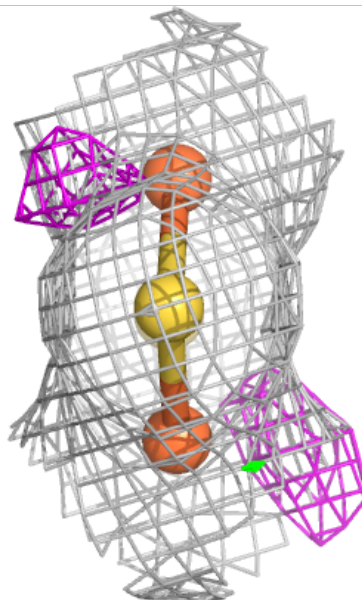
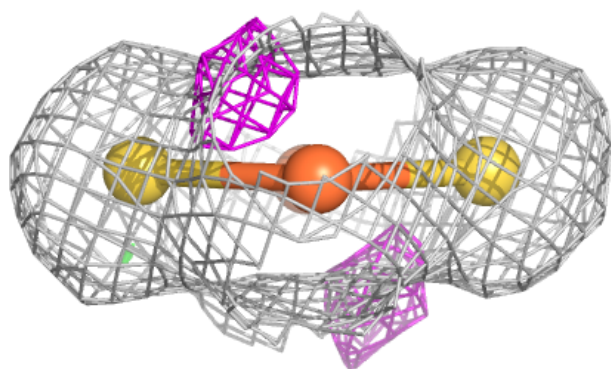
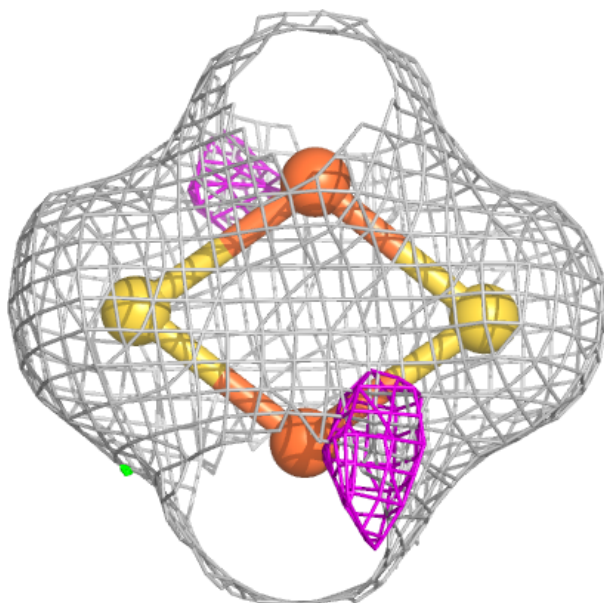
**Electron density around FES B 201:**

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



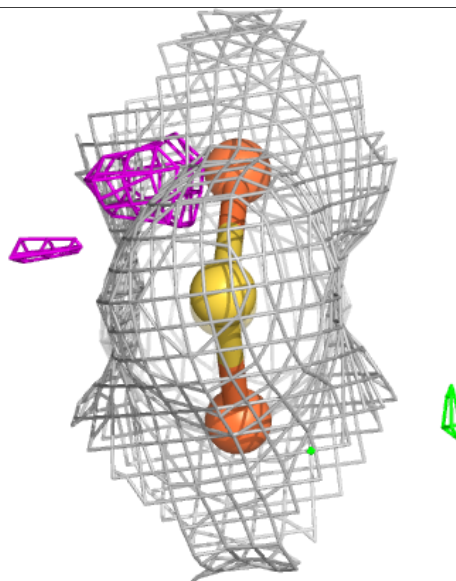
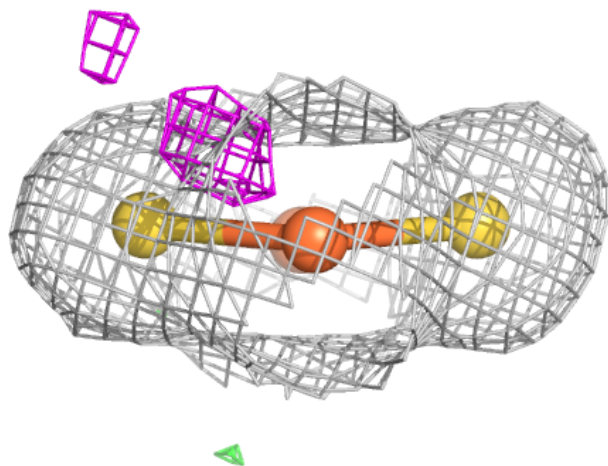
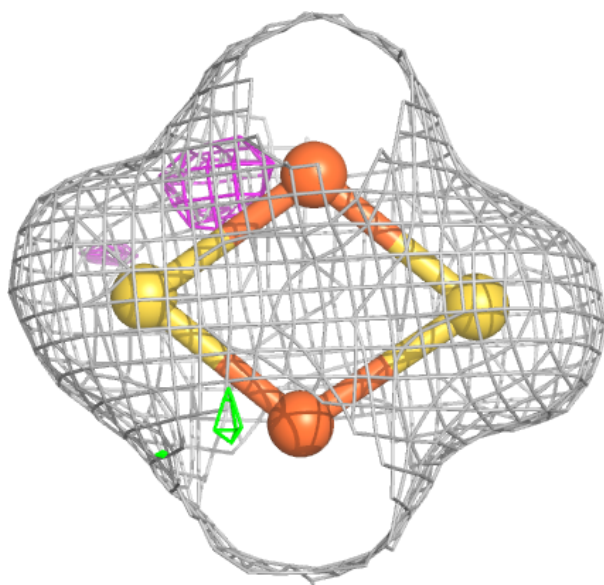
**Electron density around FES D 201:**

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



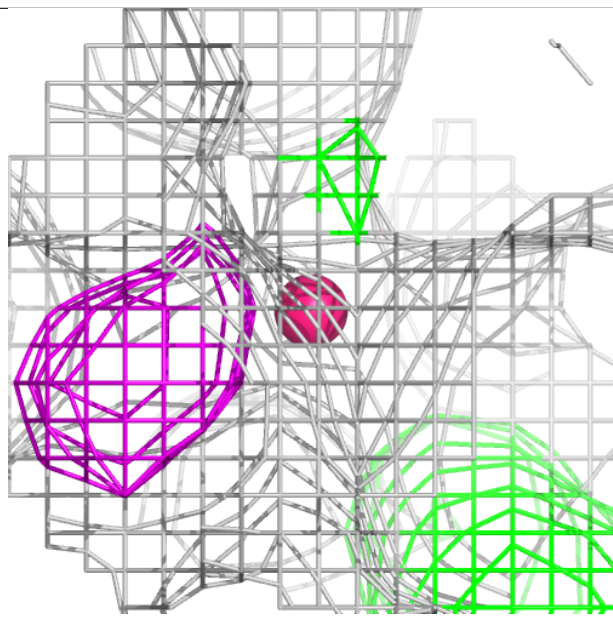
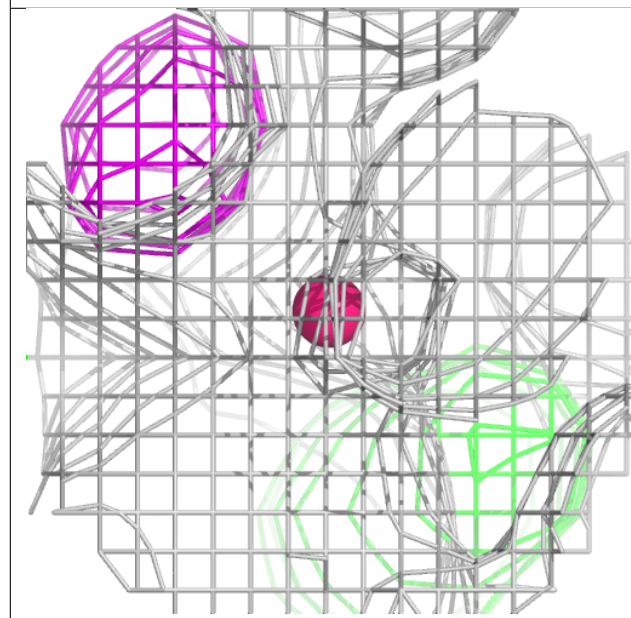
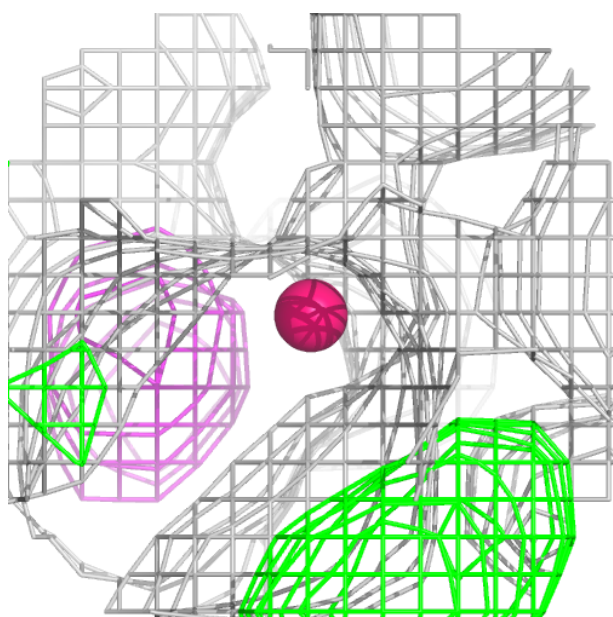
**Electron density around FES F 201:**

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



**Electron density around O A 2004:**

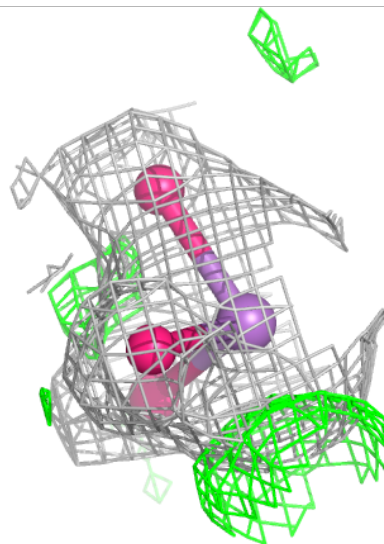
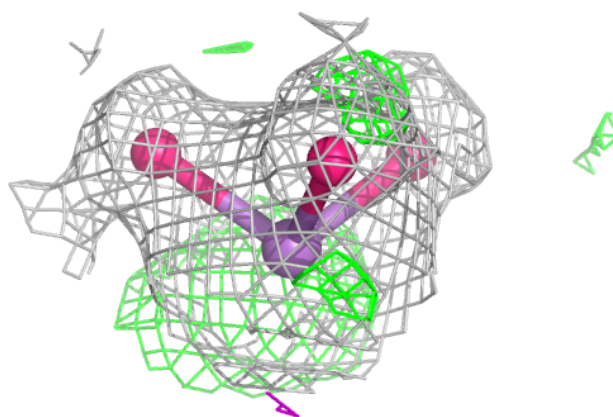
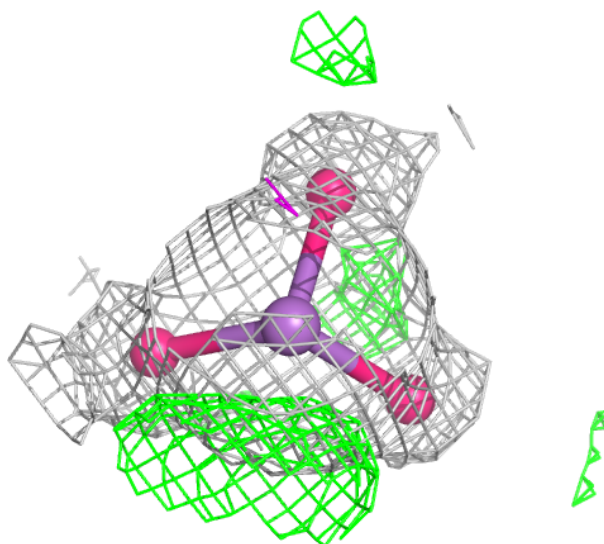
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





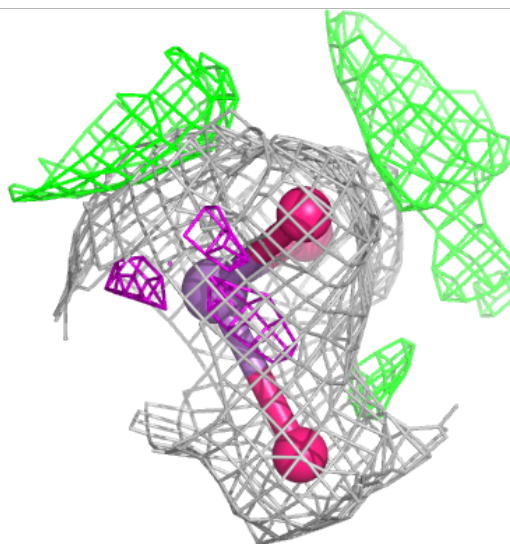
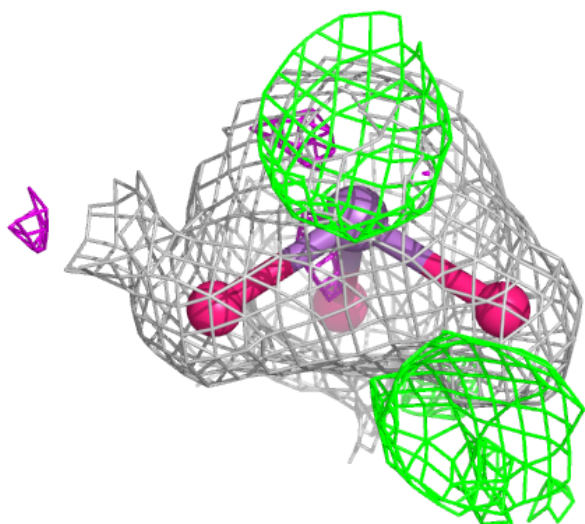
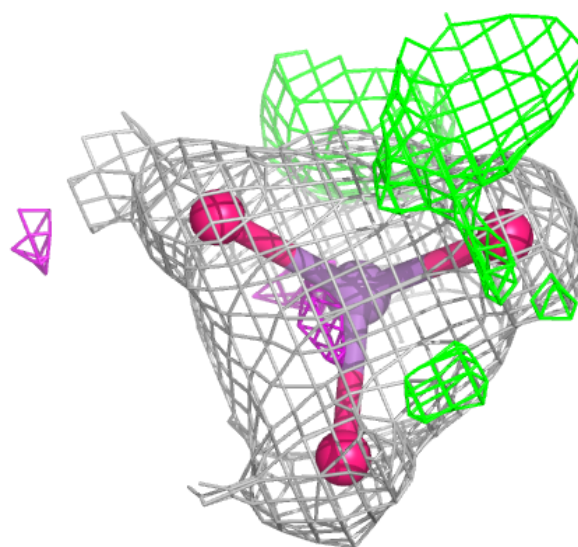
**Electron density around SBO A 2012:**

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



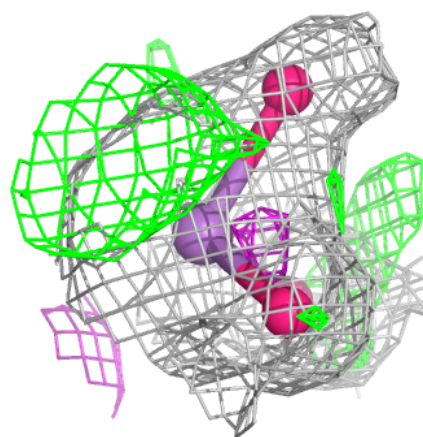
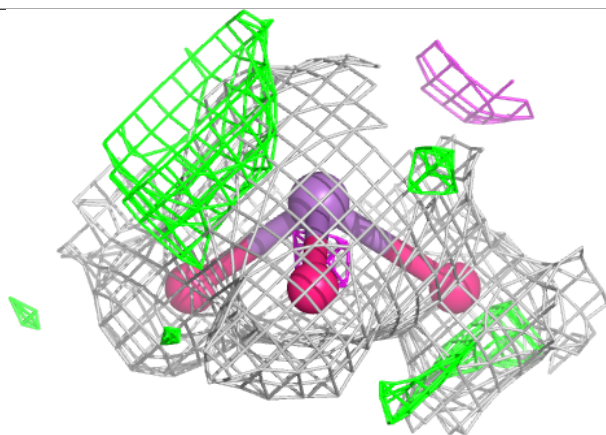
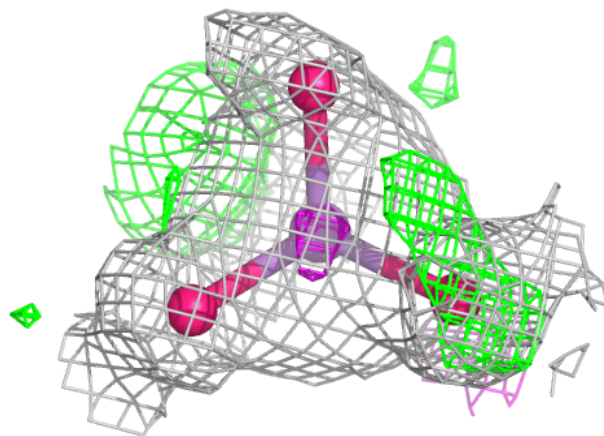
**Electron density around SBO C 2011:**

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



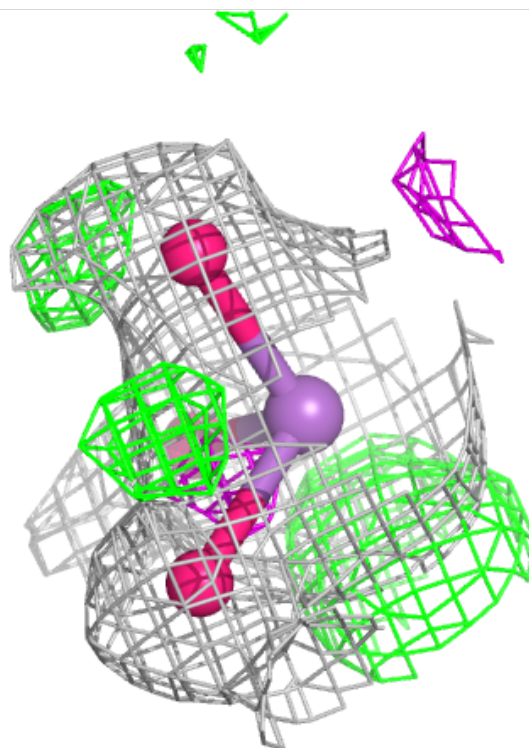
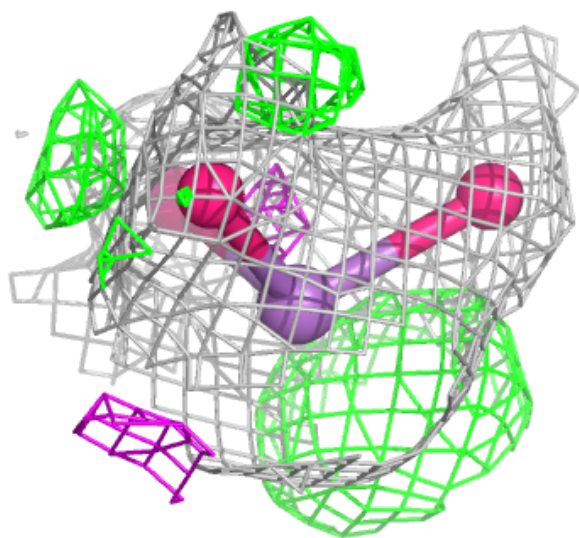
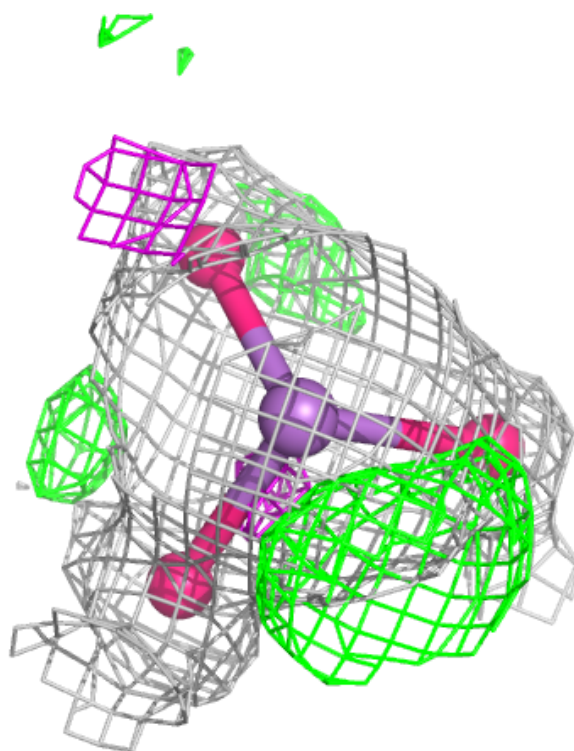
**Electron density around SBO E 2011:**

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



**Electron density around SBO G 2013:**

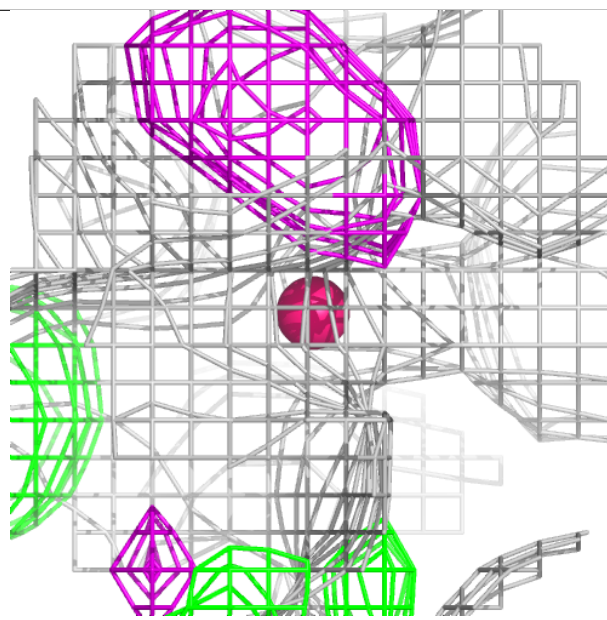
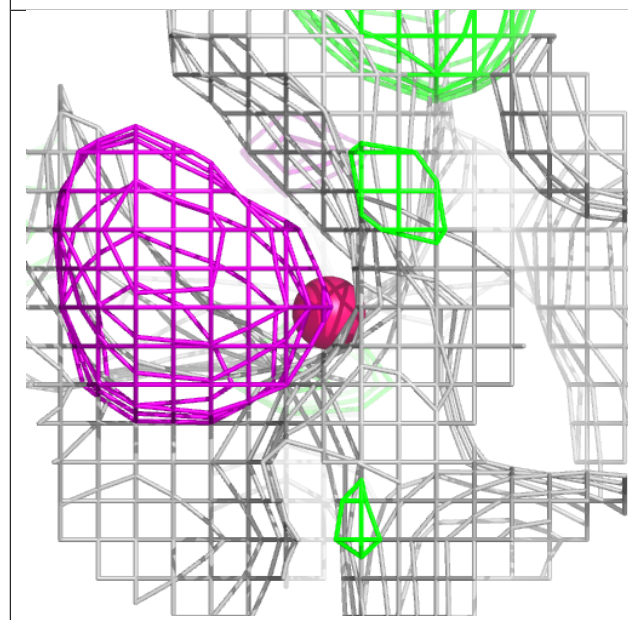
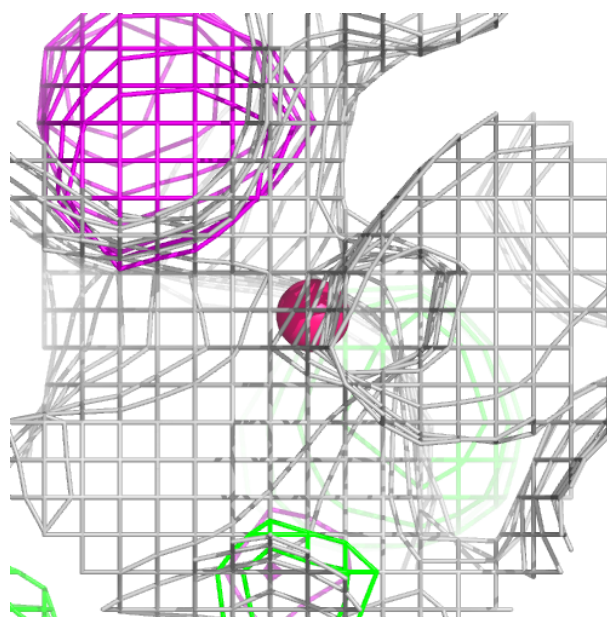
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





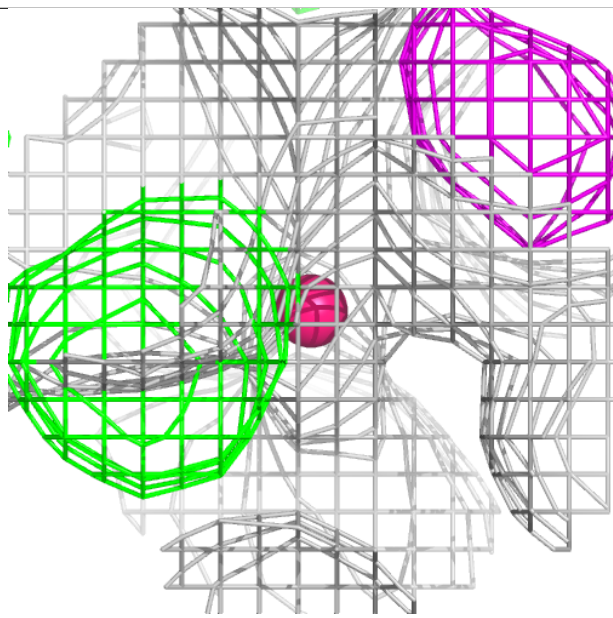
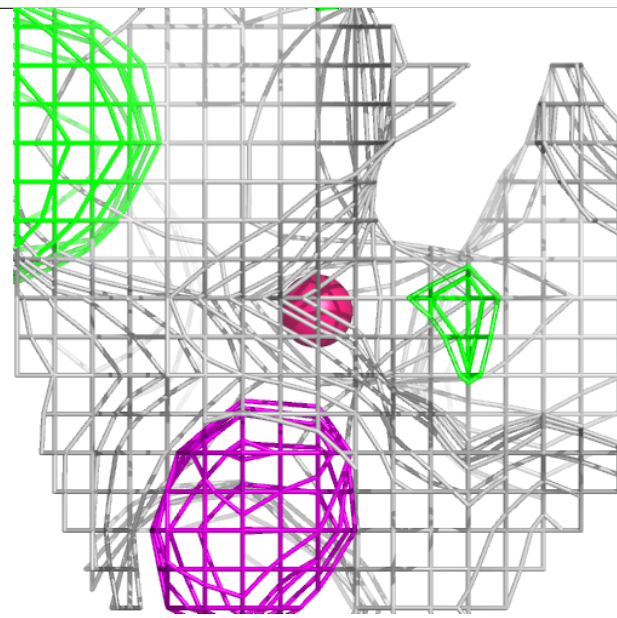
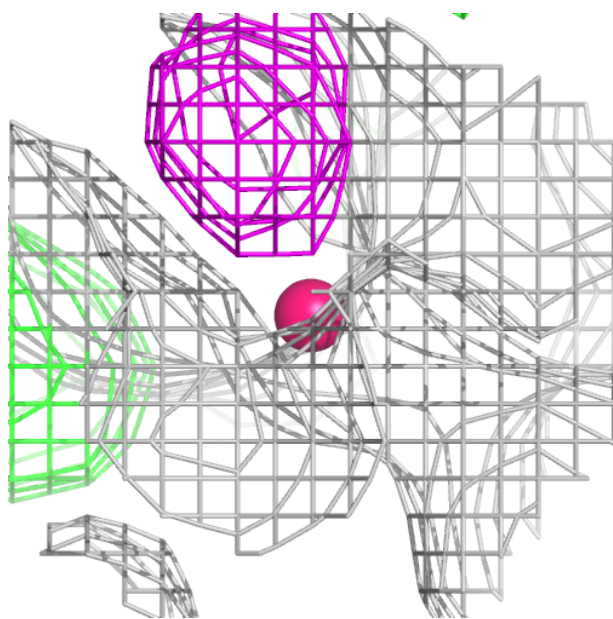
**Electron density around O G 2003:**

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



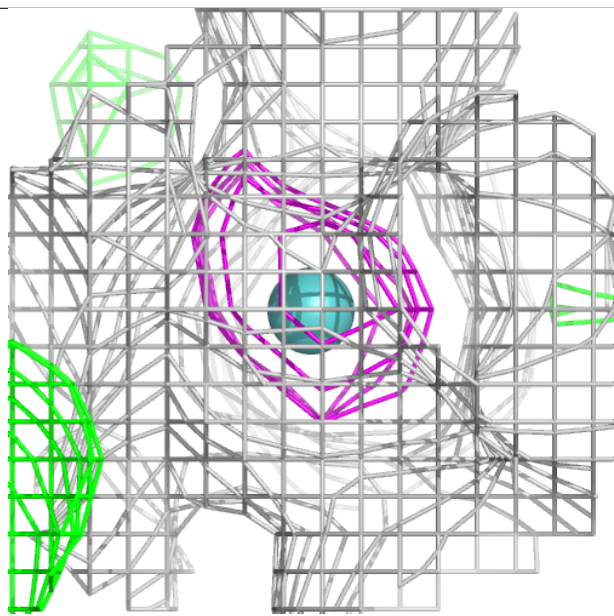
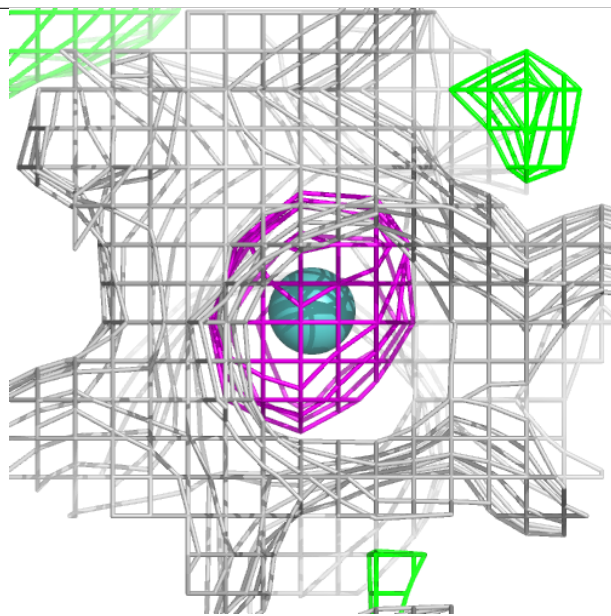
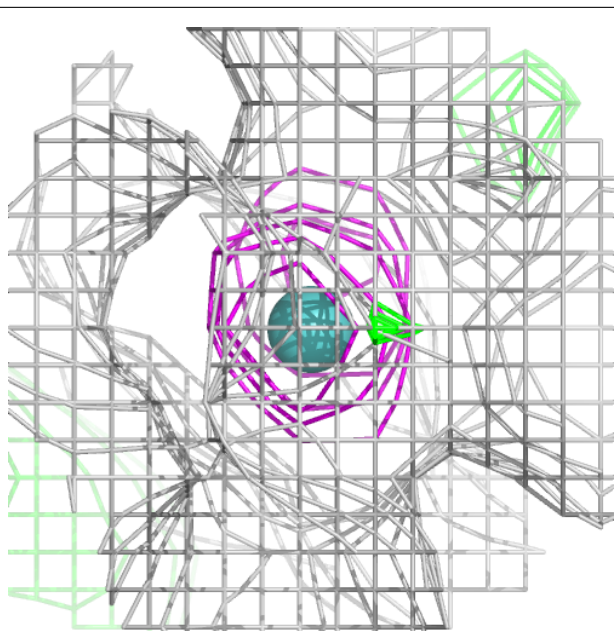
**Electron density around O A 2003:**

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



**Electron density around 4MO A 2005:**

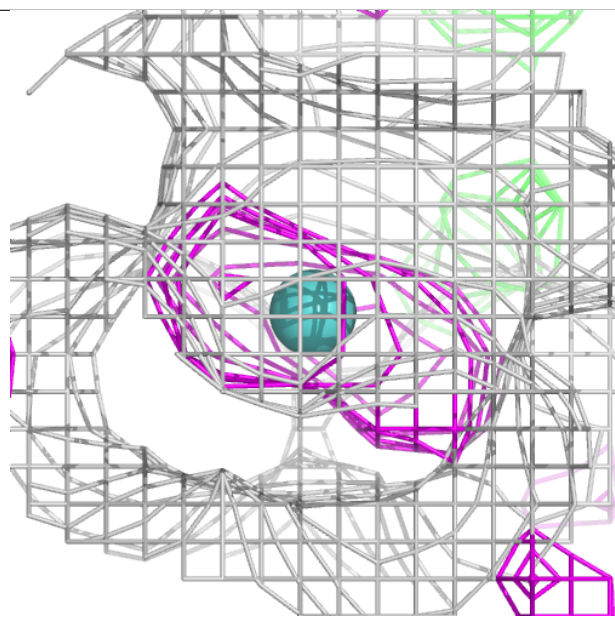
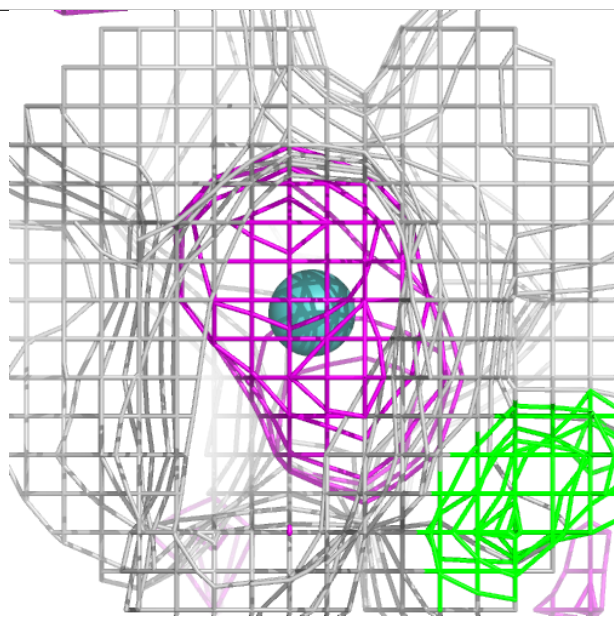
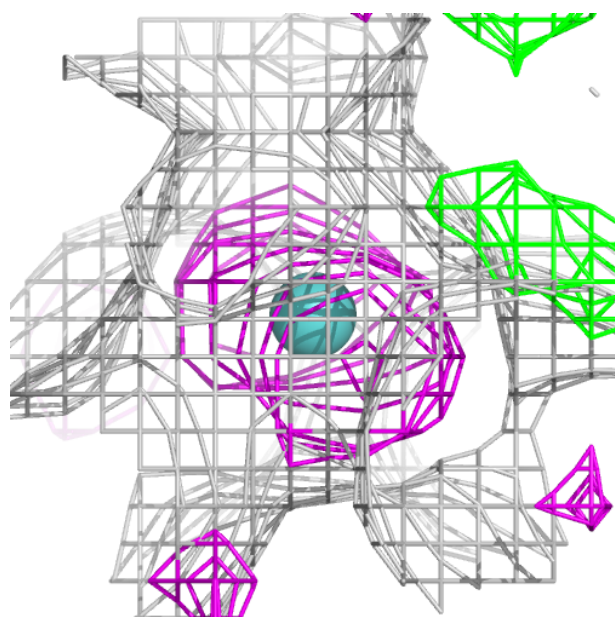
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





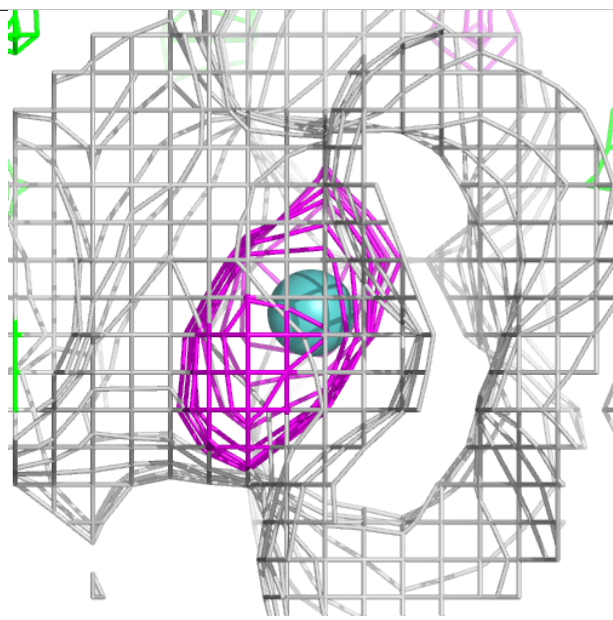
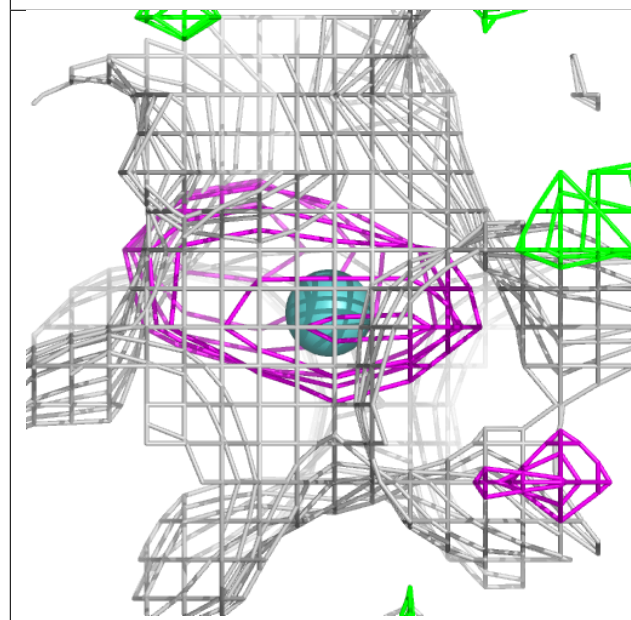
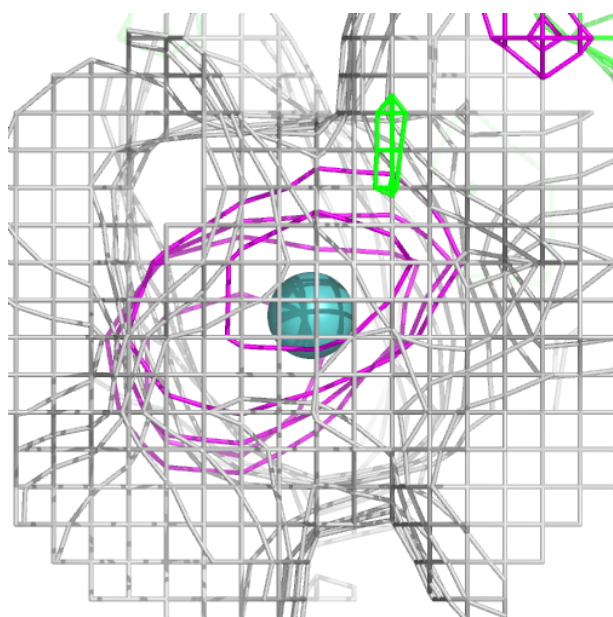
**Electron density around 4MO C 2005:**

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



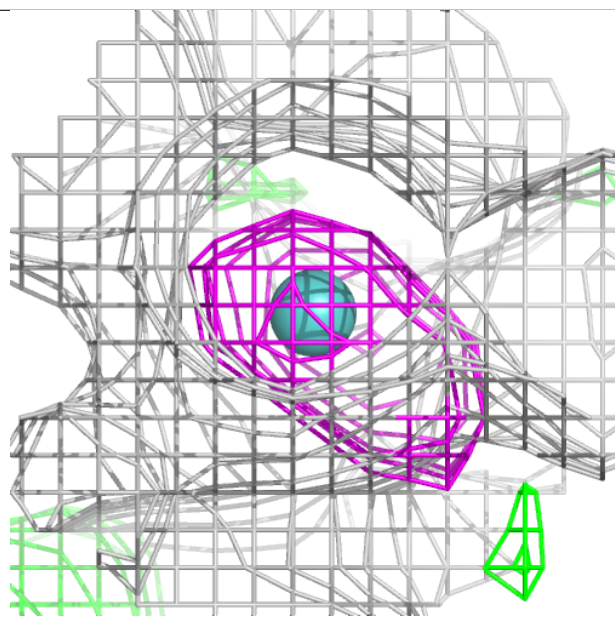
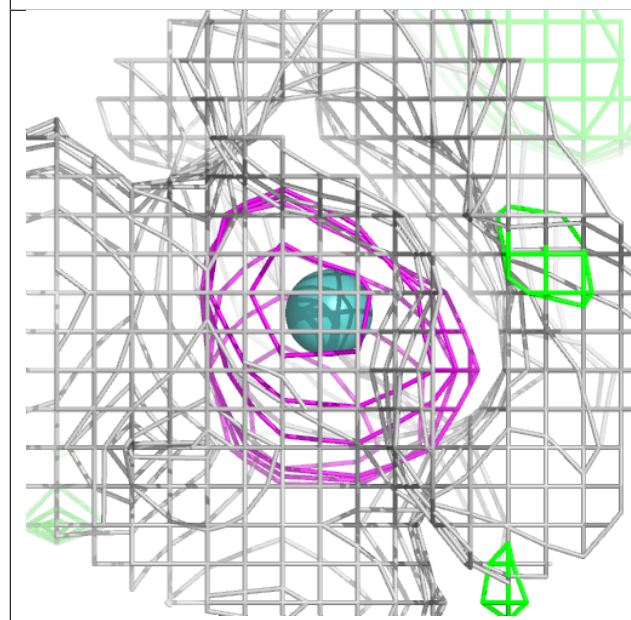
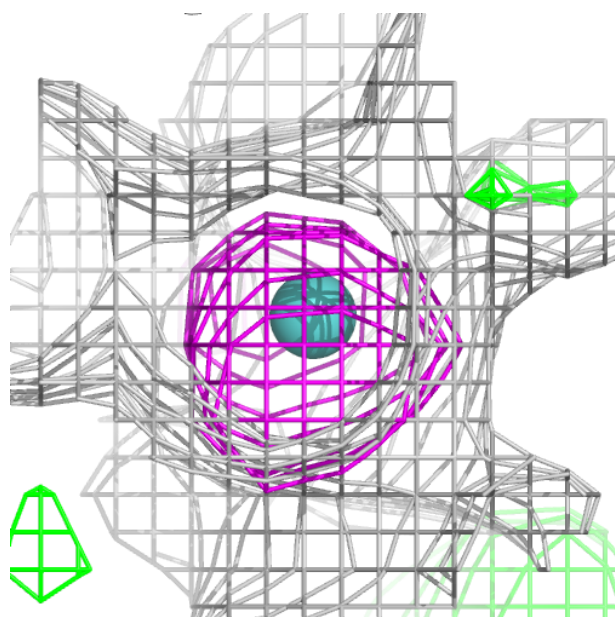
**Electron density around 4MO E 2005:**

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



**Electron density around 4MO G 2005:**

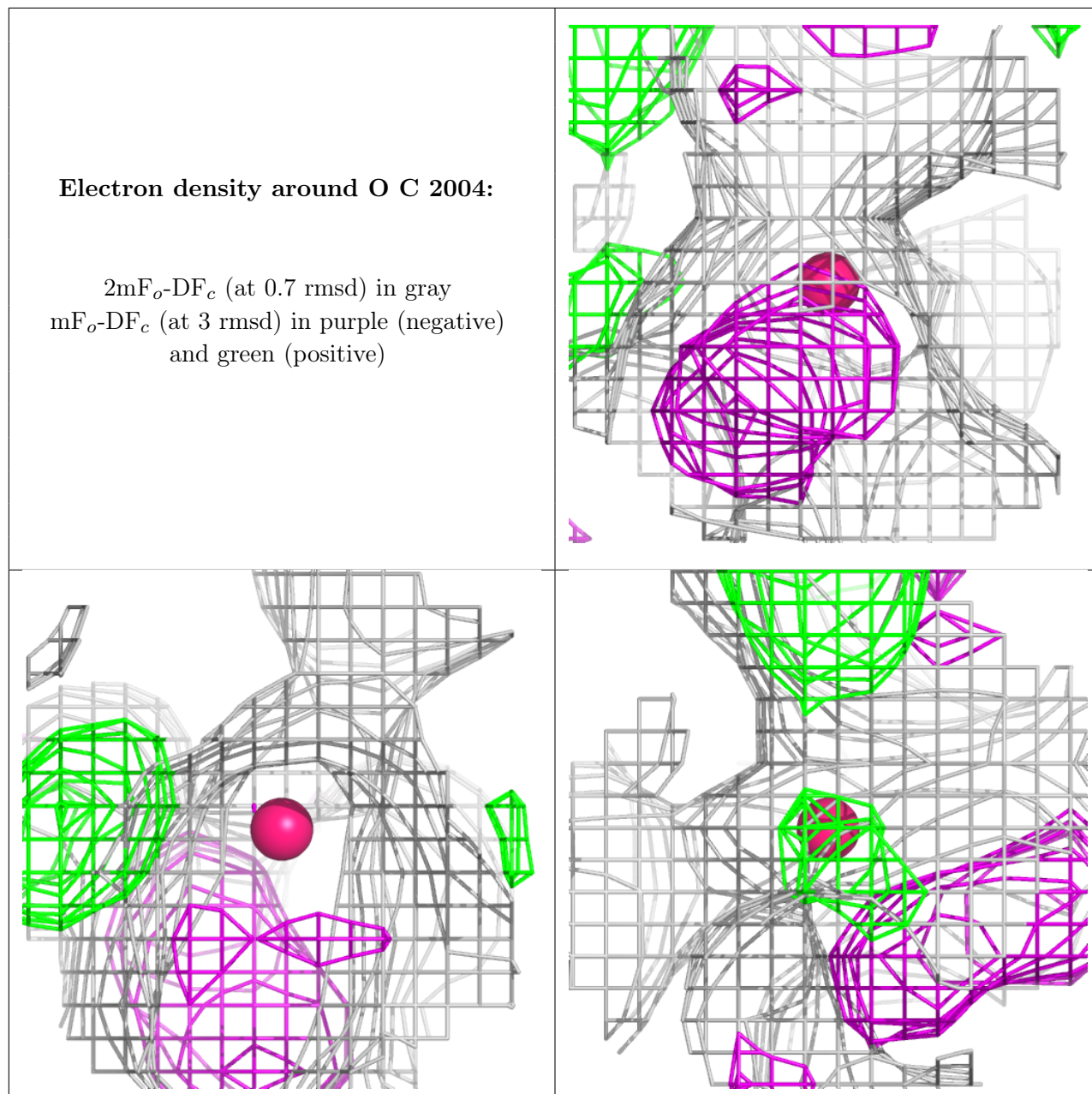
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

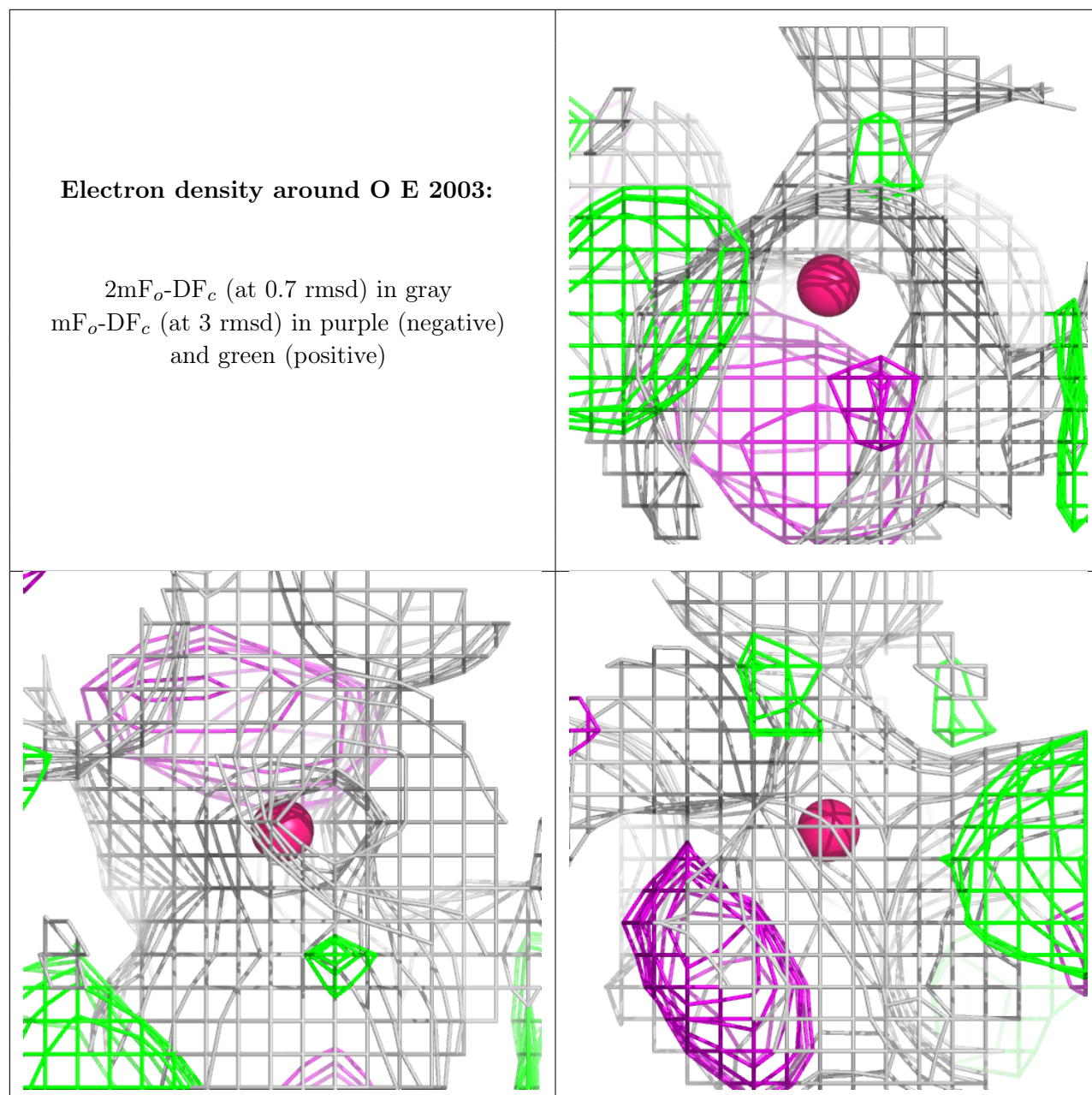




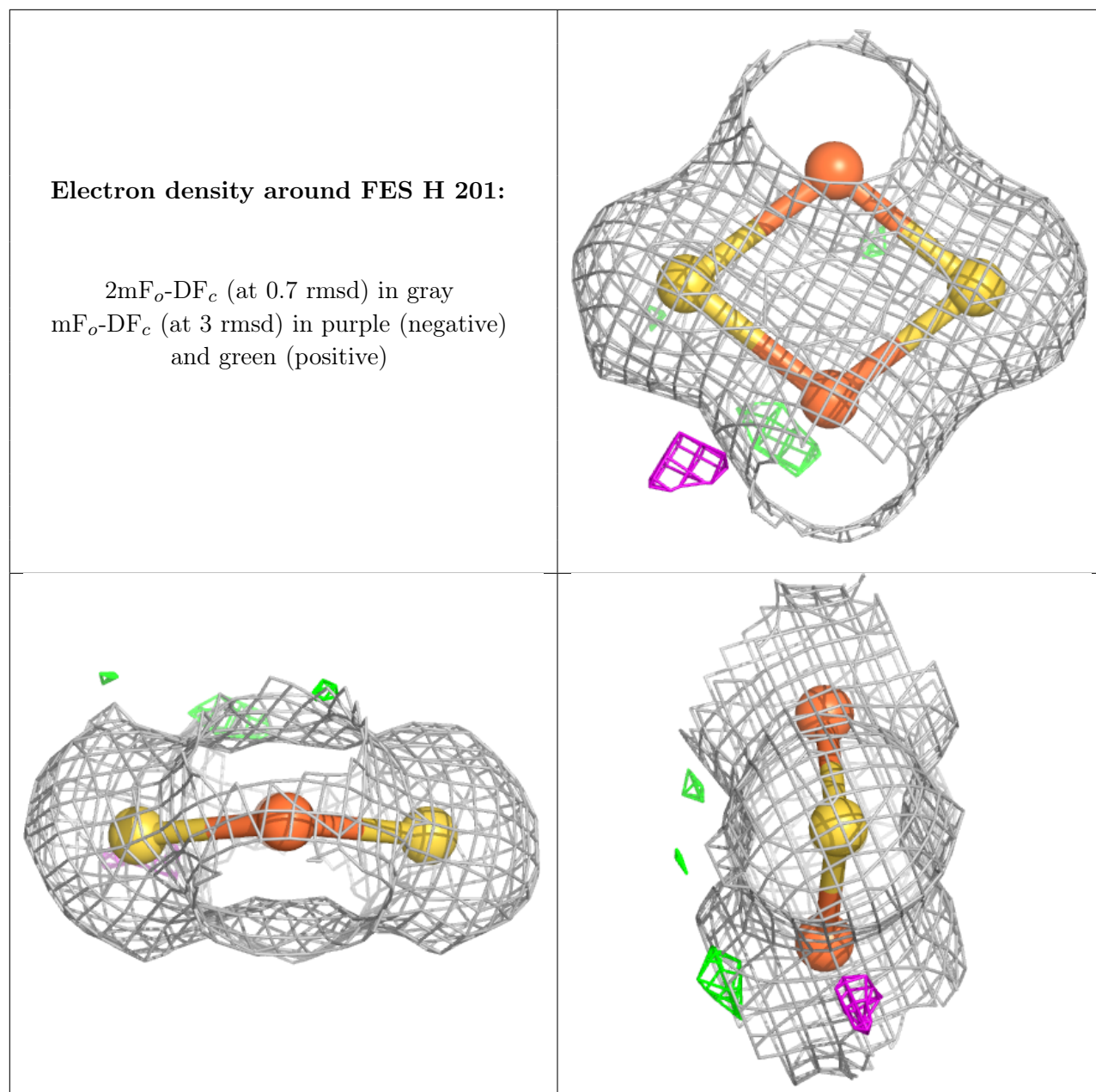
**Electron density around O C 2004:**

$2mF_o-DF_c$  (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.