



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2026 – 02:36 am BST

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 Full wwPDB X-ray Structure Validation 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 : 1.8.4, CSD as541be (2020)
Xtriage (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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

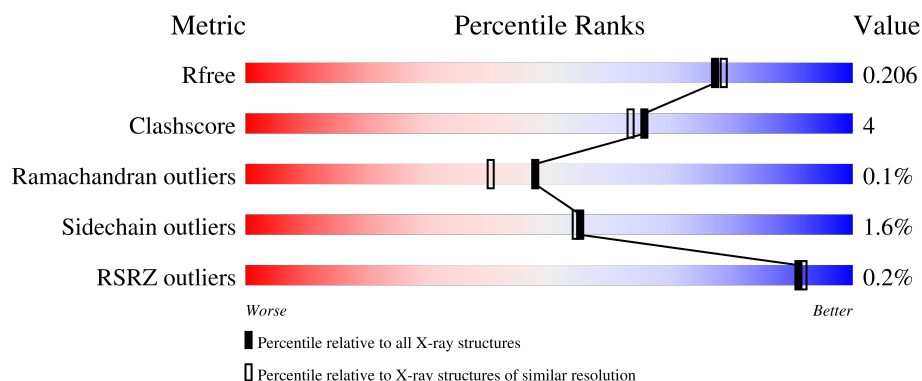
1 Overall quality at a glance

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	
1	C	845	
1	E	845	
1	G	845	
2	B	175	

Continued on next page...

Continued from previous page...

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

2 Entry composition

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.

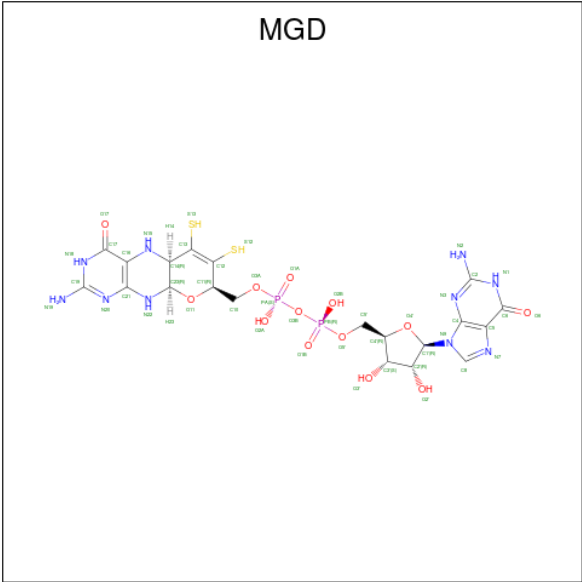
- Molecule 1 is a protein called AroA.

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

- Molecule 2 is a protein called AroB.

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

- 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
3	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- 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	0	0
			2 O		
4	C	2	Total	0	0
			2 O		
4	E	2	Total	0	0
			2 O		

Continued on next page...

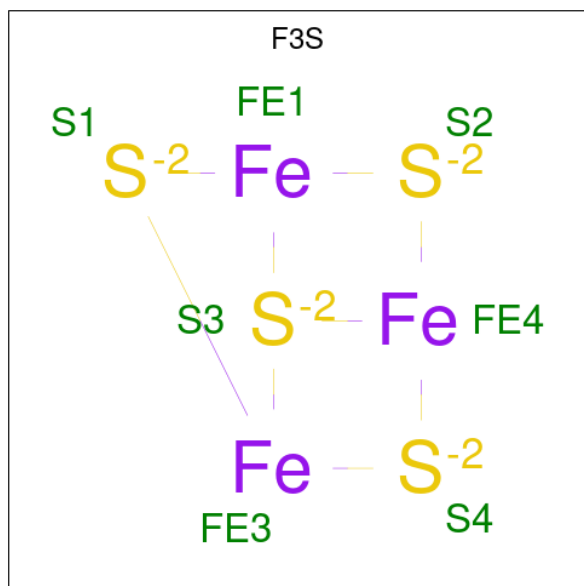
Continued from previous page...

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

- 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	0	0
			1	1		
5	C	1	Total	Mo	0	0
			1	1		
5	E	1	Total	Mo	0	0
			1	1		
5	G	1	Total	Mo	0	0
			1	1		

- Molecule 6 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄) (labeled as "Ligand of Interest" by depositor).



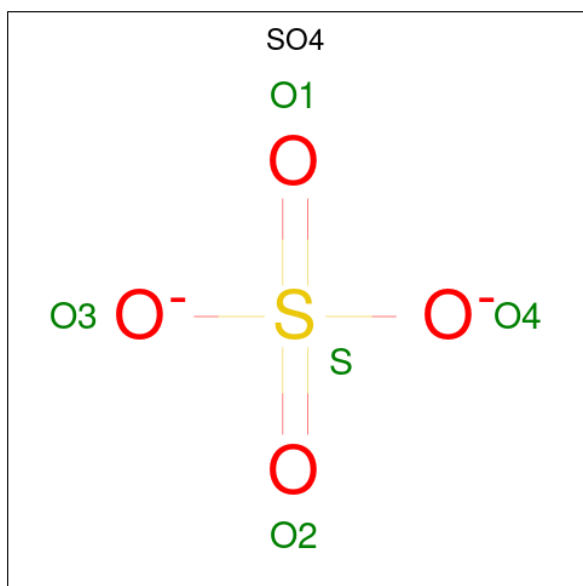
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			7	3	4		
6	C	1	Total	Fe	S	0	0
			7	3	4		
6	E	1	Total	Fe	S	0	0
			7	3	4		

Continued on next page...

Continued from previous page...

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

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



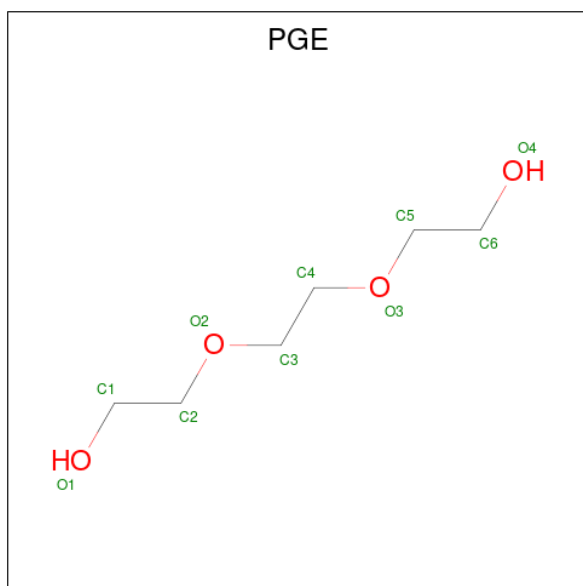
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total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

Continued on next page...

Continued from previous page...

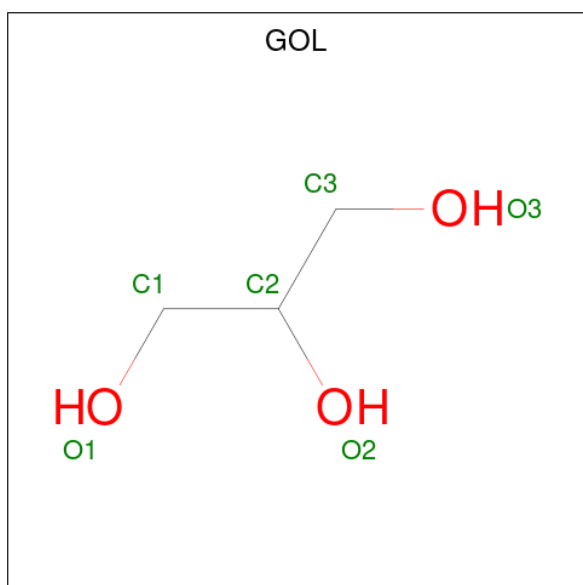
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	O	S	0	0
			5	4	1		

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



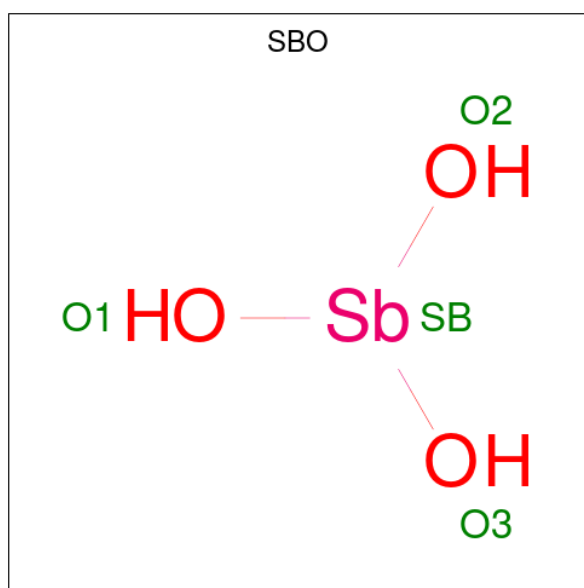
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		

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



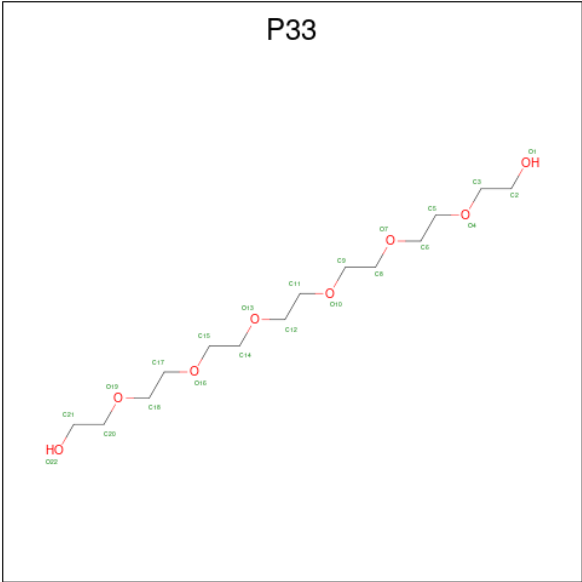
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	C	1	Total C O 6 3 3	0	0
9	E	1	Total C O 6 3 3	0	0
9	G	1	Total C O 6 3 3	0	0
9	G	1	Total C O 6 3 3	0	0

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



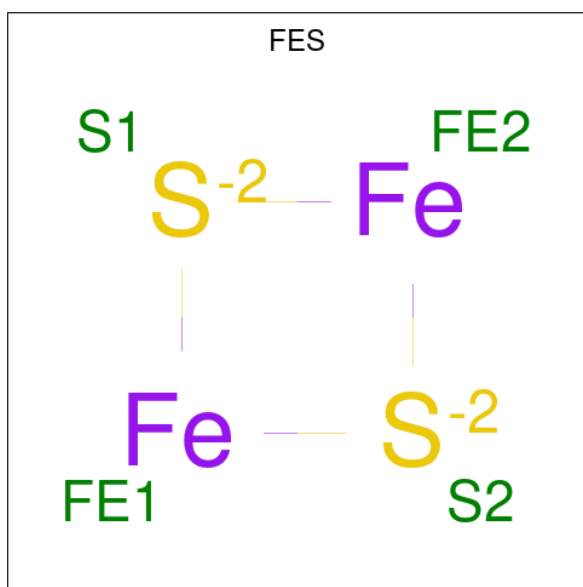
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O Sb 4 3 1	0	0
10	C	1	Total O Sb 4 3 1	0	0
10	E	1	Total O Sb 4 3 1	0	0
10	G	1	Total O Sb 4 3 1	0	0

- Molecule 11 is 3,6,9,12,15,18-HEXAOSAICOSANE-1,20-DIOL (CCD ID: 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 (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		

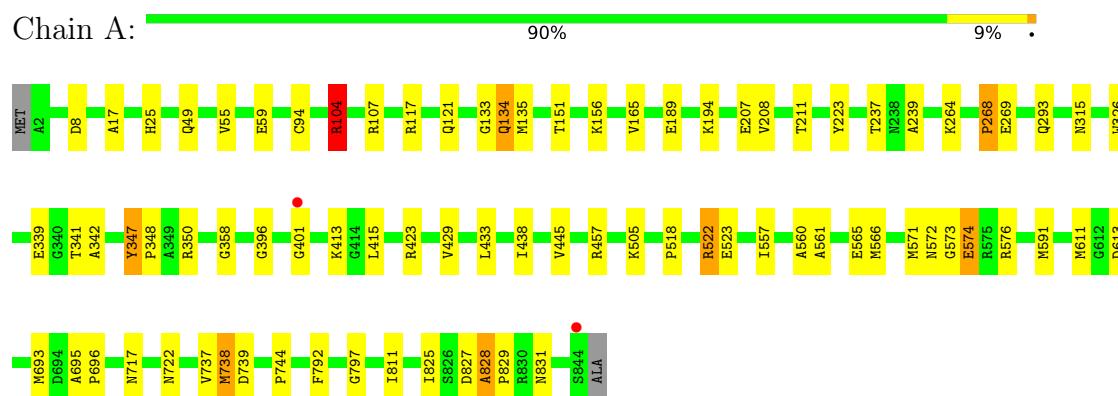
- Molecule 13 is water.

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		

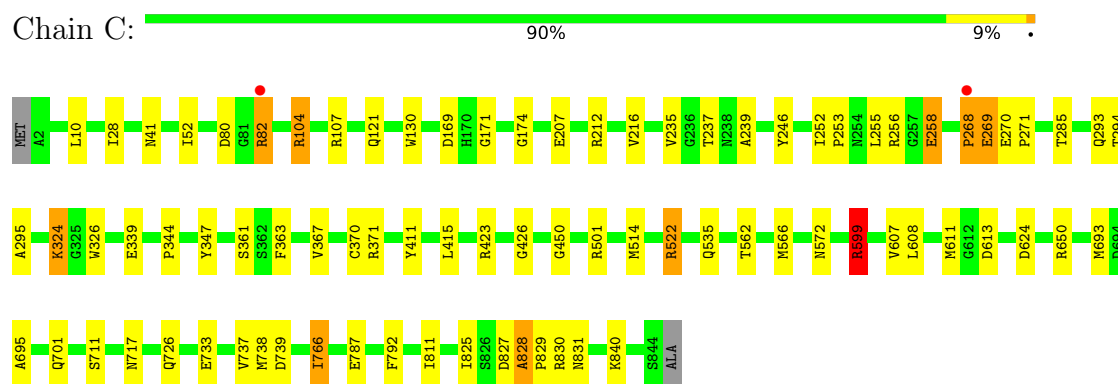
3 Residue-property plots [i](#)

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.

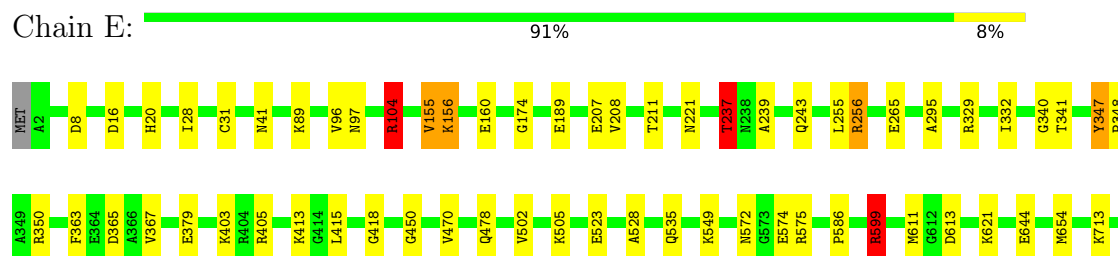
• Molecule 1: AroA



• Molecule 1: AroA



• Molecule 1: AroA





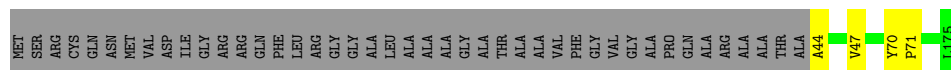
- Molecule 1: AroA

Chain G: 90% 9%



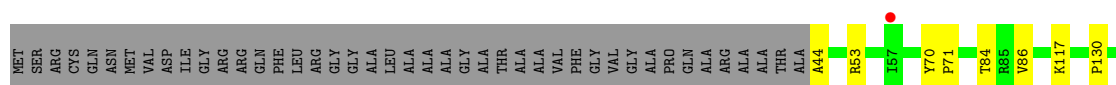
- Molecule 2: AroB

Chain B: 73% 25%



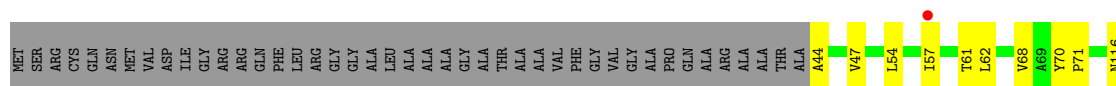
- Molecule 2: AroB

Chain D: 70% 5% 25%



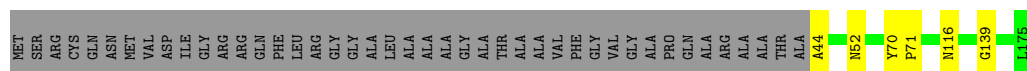
- Molecule 2: AroB

Chain F: 68% 7% 25%



- Molecule 2: AroB

Chain H: 72% 25%



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)	Xtriage
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	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

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

All (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
1	C	739	ASP	CG-OD2	7.36	1.39	1.25
1	A	104	ARG	CD-NE	-6.92	1.36	1.46
1	E	739	ASP	CG-OD2	6.91	1.38	1.25
1	C	252	ILE	CA-CB	6.79	1.57	1.54
1	C	344	PRO	CA-C	6.77	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	599	ARG	CD-NE	-6.65	1.36	1.46
1	G	189	GLU	CA-C	-6.49	1.47	1.52
1	C	121	GLN	C-O	-6.17	1.16	1.24
2	D	149	VAL	CA-C	5.98	1.58	1.53
1	C	787	GLU	CD-OE1	5.98	1.36	1.25
1	G	586	PRO	CA-C	5.98	1.57	1.52
1	A	94	CYS	CA-C	-5.90	1.45	1.52
1	A	17	ALA	C-O	-5.85	1.16	1.23
1	E	332	ILE	C-O	5.85	1.30	1.24
1	A	522	ARG	CZ-NH1	5.84	1.41	1.32
1	G	69	TYR	C-O	5.79	1.30	1.23
1	C	271	PRO	CA-C	5.76	1.59	1.52
1	G	532	ALA	N-CA	5.70	1.53	1.46
1	A	457	ARG	N-CA	-5.69	1.40	1.45
1	C	82	ARG	CZ-NH1	5.68	1.40	1.32
1	E	20	HIS	CA-C	-5.61	1.45	1.52
1	A	738	MET	N-CA	5.61	1.53	1.46
1	C	171	GLY	N-CA	5.58	1.50	1.44
1	E	586	PRO	CA-C	5.55	1.57	1.52
1	A	696	PRO	N-CA	-5.51	1.40	1.47
1	A	401	GLY	N-CA	5.50	1.53	1.45
1	C	650	ARG	C-O	5.50	1.30	1.24
1	C	10	LEU	CA-C	-5.49	1.45	1.52
1	E	403	LYS	CA-C	5.45	1.59	1.52
2	H	52	ASN	CA-C	-5.42	1.46	1.52
1	E	803	THR	CA-C	-5.42	1.45	1.52
1	E	418	GLY	N-CA	5.41	1.50	1.44
1	E	528	ALA	CA-C	5.38	1.59	1.52
1	A	165	VAL	N-CA	-5.35	1.40	1.46
1	C	701	GLN	C-O	-5.30	1.17	1.24
1	E	824	LYS	CA-C	5.27	1.59	1.52
1	G	32	GLY	C-O	-5.26	1.16	1.23
1	C	285	THR	CA-C	-5.26	1.46	1.52
1	G	725	TRP	N-CA	-5.23	1.39	1.46
1	E	16	ASP	CA-C	5.21	1.61	1.52
1	G	425	ASN	CA-C	5.21	1.59	1.52
1	C	52	ILE	C-O	-5.20	1.17	1.24
1	A	121	GLN	C-O	-5.19	1.17	1.24
1	C	80	ASP	C-O	-5.17	1.17	1.23
1	C	726	GLN	CA-C	5.14	1.57	1.53
1	A	429	VAL	CA-C	5.09	1.59	1.52
1	E	405	ARG	CA-C	5.09	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	329	ARG	CA-C	-5.08	1.46	1.52
1	C	608	LEU	CA-C	5.07	1.59	1.52
1	G	270	GLU	CA-C	-5.05	1.46	1.52
1	A	315	ASN	N-CA	-5.03	1.40	1.46
1	E	502	VAL	N-CA	-5.03	1.40	1.46

All (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
1	G	832	VAL	N-CA-CB	-8.07	101.87	112.36
1	E	237	THR	CB-CA-C	-7.66	94.18	109.35
1	G	104	ARG	NE-CZ-NH2	-7.61	112.35	119.20
1	A	104	ARG	NE-CZ-NH2	-7.51	112.44	119.20
1	G	635	GLY	N-CA-C	7.17	116.74	110.21
1	C	104	ARG	NE-CZ-NH2	-7.08	112.83	119.20
1	A	574	GLU	CB-CA-C	-7.01	98.33	110.17
1	E	574	GLU	CG-CD-OE2	-7.01	102.28	118.40
1	C	268	PRO	N-CA-C	-6.79	101.72	111.22
1	E	599	ARG	CG-CD-NE	-6.71	97.25	112.00
1	A	239	ALA	N-CA-C	6.62	119.34	111.33
1	G	832	VAL	CB-CA-C	6.55	118.13	110.93
1	C	239	ALA	N-CA-C	6.53	119.23	111.33
1	A	104	ARG	CG-CD-NE	-6.31	98.11	112.00
1	G	591	MET	CB-CA-C	6.22	118.47	109.45
1	E	599	ARG	NE-CZ-NH1	6.11	127.61	121.50
1	C	825	ILE	CB-CA-C	-6.07	104.64	111.80
1	E	654	MET	CA-CB-CG	-6.02	102.06	114.10
1	G	38	TRP	N-CA-C	6.02	113.42	108.07
1	C	246	TYR	N-CA-C	-6.01	104.64	111.14
1	C	825	ILE	N-CA-C	-6.01	105.96	111.67
1	E	104	ARG	NE-CZ-NH2	-5.97	113.83	119.20
1	E	574	GLU	CG-CD-OE1	5.91	131.99	118.40
1	A	133	GLY	N-CA-C	5.84	123.37	115.32
1	C	599	ARG	CG-CD-NE	-5.70	99.45	112.00
1	G	825	ILE	CB-CA-C	-5.63	105.15	111.80
1	A	574	GLU	CG-CD-OE2	-5.61	105.49	118.40
1	A	268	PRO	N-CA-C	-5.55	103.45	111.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	825	ILE	CB-CA-C	-5.54	105.26	111.80
1	C	216	VAL	N-CA-C	5.52	114.69	106.85
1	C	828	ALA	CA-C-N	-5.49	114.59	120.03
1	C	828	ALA	C-N-CA	-5.49	114.59	120.03
1	E	574	GLU	N-CA-CB	-5.48	102.24	110.73
1	E	713	LYS	N-CA-C	5.47	118.42	111.69
1	G	334	LYS	N-CA-C	5.46	119.11	112.23
1	G	717	ASN	N-CA-C	-5.44	103.35	110.53
1	A	151	THR	N-CA-C	-5.43	105.27	111.14
1	A	739	ASP	CB-CG-OD1	-5.42	105.93	118.40
2	F	139	GLY	N-CA-C	5.42	117.89	110.69
1	E	104	ARG	CG-CD-NE	-5.39	100.14	112.00
2	F	116	ASN	N-CA-CB	-5.39	103.42	110.59
1	G	104	ARG	CG-CD-NE	-5.37	100.19	112.00
1	G	825	ILE	N-CA-C	-5.33	106.61	111.67
1	G	802	VAL	N-CA-C	5.25	117.22	112.29
2	H	139	GLY	N-CA-C	5.24	117.66	110.69
1	A	573	GLY	CA-C-N	5.18	130.52	122.49
1	A	573	GLY	C-N-CA	5.18	130.52	122.49
1	A	828	ALA	CA-C-N	-5.18	114.90	120.03
1	A	828	ALA	C-N-CA	-5.18	114.90	120.03
1	E	825	ILE	CB-CA-C	-5.16	105.62	111.55
1	C	270	GLU	CA-C-N	-5.10	115.31	120.21
1	C	270	GLU	C-N-CA	-5.10	115.31	120.21
1	A	104	ARG	CD-NE-CZ	5.10	131.54	124.40
1	E	470	VAL	N-CA-C	5.09	115.31	110.42
1	E	239	ALA	N-CA-C	5.08	117.47	111.33
1	C	361	SER	N-CA-C	5.01	114.66	108.19
1	A	565	GLU	N-CA-C	-5.00	107.23	113.38

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

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
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
1:E:478:GLN:OE1	13:E:2101:HOH:O	1.83	0.94
1:C:613[B]:ASP:OD1	13:C:2101:HOH:O	1.85	0.94
1:G:522:ARG:NH1	13:G:2101:HOH:O	2.01	0.93
1:A:107:ARG:HD3	13:A:2514:HOH:O	1.69	0.92
1:C:566:MET:HE1	13:C:2579:HOH:O	1.70	0.91
1:C:693:MET:HE3	1:C:695:ALA:HB2	1.54	0.90
1:E:96:VAL:HG12	13:E:2281:HOH:O	1.75	0.86
1:C:423:ARG:HA	1:C:693:MET:HE1	1.59	0.84
1:A:566:MET:HE1	13:A:2116:HOH:O	1.79	0.82
1:C:522:ARG:HD3	13:C:2474:HOH:O	1.78	0.81
1:C:107:ARG:HD3	13:C:2493:HOH:O	1.81	0.79
1:A:561:ALA:O	1:A:566:MET:CE	2.31	0.79
1:A:134[B]:GLN:HG2	13:A:2193:HOH:O	1.83	0.78
1:A:611:MET:CE	13:A:2238:HOH:O	2.32	0.78
1:A:341:THR:HB	13:A:2755:HOH:O	1.85	0.76
1:G:737:VAL:HG12	1:G:738:MET:HE2	1.70	0.73
1:C:611:MET:SD	13:C:2609:HOH:O	2.46	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:GLU:HG2	13:E:2285:HOH:O	1.91	0.71
1:E:737:VAL:HG12	1:E:738:MET:HE2	1.73	0.70
11:E:2012:P33:H201	13:E:2641:HOH:O	1.91	0.70
11:G:2009:P33:O22	13:G:2103:HOH:O	2.10	0.70
1:G:566:MET:HE1	1:G:592:PRO:HA	1.73	0.69
1:C:737:VAL:HG12	1:C:738:MET:HE2	1.75	0.69
1:E:478:GLN:CD	13:E:2101:HOH:O	2.32	0.69
2:F:44:ALA:CA	13:F:347:HOH:O	2.40	0.68
1:C:693:MET:HE3	1:C:695:ALA:CB	2.23	0.68
11:A:2013:P33:O1	13:A:2101:HOH:O	2.10	0.68
1:A:423:ARG:HA	1:A:693:MET:HE1	1.75	0.67
1:E:840:LYS:HE3	13:E:2653:HOH:O	1.94	0.67
1:G:505:LYS:HE2	13:G:2775:HOH:O	1.99	0.63
13:G:2268:HOH:O	2:H:116:ASN:HB2	1.98	0.63
1:G:566:MET:HE2	1:G:592:PRO:HG3	1.81	0.62
1:C:423:ARG:HA	1:C:693:MET:CE	2.28	0.62
1:A:135:MET:HE2	1:A:557:ILE:HD12	1.82	0.62
1:A:611:MET:HE2	13:A:2238:HOH:O	1.99	0.62
1:C:41:ASN:HB3	13:H:401:HOH:O	1.99	0.61
1:A:49[B]:GLN:HG2	13:A:2854:HOH:O	1.99	0.61
1:C:501:ARG:NH1	13:C:2104:HOH:O	2.33	0.60
2:B:44:ALA:N	13:B:301:HOH:O	2.34	0.60
2:F:44:ALA:HB1	13:F:347:HOH:O	2.02	0.60
1:A:557:ILE:CG1	13:A:2693:HOH:O	2.21	0.59
1:G:611:MET:CE	13:G:2251:HOH:O	2.49	0.59
1:A:693:MET:HE2	1:A:695:ALA:HB2	1.84	0.59
1:A:561:ALA:O	1:A:566:MET:HE3	2.01	0.59
1:G:361:SER:HB2	13:G:2358:HOH:O	2.03	0.58
1:A:341:THR:OG1	1:A:342:ALA:N	2.37	0.58
1:A:523:GLU:HG2	13:A:2686:HOH:O	2.02	0.57
2:B:70:TYR:CD1	2:B:71:PRO:HA	2.39	0.57
1:G:379:GLU:HG2	13:G:2813:HOH:O	2.03	0.57
1:E:96:VAL:CG1	13:E:2281:HOH:O	2.41	0.57
1:A:223:TYR:CD1	1:A:574:GLU:HG3	2.40	0.56
1:C:562:THR:C	1:C:566:MET:HE2	2.30	0.56
1:G:155:VAL:HG22	1:G:160:GLU:HA	1.87	0.56
1:A:561:ALA:O	1:A:566:MET:HE1	2.06	0.56
1:C:324:LYS:HG2	1:C:326:TRP:CE2	2.40	0.56
1:G:368:GLU:OE1	1:G:371:ARG:NH1	2.37	0.56
1:C:212:ARG:HH12	11:C:2012:P33:H51	1.70	0.55
1:A:223:TYR:CG	1:A:574:GLU:HG3	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ARG:HA	1:A:693:MET:CE	2.36	0.54
1:A:737:VAL:HG12	1:A:738:MET:HE2	1.90	0.54
1:G:557:ILE:HD13	13:G:2812:HOH:O	2.08	0.53
2:F:44:ALA:HA	13:F:347:HOH:O	2.03	0.53
1:A:413:LYS:HE2	3:A:2001:MGD:S13	2.49	0.53
1:C:766:ILE:N	1:C:766:ILE:HD13	2.23	0.53
1:A:423:ARG:HG2	1:A:693:MET:CE	2.39	0.53
1:C:733:GLU:CG	13:C:2495:HOH:O	2.56	0.53
1:G:207:GLU:OE2	10:G:2013:SBO:O2	2.26	0.53
1:G:363:PHE:O	1:G:367:VAL:HG23	2.08	0.53
1:A:518:PRO:HA	13:A:2470:HOH:O	2.08	0.53
2:H:70:TYR:CD1	2:H:71:PRO:HA	2.43	0.53
1:A:347:TYR:CG	1:A:348:PRO:HA	2.44	0.53
1:C:212:ARG:HH22	11:C:2012:P33:H82	1.74	0.52
1:A:135:MET:HE2	1:A:557:ILE:CD1	2.38	0.52
1:C:840:LYS:HE2	13:C:2678:HOH:O	2.09	0.52
2:D:53:ARG:NH1	13:D:301:HOH:O	2.42	0.52
1:E:97:ASN:HB3	13:E:2281:HOH:O	2.08	0.52
1:E:31:CYS:HA	13:E:2281:HOH:O	2.09	0.52
1:E:156:LYS:HE2	1:E:613[B]:ASP:OD2	2.10	0.52
11:A:2013:P33:H141	13:A:2420:HOH:O	2.09	0.51
1:C:693:MET:CE	1:C:695:ALA:HB2	2.34	0.51
1:E:41:ASN:HB2	13:E:2381:HOH:O	2.09	0.51
2:B:44:ALA:N	13:B:302:HOH:O	2.43	0.51
1:C:830:ARG:HD3	13:C:2765:HOH:O	2.11	0.51
1:E:221:ASN:O	1:E:575:ARG:NH2	2.44	0.51
2:F:44:ALA:CB	13:F:347:HOH:O	2.57	0.51
1:C:82:ARG:CZ	1:C:82:ARG:HB2	2.40	0.50
2:H:44:ALA:N	13:H:303:HOH:O	2.44	0.50
1:C:293:GLN:HG3	13:C:2506:HOH:O	2.11	0.50
1:G:832:VAL:HG22	1:G:835:LEU:HD22	1.93	0.50
1:E:208:VAL:HB	1:E:211:THR:HG22	1.93	0.50
1:E:523:GLU:CG	13:E:2829:HOH:O	2.59	0.50
2:F:44:ALA:C	13:F:347:HOH:O	2.53	0.50
1:A:134[B]:GLN:NE2	1:E:549:LYS:HE3	2.26	0.50
1:A:522:ARG:NE	13:A:2107:HOH:O	2.29	0.50
11:C:2012:P33:H111	13:C:2690:HOH:O	2.11	0.50
1:A:717:ASN:OD1	3:A:2002:MGD:H8	2.12	0.50
1:C:829:PRO:HB2	1:C:831:ASN:OD1	2.12	0.49
1:C:324:LYS:HG2	1:C:326:TRP:CZ2	2.47	0.49
1:A:827:ASP:O	1:A:828:ALA:C	2.56	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:TYR:CD1	2:D:71:PRO:HA	2.48	0.49
1:A:433:LEU:HD23	1:A:438:ILE:HD12	1.95	0.49
1:E:415:LEU:HD23	1:E:415:LEU:C	2.37	0.49
1:G:739:ASP:OD1	13:G:2104:HOH:O	2.20	0.49
1:E:256:ARG:HD3	13:E:2620:HOH:O	2.11	0.49
1:A:339:GLU:HB2	13:A:2276:HOH:O	2.13	0.49
1:A:693:MET:HE2	1:A:695:ALA:CB	2.43	0.48
1:E:237:THR:CG2	1:E:243:GLN:OE1	2.61	0.48
1:A:415:LEU:HD23	1:A:415:LEU:C	2.39	0.48
1:C:363:PHE:O	1:C:367:VAL:HG23	2.13	0.48
1:G:737:VAL:HG12	1:G:738:MET:CE	2.39	0.48
1:G:59:GLU:HG2	13:G:2856:HOH:O	2.14	0.47
1:C:415:LEU:C	1:C:415:LEU:HD23	2.38	0.47
2:D:44:ALA:N	13:D:302:HOH:O	2.47	0.47
1:A:104:ARG:NH1	13:A:2122:HOH:O	2.46	0.47
1:C:255:LEU:HB3	1:C:295:ALA:HB2	1.95	0.47
1:G:212:ARG:HH22	11:G:2009:P33:H62	1.80	0.47
1:C:207:GLU:OE2	10:C:2011:SBO:O2	2.33	0.47
1:A:156:LYS:HE3	1:A:613[A]:ASP:OD2	2.15	0.47
1:G:174:GLY:HA2	3:G:2001:MGD:C6	2.44	0.47
1:C:599:ARG:HD3	1:C:599:ARG:HA	1.62	0.46
2:F:44:ALA:N	13:F:303:HOH:O	2.47	0.46
1:G:208:VAL:HB	1:G:211:THR:HG22	1.97	0.46
1:A:572:ASN:OD1	1:A:574:GLU:HB2	2.16	0.46
1:G:135:MET:HE2	1:G:557:ILE:HD12	1.97	0.46
1:A:49[B]:GLN:NE2	13:A:2128:HOH:O	2.48	0.46
1:C:737:VAL:CG1	1:C:738:MET:HE2	2.44	0.46
1:E:599:ARG:HD3	1:E:599:ARG:HA	1.74	0.46
1:E:255:LEU:HB3	1:E:295:ALA:HB2	1.98	0.46
1:A:350:ARG:HD3	13:A:2810:HOH:O	2.15	0.46
1:E:363:PHE:O	1:E:367:VAL:HG23	2.16	0.46
1:E:717:ASN:OD1	3:E:2002:MGD:H8	2.16	0.46
1:E:840:LYS:CE	13:E:2653:HOH:O	2.57	0.46
1:C:174:GLY:HA2	3:C:2001:MGD:C6	2.46	0.45
1:C:566:MET:CE	13:C:2579:HOH:O	2.44	0.45
1:A:423:ARG:HG2	1:A:693:MET:HE1	1.99	0.45
2:F:70:TYR:CD1	2:F:71:PRO:HA	2.51	0.45
1:A:117:ARG:HG2	8:A:2010:PGE:H4	1.99	0.45
1:A:522:ARG:NH2	13:A:2107:HOH:O	2.42	0.45
1:C:256:ARG:HB3	1:C:258:GLU:HG2	1.98	0.45
1:E:207:GLU:OE2	10:E:2011:SBO:O2	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:ALA:O	1:G:156:LYS:HG3	2.17	0.45
1:A:611:MET:HE1	13:A:2238:HOH:O	2.05	0.45
1:C:733:GLU:HG3	13:C:2495:HOH:O	2.15	0.45
2:D:84:THR:O	2:D:86:VAL:HG13	2.17	0.45
1:E:28:ILE:O	1:E:572:ASN:HB2	2.17	0.45
1:C:235:VAL:O	1:C:411:TYR:HA	2.17	0.44
1:C:624:ASP:HB2	13:C:2575:HOH:O	2.17	0.44
1:E:347:TYR:CG	1:E:348:PRO:HA	2.53	0.44
1:C:253:PRO:HA	1:C:258:GLU:HG3	1.98	0.44
1:E:174:GLY:HA2	3:E:2001:MGD:C6	2.48	0.44
1:E:350:ARG:HD2	13:E:2672:HOH:O	2.16	0.44
1:A:59:GLU:HG3	13:A:2730:HOH:O	2.16	0.44
1:A:208:VAL:HB	1:A:211:THR:HG22	2.00	0.44
1:G:729:TYR:CD2	3:G:2001:MGD:H2'	2.53	0.44
1:A:341:THR:HG22	13:A:2179:HOH:O	2.17	0.44
1:A:268:PRO:O	1:A:269:GLU:CB	2.64	0.44
1:A:8:ASP:HB3	2:B:47:VAL:HG21	2.00	0.44
1:G:723:VAL:HG21	13:G:2778:HOH:O	2.18	0.44
1:C:717:ASN:OD1	3:C:2002:MGD:H8	2.18	0.43
1:E:478:GLN:NE2	13:E:2128:HOH:O	2.50	0.43
1:E:737:VAL:CG1	1:E:738:MET:HE2	2.45	0.43
1:E:31:CYS:SG	1:E:97:ASN:HB3	2.58	0.43
1:G:110:GLU:CD	9:G:2011:GOL:H31	2.43	0.43
1:G:450:GLY:HA2	3:G:2002:MGD:H23	2.00	0.43
1:E:8:ASP:HB3	2:F:47:VAL:HG21	2.01	0.43
1:G:687:ASP:OD1	1:G:691:ARG:NH2	2.52	0.43
1:C:426:GLY:HA3	1:C:693:MET:HE2	2.00	0.43
1:G:347:TYR:OH	1:G:694:ASP:O	2.37	0.43
1:C:268:PRO:O	1:C:269:GLU:CB	2.65	0.43
1:G:501:ARG:NH2	13:G:2143:HOH:O	2.52	0.43
1:A:744:PRO:HG3	1:A:797:GLY:O	2.18	0.42
1:C:169:ASP:OD1	1:C:169:ASP:C	2.62	0.42
2:D:44:ALA:HB3	13:D:368:HOH:O	2.19	0.42
1:G:347:TYR:CG	1:G:348:PRO:HA	2.54	0.42
1:C:827:ASP:O	1:C:828:ALA:C	2.61	0.42
2:B:70:TYR:CG	2:B:71:PRO:HA	2.53	0.42
1:E:413:LYS:HE2	3:E:2001:MGD:S13	2.59	0.42
1:G:566:MET:HE1	1:G:592:PRO:CA	2.46	0.42
1:A:341:THR:CG2	13:A:2755:HOH:O	2.67	0.42
1:A:268:PRO:O	13:A:2102:HOH:O	2.21	0.42
1:A:829:PRO:HB2	1:A:831:ASN:OD1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:389:HOH:O	1:E:41:ASN:HB2	2.18	0.42
2:D:117:LYS:O	2:D:130:PRO:HD2	2.19	0.42
1:C:28:ILE:O	1:C:572:ASN:HB2	2.18	0.42
1:G:270:GLU:OE2	1:G:399:LYS:NZ	2.41	0.42
1:E:340:GLY:HA3	1:E:365:ASP:OD2	2.19	0.42
1:G:445:VAL:O	1:G:445:VAL:HG13	2.19	0.42
1:A:560:ALA:HA	1:A:591:MET:O	2.20	0.42
1:G:220:ASN:H	1:G:446:VAL:HG12	1.85	0.42
1:A:505:LYS:NZ	13:C:2120:HOH:O	2.51	0.42
11:G:2009:P33:O1	13:G:2102:HOH:O	2.09	0.42
1:E:535:GLN:HB3	13:E:2179:HOH:O	2.20	0.42
1:A:207:GLU:OE2	10:A:2012:SBO:O2	2.38	0.41
1:A:194:LYS:HE2	1:A:194:LYS:HB2	1.84	0.41
1:C:256:ARG:HG3	1:C:294:THR:HG23	2.02	0.41
1:C:535:GLN:HB3	13:C:2120:HOH:O	2.19	0.41
1:E:155:VAL:HG22	1:E:160:GLU:HA	2.02	0.41
1:A:104:ARG:NH2	1:A:722:ASN:OD1	2.53	0.41
1:A:557:ILE:CD1	13:A:2693:HOH:O	2.62	0.41
1:E:89:LYS:CE	13:E:2380:HOH:O	2.68	0.41
1:G:31:CYS:SG	1:G:97:ASN:HB3	2.61	0.41
1:G:744:PRO:HG3	1:G:797:GLY:O	2.20	0.41
1:A:445:VAL:HG13	1:A:445:VAL:O	2.21	0.41
1:E:89:LYS:HE3	13:E:2380:HOH:O	2.19	0.41
1:E:156:LYS:HE3	1:E:156:LYS:HB2	1.85	0.41
2:F:61:THR:O	2:F:62:LEU:C	2.63	0.41
1:A:326:TRP:HB3	1:A:396:GLY:O	2.21	0.41
2:F:54:LEU:HD11	2:F:160:ALA:HB2	2.02	0.41
1:C:370:CYS:O	1:C:371:ARG:C	2.64	0.41
13:C:2495:HOH:O	1:G:121:GLN:HG3	2.21	0.41
1:E:156:LYS:NZ	1:E:611:MET:SD	2.88	0.41
1:E:621:LYS:HE3	13:E:2721:HOH:O	2.19	0.41
1:G:706:GLN:HB3	9:G:2012:GOL:H31	2.03	0.41
1:C:450:GLY:HA2	3:C:2002:MGD:H23	2.03	0.41
1:E:450:GLY:HA2	3:E:2002:MGD:H23	2.01	0.41
1:G:827:ASP:O	1:G:828:ALA:C	2.64	0.41
1:A:557:ILE:HD11	13:A:2696:HOH:O	2.21	0.40
1:G:415:LEU:C	1:G:415:LEU:HD23	2.46	0.40
1:A:571:MET:HA	1:A:576:ARG:O	2.22	0.40
1:A:25:HIS:HD2	13:A:2159:HOH:O	2.04	0.40
1:G:153:LYS:HE2	1:G:527:ASN:OD1	2.21	0.40
1:C:130:TRP:O	1:C:514:MET:HE2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:ARG:NH2	1:E:722:ASN:OD1	2.54	0.40
1:G:293:GLN:HG3	13:G:2319:HOH:O	2.21	0.40

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 ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	104	ARG
1	A	134[A]	GLN
1	A	134[B]	GLN
1	A	189	GLU
1	A	237	THR
1	A	264	LYS
1	A	293	GLN
1	A	347	TYR
1	A	792	PHE
1	C	104	ARG
1	C	237	THR
1	C	258	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	269	GLU
1	C	324	LYS
1	C	339	GLU
1	C	347	TYR
1	C	607	VAL
1	C	711	SER
1	C	766	ILE
1	C	792	PHE
1	E	104	ARG
1	E	155	VAL
1	E	156	LYS
1	E	237	THR
1	E	256	ARG
1	E	265	GLU
1	E	341	THR
1	E	347	TYR
1	E	379	GLU
1	E	505	LYS
1	E	599	ARG
1	E	644	GLU
1	E	792	PHE
2	F	57	ILE
2	F	68	VAL
2	F	161	GLU
1	G	55	VAL
1	G	110	GLU
1	G	155	VAL
1	G	156	LYS
1	G	237	THR
1	G	269	GLU
1	G	400	GLU
1	G	591	MET
1	G	751	GLU
1	G	785	ARG
1	G	792	PHE
1	G	832	VAL
1	G	844	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	220	ASN
1	A	535	GLN
1	A	589	GLN
1	A	619	GLN
1	A	732	GLN
1	C	79	GLN
1	C	118	ASN
1	C	289	ASN
1	C	589	GLN
1	E	6	HIS
1	E	220	ASN
1	E	478	GLN
1	E	535	GLN
2	F	116	ASN
2	F	143	GLN
1	G	21	ASN
1	G	118	ASN
1	G	220	ASN
1	G	293	GLN
1	G	535	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 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
6	F3S	A	2006	1	0,9,9	-	-	-		
11	P33	G	2010	-	21,21,21	0.67	0	20,20,20	1.16	2 (10%)
9	GOL	C	2010	-	5,5,5	1.35	0	5,5,5	0.89	0
3	MGD	E	2002	5	45,52,52	1.47	6 (13%)	54,81,81	1.77	12 (22%)
3	MGD	G	2002	5	45,52,52	1.72	9 (20%)	54,81,81	1.76	14 (25%)
7	SO4	E	2007	-	4,4,4	0.39	0	6,6,6	0.61	0
10	SBO	A	2012	4	0,3,3	-	-	-		
3	MGD	E	2001	5	45,52,52	1.44	6 (13%)	54,81,81	1.72	12 (22%)
3	MGD	G	2001	5	45,52,52	1.39	9 (20%)	54,81,81	1.74	14 (25%)
7	SO4	A	2008	-	4,4,4	0.38	0	6,6,6	0.78	0
7	SO4	G	2007	-	4,4,4	0.59	0	6,6,6	0.92	0
9	GOL	G	2011	-	5,5,5	1.07	0	5,5,5	1.65	1 (20%)
12	FES	F	201	2	0,4,4	-	-	-		
6	F3S	C	2006	1	0,9,9	-	-	-		
3	MGD	C	2002	5	45,52,52	1.73	10 (22%)	54,81,81	1.73	9 (16%)
7	SO4	C	2008	-	4,4,4	0.36	0	6,6,6	0.84	0
11	P33	C	2012	-	21,21,21	0.73	0	20,20,20	1.44	4 (20%)
6	F3S	E	2006	1	0,9,9	-	-	-		
8	PGE	A	2010	-	9,9,9	1.01	0	8,8,8	1.89	4 (50%)
12	FES	D	201	2	0,4,4	-	-	-		
11	P33	E	2012	-	21,21,21	0.76	0	20,20,20	1.14	1 (5%)
7	SO4	A	2009	-	4,4,4	0.77	0	6,6,6	0.92	0
10	SBO	E	2011	4	0,3,3	-	-	-		
3	MGD	A	2001	5	45,52,52	1.59	6 (13%)	54,81,81	1.70	13 (24%)
11	P33	G	2009	-	21,21,21	1.03	1 (4%)	20,20,20	1.69	6 (30%)
3	MGD	C	2001	5	45,52,52	1.52	10 (22%)	54,81,81	1.98	14 (25%)
9	GOL	E	2010	-	5,5,5	0.91	0	5,5,5	1.72	1 (20%)
9	GOL	G	2012	-	5,5,5	1.33	0	5,5,5	2.46	3 (60%)
9	GOL	A	2011	-	5,5,5	0.71	0	5,5,5	1.47	0
7	SO4	A	2007	-	4,4,4	0.46	0	6,6,6	1.05	0
12	FES	B	201	2	0,4,4	-	-	-		
7	SO4	C	2009	-	4,4,4	0.45	0	6,6,6	0.53	0
12	FES	H	201	2	0,4,4	-	-	-		
6	F3S	G	2006	1	0,9,9	-	-	-		
7	SO4	E	2009	-	4,4,4	0.34	0	6,6,6	0.40	0
3	MGD	A	2002	5	45,52,52	1.53	6 (13%)	54,81,81	1.62	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SBO	G	2013	4	0,3,3	-	-	-		
7	SO4	C	2007	-	4,4,4	0.73	0	6,6,6	0.93	0
7	SO4	E	2008	-	4,4,4	0.75	0	6,6,6	1.25	1 (16%)
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
10	SBO	C	2011	4	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. '-' means no outliers of that kind were identified.

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MGD	A	2002	5	-	3/22/66/66	0/6/6/6
11	P33	A	2013	-	-	5/19/19/19	-

All (63) 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
3	E	2002	MGD	C16-C21	4.82	1.46	1.38
3	C	2001	MGD	C16-C21	4.60	1.46	1.38
3	A	2001	MGD	C6-N1	-4.46	1.30	1.38
3	E	2002	MGD	C21-N22	-4.15	1.31	1.35
3	C	2002	MGD	C21-N22	-3.91	1.31	1.35
3	G	2002	MGD	C4-N9	-3.68	1.28	1.38
3	G	2002	MGD	C17-N18	-3.60	1.32	1.38
3	E	2001	MGD	C6-N1	-3.37	1.32	1.38
3	A	2002	MGD	C14-N15	-3.36	1.42	1.46
3	G	2002	MGD	C5-N7	-3.25	1.32	1.39
3	G	2001	MGD	C16-C21	3.23	1.44	1.38
3	G	2002	MGD	C16-C17	3.18	1.50	1.42
3	C	2002	MGD	C6-N1	-3.17	1.32	1.38
3	C	2001	MGD	C14-N15	-3.12	1.42	1.46
3	C	2001	MGD	C21-N22	-3.08	1.32	1.35
3	G	2001	MGD	C6-N1	-2.92	1.33	1.38
3	G	2001	MGD	O6-C6	2.88	1.29	1.23
3	G	2002	MGD	C5-C4	2.86	1.46	1.38
3	G	2002	MGD	C21-N20	-2.83	1.32	1.36
3	E	2001	MGD	C5-N7	-2.78	1.33	1.39
3	A	2002	MGD	C17-N18	-2.78	1.33	1.38
3	E	2002	MGD	C6-N1	-2.69	1.33	1.38
3	A	2002	MGD	C4-N9	-2.65	1.31	1.38
3	A	2002	MGD	C21-N22	-2.63	1.32	1.35
3	C	2002	MGD	C17-N18	-2.60	1.34	1.38
3	C	2002	MGD	C5-N7	-2.60	1.34	1.39
3	A	2001	MGD	C23-N22	-2.60	1.40	1.45
3	E	2002	MGD	C17-N18	-2.58	1.34	1.38
3	E	2001	MGD	C4-N9	-2.58	1.31	1.38
3	C	2001	MGD	C17-N18	-2.56	1.34	1.38
3	G	2001	MGD	C4-N9	-2.52	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	MGD	C4-N9	-2.51	1.31	1.38
3	C	2002	MGD	C23-N22	-2.50	1.41	1.45
3	C	2001	MGD	C2-N1	-2.49	1.31	1.37
3	G	2001	MGD	C21-N22	-2.48	1.32	1.35
3	C	2002	MGD	C14-N15	-2.46	1.43	1.46
3	A	2001	MGD	O11-C23	-2.46	1.40	1.43
3	E	2002	MGD	C4-N9	-2.44	1.31	1.38
3	C	2001	MGD	C6-N1	-2.41	1.34	1.38
3	C	2001	MGD	C4-N9	-2.41	1.31	1.38
3	C	2001	MGD	C5-C4	2.40	1.45	1.38
3	G	2001	MGD	C17-N18	-2.38	1.34	1.38
3	G	2001	MGD	C5-C4	2.38	1.45	1.38
3	C	2001	MGD	O11-C23	-2.36	1.40	1.43
3	C	2002	MGD	C4-N9	-2.34	1.32	1.38
3	A	2002	MGD	C6-N1	-2.31	1.34	1.38
3	C	2002	MGD	C5-C4	2.30	1.45	1.38
3	E	2001	MGD	C2-N1	-2.30	1.32	1.37
3	E	2002	MGD	C5-C4	2.30	1.45	1.38
3	E	2001	MGD	O17-C17	2.29	1.27	1.23
3	G	2002	MGD	C2-N3	2.16	1.38	1.33
11	G	2009	P33	O10-C11	2.13	1.51	1.42
3	G	2002	MGD	PA-O1A	-2.13	1.43	1.50
3	G	2001	MGD	O17-C17	2.11	1.27	1.23
3	C	2002	MGD	O11-C11	-2.07	1.41	1.43
3	A	2001	MGD	C5-C4	2.06	1.44	1.38
3	C	2001	MGD	O4'-C4'	-2.05	1.40	1.45
3	G	2001	MGD	O4'-C4'	-2.04	1.40	1.45

All (119) 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	C	2001	MGD	N9-C4-N3	5.19	136.37	125.94
3	C	2001	MGD	C5-C4-N3	-4.98	120.38	128.46
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	2002	MGD	C5-C4-N3	-4.43	121.27	128.46
3	C	2001	MGD	O17-C17-C16	-4.30	117.39	127.24
3	A	2002	MGD	O11-C23-C14	4.23	111.78	108.96
3	E	2002	MGD	C4'-O4'-C1'	-4.11	100.40	109.47
3	A	2002	MGD	O17-C17-C16	-4.07	117.90	127.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	MGD	O11-C23-N22	-4.07	104.39	108.57
3	E	2002	MGD	O11-C23-C14	4.00	111.63	108.96
3	E	2002	MGD	O11-C23-N22	-3.76	104.70	108.57
3	C	2001	MGD	C19-N20-C21	3.75	120.20	113.43
3	A	2001	MGD	C17-C16-N15	3.72	126.75	116.76
3	E	2001	MGD	C2-N3-C4	3.71	118.91	112.30
3	G	2001	MGD	N9-C4-N3	3.69	133.36	125.94
3	C	2001	MGD	C2-N3-C4	3.65	118.80	112.30
3	G	2001	MGD	O11-C23-C14	3.64	111.39	108.96
9	G	2012	GOL	O3-C3-C2	3.56	127.28	110.20
3	E	2001	MGD	C17-C16-N15	3.55	126.28	116.76
3	A	2001	MGD	C5-C4-N3	-3.46	122.84	128.46
11	C	2012	P33	O10-C11-C12	3.39	125.69	110.39
3	C	2002	MGD	C2-N3-C4	3.39	118.33	112.30
3	E	2001	MGD	C5-C4-N3	-3.39	122.97	128.46
3	A	2001	MGD	C19-N20-C21	3.38	119.53	113.43
3	E	2001	MGD	C19-N20-C21	3.37	119.52	113.43
3	E	2002	MGD	N9-C4-N3	3.34	132.64	125.94
9	G	2012	GOL	O2-C2-C1	3.30	123.65	109.12
3	E	2002	MGD	C5-C4-N3	-3.29	123.12	128.46
3	G	2002	MGD	C19-N20-C21	3.28	119.35	113.43
3	G	2001	MGD	C5-C4-N3	-3.27	123.16	128.46
3	A	2001	MGD	N9-C4-N3	3.23	132.42	125.94
3	A	2002	MGD	C4'-O4'-C1'	-3.21	102.38	109.47
3	G	2002	MGD	C5-C4-N3	-3.15	123.34	128.46
3	E	2001	MGD	N9-C4-N3	3.13	132.23	125.94
3	G	2001	MGD	C8-N9-C4	3.13	112.01	106.05
3	C	2002	MGD	N9-C4-N3	3.13	132.22	125.94
3	C	2001	MGD	O6-C6-C5	-3.11	118.36	126.60
3	E	2002	MGD	C19-N20-C21	3.08	118.98	113.43
3	E	2001	MGD	C6-C5-N7	3.07	135.97	130.25
3	C	2002	MGD	O17-C17-C16	-3.07	120.20	127.24
3	A	2002	MGD	C5-C4-N3	-3.03	123.55	128.46
9	G	2011	GOL	O3-C3-C2	3.02	124.70	110.20
3	E	2001	MGD	C6-C5-C4	-3.00	114.15	118.77
3	G	2002	MGD	O17-C17-C16	-2.96	120.46	127.24
9	E	2010	GOL	O3-C3-C2	2.95	124.36	110.20
3	G	2002	MGD	C2-N3-C4	2.95	117.55	112.30
8	A	2010	PGE	O3-C4-C3	2.86	123.29	110.39
11	C	2012	P33	O7-C8-C9	2.85	123.26	110.39
3	G	2001	MGD	C2-N3-C4	2.83	117.33	112.30
3	G	2002	MGD	O6-C6-C5	-2.82	119.12	126.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2001	MGD	O11-C23-N22	2.81	111.46	108.57
3	A	2002	MGD	C6-C5-N7	2.80	135.45	130.25
3	G	2002	MGD	N9-C4-N3	2.76	131.49	125.94
11	G	2009	P33	O19-C20-C21	2.73	122.05	110.07
3	C	2001	MGD	C2'-C1'-N9	2.73	120.94	113.22
3	E	2001	MGD	O2B-PB-O1B	2.72	125.67	112.24
3	G	2002	MGD	C6-C5-N7	2.69	135.25	130.25
11	G	2009	P33	O10-C9-C8	2.68	122.47	110.39
3	G	2001	MGD	C17-C16-N15	2.68	123.94	116.76
3	E	2001	MGD	O2A-PA-O1A	2.67	125.42	112.24
3	G	2002	MGD	C4'-O4'-C1'	-2.64	103.64	109.47
3	G	2001	MGD	O6-C6-C5	-2.63	119.62	126.60
3	C	2001	MGD	C17-C16-N15	2.60	123.74	116.76
3	C	2002	MGD	C6-C5-N7	2.59	135.07	130.25
8	A	2010	PGE	O2-C2-C1	2.56	121.30	110.07
3	A	2001	MGD	C2-N3-C4	2.55	116.84	112.30
11	E	2012	P33	O4-C3-C2	-2.53	98.94	110.07
3	E	2002	MGD	C16-C17-N18	2.52	119.82	112.31
8	A	2010	PGE	O2-C3-C4	2.48	121.57	110.39
3	A	2001	MGD	C8-N9-C4	2.44	110.70	106.05
3	G	2001	MGD	O2A-PA-O1A	2.42	124.23	112.24
3	C	2001	MGD	C23-C14-C13	2.38	115.86	110.53
3	E	2001	MGD	O6-C6-C5	-2.38	120.30	126.60
11	G	2009	P33	O13-C12-C11	2.36	121.03	110.39
3	C	2001	MGD	C8-N9-C4	2.35	110.53	106.05
3	C	2002	MGD	C4-C5-N7	-2.35	107.01	110.72
3	G	2001	MGD	C1'-N9-C4	-2.34	119.54	126.50
11	G	2010	P33	C9-O10-C11	2.34	123.42	113.29
11	G	2009	P33	O7-C6-C5	2.34	120.94	110.39
3	C	2001	MGD	C16-C17-N18	2.33	119.25	112.31
11	G	2009	P33	O10-C11-C12	2.32	120.85	110.39
3	A	2002	MGD	C16-C17-N18	2.31	119.19	112.31
3	A	2001	MGD	N19-C19-N18	2.27	121.54	116.71
3	A	2001	MGD	O6-C6-C5	-2.26	120.60	126.60
3	G	2001	MGD	N19-C19-N18	2.26	121.52	116.71
3	G	2001	MGD	O17-C17-C16	-2.25	122.09	127.24
3	C	2001	MGD	C5-C6-N1	2.24	118.87	113.19
11	G	2009	P33	O16-C17-C18	2.22	120.41	110.39
3	G	2002	MGD	O2A-PA-O1A	2.21	123.15	112.24
3	E	2001	MGD	N9-C8-N7	-2.19	109.27	113.39
3	G	2002	MGD	O3A-PA-O1A	2.18	117.59	109.07
3	G	2002	MGD	C17-C16-N15	2.18	122.61	116.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	MGD	O4'-C4'-C3'	2.18	109.42	105.11
3	E	2002	MGD	C2-N3-C4	2.18	116.17	112.30
9	G	2012	GOL	C3-C2-C1	-2.16	103.32	111.70
3	C	2001	MGD	N19-C19-N18	2.15	121.29	116.71
3	G	2001	MGD	C6-C5-C4	-2.11	115.52	118.77
3	A	2002	MGD	C19-N20-C21	2.11	117.24	113.43
3	E	2002	MGD	C6-C5-N7	2.11	134.17	130.25
11	C	2012	P33	C15-O16-C17	2.10	122.39	113.29
8	A	2010	PGE	O3-C5-C6	2.10	119.28	110.07
3	E	2002	MGD	C17-C16-N15	2.10	122.39	116.76
3	C	2002	MGD	C19-N20-C21	2.09	117.21	113.43
3	E	2002	MGD	O6-C6-C5	-2.09	121.05	126.60
3	A	2002	MGD	N9-C4-N3	2.08	130.12	125.94
7	E	2008	SO4	O3-S-O1	2.07	120.14	109.31
3	A	2001	MGD	O17-C17-C16	-2.07	122.49	127.24
3	G	2002	MGD	O6-C6-N1	2.07	124.08	120.12
3	A	2001	MGD	C1'-N9-C4	-2.07	120.36	126.50
3	G	2002	MGD	O4'-C1'-C2'	-2.05	102.17	106.64
11	G	2010	P33	C18-O19-C20	2.05	122.16	113.29
3	G	2001	MGD	C6-C5-N7	2.04	134.05	130.25
3	C	2002	MGD	C4'-O4'-C1'	-2.04	104.97	109.47
11	C	2012	P33	O4-C5-C6	2.02	119.49	110.39
3	A	2001	MGD	N19-C19-N20	-2.01	115.82	119.73
3	E	2001	MGD	O4'-C4'-C3'	2.00	109.07	105.11

There are no chirality outliers.

All (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
3	C	2002	MGD	C5'-O5'-PB-O3B
3	E	2001	MGD	C5'-O5'-PB-O3B
3	E	2002	MGD	PA-O3B-PB-O5'
3	E	2002	MGD	C5'-O5'-PB-O1B
3	E	2002	MGD	C5'-O5'-PB-O3B
3	G	2001	MGD	PA-O3B-PB-O5'
3	G	2001	MGD	C5'-O5'-PB-O3B
3	G	2002	MGD	PA-O3B-PB-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	2002	MGD	C5'-O5'-PB-O3B
9	E	2010	GOL	C1-C2-C3-O3
9	G	2011	GOL	O1-C1-C2-O2
9	G	2011	GOL	O1-C1-C2-C3
11	G	2009	P33	C18-C17-O16-C15
11	G	2010	P33	C8-C9-O10-C11
8	A	2010	PGE	O1-C1-C2-O2
11	G	2009	P33	C12-C11-O10-C9
11	G	2009	P33	O4-C5-C6-O7
11	A	2013	P33	O16-C17-C18-O19
8	A	2010	PGE	O2-C3-C4-O3
11	G	2010	P33	O4-C5-C6-O7
11	A	2013	P33	O13-C14-C15-O16
9	A	2011	GOL	O1-C1-C2-O2
9	E	2010	GOL	O2-C2-C3-O3
11	C	2012	P33	O19-C20-C21-O22
11	G	2010	P33	O19-C20-C21-O22
11	G	2010	P33	O1-C2-C3-O4
11	G	2010	P33	O7-C8-C9-O10
11	C	2012	P33	O4-C5-C6-O7
8	A	2010	PGE	O3-C5-C6-O4
11	G	2009	P33	O19-C20-C21-O22
11	G	2009	P33	O1-C2-C3-O4
11	G	2010	P33	O13-C14-C15-O16
11	G	2009	P33	O7-C8-C9-O10
9	A	2011	GOL	O1-C1-C2-C3
9	C	2010	GOL	O1-C1-C2-C3
9	E	2010	GOL	O1-C1-C2-C3
9	G	2012	GOL	C1-C2-C3-O3
11	G	2009	P33	O10-C11-C12-O13
9	E	2010	GOL	O1-C1-C2-O2
11	G	2010	P33	O16-C17-C18-O19
11	G	2009	P33	O16-C17-C18-O19
11	E	2012	P33	O16-C17-C18-O19
9	C	2010	GOL	O1-C1-C2-O2
11	E	2012	P33	O7-C8-C9-O10
11	E	2012	P33	O4-C5-C6-O7
11	C	2012	P33	C2-C3-O4-C5
3	A	2001	MGD	PA-O3B-PB-O5'
3	A	2002	MGD	PA-O3B-PB-O5'
3	C	2002	MGD	PA-O3B-PB-O5'
3	E	2001	MGD	PA-O3B-PB-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	G	2009	P33	O13-C14-C15-O16
11	C	2012	P33	C17-C18-O19-C20
11	G	2009	P33	C6-C5-O4-C3
11	A	2013	P33	C12-C11-O10-C9
8	A	2010	PGE	C6-C5-O3-C4
11	A	2013	P33	C11-C12-O13-C14
9	G	2012	GOL	O1-C1-C2-O2
8	A	2010	PGE	C1-C2-O2-C3
3	C	2001	MGD	O4'-C4'-C5'-O5'
11	C	2012	P33	C14-C15-O16-C17
3	E	2002	MGD	PB-O3B-PA-O1A
3	G	2002	MGD	PB-O3B-PA-O1A
11	E	2012	P33	C17-C18-O19-C20
11	C	2012	P33	O16-C17-C18-O19
3	A	2001	MGD	C5'-O5'-PB-O1B
3	C	2001	MGD	C5'-O5'-PB-O1B
3	E	2001	MGD	C5'-O5'-PB-O1B
3	G	2001	MGD	C5'-O5'-PB-O1B
11	C	2012	P33	O10-C11-C12-O13
11	C	2012	P33	C18-C17-O16-C15
11	E	2012	P33	C21-C20-O19-C18
11	G	2009	P33	C2-C3-O4-C5
11	E	2012	P33	C9-C8-O7-C6
11	E	2012	P33	O1-C2-C3-O4
11	G	2009	P33	C9-C8-O7-C6
3	E	2001	MGD	O4'-C4'-C5'-O5'
11	E	2012	P33	O19-C20-C21-O22
11	C	2012	P33	C5-C6-O7-C8
11	G	2009	P33	C11-C12-O13-C14
11	G	2010	P33	C5-C6-O7-C8
11	E	2012	P33	O13-C14-C15-O16
3	C	2001	MGD	C3'-C4'-C5'-O5'
11	C	2012	P33	C8-C9-O10-C11
3	G	2001	MGD	O4'-C4'-C5'-O5'
3	A	2001	MGD	PB-O3B-PA-O2A
11	G	2010	P33	C11-C12-O13-C14
3	A	2002	MGD	C5'-O5'-PB-O1B
3	G	2002	MGD	C5'-O5'-PB-O1B
3	A	2001	MGD	O4'-C4'-C5'-O5'
11	A	2013	P33	C15-C14-O13-C12
11	G	2010	P33	O10-C11-C12-O13
11	C	2012	P33	O7-C8-C9-O10

Continued on next page...

Continued from previous page...

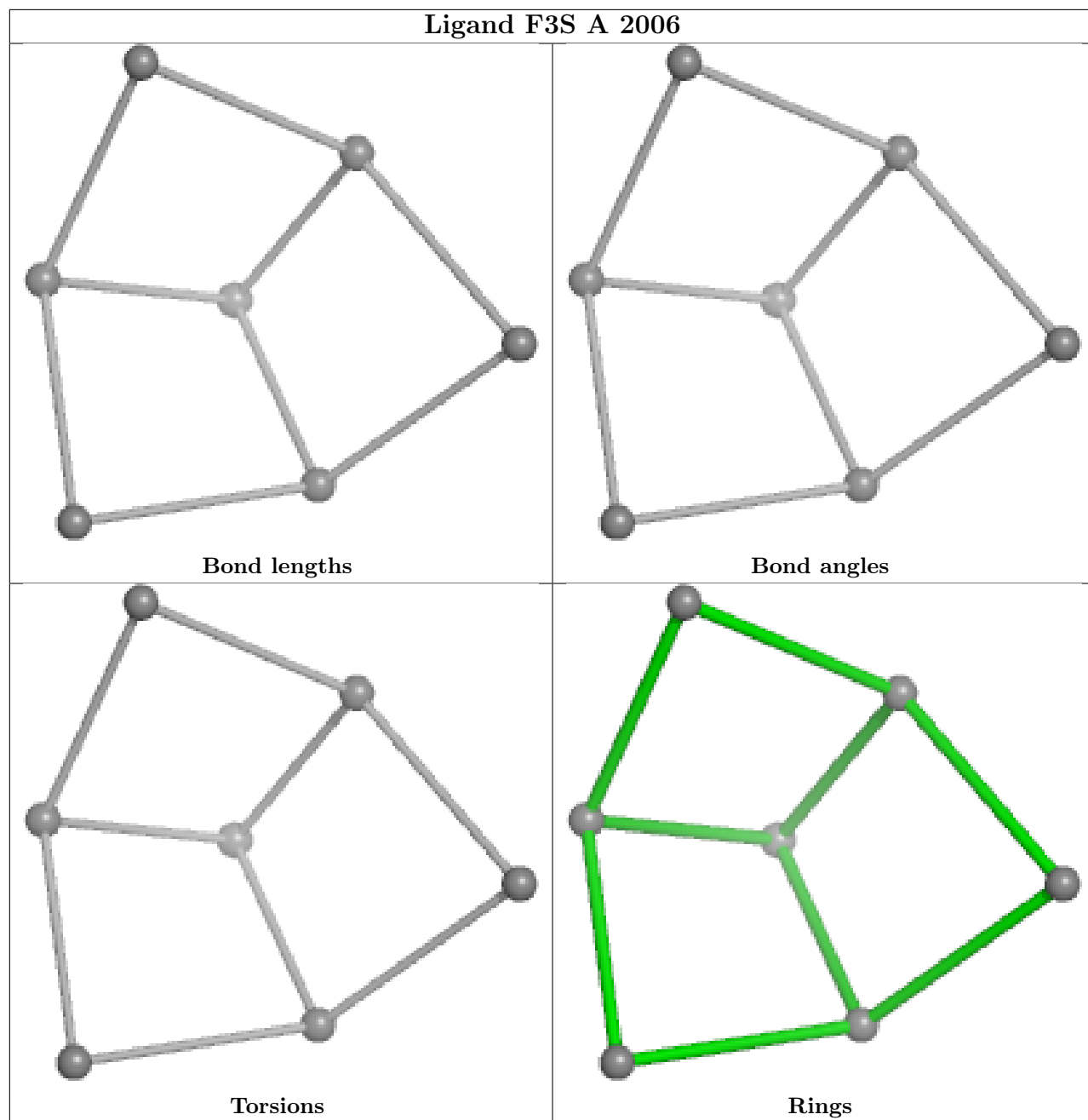
Mol	Chain	Res	Type	Atoms
11	E	2012	P33	C14-C15-O16-C17

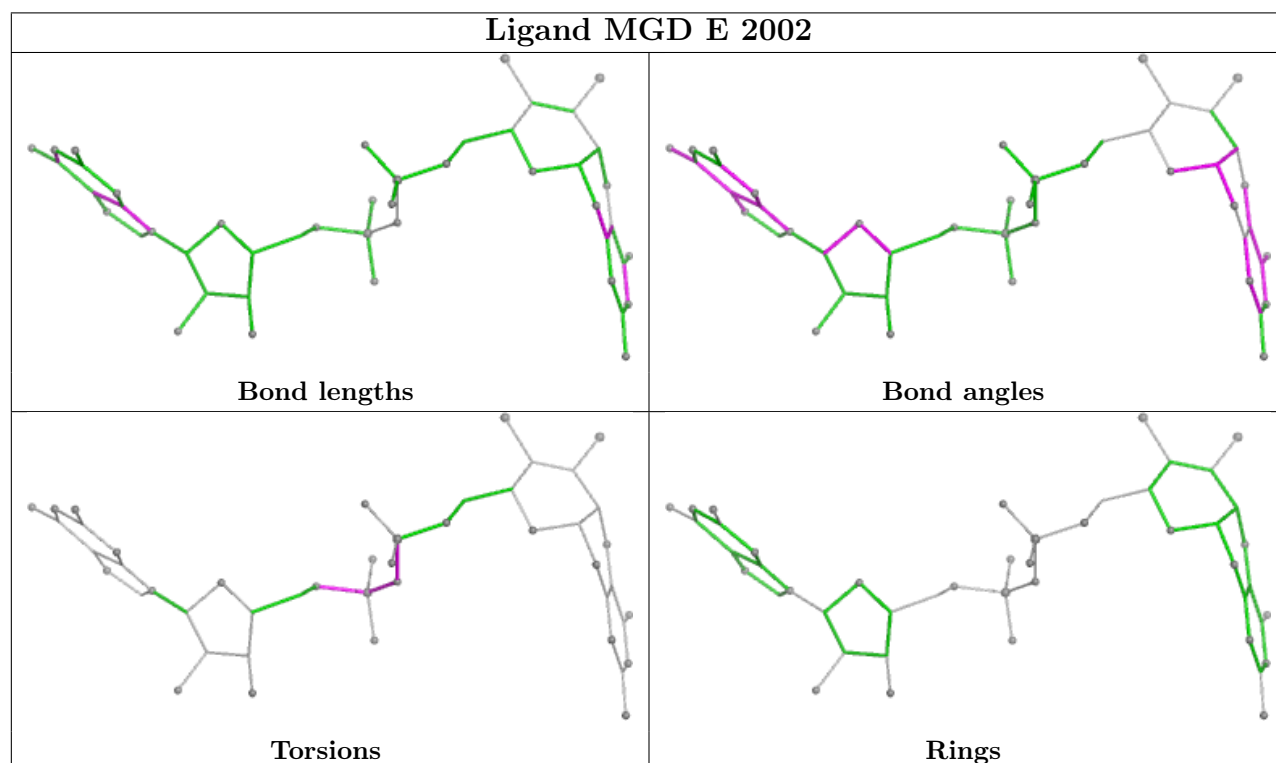
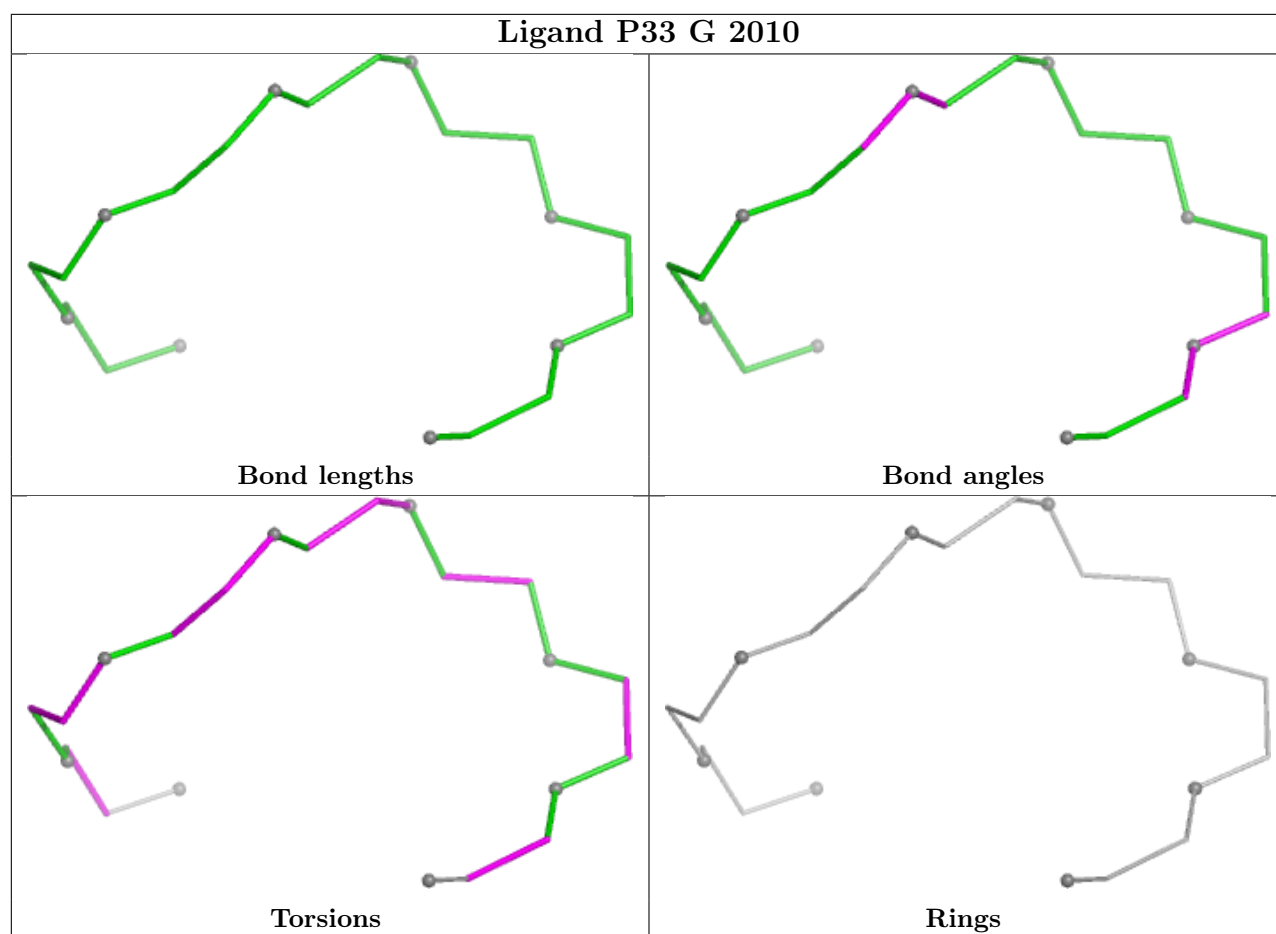
There are no ring outliers.

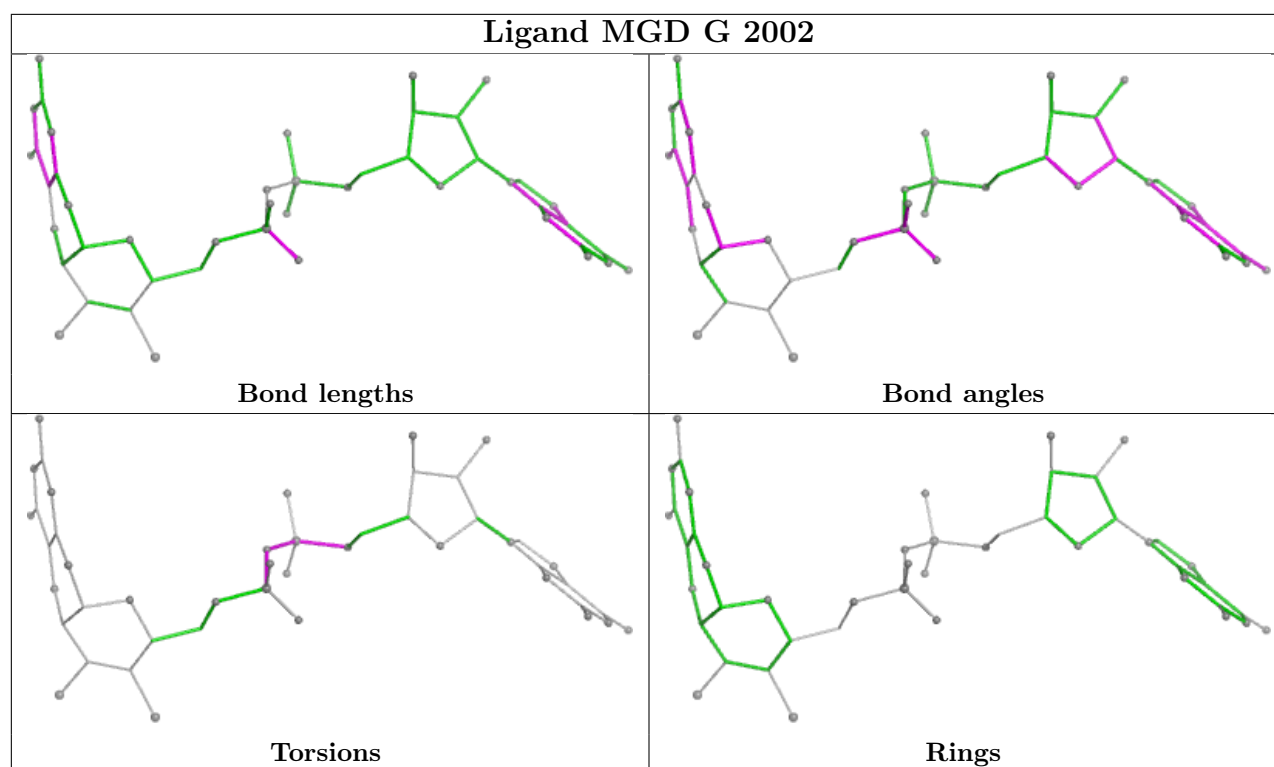
19 monomers are involved in 28 short contacts:

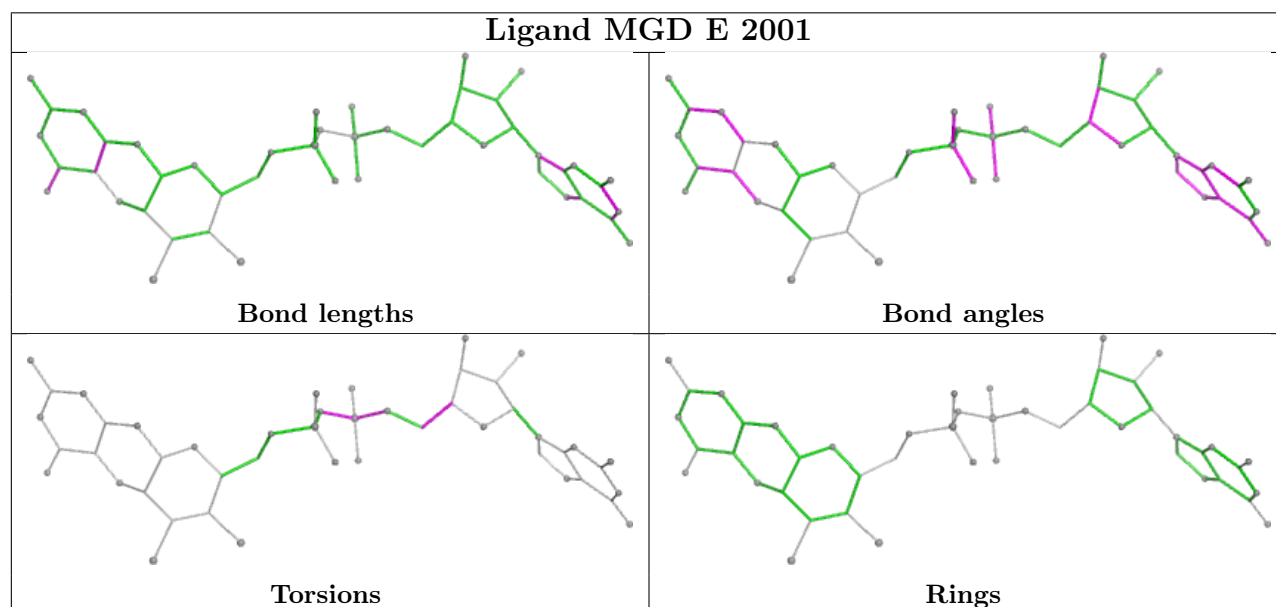
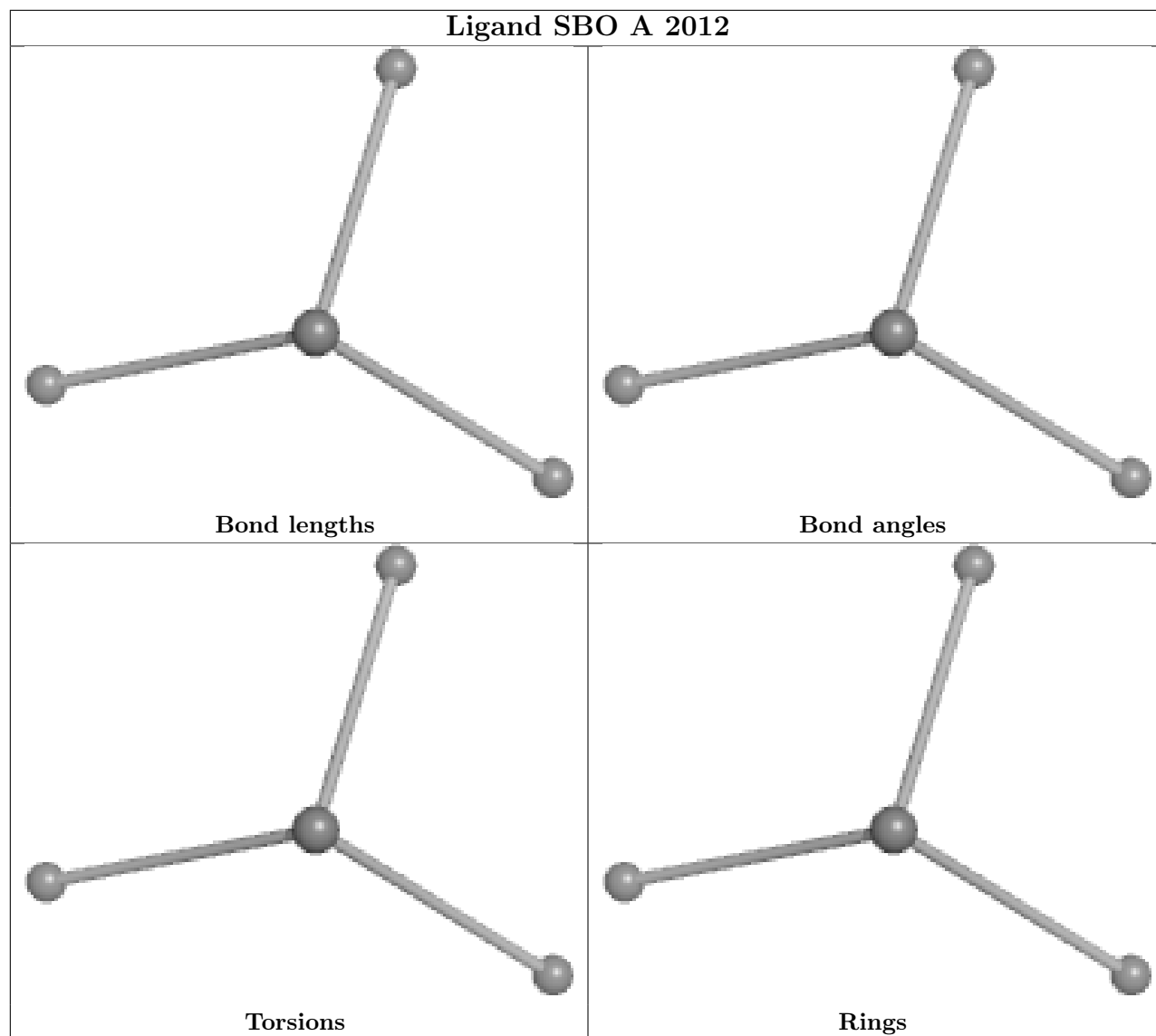
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2002	MGD	2	0
3	G	2002	MGD	1	0
10	A	2012	SBO	1	0
3	E	2001	MGD	2	0
3	G	2001	MGD	2	0
9	G	2011	GOL	1	0
3	C	2002	MGD	2	0
11	C	2012	P33	3	0
8	A	2010	PGE	1	0
11	E	2012	P33	1	0
10	E	2011	SBO	1	0
3	A	2001	MGD	1	0
11	G	2009	P33	3	0
3	C	2001	MGD	1	0
9	G	2012	GOL	1	0
3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

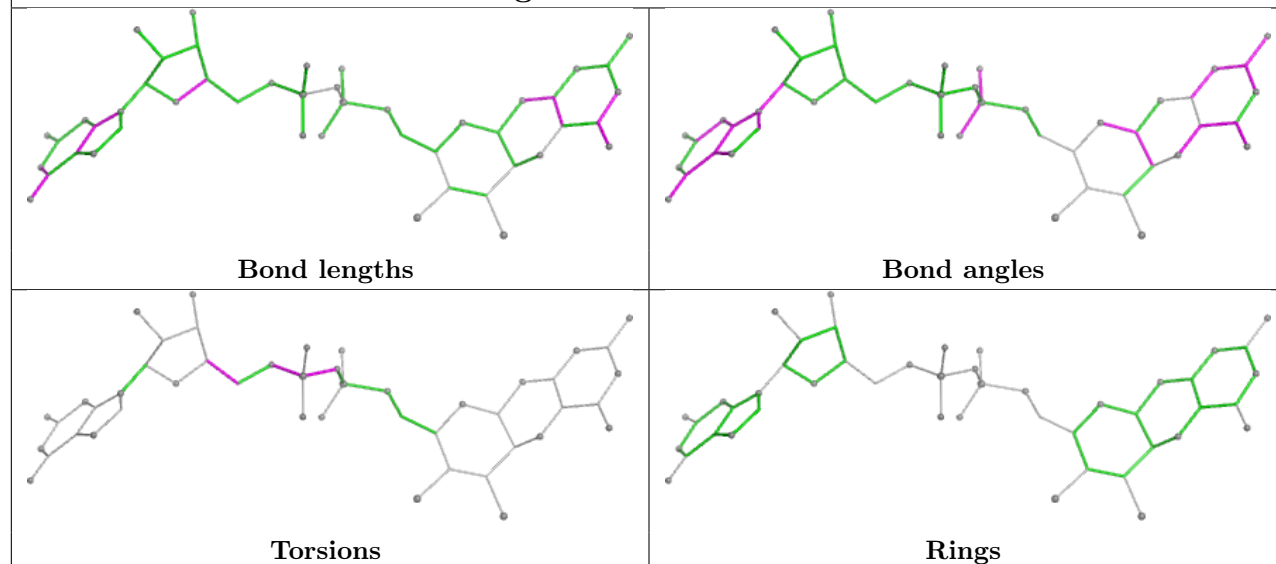




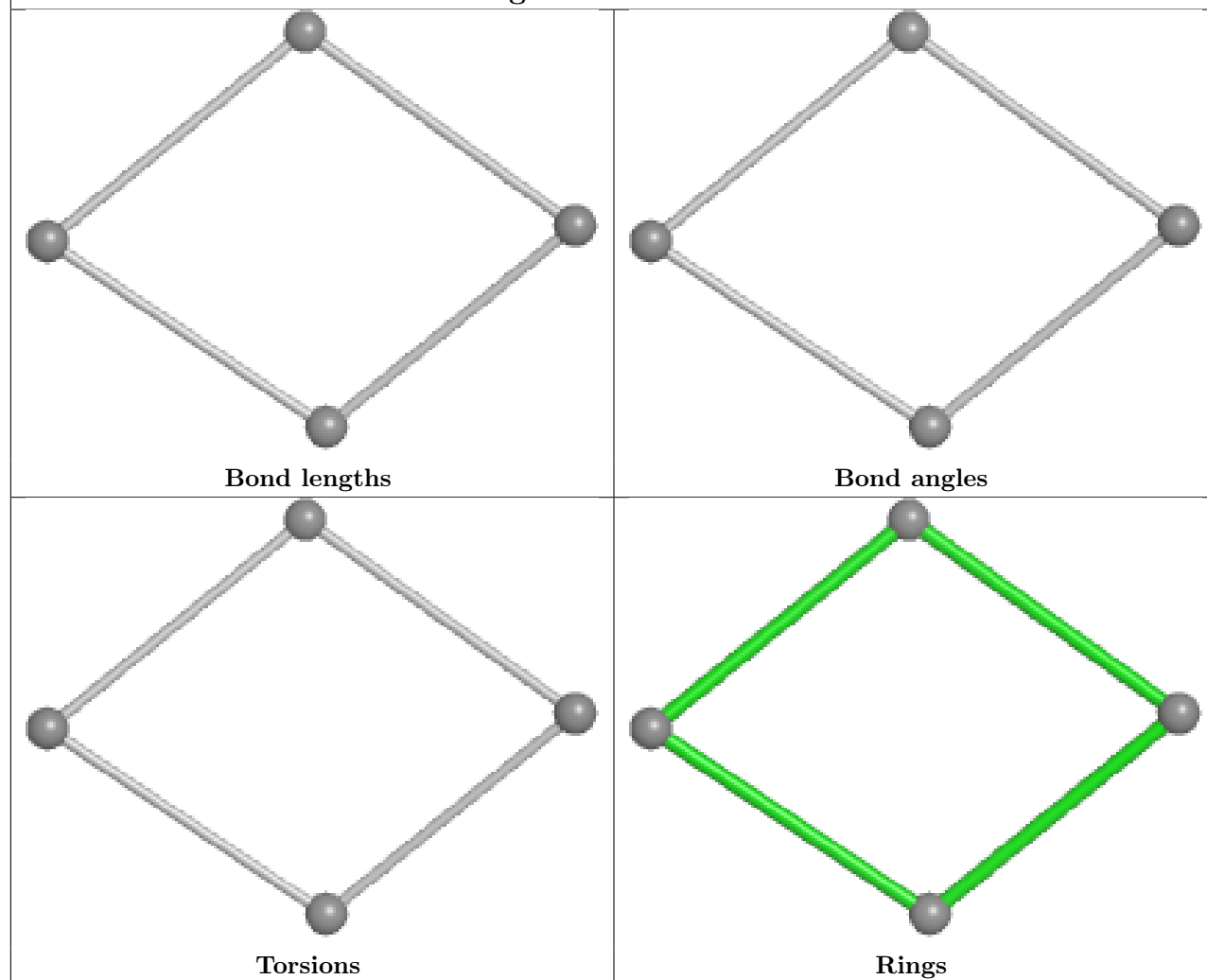


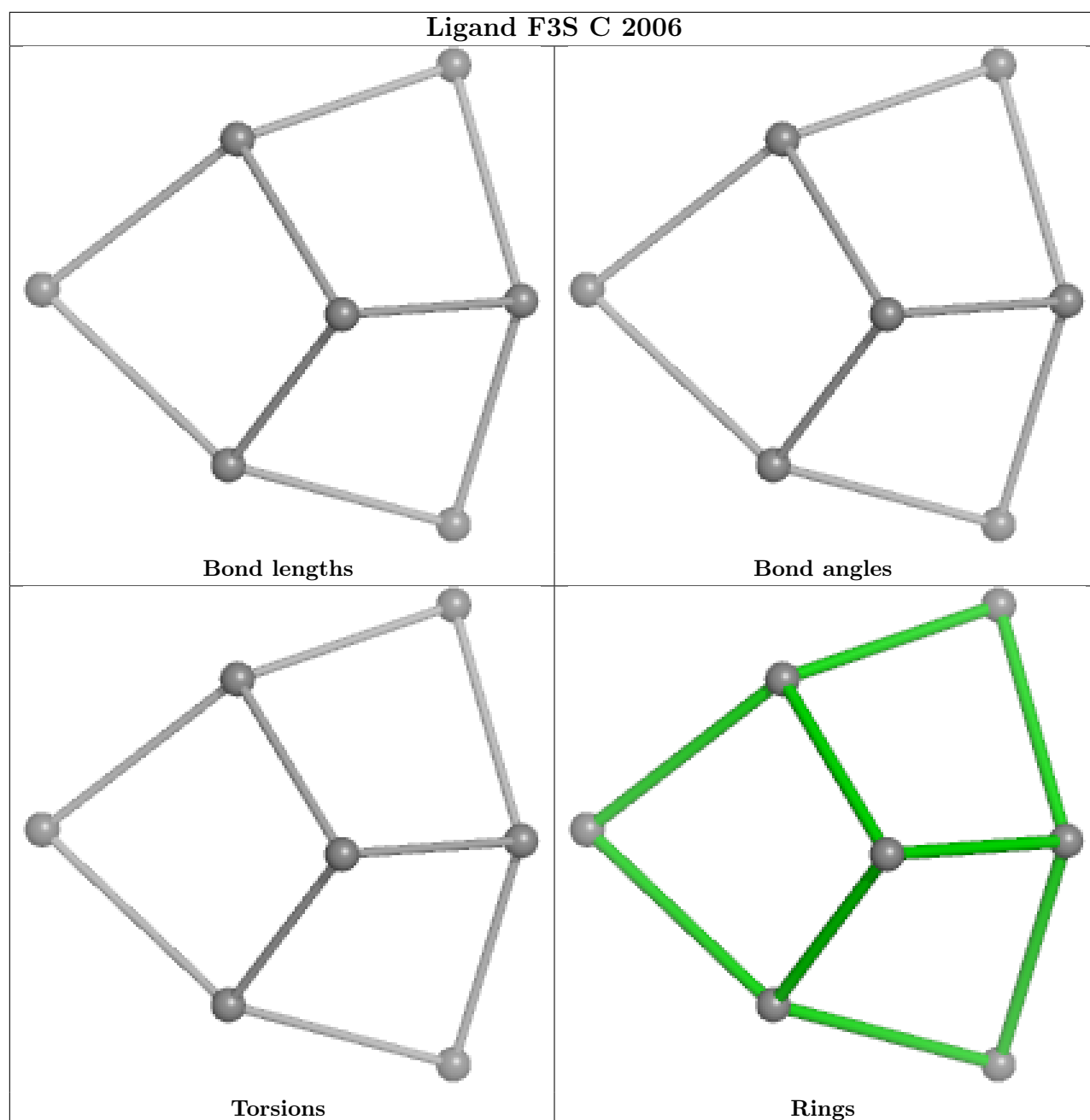


Ligand MGD G 2001

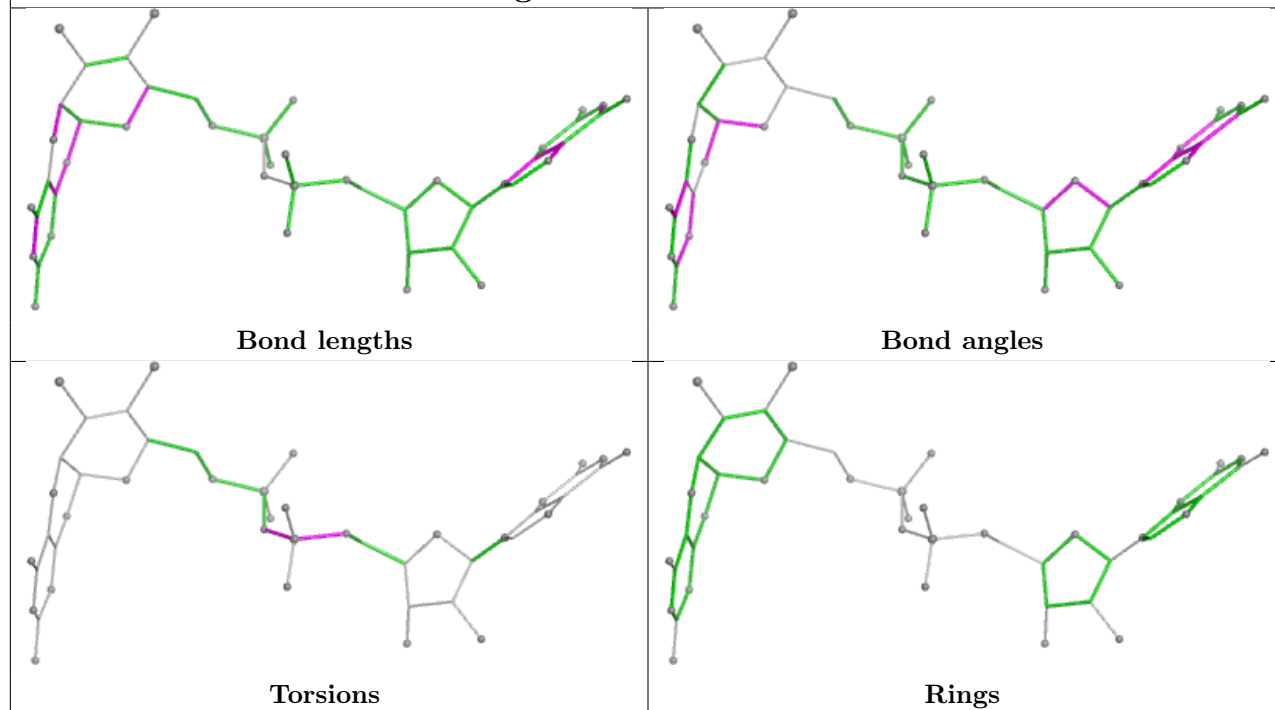


Ligand FES F 201

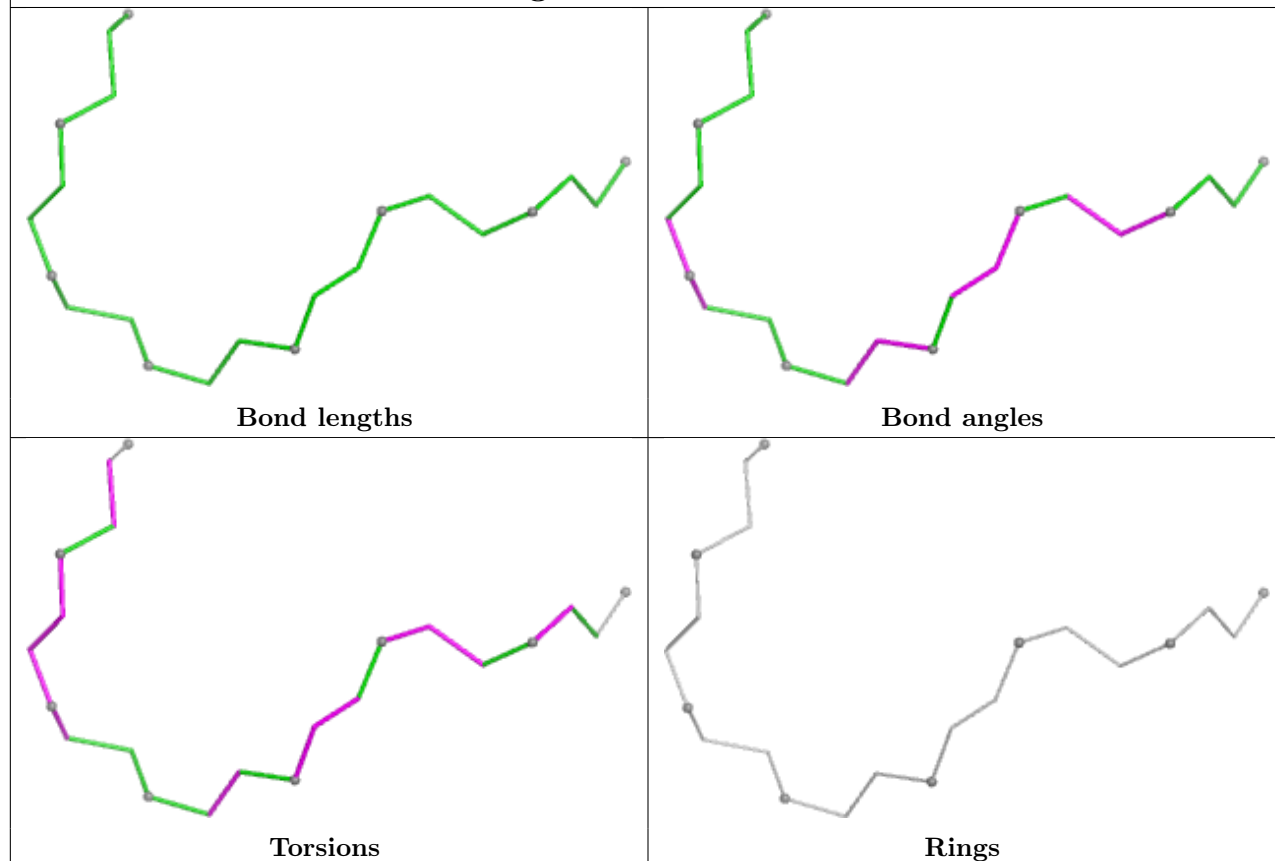


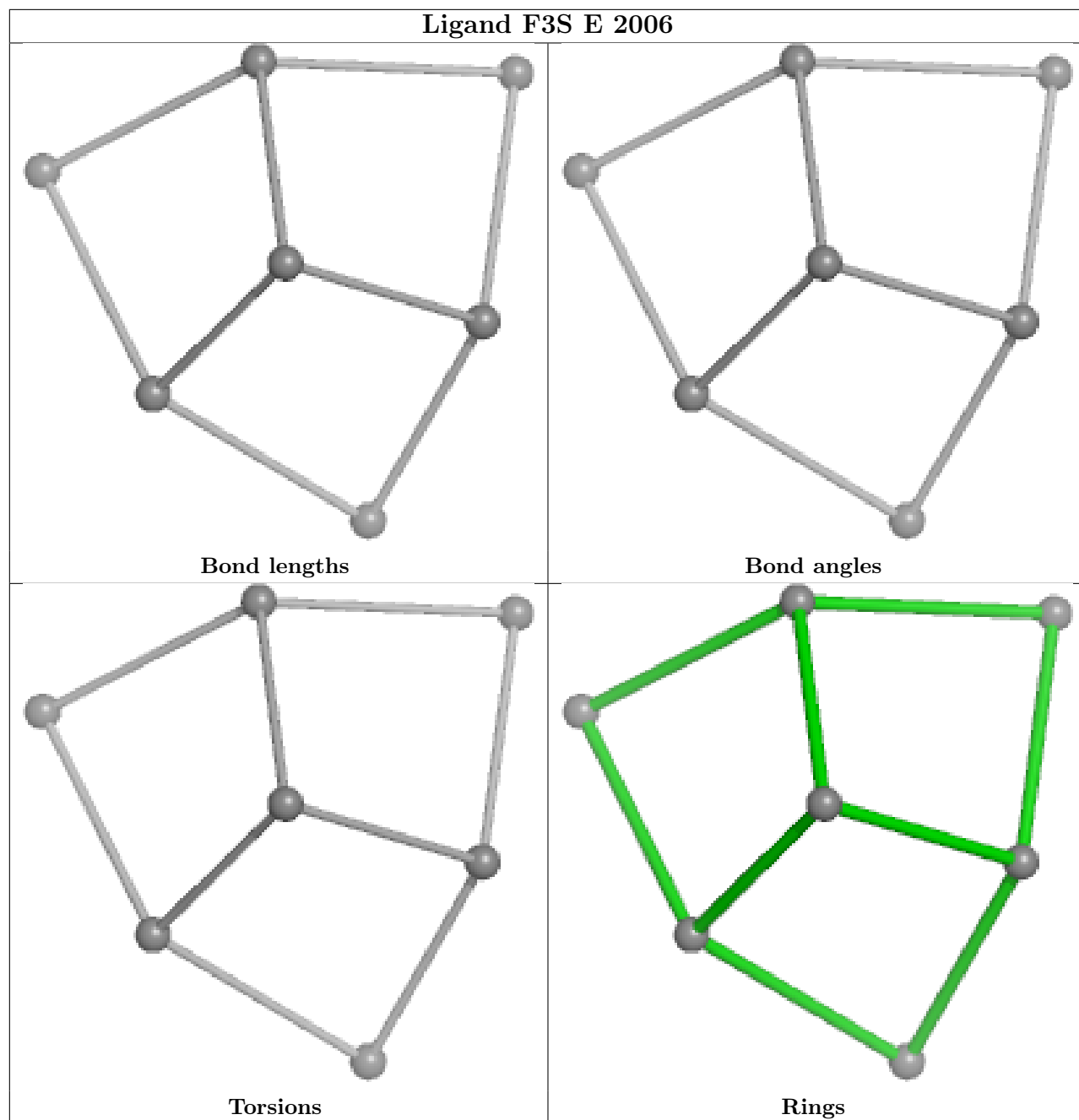


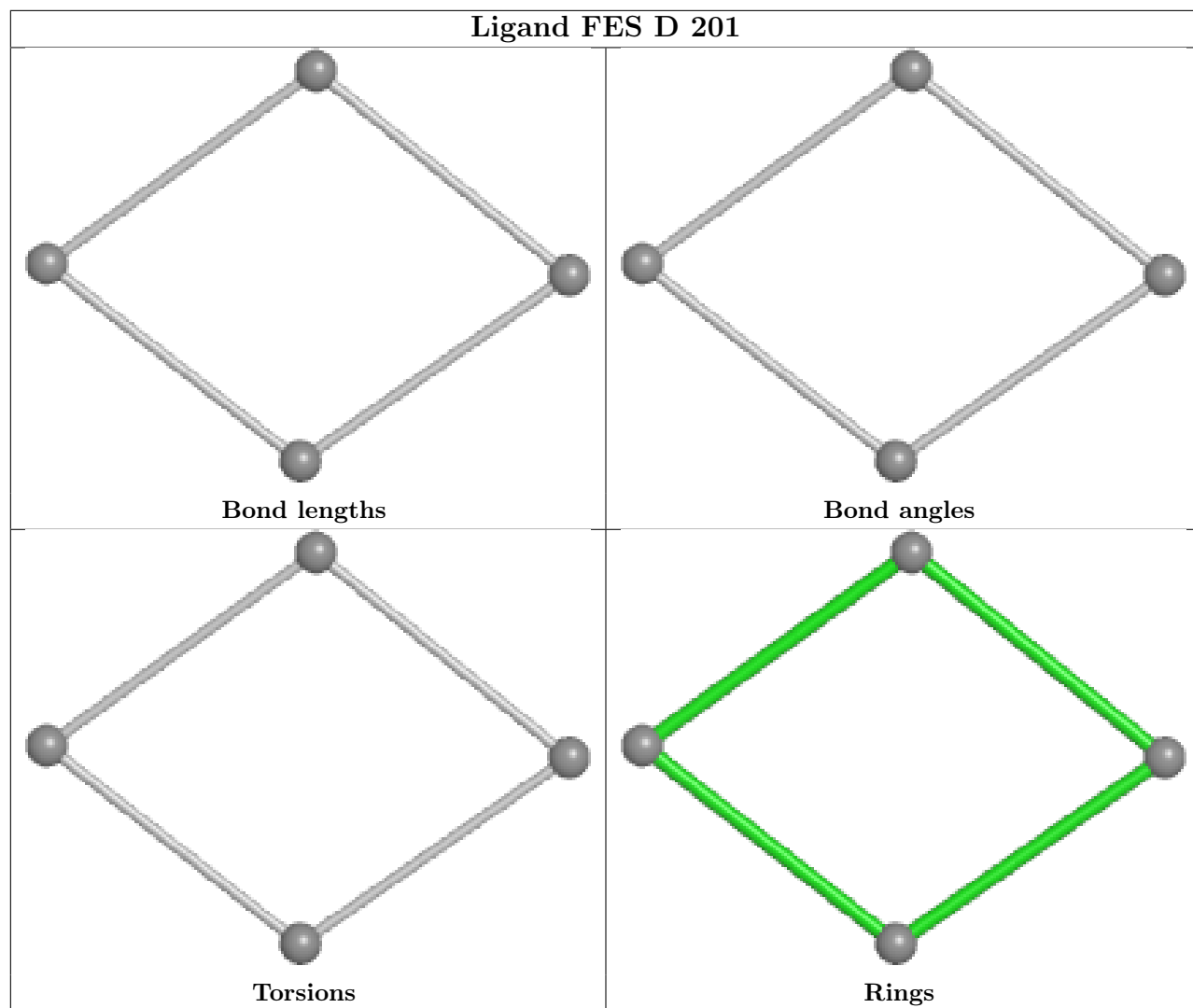
Ligand MGD C 2002

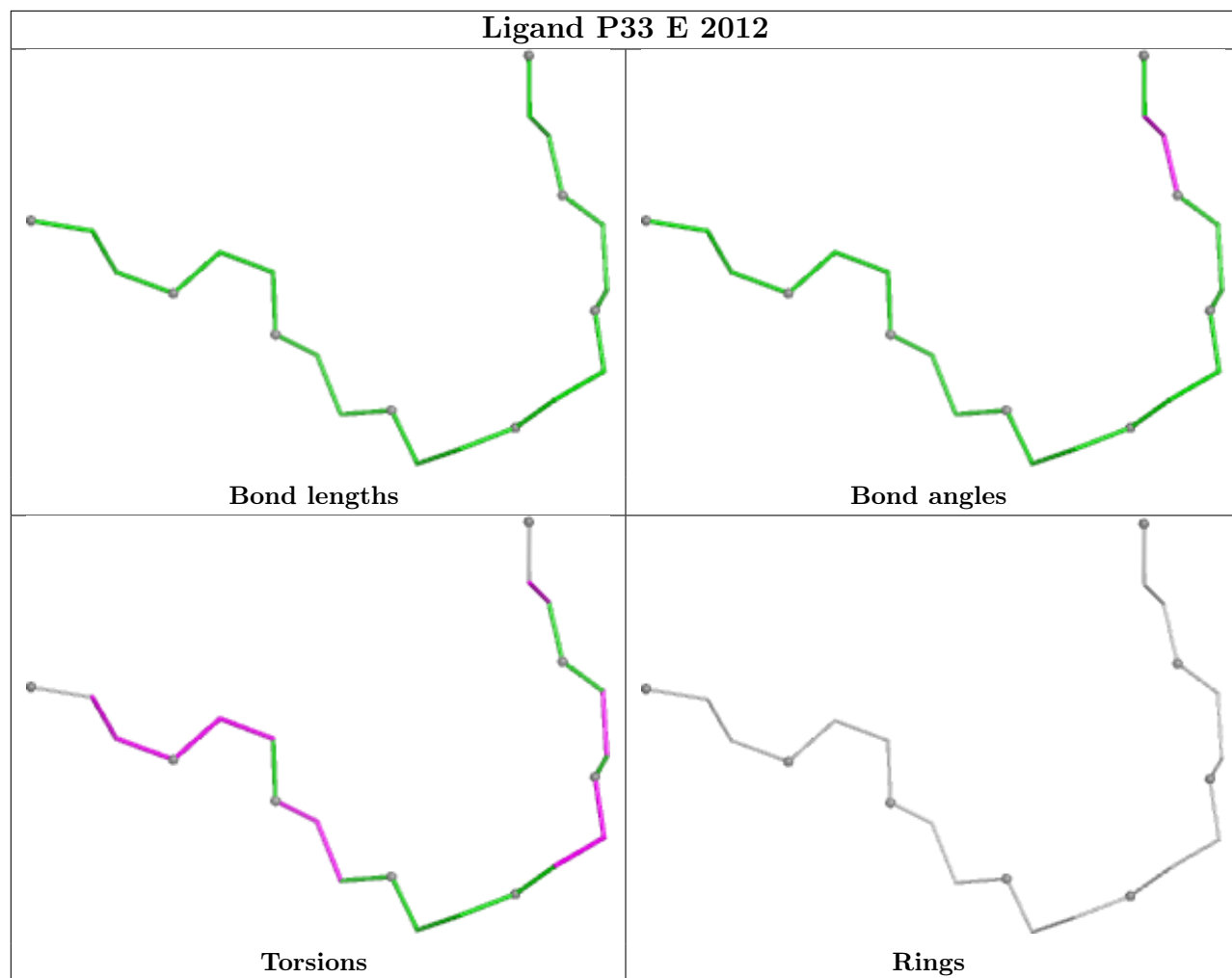


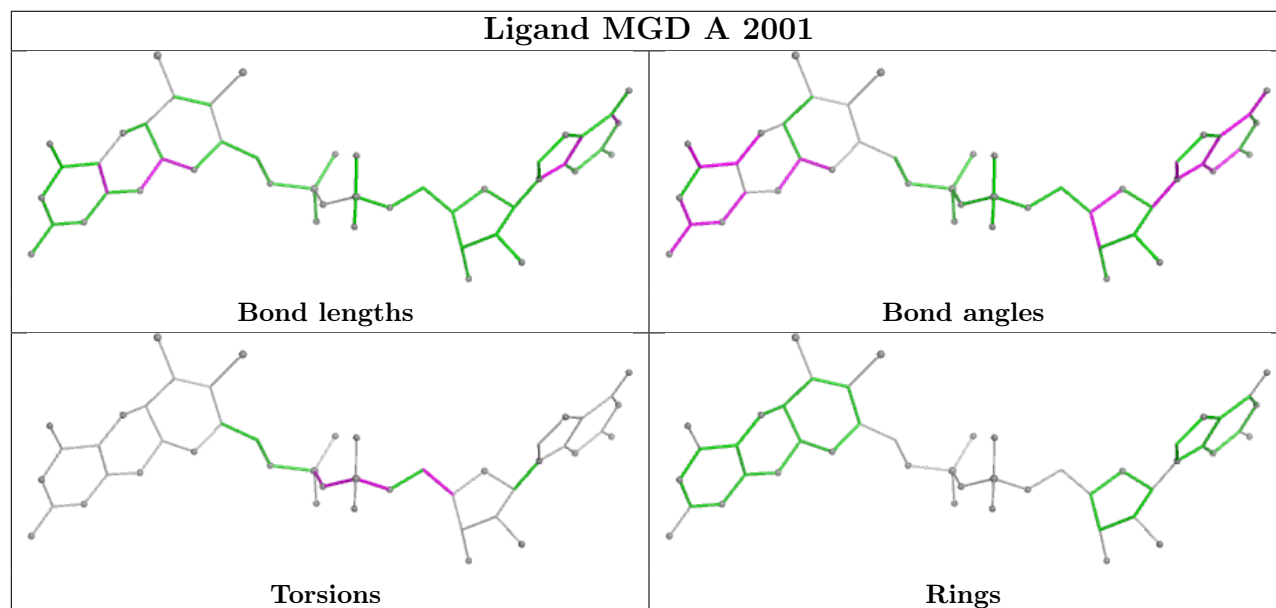
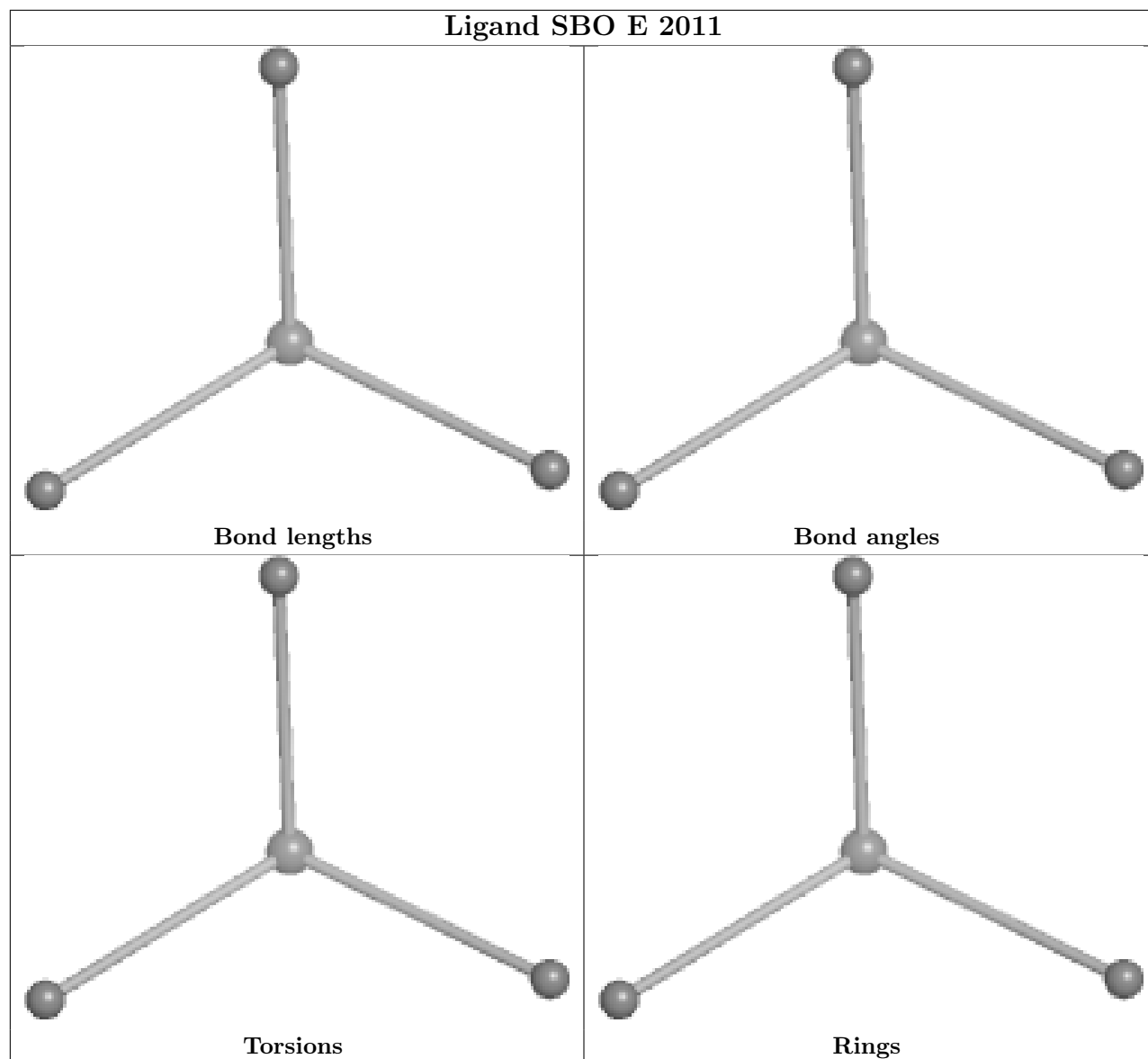
Ligand P33 C 2012

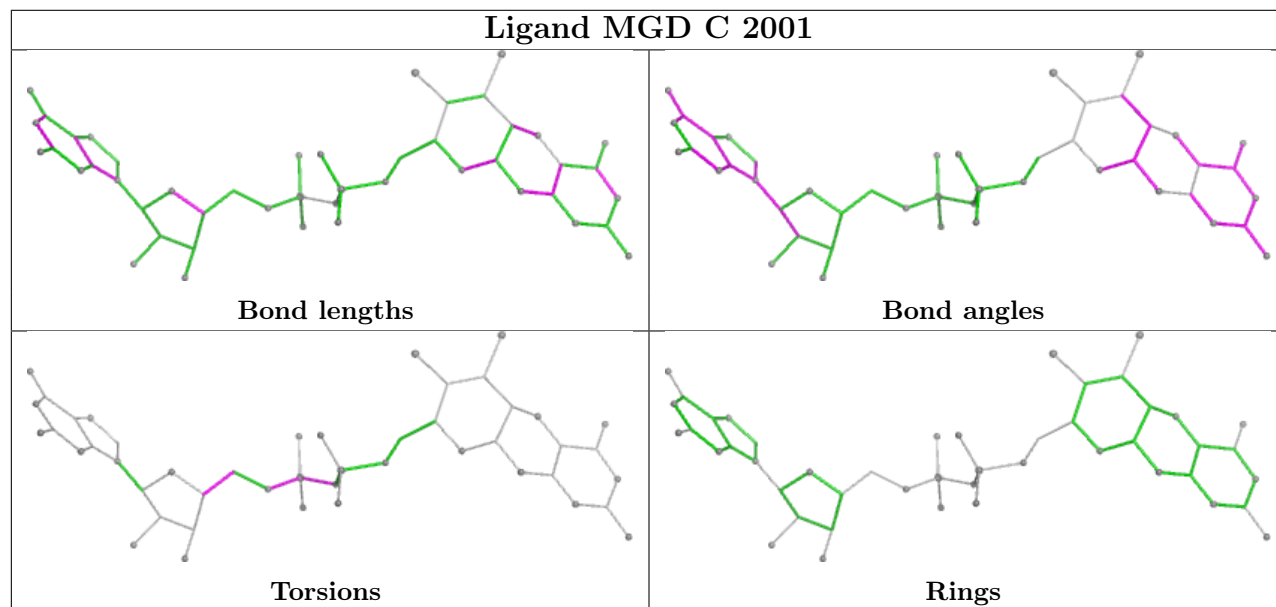
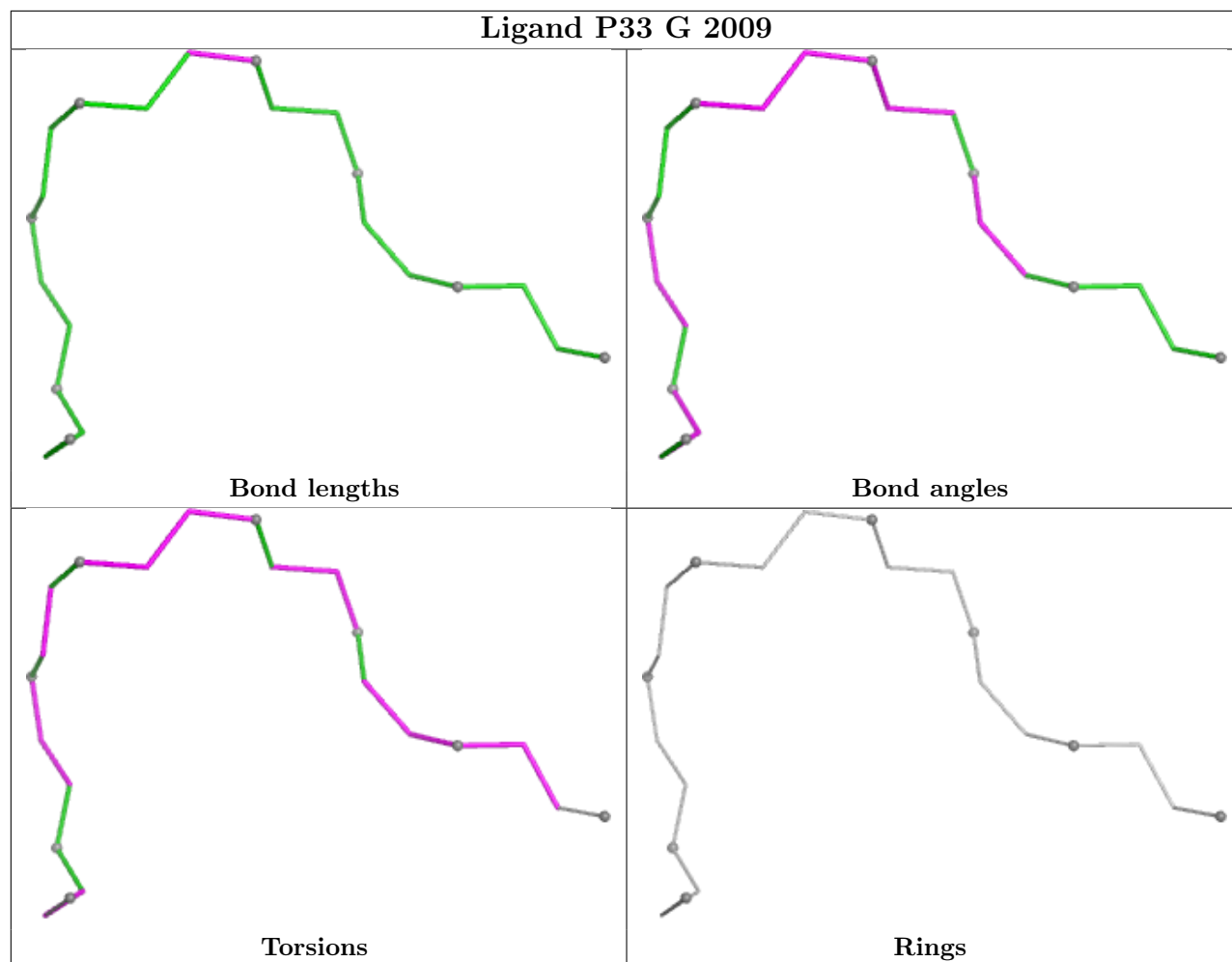


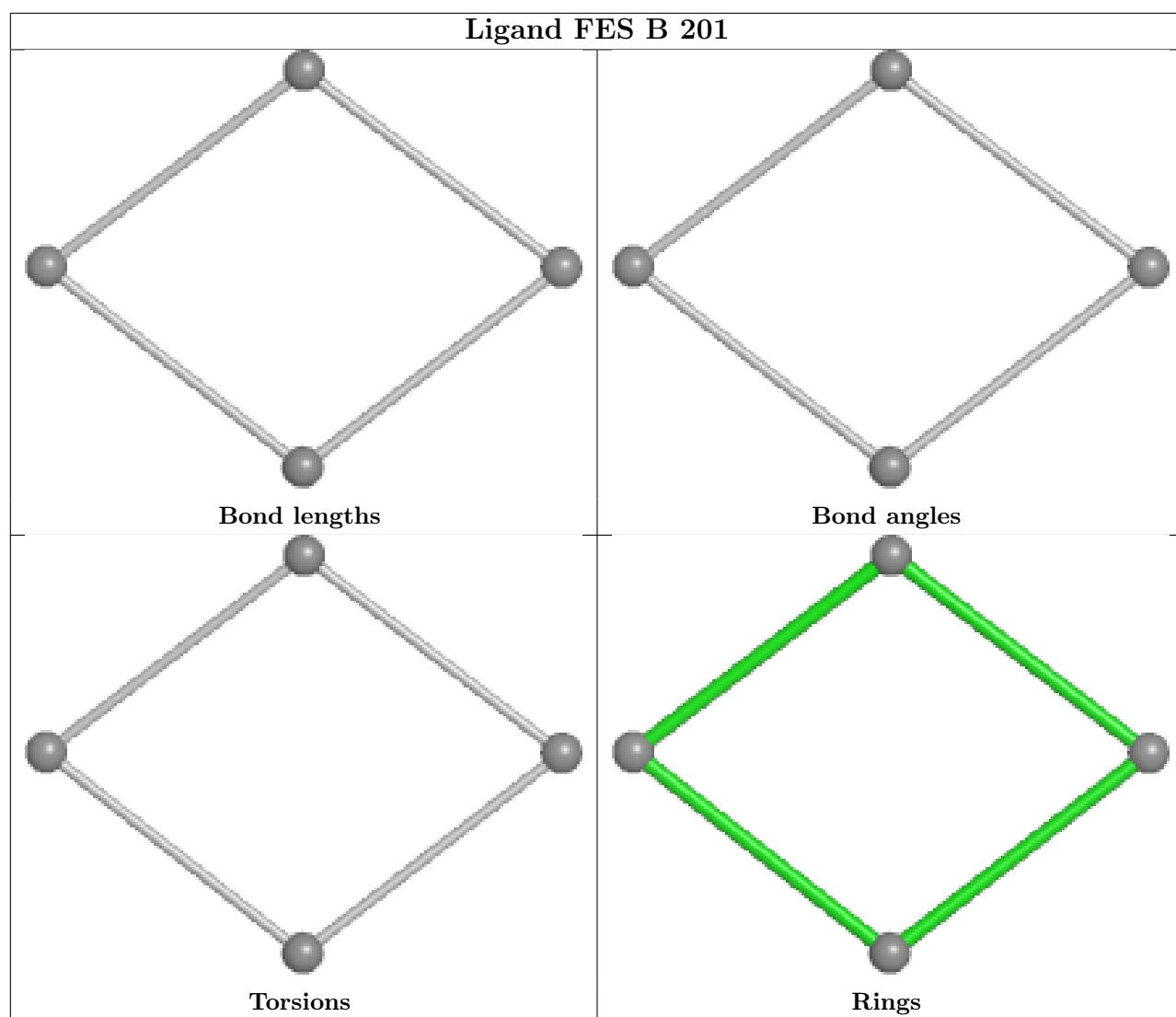


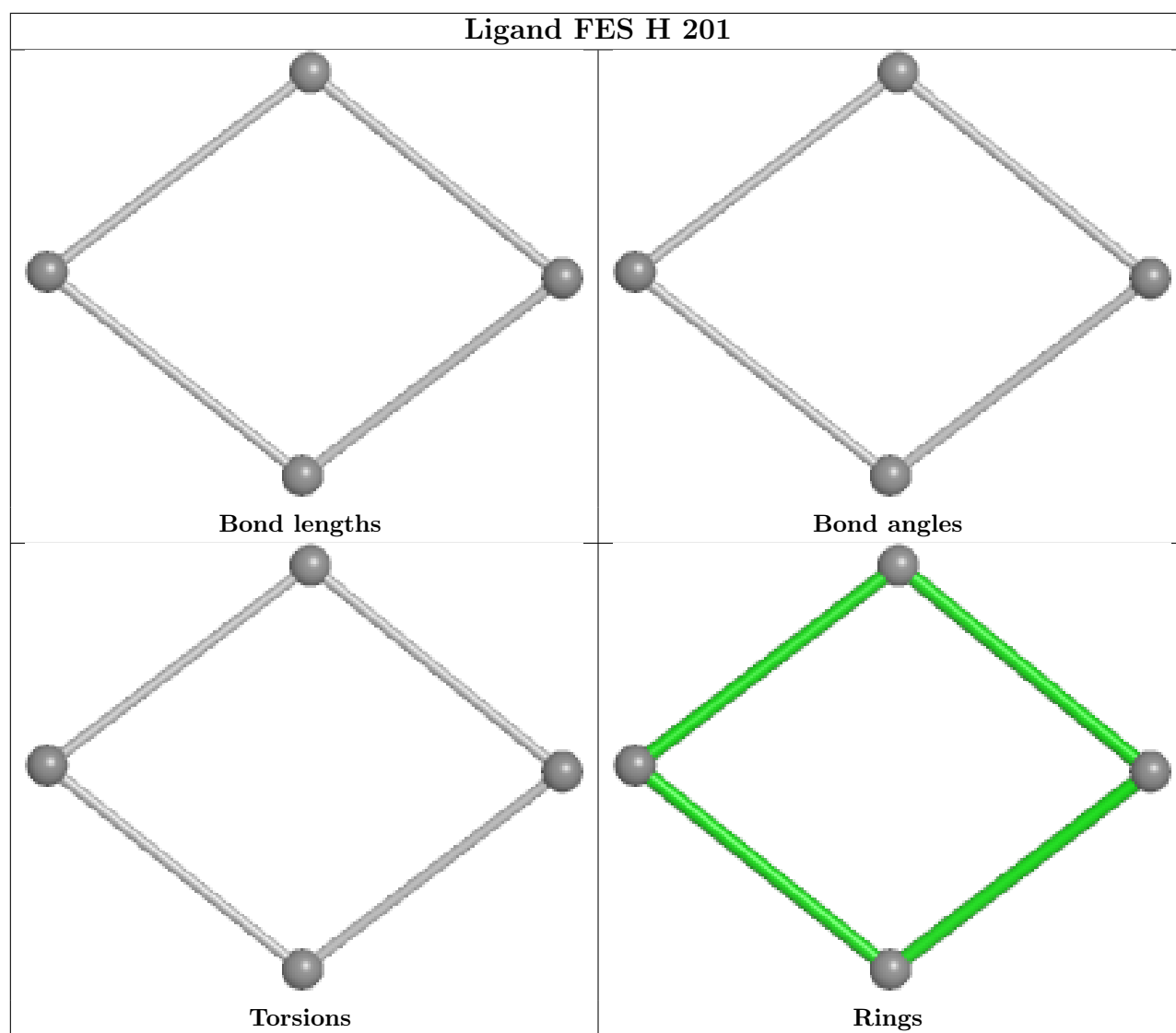


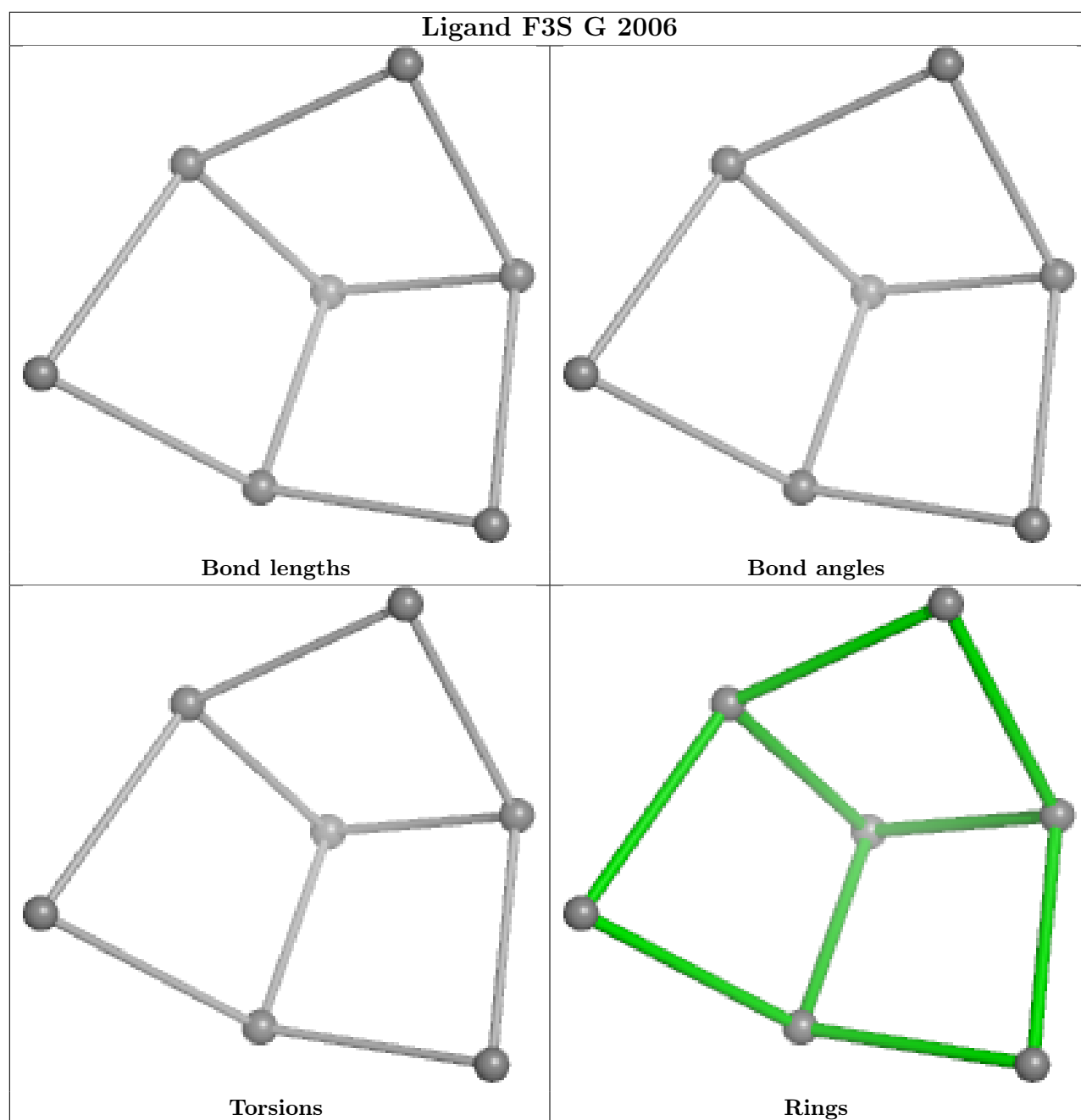


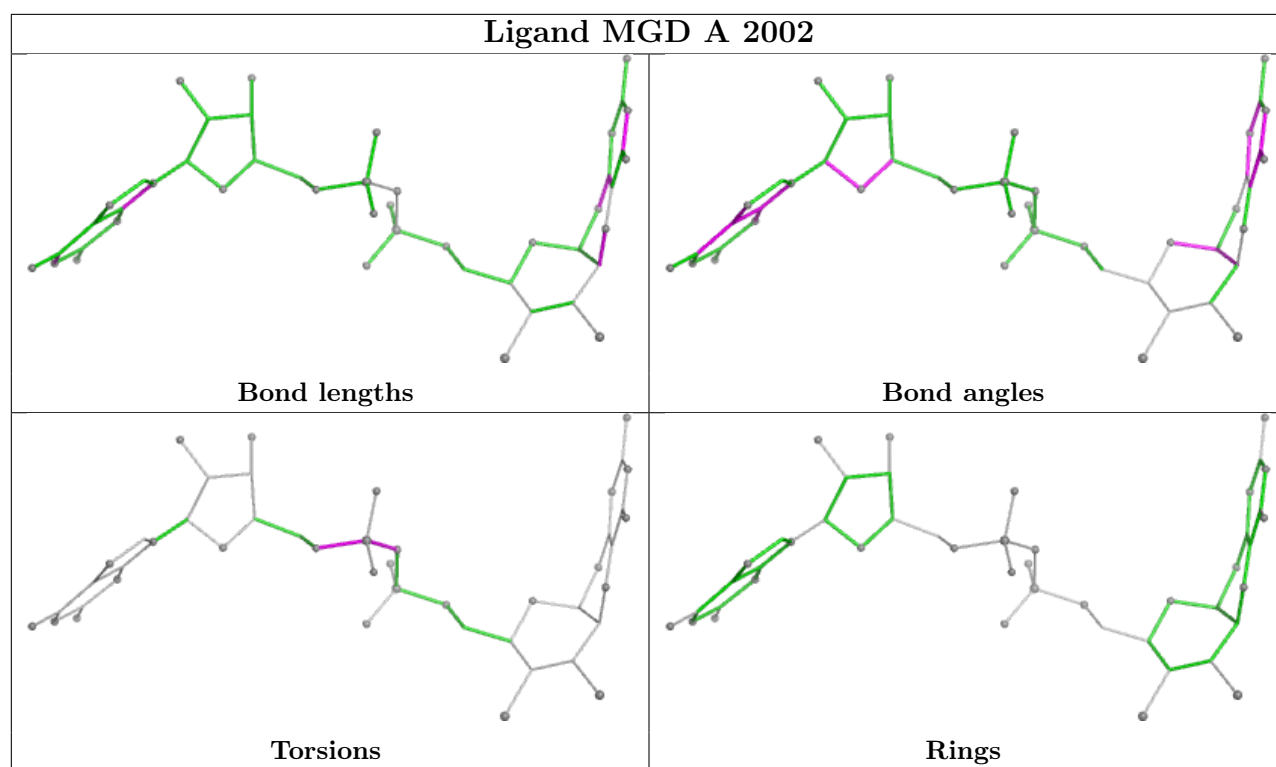


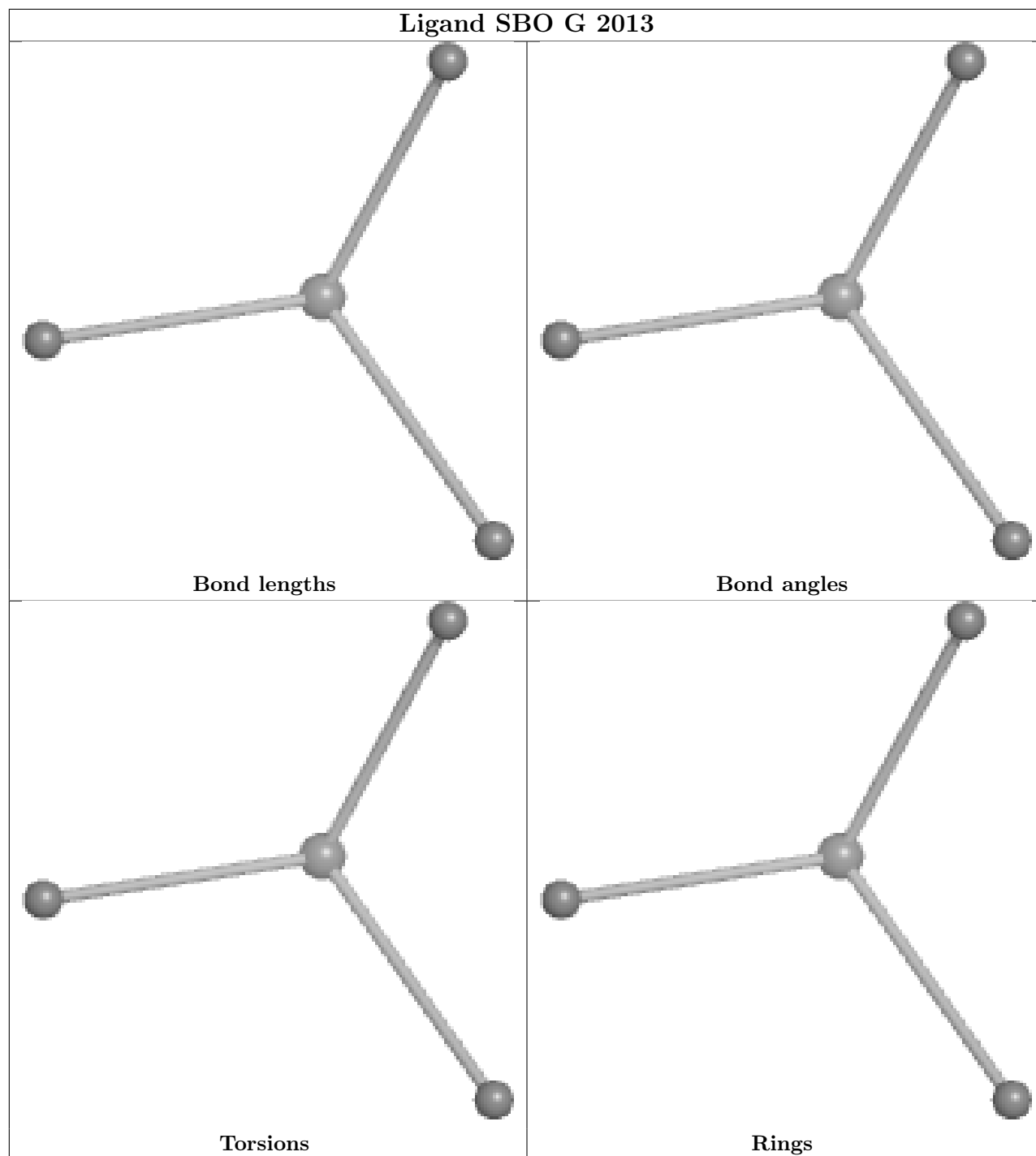


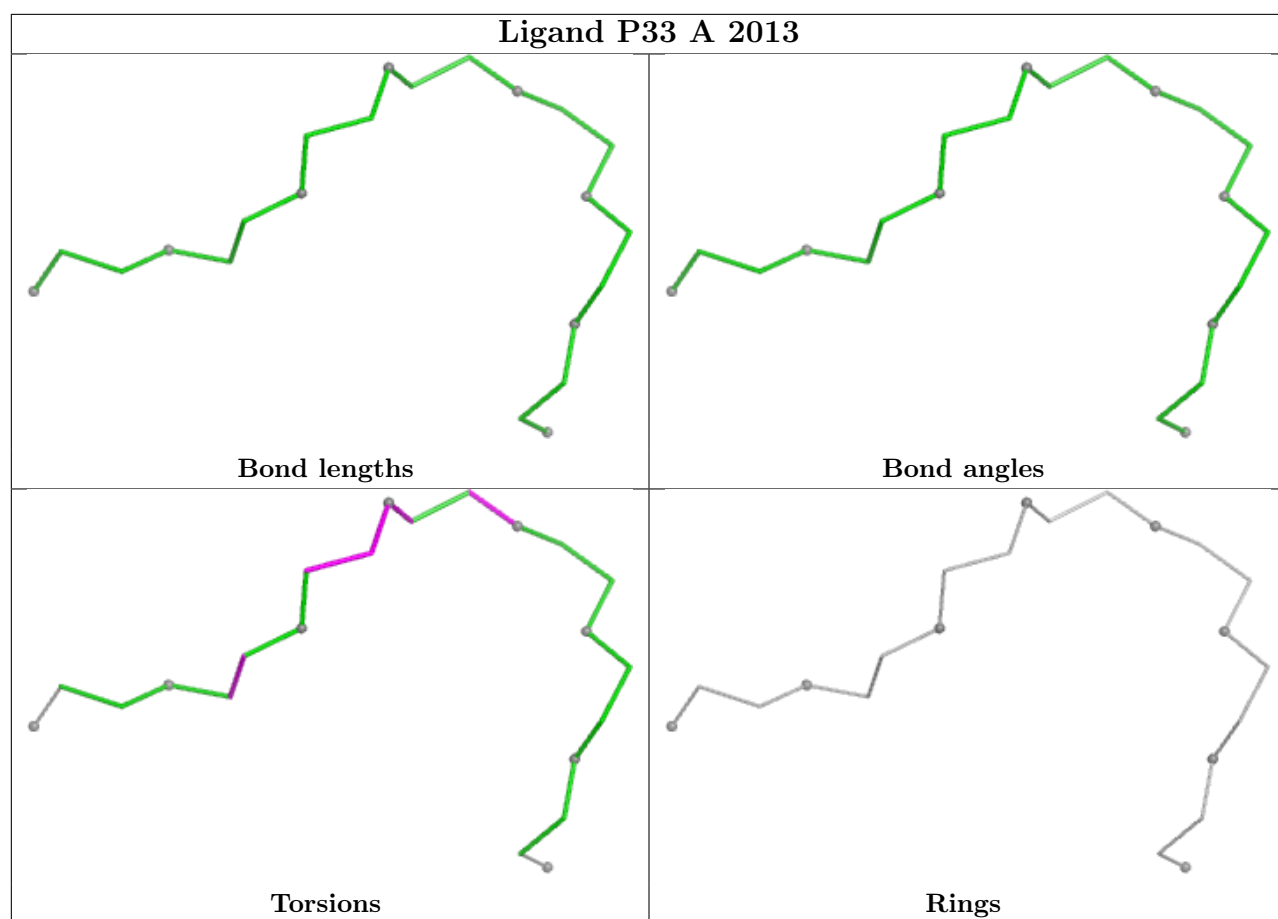


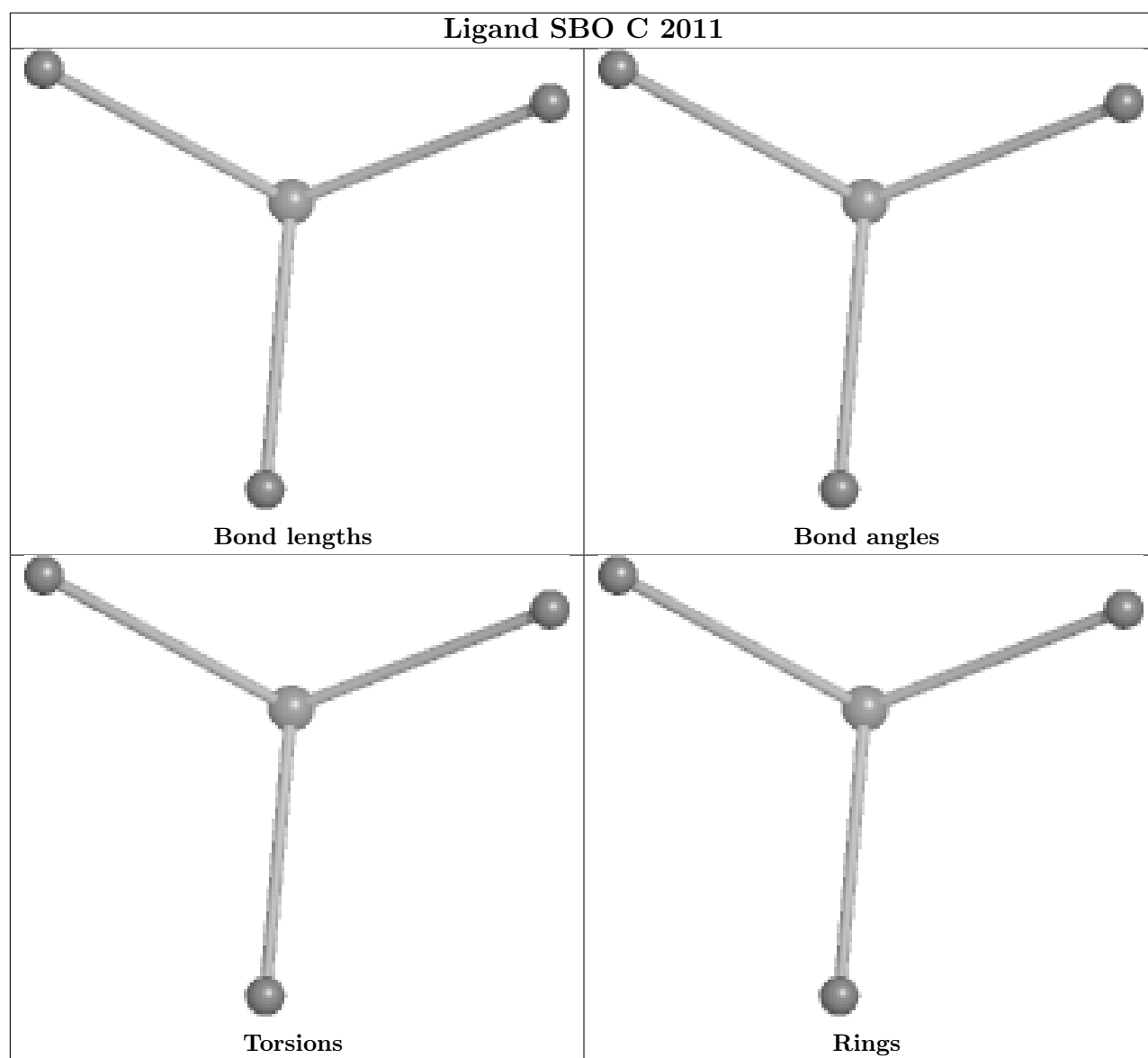












5.7 Other polymers [i](#)

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, 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%)

All (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
1	G	844	SER	2.0
1	C	82	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Continued on next page...

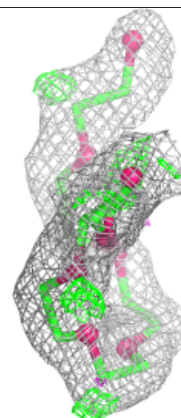
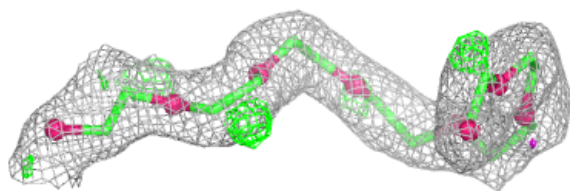
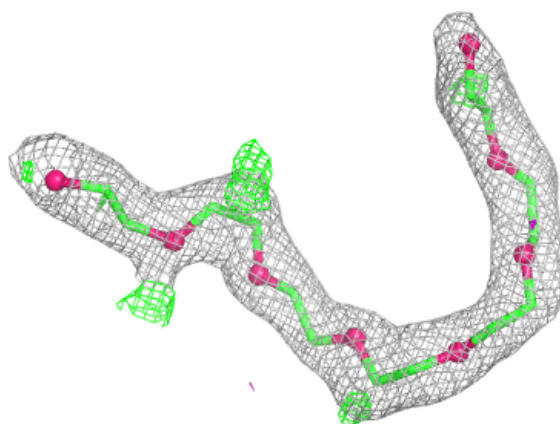
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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.

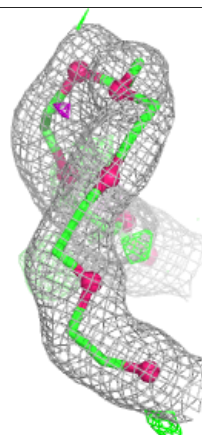
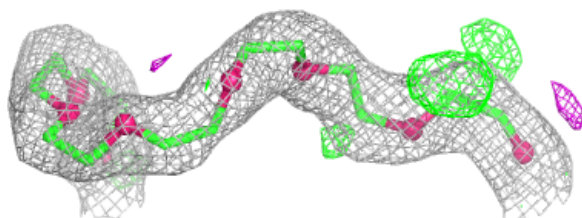
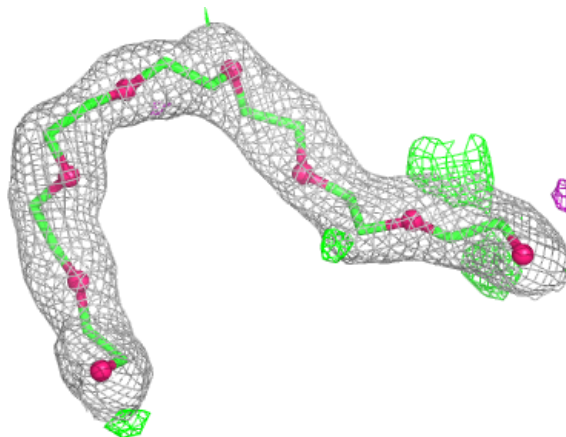
Electron density around P33 E 2012:

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

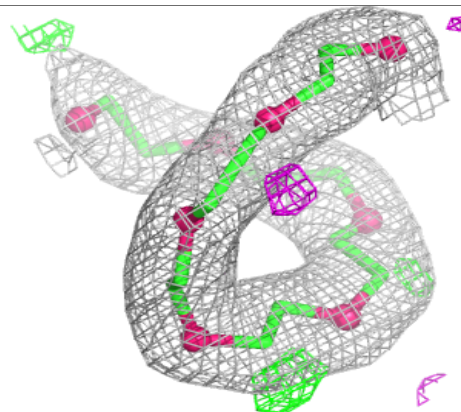
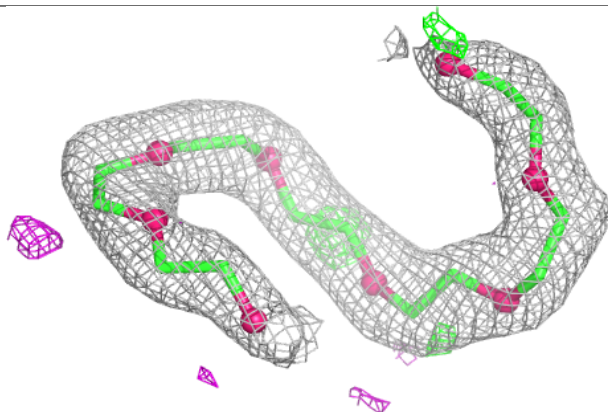
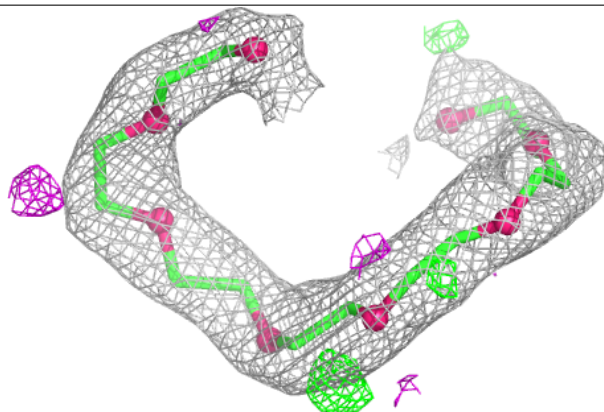


Electron density around P33 A 2013:

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

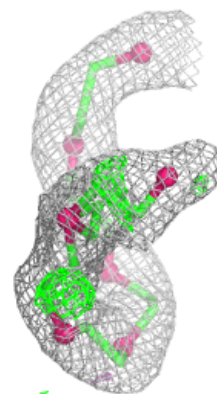
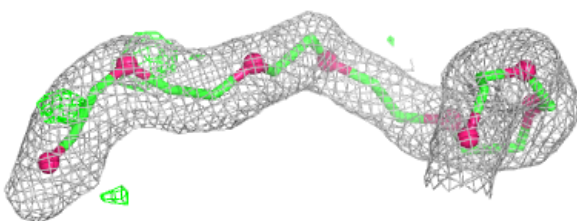
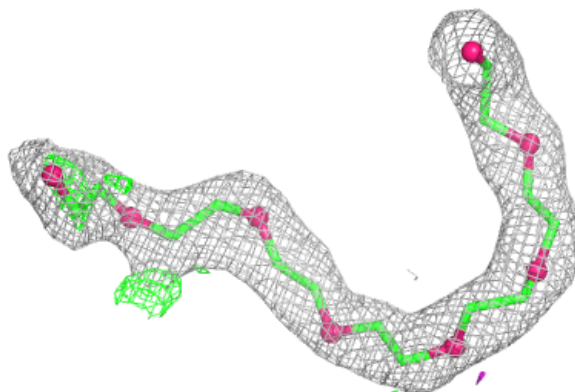
**Electron density around P33 G 2010:**

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

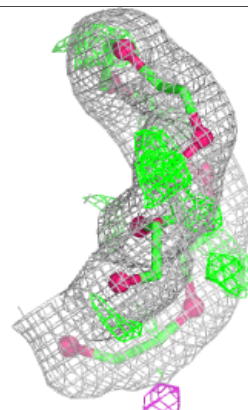
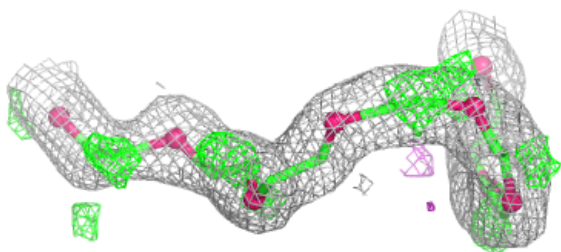
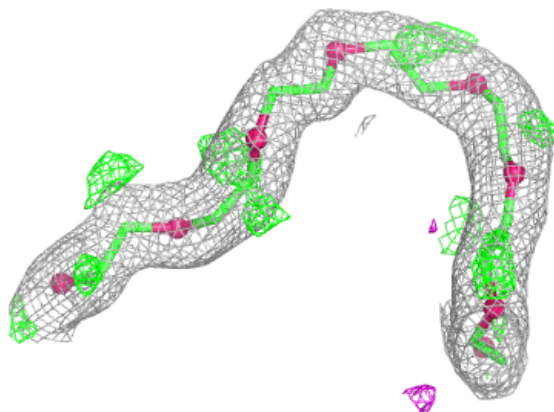


Electron density around P33 C 2012:

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

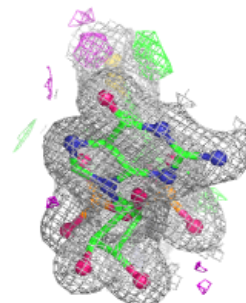
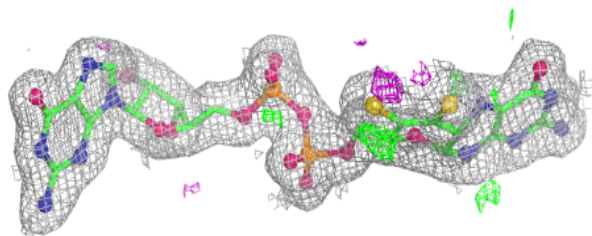
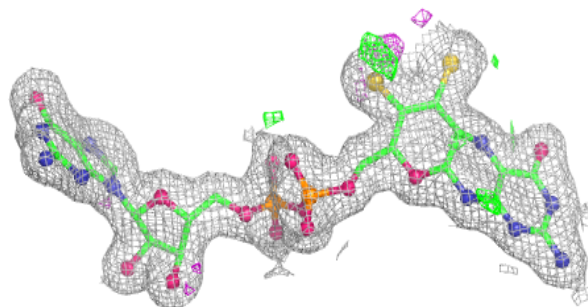
**Electron density around P33 G 2009:**

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

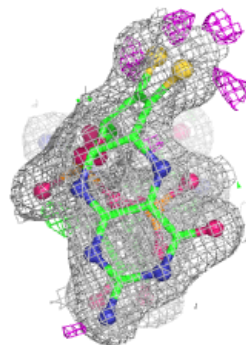
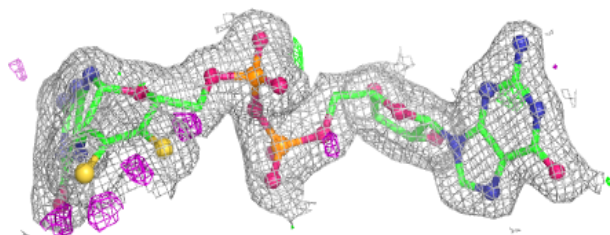
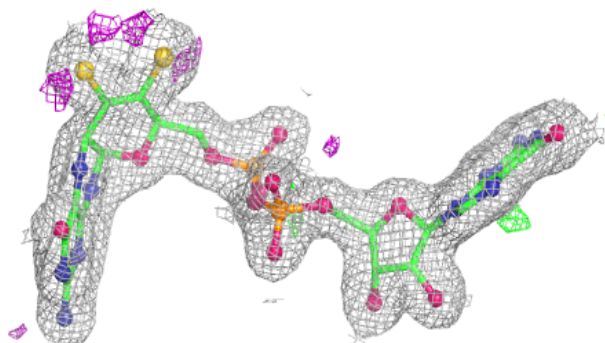


Electron density around MGD C 2001:

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

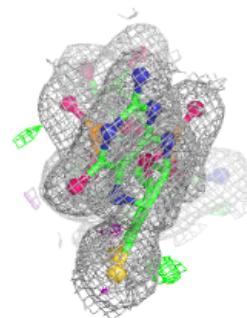
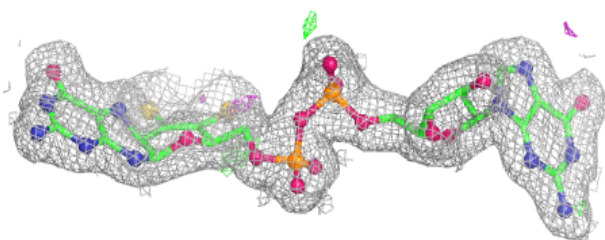
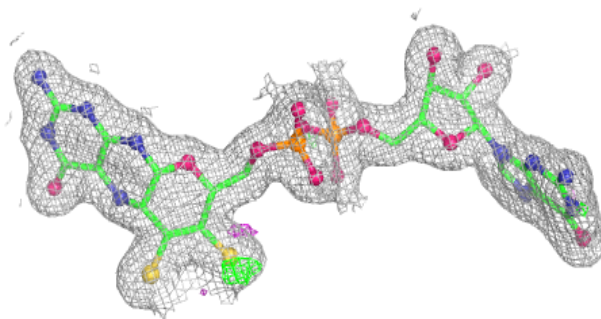
**Electron density around MGD C 2002:**

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

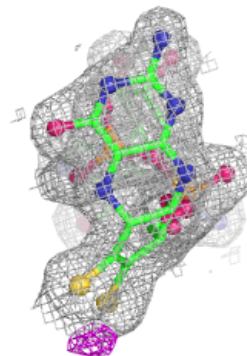
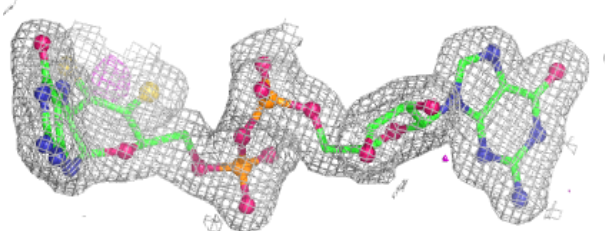
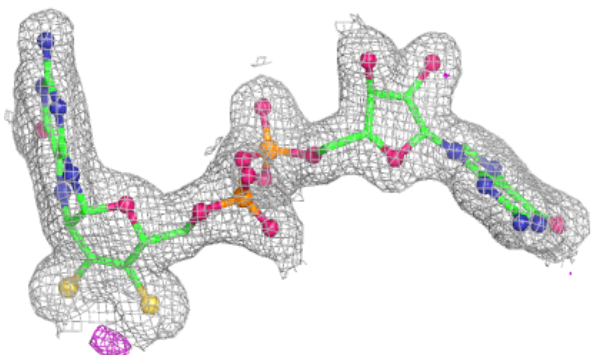


Electron density around MGD E 2001:

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

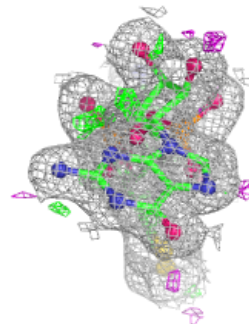
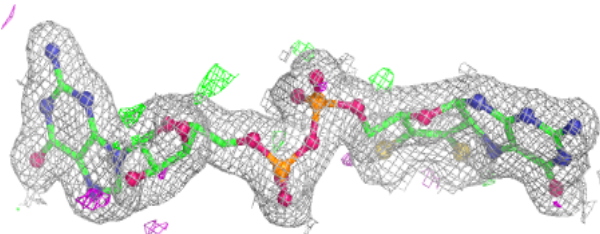
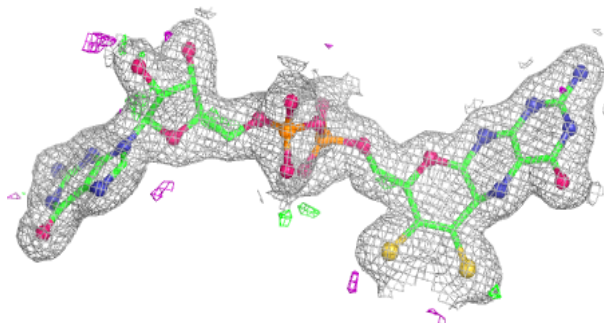
**Electron density around MGD E 2002:**

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

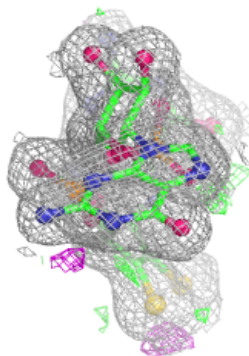
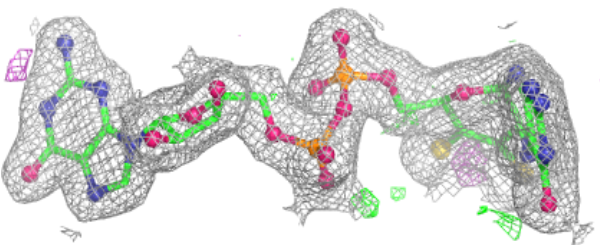
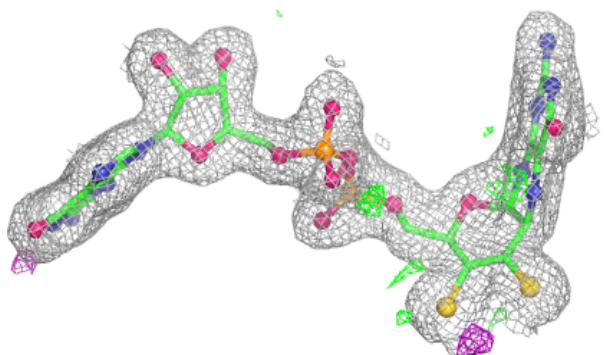


Electron density around MGD G 2001:

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

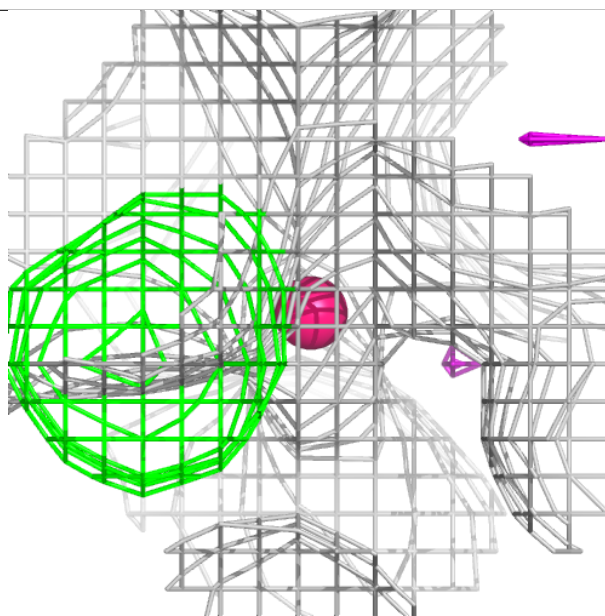
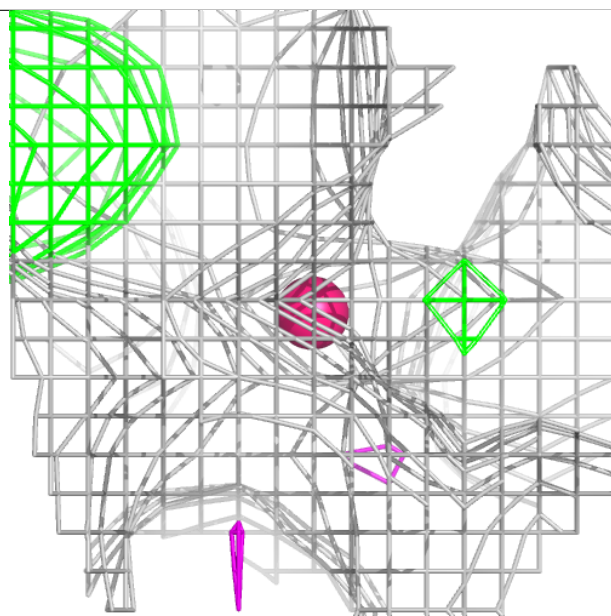
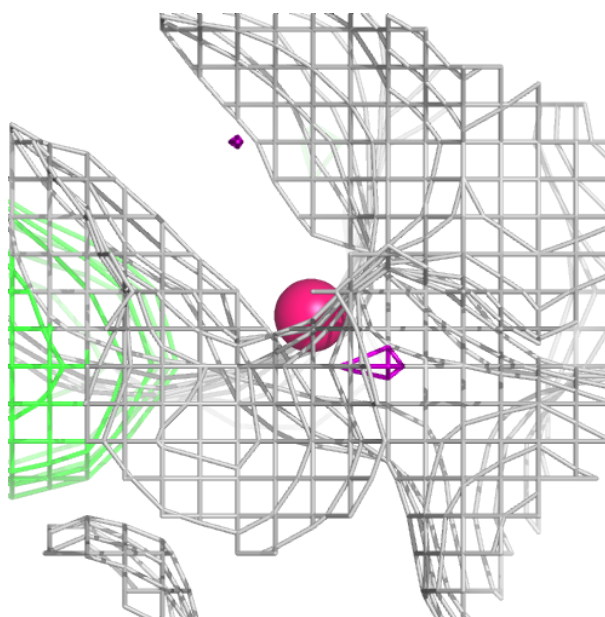
**Electron density around MGD G 2002:**

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



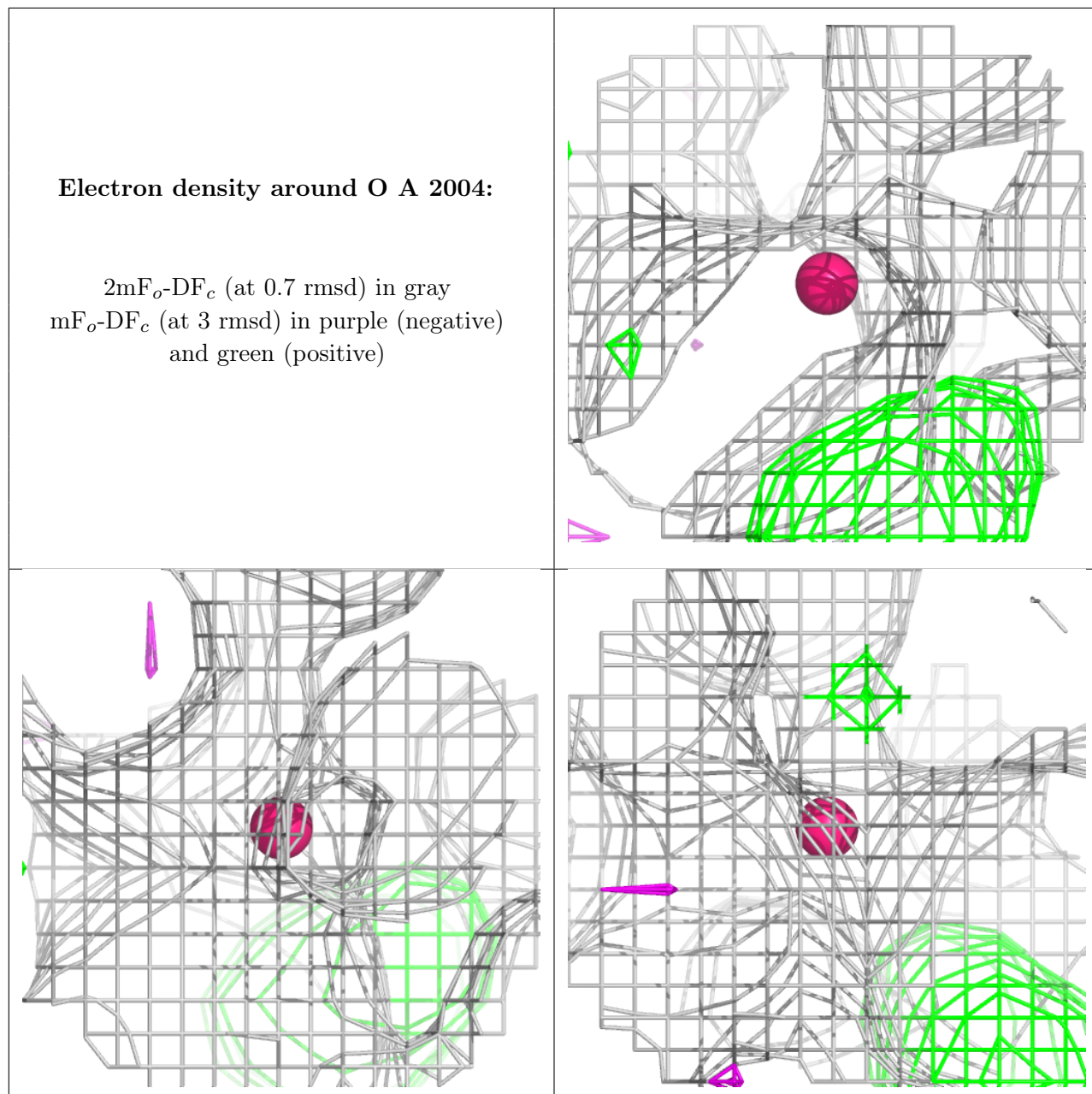
Electron density around O A 2003:

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



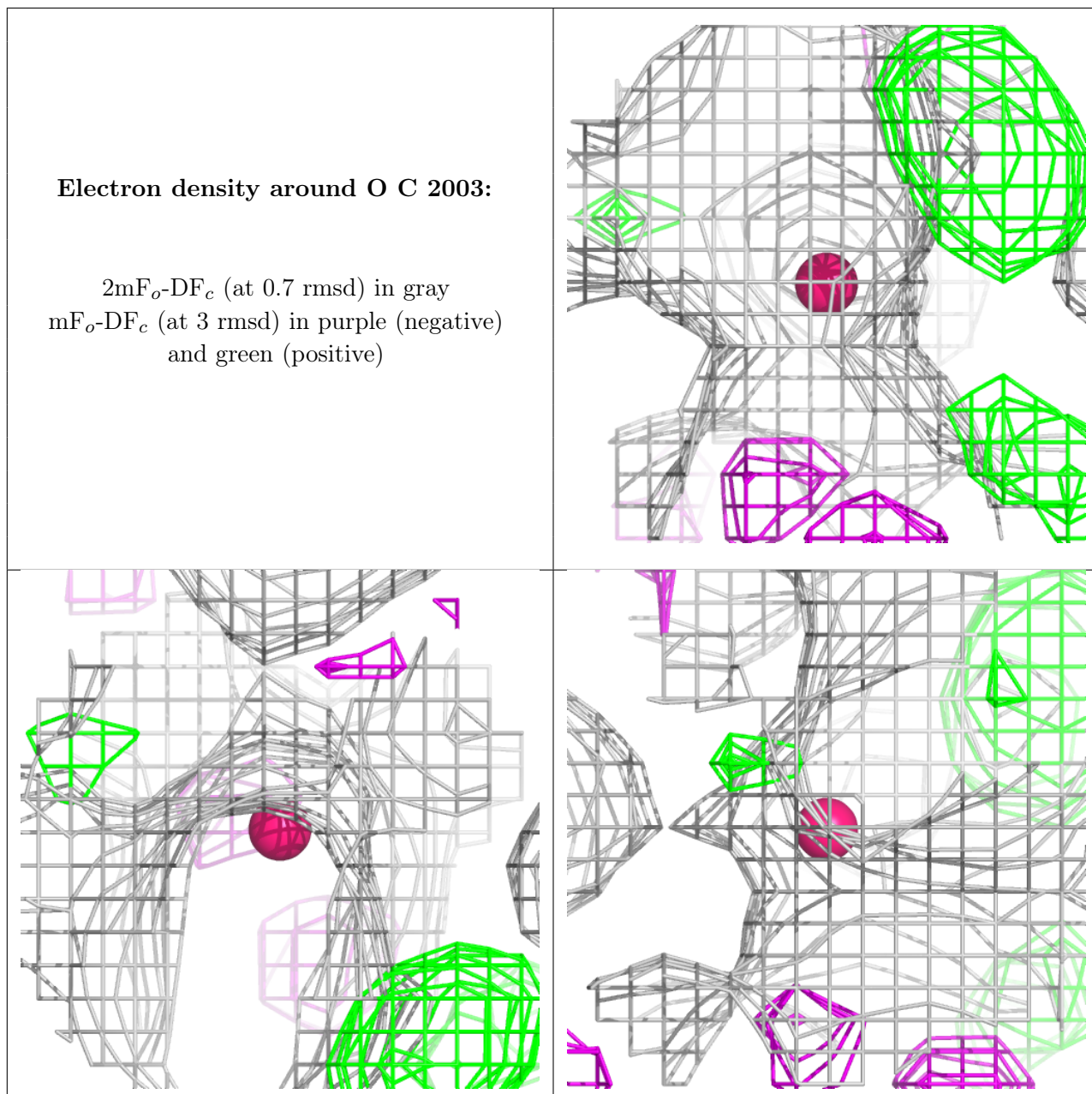
Electron density around O A 2004:

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



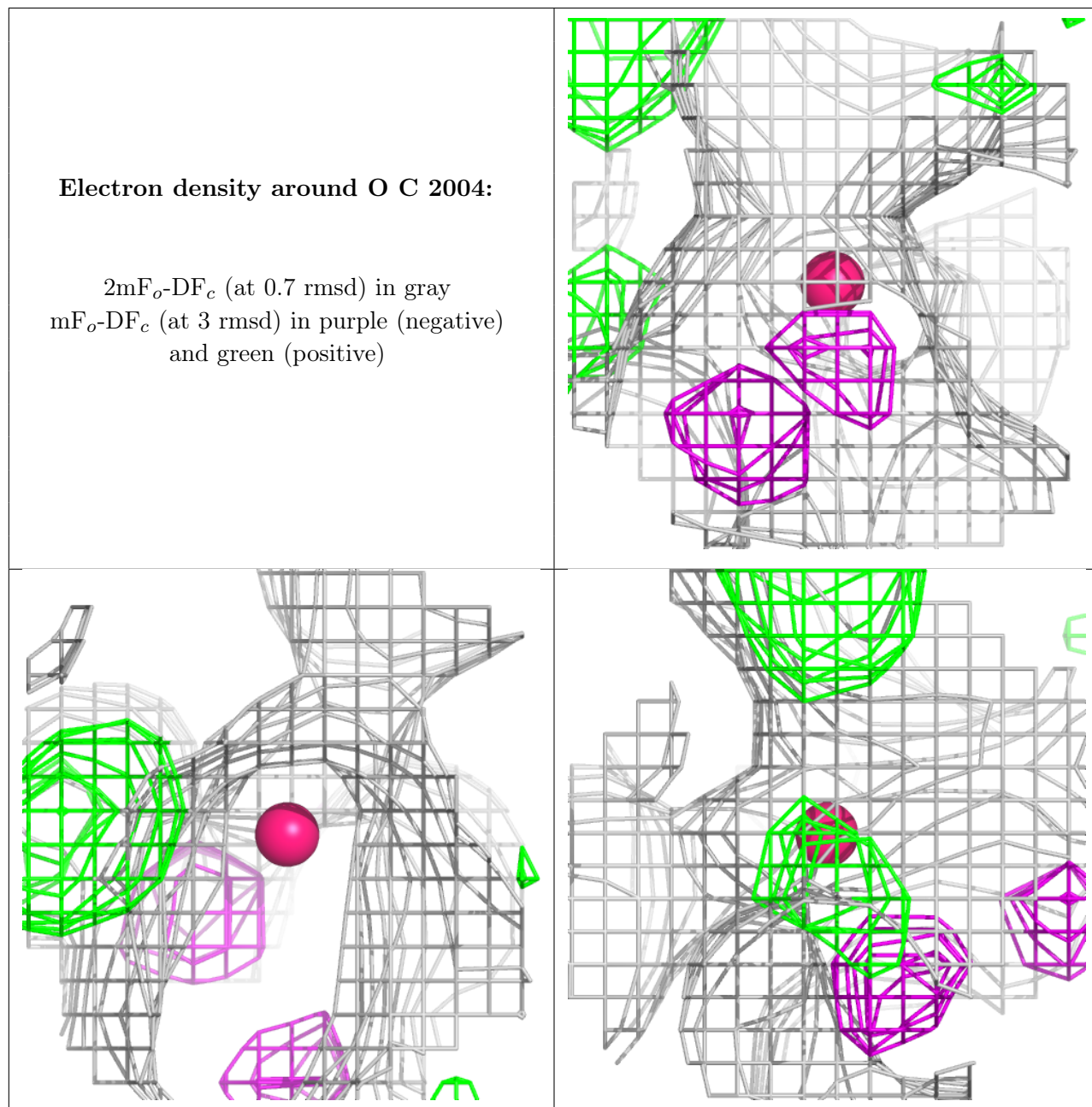
Electron density around O C 2003:

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



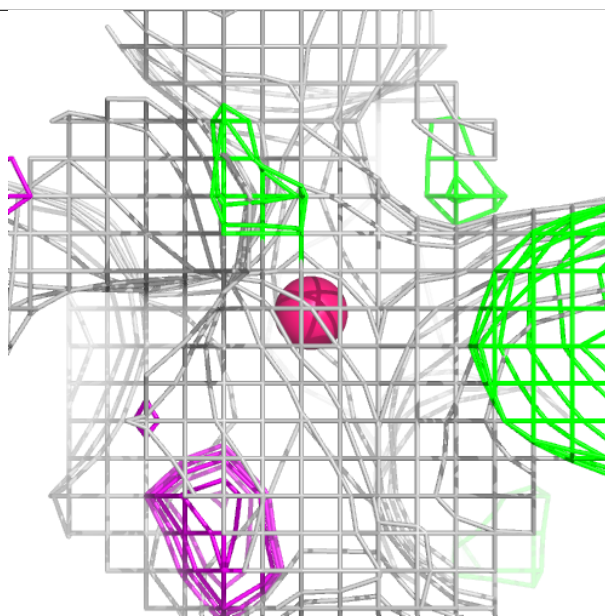
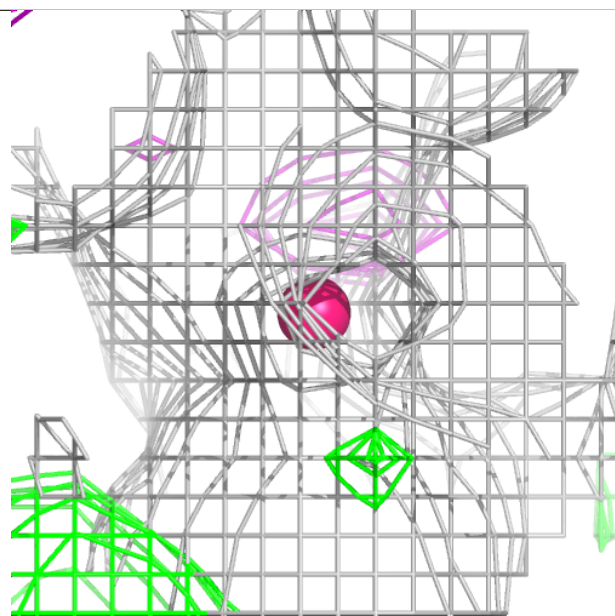
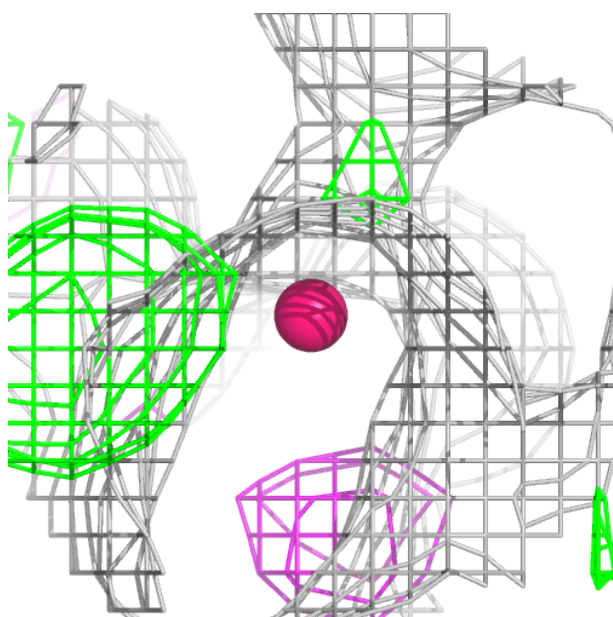
Electron density around O C 2004:

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



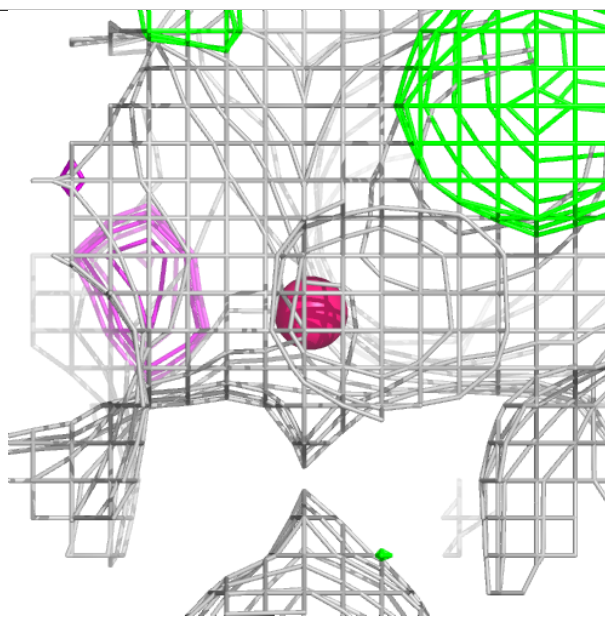
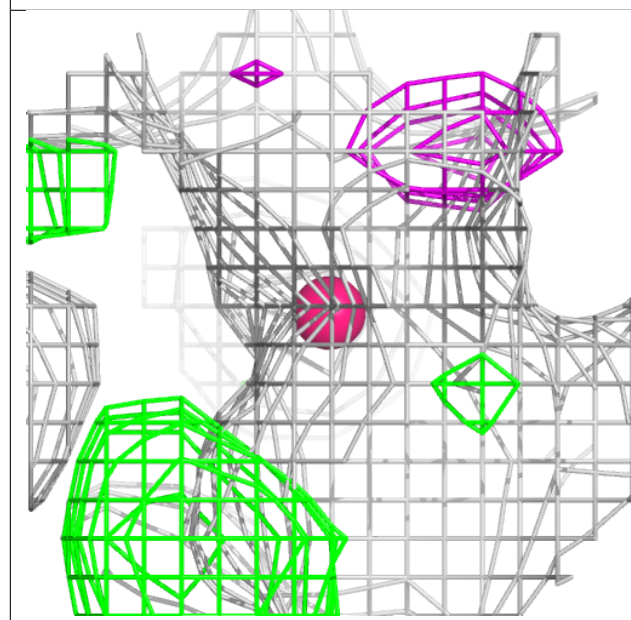
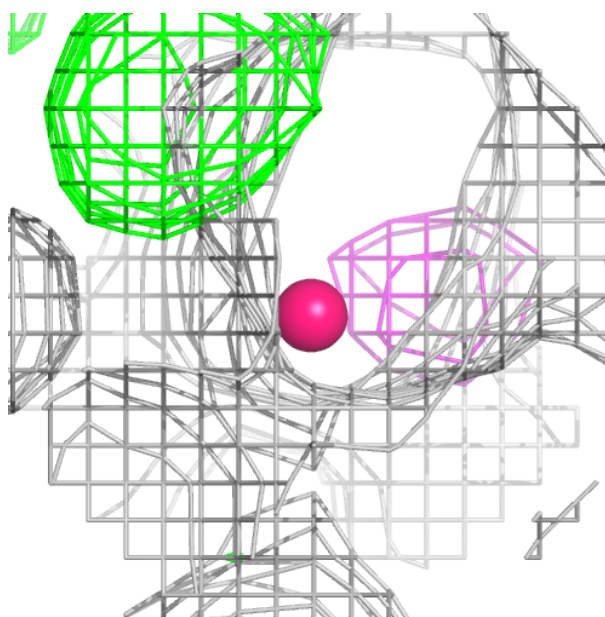
Electron density around O E 2003:

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



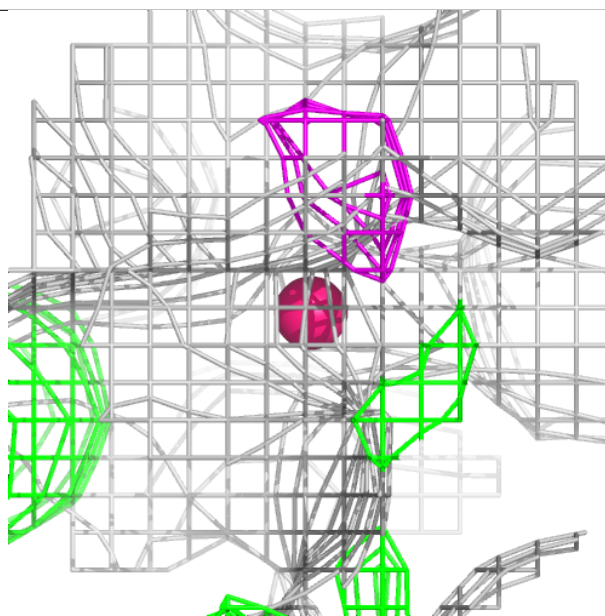
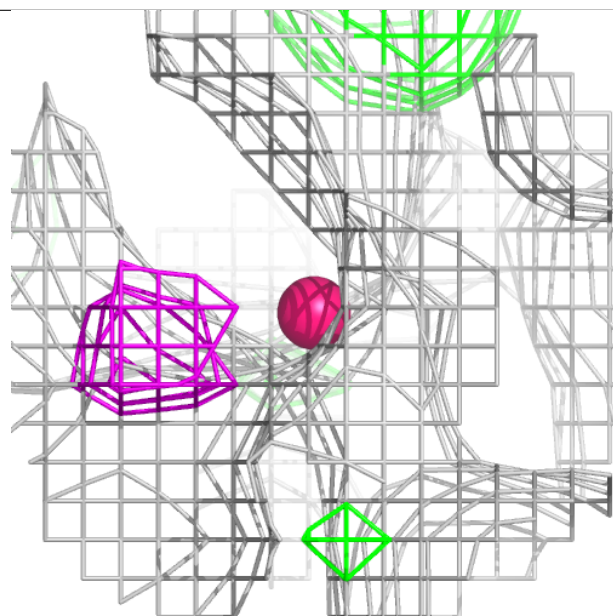
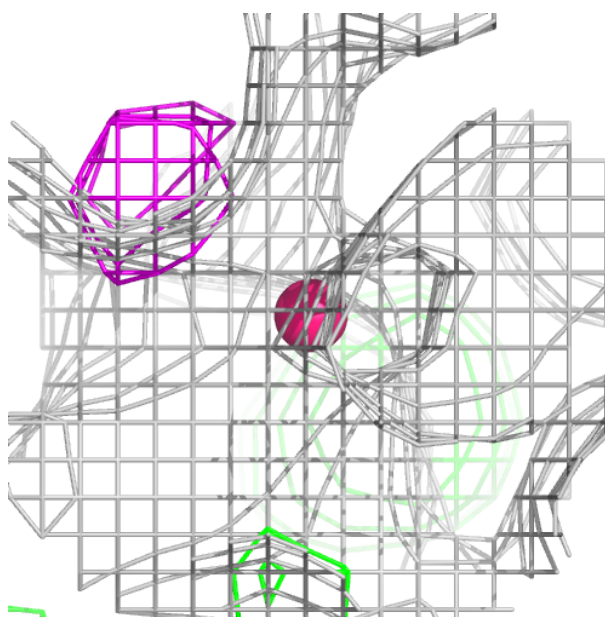
Electron density around O E 2004:

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



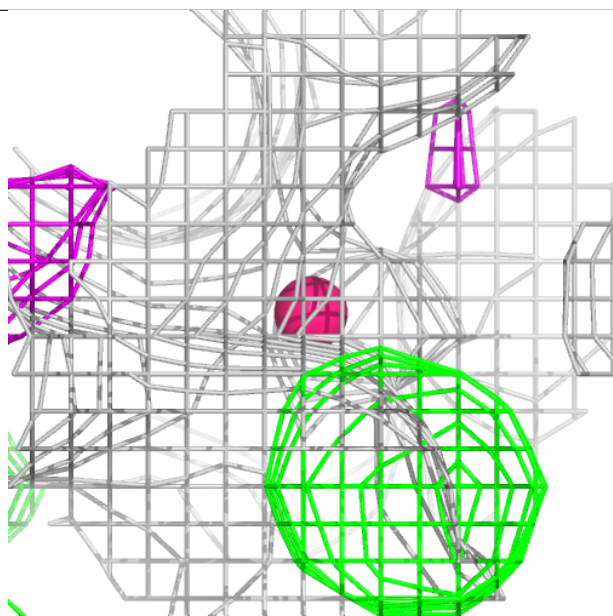
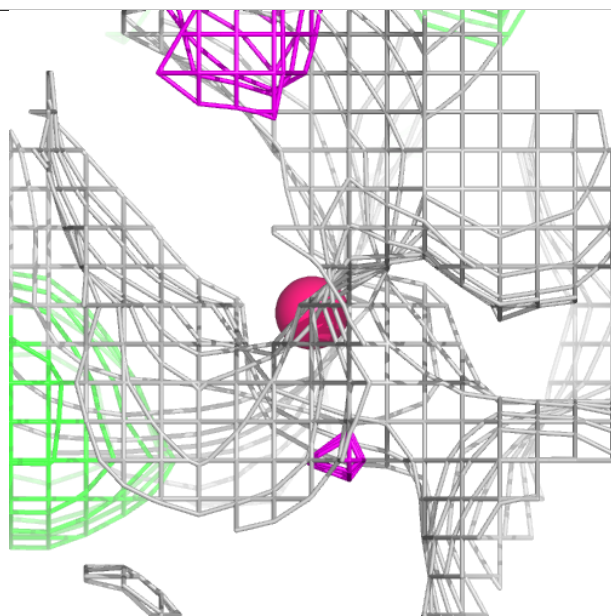
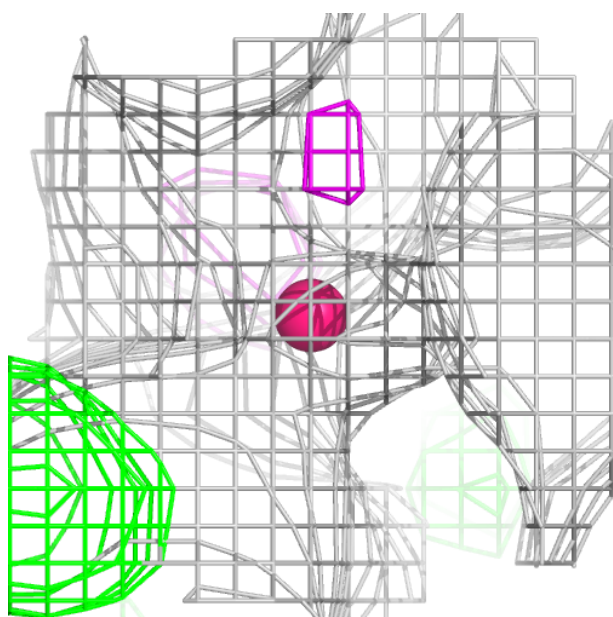
Electron density around O G 2003:

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



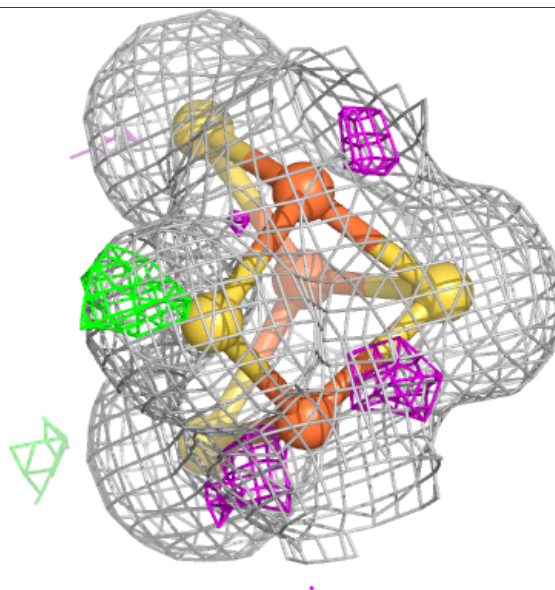
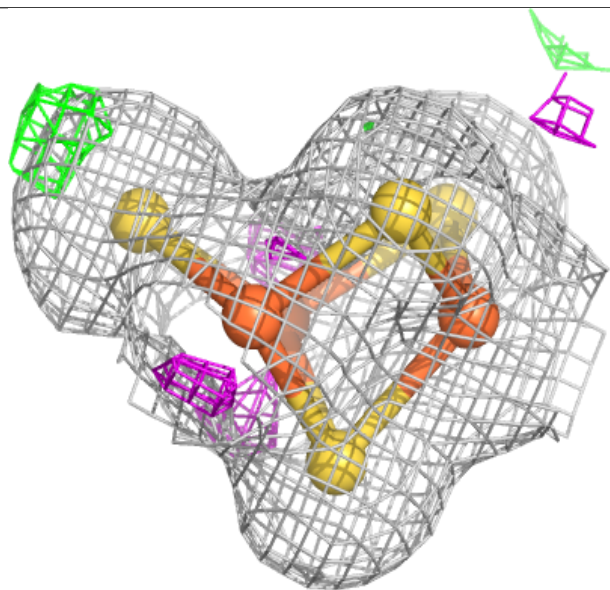
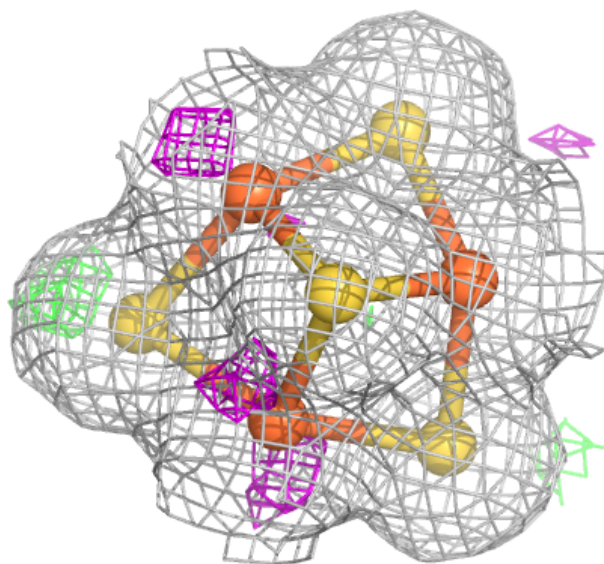
Electron density around O G 2004:

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



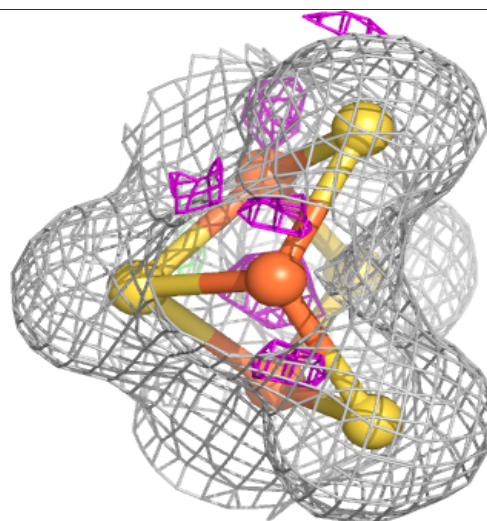
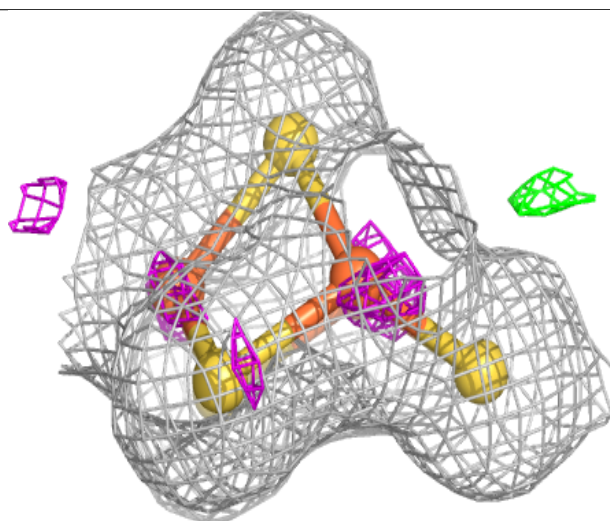
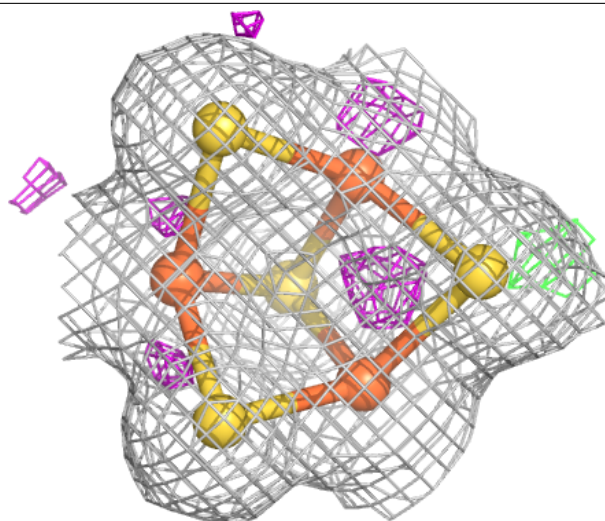
Electron density around F3S A 2006:

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



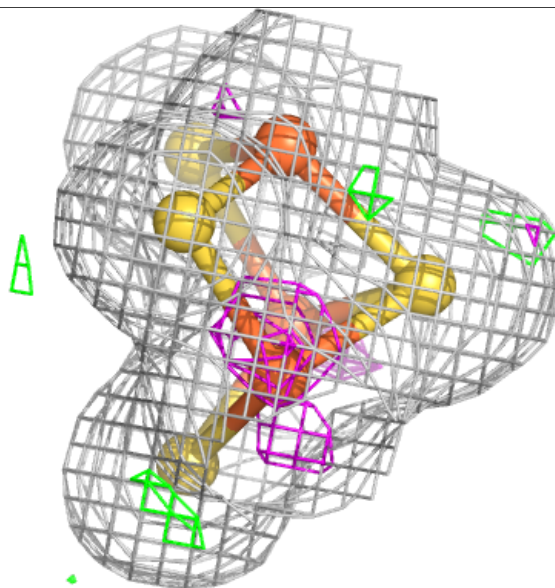
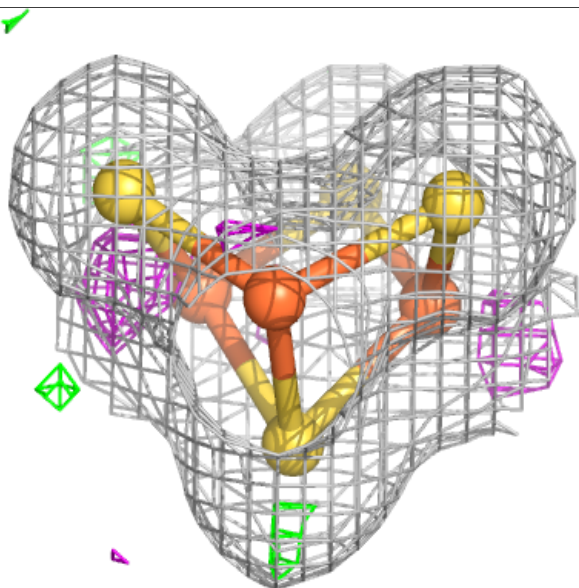
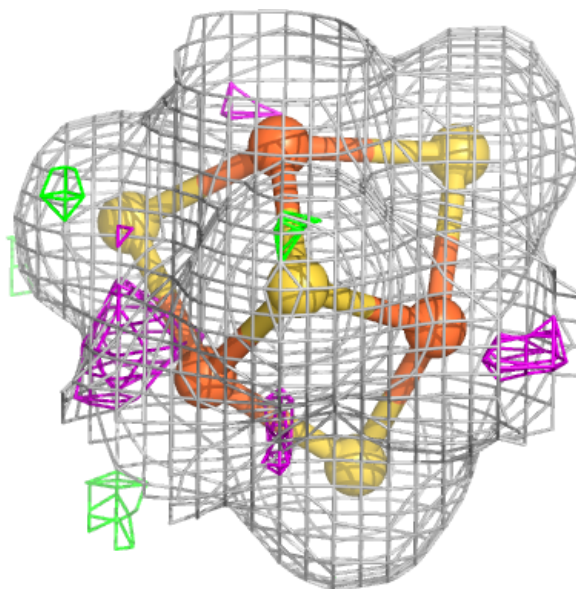
Electron density around F3S C 2006:

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



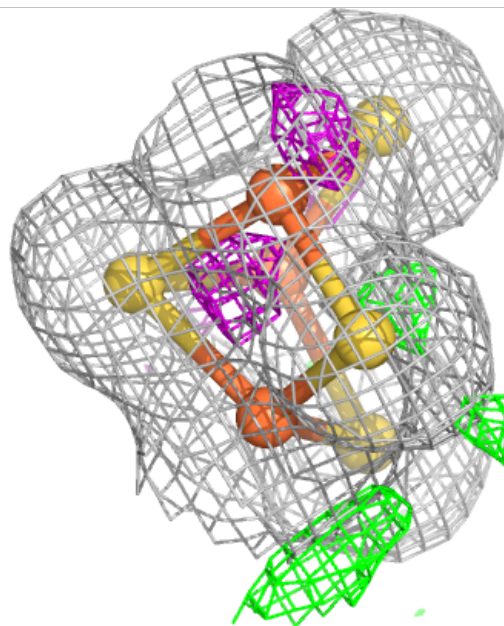
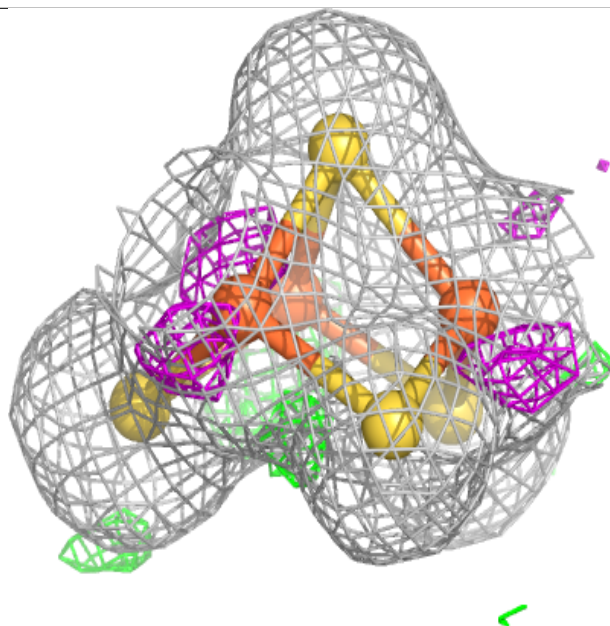
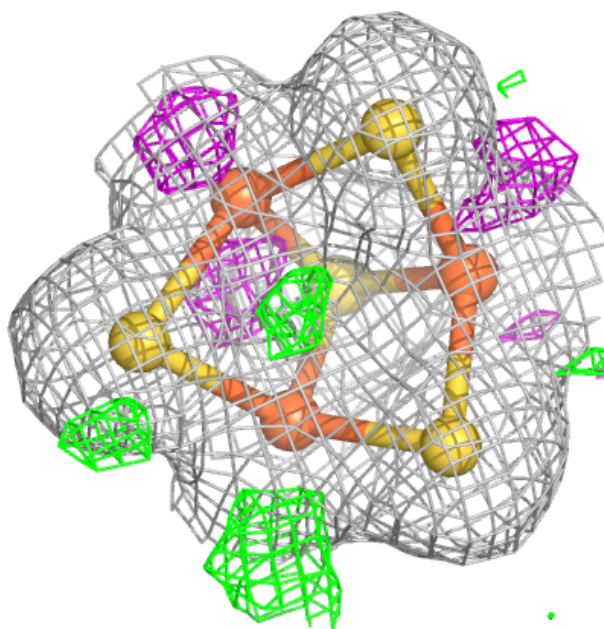
Electron density around F3S E 2006:

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



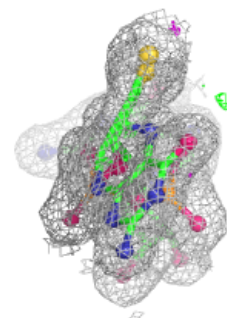
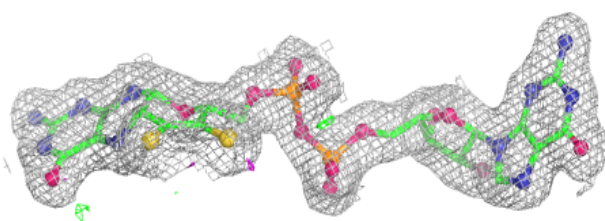
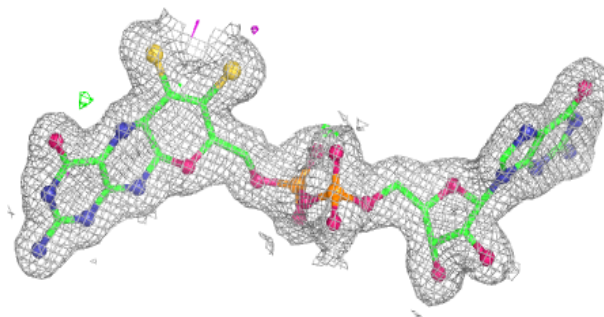
Electron density around F3S G 2006:

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

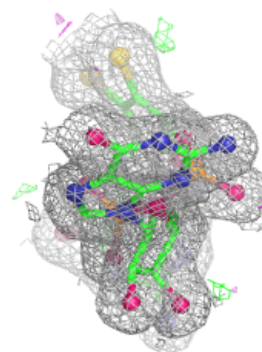
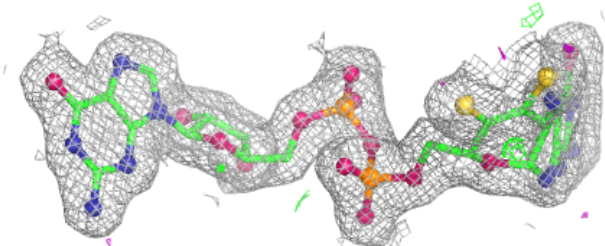
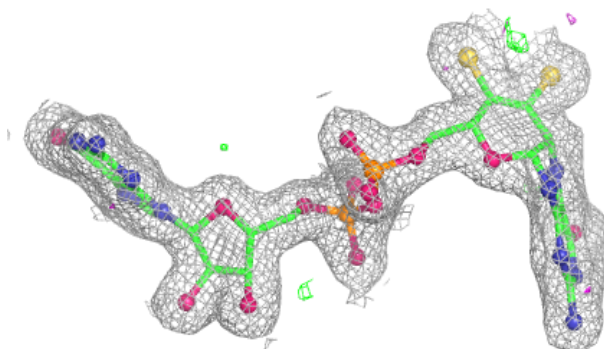


Electron density around MGD A 2001:

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

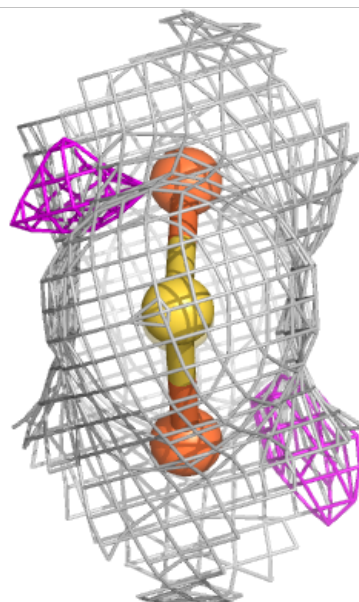
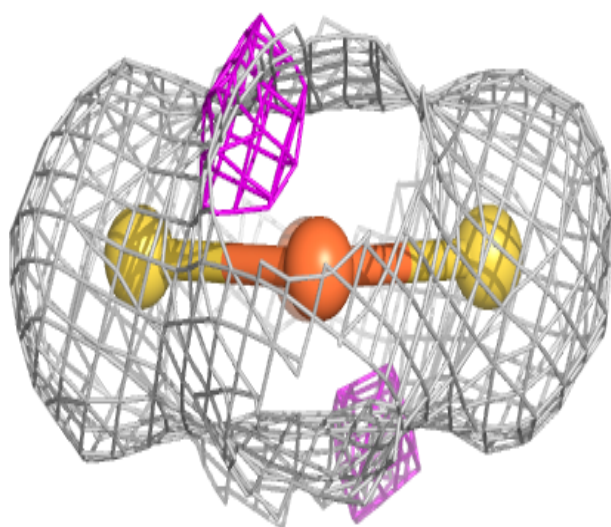
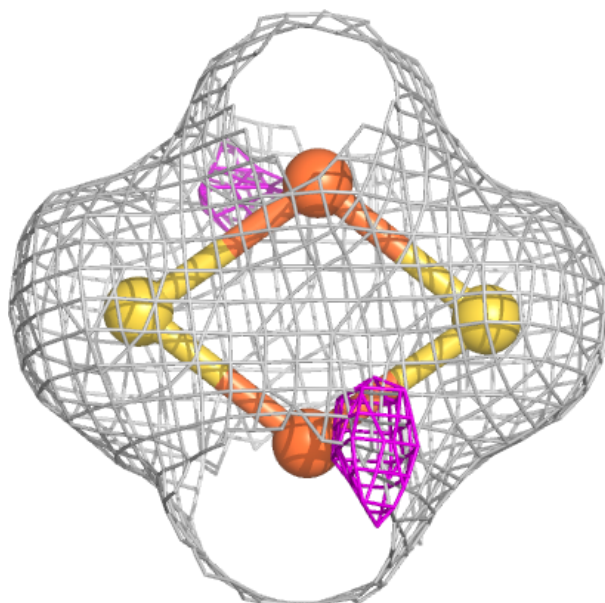
**Electron density around MGD A 2002:**

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



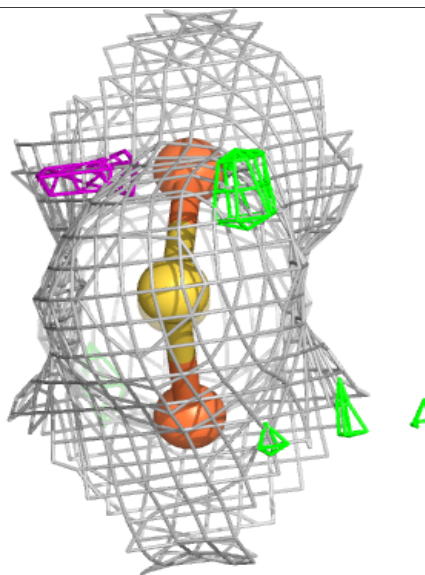
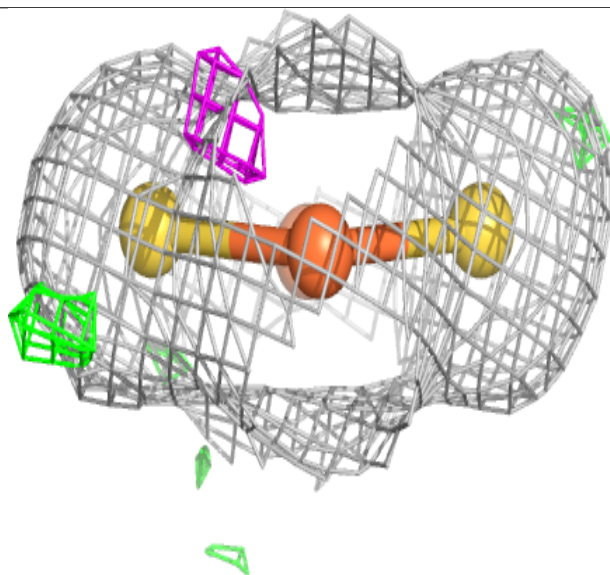
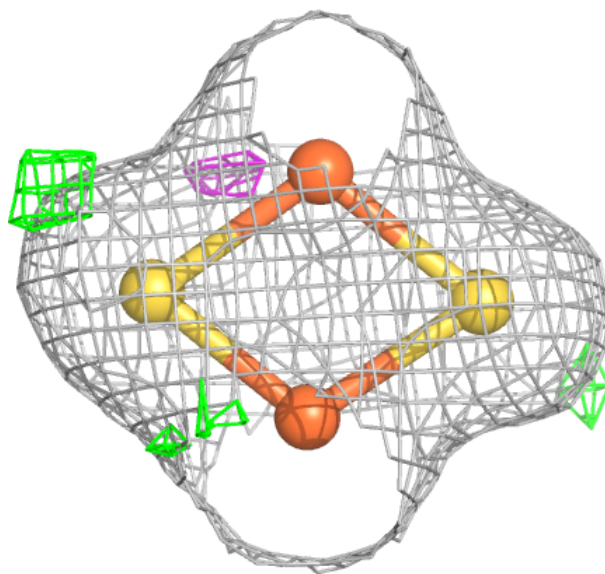
Electron density around FES D 201:

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



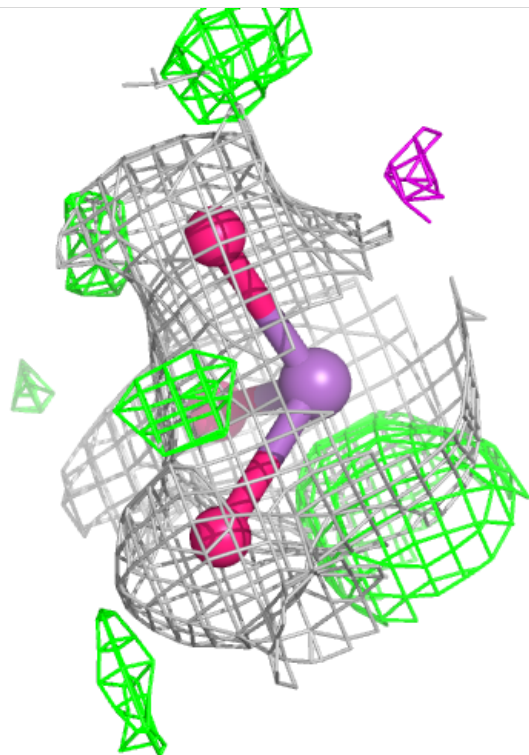
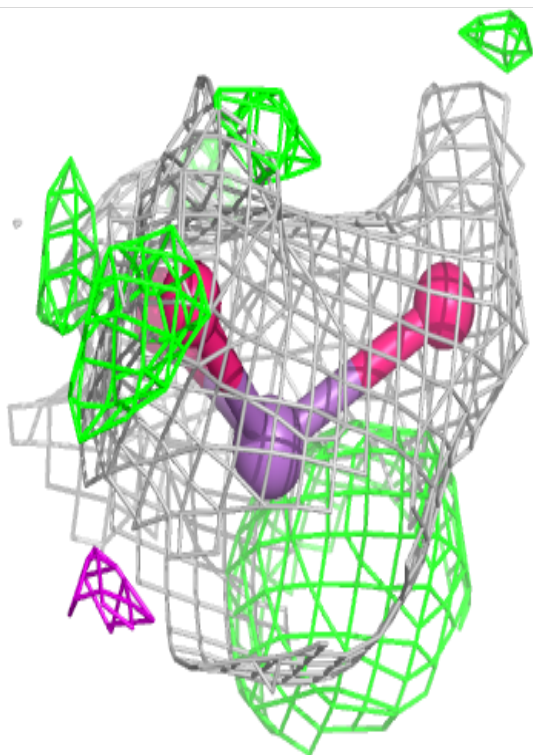
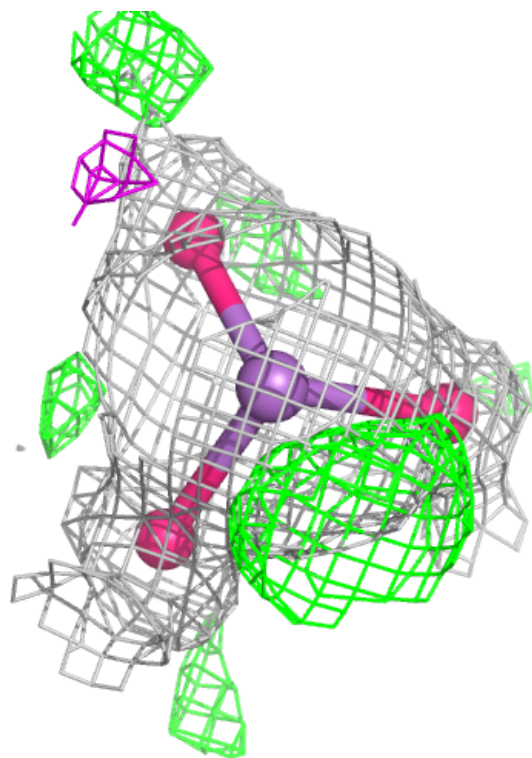
Electron density around FES F 201:

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



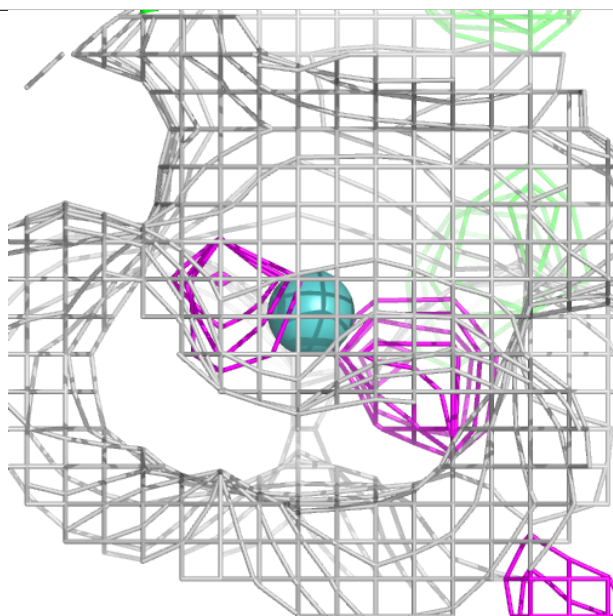
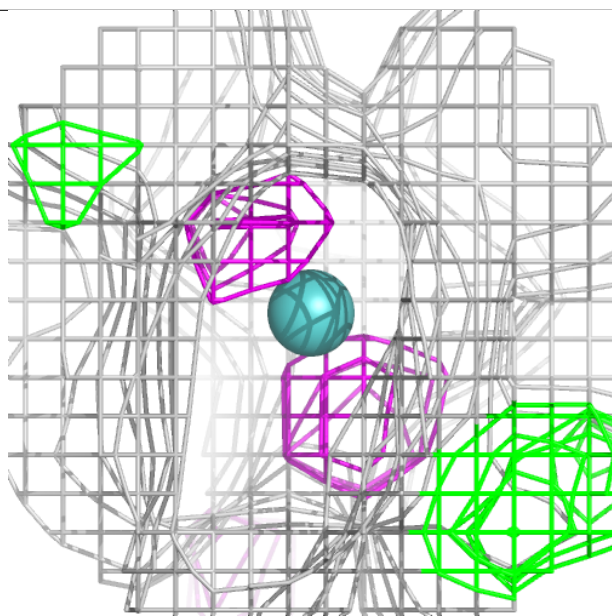
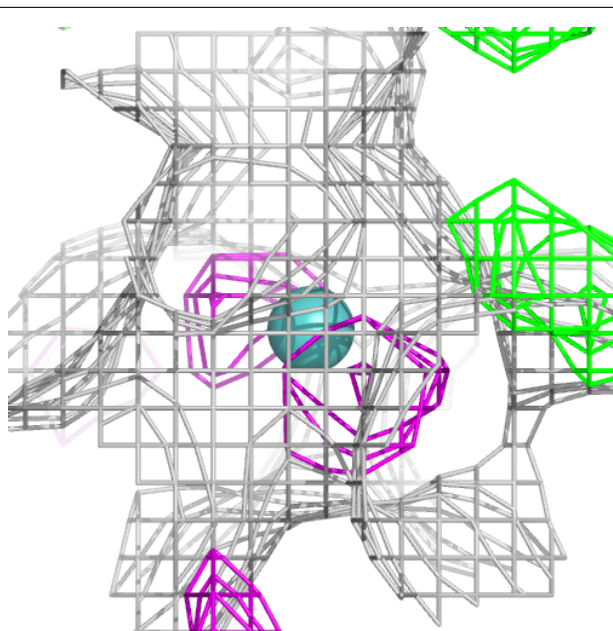
Electron density around SBO G 2013:

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



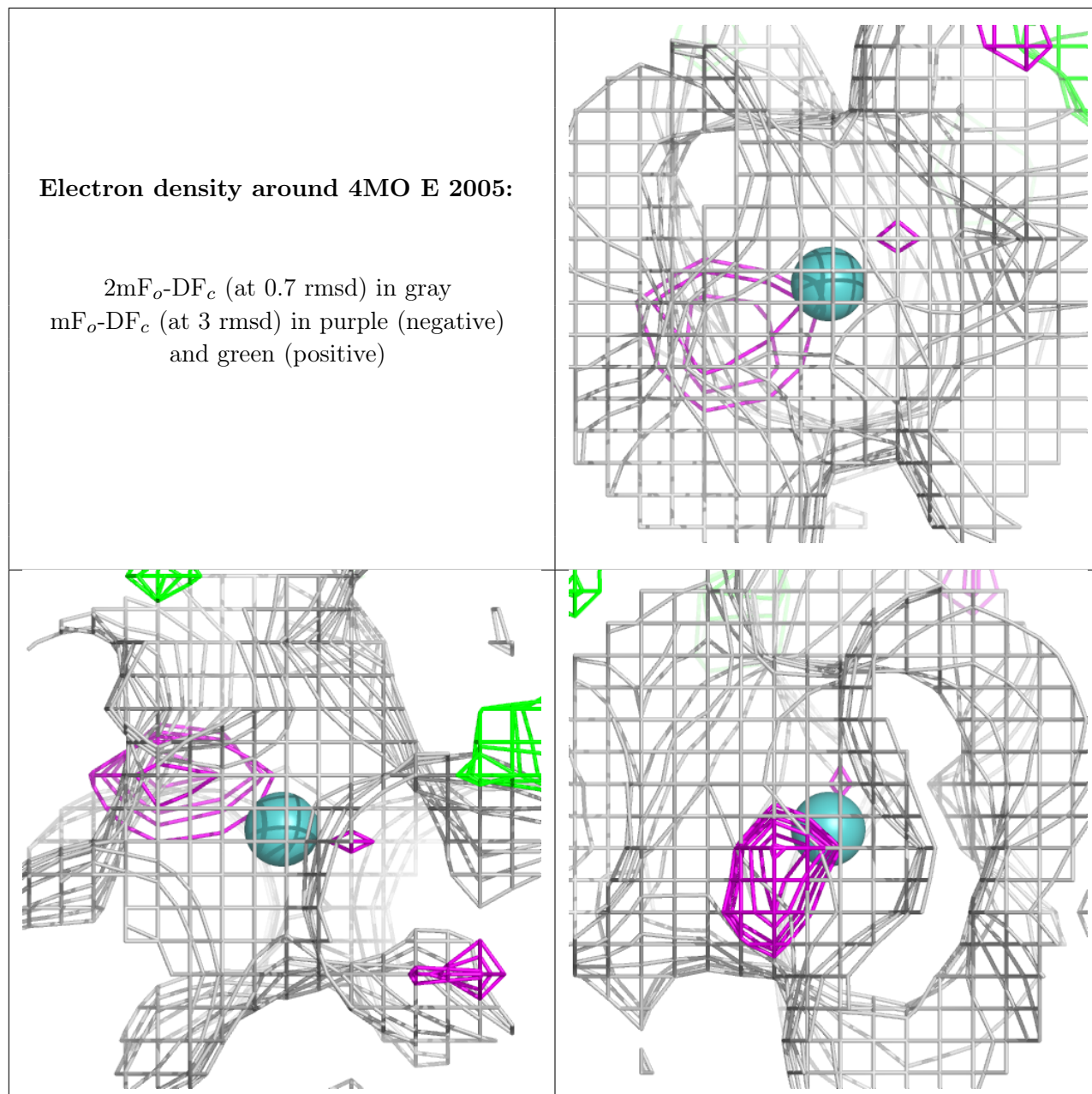
Electron density around 4MO C 2005:

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



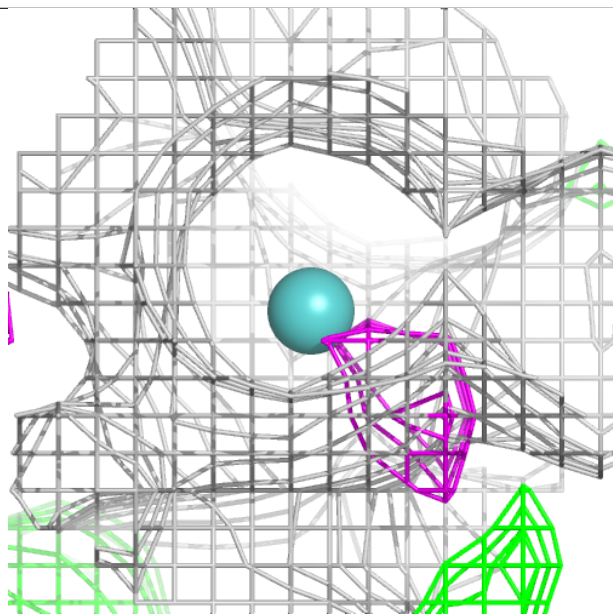
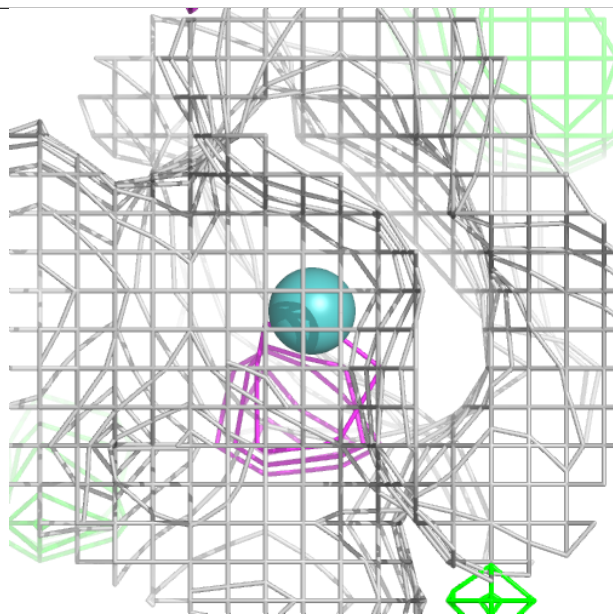
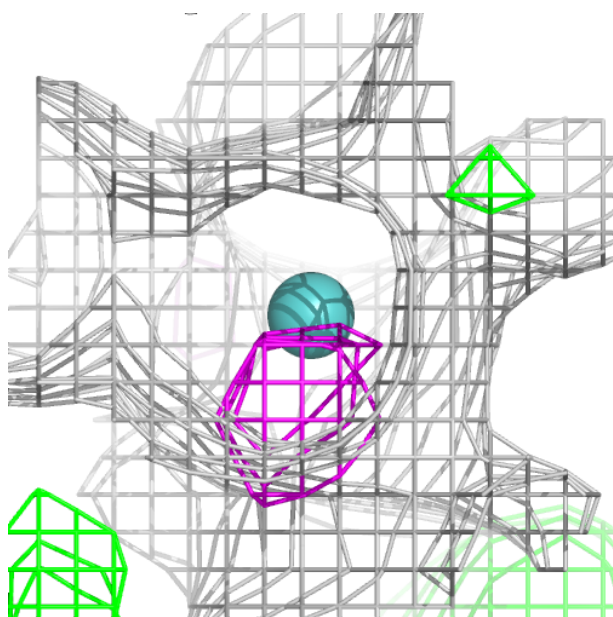
Electron density around 4MO E 2005:

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



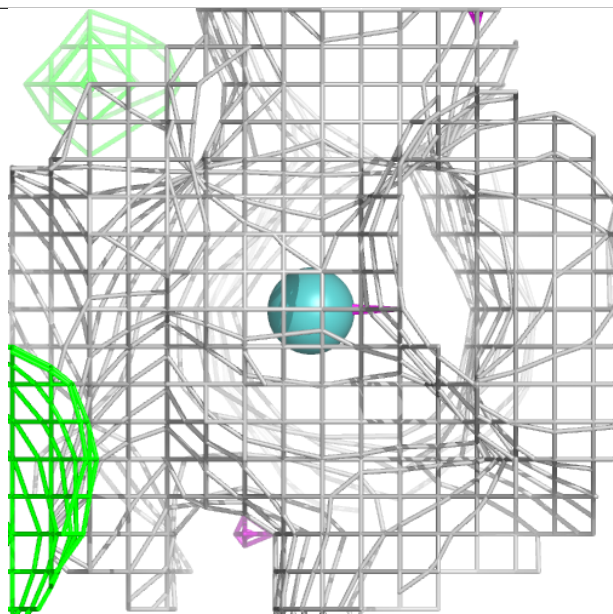
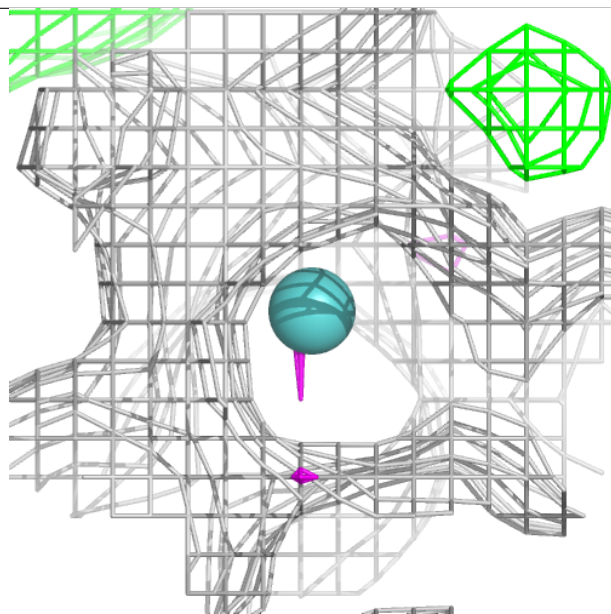
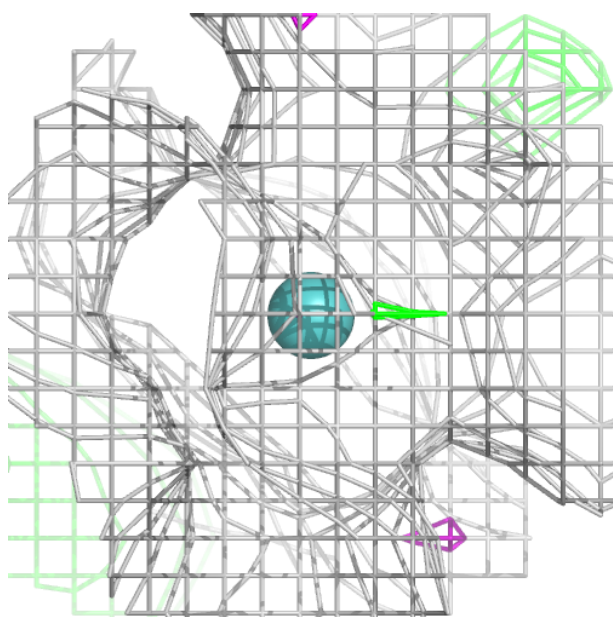
Electron density around 4MO G 2005:

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



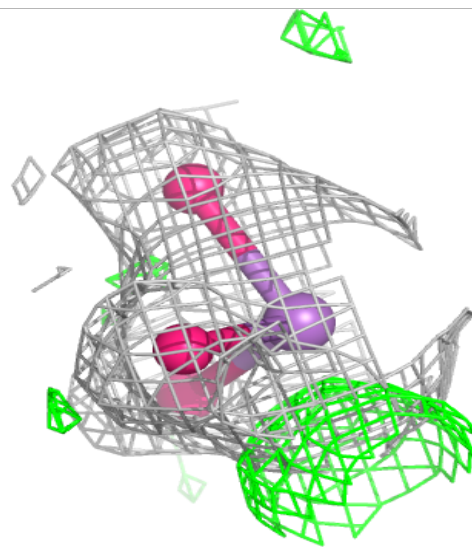
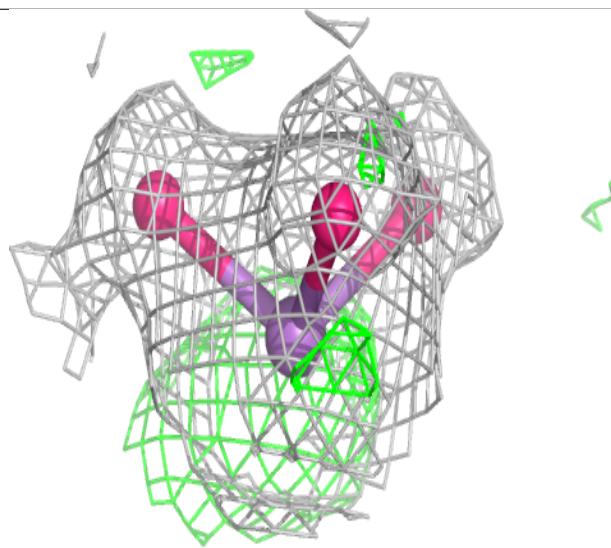
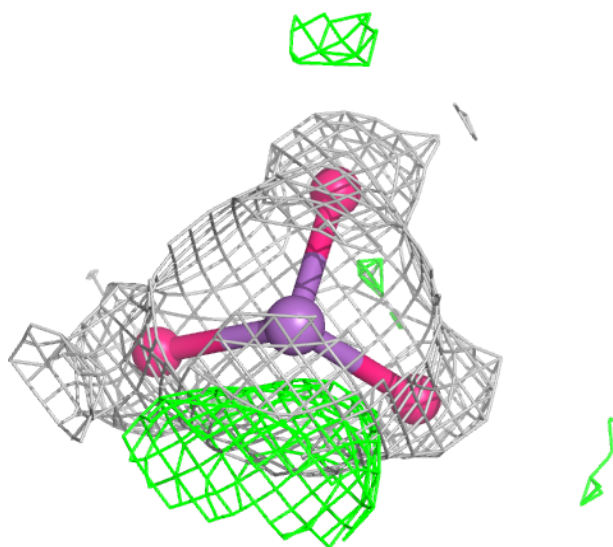
Electron density around 4MO A 2005:

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



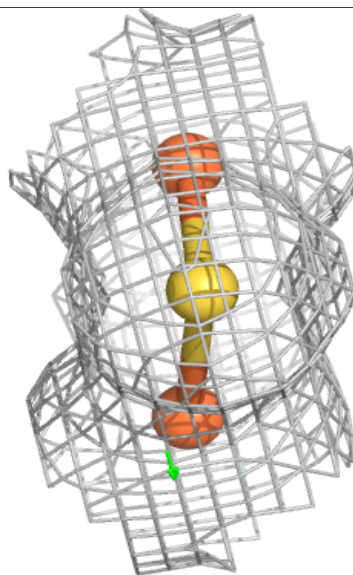
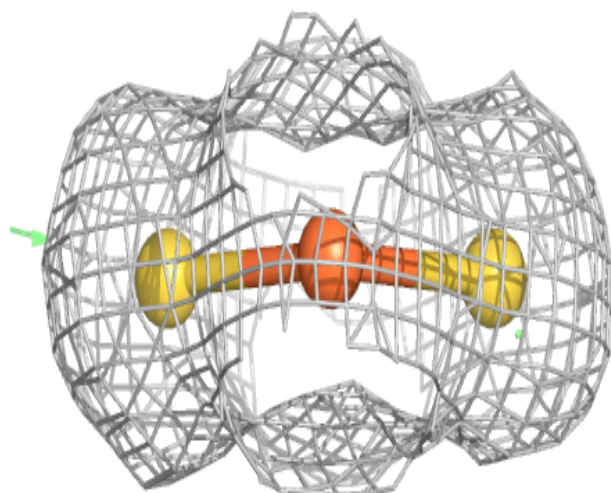
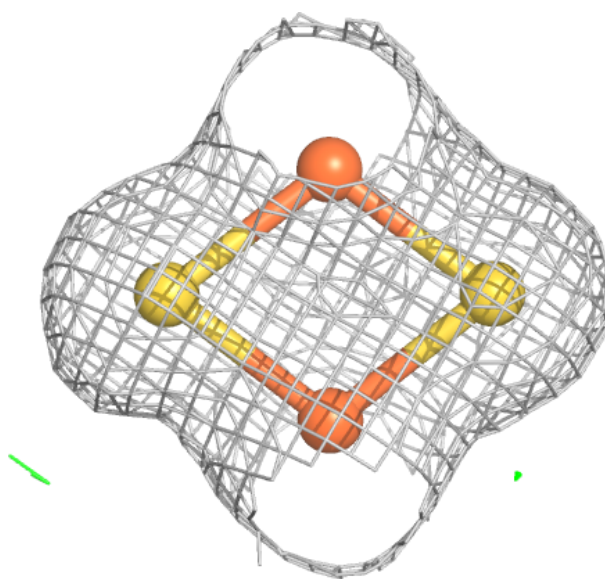
Electron density around SBO A 2012:

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



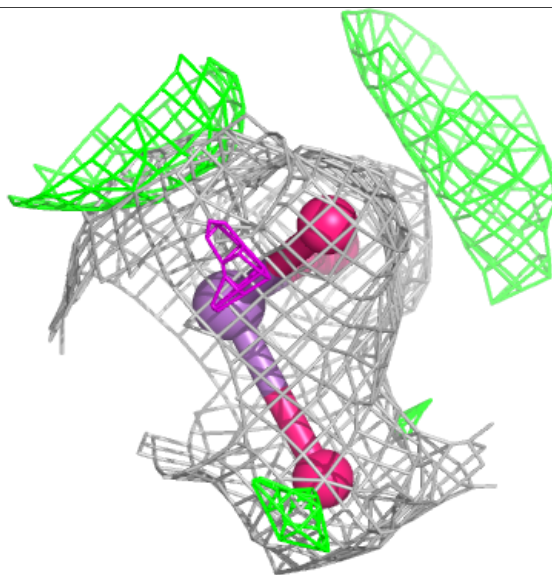
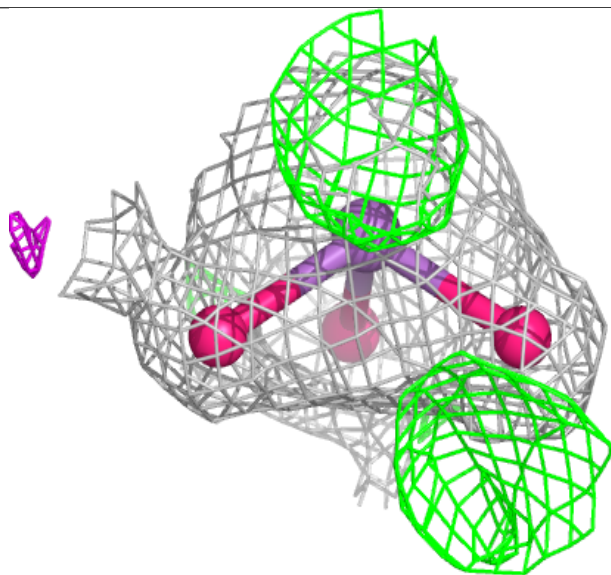
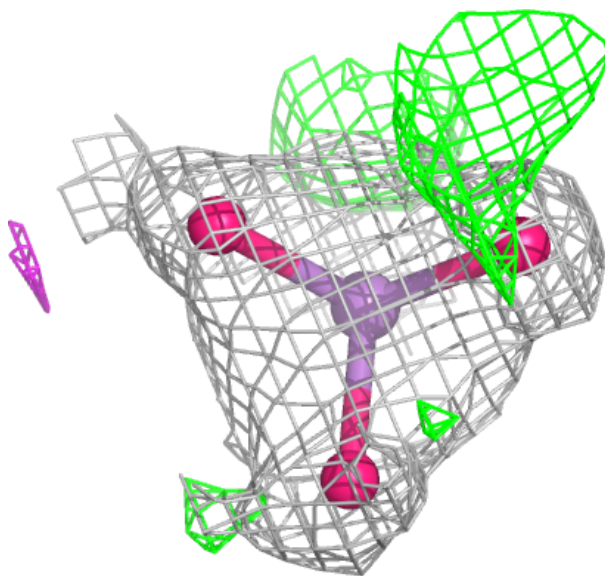
Electron density around FES B 201:

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



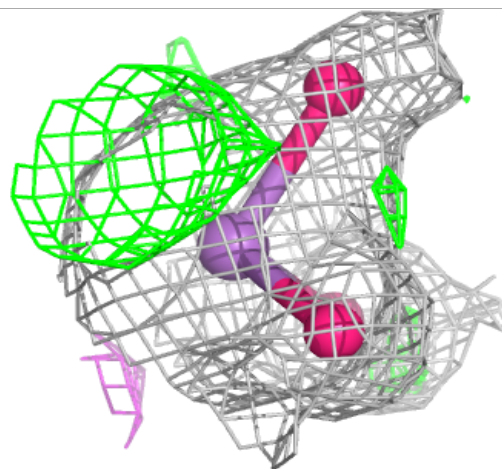
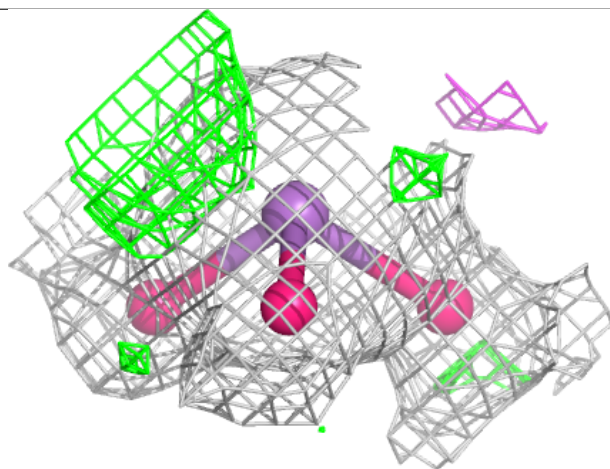
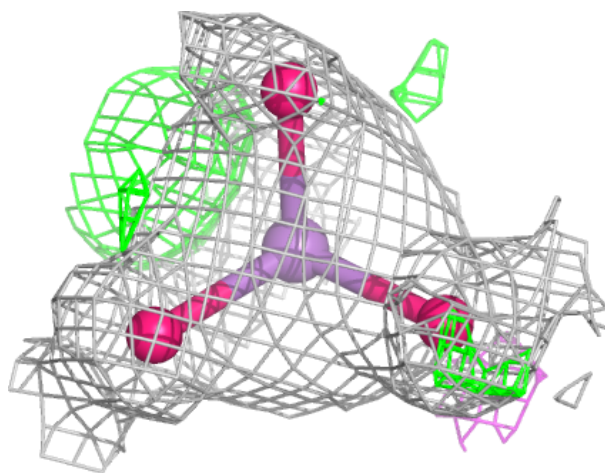
Electron density around SBO C 2011:

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



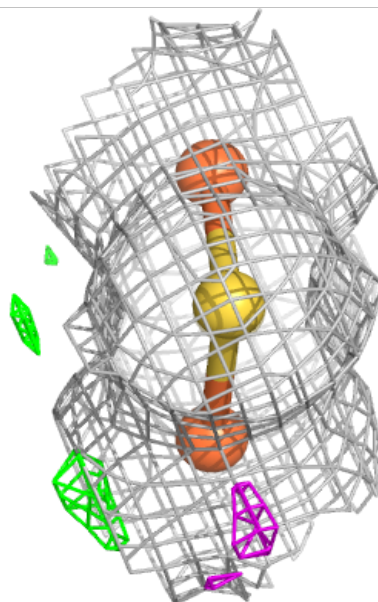
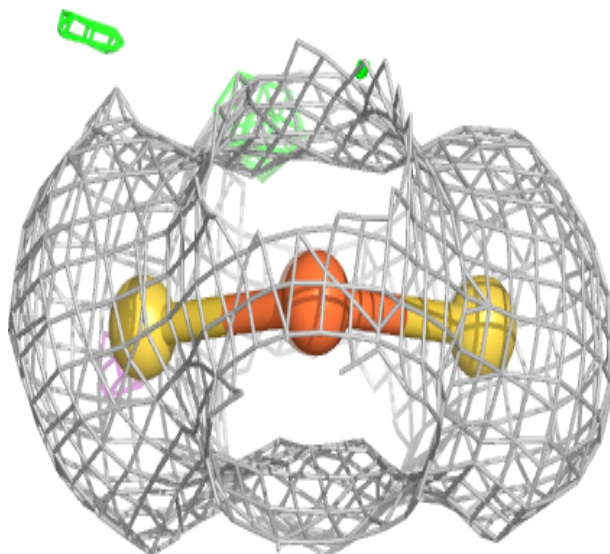
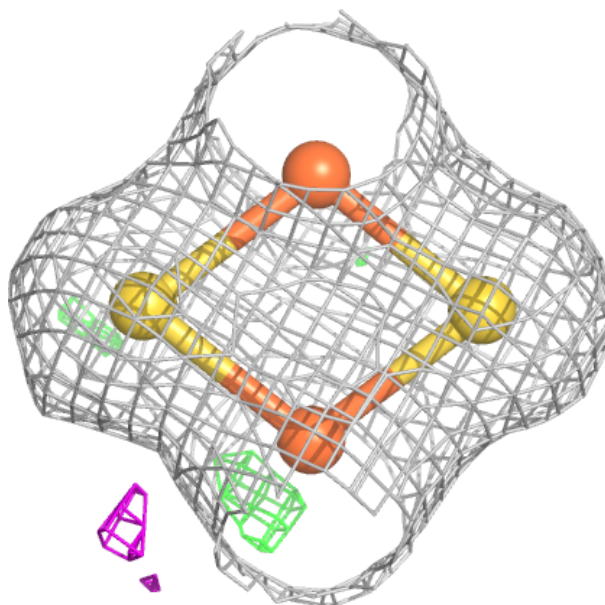
Electron density around SBO E 2011:

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



Electron density around FES H 201:

$2mF_o-DF_c$ (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.