



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 08:18 AM UTC

PDB ID : 8CCQ / pdb_00008ccq
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

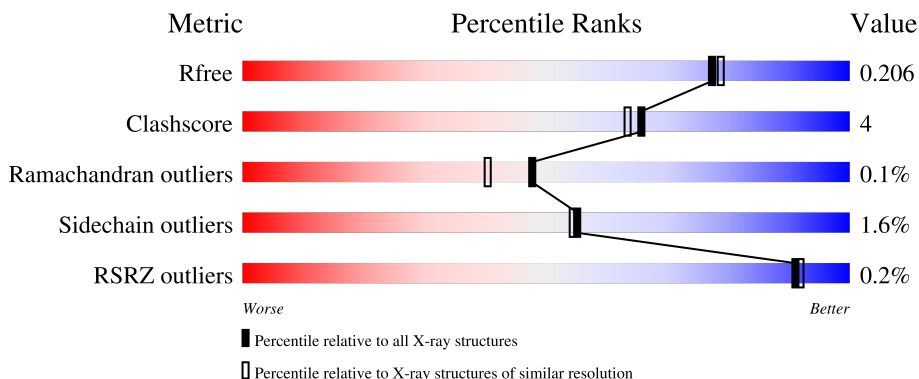
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

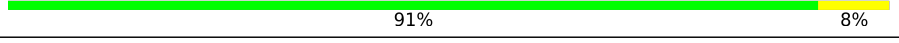

The reported resolution of this entry is 1.89 Å.

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 ≥ 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	 90% 9%
1	E	845	 91% 8%
1	G	845	 90% 9%
2	B	175	 73% 25%

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Mol	Chain	Length	Quality of chain
2	D	175	 <p>% 70% 5% 25%</p>
2	F	175	 <p>% 68% 7% 25%</p>
2	H	175	 <p>72% • 25%</p>

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.

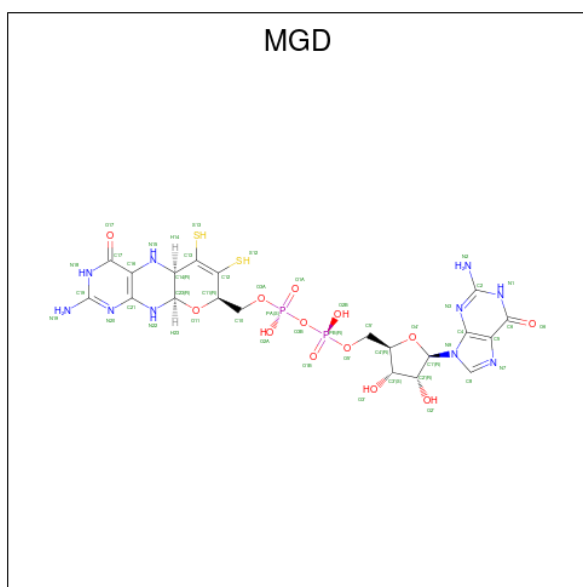
- Molecule 1 is a protein called AroA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	843	6570	4104	1172	1257	37	0	4	0
1	C	843	6564	4100	1171	1256	37	0	3	0
1	E	843	6564	4100	1171	1256	37	0	3	0
1	G	843	6559	4097	1171	1254	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	995	629	166	198	2	0	0	0
2	D	132	995	629	166	198	2	0	0	0
2	F	132	995	629	166	198	2	0	0	0
2	H	132	995	629	166	198	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 (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂) (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 (CCD ID: O) (formula: O) (labeled as "Ligand of Interest" by depositor).

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

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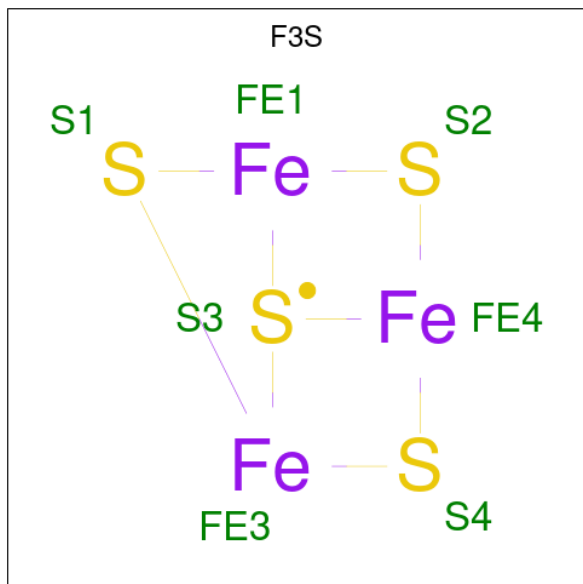
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	2	Total O 2 2	0	0

- Molecule 5 is MOLYBDENUM(IV) ION (CCD ID: 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 (CCD ID: F3S) (formula: Fe₃S₄) (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

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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



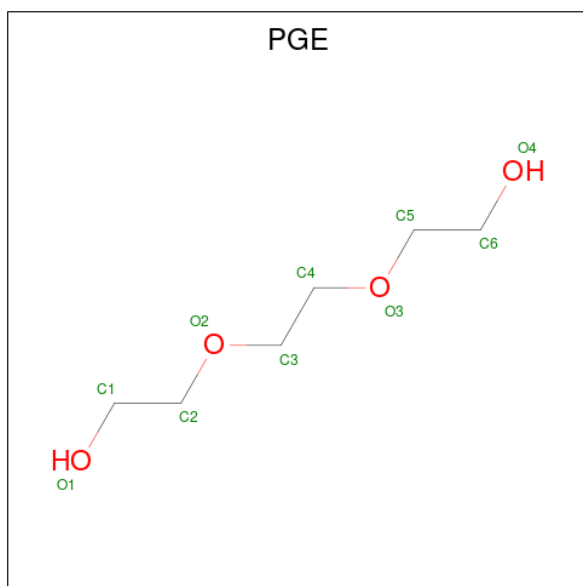
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	A	1	5	4	1	0	0
7	A	1	5	4	1	0	0
7	A	1	5	4	1	0	0
7	C	1	5	4	1	0	0
7	C	1	5	4	1	0	0
7	C	1	5	4	1	0	0
7	E	1	5	4	1	0	0
7	E	1	5	4	1	0	0
7	E	1	5	4	1	0	0
7	G	1	5	4	1	0	0

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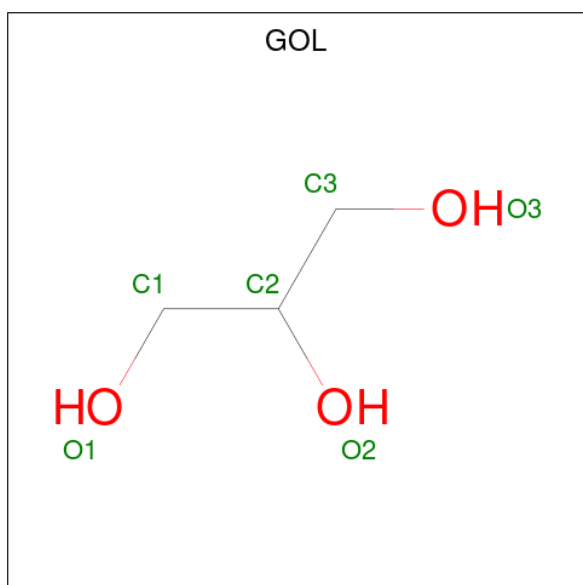
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	G	1	5	4	1	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



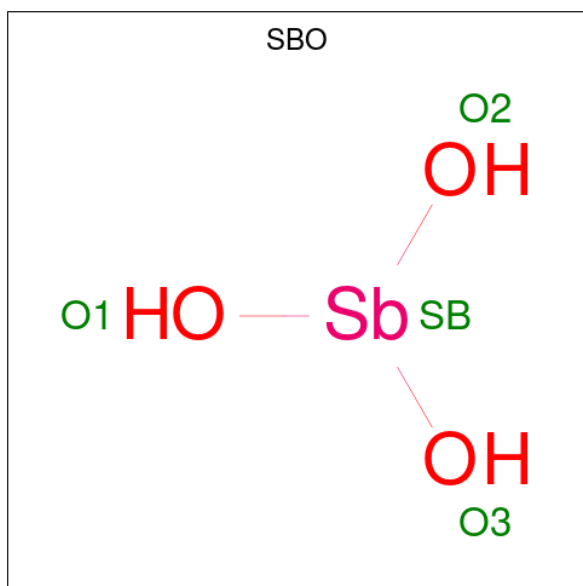
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	10	6	4	0	0

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



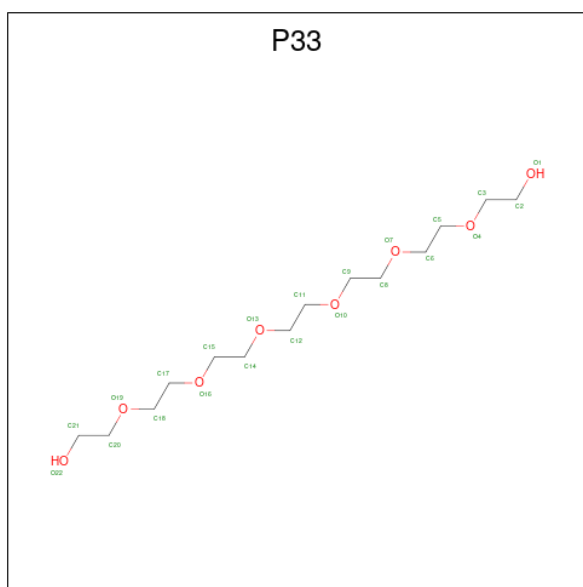
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	C	1	Total C O 6 3 3	0	0
9	E	1	Total C O 6 3 3	0	0
9	G	1	Total C O 6 3 3	0	0
9	G	1	Total C O 6 3 3	0	0

- Molecule 10 is TRIHYDROXYANTIMONITE(III) (CCD ID: SBO) (formula: H_3O_3Sb) (labeled as "Ligand of Interest" by depositor).



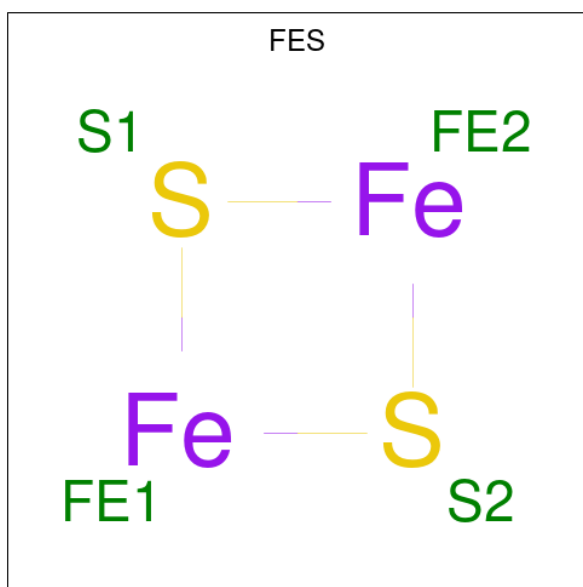
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O Sb 4 3 1	0	0
10	C	1	Total O Sb 4 3 1	0	0
10	E	1	Total O Sb 4 3 1	0	0
10	G	1	Total O Sb 4 3 1	0	0

- Molecule 11 is 3,6,9,12,15,18-HEXA-OXAICOSANE-1,20-DIOL (CCD ID: P33) (formula: $C_{14}H_{30}O_8$).



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 (CCD ID: FES) (formula: Fe₂S₂) (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		

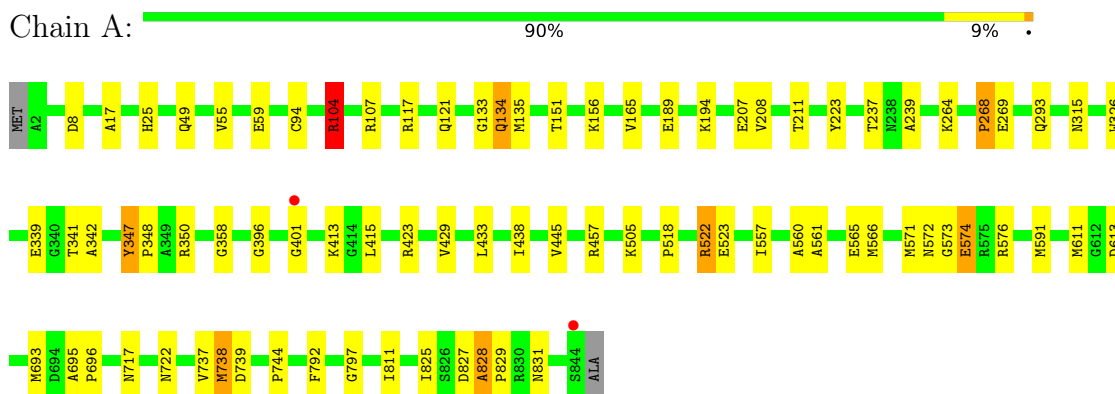
- Molecule 13 is water.

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		

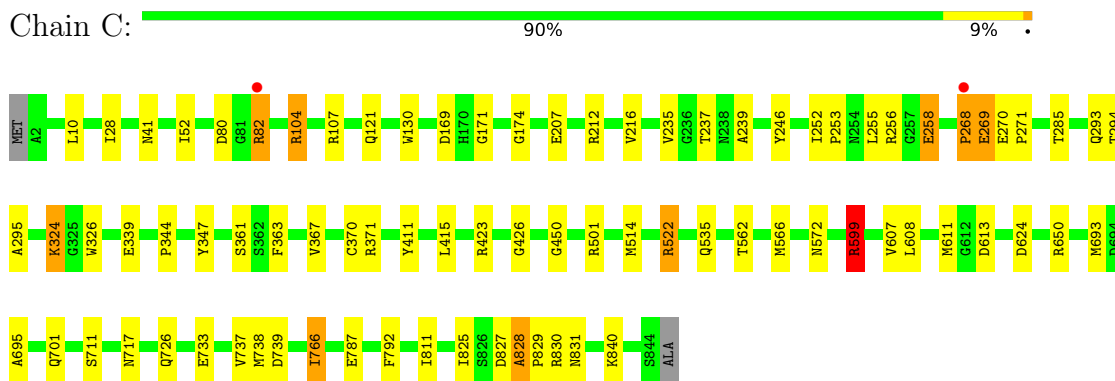
3 Residue-property plots [i](#)

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.

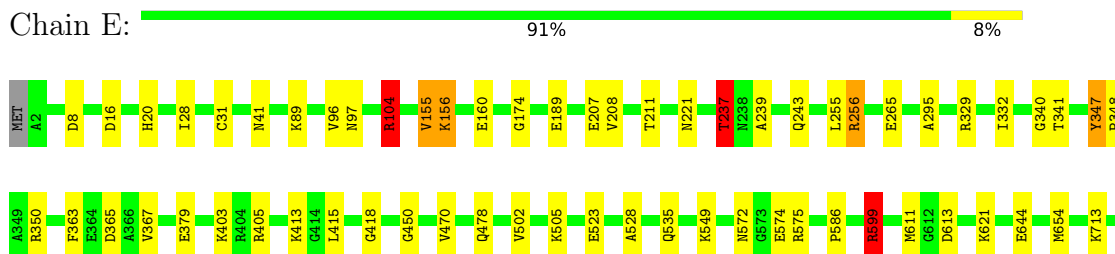
- Molecule 1: AroA



- Molecule 1: AroA

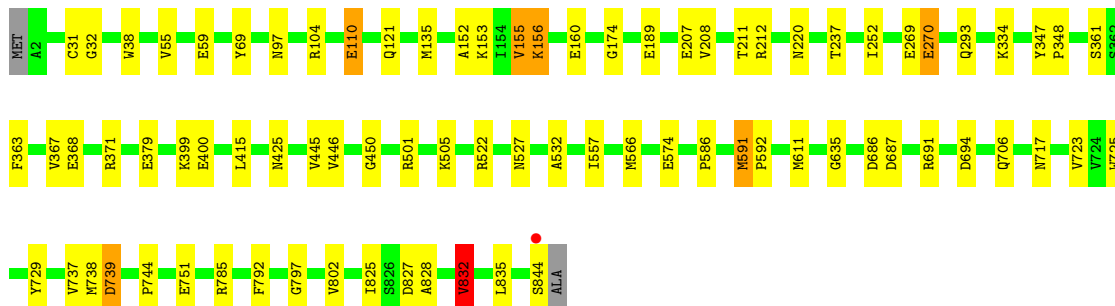
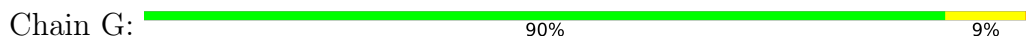


- Molecule 1: AroA

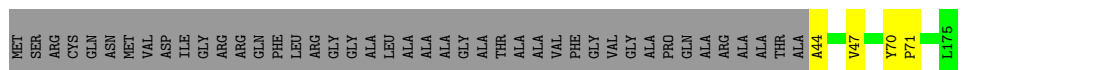




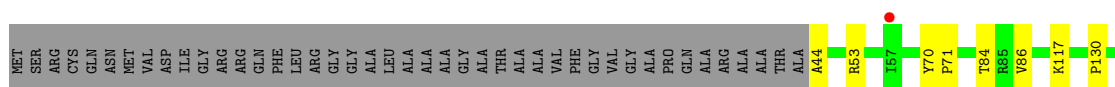
• Molecule 1: AroA



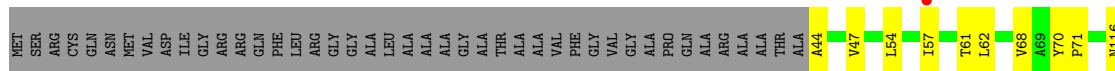
• Molecule 2: AroB



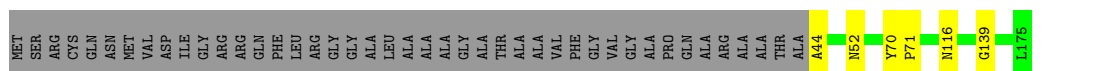
• Molecule 2: AroB



• Molecule 2: AroB



• Molecule 2: AroB



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.53Å 148.40Å 232.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.53 – 1.89 141.53 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.8 (141.53-1.89) 99.8 (141.53-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.24	13/6730 (0.2%)	1.11	16/9117 (0.2%)
1	C	1.23	18/6721 (0.3%)	1.11	16/9105 (0.2%)
1	E	1.22	14/6721 (0.2%)	1.11	14/9105 (0.2%)
1	G	1.22	10/6713 (0.1%)	1.10	13/9094 (0.1%)
2	B	1.12	0/1018	1.02	0/1387
2	D	1.10	1/1018 (0.1%)	0.99	0/1387
2	F	1.15	0/1018	1.09	2/1387 (0.1%)
2	H	1.11	1/1018 (0.1%)	1.01	1/1387 (0.1%)
All	All	1.22	57/30957 (0.2%)	1.09	62/41969 (0.1%)

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

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

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	739	ASP	CG-OD2	9.06	1.42	1.25
1	G	739	ASP	CG-OD2	7.89	1.40	1.25
1	C	522	ARG	CZ-NH1	7.59	1.43	1.32
1	C	599	ARG	CD-NE	-7.56	1.35	1.46
1	G	252	ILE	CA-CB	7.55	1.58	1.54

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	599	ARG	NE-CZ-NH2	-13.59	106.97	119.20
1	E	599	ARG	NE-CZ-NH2	-11.02	109.28	119.20
1	G	574	GLU	CB-CA-C	-9.17	95.22	110.72
1	C	599	ARG	NE-CZ-NH1	8.73	130.23	121.50
1	C	599	ARG	CD-NE-CZ	8.45	136.22	124.40

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	65	0
1	C	6564	0	6321	51	0
1	E	6564	0	6321	44	0
1	G	6559	0	6317	42	1
2	B	995	0	947	5	0
2	D	995	0	947	6	0
2	F	995	0	947	10	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

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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	2	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	28	0
13	B	111	0	0	3	0
13	C	730	0	0	19	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	14	2
13	H	123	0	0	2	0
All	All	34457	0	29456	229	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 229 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

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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:A:358:GLY:HA3	1:A:693:MET:HE3	1.46	0.97

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%)	48 40
1	C	844/845 (100%)	810 (96%)	33 (4%)	1 (0%)	48 40
1	E	844/845 (100%)	815 (97%)	28 (3%)	1 (0%)	48 40
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%)	48 40

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%)	671 (98%)	10 (2%)	57	56
1	C	680/678 (100%)	669 (98%)	11 (2%)	55	54
1	E	680/678 (100%)	667 (98%)	13 (2%)	50	47
1	G	679/678 (100%)	666 (98%)	13 (2%)	50	47
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%)	102 (97%)	3 (3%)	37	31
2	H	105/130 (81%)	105 (100%)	0	100	100
All	All	3140/3232 (97%)	3090 (98%)	50 (2%)	55	54

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	347	TYR
2	F	68	VAL
1	G	844	SER
1	E	379	GLU
1	E	644	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	116	ASN
1	G	118	ASN
1	G	535	GLN

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Mol	Chain	Res	Type
1	G	220	ASN
1	G	21	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
7	SO4	C	2007	-	4,4,4	0.76	0	6,6,6	0.91	0
6	F3S	G	2006	1	0,9,9	-	-	-		
7	SO4	A	2008	-	4,4,4	0.48	0	6,6,6	0.71	0
3	MGD	A	2001	5	47,52,52	1.57	7 (14%)	58,81,81	1.78	14 (24%)
11	P33	A	2013	-	21,21,21	0.58	0	20,20,20	0.74	0
7	SO4	E	2008	-	4,4,4	0.80	0	6,6,6	1.21	1 (16%)
7	SO4	C	2009	-	4,4,4	0.54	0	6,6,6	0.55	0
3	MGD	E	2002	5	47,52,52	1.60	8 (17%)	58,81,81	1.89	15 (25%)
3	MGD	C	2002	5	47,52,52	1.75	10 (21%)	58,81,81	1.88	12 (20%)
9	GOL	C	2010	-	5,5,5	1.40	1 (20%)	5,5,5	0.94	0
7	SO4	G	2007	-	4,4,4	0.67	0	6,6,6	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	A	2011	-	5,5,5	0.74	0	5,5,5	1.55	1 (20%)
7	SO4	G	2008	-	4,4,4	0.58	0	6,6,6	0.41	0
11	P33	C	2012	-	21,21,21	0.73	0	20,20,20	1.43	4 (20%)
3	MGD	G	2001	5	47,52,52	1.39	9 (19%)	58,81,81	1.84	17 (29%)
12	FES	H	201	2	0,4,4	-	-	-	-	-
8	PGE	A	2010	-	9,9,9	1.01	0	8,8,8	1.87	4 (50%)
9	GOL	G	2012	-	5,5,5	1.37	0	5,5,5	2.61	3 (60%)
3	MGD	C	2001	5	47,52,52	1.50	10 (21%)	58,81,81	2.02	15 (25%)
10	SBO	A	2012	-	0,3,3	-	-	-	-	-
10	SBO	E	2011	-	0,3,3	-	-	-	-	-
11	P33	G	2010	-	21,21,21	0.68	0	20,20,20	1.16	2 (10%)
7	SO4	C	2008	-	4,4,4	0.44	0	6,6,6	0.80	0
7	SO4	A	2009	-	4,4,4	0.83	0	6,6,6	0.77	0
10	SBO	C	2011	-	0,3,3	-	-	-	-	-
3	MGD	A	2002	5	47,52,52	1.60	7 (14%)	58,81,81	1.77	12 (20%)
3	MGD	E	2001	5	47,52,52	1.45	8 (17%)	58,81,81	1.80	12 (20%)
6	F3S	A	2006	1	0,9,9	-	-	-	-	-
12	FES	F	201	2	0,4,4	-	-	-	-	-
3	MGD	G	2002	5	47,52,52	1.79	11 (23%)	58,81,81	1.98	17 (29%)
9	GOL	E	2010	-	5,5,5	0.93	0	5,5,5	1.82	1 (20%)
12	FES	D	201	2	0,4,4	-	-	-	-	-
7	SO4	E	2009	-	4,4,4	0.43	0	6,6,6	0.38	0
11	P33	G	2009	-	21,21,21	1.03	1 (4%)	20,20,20	1.68	6 (30%)
6	F3S	E	2006	1	0,9,9	-	-	-	-	-
6	F3S	C	2006	1	0,9,9	-	-	-	-	-
12	FES	B	201	2	0,4,4	-	-	-	-	-
11	P33	E	2012	-	21,21,21	0.77	0	20,20,20	1.13	1 (5%)
7	SO4	A	2007	-	4,4,4	0.56	0	6,6,6	1.05	0
9	GOL	G	2011	-	5,5,5	1.09	0	5,5,5	1.74	1 (20%)
7	SO4	E	2007	-	4,4,4	0.48	0	6,6,6	0.61	0
10	SBO	G	2013	-	0,3,3	-	-	-	-	-

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	F3S	G	2006	1	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MGD	A	2001	5	-	4/22/66/66	0/6/6/6
11	P33	A	2013	-	-	5/19/19/19	-
3	MGD	E	2002	5	-	5/22/66/66	0/6/6/6
3	MGD	C	2002	5	-	4/22/66/66	0/6/6/6
9	GOL	C	2010	-	-	2/4/4/4	-
9	GOL	A	2011	-	-	2/4/4/4	-
11	P33	C	2012	-	-	10/19/19/19	-
3	MGD	G	2001	5	-	3/22/66/66	0/6/6/6
12	FES	H	201	2	-	-	0/1/1/1
8	PGE	A	2010	-	-	5/7/7/7	-
9	GOL	G	2012	-	-	2/4/4/4	-
3	MGD	C	2001	5	-	5/22/66/66	0/6/6/6
11	P33	G	2010	-	-	10/19/19/19	-
3	MGD	A	2002	5	-	4/22/66/66	0/6/6/6
3	MGD	E	2001	5	-	4/22/66/66	0/6/6/6
6	F3S	A	2006	1	-	-	0/3/3/3
12	FES	F	201	2	-	-	0/1/1/1
3	MGD	G	2002	5	-	4/22/66/66	0/6/6/6
9	GOL	E	2010	-	-	4/4/4/4	-
12	FES	D	201	2	-	-	0/1/1/1
11	P33	G	2009	-	-	13/19/19/19	-
6	F3S	C	2006	1	-	-	0/3/3/3
6	F3S	E	2006	1	-	-	0/3/3/3
12	FES	B	201	2	-	-	0/1/1/1
11	P33	E	2012	-	-	10/19/19/19	-
9	GOL	G	2011	-	-	2/4/4/4	-

The worst 5 of 72 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 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2002	MGD	O11-C23-N22	-6.89	102.35	108.61
3	G	2002	MGD	O11-C23-N22	-6.60	102.62	108.61
3	C	2001	MGD	N9-C4-N3	5.21	136.37	125.95
3	G	2002	MGD	C23-C14-N15	5.08	112.86	107.87
3	C	2001	MGD	C5-C4-N3	-5.04	120.38	128.39

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

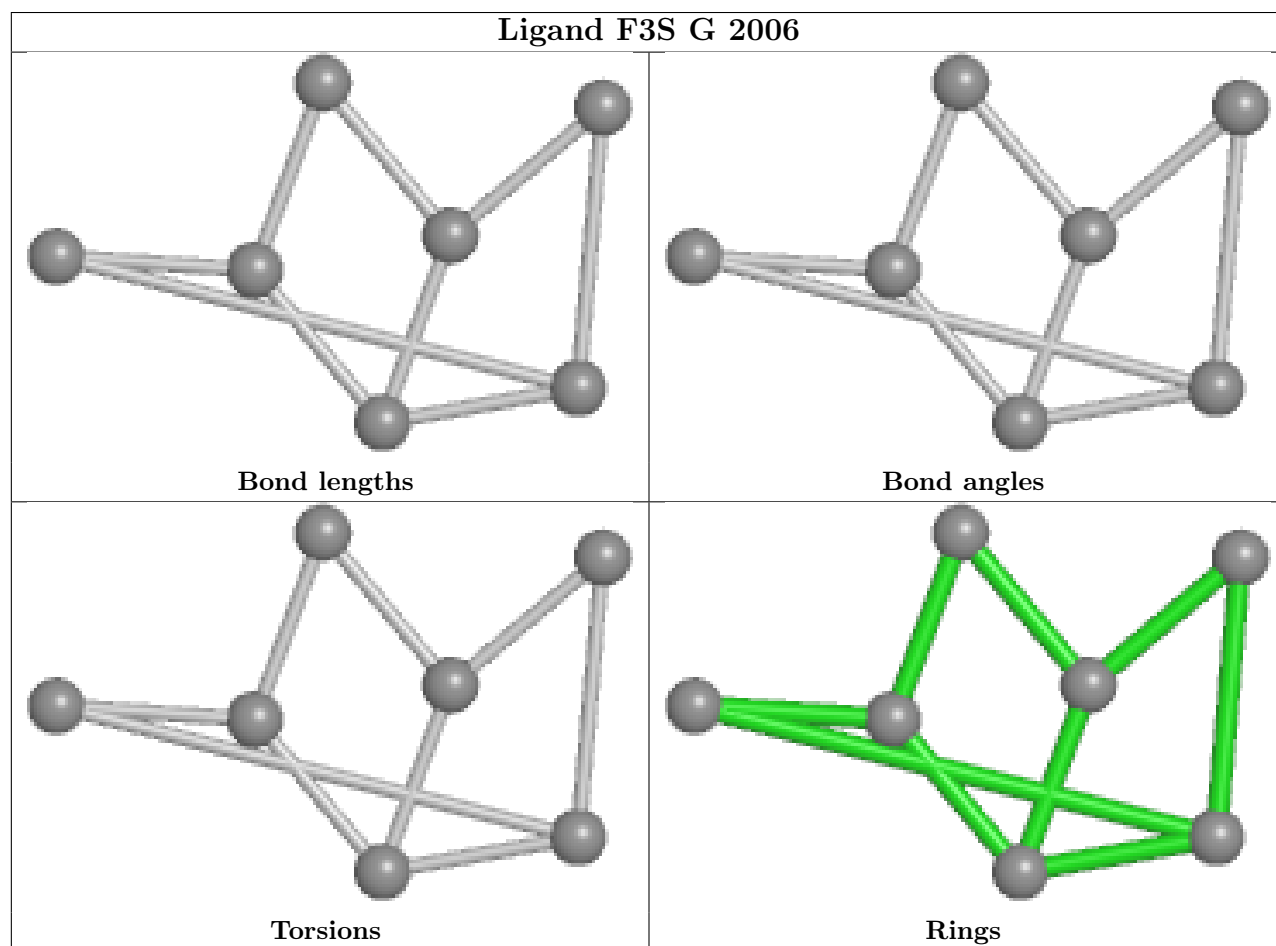
There are no ring outliers.

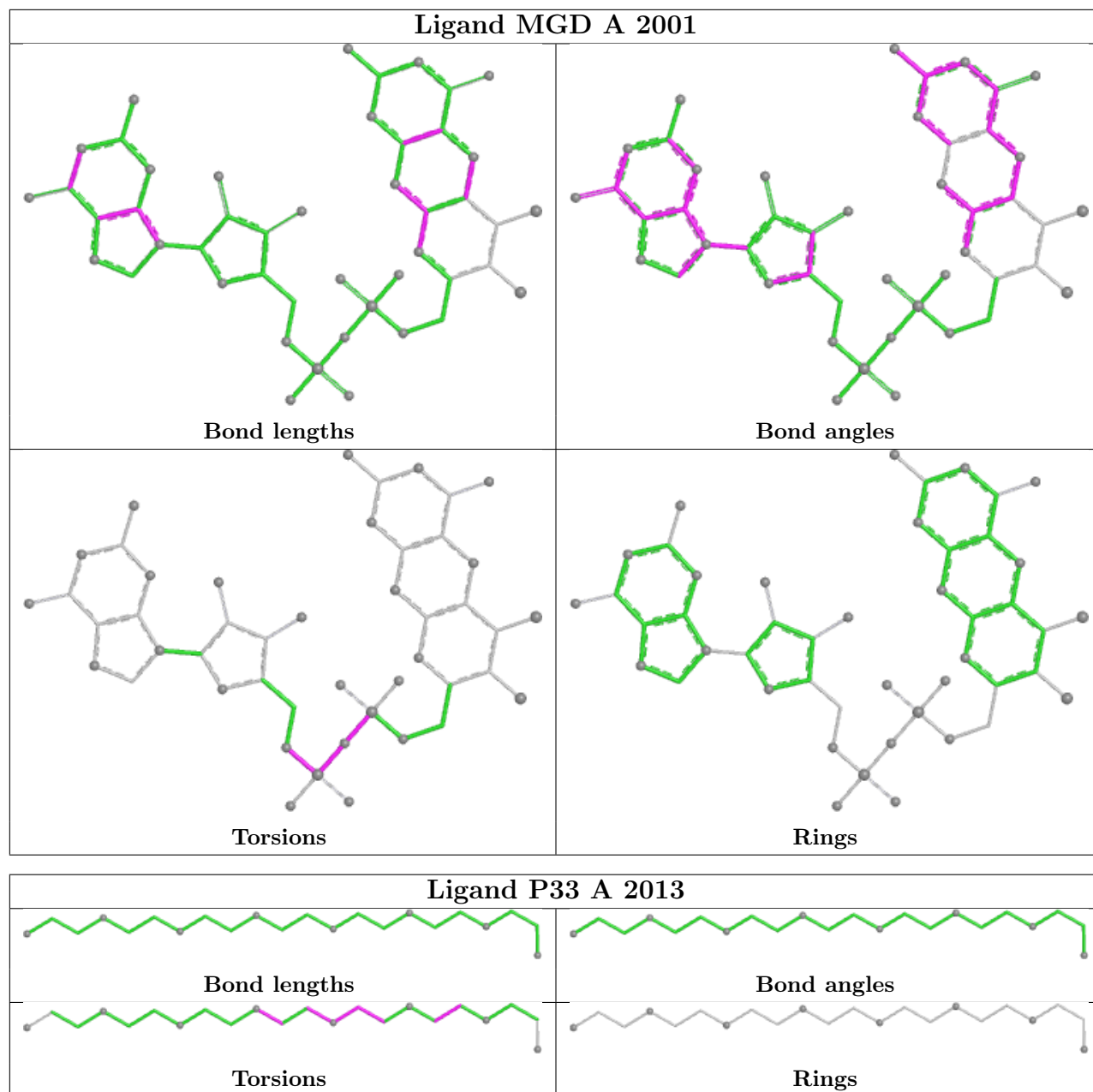
19 monomers are involved in 28 short contacts:

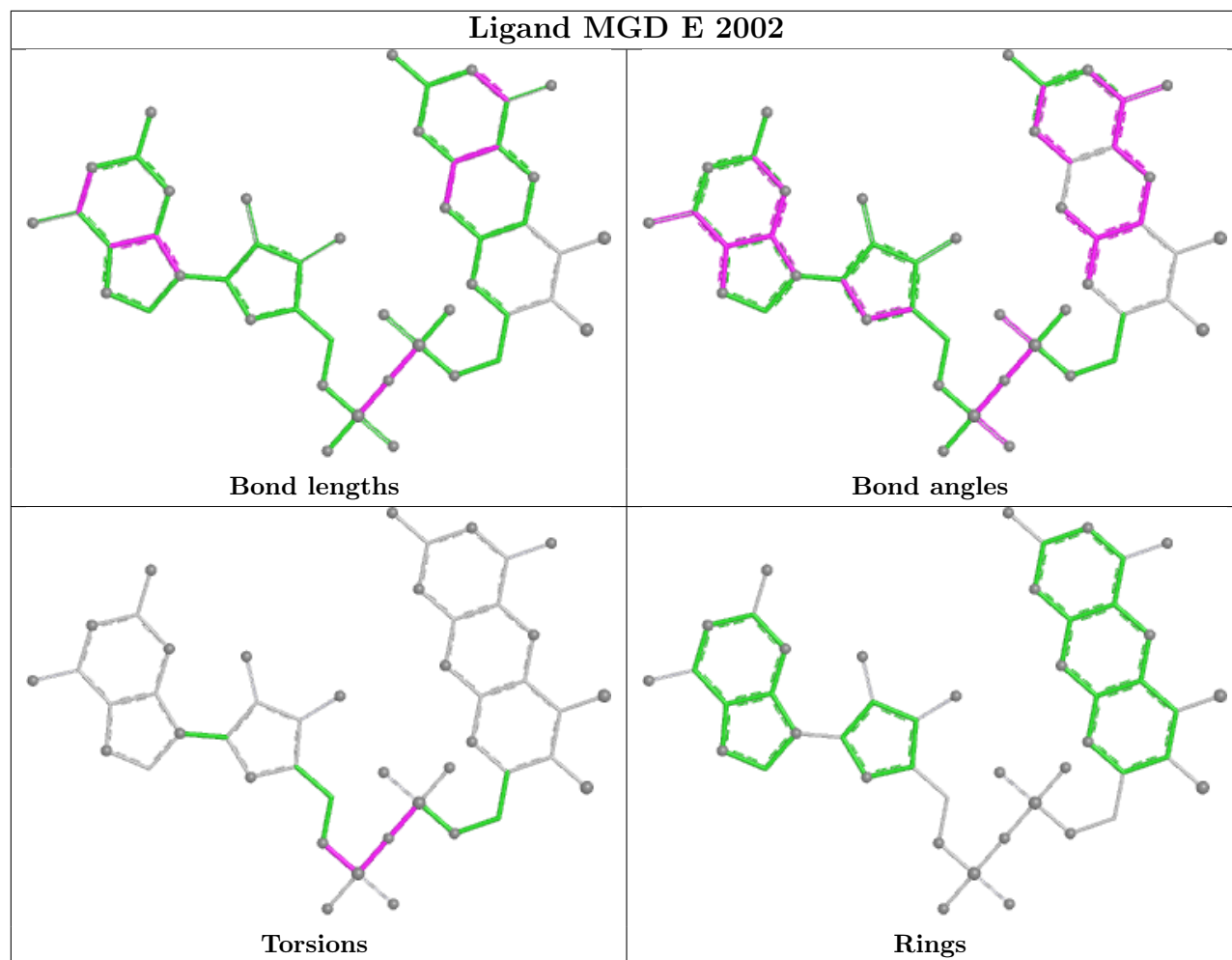
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	MGD	1	0
11	A	2013	P33	2	0
3	E	2002	MGD	2	0
3	C	2002	MGD	2	0
11	C	2012	P33	3	0
3	G	2001	MGD	2	0
8	A	2010	PGE	1	0
9	G	2012	GOL	1	0
3	C	2001	MGD	1	0
10	A	2012	SBO	1	0
10	E	2011	SBO	1	0
10	C	2011	SBO	1	0
3	A	2002	MGD	1	0
3	E	2001	MGD	2	0
3	G	2002	MGD	1	0
11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

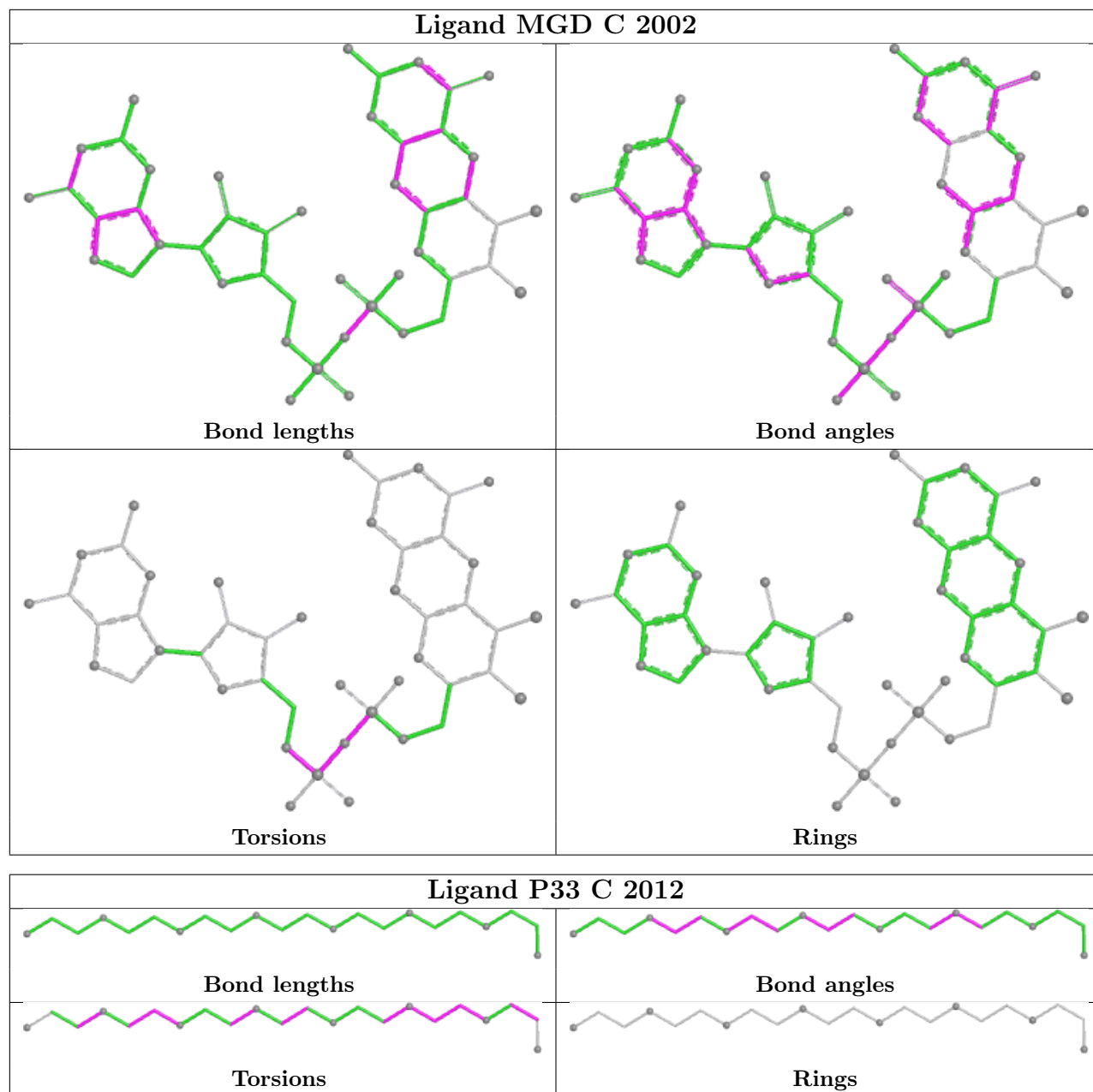
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

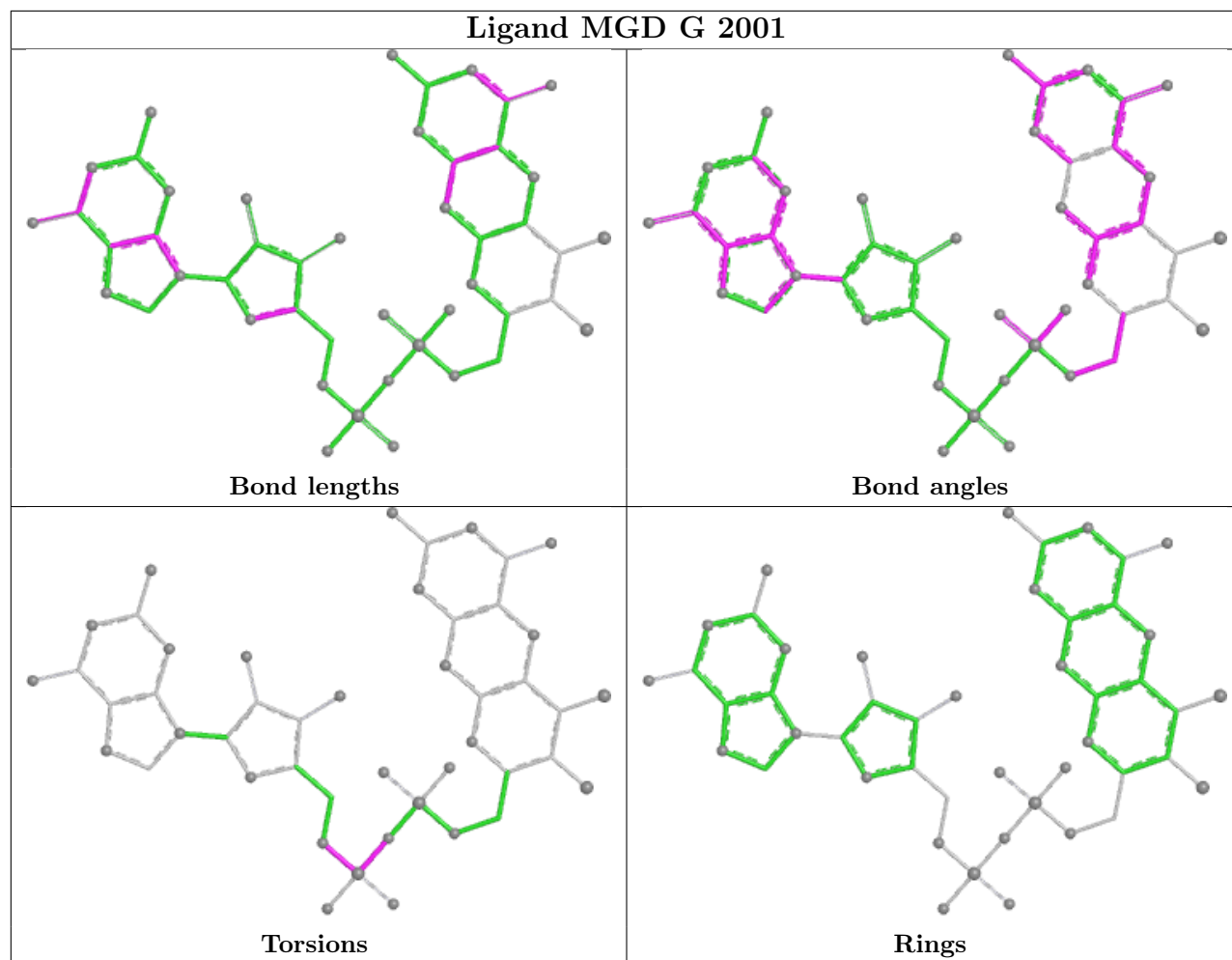
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

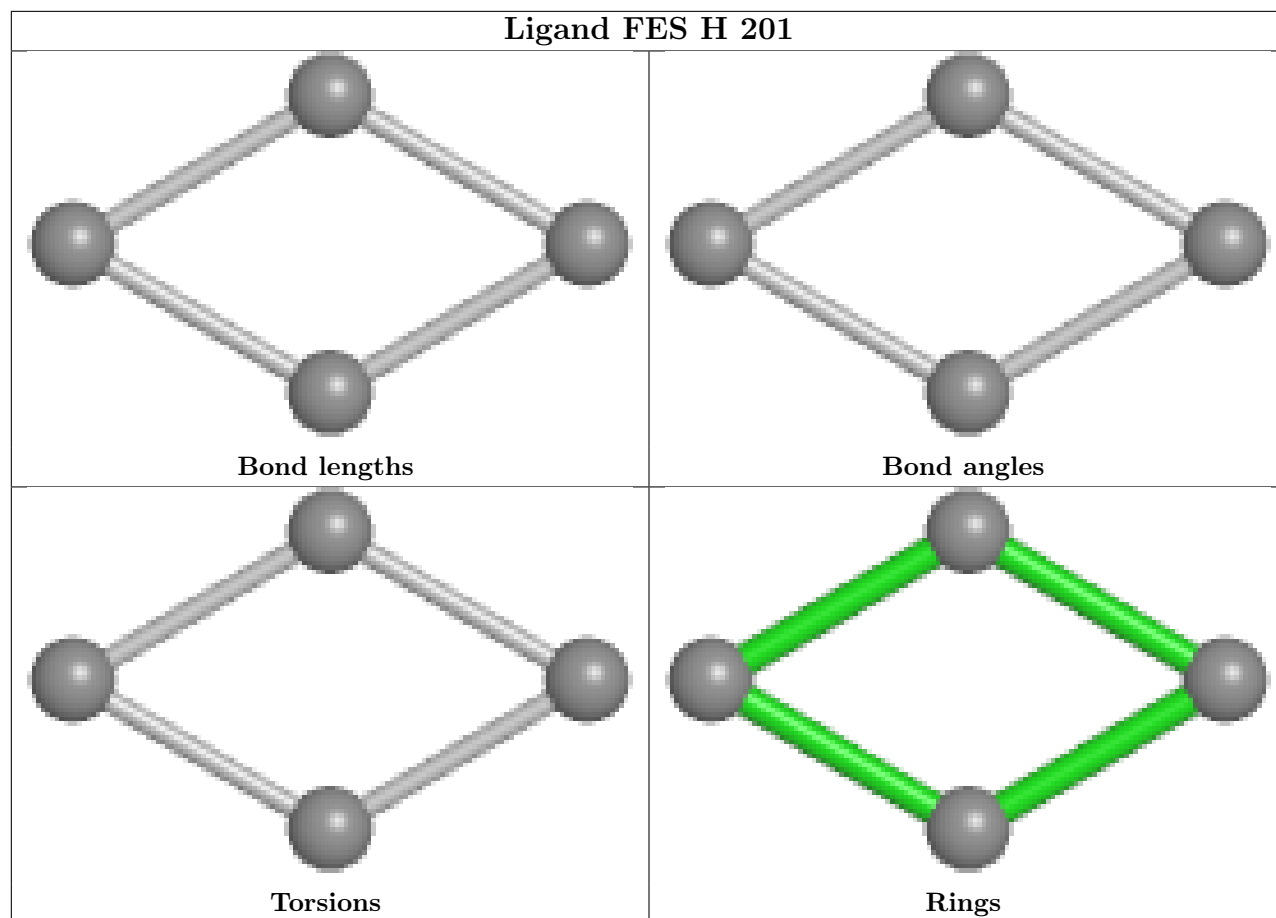


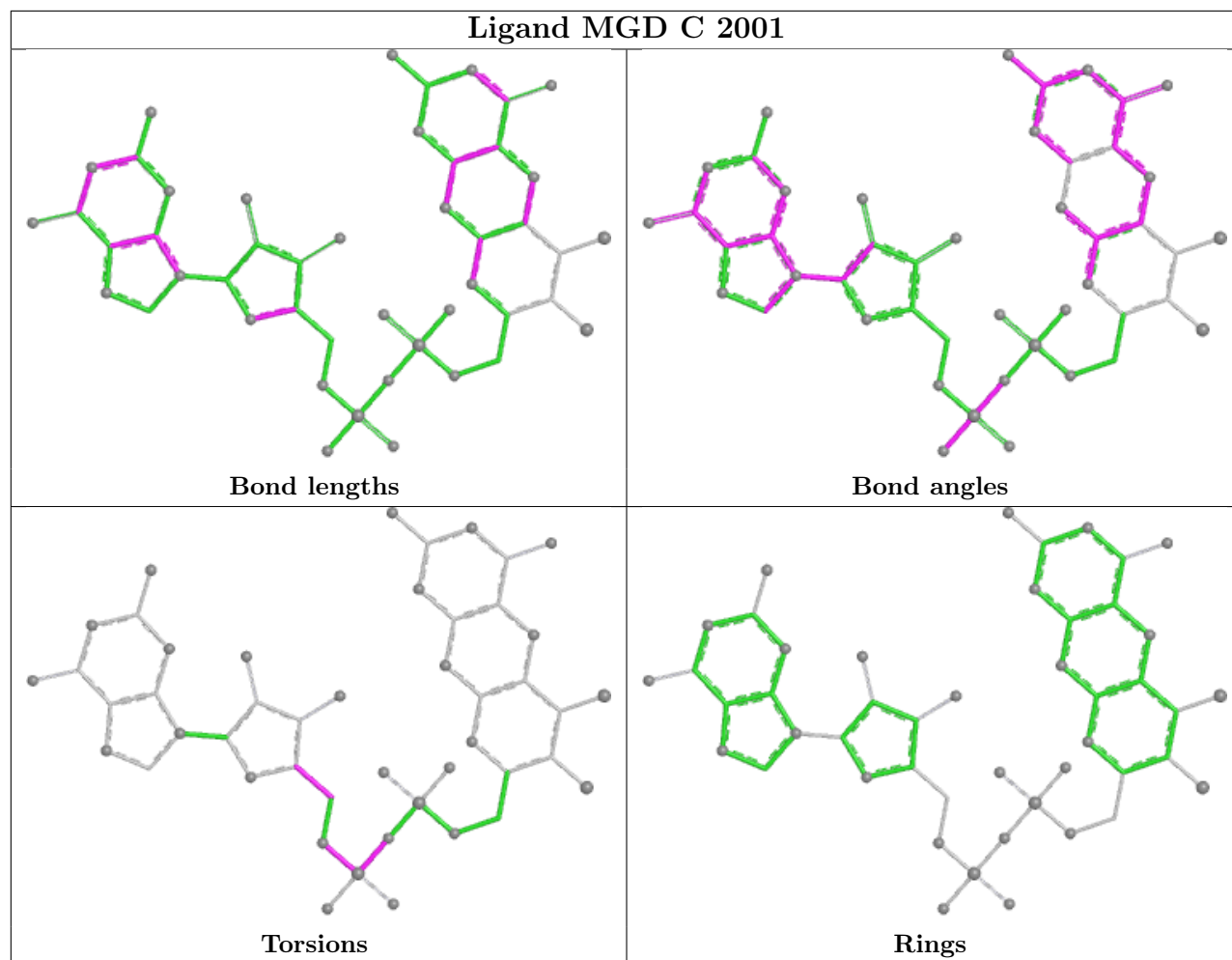


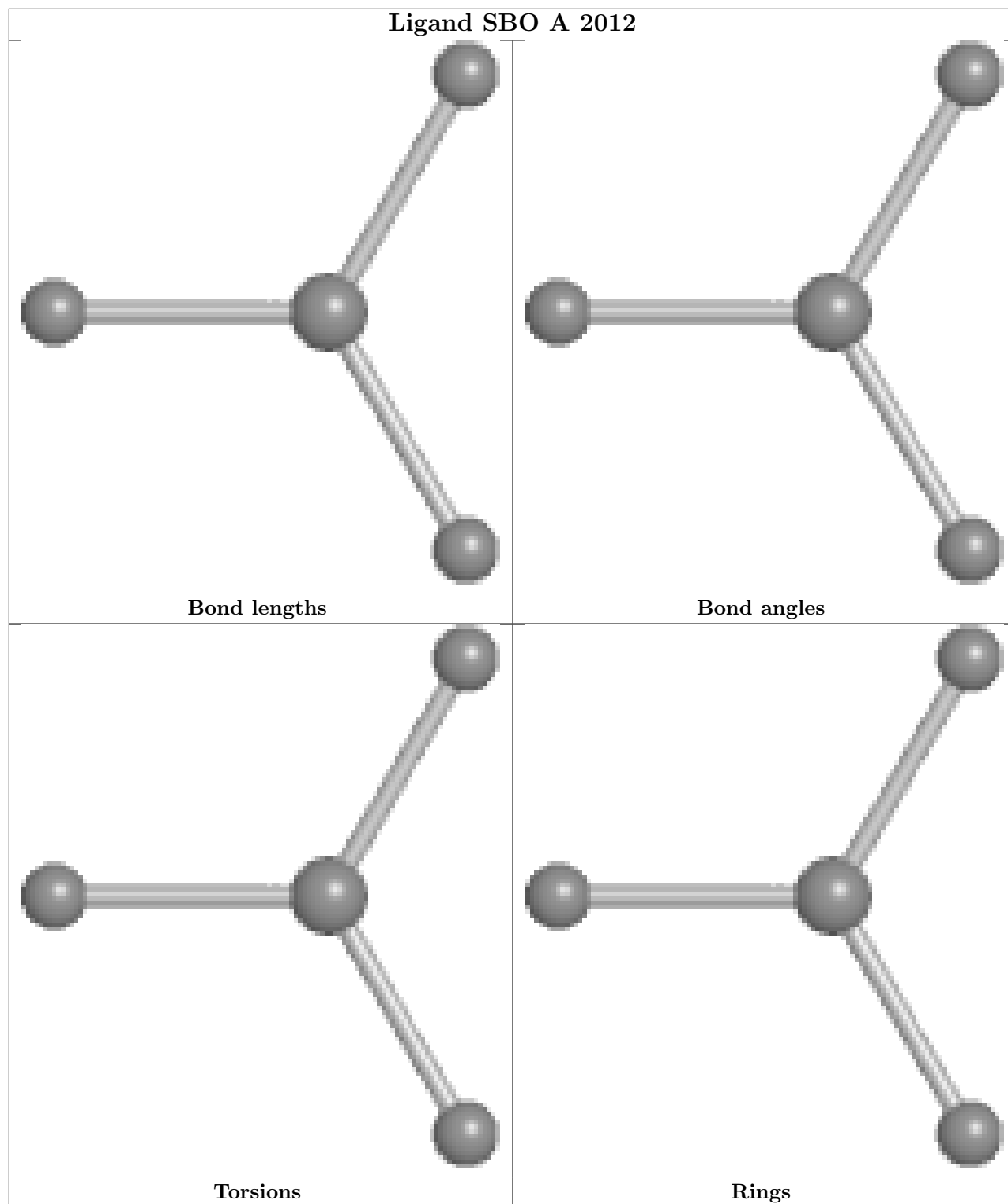


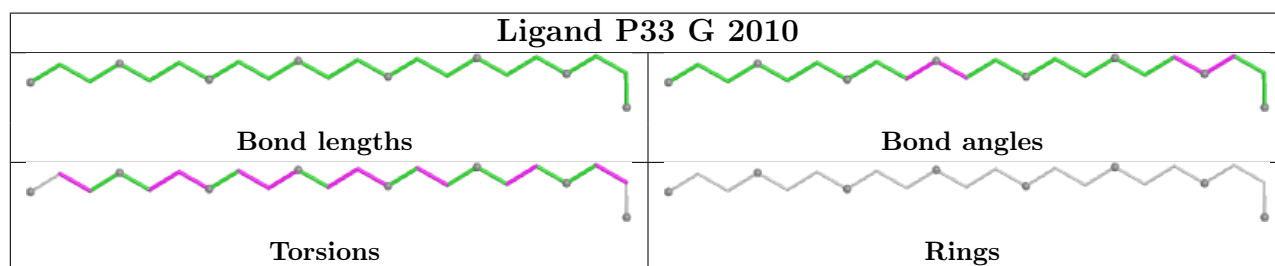
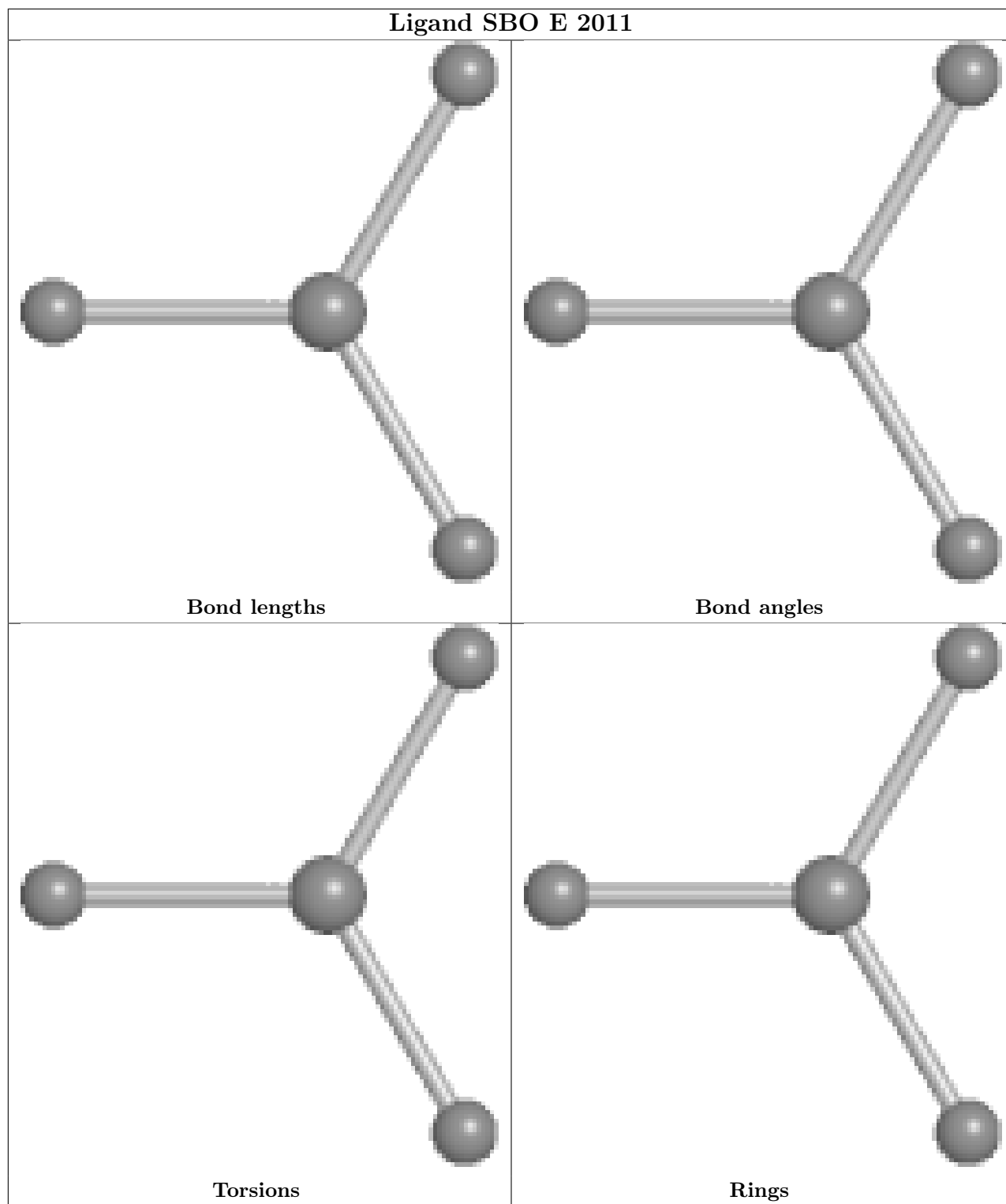


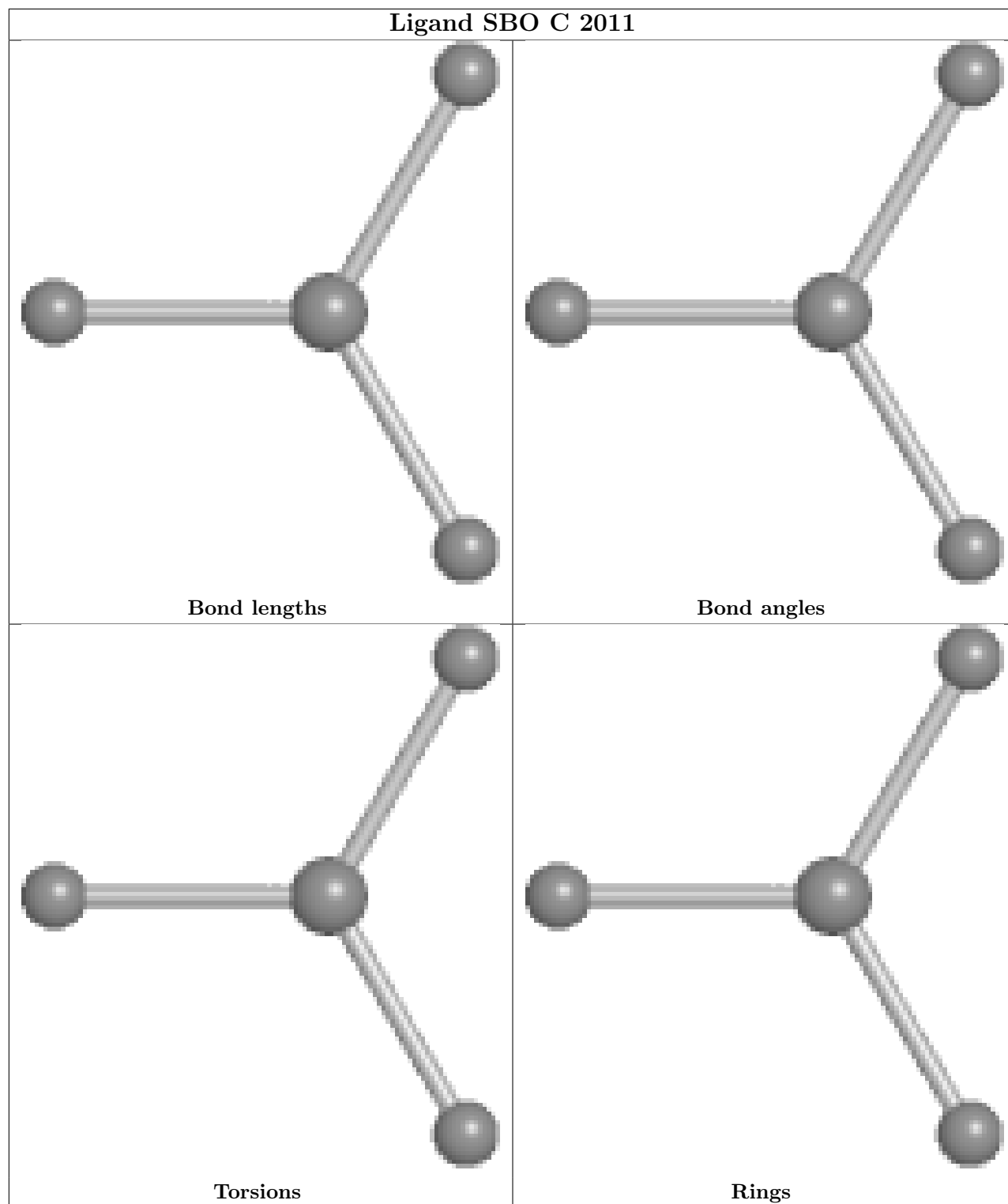


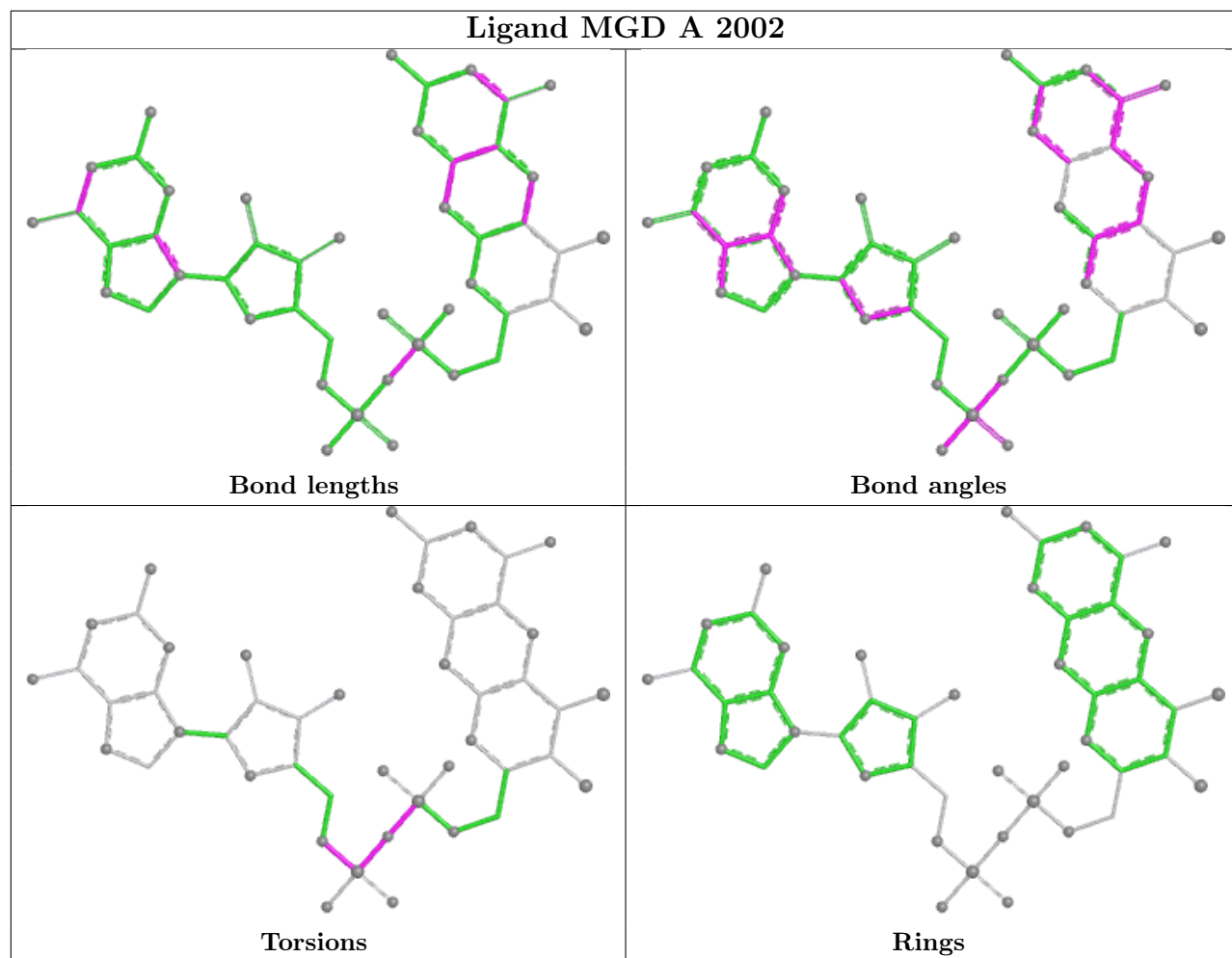


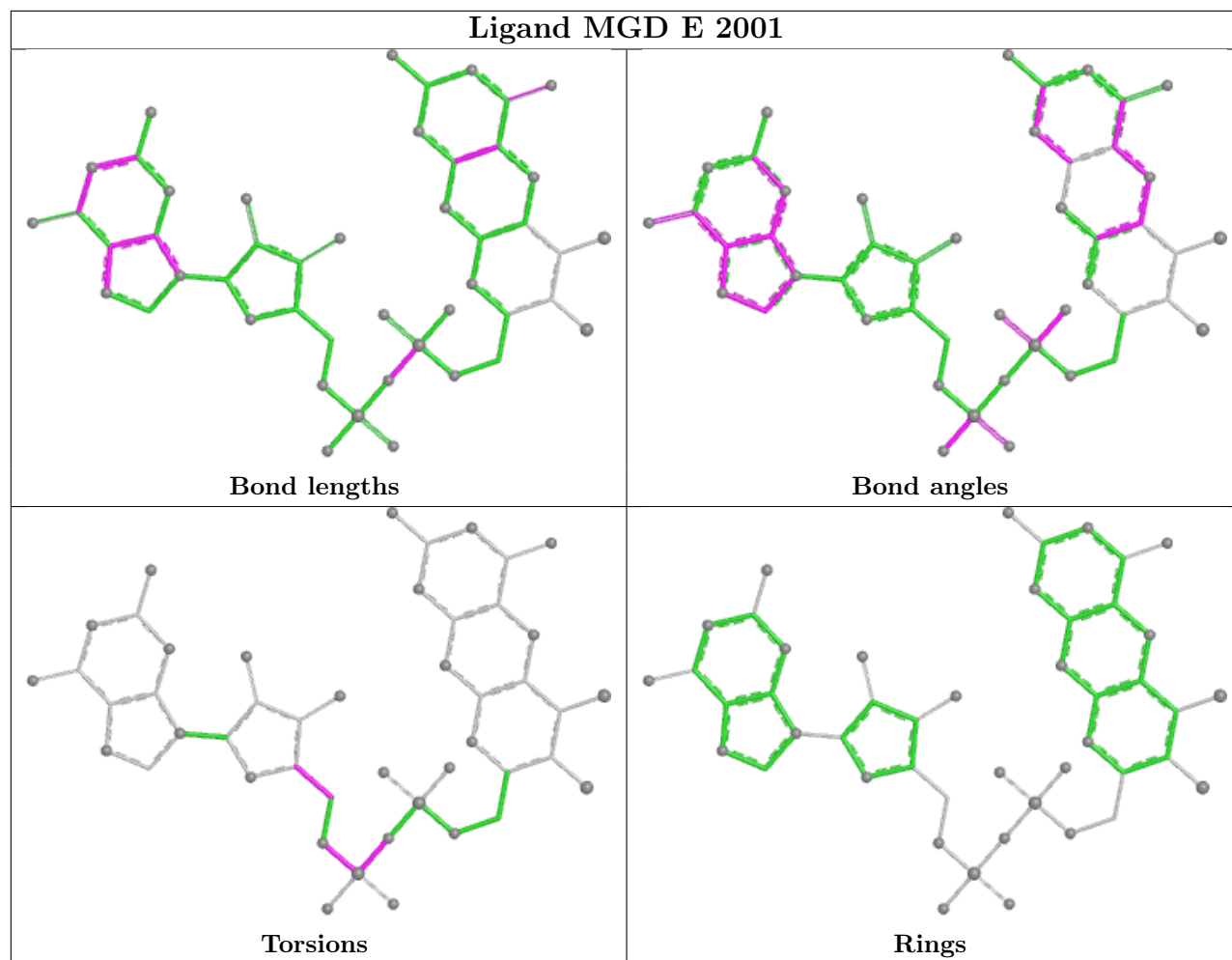


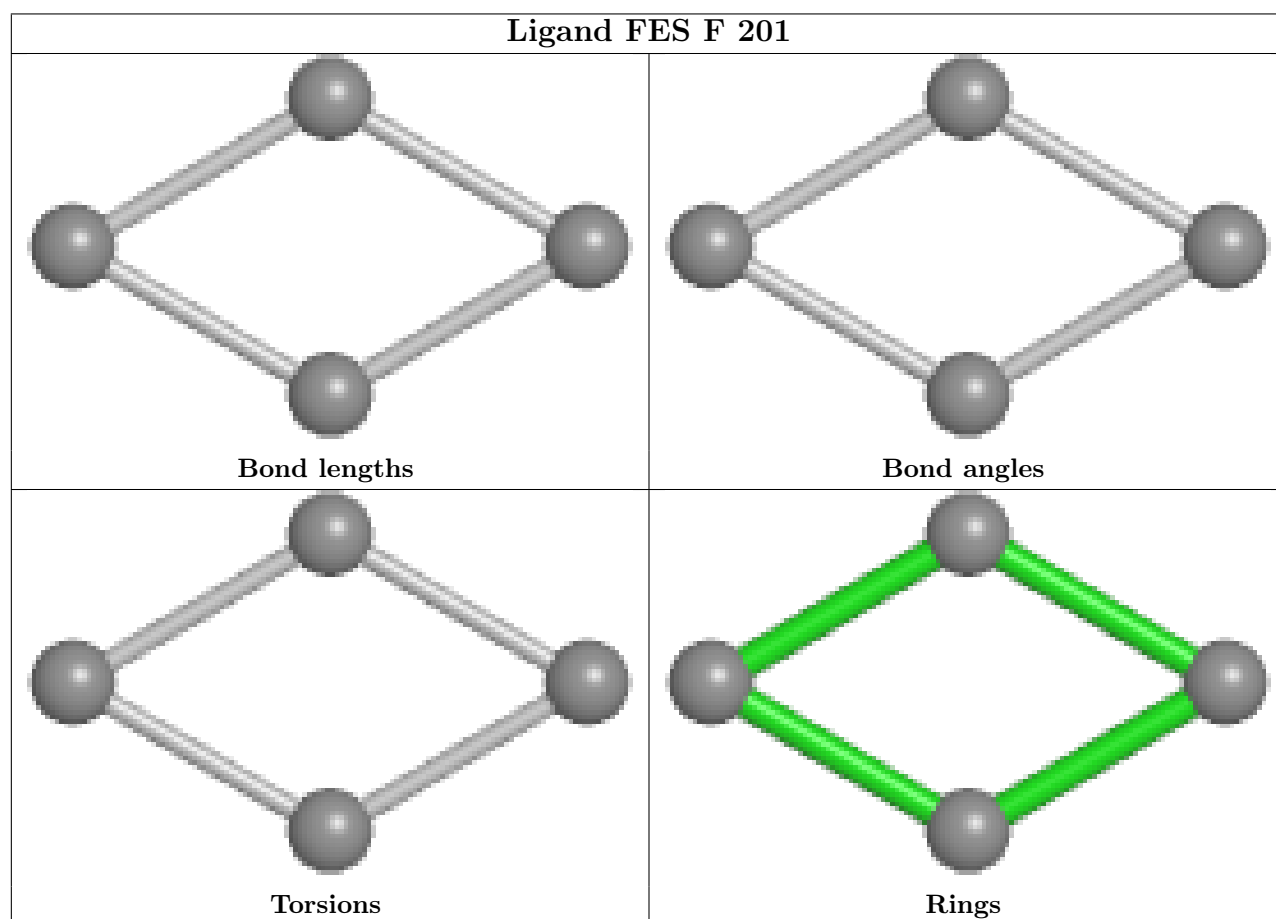
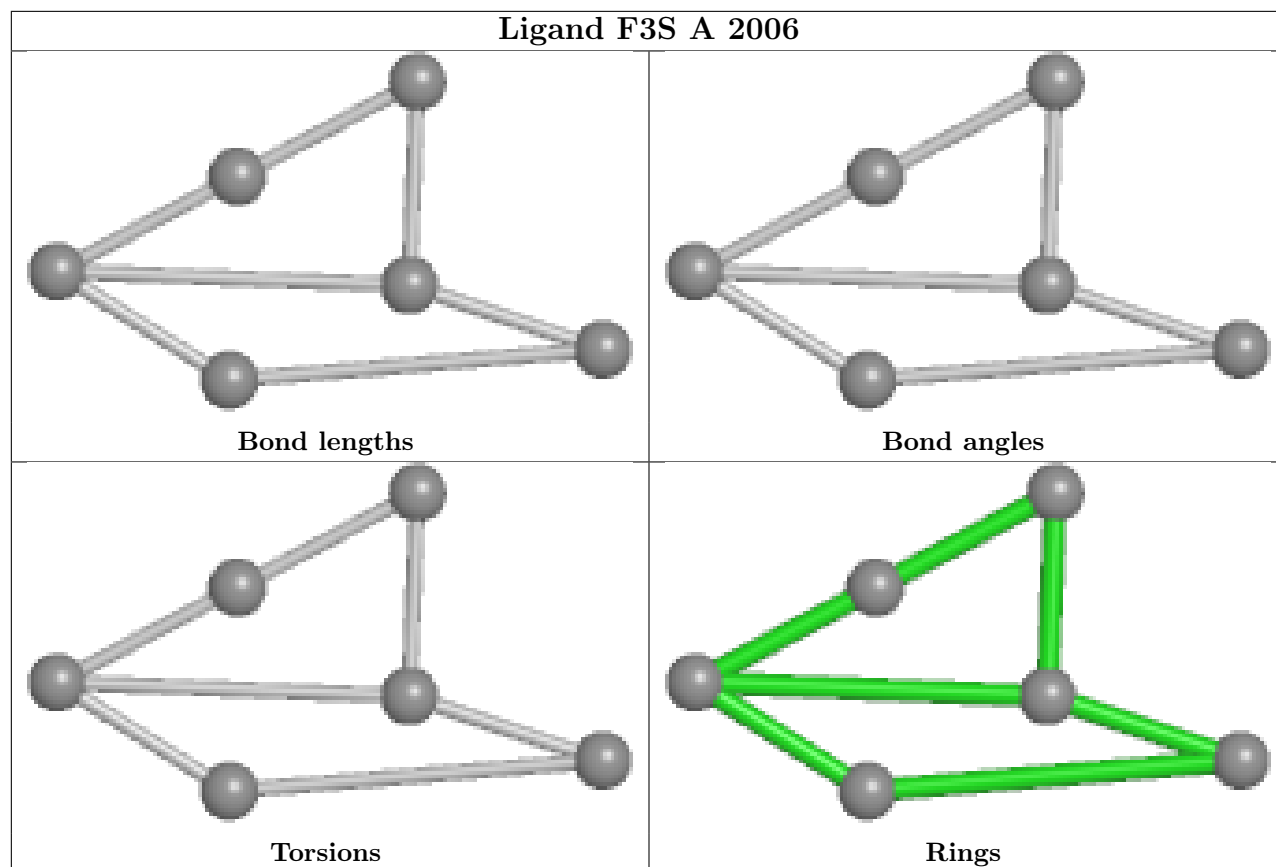


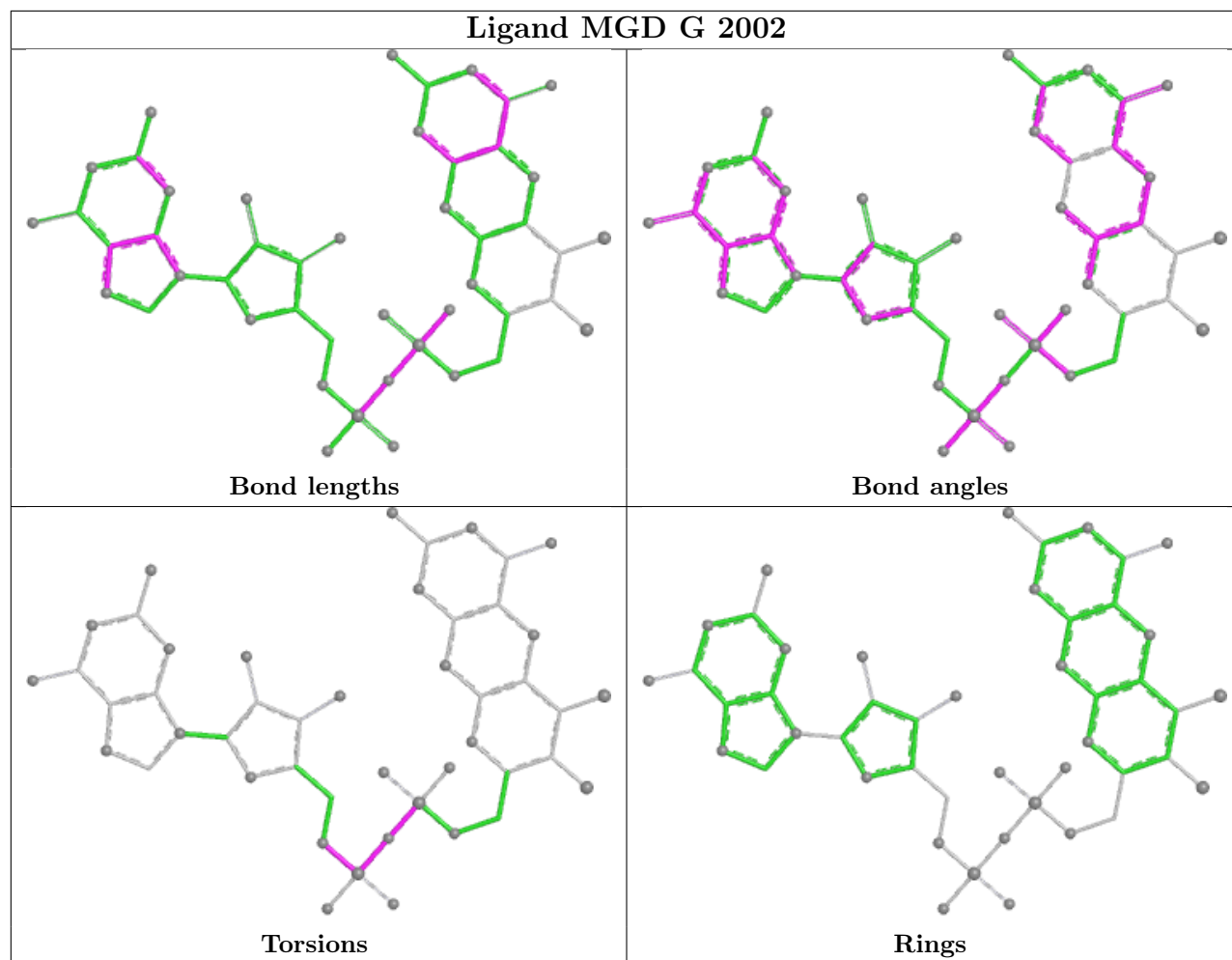


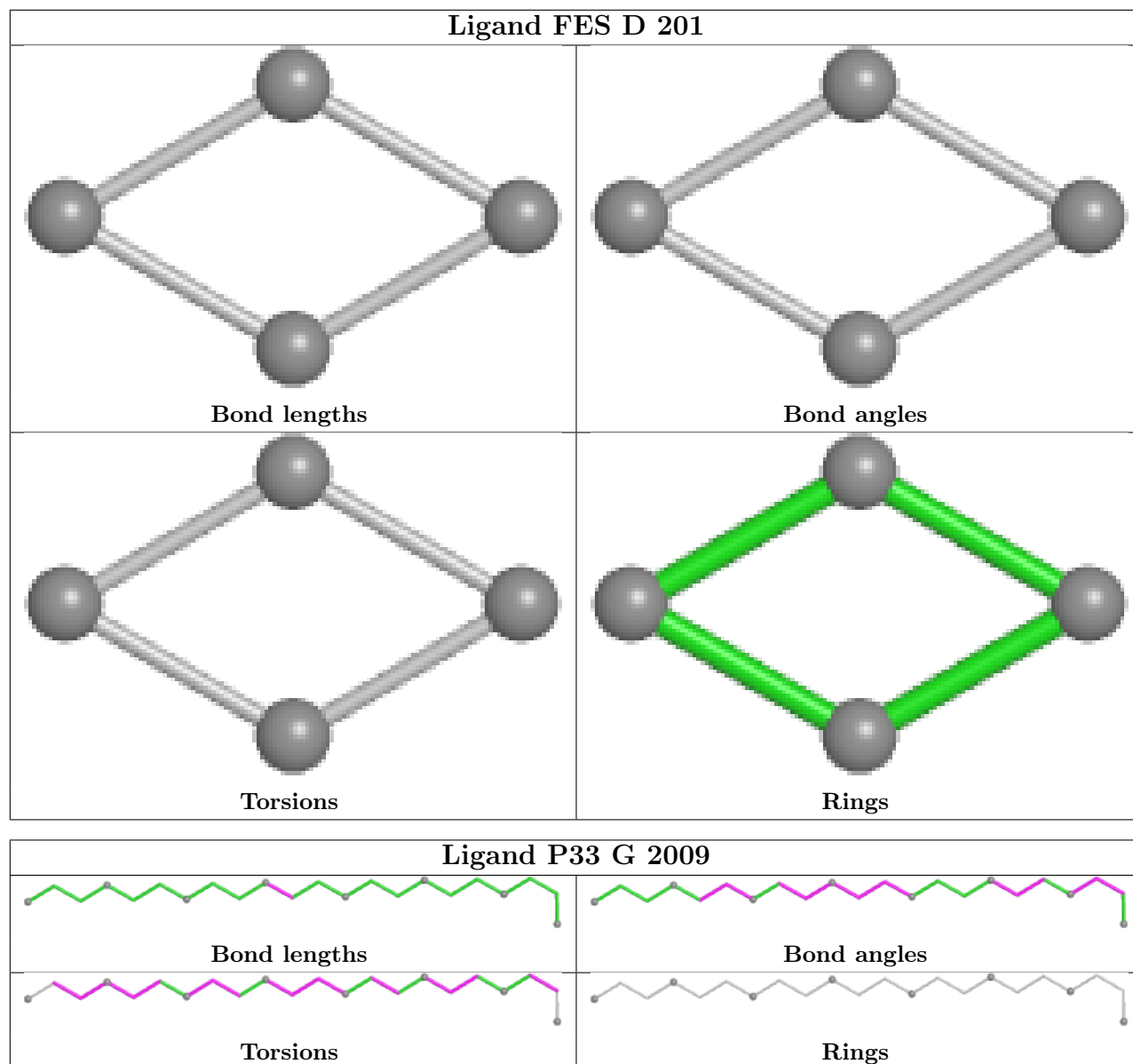


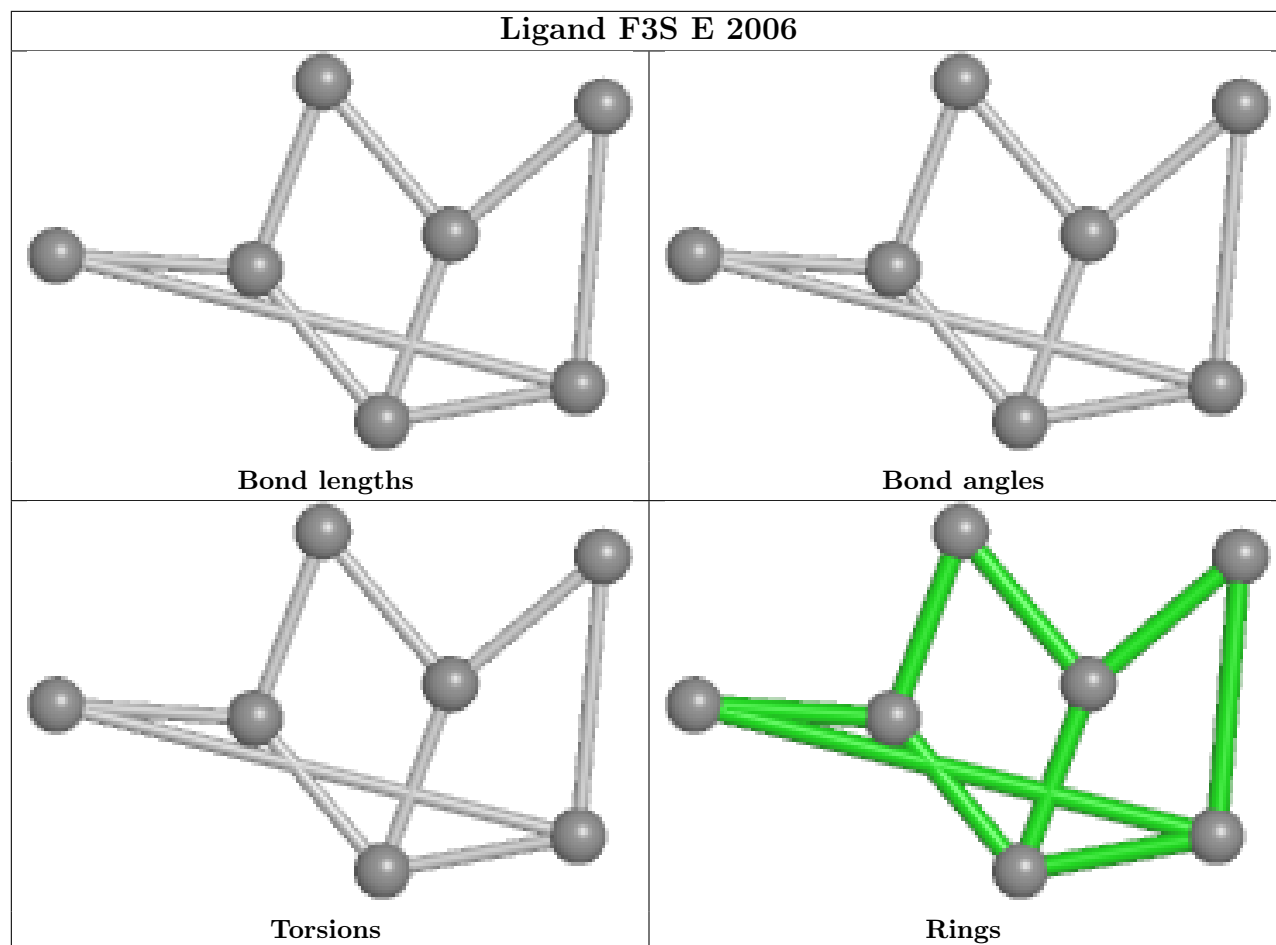


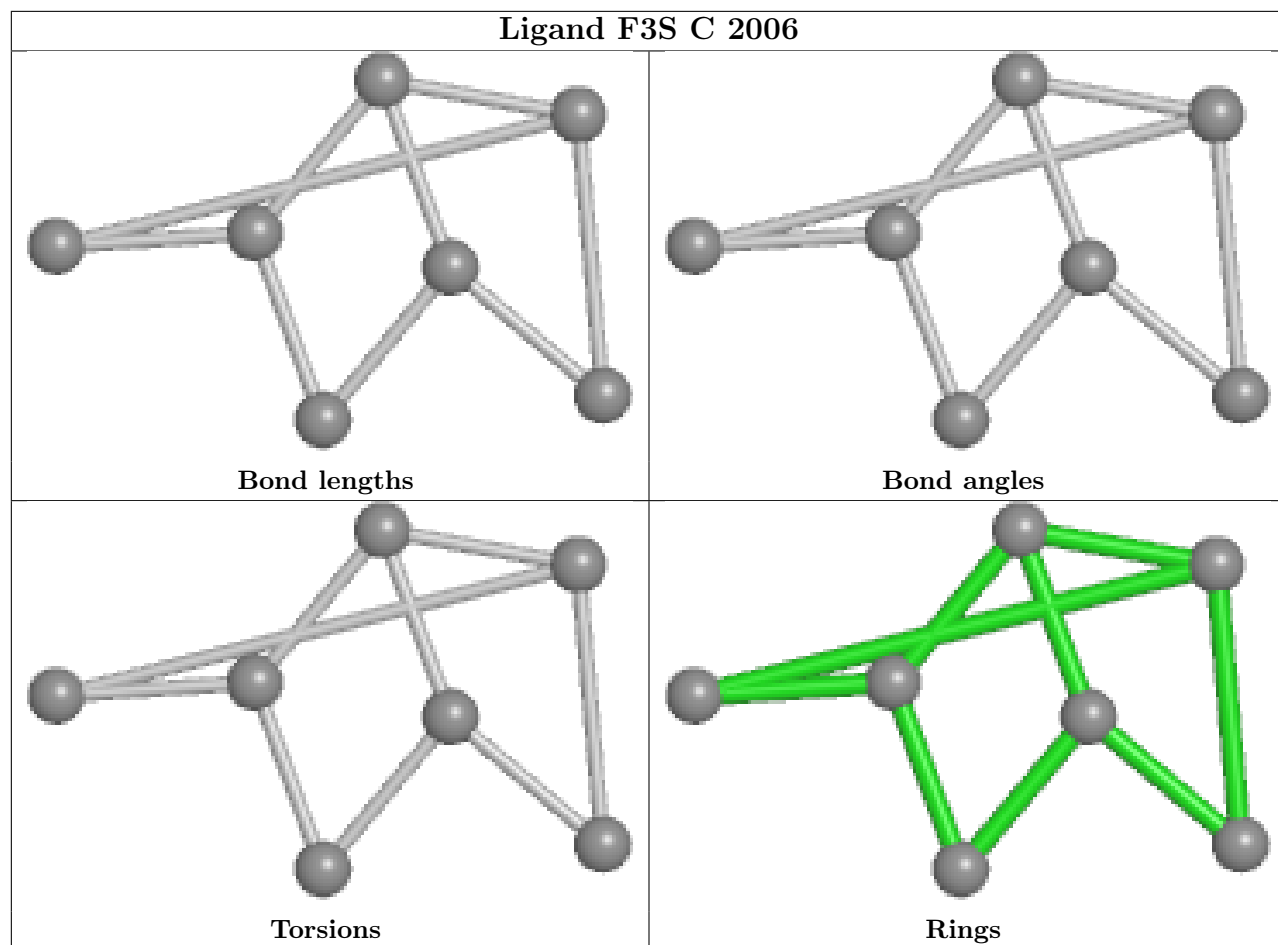


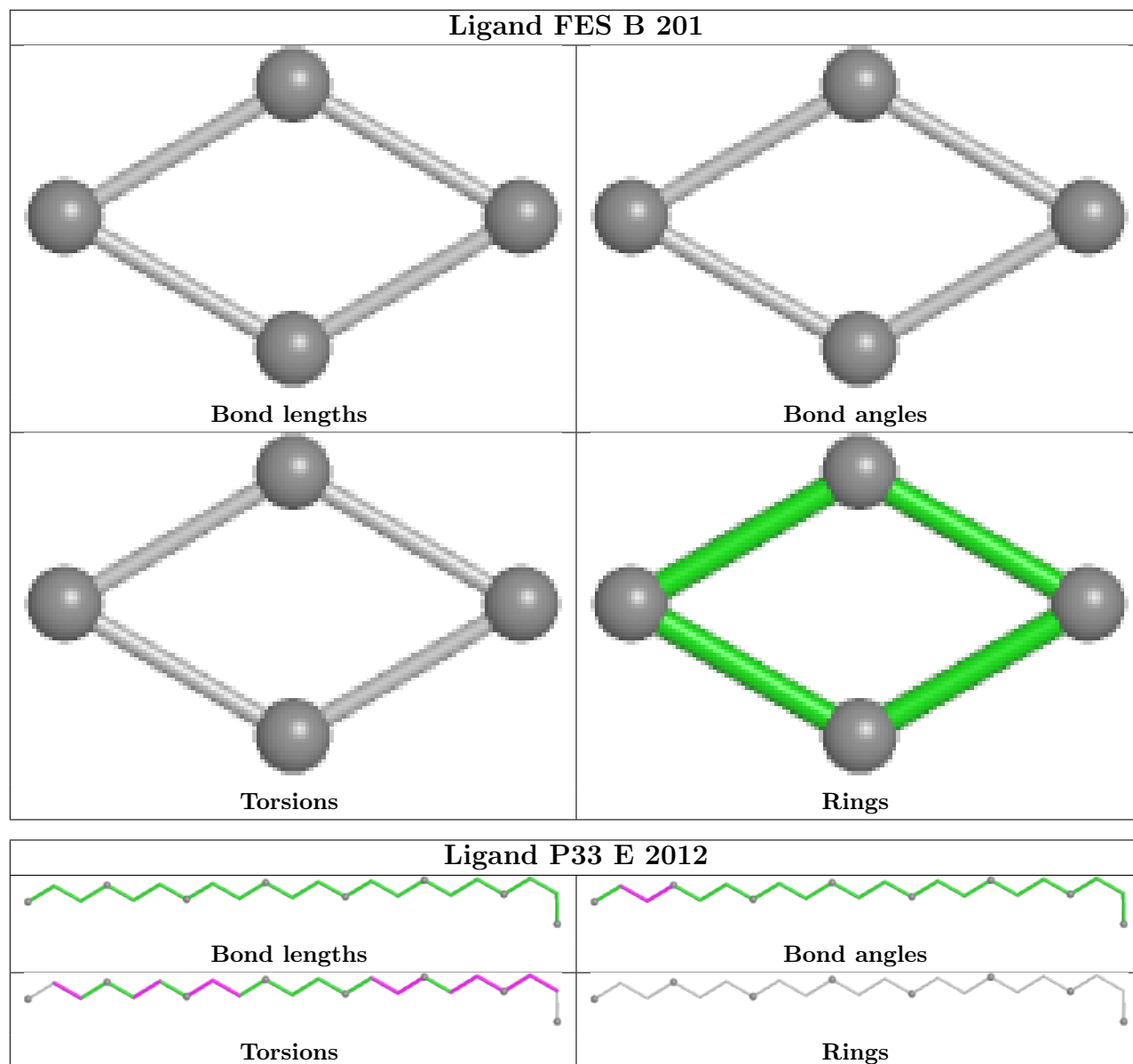


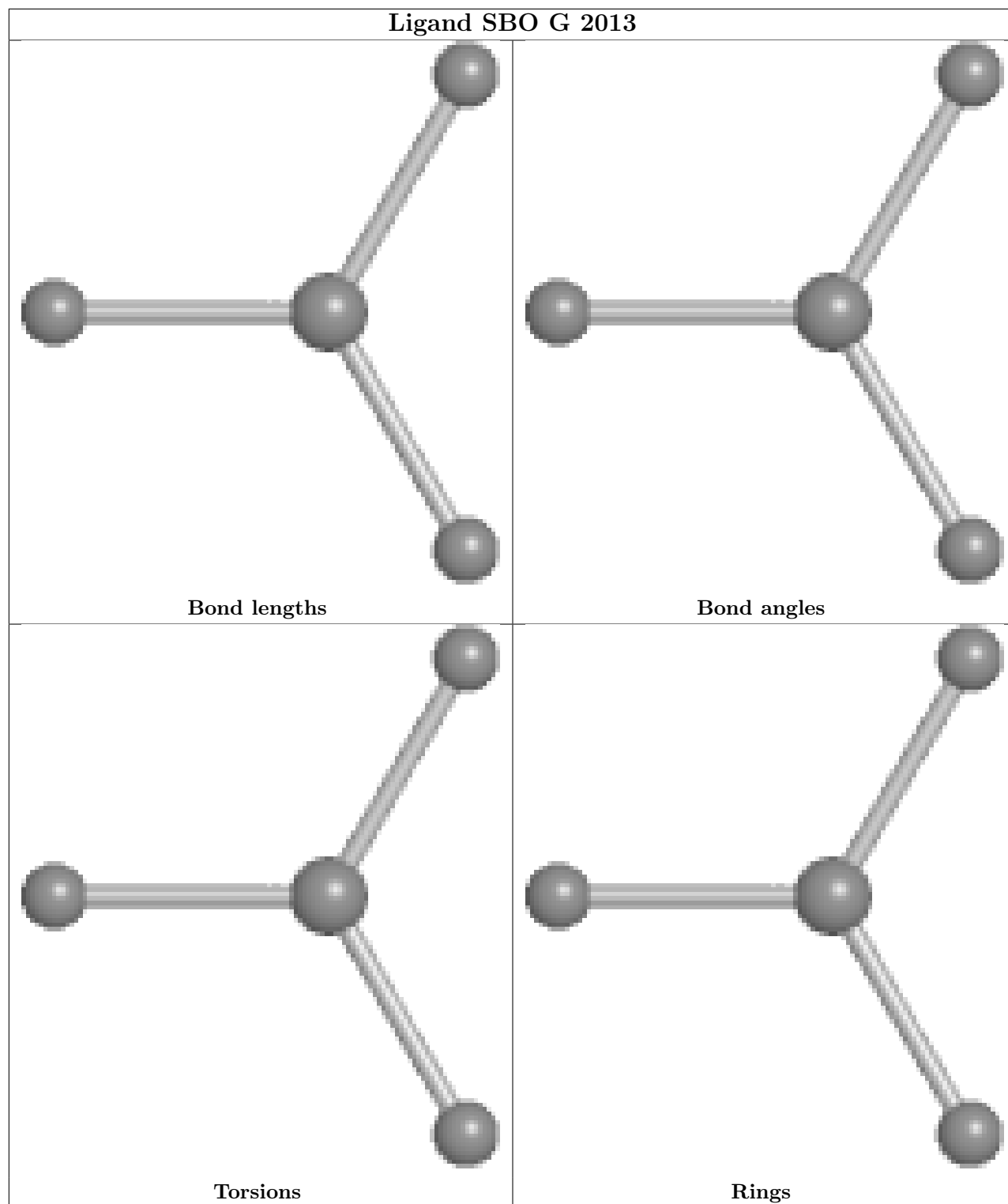












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	843/845 (99%)	-0.57	2 (0%) 91 92	13, 23, 41, 66	4 (0%)
1	C	843/845 (99%)	-0.40	2 (0%) 91 92	14, 27, 45, 75	3 (0%)
1	E	843/845 (99%)	-0.38	0 100 100	13, 27, 46, 81	3 (0%)
1	G	843/845 (99%)	-0.49	1 (0%) 92 92	14, 25, 42, 71	2 (0%)
2	B	132/175 (75%)	-0.11	0 100 100	20, 33, 50, 67	0
2	D	132/175 (75%)	-0.05	1 (0%) 82 85	23, 34, 56, 69	0
2	F	132/175 (75%)	0.14	1 (0%) 82 85	25, 38, 56, 69	0
2	H	132/175 (75%)	-0.29	0 100 100	20, 30, 50, 65	0
All	All	3900/4080 (95%)	-0.41	7 (0%) 91 92	13, 26, 47, 81	12 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	GLY	3.0
1	C	268	PRO	2.3
2	D	57	ILE	2.3
2	F	57	ILE	2.1
1	A	844	SER	2.1

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 oligosaccharides in this entry.

6.4 Ligands i

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

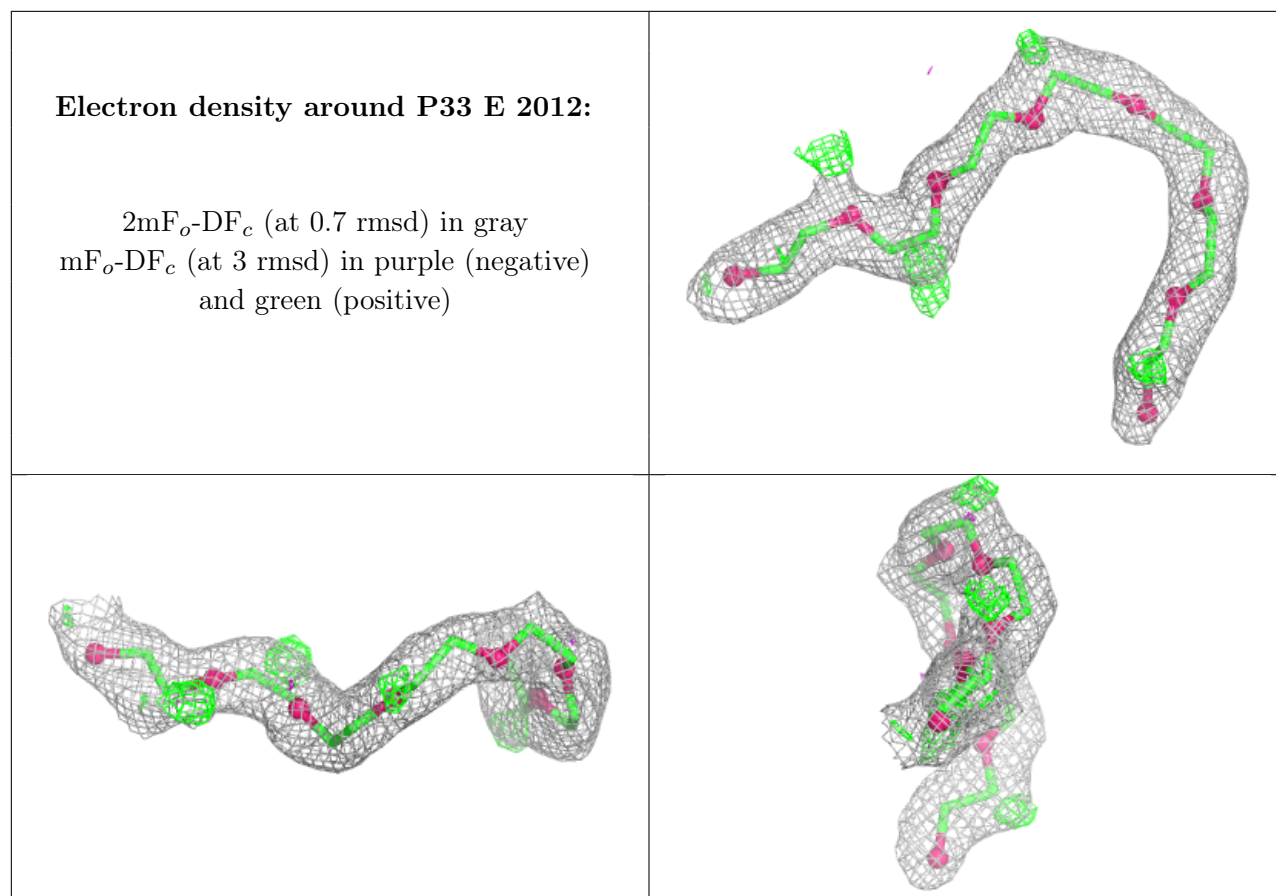
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SO4	E	2009	5/5	0.83	0.10	81,82,96,98	0
7	SO4	G	2008	5/5	0.87	0.09	70,75,83,98	0
9	GOL	C	2010	6/6	0.87	0.14	32,40,50,51	0
7	SO4	C	2009	5/5	0.89	0.08	76,78,83,90	0
7	SO4	C	2008	5/5	0.89	0.09	65,69,74,78	0
9	GOL	G	2012	6/6	0.89	0.13	34,44,48,51	0
9	GOL	G	2011	6/6	0.90	0.13	32,42,45,48	0
7	SO4	E	2007	5/5	0.90	0.09	71,72,76,86	0
11	P33	E	2012	22/22	0.90	0.12	35,45,51,53	0
9	GOL	E	2010	6/6	0.92	0.12	34,43,46,59	0
11	P33	A	2013	22/22	0.92	0.11	37,41,48,52	0
7	SO4	A	2007	5/5	0.92	0.10	58,59,74,74	0
11	P33	G	2010	22/22	0.92	0.12	38,48,54,57	0
8	PGE	A	2010	10/10	0.93	0.11	32,39,43,43	0
11	P33	C	2012	22/22	0.93	0.12	39,47,55,57	0
9	GOL	A	2011	6/6	0.93	0.10	31,39,44,54	0
11	P33	G	2009	22/22	0.93	0.10	26,37,42,47	0
7	SO4	A	2008	5/5	0.93	0.09	57,66,74,85	0
7	SO4	E	2008	5/5	0.97	0.09	30,32,45,45	0
7	SO4	C	2007	5/5	0.98	0.09	27,29,37,43	0
7	SO4	A	2009	5/5	0.98	0.07	27,30,37,39	0
7	SO4	G	2007	5/5	0.98	0.07	29,31,38,40	0
3	MGD	C	2001	47/47	0.99	0.04	18,20,25,27	0
3	MGD	C	2002	47/47	0.99	0.04	19,22,26,27	0
3	MGD	E	2001	47/47	0.99	0.04	15,20,23,29	0
3	MGD	E	2002	47/47	0.99	0.04	17,22,28,31	0
3	MGD	G	2001	47/47	0.99	0.04	17,20,25,26	0
3	MGD	G	2002	47/47	0.99	0.04	17,22,24,26	0
4	O	A	2003	1/1	0.99	0.06	29,29,29,29	0
4	O	A	2004	1/1	0.99	0.05	25,25,25,25	0
4	O	C	2003	1/1	0.99	0.04	19,19,19,19	0
4	O	C	2004	1/1	0.99	0.04	25,25,25,25	0
4	O	E	2003	1/1	0.99	0.05	28,28,28,28	0
4	O	E	2004	1/1	0.99	0.05	26,26,26,26	0
4	O	G	2003	1/1	0.99	0.07	27,27,27,27	0
4	O	G	2004	1/1	0.99	0.06	33,33,33,33	0
6	F3S	A	2006	7/7	0.99	0.02	21,22,23,24	0

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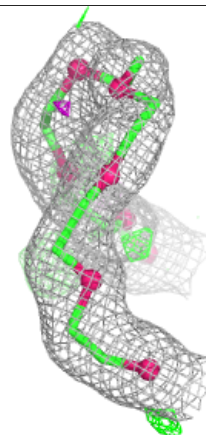
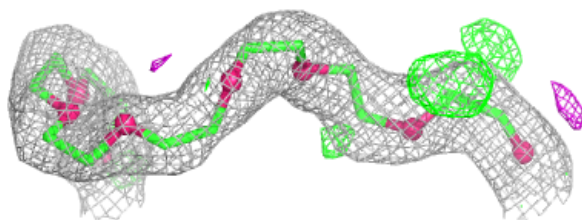
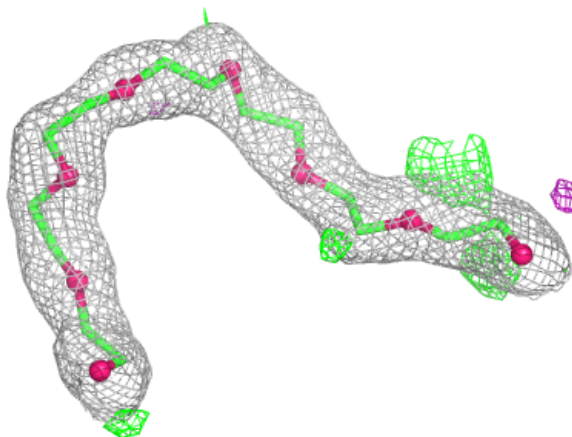
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	F3S	C	2006	7/7	0.99	0.03	23,25,26,26	0
6	F3S	E	2006	7/7	0.99	0.03	24,26,27,28	0
6	F3S	G	2006	7/7	0.99	0.03	22,23,26,26	0
3	MGD	A	2001	47/47	0.99	0.03	14,17,21,23	0
3	MGD	A	2002	47/47	0.99	0.03	15,17,20,22	0
12	FES	D	201	4/4	0.99	0.03	27,29,29,30	0
12	FES	F	201	4/4	0.99	0.02	28,29,30,30	0
10	SBO	G	2013	4/4	1.00	0.04	25,26,27,28	4
5	4MO	C	2005	1/1	1.00	0.02	24,24,24,24	0
5	4MO	E	2005	1/1	1.00	0.02	25,25,25,25	0
5	4MO	G	2005	1/1	1.00	0.02	22,22,22,22	0
5	4MO	A	2005	1/1	1.00	0.01	21,21,21,21	0
10	SBO	A	2012	4/4	1.00	0.03	22,22,24,30	4
12	FES	B	201	4/4	1.00	0.02	23,24,25,25	0
10	SBO	C	2011	4/4	1.00	0.03	27,27,27,29	4
10	SBO	E	2011	4/4	1.00	0.04	26,26,27,29	4
12	FES	H	201	4/4	1.00	0.02	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.

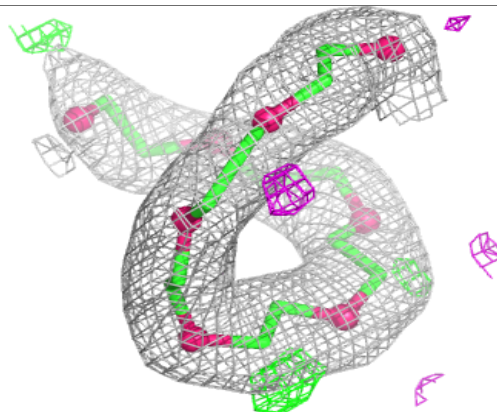
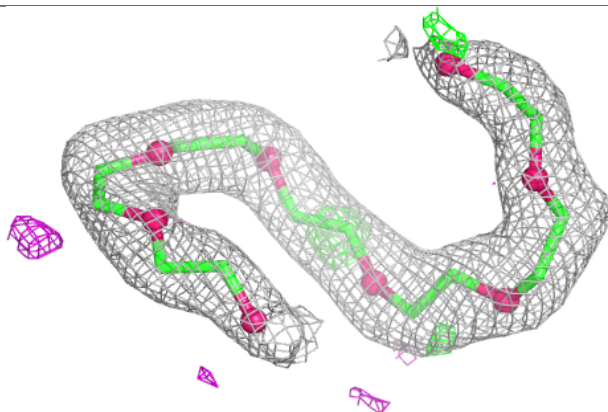
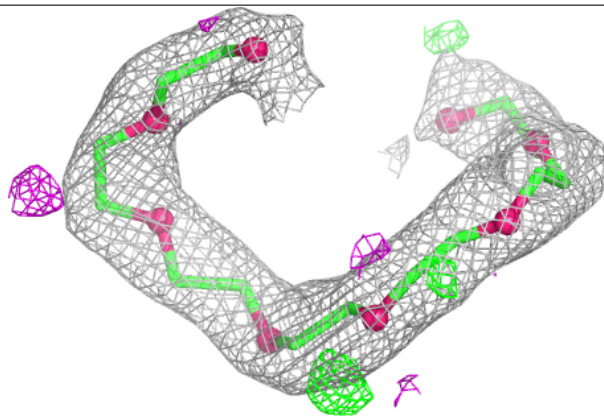


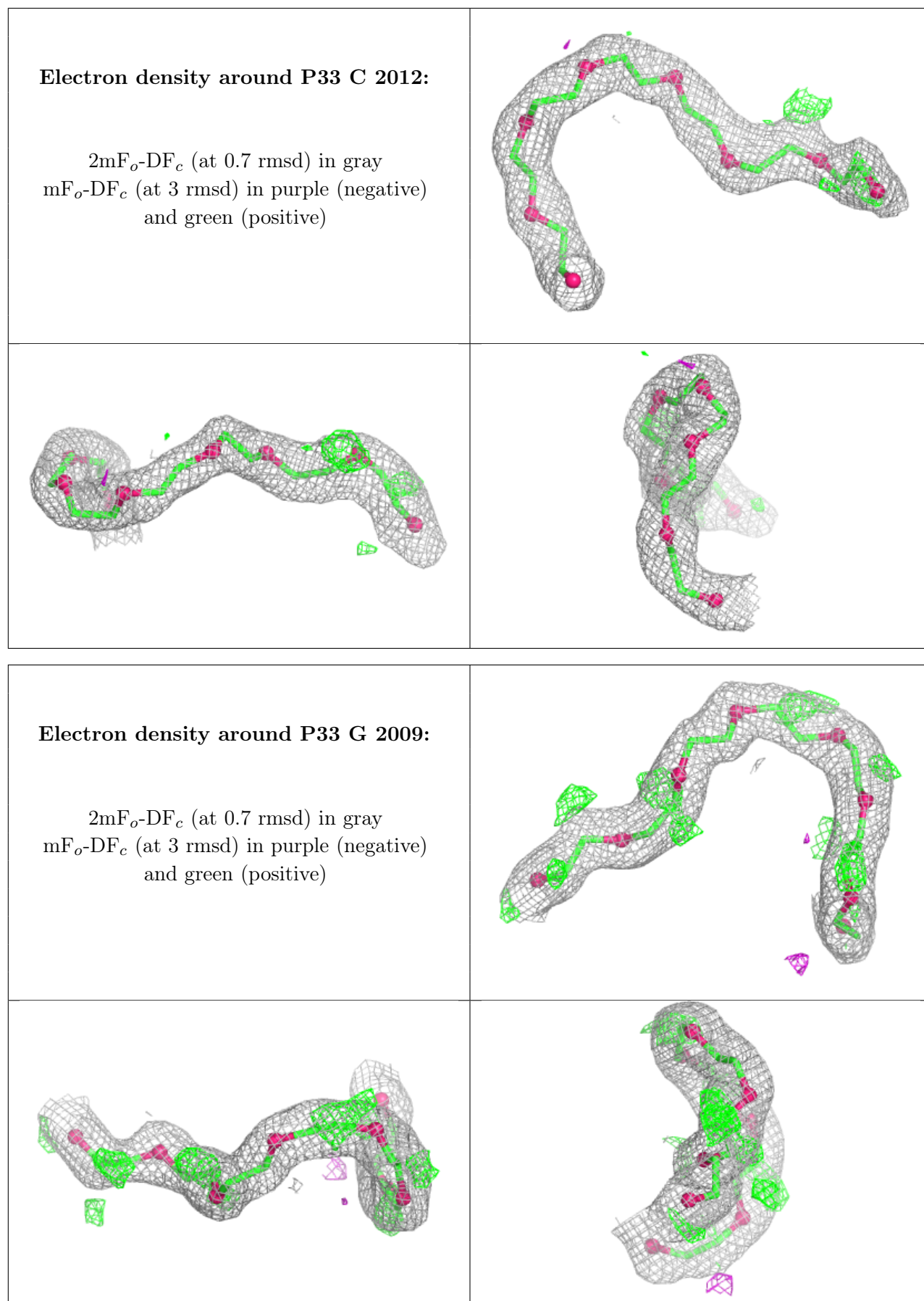
Electron density around P33 A 2013:

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

**Electron density around P33 G 2010:**

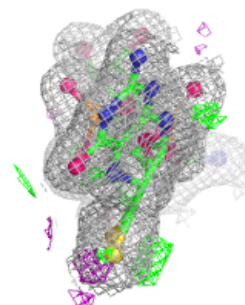
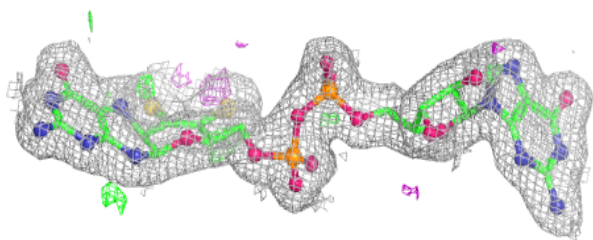
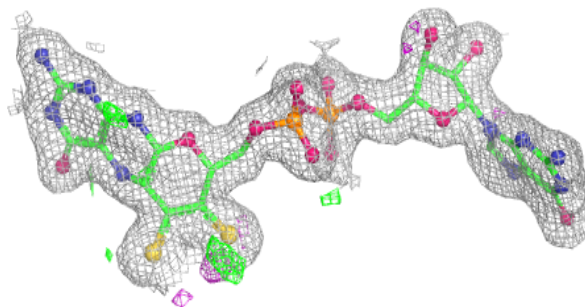
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 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



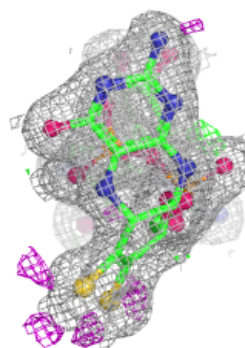
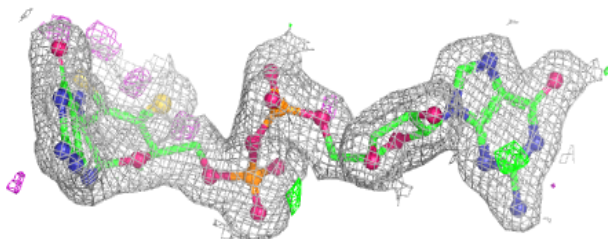
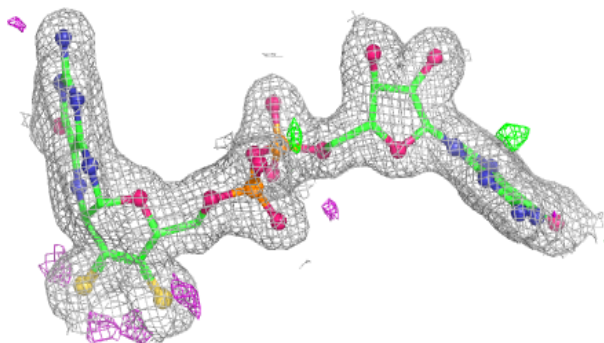


Electron density around MGD C 2001:

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and green (positive)

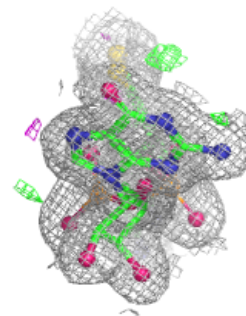
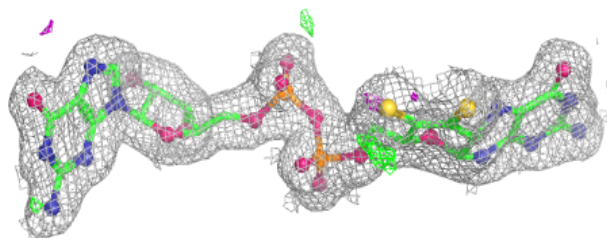
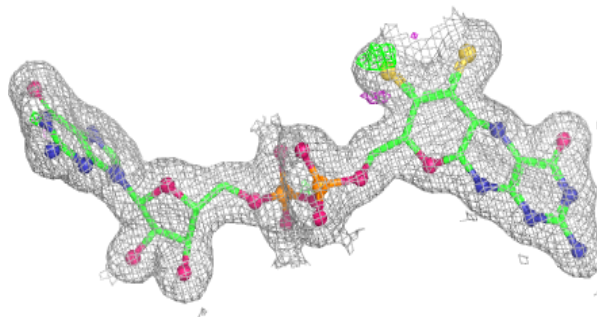
**Electron density around MGD C 2002:**

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

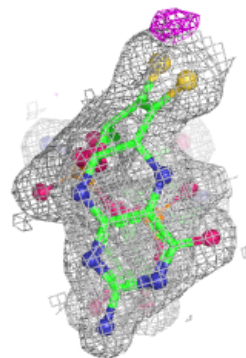
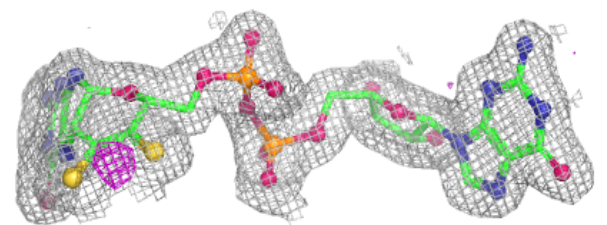
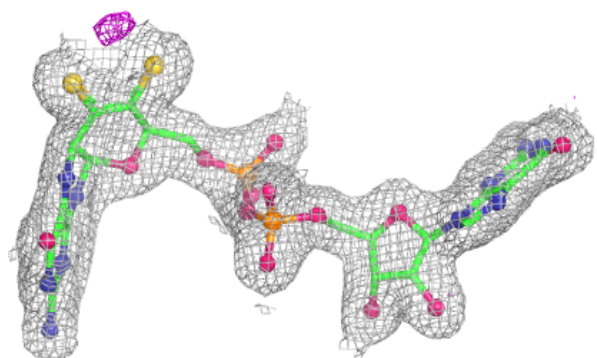


Electron density around MGD E 2001:

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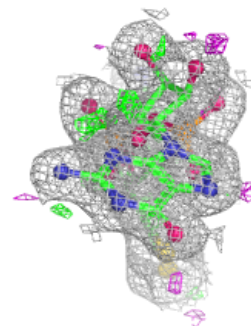
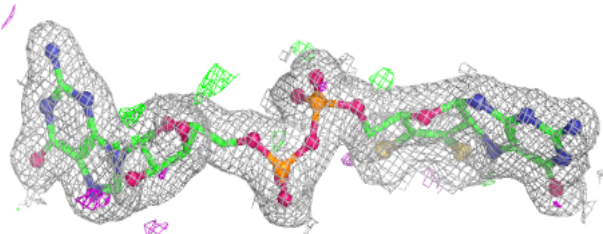
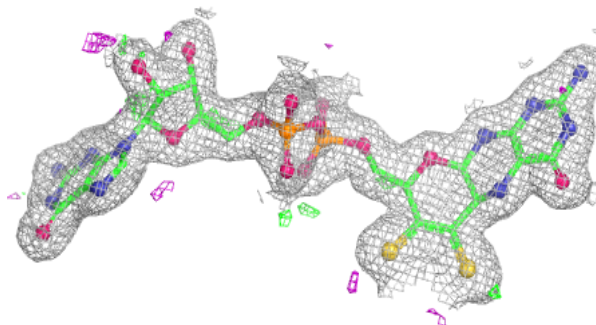
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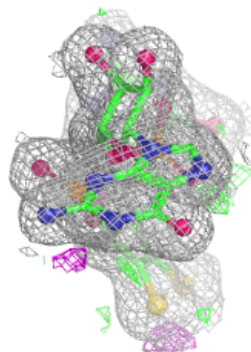
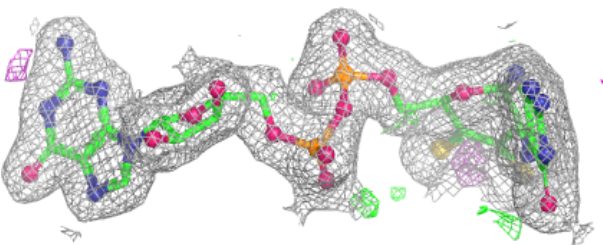
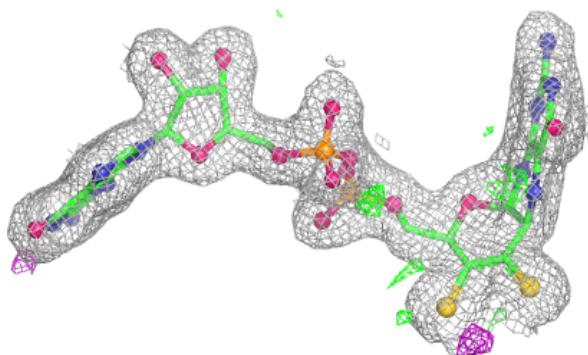


Electron density around MGD G 2001:

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

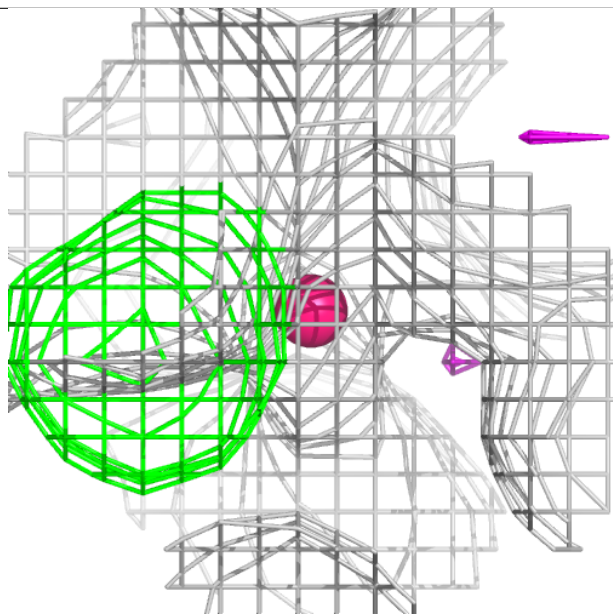
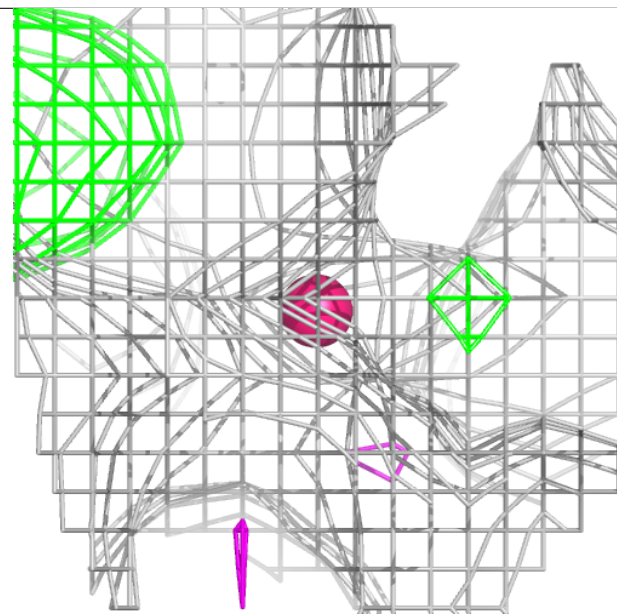
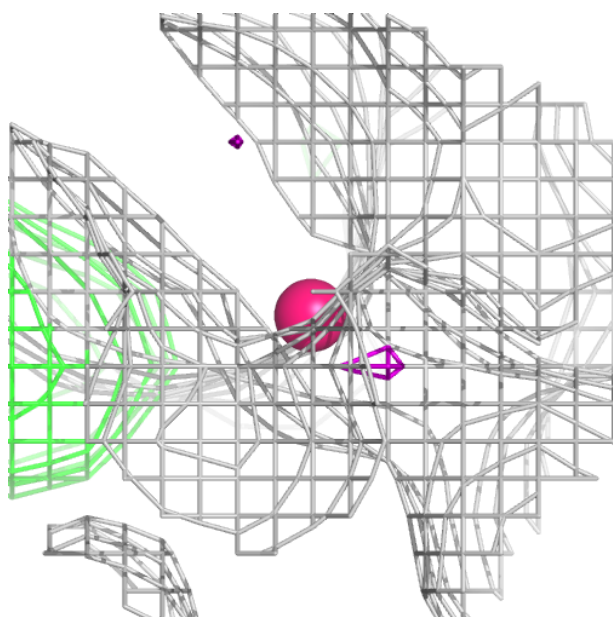
**Electron density around MGD G 2002:**

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and green (positive)



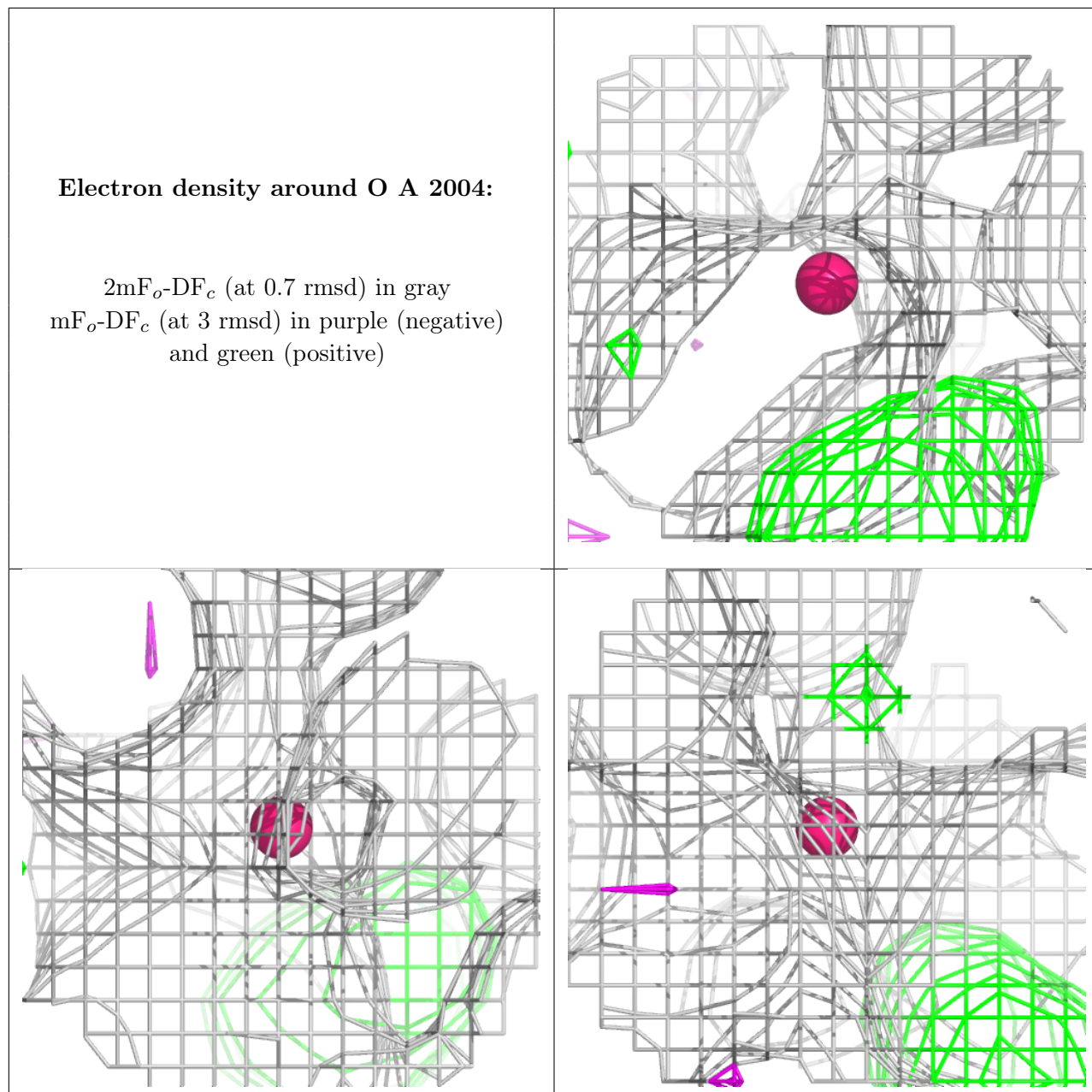
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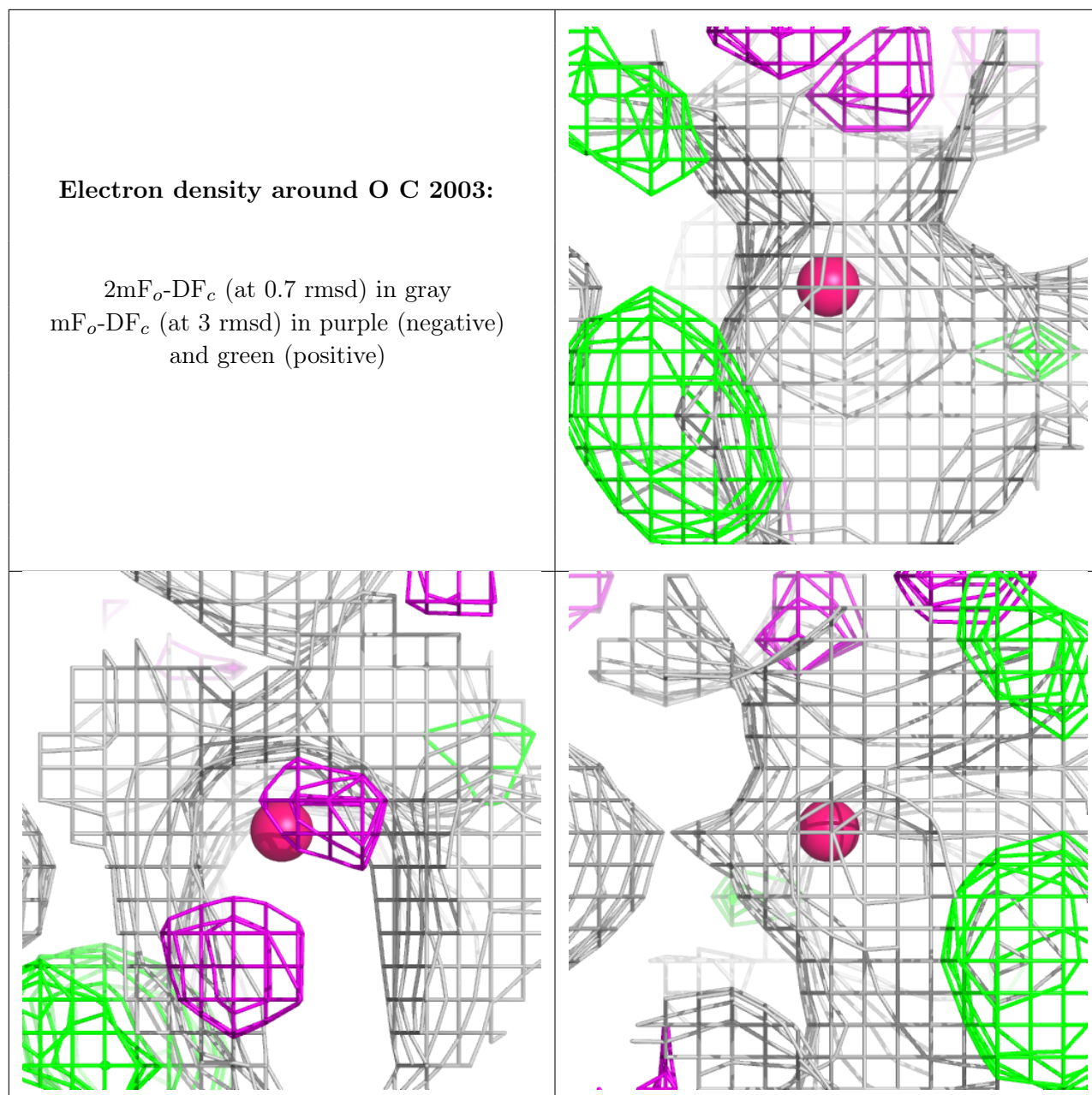
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and green (positive)



Electron density around O A 2004:

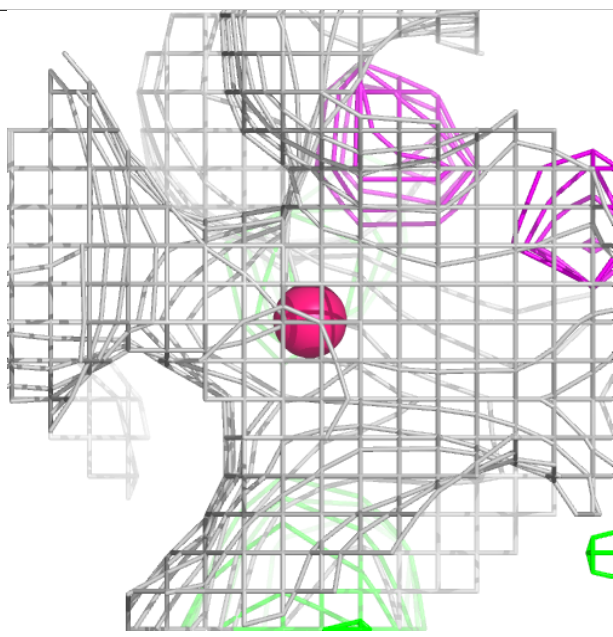
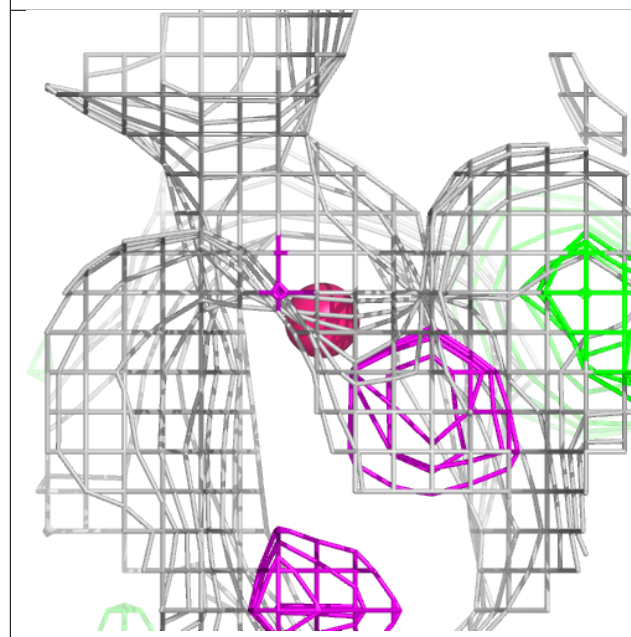
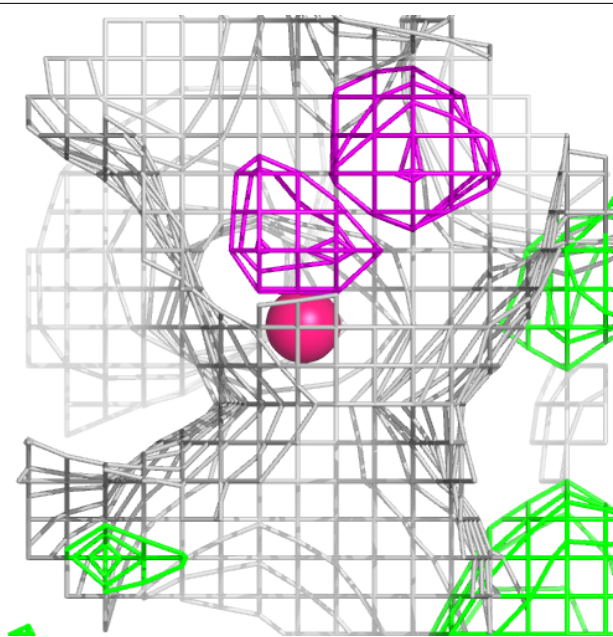
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and green (positive)

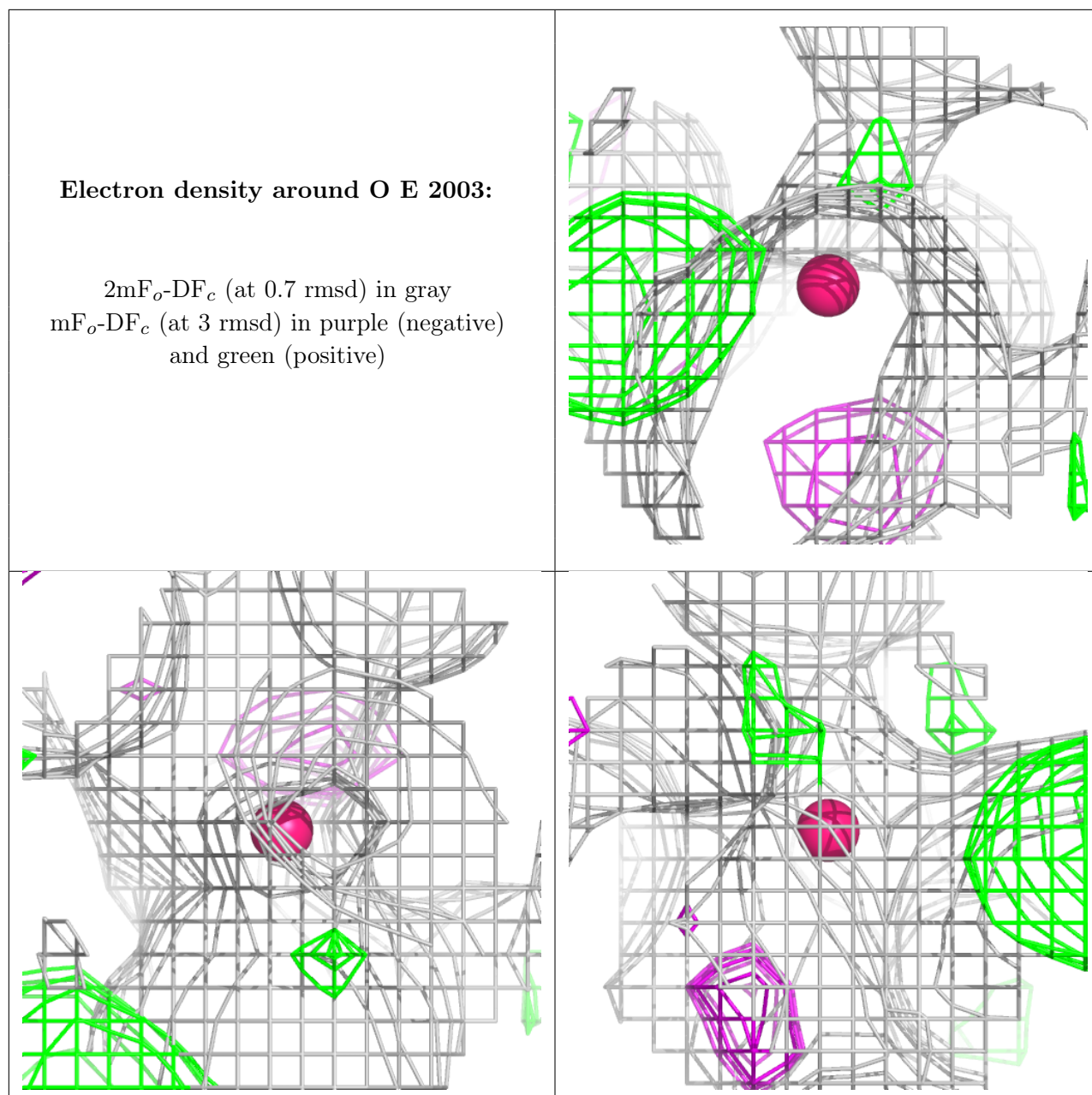


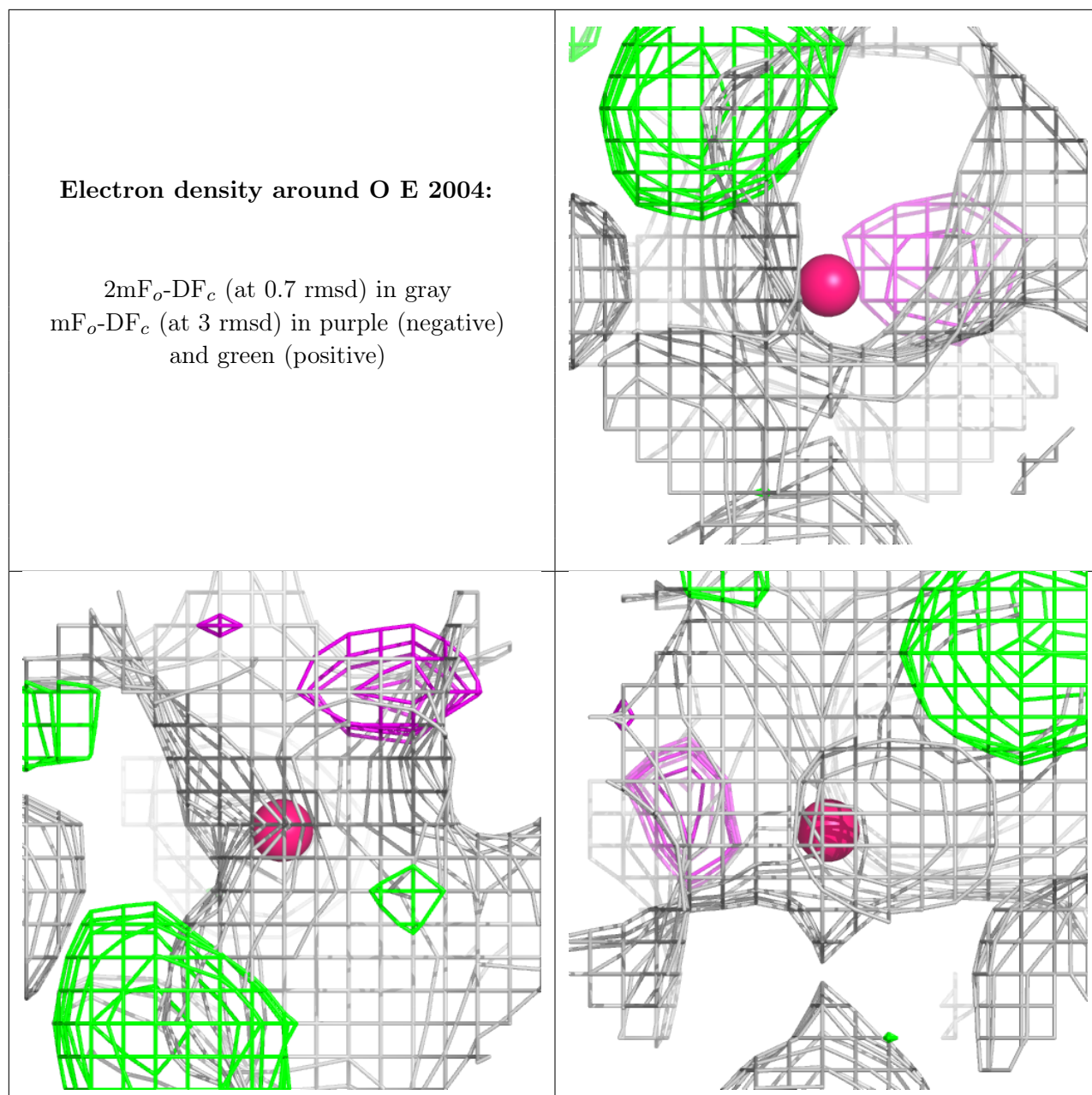


Electron density around O C 2004:

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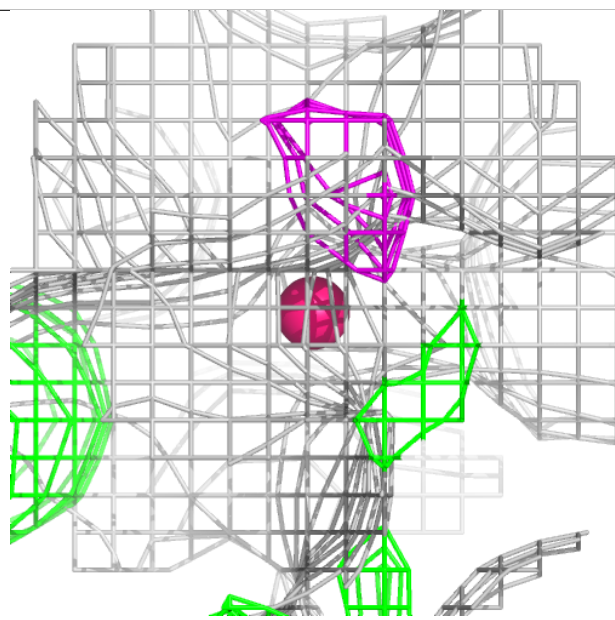
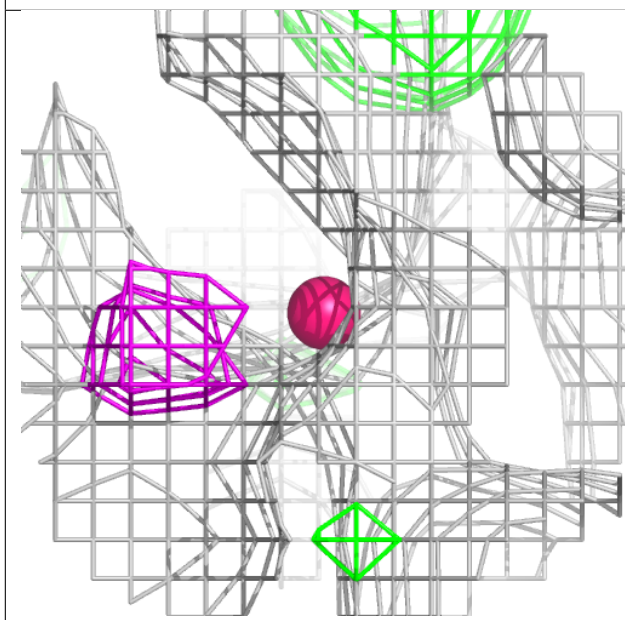
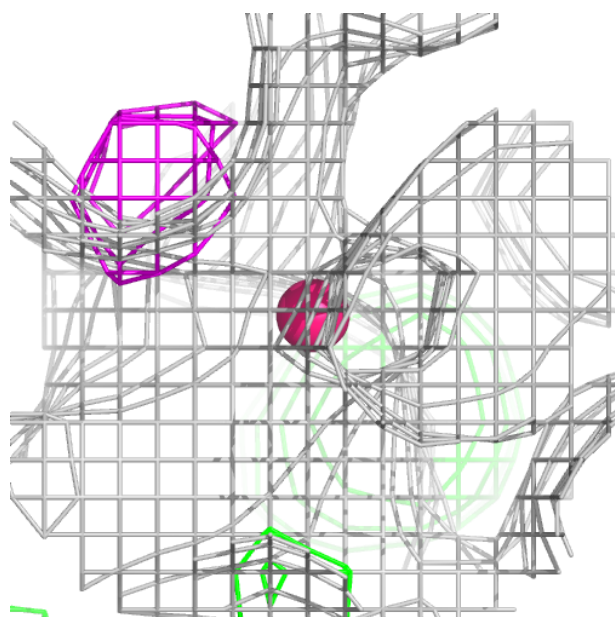






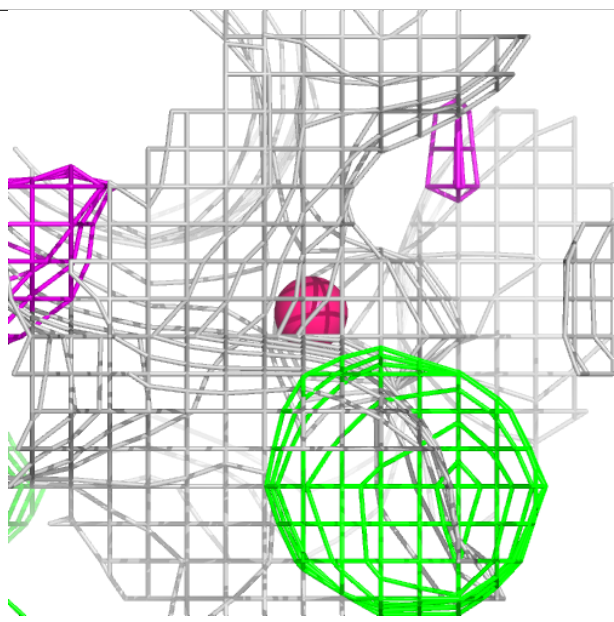
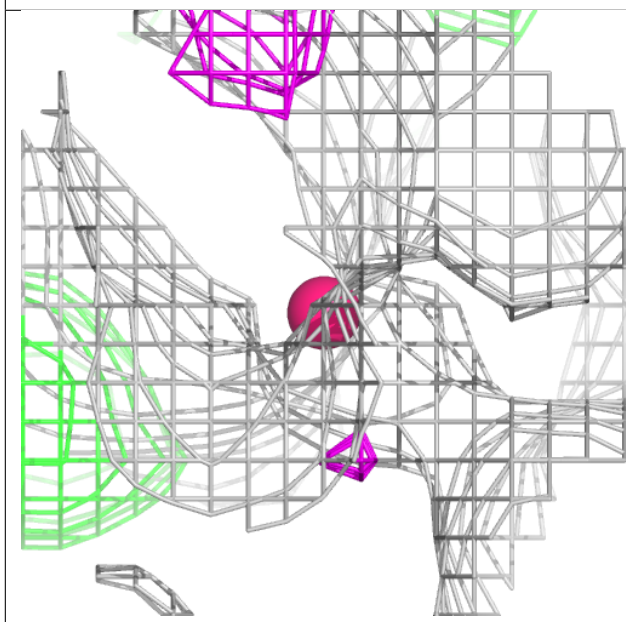
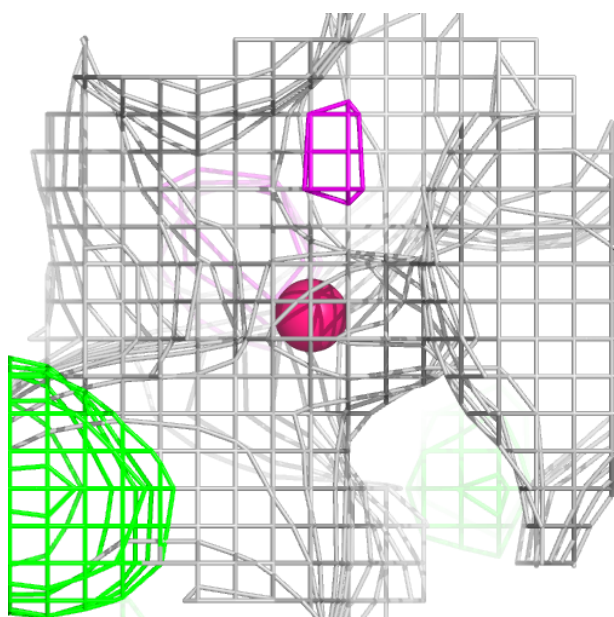
Electron density around O G 2003:

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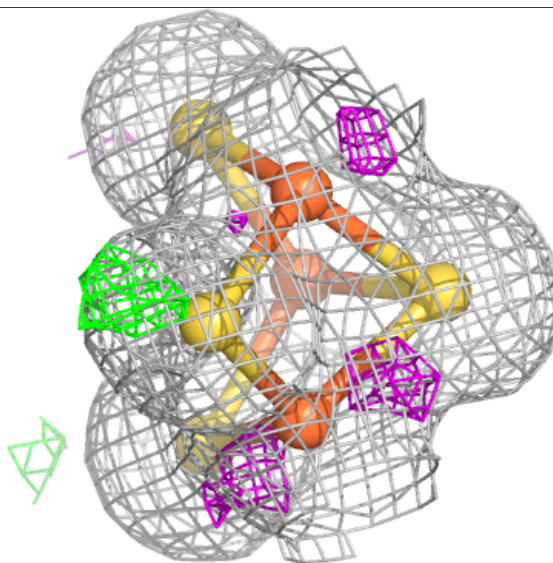
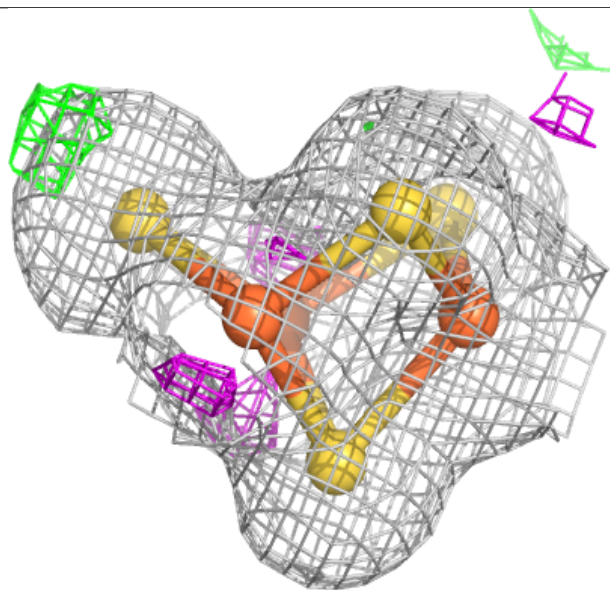
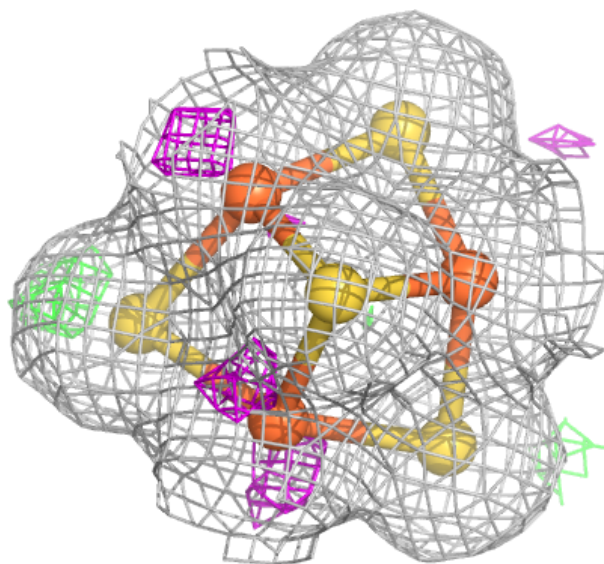
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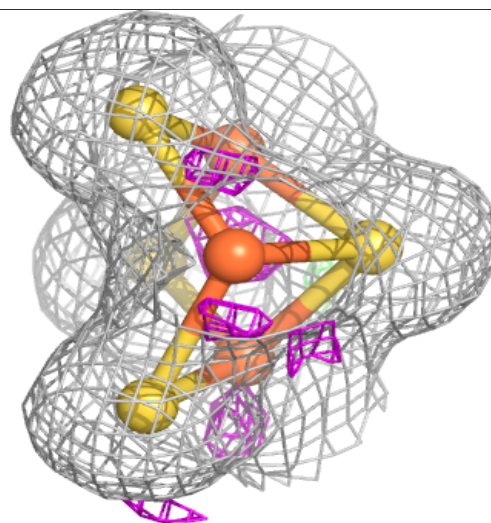
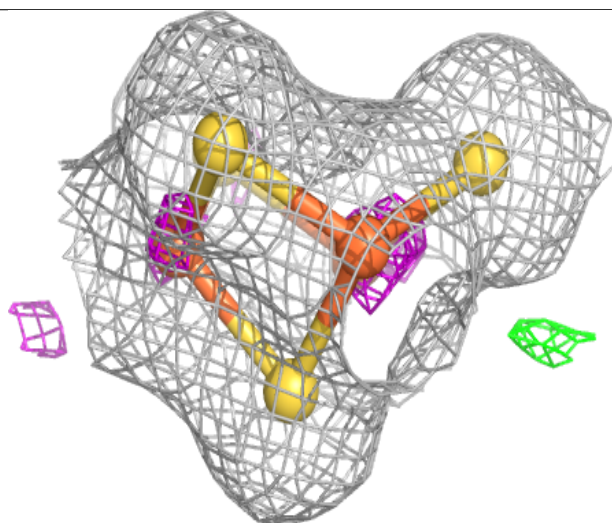
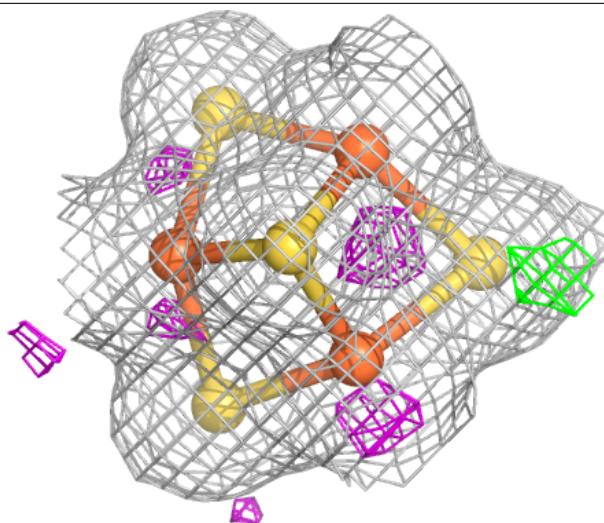
Electron density around F3S A 2006:

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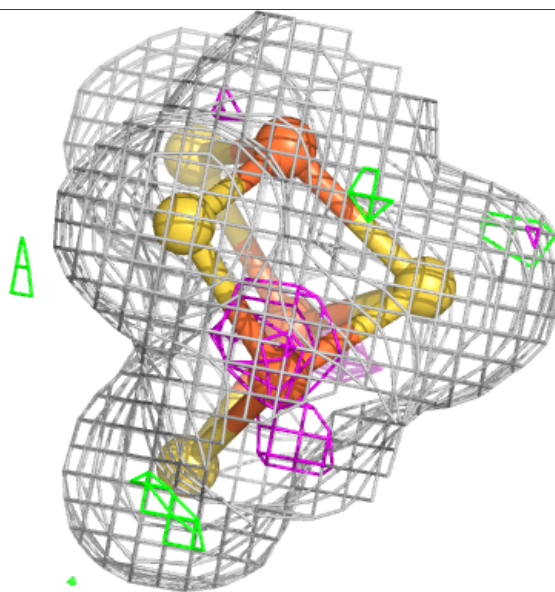
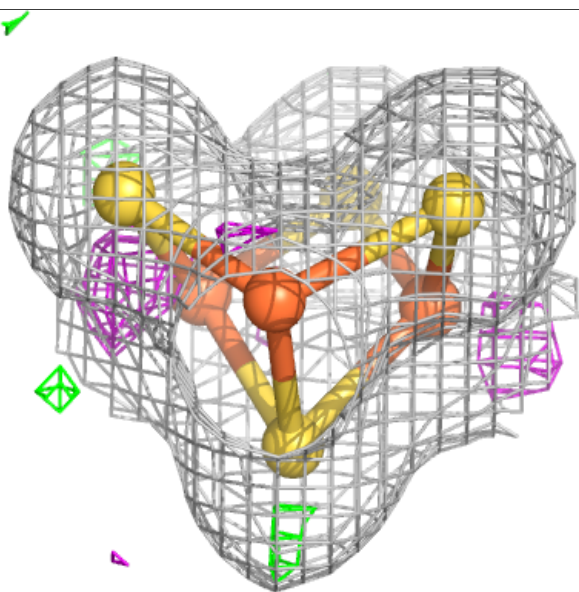
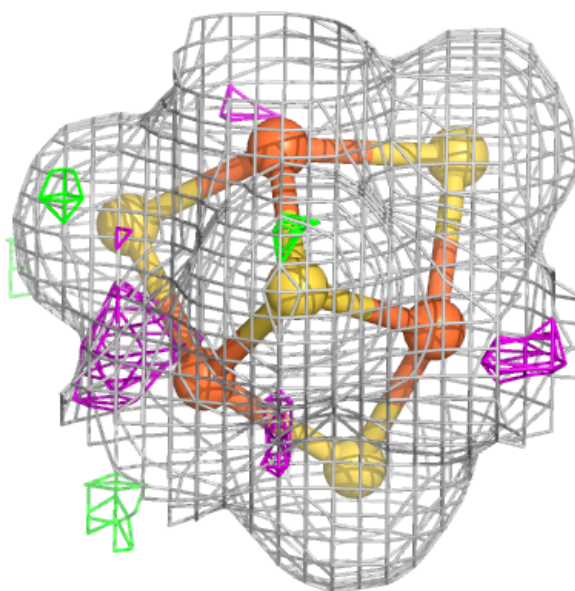
Electron density around F3S C 2006:

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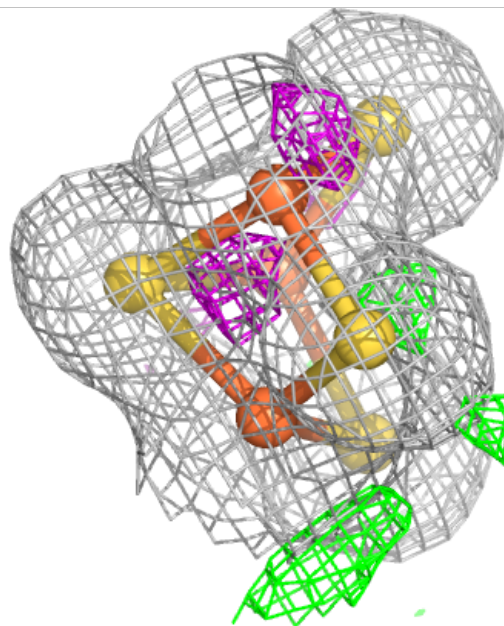
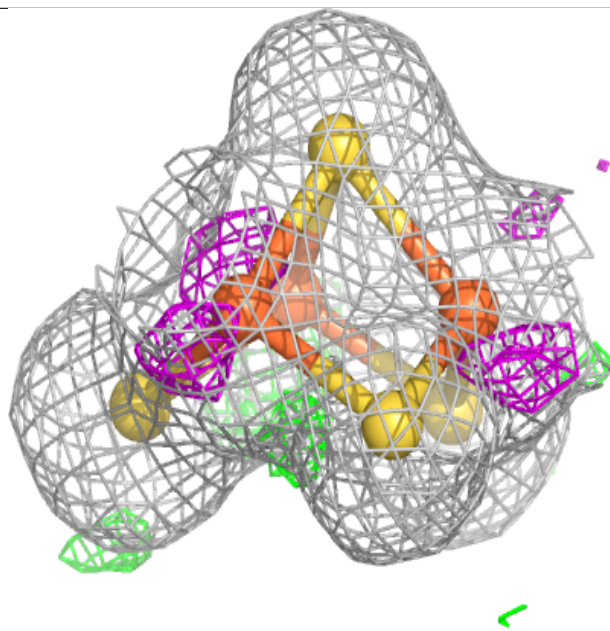
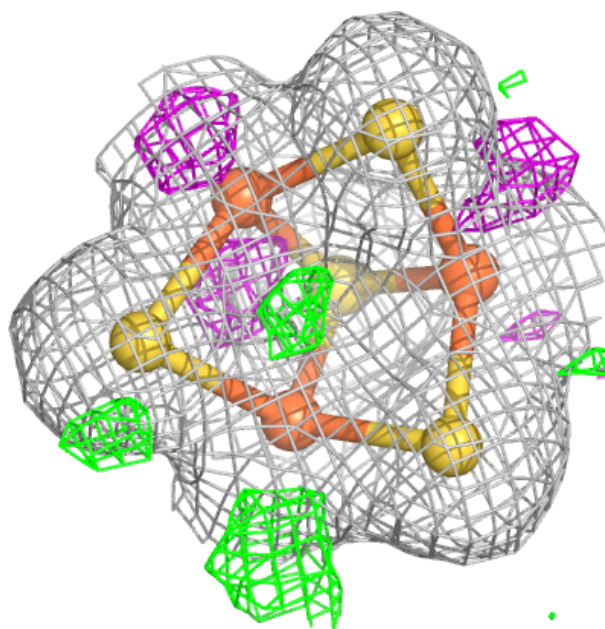
Electron density around F3S E 2006:

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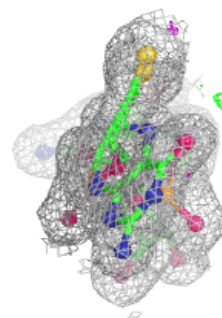
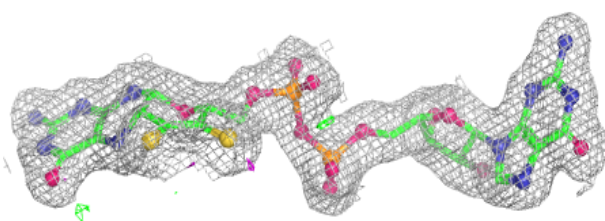
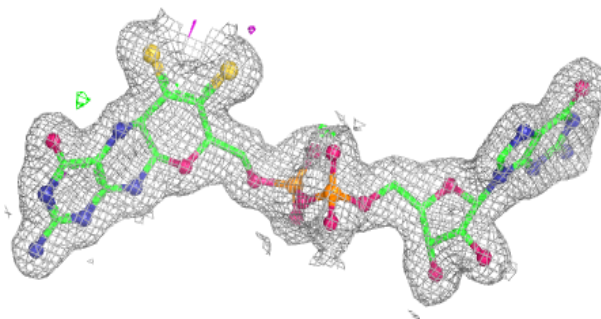
Electron density around F3S G 2006:

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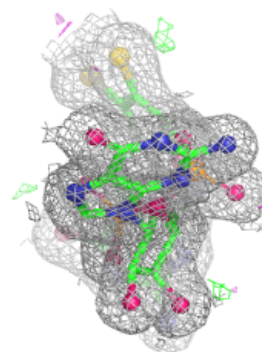
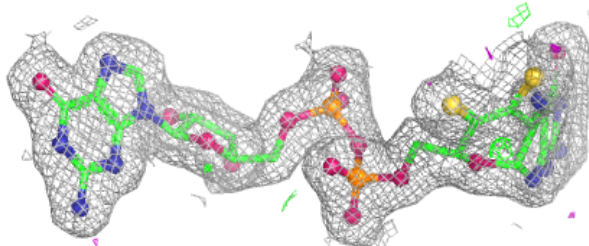
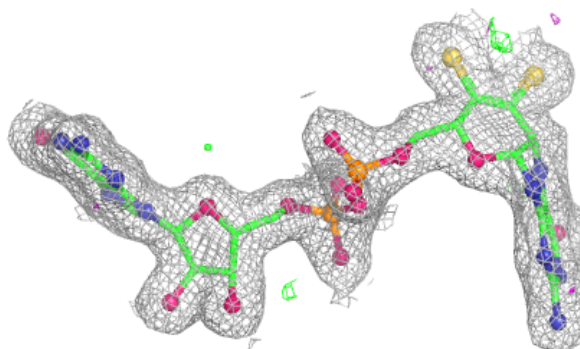


Electron density around MGD A 2001:

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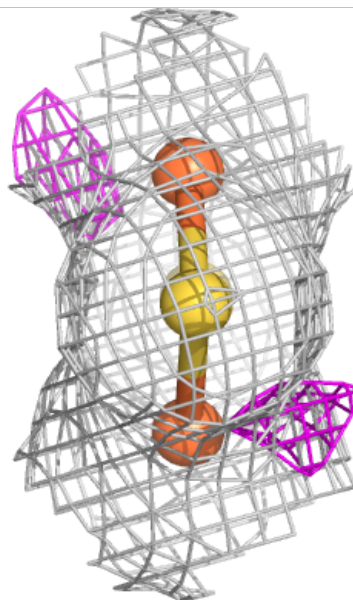
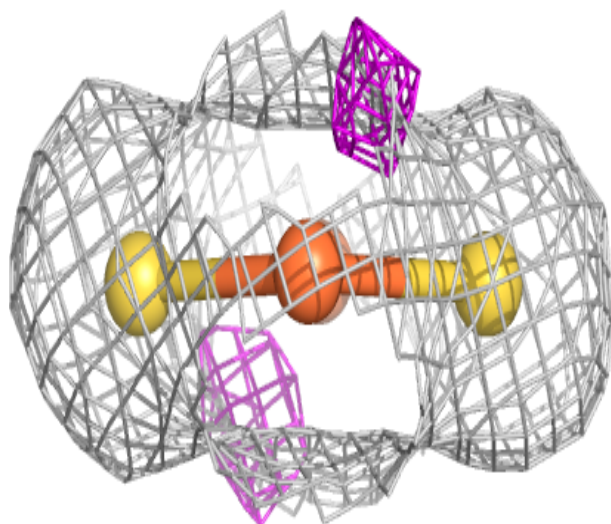
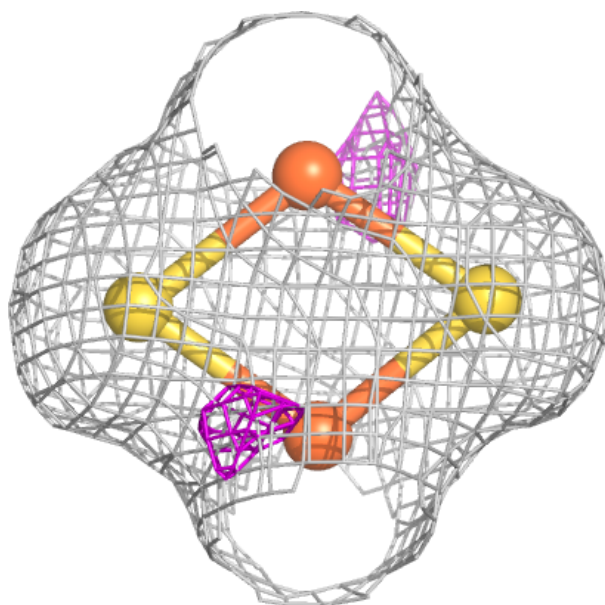
**Electron density around MGD A 2002:**

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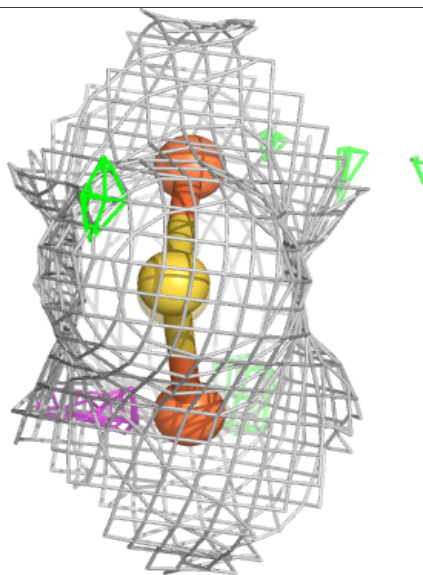
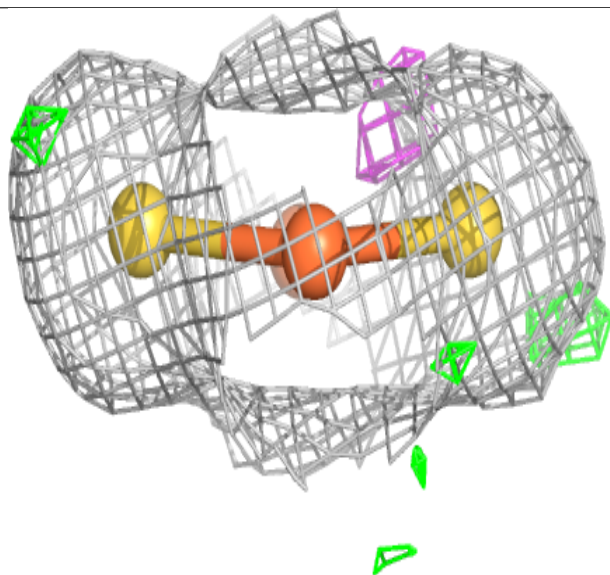
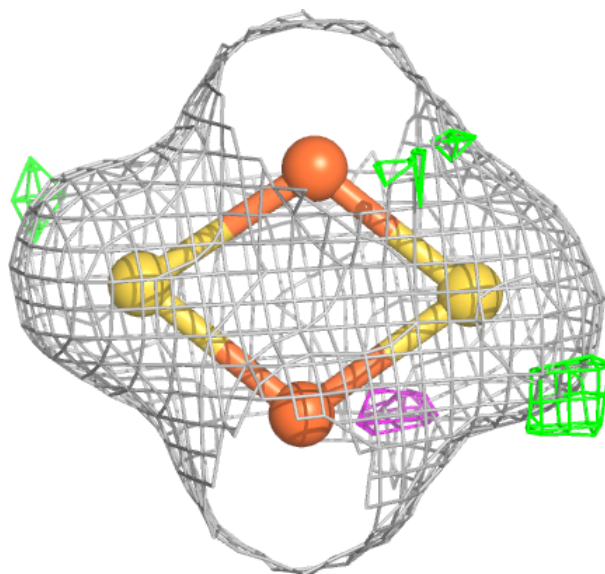
Electron density around FES D 201:

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



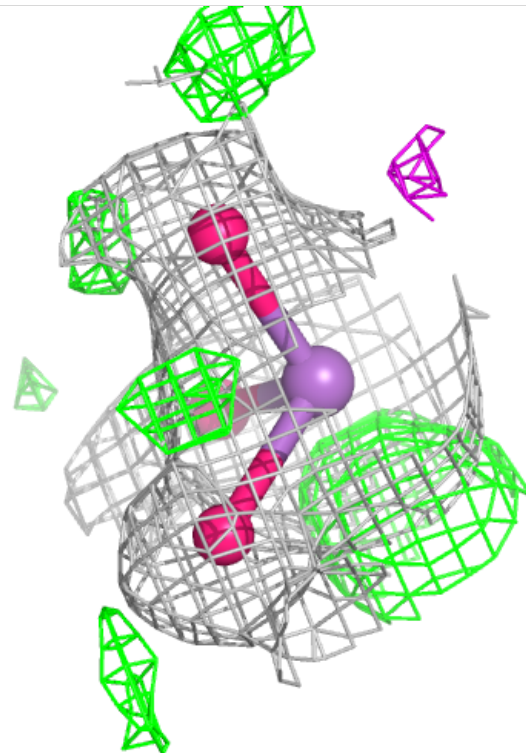
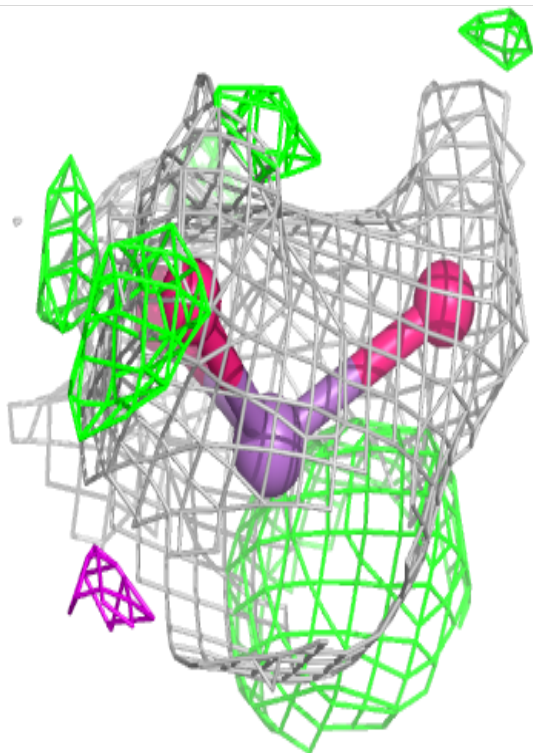
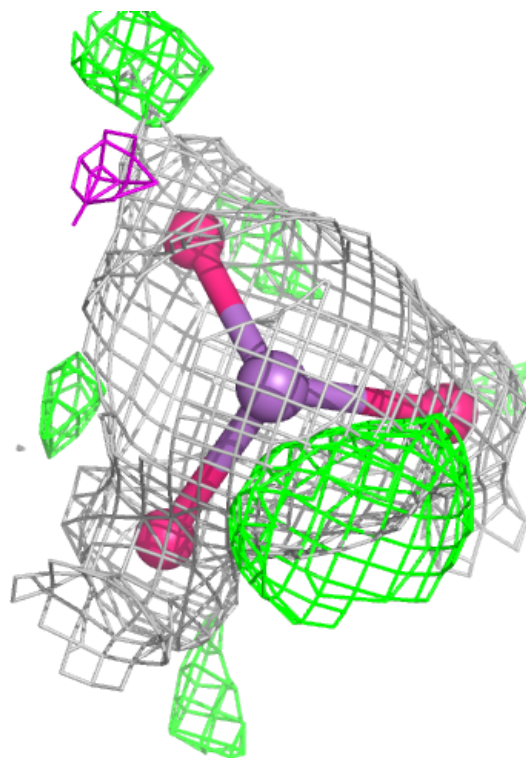
Electron density around FES F 201:

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



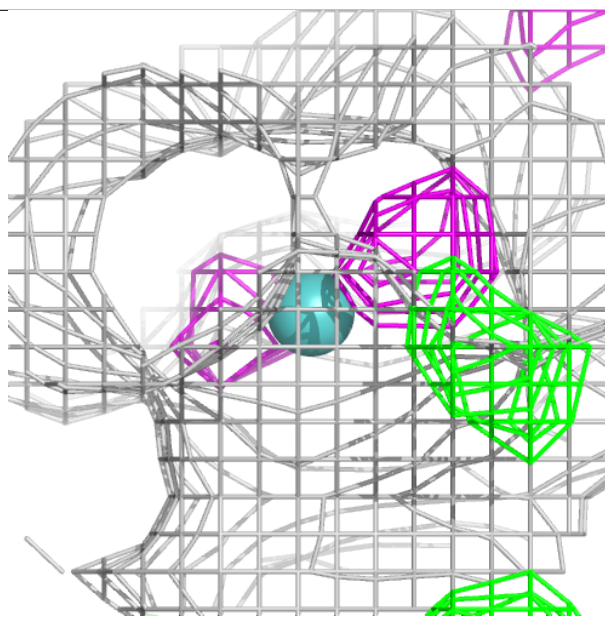
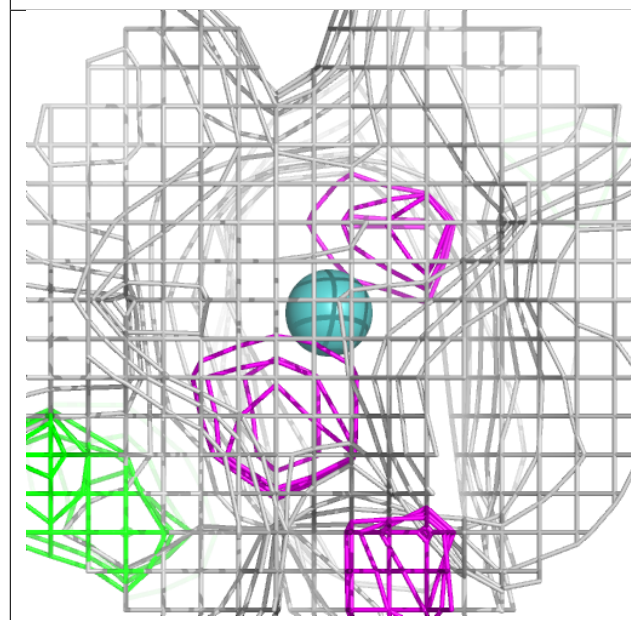
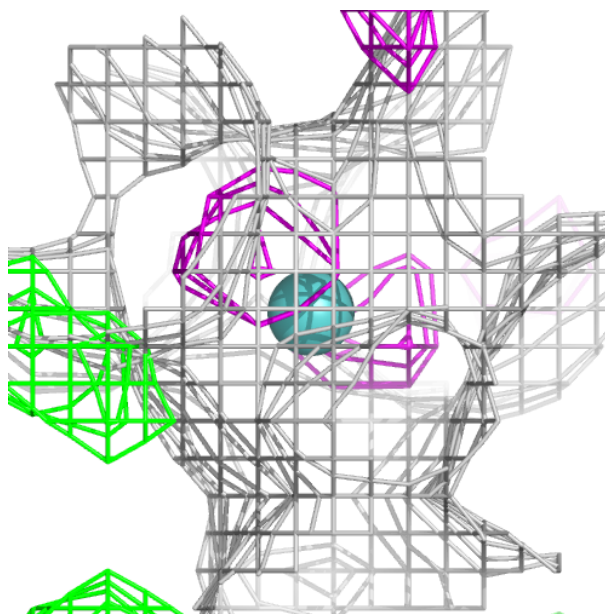
Electron density around SBO G 2013:

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



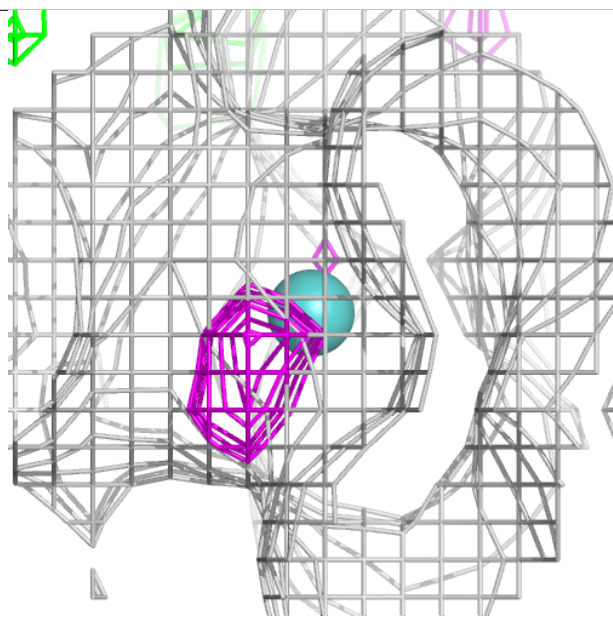
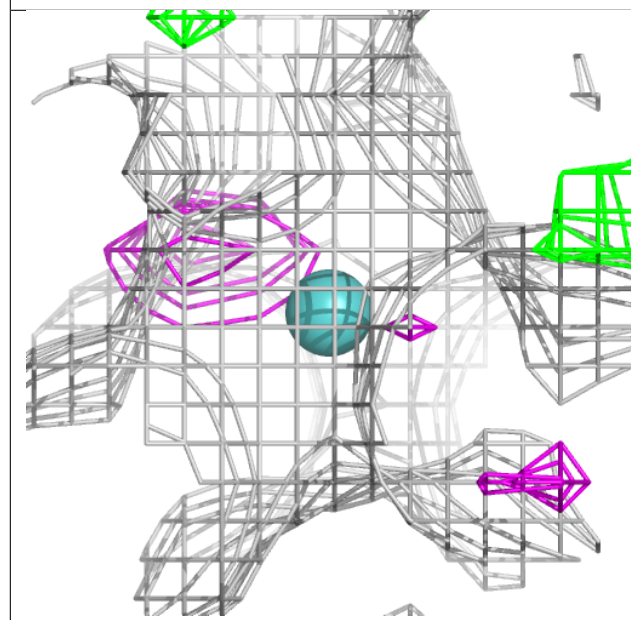
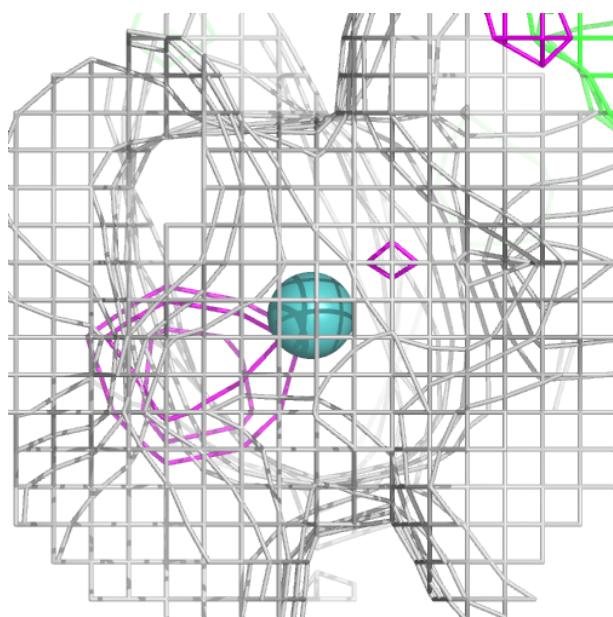
Electron density around 4MO C 2005:

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



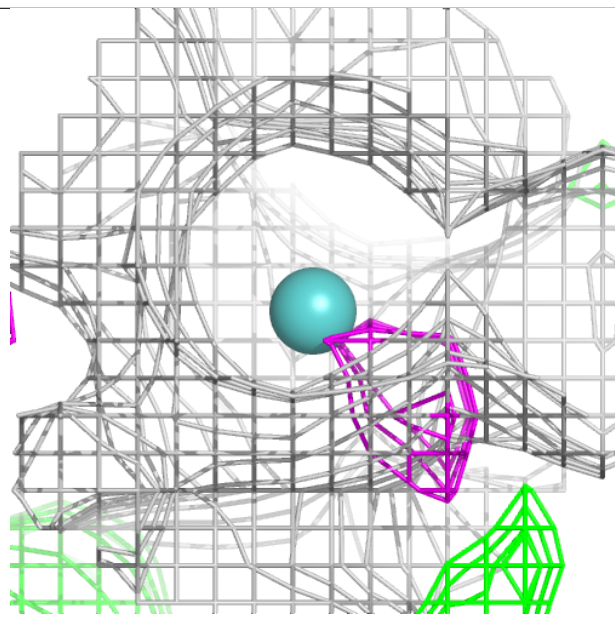
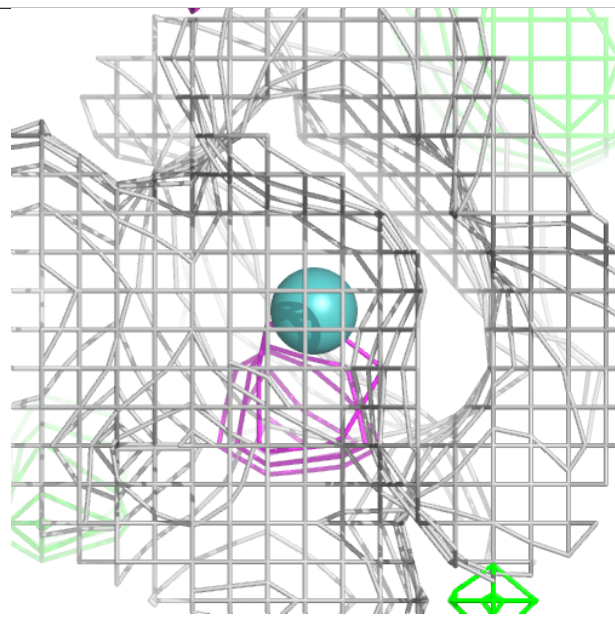
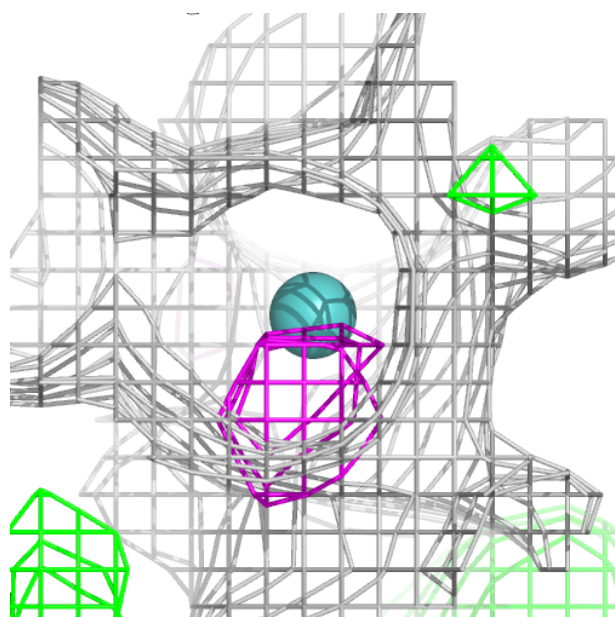
Electron density around 4MO E 2005:

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



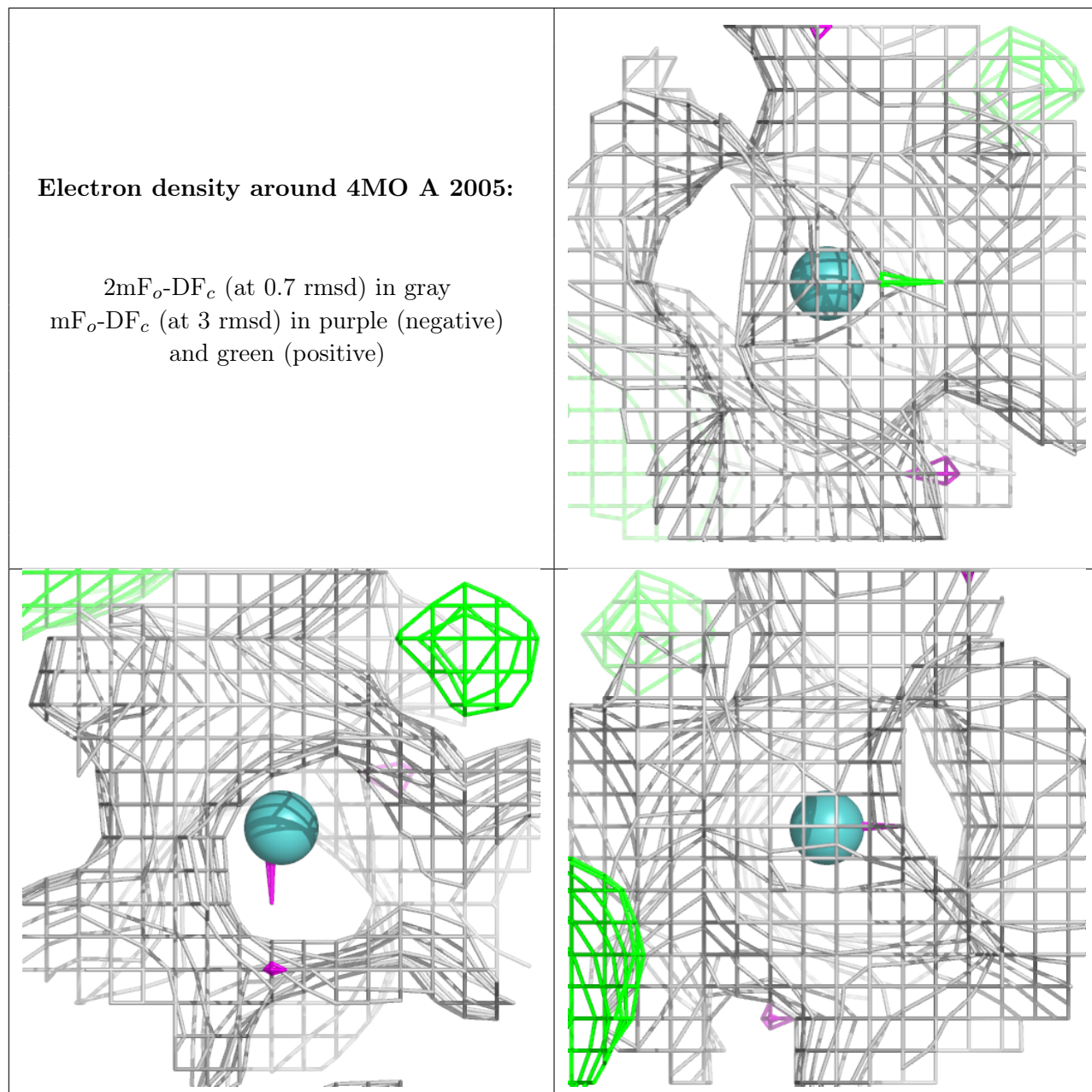
Electron density around 4MO G 2005:

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



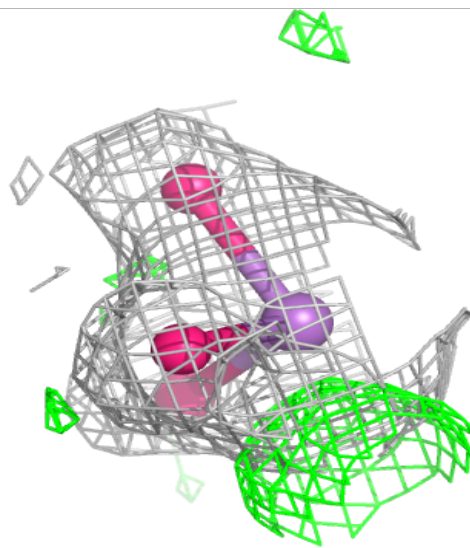
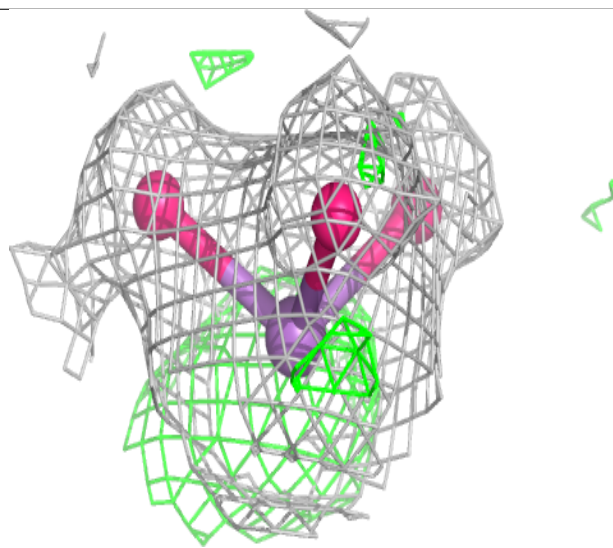
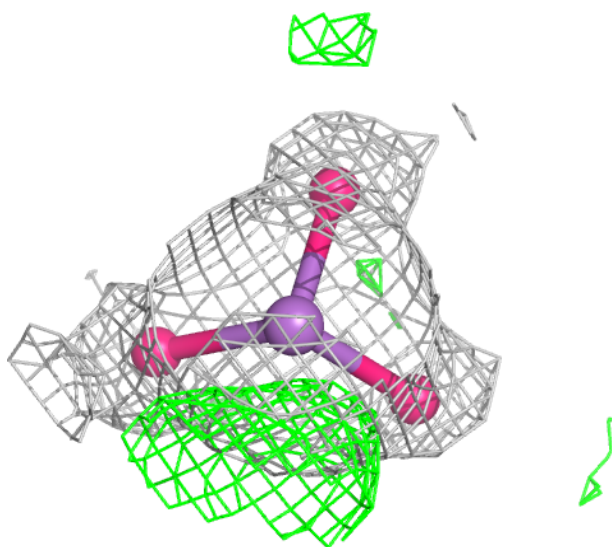
Electron density around 4MO A 2005:

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



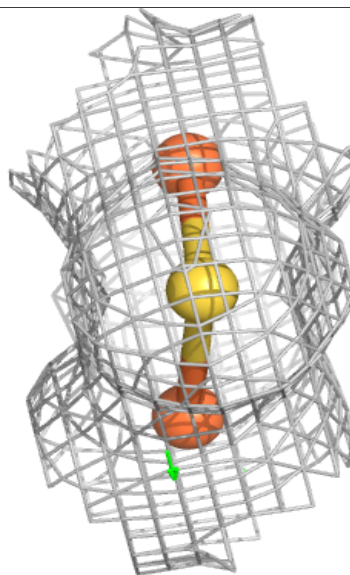
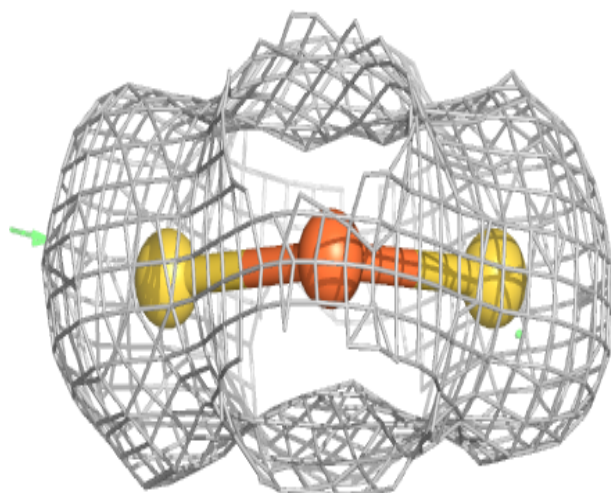
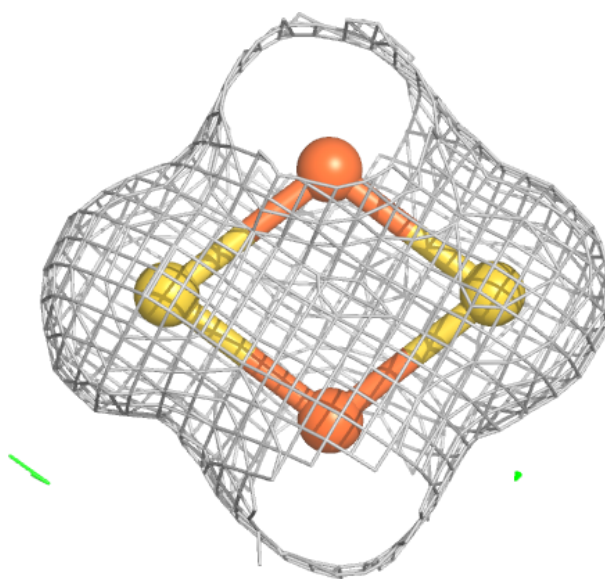
Electron density around SBO A 2012:

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



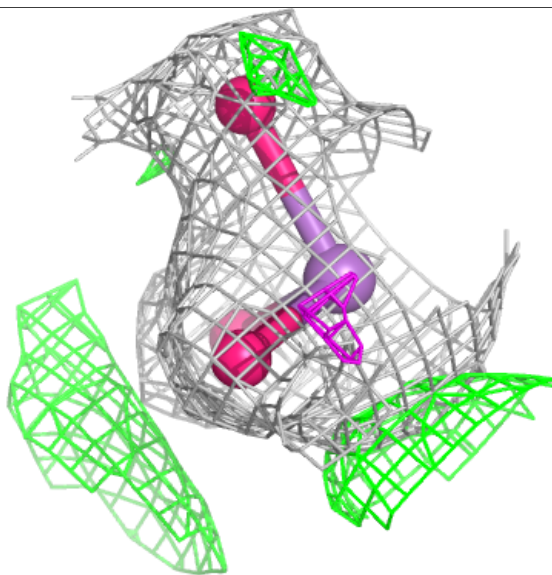
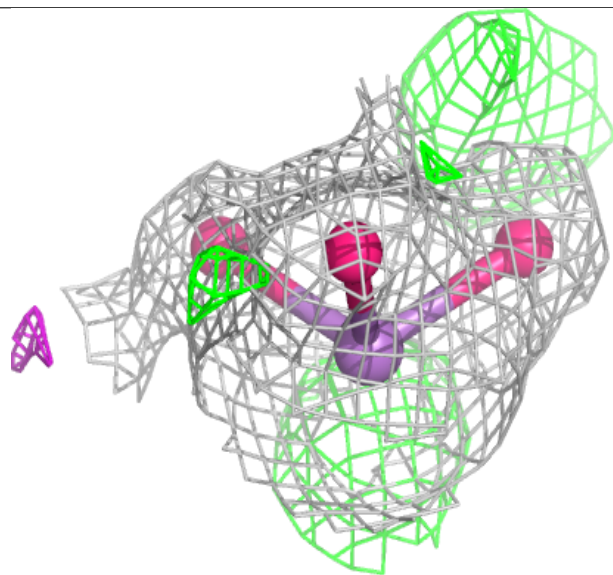
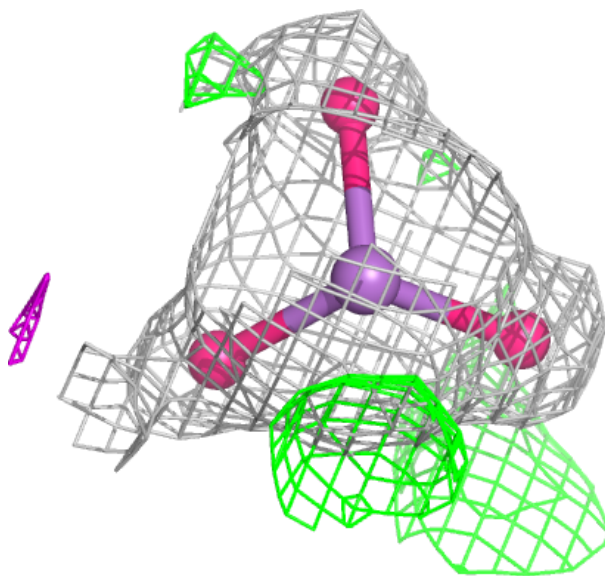
Electron density around FES B 201:

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



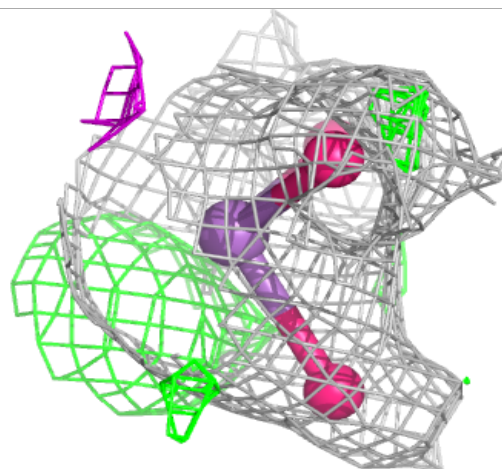
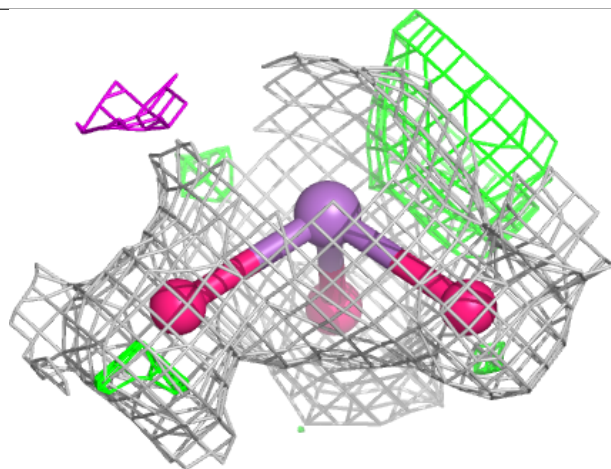
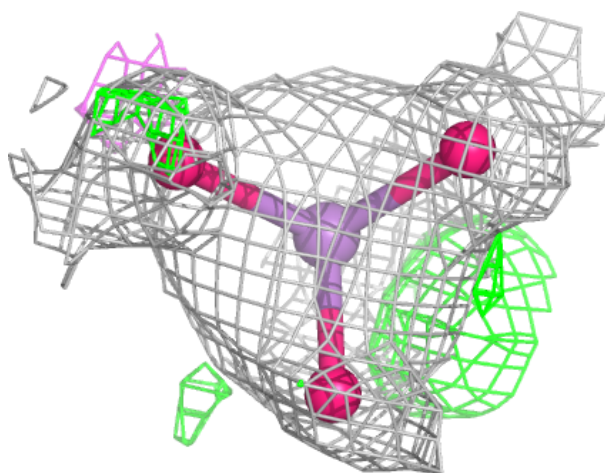
Electron density around SBO C 2011:

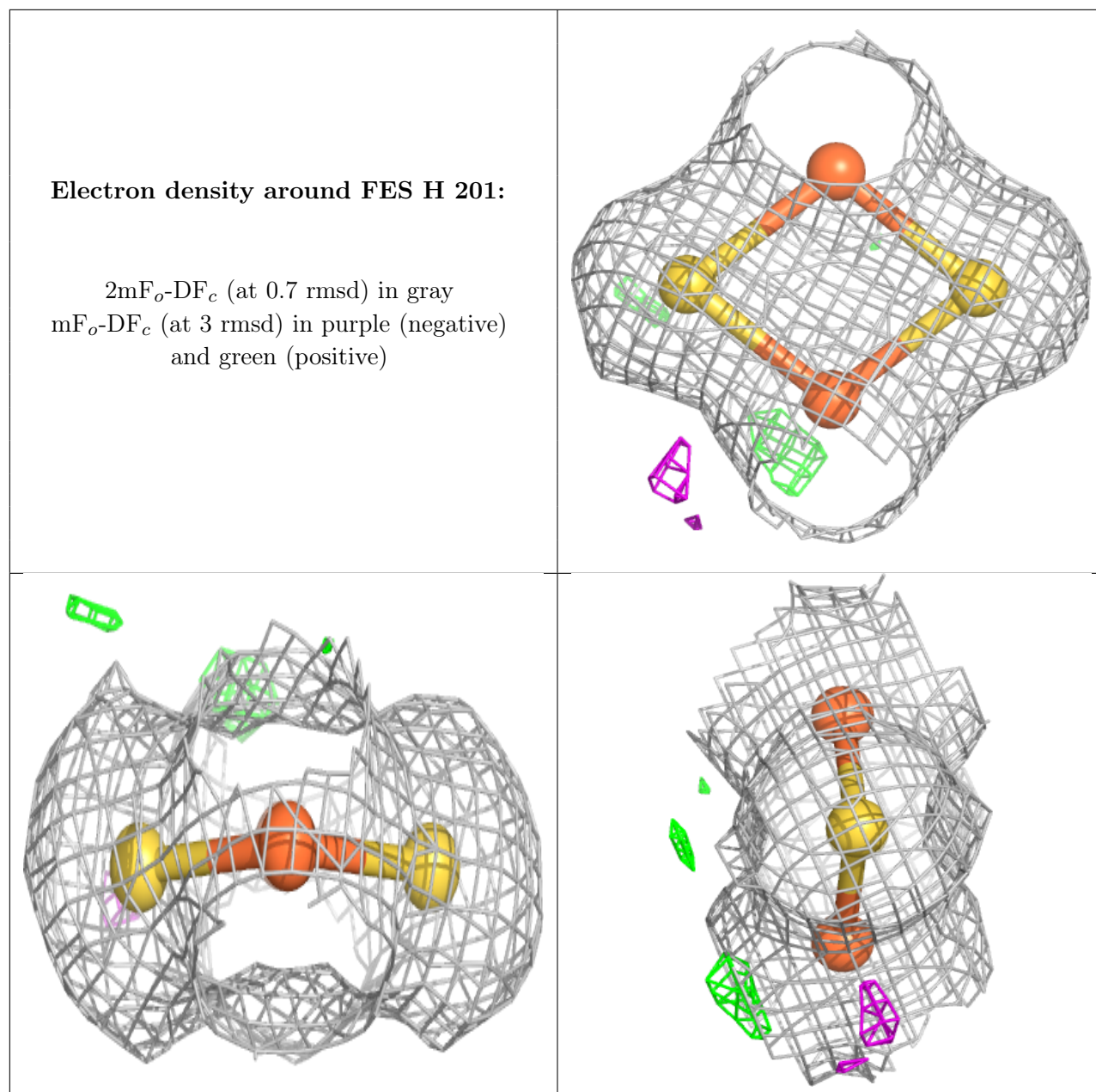
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.