



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:15 PM UTC

PDB ID : 8HMG / pdb_00008hmg
Title : The open state of RGLG2-VWA
Authors : Wang, Q.
Deposited on : 2022-12-03
Resolution : 2.81 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 : 2022.3.0, CSD as543be (2022)
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 : 9.0.010 (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

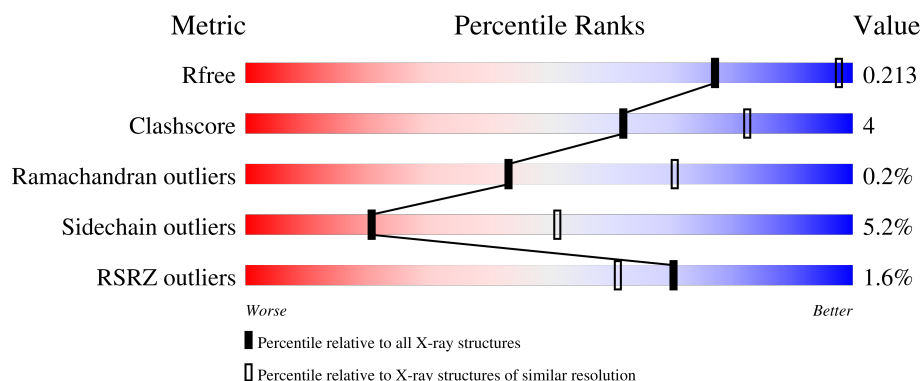
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

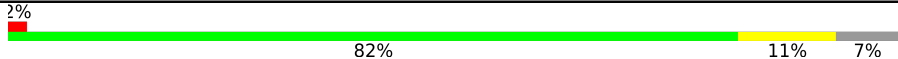
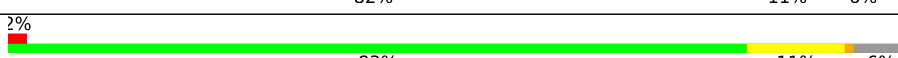
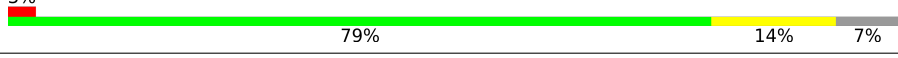
The reported resolution of this entry is 2.81 Å.

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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	307	
1	B	307	
1	C	307	
1	D	307	
1	E	307	

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Mol	Chain	Length	Quality of chain
1	F	307	% 82% 11% • 6%
1	G	307	2% 81% 11% • 7%
1	H	307	2% 84% 10% • 6%
1	I	307	% 82% 12% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21046 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 E3 ubiquitin-protein ligase RGLG2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2258	1430	380	439	9			
1	B	290	Total	C	N	O	S	0	0	0
			2280	1441	384	446	9			
1	C	289	Total	C	N	O	S	0	0	0
			2272	1436	383	445	8			
1	D	290	Total	C	N	O	S	0	0	0
			2280	1441	384	446	9			
1	E	287	Total	C	N	O	S	0	0	0
			2259	1430	380	440	9			
1	F	289	Total	C	N	O	S	0	0	0
			2274	1438	383	444	9			
1	G	287	Total	C	N	O	S	0	0	0
			2258	1430	380	439	9			
1	H	289	Total	C	N	O	S	0	0	0
			2272	1436	383	445	8			
1	I	290	Total	C	N	O	S	0	0	0
			2280	1441	384	446	9			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	GLY	-	expression tag	UNP Q9LY87
A	75	THR	-	expression tag	UNP Q9LY87
A	76	SER	-	expression tag	UNP Q9LY87
A	77	SER	-	expression tag	UNP Q9LY87
A	78	MET	-	expression tag	UNP Q9LY87
A	79	ALA	-	expression tag	UNP Q9LY87
A	80	ASP	-	expression tag	UNP Q9LY87
A	81	ILE	-	expression tag	UNP Q9LY87
A	82	GLY	-	expression tag	UNP Q9LY87
A	83	SER	-	expression tag	UNP Q9LY87
A	84	GLU	-	expression tag	UNP Q9LY87

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Chain	Residue	Modelled	Actual	Comment	Reference
A	85	PHE	-	expression tag	UNP Q9LY87
B	74	GLY	-	expression tag	UNP Q9LY87
B	75	THR	-	expression tag	UNP Q9LY87
B	76	SER	-	expression tag	UNP Q9LY87
B	77	SER	-	expression tag	UNP Q9LY87
B	78	MET	-	expression tag	UNP Q9LY87
B	79	ALA	-	expression tag	UNP Q9LY87
B	80	ASP	-	expression tag	UNP Q9LY87
B	81	ILE	-	expression tag	UNP Q9LY87
B	82	GLY	-	expression tag	UNP Q9LY87
B	83	SER	-	expression tag	UNP Q9LY87
B	84	GLU	-	expression tag	UNP Q9LY87
B	85	PHE	-	expression tag	UNP Q9LY87
C	74	GLY	-	expression tag	UNP Q9LY87
C	75	THR	-	expression tag	UNP Q9LY87
C	76	SER	-	expression tag	UNP Q9LY87
C	77	SER	-	expression tag	UNP Q9LY87
C	78	MET	-	expression tag	UNP Q9LY87
C	79	ALA	-	expression tag	UNP Q9LY87
C	80	ASP	-	expression tag	UNP Q9LY87
C	81	ILE	-	expression tag	UNP Q9LY87
C	82	GLY	-	expression tag	UNP Q9LY87
C	83	SER	-	expression tag	UNP Q9LY87
C	84	GLU	-	expression tag	UNP Q9LY87
C	85	PHE	-	expression tag	UNP Q9LY87
D	74	GLY	-	expression tag	UNP Q9LY87
D	75	THR	-	expression tag	UNP Q9LY87
D	76	SER	-	expression tag	UNP Q9LY87
D	77	SER	-	expression tag	UNP Q9LY87
D	78	MET	-	expression tag	UNP Q9LY87
D	79	ALA	-	expression tag	UNP Q9LY87
D	80	ASP	-	expression tag	UNP Q9LY87
D	81	ILE	-	expression tag	UNP Q9LY87
D	82	GLY	-	expression tag	UNP Q9LY87
D	83	SER	-	expression tag	UNP Q9LY87
D	84	GLU	-	expression tag	UNP Q9LY87
D	85	PHE	-	expression tag	UNP Q9LY87
E	74	GLY	-	expression tag	UNP Q9LY87
E	75	THR	-	expression tag	UNP Q9LY87
E	76	SER	-	expression tag	UNP Q9LY87
E	77	SER	-	expression tag	UNP Q9LY87
E	78	MET	-	expression tag	UNP Q9LY87

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Chain	Residue	Modelled	Actual	Comment	Reference
E	79	ALA	-	expression tag	UNP Q9LY87
E	80	ASP	-	expression tag	UNP Q9LY87
E	81	ILE	-	expression tag	UNP Q9LY87
E	82	GLY	-	expression tag	UNP Q9LY87
E	83	SER	-	expression tag	UNP Q9LY87
E	84	GLU	-	expression tag	UNP Q9LY87
E	85	PHE	-	expression tag	UNP Q9LY87
F	74	GLY	-	expression tag	UNP Q9LY87
F	75	THR	-	expression tag	UNP Q9LY87
F	76	SER	-	expression tag	UNP Q9LY87
F	77	SER	-	expression tag	UNP Q9LY87
F	78	MET	-	expression tag	UNP Q9LY87
F	79	ALA	-	expression tag	UNP Q9LY87
F	80	ASP	-	expression tag	UNP Q9LY87
F	81	ILE	-	expression tag	UNP Q9LY87
F	82	GLY	-	expression tag	UNP Q9LY87
F	83	SER	-	expression tag	UNP Q9LY87
F	84	GLU	-	expression tag	UNP Q9LY87
F	85	PHE	-	expression tag	UNP Q9LY87
G	74	GLY	-	expression tag	UNP Q9LY87
G	75	THR	-	expression tag	UNP Q9LY87
G	76	SER	-	expression tag	UNP Q9LY87
G	77	SER	-	expression tag	UNP Q9LY87
G	78	MET	-	expression tag	UNP Q9LY87
G	79	ALA	-	expression tag	UNP Q9LY87
G	80	ASP	-	expression tag	UNP Q9LY87
G	81	ILE	-	expression tag	UNP Q9LY87
G	82	GLY	-	expression tag	UNP Q9LY87
G	83	SER	-	expression tag	UNP Q9LY87
G	84	GLU	-	expression tag	UNP Q9LY87
G	85	PHE	-	expression tag	UNP Q9LY87
H	74	GLY	-	expression tag	UNP Q9LY87
H	75	THR	-	expression tag	UNP Q9LY87
H	76	SER	-	expression tag	UNP Q9LY87
H	77	SER	-	expression tag	UNP Q9LY87
H	78	MET	-	expression tag	UNP Q9LY87
H	79	ALA	-	expression tag	UNP Q9LY87
H	80	ASP	-	expression tag	UNP Q9LY87
H	81	ILE	-	expression tag	UNP Q9LY87
H	82	GLY	-	expression tag	UNP Q9LY87
H	83	SER	-	expression tag	UNP Q9LY87
H	84	GLU	-	expression tag	UNP Q9LY87

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Chain	Residue	Modelled	Actual	Comment	Reference
H	85	PHE	-	expression tag	UNP Q9LY87
I	74	GLY	-	expression tag	UNP Q9LY87
I	75	THR	-	expression tag	UNP Q9LY87
I	76	SER	-	expression tag	UNP Q9LY87
I	77	SER	-	expression tag	UNP Q9LY87
I	78	MET	-	expression tag	UNP Q9LY87
I	79	ALA	-	expression tag	UNP Q9LY87
I	80	ASP	-	expression tag	UNP Q9LY87
I	81	ILE	-	expression tag	UNP Q9LY87
I	82	GLY	-	expression tag	UNP Q9LY87
I	83	SER	-	expression tag	UNP Q9LY87
I	84	GLU	-	expression tag	UNP Q9LY87
I	85	PHE	-	expression tag	UNP Q9LY87

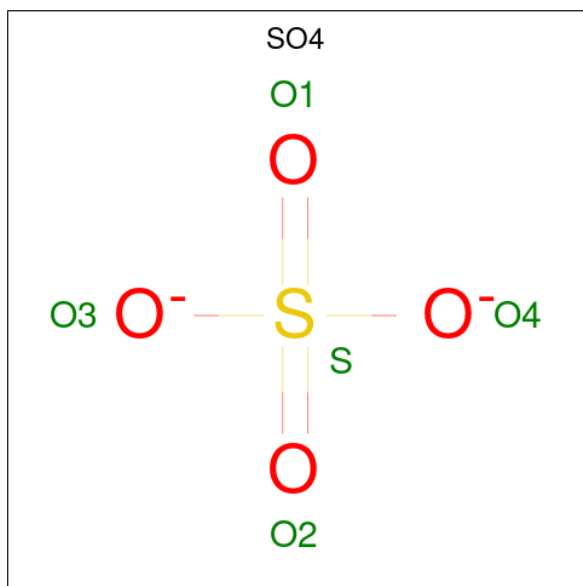
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total 3 Ca 3	0	0
2	B	3	Total 3 Ca 3	0	0
2	C	3	Total 3 Ca 3	0	0
2	D	3	Total 3 Ca 3	0	0
2	E	3	Total 3 Ca 3	0	0
2	F	3	Total 3 Ca 3	0	0
2	G	3	Total 3 Ca 3	0	0
2	H	3	Total 3 Ca 3	0	0
2	I	3	Total 3 Ca 3	0	0

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

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		

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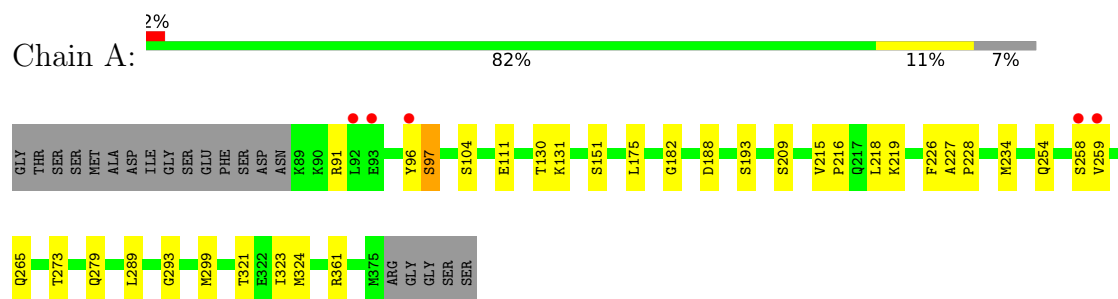
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	66	Total 66	O 66	0	0
5	C	58	Total 58	O 58	0	0
5	D	68	Total 68	O 68	0	0
5	E	45	Total 45	O 45	0	0
5	F	44	Total 44	O 44	0	0
5	G	46	Total 46	O 46	0	0
5	H	41	Total 41	O 41	0	0
5	I	44	Total 44	O 44	0	0

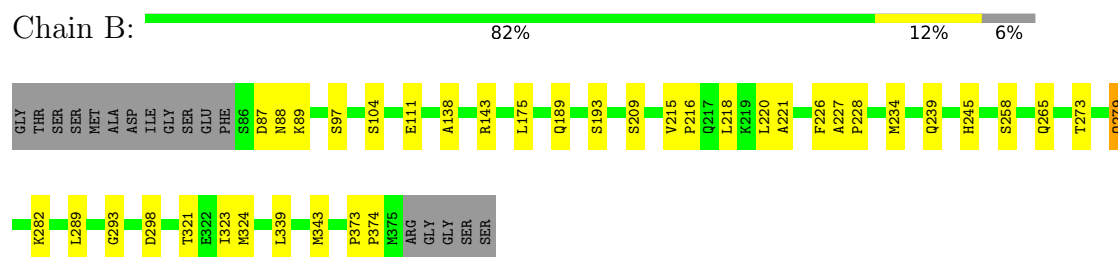
3 Residue-property plots [i](#)

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

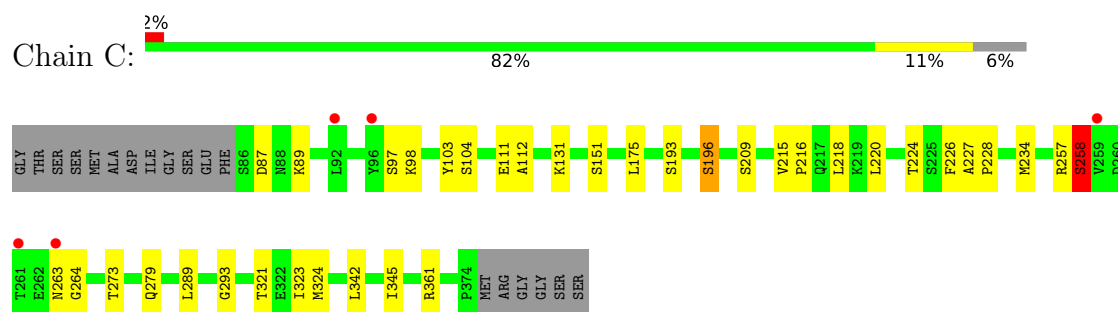
- Molecule 1: E3 ubiquitin-protein ligase RGLG2



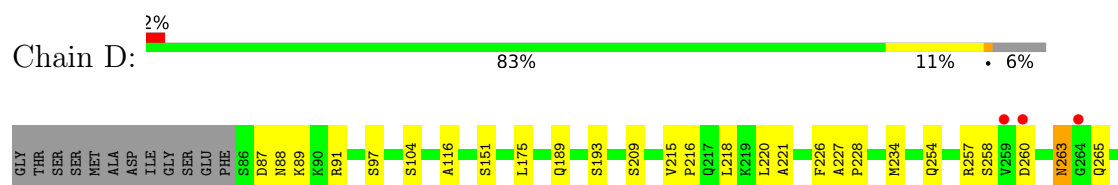
- Molecule 1: E3 ubiquitin-protein ligase RGLG2



- Molecule 1: E3 ubiquitin-protein ligase RGLG2

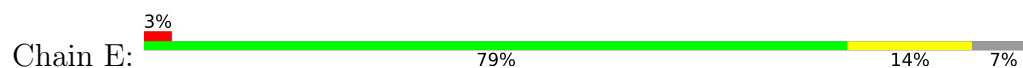


- Molecule 1: E3 ubiquitin-protein ligase RGLG2

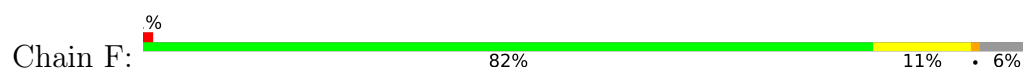




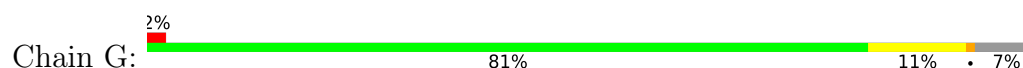
- Molecule 1: E3 ubiquitin-protein ligase RGLG2



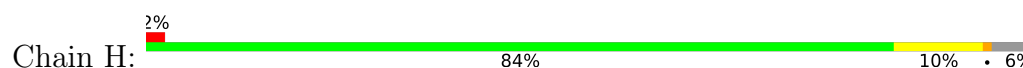
- Molecule 1: E3 ubiquitin-protein ligase RGLG2



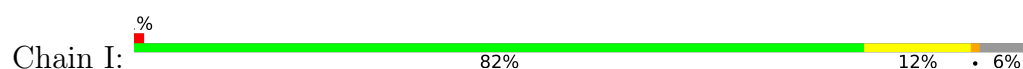
- Molecule 1: E3 ubiquitin-protein ligase RGLG2

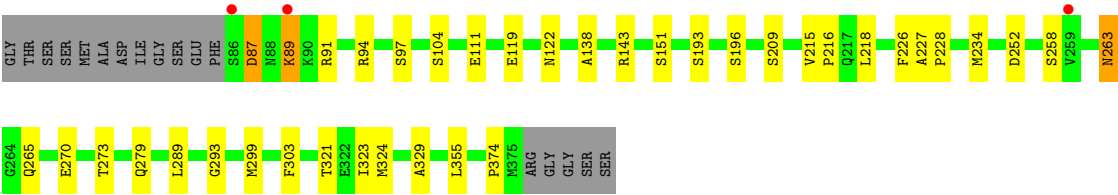


- Molecule 1: E3 ubiquitin-protein ligase RGLG2



- Molecule 1: E3 ubiquitin-protein ligase RGLG2





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	244.41Å 244.41Å 63.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.81 – 2.81 49.81 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.81-2.81) 99.9 (49.81-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.183 , 0.208 0.194 , 0.213	Depositor DCC
R_{free} test set	5115 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.010 for h,-h-k,-l 0.004 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21046	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: SO4, MG, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.98	0/2305	1.36	1/3121 (0.0%)
1	B	1.00	1/2327 (0.0%)	1.38	2/3151 (0.1%)
1	C	0.98	0/2319	1.37	3/3141 (0.1%)
1	D	1.01	0/2327	1.40	4/3151 (0.1%)
1	E	0.98	0/2305	1.38	2/3120 (0.1%)
1	F	1.00	0/2321	1.38	6/3143 (0.2%)
1	G	1.00	0/2305	1.36	0/3121
1	H	1.00	0/2319	1.38	2/3141 (0.1%)
1	I	0.98	0/2327	1.38	4/3151 (0.1%)
All	All	0.99	1/20855 (0.0%)	1.38	24/28240 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	245	HIS	CE1-NE2	5.59	1.38	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	279	GLN	CB-CG-CD	-6.53	101.50	112.60
1	C	258	SER	CA-C-O	-6.30	113.87	121.05
1	F	205	GLU	N-CA-CB	6.29	119.32	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	374	PRO	CA-C-N	5.46	131.52	121.70
1	I	374	PRO	C-N-CA	5.46	131.52	121.70
1	D	326	LYS	CA-C-N	5.43	128.57	120.31
1	D	326	LYS	C-N-CA	5.43	128.57	120.31
1	D	87	ASP	CA-C-N	5.41	127.80	120.65
1	D	87	ASP	C-N-CA	5.41	127.80	120.65
1	C	87	ASP	CA-C-N	5.38	127.75	120.65
1	C	87	ASP	C-N-CA	5.38	127.75	120.65
1	H	87	ASP	CA-C-N	5.22	127.55	120.65
1	H	87	ASP	C-N-CA	5.22	127.55	120.65
1	E	87	ASP	CA-C-N	5.20	127.51	120.65
1	E	87	ASP	C-N-CA	5.20	127.51	120.65
1	A	188	ASP	CA-CB-CG	5.13	117.73	112.60
1	I	87	ASP	CA-C-N	5.12	127.41	120.65
1	I	87	ASP	C-N-CA	5.12	127.41	120.65
1	F	290	VAL	CA-C-N	5.10	125.57	120.98
1	F	290	VAL	C-N-CA	5.10	125.57	120.98
1	B	88	ASN	CA-C-N	5.08	127.35	120.38
1	B	88	ASN	C-N-CA	5.08	127.35	120.38
1	F	87	ASP	CA-C-N	5.01	127.26	120.65
1	F	87	ASP	C-N-CA	5.01	127.26	120.65

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	258	SER	Mainchain

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	2258	0	2213	19	0
1	B	2280	0	2228	16	0
1	C	2272	0	2219	19	0
1	D	2280	0	2228	23	0
1	E	2259	0	2212	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2274	0	2223	20	0
1	G	2258	0	2213	22	0
1	H	2272	0	2220	18	0
1	I	2280	0	2228	21	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	20	0	0	0	0
4	D	15	0	0	0	0
4	E	10	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	10	0	0	0	0
4	I	15	0	0	1	0
5	A	65	0	0	8	0
5	B	66	0	0	2	0
5	C	58	0	0	8	0
5	D	68	0	0	6	0
5	E	45	0	0	7	0
5	F	44	0	0	5	0
5	G	46	0	0	6	0
5	H	41	0	0	3	0
5	I	44	0	0	6	0
All	All	21046	0	19984	165	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 4.

All (165) 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:D:260:ASP:OD1	1:G:104:SER:OG	1.56	1.22
1:A:96:TYR:HD2	5:A:501:HOH:O	1.43	1.02
1:D:257:ARG:HD3	5:D:539:HOH:O	1.68	0.94
1:I:270:GLU:HG2	1:I:299:MET:HE2	1.57	0.85
1:D:279:GLN:OE1	5:D:501:HOH:O	1.96	0.83
1:H:257:ARG:HD3	5:H:524:HOH:O	1.78	0.83
1:I:87:ASP:HB3	5:I:523:HOH:O	1.79	0.82
1:F:117:GLY:HA2	5:F:518:HOH:O	1.79	0.82
1:E:254:GLN:O	5:E:501:HOH:O	2.01	0.78
1:A:259:VAL:HG21	1:D:116:ALA:HA	1.67	0.75
1:A:131:LYS:HE2	5:D:540:HOH:O	1.88	0.74
1:G:234:MET:HE1	1:G:279:GLN:HG3	1.71	0.72
1:F:187:HIS:ND1	5:F:502:HOH:O	2.24	0.70
1:C:264:GLY:HA2	5:C:538:HOH:O	1.91	0.69
1:I:299:MET:HE3	1:I:303:PHE:CE1	2.30	0.67
1:A:97:SER:O	5:A:502:HOH:O	2.11	0.67
1:I:196:SER:N	4:I:407:SO4:O4	2.28	0.67
1:D:234:MET:HE1	1:D:279:GLN:HG3	1.76	0.66
1:I:94:ARG:HB3	5:I:535:HOH:O	1.95	0.66
1:H:122:ASN:HB3	5:H:519:HOH:O	1.95	0.65
1:B:234:MET:HE1	1:B:279:GLN:HG3	1.77	0.64
1:H:89:LYS:NZ	1:H:93:GLU:OE1	2.29	0.64
1:A:361:ARG:HD2	5:A:545:HOH:O	1.97	0.64
1:G:176:ILE:HG12	1:G:204:PHE:CE1	2.32	0.64
1:C:98:LYS:HE2	5:C:545:HOH:O	1.96	0.64
1:E:375:MET:HA	5:E:520:HOH:O	1.98	0.63
1:G:327:ASN:HB2	5:G:512:HOH:O	1.99	0.62
1:E:176:ILE:HG12	1:E:204:PHE:CE1	2.35	0.62
1:C:342:LEU:HD23	1:C:345:ILE:HD12	1.82	0.61
1:I:329:ALA:HA	5:I:517:HOH:O	2.00	0.61
1:D:254:GLN:O	5:D:502:HOH:O	2.16	0.60
1:G:342:LEU:HD23	1:G:345:ILE:HD12	1.82	0.60
1:D:361:ARG:HD2	5:D:562:HOH:O	2.00	0.60
1:A:254:GLN:O	5:A:503:HOH:O	2.16	0.60
1:E:243:GLN:HA	5:E:541:HOH:O	2.02	0.59
1:D:263:ASN:HD22	1:D:263:ASN:H	1.47	0.59
1:F:263:ASN:H	1:F:263:ASN:HD22	1.51	0.59
1:G:263:ASN:HD22	1:G:263:ASN:H	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:263:ASN:H	1:I:263:ASN:HD22	1.50	0.58
1:H:218:LEU:CD1	1:H:374:PRO:HG2	2.35	0.57
1:E:221:ALA:O	1:G:119:GLU:HB3	2.05	0.57
1:A:96:TYR:CD2	5:A:501:HOH:O	2.31	0.56
1:F:234:MET:HE1	1:F:279:GLN:HB3	1.90	0.54
1:E:361:ARG:HD2	5:E:536:HOH:O	2.06	0.54
1:F:104:SER:HB2	5:F:538:HOH:O	2.07	0.54
1:C:103:TYR:HE2	1:C:112:ALA:HB2	1.72	0.54
1:F:322:GLU:HG3	5:F:541:HOH:O	2.08	0.54
1:I:89:LYS:HE2	1:I:355:LEU:HD22	1.88	0.54
1:E:234:MET:HE1	1:E:279:GLN:HB3	1.90	0.53
1:H:234:MET:HE1	1:H:279:GLN:HB3	1.91	0.52
1:I:252:ASP:OD1	5:I:501:HOH:O	2.19	0.52
1:D:263:ASN:HD22	1:D:263:ASN:N	2.07	0.52
1:G:333:LYS:HA	5:G:506:HOH:O	2.10	0.52
1:A:219:LYS:NZ	5:A:507:HOH:O	2.43	0.51
1:D:215:VAL:HG12	1:D:216:PRO:HD3	1.93	0.51
1:A:234:MET:HE1	1:A:279:GLN:HB3	1.91	0.51
1:B:215:VAL:HG12	1:B:216:PRO:HD3	1.93	0.51
1:H:215:VAL:HG12	1:H:216:PRO:HD3	1.92	0.51
1:I:263:ASN:HD22	1:I:263:ASN:N	2.08	0.51
1:E:215:VAL:HG12	1:E:216:PRO:HD3	1.93	0.51
1:F:215:VAL:HG12	1:F:216:PRO:HD3	1.93	0.51
1:F:263:ASN:HD22	1:F:263:ASN:N	2.09	0.51
1:G:215:VAL:HG12	1:G:216:PRO:HD3	1.93	0.51
1:C:234:MET:HE1	1:C:279:GLN:HB3	1.92	0.51
1:E:119:GLU:CD	5:E:502:HOH:O	2.52	0.51
1:G:263:ASN:HD22	1:G:263:ASN:N	2.08	0.50
1:I:215:VAL:HG12	1:I:216:PRO:HD3	1.92	0.50
1:I:234:MET:HE1	1:I:279:GLN:HB3	1.92	0.50
1:E:227:ALA:HB3	1:E:228:PRO:HD3	1.93	0.50
1:I:227:ALA:HB3	1:I:228:PRO:HD3	1.94	0.50
1:D:258:SER:HA	5:D:516:HOH:O	2.11	0.50
1:A:215:VAL:HG12	1:A:216:PRO:HD3	1.94	0.50
1:F:117:GLY:CA	5:F:518:HOH:O	2.51	0.49
1:H:323:ILE:HG22	1:H:324:MET:HE2	1.95	0.49
1:D:260:ASP:CB	1:H:95:LYS:HZ1	2.26	0.49
1:G:227:ALA:HB3	1:G:228:PRO:HD3	1.95	0.49
1:C:227:ALA:HB3	1:C:228:PRO:HD3	1.94	0.49
1:C:215:VAL:HG12	1:C:216:PRO:HD3	1.93	0.49
1:H:227:ALA:HB3	1:H:228:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:ALA:HB3	1:F:228:PRO:HD3	1.93	0.48
1:C:361:ARG:HD2	5:C:532:HOH:O	2.13	0.48
1:B:227:ALA:HB3	1:B:228:PRO:HD3	1.93	0.48
1:D:323:ILE:HG22	1:D:324:MET:HE2	1.95	0.48
1:D:227:ALA:HB3	1:D:228:PRO:HD3	1.95	0.48
1:D:221:ALA:O	1:H:119:GLU:HB3	2.13	0.48
1:D:226:PHE:HB2	1:D:273:THR:HG23	1.96	0.48
1:F:226:PHE:HB2	1:F:273:THR:HG23	1.96	0.48
1:I:226:PHE:HB2	1:I:273:THR:HG23	1.96	0.48
1:B:226:PHE:HB2	1:B:273:THR:HG23	1.96	0.48
1:C:226:PHE:HB2	1:C:273:THR:HG23	1.96	0.47
1:F:323:ILE:HG22	1:F:324:MET:HE2	1.96	0.47
1:B:87:ASP:HB3	1:F:327:ASN:ND2	2.28	0.47
1:G:361:ARG:HD2	5:G:528:HOH:O	2.15	0.47
1:A:321:THR:HG22	5:A:551:HOH:O	2.13	0.47
1:A:227:ALA:HB3	1:A:228:PRO:HD3	1.95	0.47
1:A:226:PHE:HB2	1:A:273:THR:HG23	1.96	0.47
1:B:87:ASP:C	1:F:327:ASN:HD22	2.22	0.47
1:E:226:PHE:HB2	1:E:273:THR:HG23	1.96	0.47
1:E:323:ILE:HG22	1:E:324:MET:HE2	1.97	0.47
1:G:226:PHE:HB2	1:G:273:THR:HG23	1.96	0.47
1:B:87:ASP:O	1:F:327:ASN:ND2	2.44	0.47
1:B:239:GLN:HG3	5:B:551:HOH:O	2.14	0.46
1:C:224:THR:HG21	5:C:505:HOH:O	2.15	0.46
1:D:258:SER:CB	1:H:354:GLU:HG2	2.45	0.46
1:G:89:LYS:HE3	5:G:536:HOH:O	2.15	0.46
1:H:226:PHE:HB2	1:H:273:THR:HG23	1.96	0.46
1:B:323:ILE:HG22	1:B:324:MET:HE2	1.97	0.46
1:C:323:ILE:HG22	1:C:324:MET:HE2	1.97	0.46
1:D:258:SER:HB3	1:H:354:GLU:HG2	1.97	0.46
1:G:163:ILE:HG22	1:G:204:PHE:CE2	2.51	0.46
1:G:323:ILE:HG22	1:G:324:MET:HE2	1.97	0.46
1:I:323:ILE:HG22	1:I:324:MET:HE2	1.98	0.46
1:A:323:ILE:HG22	1:A:324:MET:HE2	1.97	0.45
1:D:215:VAL:N	1:D:216:PRO:CD	2.80	0.45
1:F:215:VAL:N	1:F:216:PRO:CD	2.80	0.45
1:G:323:ILE:HG13	5:G:535:HOH:O	2.17	0.45
1:G:215:VAL:N	1:G:216:PRO:CD	2.79	0.45
1:I:87:ASP:HB2	5:I:505:HOH:O	2.17	0.45
1:A:215:VAL:N	1:A:216:PRO:CD	2.80	0.45
1:C:215:VAL:N	1:C:216:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:ILE:HG22	1:E:204:PHE:CE2	2.51	0.44
1:H:215:VAL:N	1:H:216:PRO:CD	2.80	0.44
1:I:215:VAL:N	1:I:216:PRO:CD	2.80	0.44
1:B:215:VAL:N	1:B:216:PRO:CD	2.80	0.44
1:C:257:ARG:NH2	5:C:507:HOH:O	2.51	0.44
1:E:215:VAL:N	1:E:216:PRO:CD	2.80	0.44
1:B:221:ALA:O	1:I:119:GLU:HB3	2.17	0.44
1:C:131:LYS:CE	5:C:546:HOH:O	2.65	0.44
1:E:88:ASN:OD1	1:E:91:ARG:NH2	2.51	0.44
1:B:339:LEU:HD11	1:B:343:MET:HE1	2.00	0.43
1:E:87:ASP:CB	5:E:542:HOH:O	2.66	0.43
1:B:293:GLY:H	1:B:321:THR:HG21	1.84	0.43
1:B:282:LYS:HA	5:B:512:HOH:O	2.19	0.43
1:E:293:GLY:H	1:E:321:THR:HG21	1.84	0.43
1:D:88:ASN:OD1	1:D:91:ARG:NH2	2.51	0.42
1:H:293:GLY:H	1:H:321:THR:HG21	1.84	0.42
1:H:282:LYS:HA	5:H:510:HOH:O	2.18	0.42
1:C:293:GLY:H	1:C:321:THR:HG21	1.85	0.42
1:A:96:TYR:HB2	5:A:501:HOH:O	2.19	0.42
1:I:293:GLY:H	1:I:321:THR:HG21	1.85	0.42
1:C:196:SER:N	5:C:509:HOH:O	2.52	0.42
1:E:373:PRO:HA	1:E:374:PRO:HD3	1.90	0.42
1:G:131:LYS:HA	1:G:220:LEU:HB3	2.02	0.42
1:D:293:GLY:H	1:D:321:THR:HG21	1.84	0.42
1:G:224:THR:HG21	5:G:504:HOH:O	2.20	0.42
1:A:293:GLY:H	1:A:321:THR:HG21	1.83	0.41
1:B:289:LEU:C	1:B:289:LEU:HD13	2.45	0.41
1:B:373:PRO:HA	1:B:374:PRO:HD3	1.91	0.41
1:D:260:ASP:HB3	1:H:95:LYS:NZ	2.36	0.41
1:F:293:GLY:H	1:F:321:THR:HG21	1.86	0.41
1:H:218:LEU:HD11	1:H:374:PRO:HG2	2.01	0.41
1:I:289:LEU:C	1:I:289:LEU:HD13	2.46	0.41
1:A:130:THR:HG22	1:A:182:GLY:HA3	2.02	0.41
1:C:263:ASN:HB2	1:F:326:LYS:NZ	2.36	0.41
1:E:169:ALA:CB	5:E:507:HOH:O	2.68	0.41
1:C:131:LYS:HE2	5:C:546:HOH:O	2.20	0.41
1:A:289:LEU:C	1:A:289:LEU:HD13	2.45	0.41
1:F:289:LEU:C	1:F:289:LEU:HD13	2.46	0.41
1:G:293:GLY:H	1:G:321:THR:HG21	1.86	0.41
1:E:289:LEU:C	1:E:289:LEU:HD13	2.46	0.41
1:C:289:LEU:C	1:C:289:LEU:HD13	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:ASN:HB3	5:I:510:HOH:O	2.22	0.40
1:D:260:ASP:OD1	1:G:104:SER:CB	2.60	0.40
1:E:350:LYS:HD3	1:F:260:ASP:OD2	2.21	0.40
1:E:130:THR:HG22	1:E:182:GLY:HA3	2.04	0.40

There are no symmetry-related clashes.

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	285/307 (93%)	268 (94%)	17 (6%)	0	100	100
1	B	288/307 (94%)	272 (94%)	15 (5%)	1 (0%)	36	64
1	C	287/307 (94%)	269 (94%)	18 (6%)	0	100	100
1	D	288/307 (94%)	271 (94%)	17 (6%)	0	100	100
1	E	283/307 (92%)	271 (96%)	11 (4%)	1 (0%)	30	58
1	F	287/307 (94%)	269 (94%)	17 (6%)	1 (0%)	36	64
1	G	285/307 (93%)	269 (94%)	15 (5%)	1 (0%)	30	58
1	H	287/307 (94%)	271 (94%)	16 (6%)	0	100	100
1	I	288/307 (94%)	271 (94%)	16 (6%)	1 (0%)	36	64
All	All	2578/2763 (93%)	2431 (94%)	142 (6%)	5 (0%)	43	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	138	ALA
1	E	138	ALA
1	F	138	ALA
1	G	138	ALA
1	I	138	ALA

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	248/263 (94%)	236 (95%)	12 (5%)	23	54
1	B	251/263 (95%)	236 (94%)	15 (6%)	17	45
1	C	250/263 (95%)	238 (95%)	12 (5%)	23	54
1	D	251/263 (95%)	238 (95%)	13 (5%)	21	51
1	E	249/263 (95%)	235 (94%)	14 (6%)	19	48
1	F	250/263 (95%)	236 (94%)	14 (6%)	19	48
1	G	248/263 (94%)	235 (95%)	13 (5%)	21	51
1	H	250/263 (95%)	239 (96%)	11 (4%)	25	58
1	I	251/263 (95%)	238 (95%)	13 (5%)	21	51
All	All	2248/2367 (95%)	2131 (95%)	117 (5%)	21	51

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	A	97	SER
1	A	104	SER
1	A	111	GLU
1	A	151	SER
1	A	175	LEU
1	A	193	SER
1	A	209	SER
1	A	218	LEU
1	A	258	SER
1	A	265	GLN
1	A	299	MET
1	B	89	LYS
1	B	97	SER
1	B	104	SER
1	B	111	GLU
1	B	143	ARG
1	B	175	LEU

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Mol	Chain	Res	Type
1	B	189	GLN
1	B	193	SER
1	B	209	SER
1	B	218	LEU
1	B	220	LEU
1	B	258	SER
1	B	265	GLN
1	B	279	GLN
1	B	298	ASP
1	C	89	LYS
1	C	97	SER
1	C	104	SER
1	C	111	GLU
1	C	151	SER
1	C	175	LEU
1	C	193	SER
1	C	196	SER
1	C	209	SER
1	C	218	LEU
1	C	220	LEU
1	C	258	SER
1	D	89	LYS
1	D	97	SER
1	D	104	SER
1	D	151	SER
1	D	175	LEU
1	D	189	GLN
1	D	193	SER
1	D	209	SER
1	D	218	LEU
1	D	220	LEU
1	D	263	ASN
1	D	265	GLN
1	D	279	GLN
1	E	87	ASP
1	E	89	LYS
1	E	97	SER
1	E	100	SER
1	E	104	SER
1	E	111	GLU
1	E	143	ARG
1	E	189	GLN

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Mol	Chain	Res	Type
1	E	193	SER
1	E	196	SER
1	E	209	SER
1	E	218	LEU
1	E	220	LEU
1	E	265	GLN
1	F	89	LYS
1	F	97	SER
1	F	104	SER
1	F	143	ARG
1	F	175	LEU
1	F	189	GLN
1	F	193	SER
1	F	209	SER
1	F	218	LEU
1	F	258	SER
1	F	263	ASN
1	F	265	GLN
1	F	279	GLN
1	F	375	MET
1	G	97	SER
1	G	104	SER
1	G	111	GLU
1	G	189	GLN
1	G	193	SER
1	G	196	SER
1	G	209	SER
1	G	218	LEU
1	G	220	LEU
1	G	258	SER
1	G	263	ASN
1	G	265	GLN
1	G	279	GLN
1	H	89	LYS
1	H	97	SER
1	H	104	SER
1	H	111	GLU
1	H	143	ARG
1	H	189	GLN
1	H	193	SER
1	H	209	SER
1	H	218	LEU

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Mol	Chain	Res	Type
1	H	220	LEU
1	H	262	GLU
1	I	89	LYS
1	I	91	ARG
1	I	97	SER
1	I	104	SER
1	I	111	GLU
1	I	143	ARG
1	I	151	SER
1	I	193	SER
1	I	209	SER
1	I	218	LEU
1	I	258	SER
1	I	263	ASN
1	I	265	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	195	ASN
1	A	254	GLN
1	B	88	ASN
1	B	195	ASN
1	B	243	GLN
1	B	254	GLN
1	C	189	GLN
1	C	195	ASN
1	C	254	GLN
1	D	174	ASN
1	D	189	GLN
1	D	195	ASN
1	D	243	GLN
1	D	254	GLN
1	D	263	ASN
1	E	195	ASN
1	E	254	GLN
1	E	265	GLN
1	F	189	GLN
1	F	195	ASN
1	F	254	GLN
1	F	263	ASN

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Mol	Chain	Res	Type
1	F	327	ASN
1	F	330	GLN
1	G	108	GLN
1	G	174	ASN
1	G	187	HIS
1	G	189	GLN
1	G	195	ASN
1	G	254	GLN
1	G	263	ASN
1	H	88	ASN
1	H	187	HIS
1	H	189	GLN
1	H	195	ASN
1	H	254	GLN
1	I	88	ASN
1	I	174	ASN
1	I	187	HIS
1	I	254	GLN
1	I	263	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 56 ligands modelled in this entry, 36 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	B	406	-	4,4,4	0.24	0	6,6,6	0.22	0
4	SO4	H	406	-	4,4,4	0.27	0	6,6,6	0.13	0
4	SO4	D	406	-	4,4,4	0.24	0	6,6,6	0.14	0
4	SO4	I	407	-	4,4,4	0.32	0	6,6,6	0.10	0
4	SO4	I	406	-	4,4,4	0.26	0	6,6,6	0.19	0
4	SO4	B	405	-	4,4,4	0.28	0	6,6,6	0.12	0
4	SO4	D	405	-	4,4,4	0.32	0	6,6,6	0.13	0
4	SO4	A	406	-	4,4,4	0.33	0	6,6,6	0.14	0
4	SO4	A	405	-	4,4,4	0.32	0	6,6,6	0.34	0
4	SO4	D	407	-	4,4,4	0.28	0	6,6,6	0.21	0
4	SO4	C	405	-	4,4,4	0.25	0	6,6,6	0.16	0
4	SO4	H	405	-	4,4,4	0.30	0	6,6,6	0.09	0
4	SO4	F	405	-	4,4,4	0.35	0	6,6,6	0.13	0
4	SO4	C	407	-	4,4,4	0.34	0	6,6,6	0.13	0
4	SO4	I	405	-	4,4,4	0.27	0	6,6,6	0.33	0
4	SO4	C	408	-	4,4,4	0.31	0	6,6,6	0.12	0
4	SO4	E	406	-	4,4,4	0.30	0	6,6,6	0.17	0
4	SO4	G	405	-	4,4,4	0.28	0	6,6,6	0.11	0
4	SO4	C	406	-	4,4,4	0.31	0	6,6,6	0.19	0
4	SO4	E	405	-	4,4,4	0.31	0	6,6,6	0.22	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

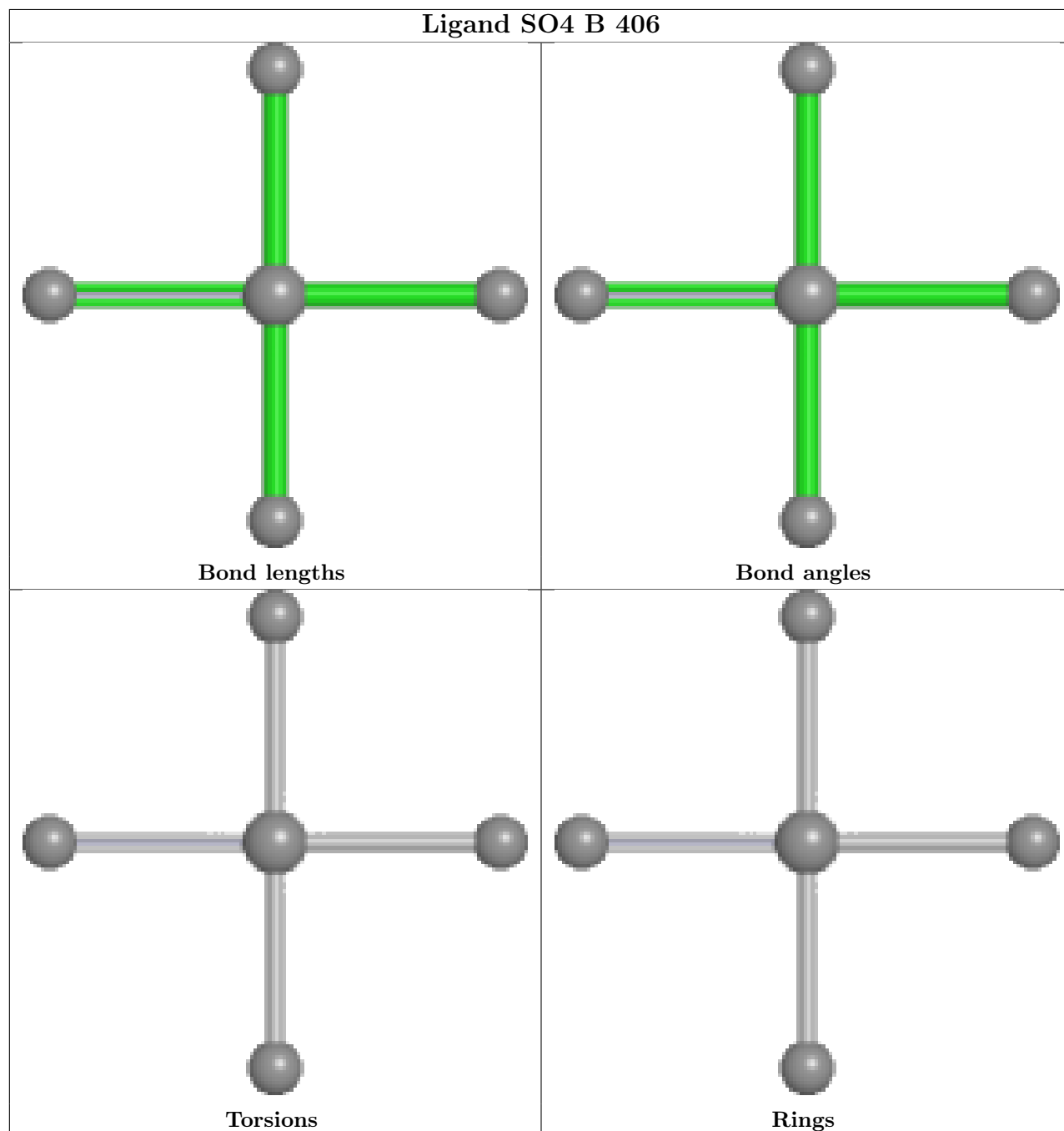
There are no ring outliers.

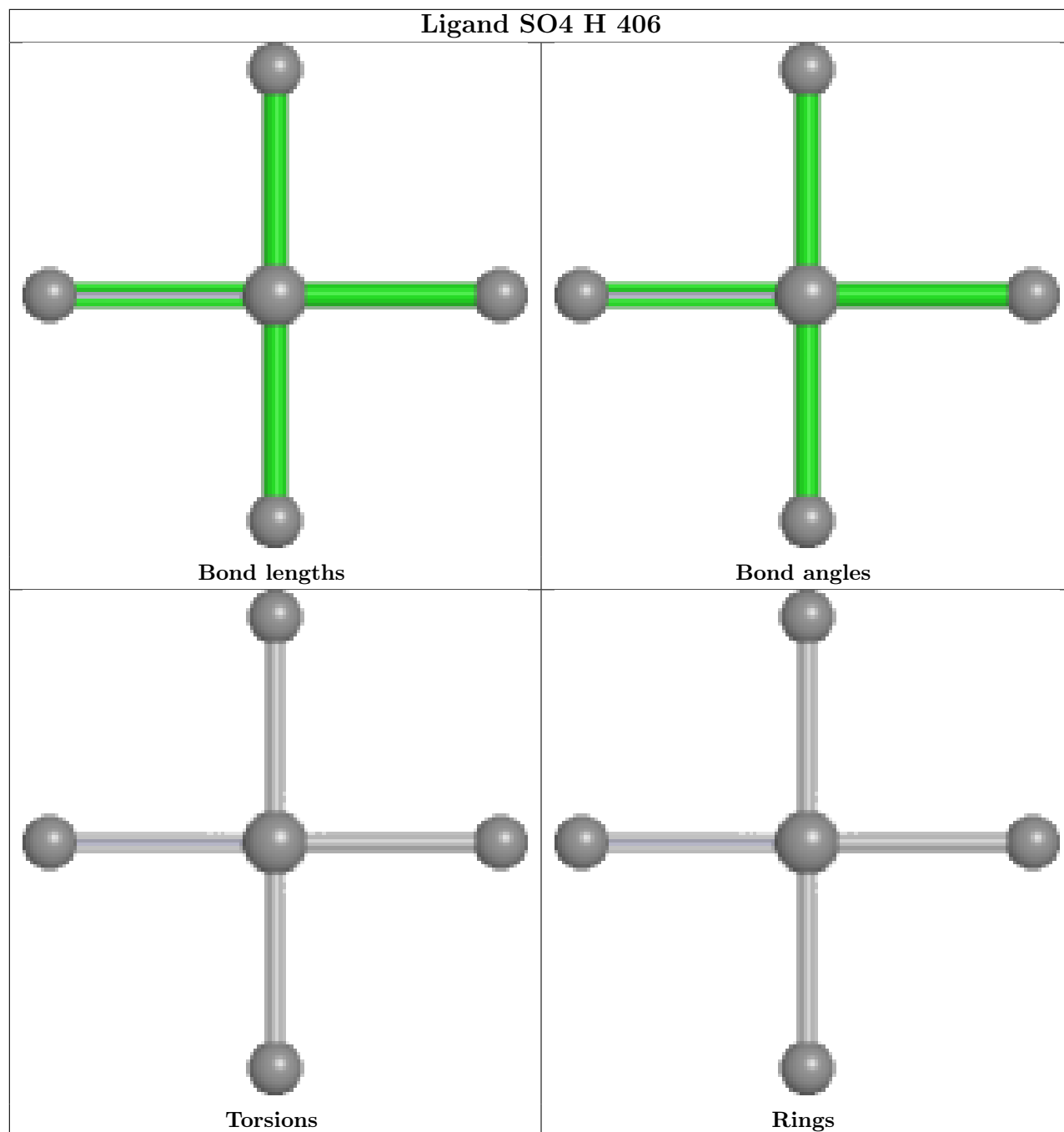
1 monomer is involved in 1 short contact:

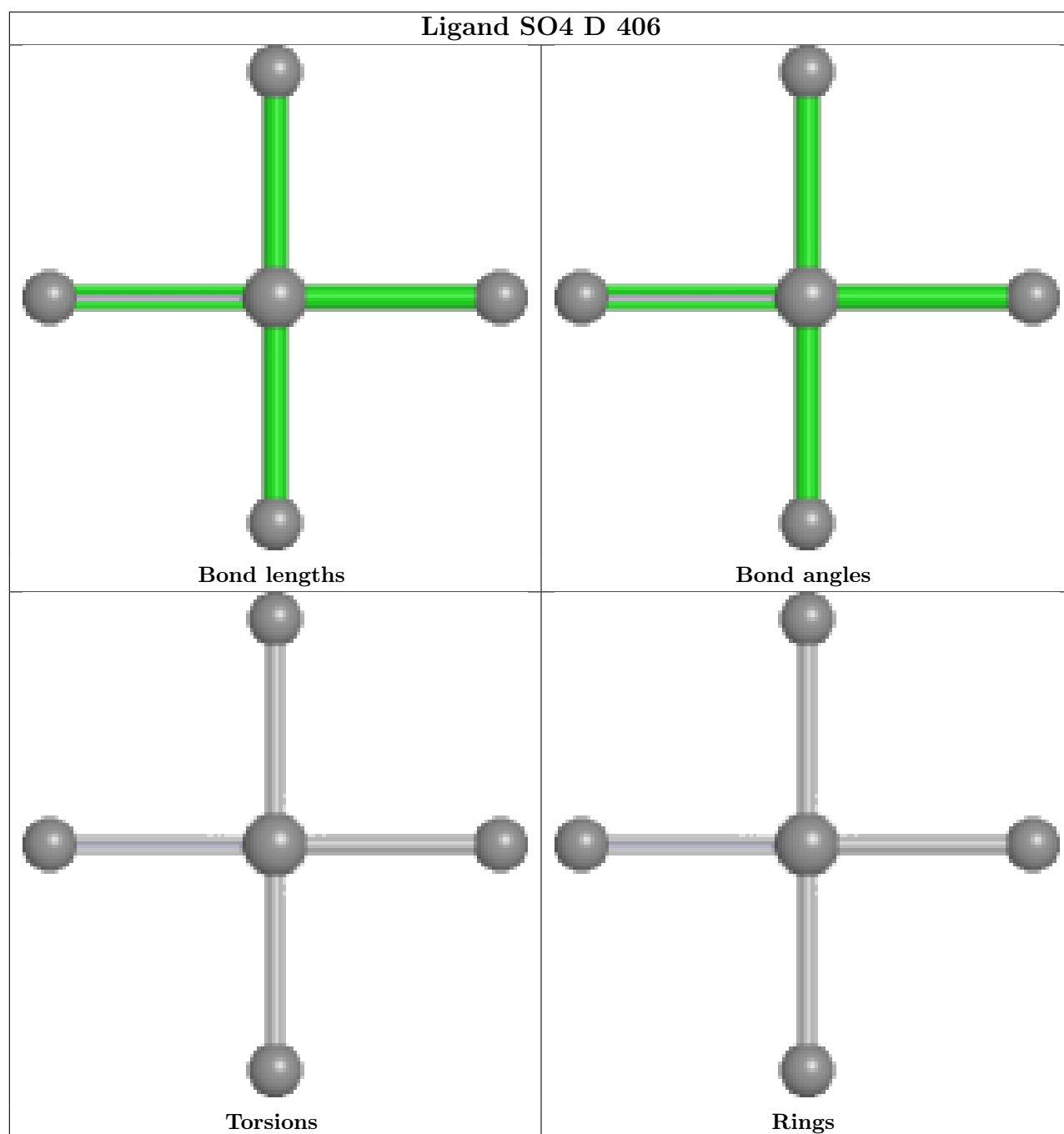
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	407	SO4	1	0

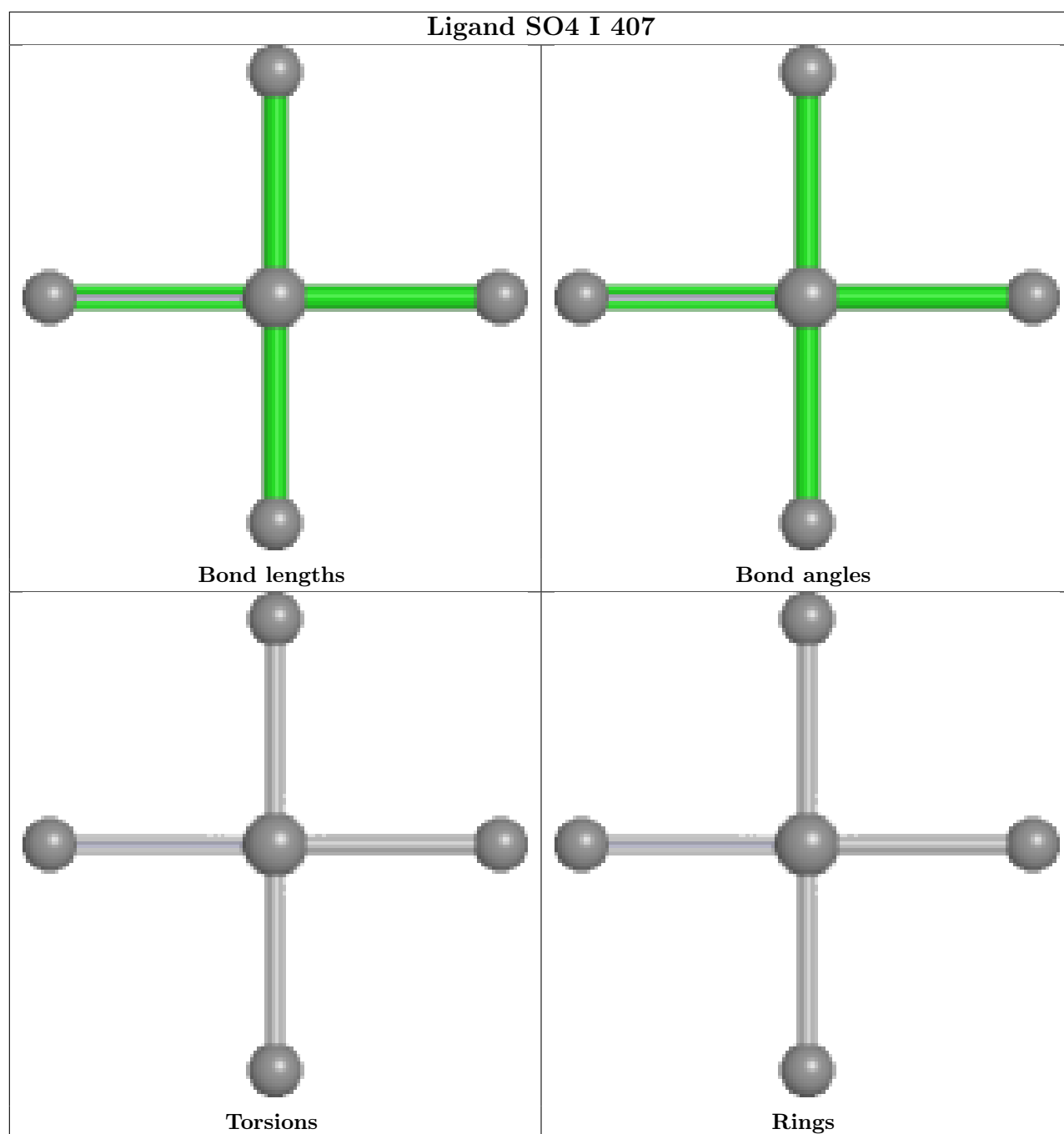
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

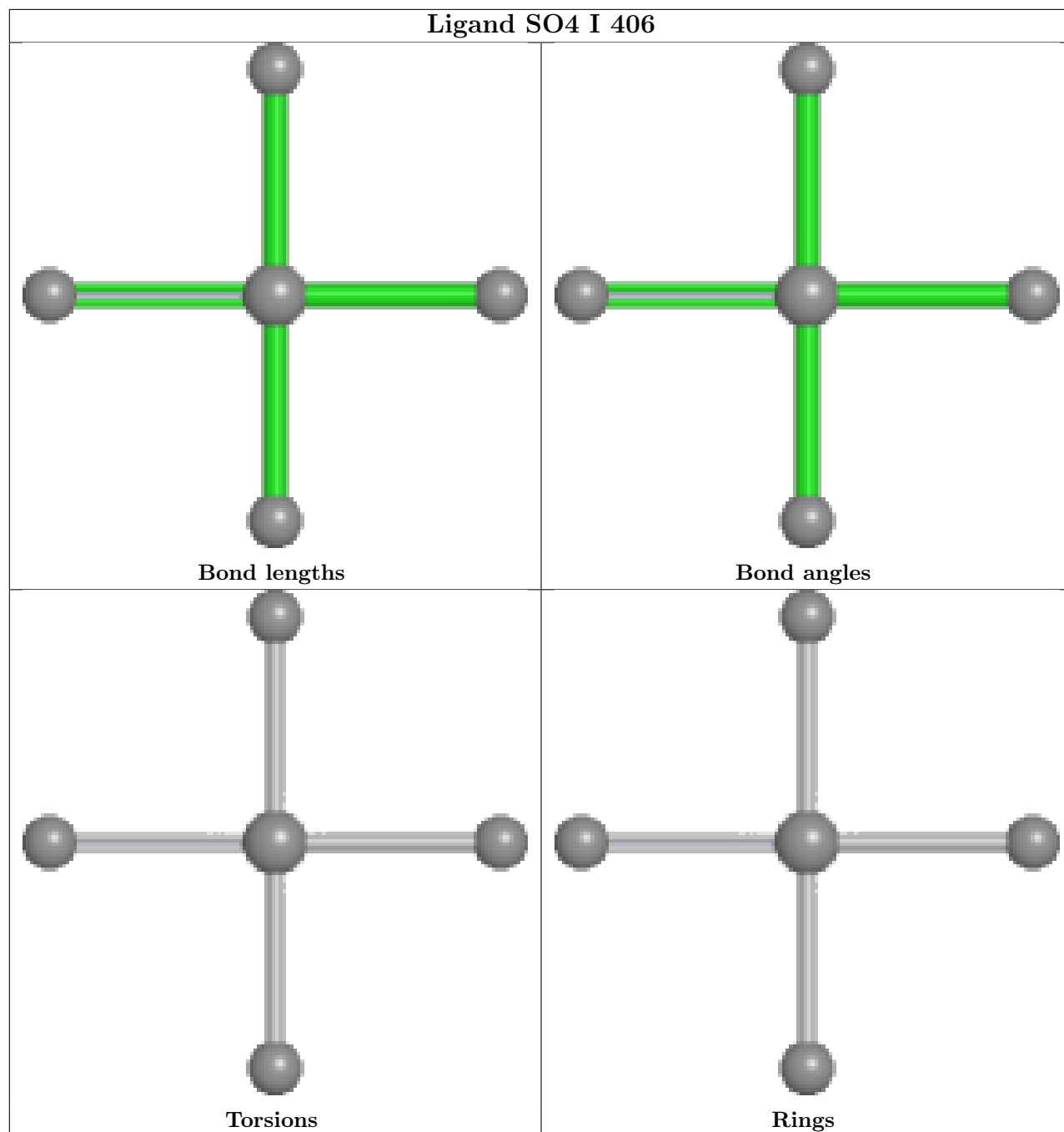
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

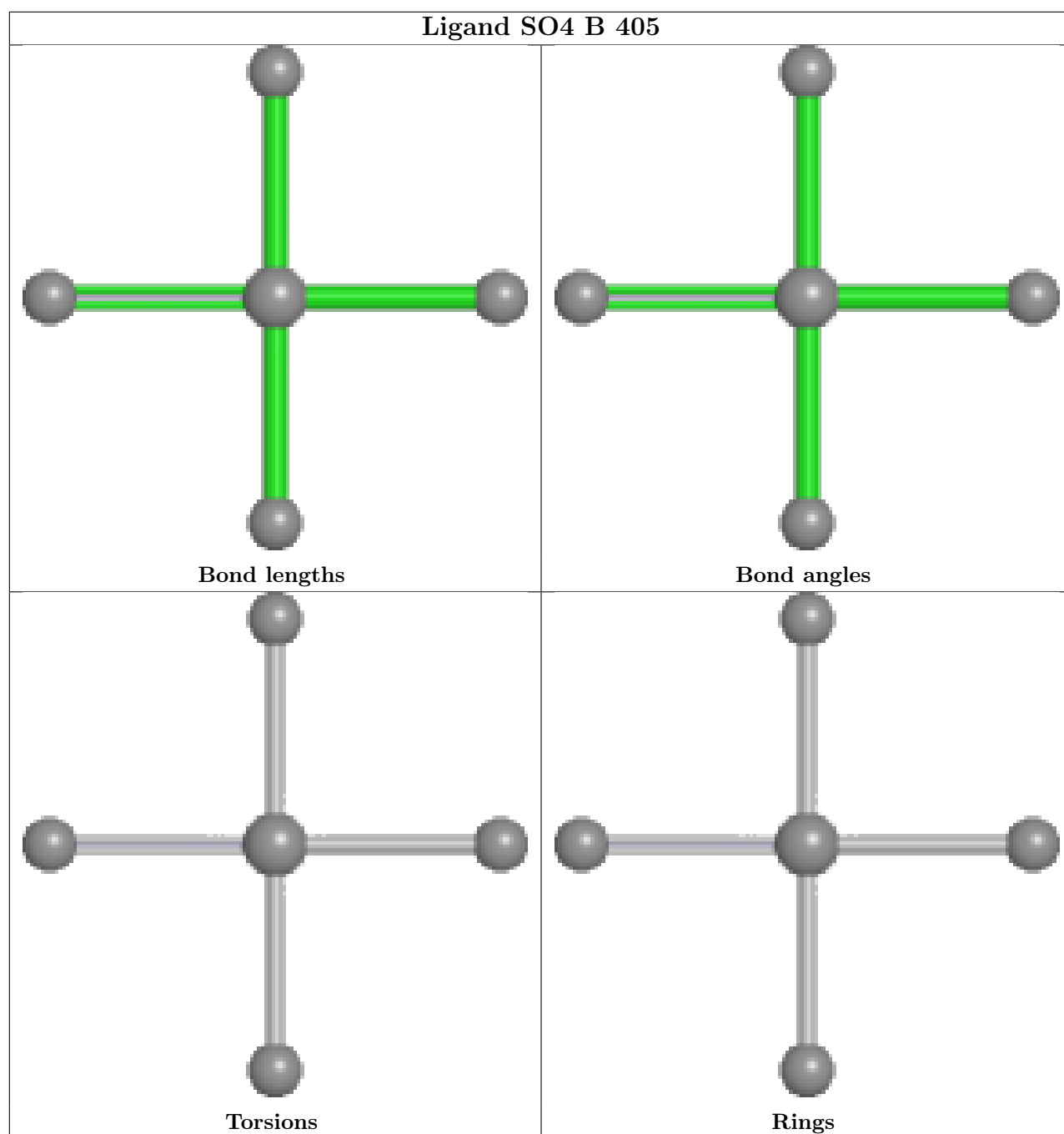


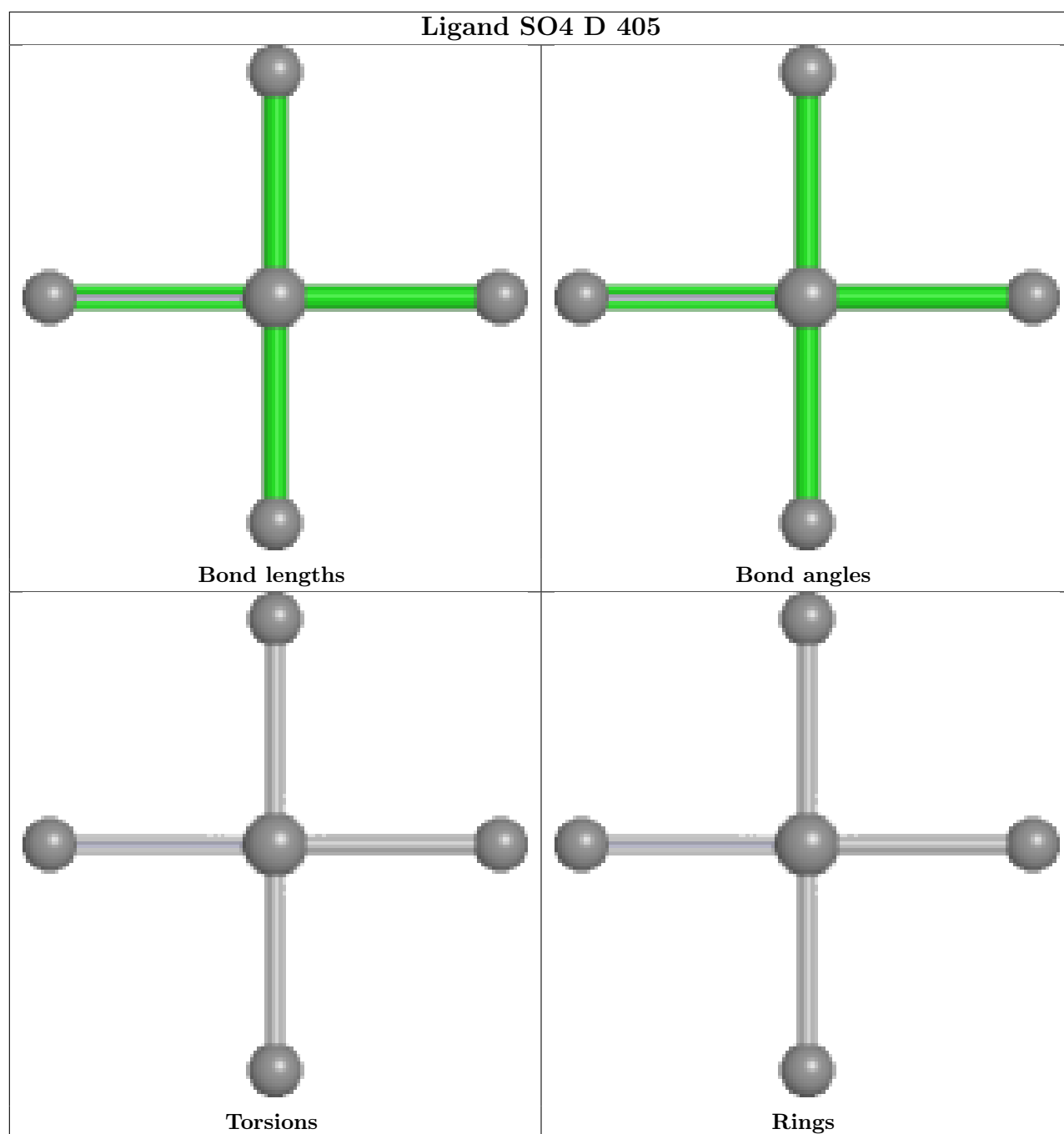


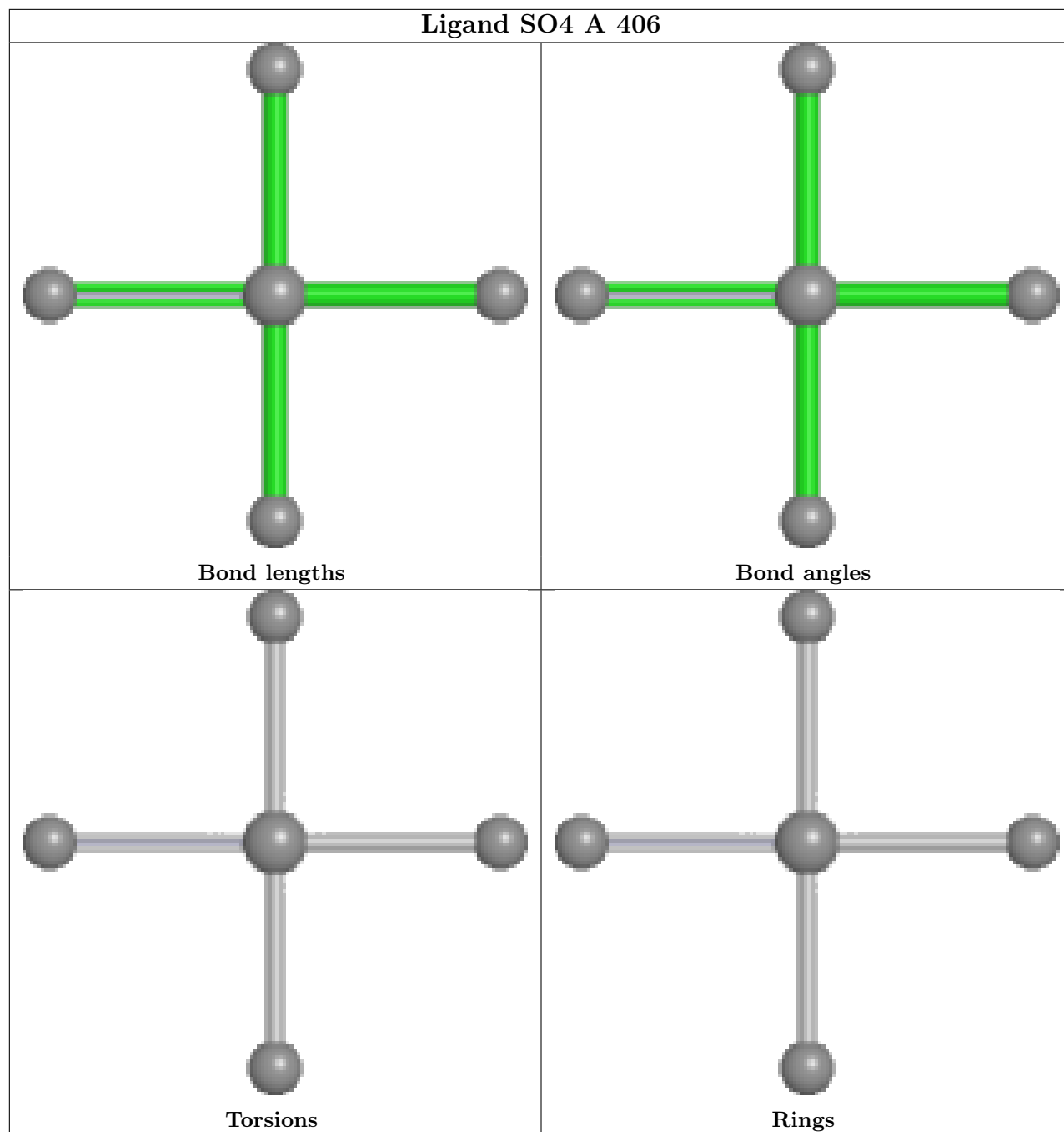


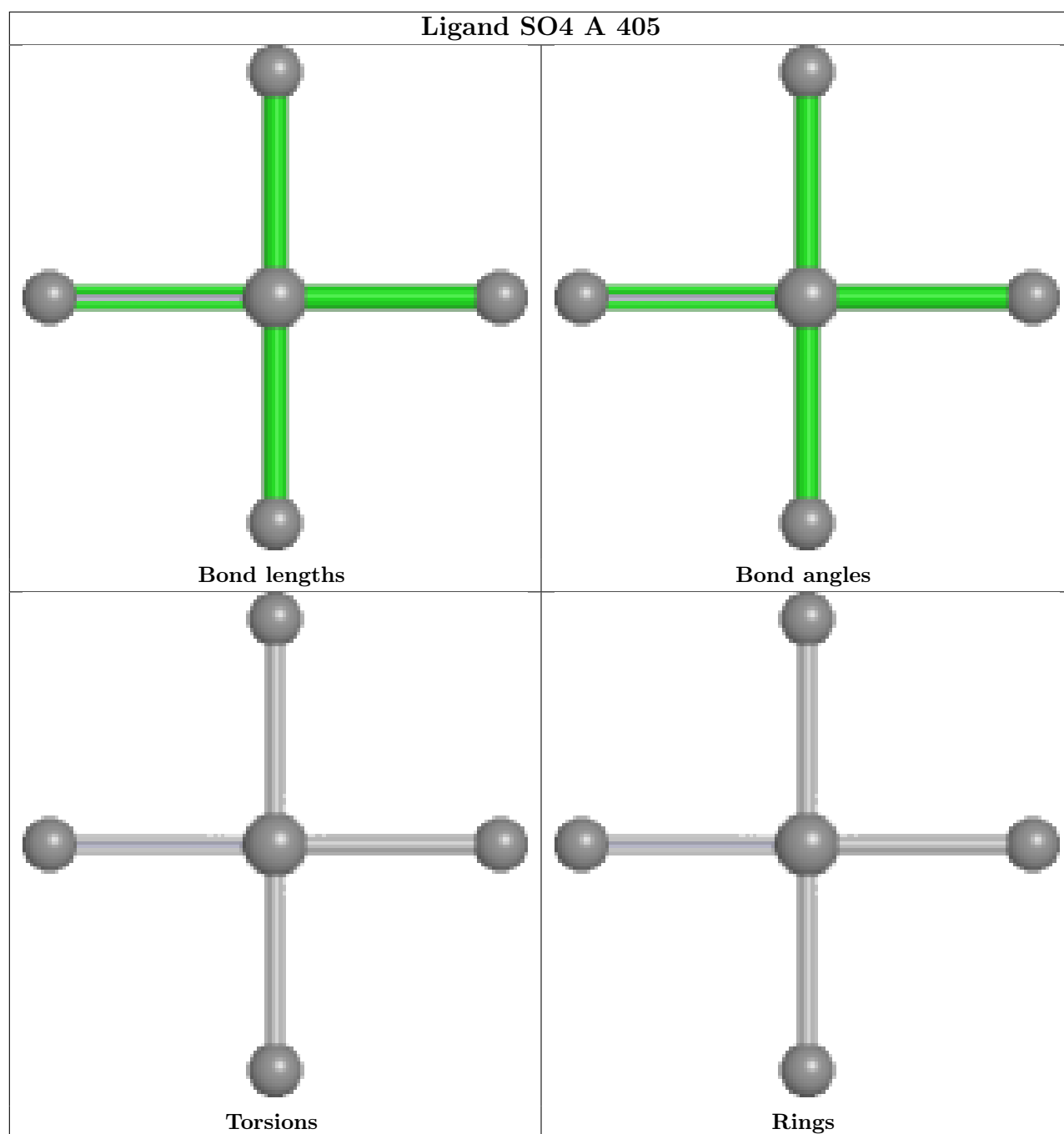


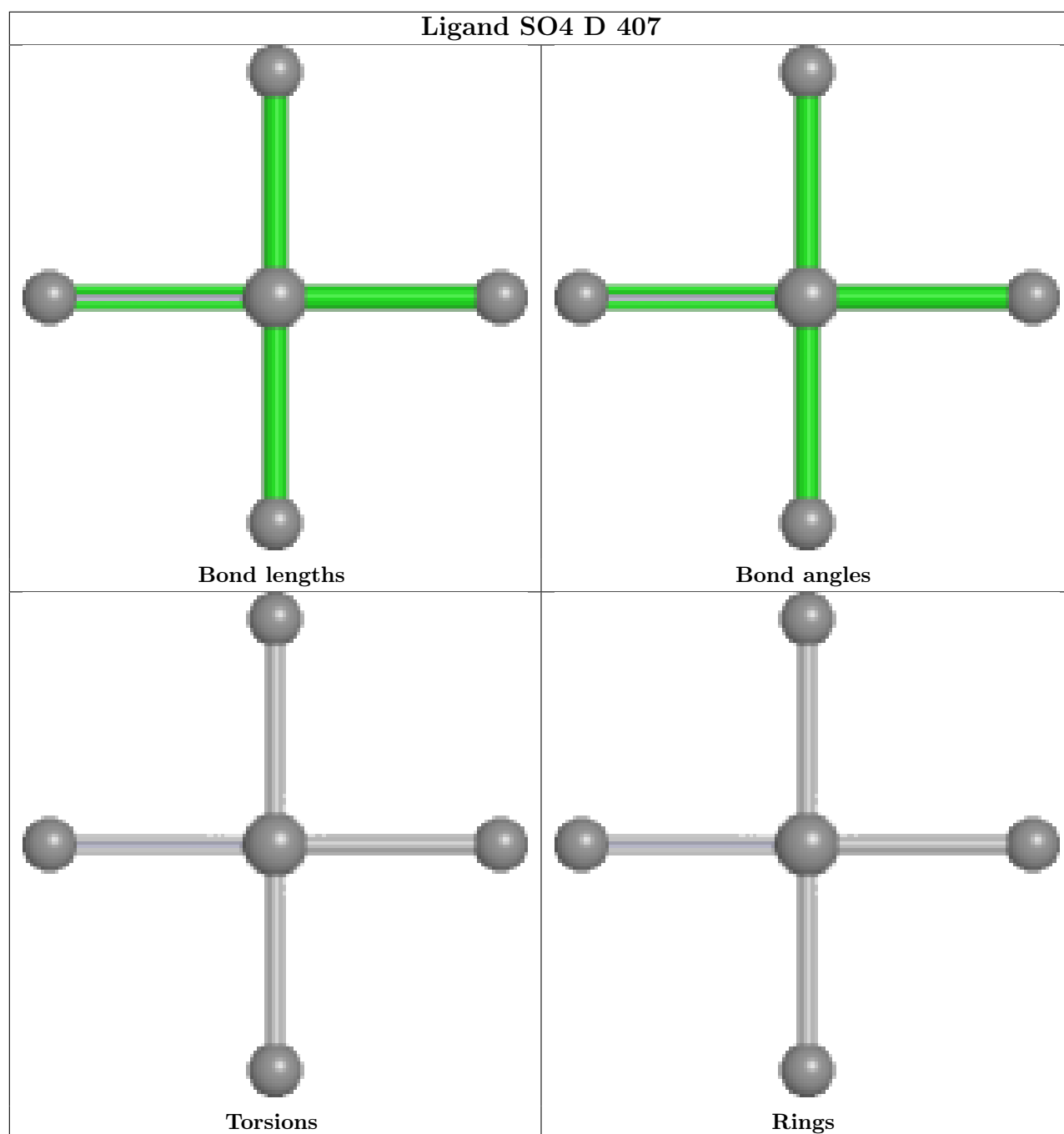


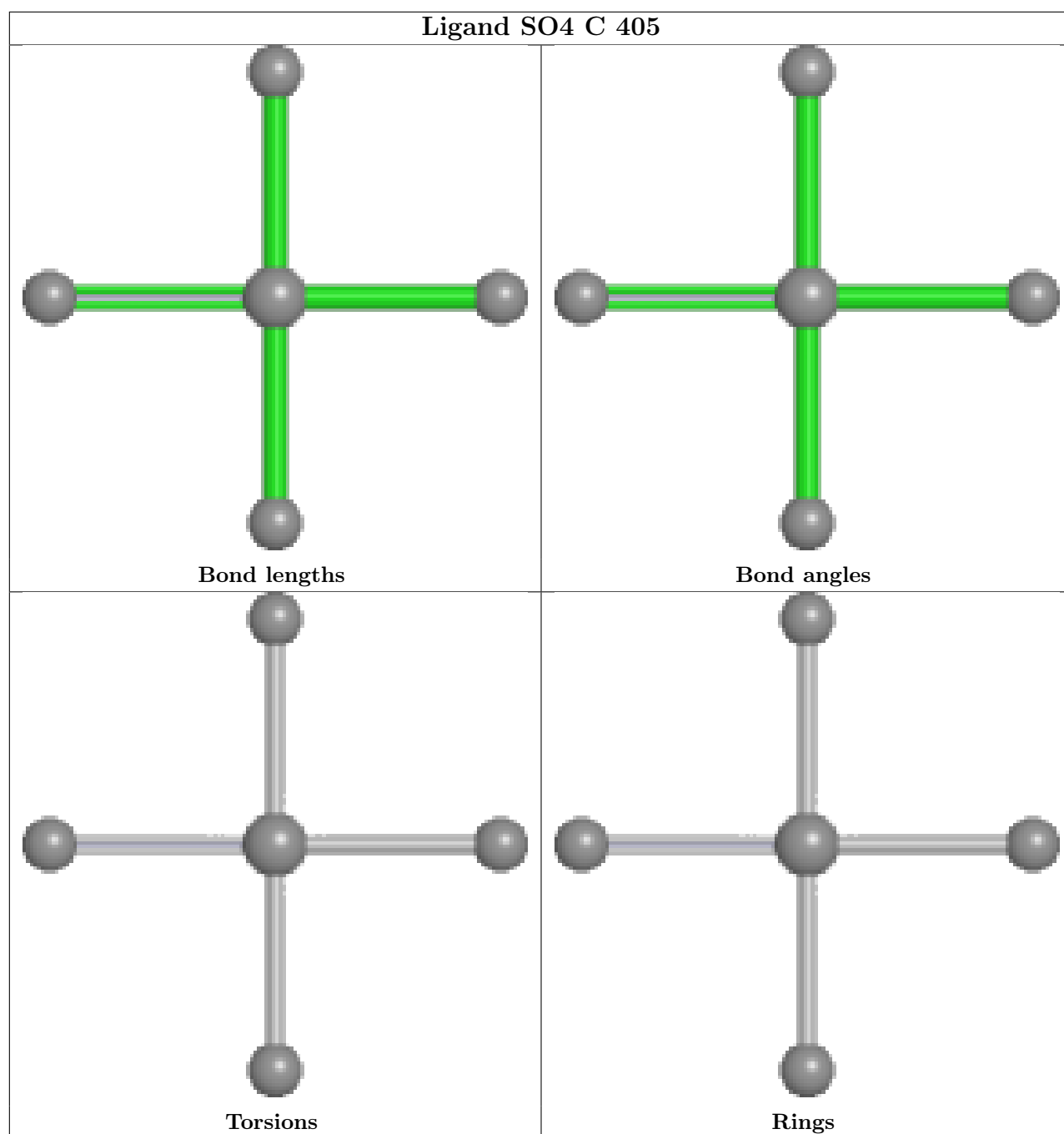


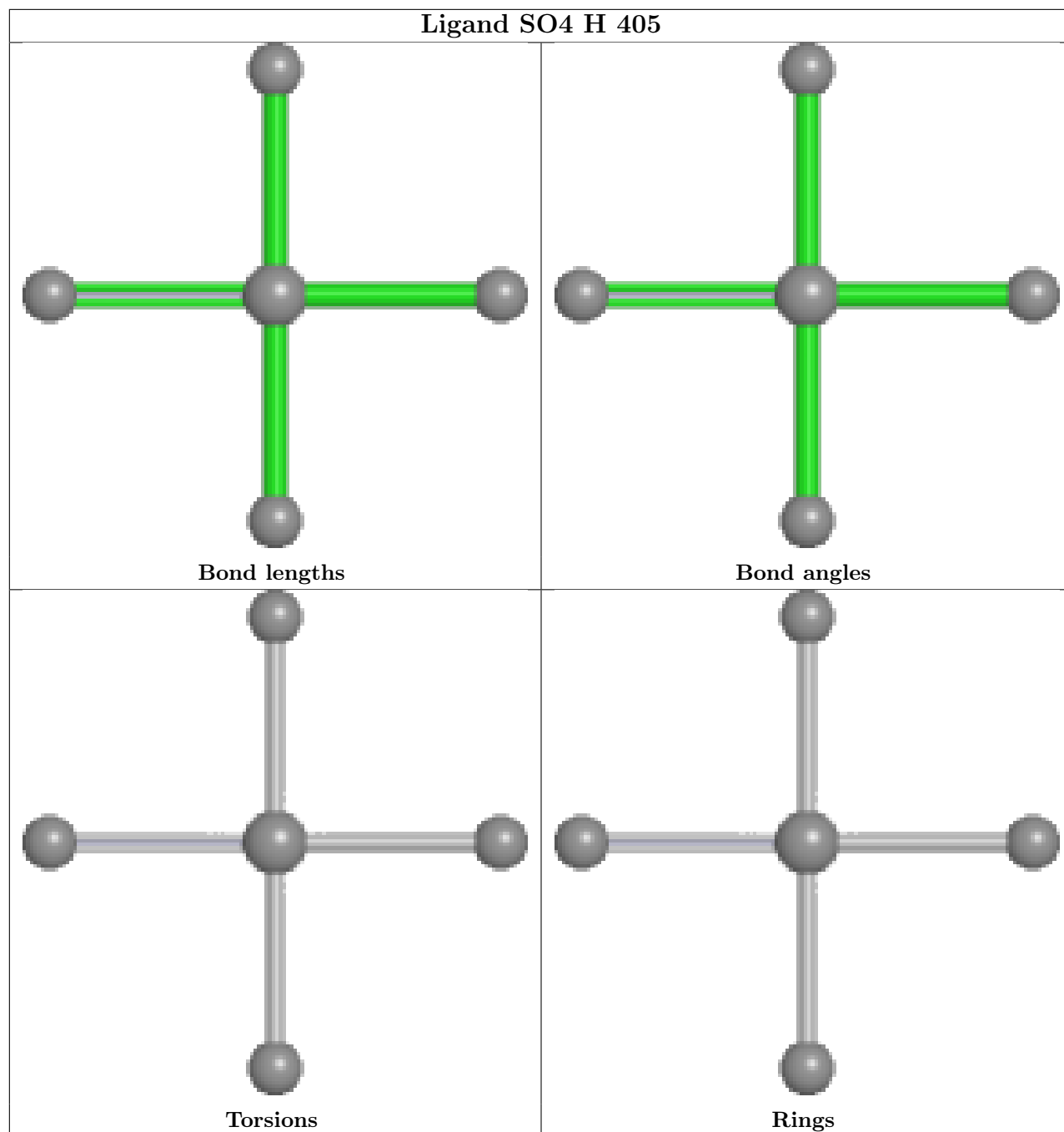


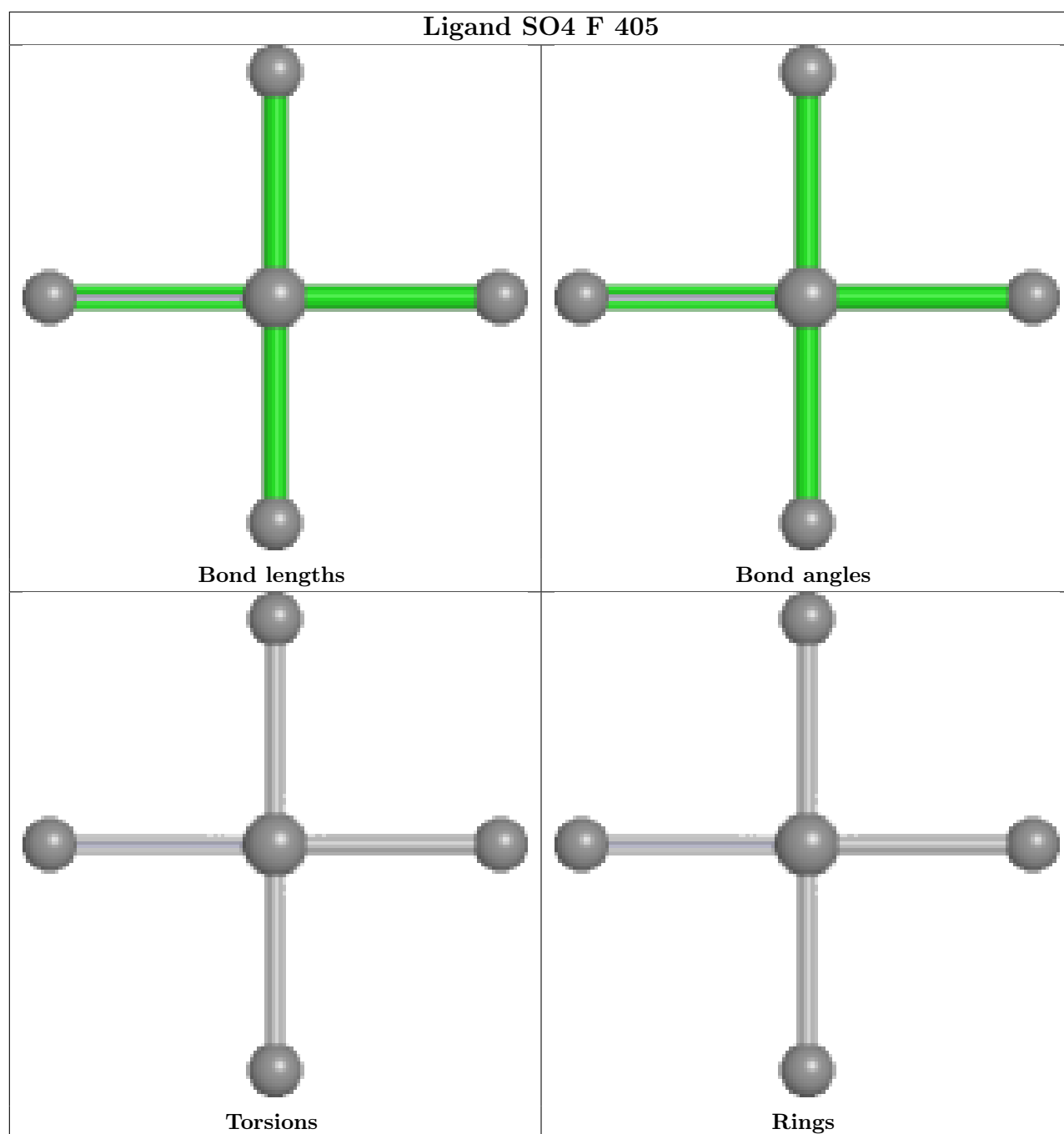


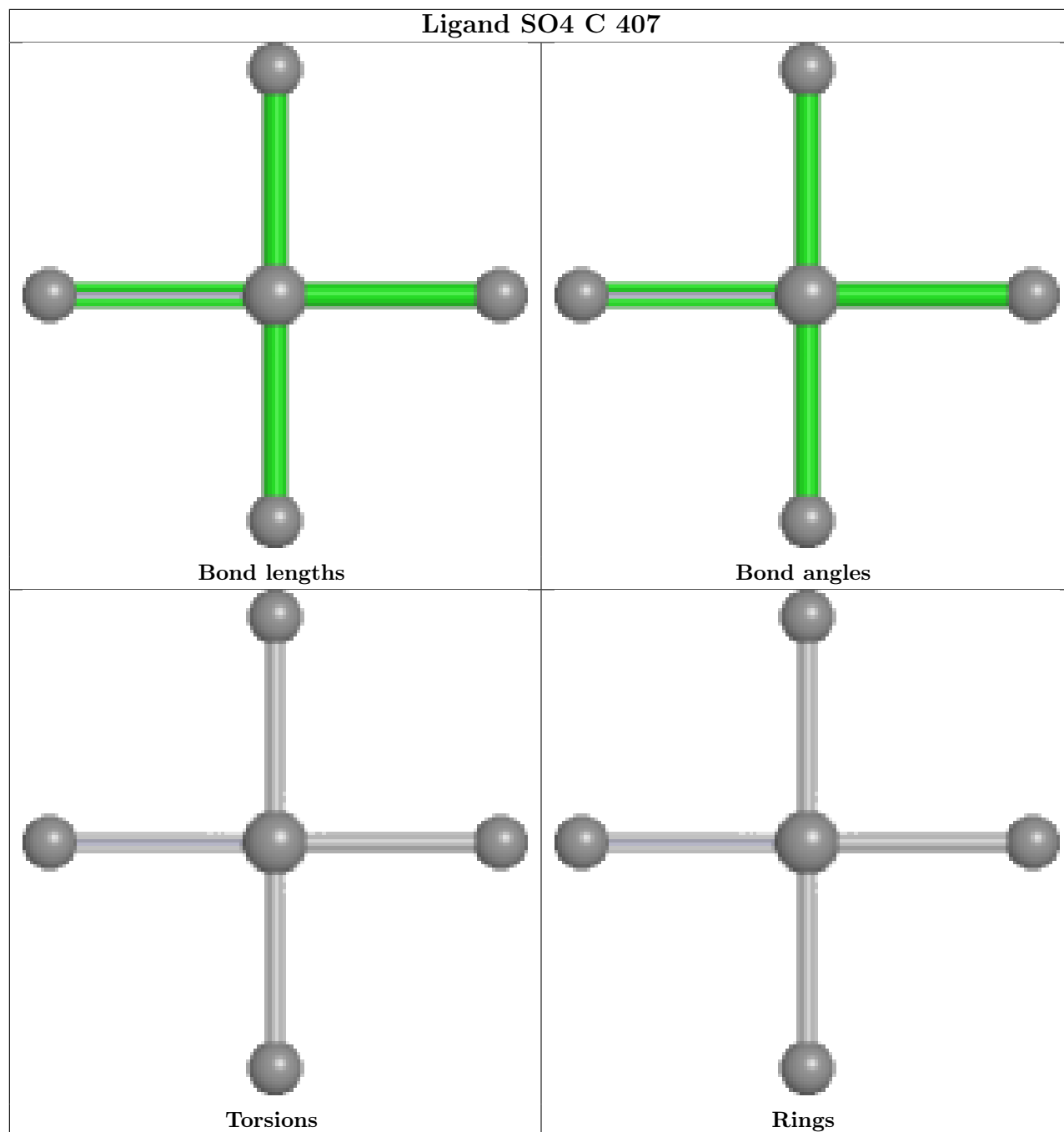


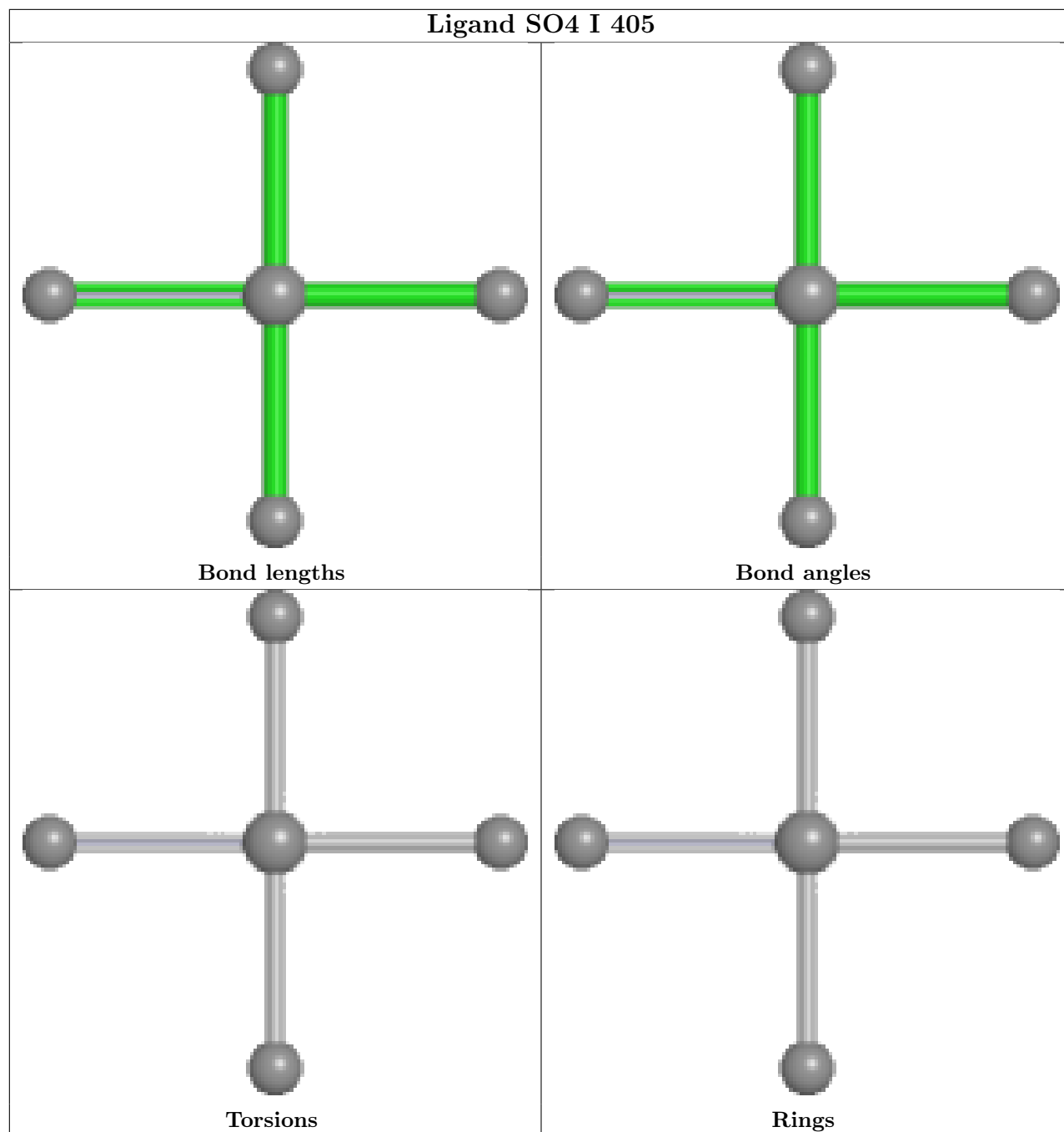


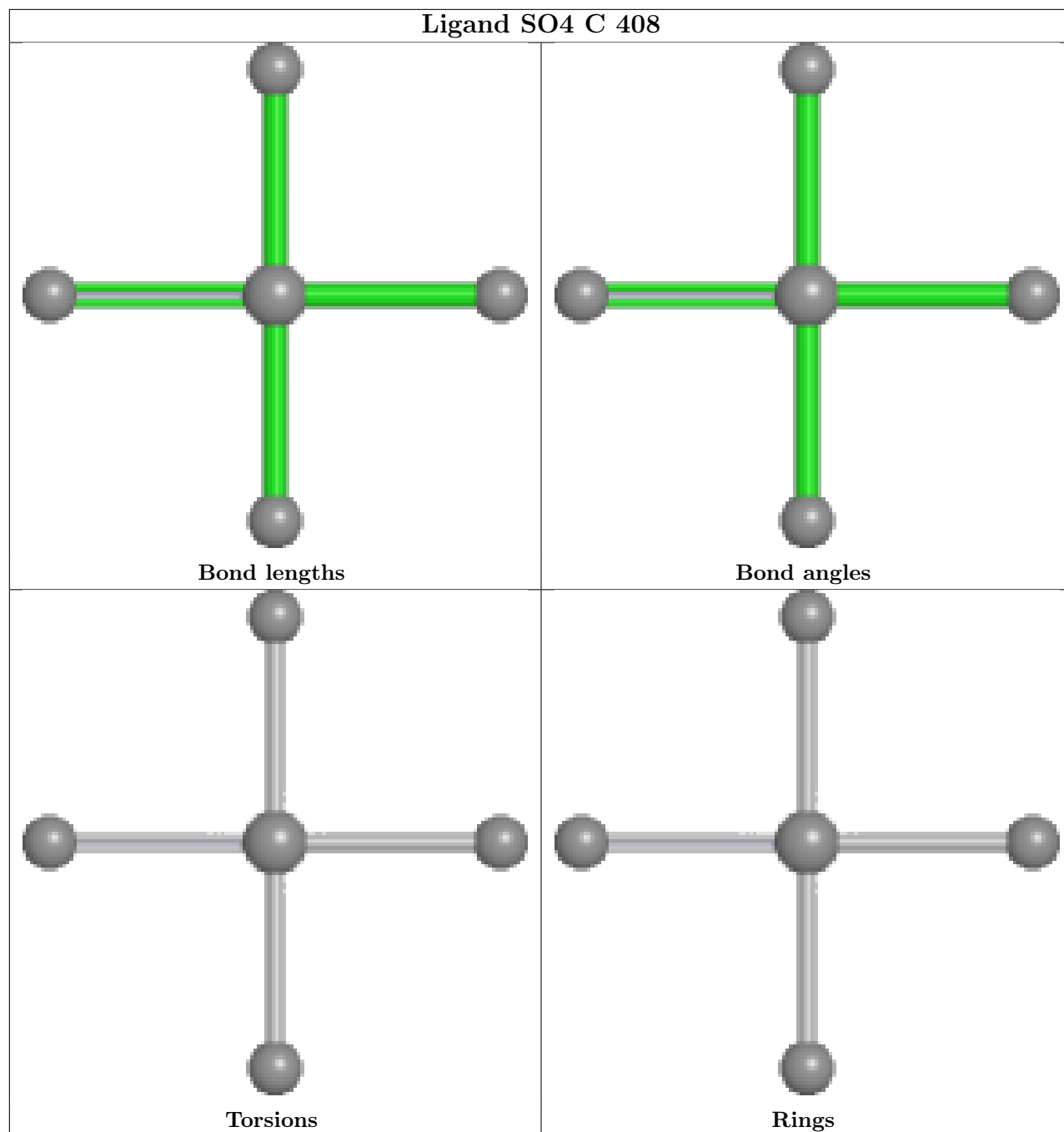


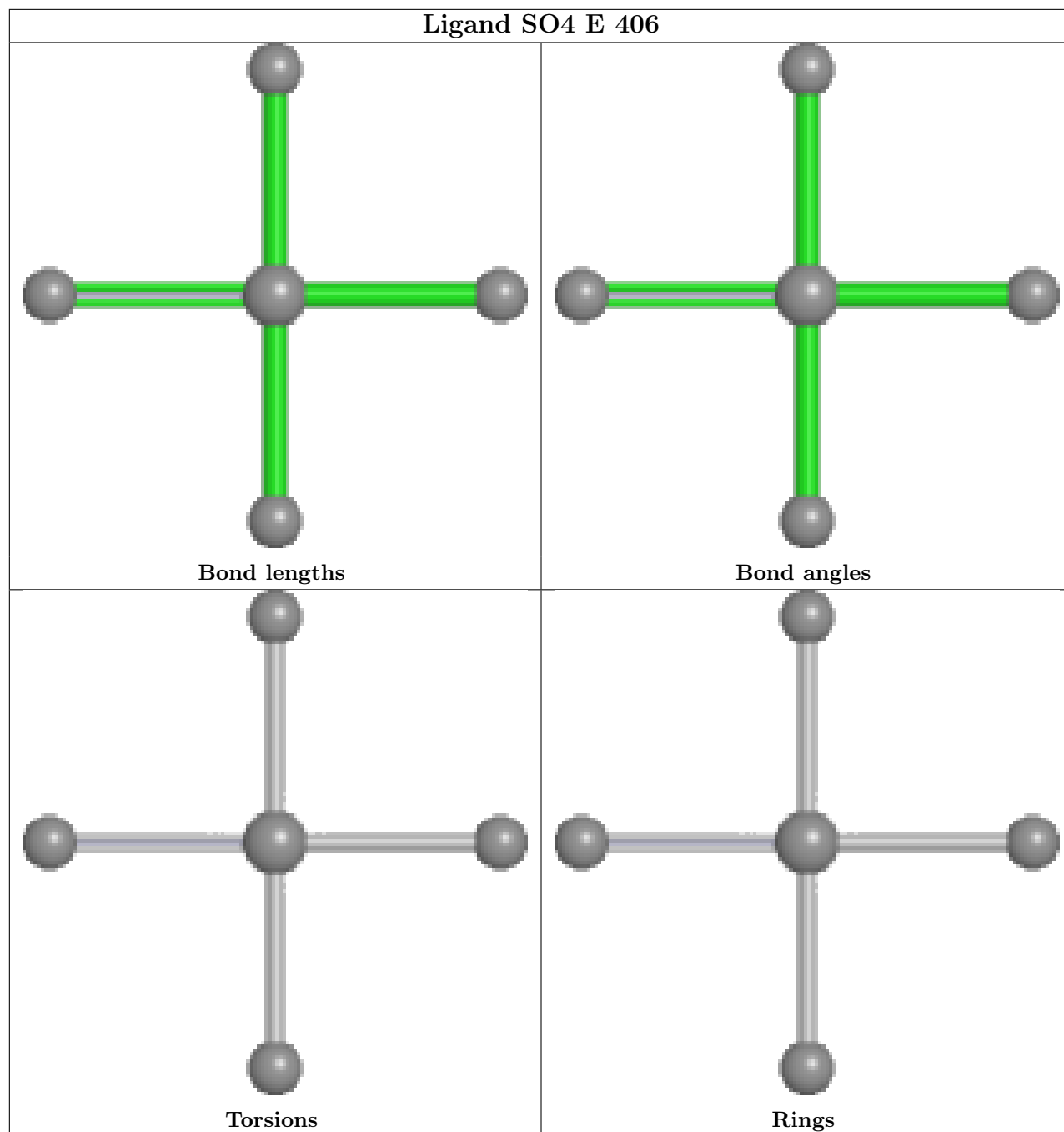


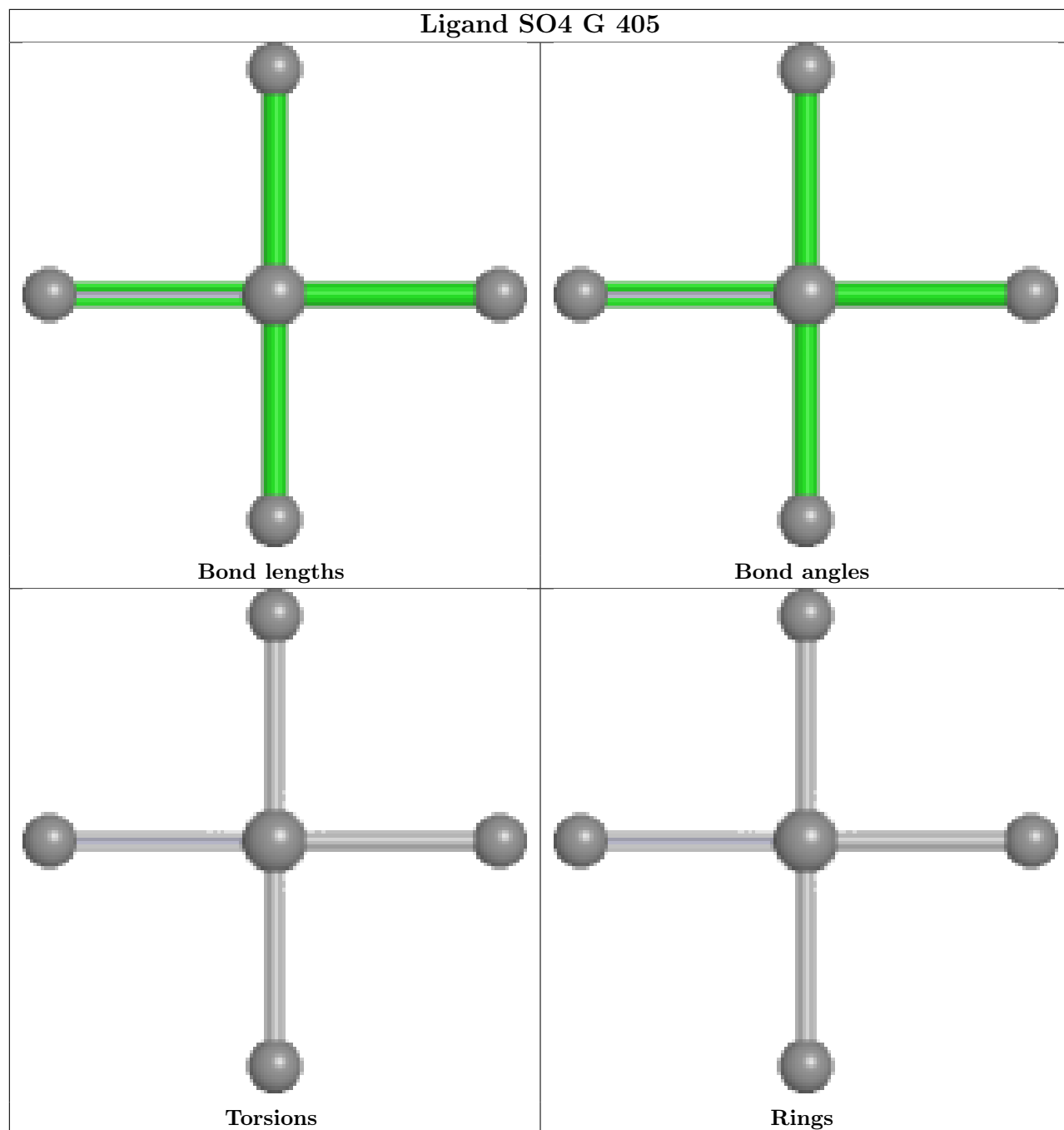


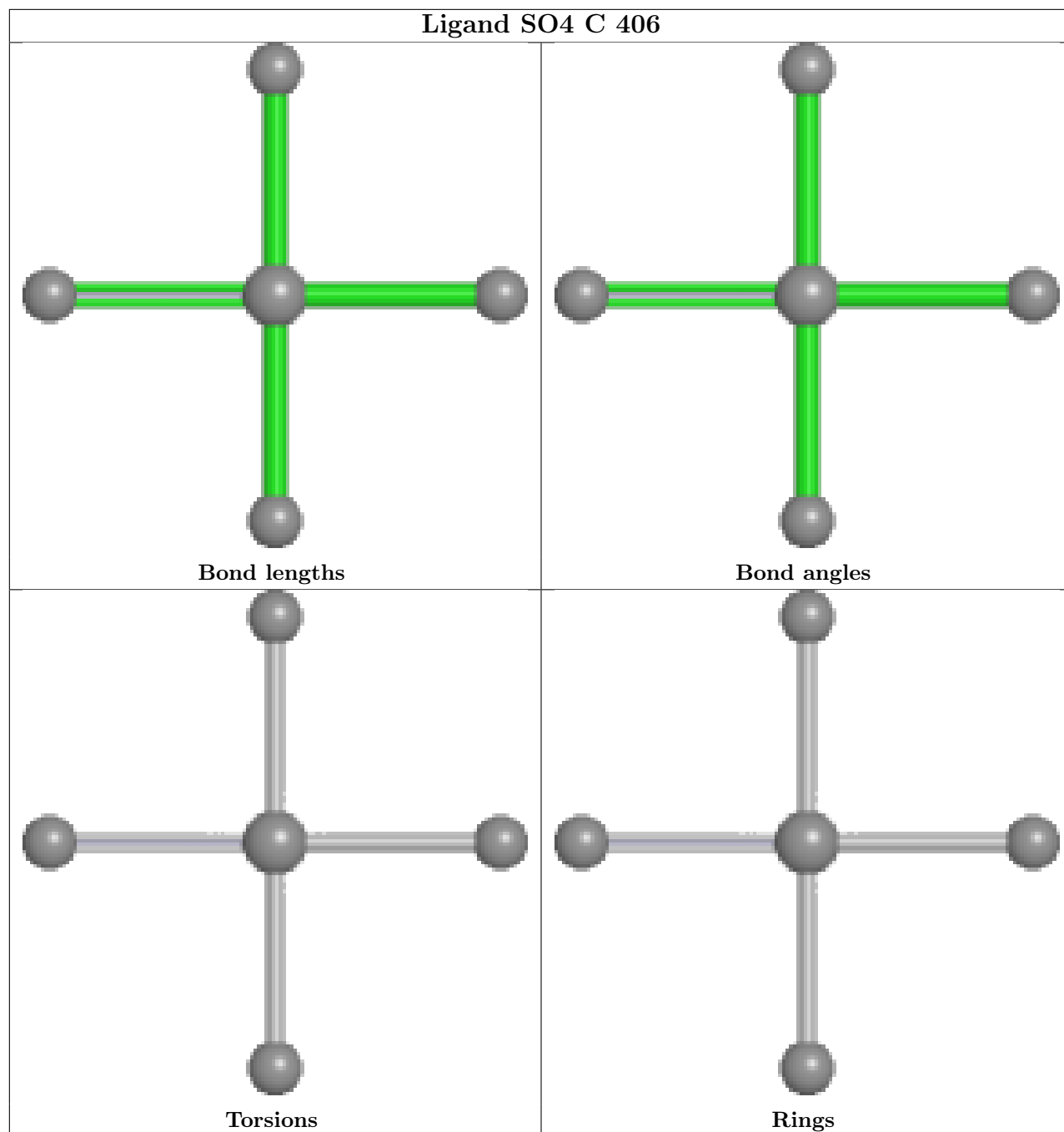


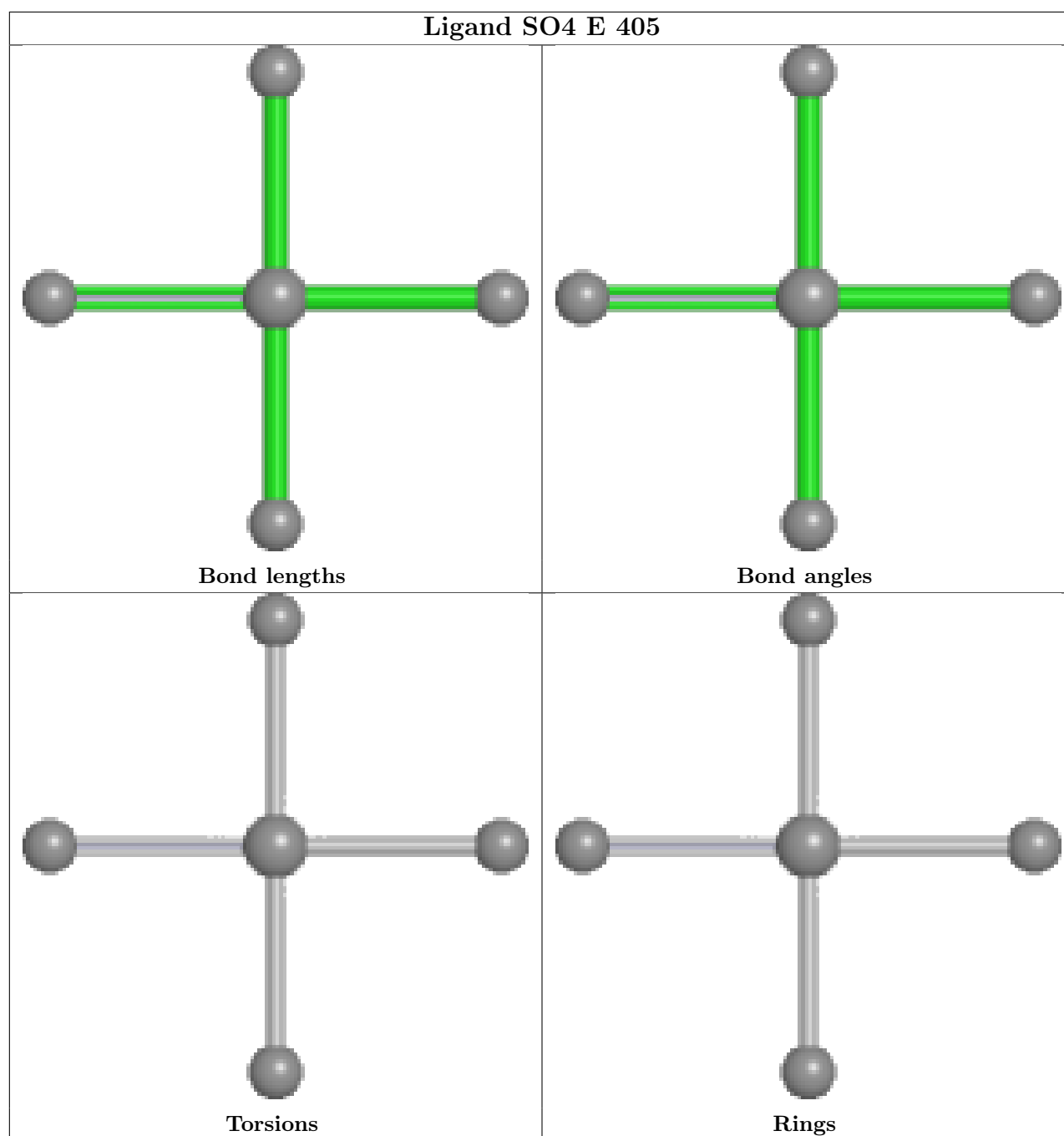












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	287/307 (93%)	-0.35	5 (1%) 69 60	40, 54, 107, 195	0
1	B	290/307 (94%)	-0.29	0 100 100	41, 58, 107, 152	0
1	C	289/307 (94%)	-0.22	5 (1%) 69 60	38, 61, 106, 162	0
1	D	290/307 (94%)	-0.15	5 (1%) 69 60	42, 60, 112, 164	0
1	E	287/307 (93%)	0.03	8 (2%) 55 44	46, 68, 122, 163	0
1	F	289/307 (94%)	0.04	4 (1%) 73 64	46, 66, 125, 167	0
1	G	287/307 (93%)	0.22	6 (2%) 63 54	50, 77, 128, 165	0
1	H	289/307 (94%)	0.04	5 (1%) 69 60	47, 66, 131, 211	0
1	I	290/307 (94%)	-0.15	3 (1%) 79 72	44, 64, 115, 158	0
All	All	2598/2763 (94%)	-0.09	41 (1%) 70 61	38, 64, 122, 211	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	92	LEU	5.1
1	A	96	TYR	4.4
1	D	259	VAL	4.1
1	A	92	LEU	4.0
1	H	96	TYR	3.8
1	E	261	THR	3.6
1	F	259	VAL	3.2
1	I	259	VAL	3.1
1	A	259	VAL	3.0
1	C	96	TYR	2.9
1	F	89	LYS	2.9
1	H	259	VAL	2.9
1	A	258	SER	2.7
1	H	260	ASP	2.7
1	E	259	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	258	SER	2.6
1	E	115	ARG	2.6
1	G	92	LEU	2.6
1	E	114	ALA	2.6
1	C	261	THR	2.6
1	G	375	MET	2.5
1	G	259	VAL	2.5
1	A	93	GLU	2.5
1	C	92	LEU	2.4
1	D	260	ASP	2.4
1	D	347	GLN	2.4
1	G	260	ASP	2.4
1	E	332	LEU	2.4
1	G	264	GLY	2.3
1	G	332	LEU	2.3
1	F	331	SER	2.3
1	C	259	VAL	2.2
1	F	299	MET	2.2
1	E	260	ASP	2.2
1	D	375	MET	2.2
1	E	265	GLN	2.1
1	C	263	ASN	2.1
1	I	89	LYS	2.1
1	D	264	GLY	2.1
1	I	86	SER	2.1
1	H	265	GLN	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 [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($\text{\AA}^2$)	Q<0.9
4	SO4	I	407	5/5	0.57	0.14	142,165,185,193	0
4	SO4	C	408	5/5	0.65	0.09	145,150,156,157	0
4	SO4	C	407	5/5	0.68	0.13	141,141,158,164	0
4	SO4	H	406	5/5	0.87	0.14	97,100,109,124	0
4	SO4	C	406	5/5	0.88	0.12	92,94,106,108	0
4	SO4	D	406	5/5	0.89	0.12	114,115,130,133	0
4	SO4	D	407	5/5	0.89	0.14	91,123,132,144	0
4	SO4	I	406	5/5	0.90	0.16	101,102,112,121	0
4	SO4	B	406	5/5	0.90	0.14	86,91,120,130	0
4	SO4	E	406	5/5	0.91	0.14	97,101,110,110	0
4	SO4	F	405	5/5	0.92	0.14	79,95,104,113	0
4	SO4	I	405	5/5	0.93	0.08	60,65,73,81	0
4	SO4	G	405	5/5	0.93	0.15	99,101,105,113	0
4	SO4	E	405	5/5	0.93	0.09	84,96,106,117	0
4	SO4	D	405	5/5	0.94	0.14	83,87,88,97	0
4	SO4	H	405	5/5	0.94	0.07	90,96,106,113	0
4	SO4	B	405	5/5	0.94	0.12	72,85,88,114	0
4	SO4	C	405	5/5	0.95	0.13	77,85,89,103	0
4	SO4	A	406	5/5	0.95	0.10	73,86,89,100	0
3	MG	H	404	1/1	0.96	0.10	67,67,67,67	0
4	SO4	A	405	5/5	0.97	0.07	47,52,65,78	0
3	MG	D	404	1/1	0.97	0.09	73,73,73,73	0
3	MG	G	404	1/1	0.98	0.08	80,80,80,80	0
3	MG	B	404	1/1	0.98	0.09	64,64,64,64	0
2	CA	G	403	1/1	0.99	0.05	74,74,74,74	0
2	CA	H	401	1/1	0.99	0.05	62,62,62,62	0
2	CA	I	402	1/1	0.99	0.05	51,51,51,51	0
3	MG	A	404	1/1	0.99	0.11	57,57,57,57	0
2	CA	A	401	1/1	0.99	0.03	54,54,54,54	0
3	MG	C	404	1/1	0.99	0.06	50,50,50,50	0
2	CA	D	401	1/1	0.99	0.04	56,56,56,56	0
3	MG	E	404	1/1	0.99	0.10	67,67,67,67	0
3	MG	F	404	1/1	0.99	0.07	60,60,60,60	0
2	CA	E	401	1/1	0.99	0.03	63,63,63,63	0
2	CA	E	403	1/1	0.99	0.05	62,62,62,62	0
3	MG	I	404	1/1	0.99	0.11	64,64,64,64	0
2	CA	F	401	1/1	0.99	0.05	54,54,54,54	0
2	CA	F	402	1/1	0.99	0.07	59,59,59,59	0
2	CA	G	401	1/1	0.99	0.05	70,70,70,70	0
2	CA	G	402	1/1	0.99	0.08	74,74,74,74	0
2	CA	I	401	1/1	1.00	0.03	61,61,61,61	0
2	CA	D	402	1/1	1.00	0.05	58,58,58,58	0
2	CA	I	403	1/1	1.00	0.03	52,52,52,52	0

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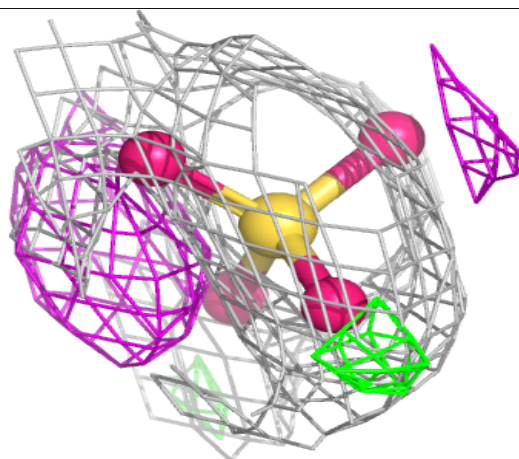
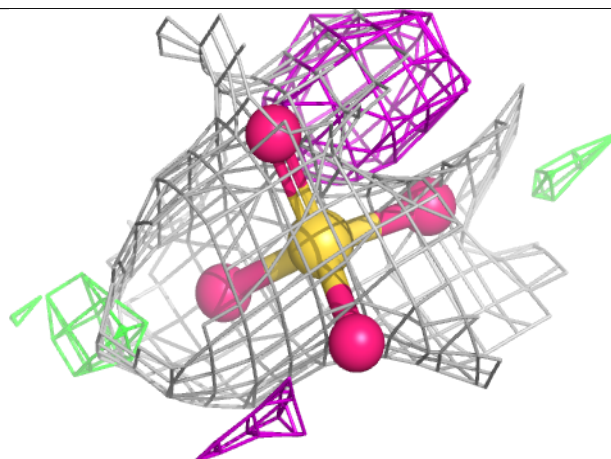
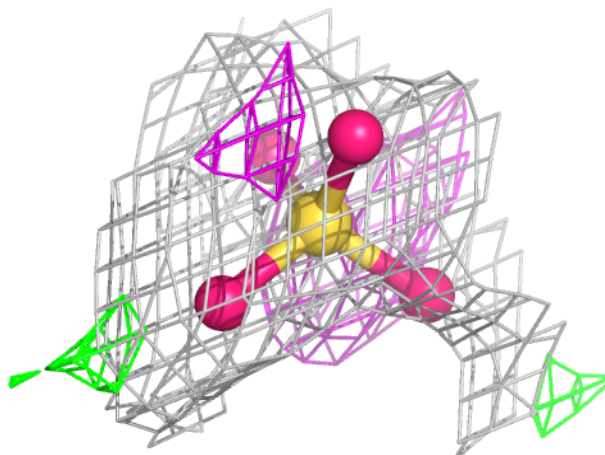
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	D	403	1/1	1.00	0.02	49,49,49,49	0
2	CA	A	403	1/1	1.00	0.04	48,48,48,48	0
2	CA	E	402	1/1	1.00	0.04	64,64,64,64	0
2	CA	B	401	1/1	1.00	0.05	49,49,49,49	0
2	CA	B	402	1/1	1.00	0.05	56,56,56,56	0
2	CA	B	403	1/1	1.00	0.03	52,52,52,52	0
2	CA	F	403	1/1	1.00	0.04	58,58,58,58	0
2	CA	C	401	1/1	1.00	0.03	52,52,52,52	0
2	CA	C	402	1/1	1.00	0.06	54,54,54,54	0
2	CA	C	403	1/1	1.00	0.06	55,55,55,55	0
2	CA	A	402	1/1	1.00	0.03	47,47,47,47	0
2	CA	H	402	1/1	1.00	0.06	60,60,60,60	0
2	CA	H	403	1/1	1.00	0.02	60,60,60,60	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.

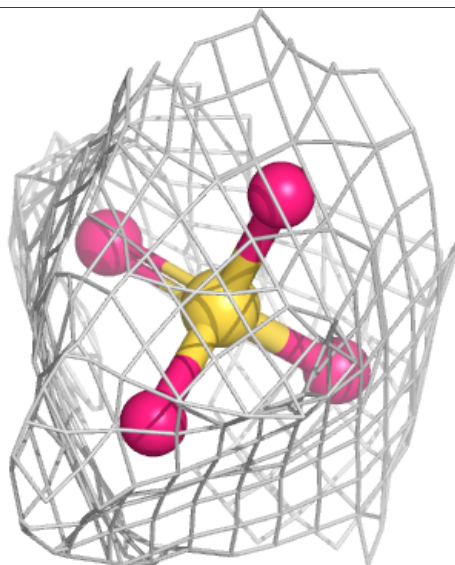
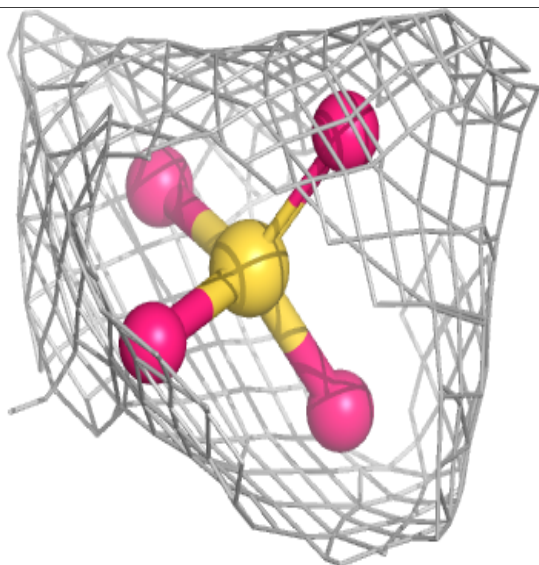
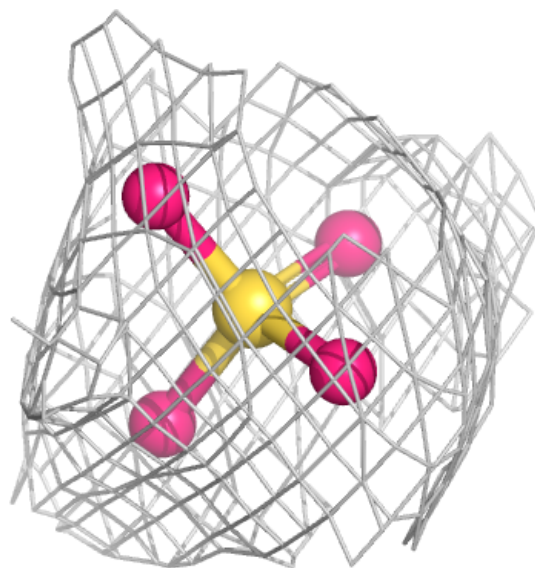
Electron density around SO4 I 407:

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



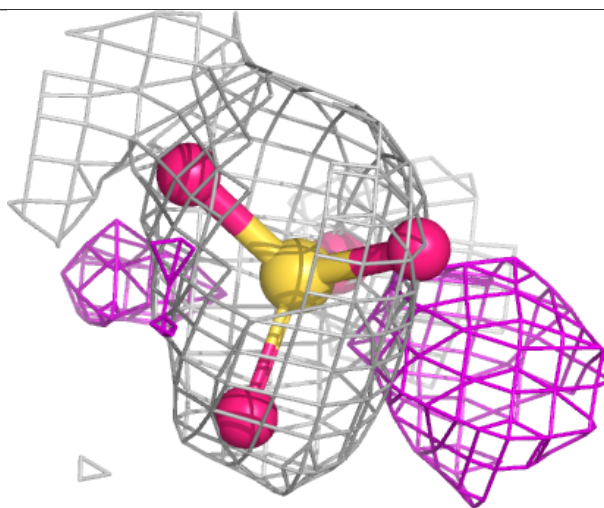
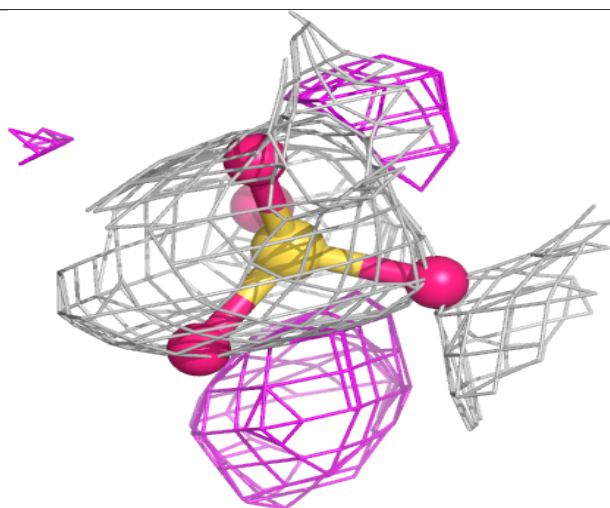
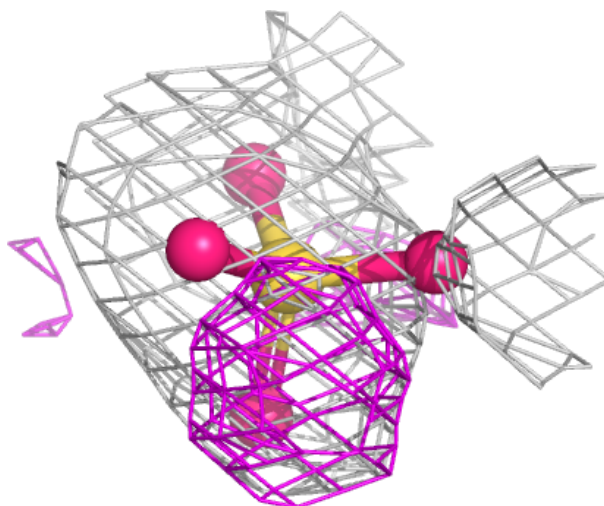
Electron density around SO4 C 408:

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



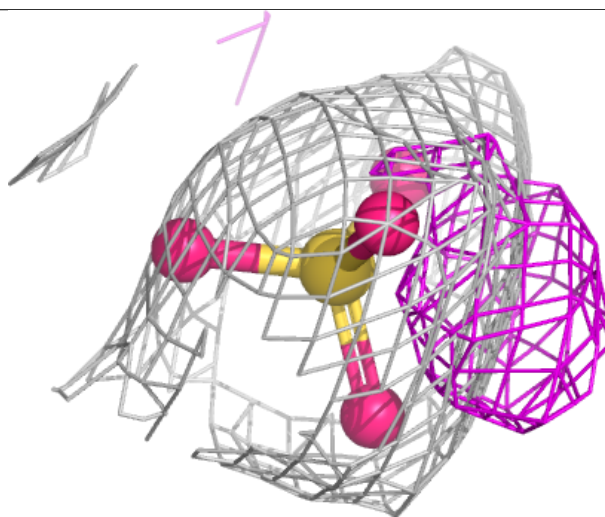
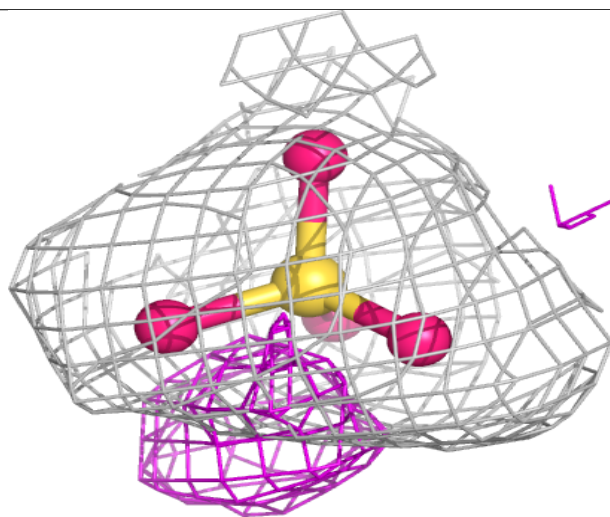
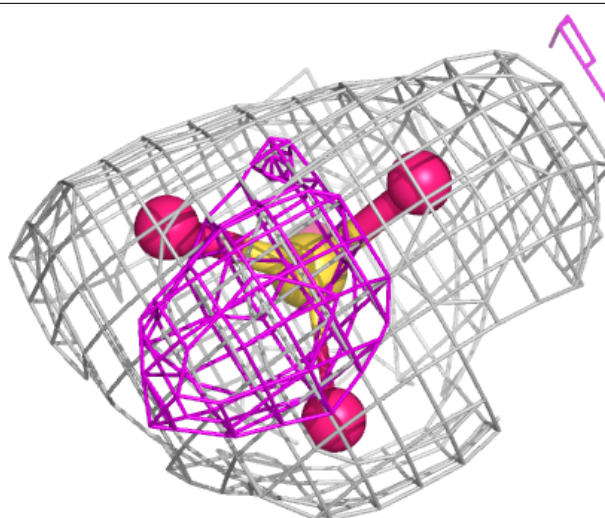
Electron density around SO4 C 407:

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



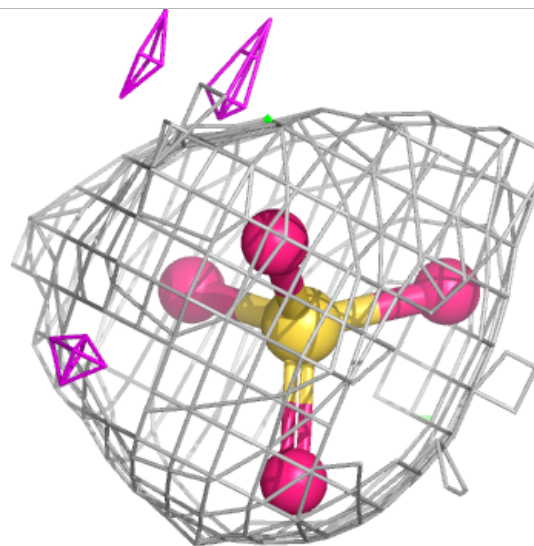
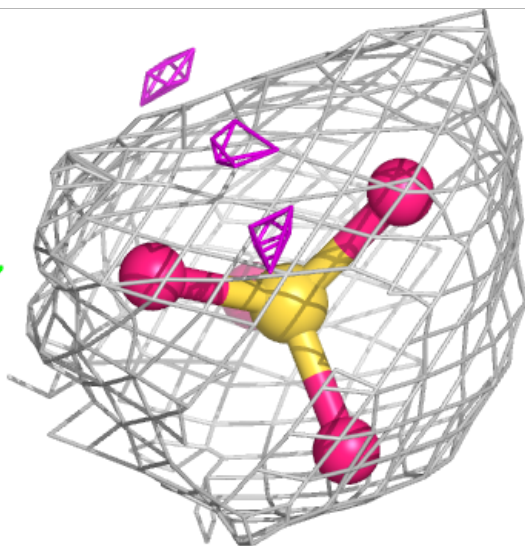
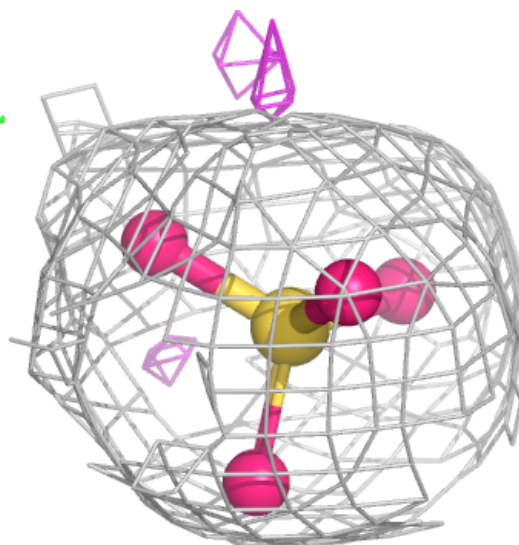
Electron density around SO4 H 406:

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



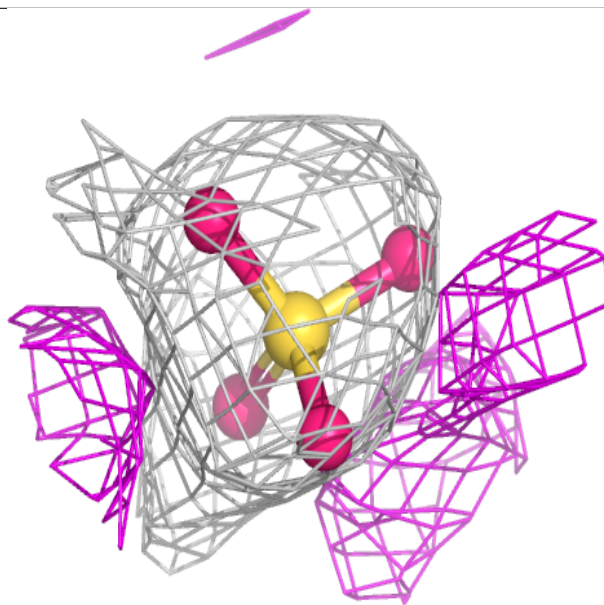
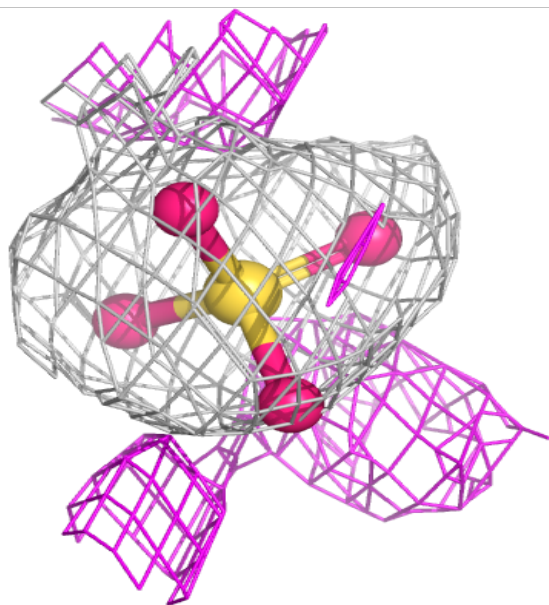
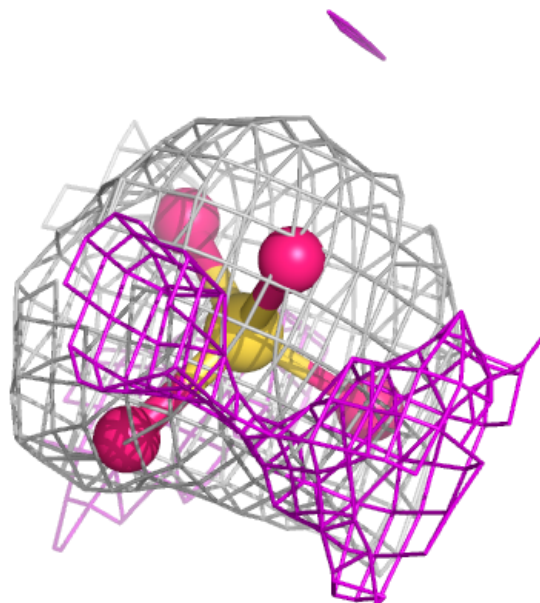
Electron density around SO4 C 406:

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



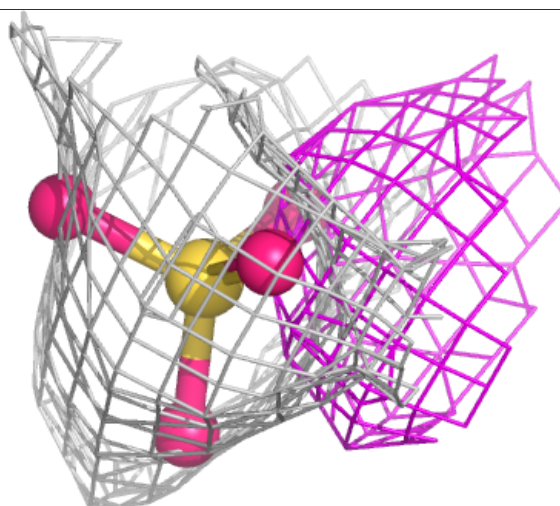
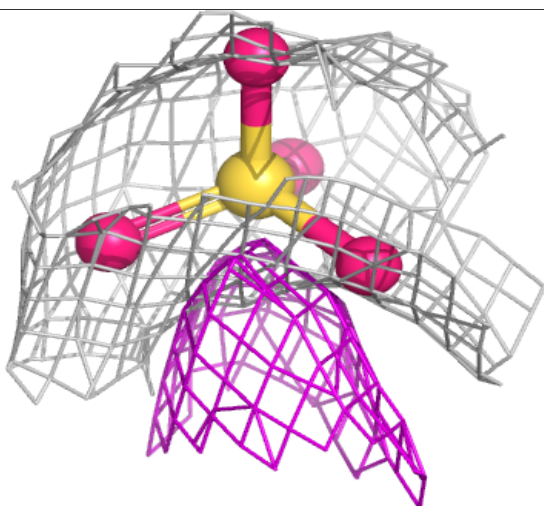
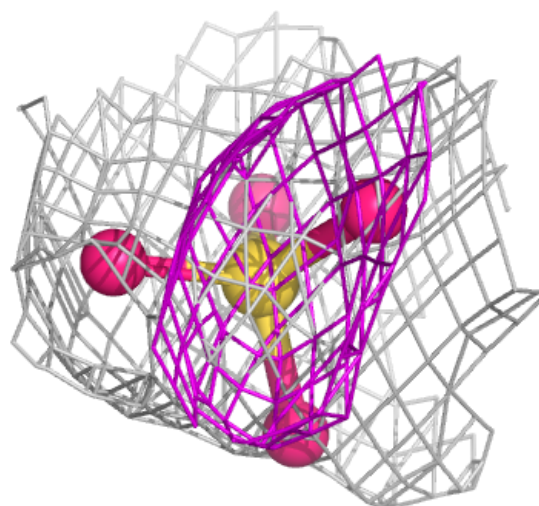
Electron density around SO4 D 406:

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



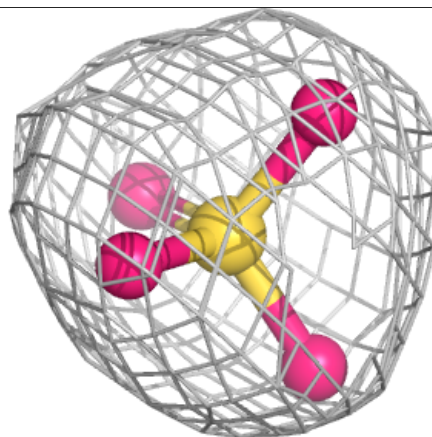
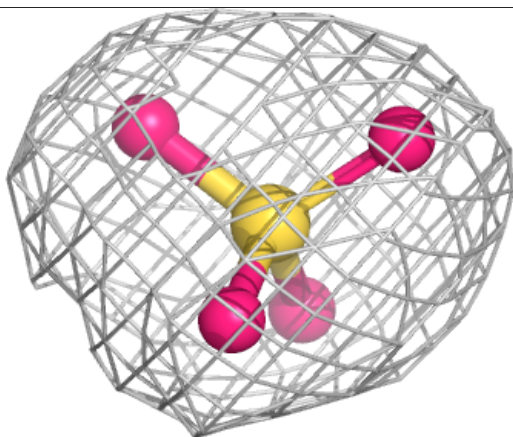
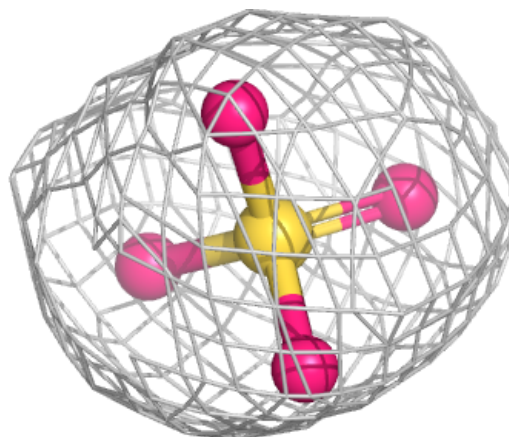
Electron density around SO4 D 407:

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



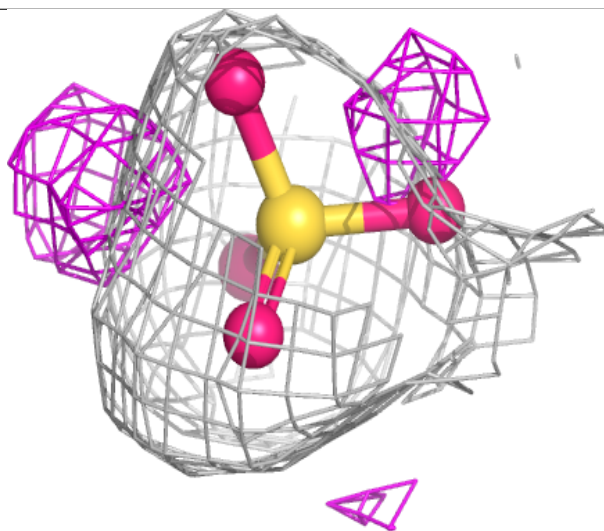
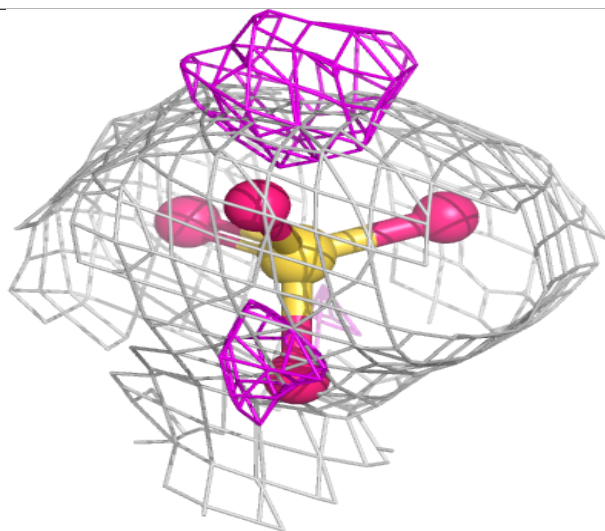
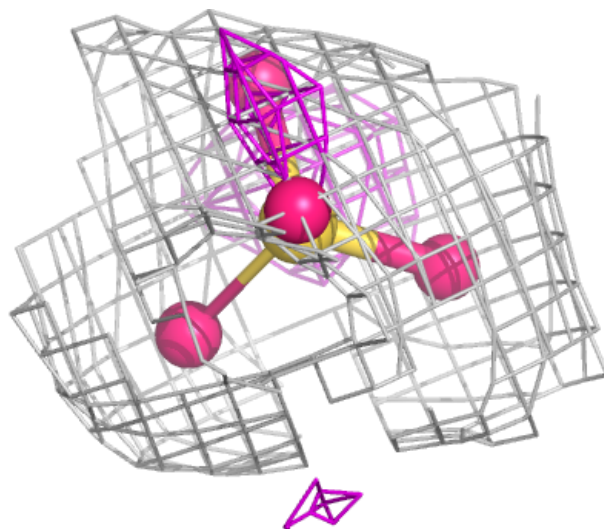
Electron density around SO4 I 406:

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



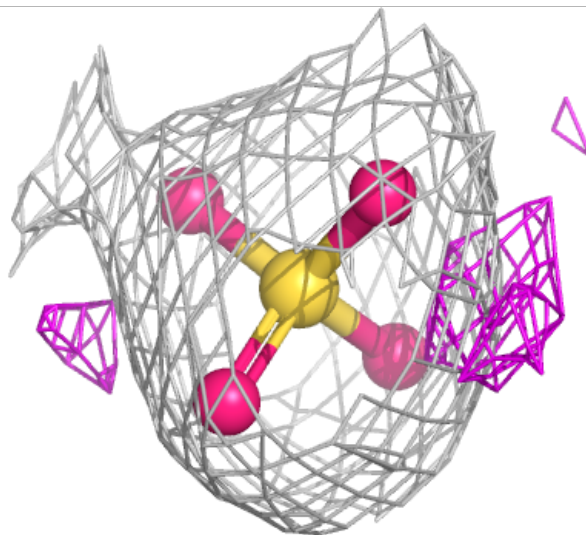
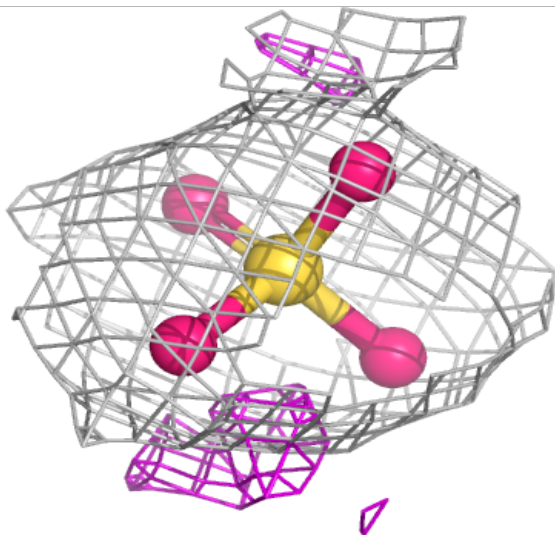
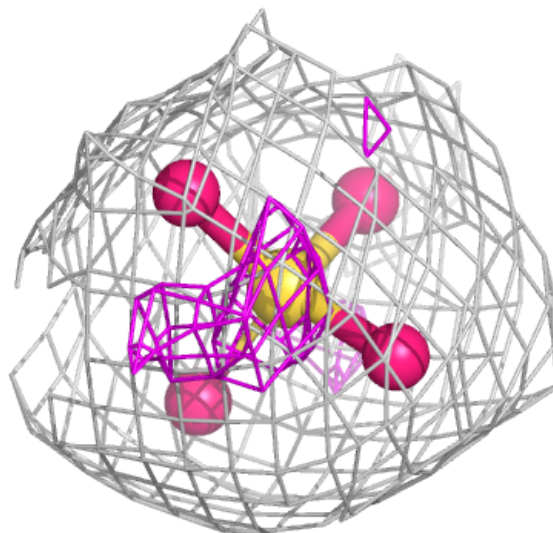
Electron density around SO4 B 406:

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



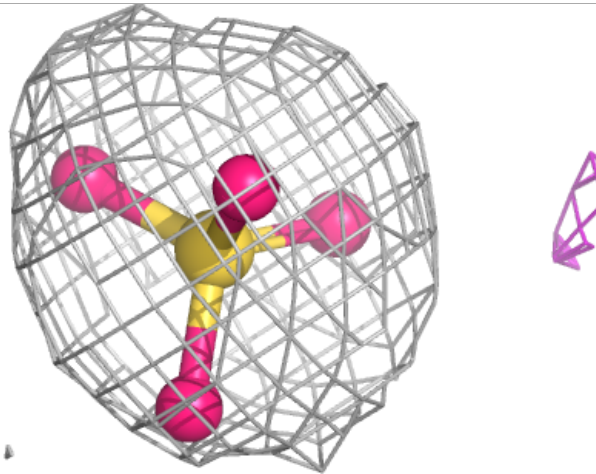
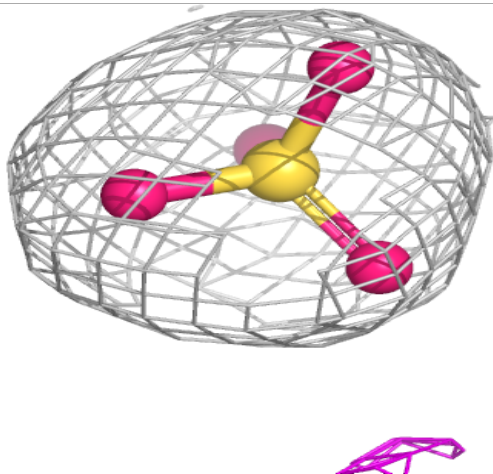
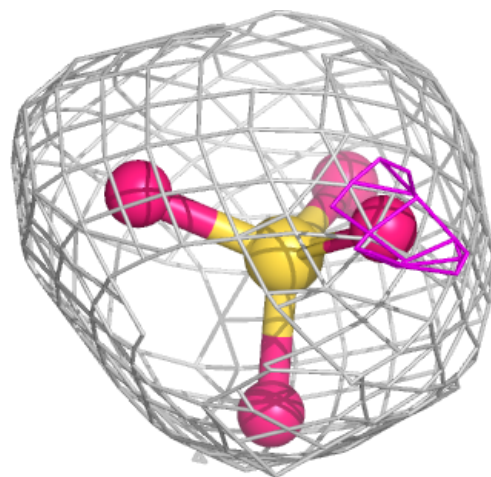
Electron density around SO4 E 406:

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



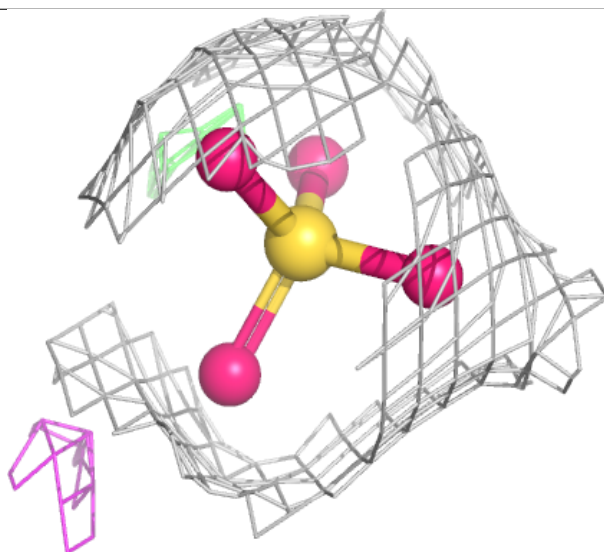
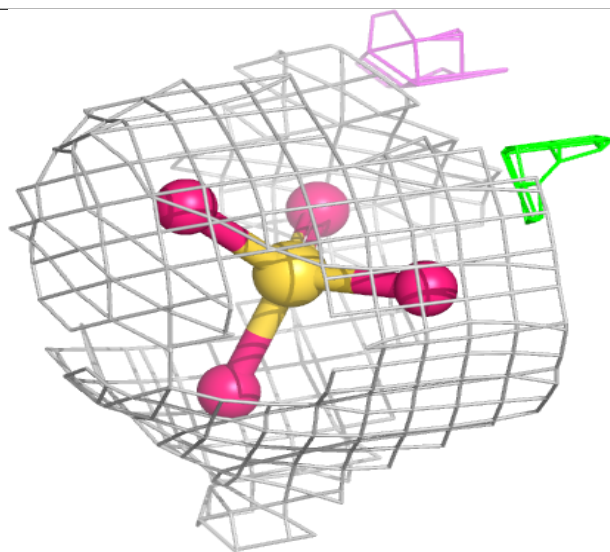
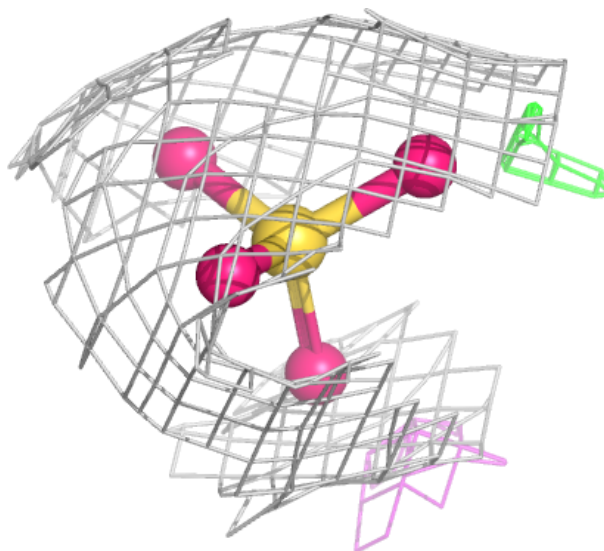
Electron density around SO4 F 405:

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



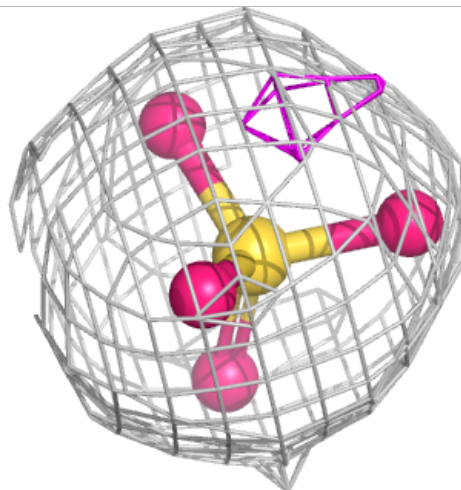
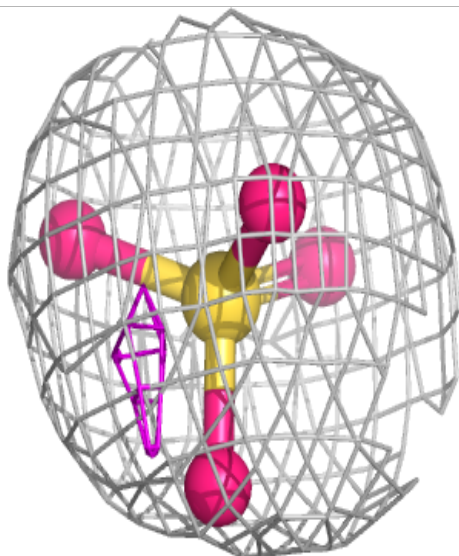
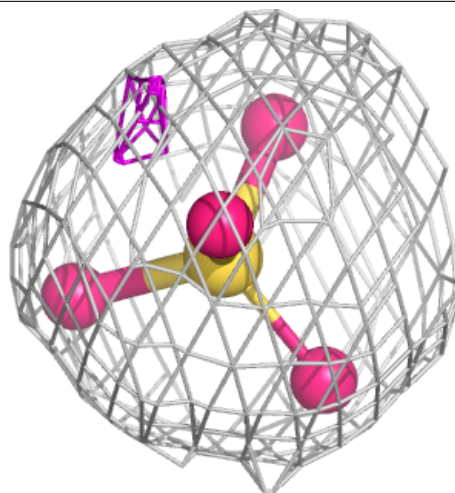
Electron density around SO4 I 405:

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



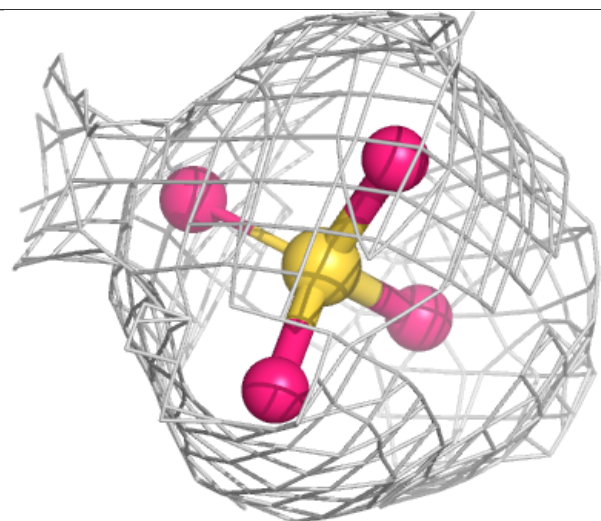
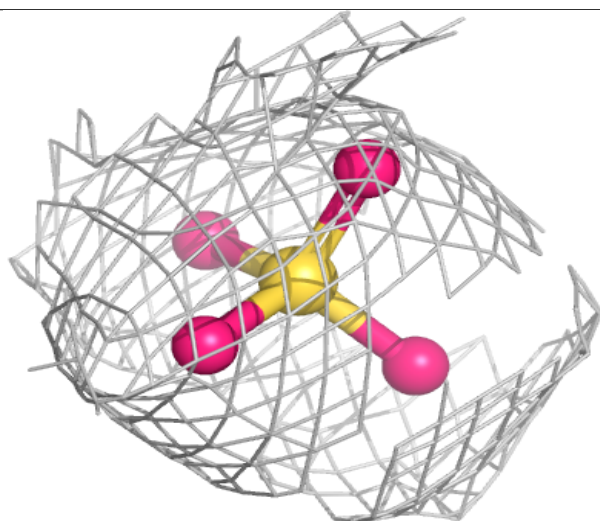
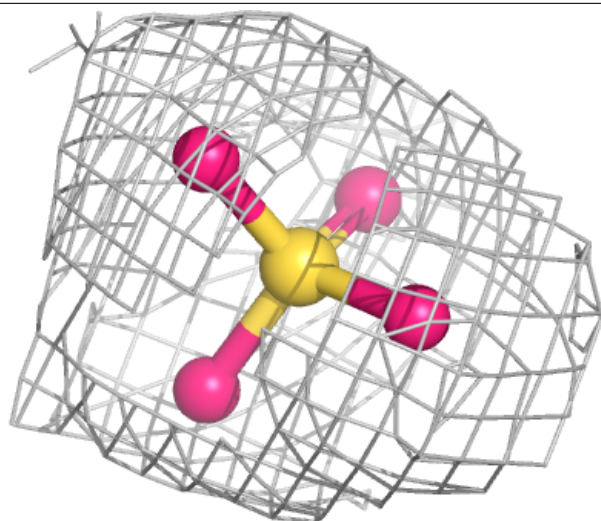
Electron density around SO4 G 405:

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



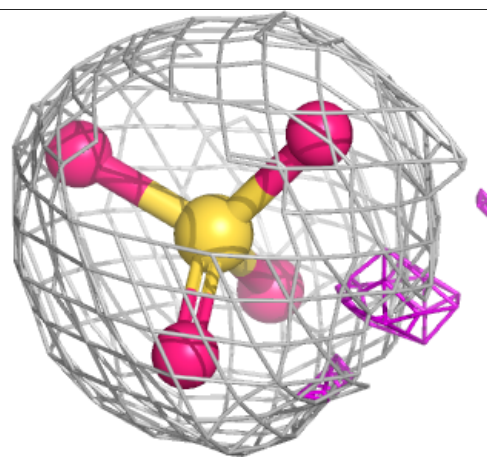
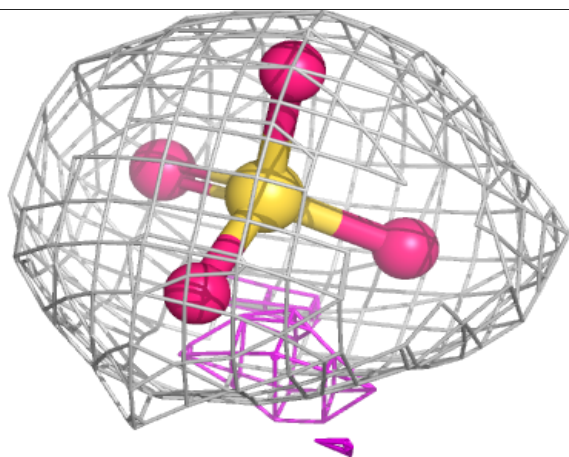
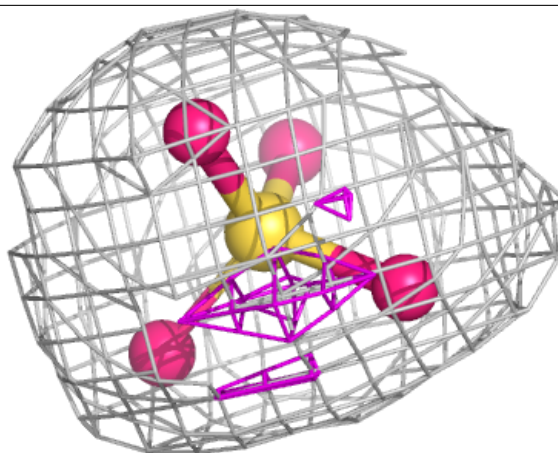
Electron density around SO4 E 405:

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



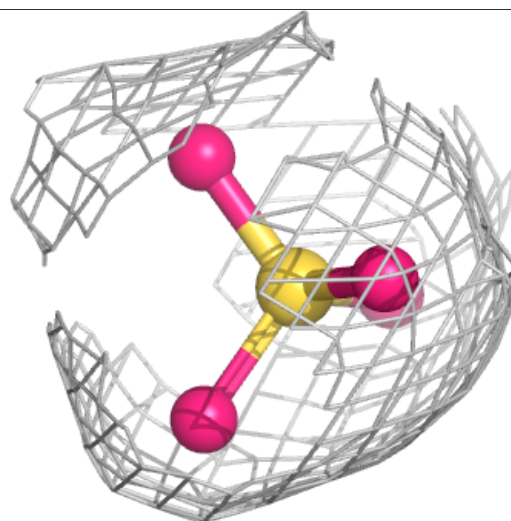
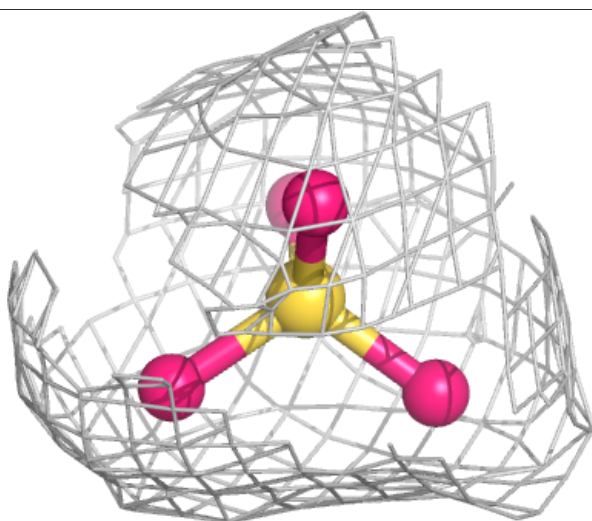
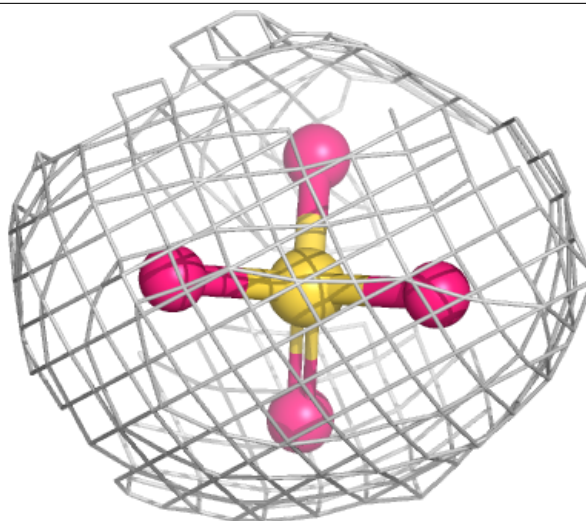
Electron density around SO4 D 405:

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



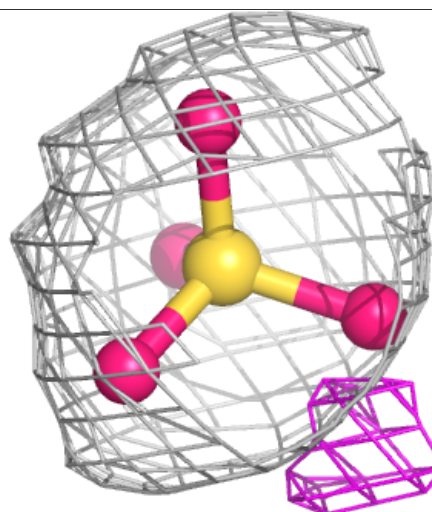
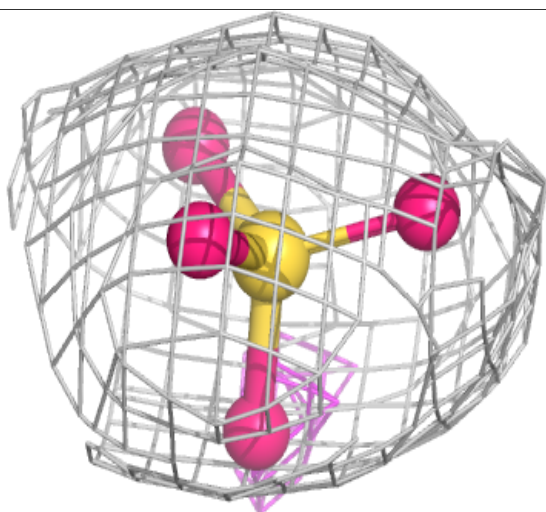
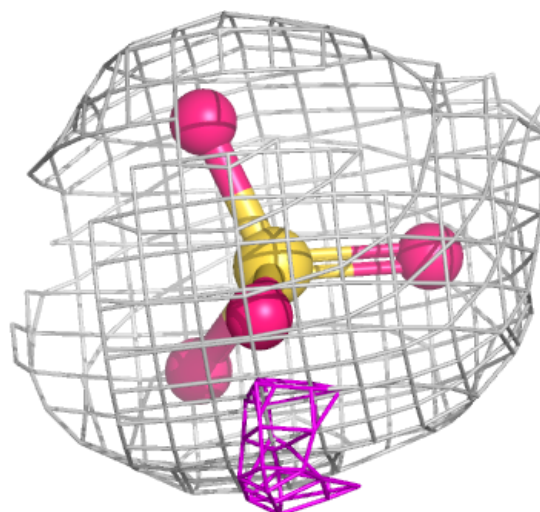
Electron density around SO4 H 405:

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



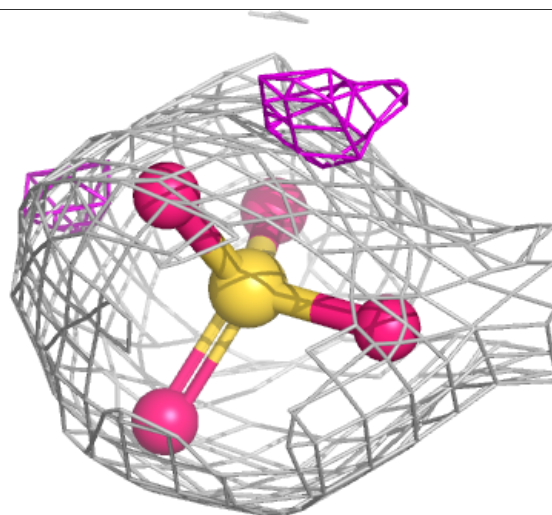
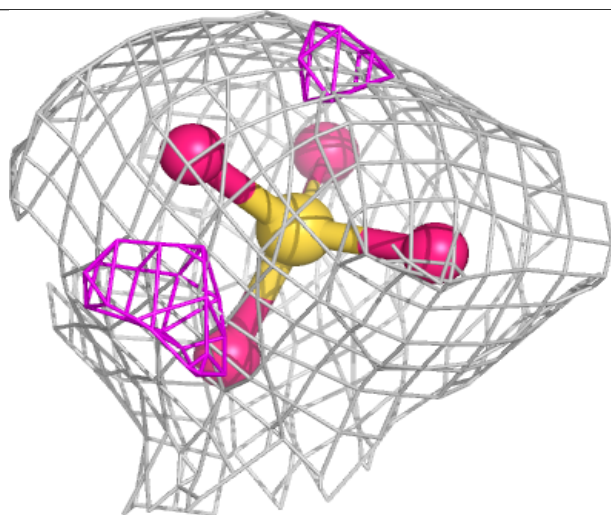
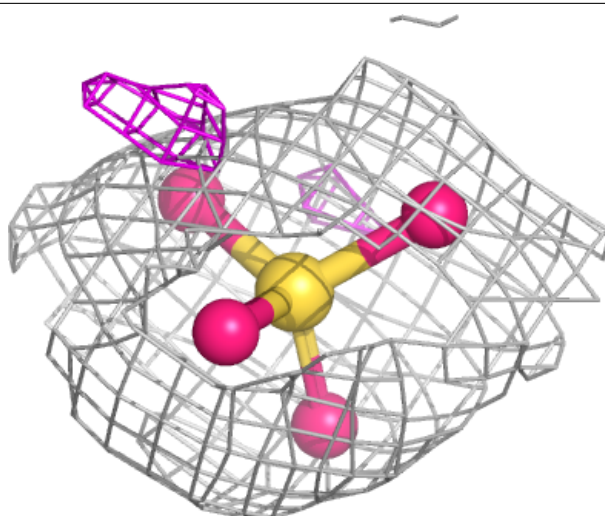
Electron density around SO4 B 405:

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



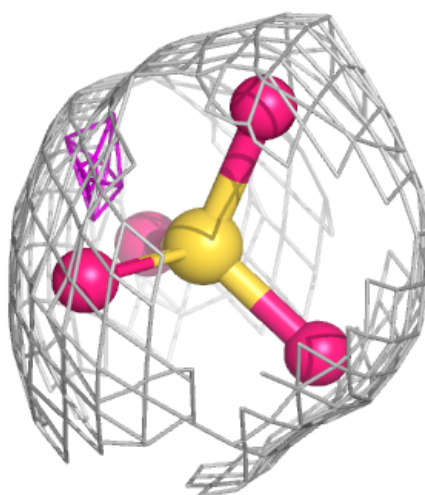
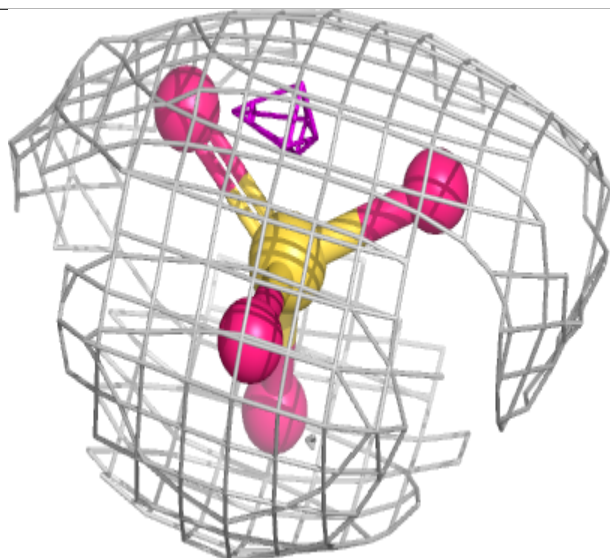
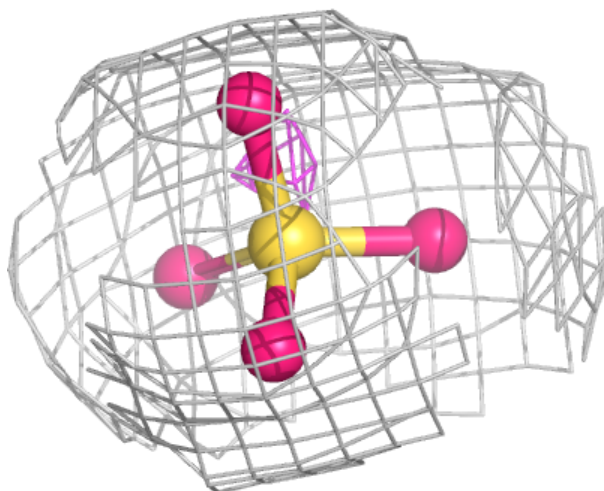
Electron density around SO4 C 405:

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



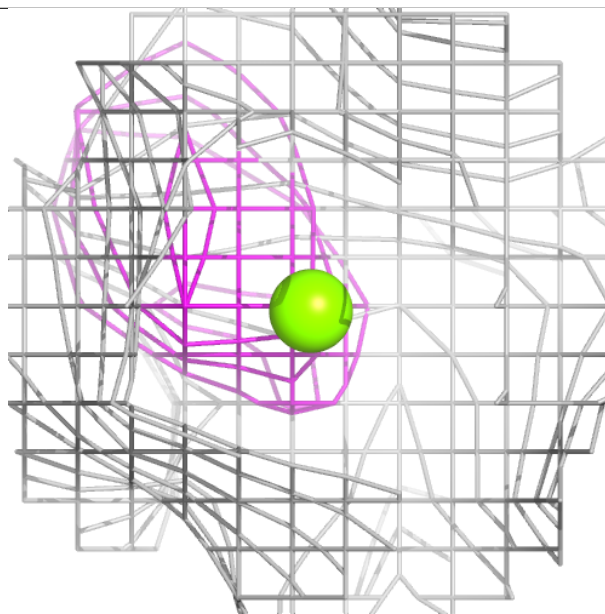
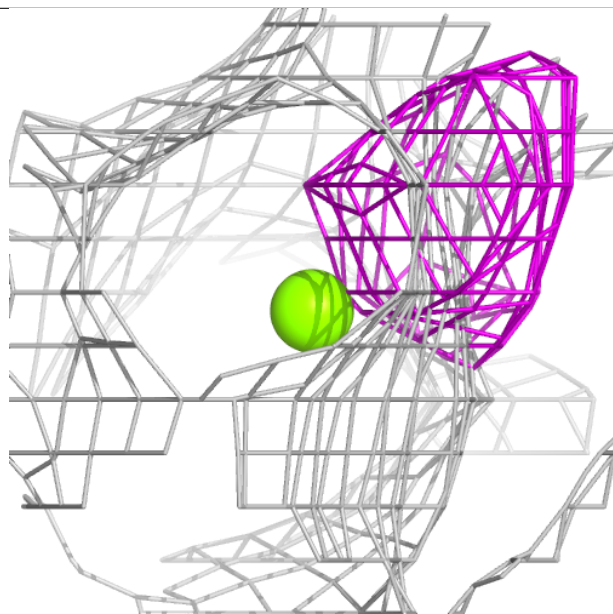
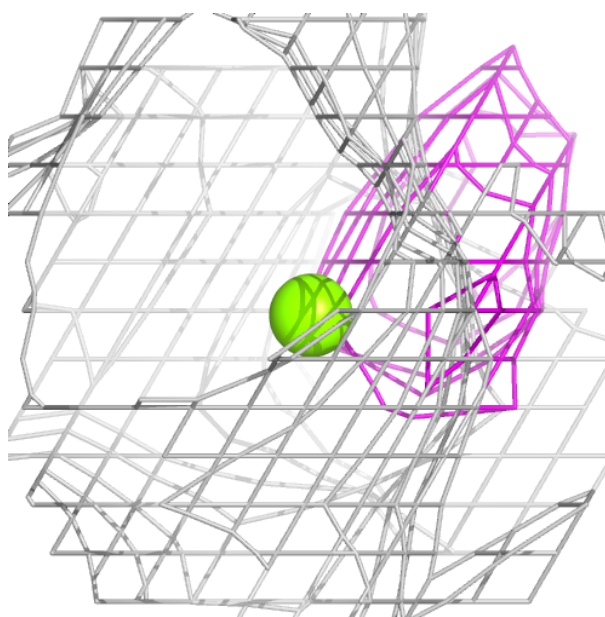
Electron density around SO4 A 406:

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



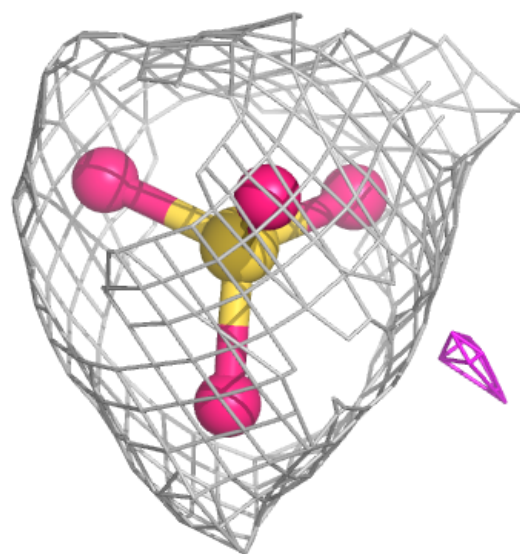
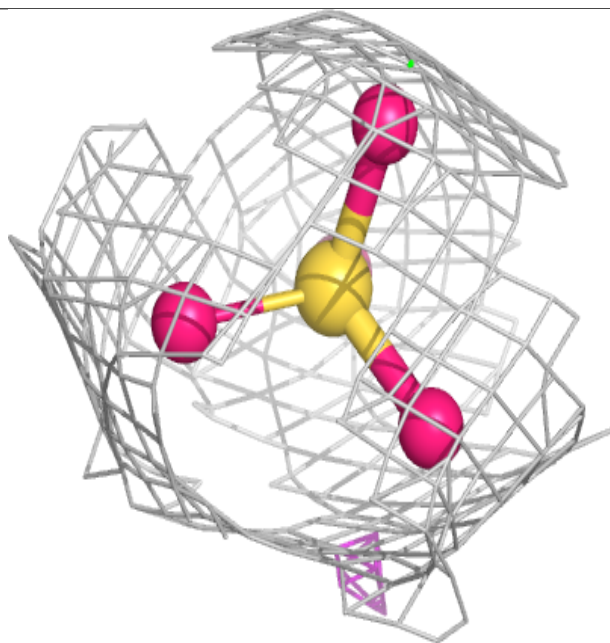
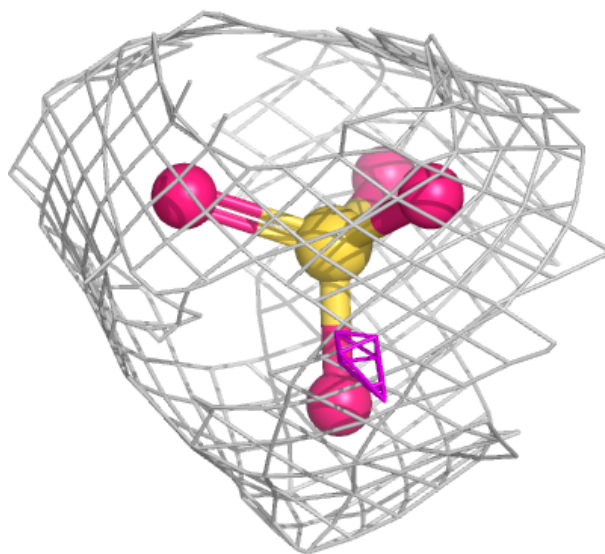
Electron density around MG H 404:

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



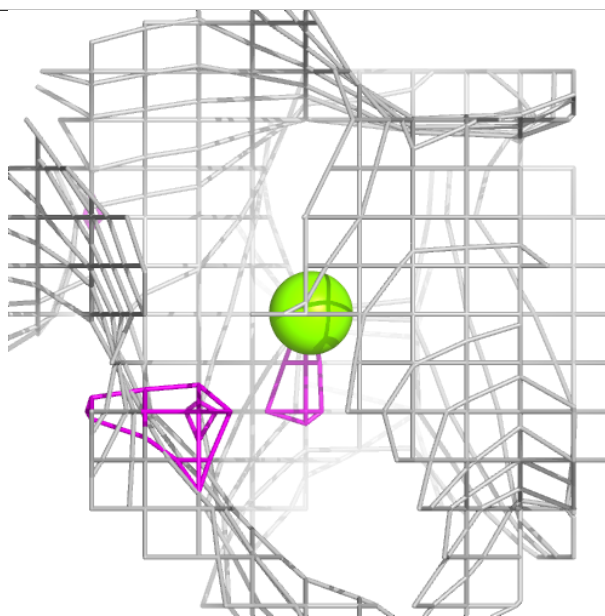
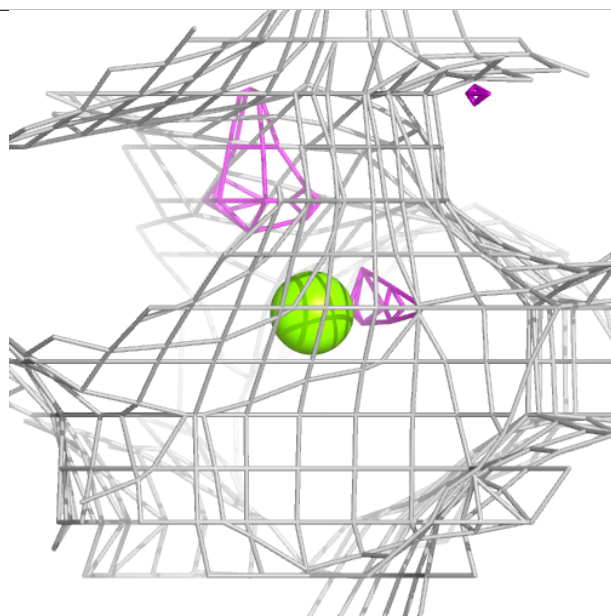
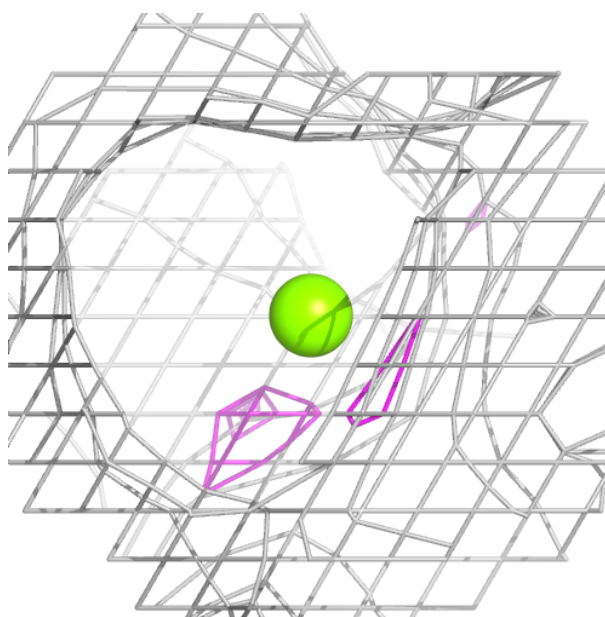
Electron density around SO4 A 405:

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



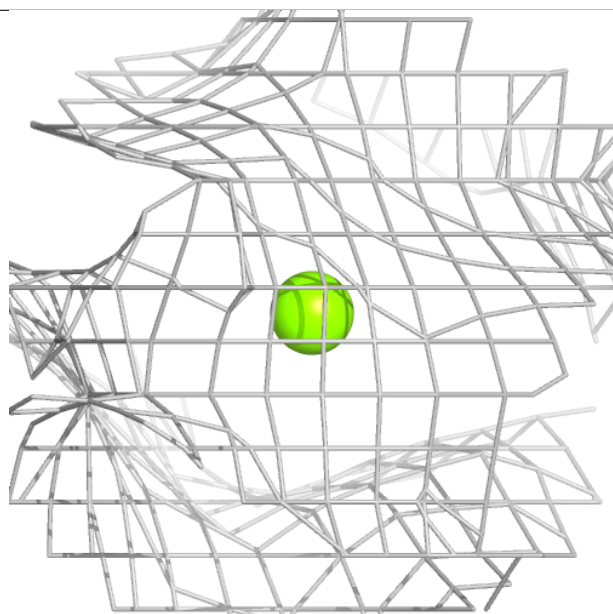
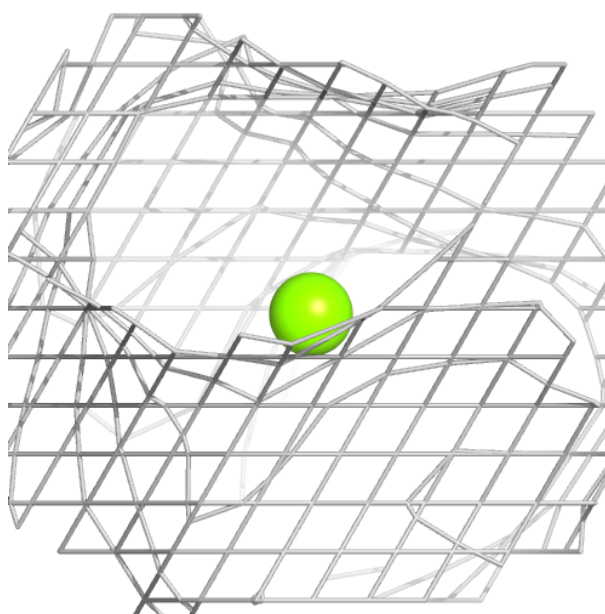
Electron density around MG D 404:

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



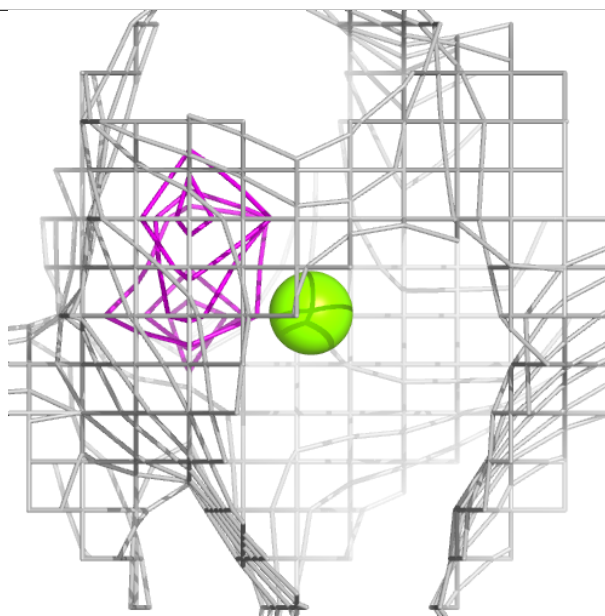
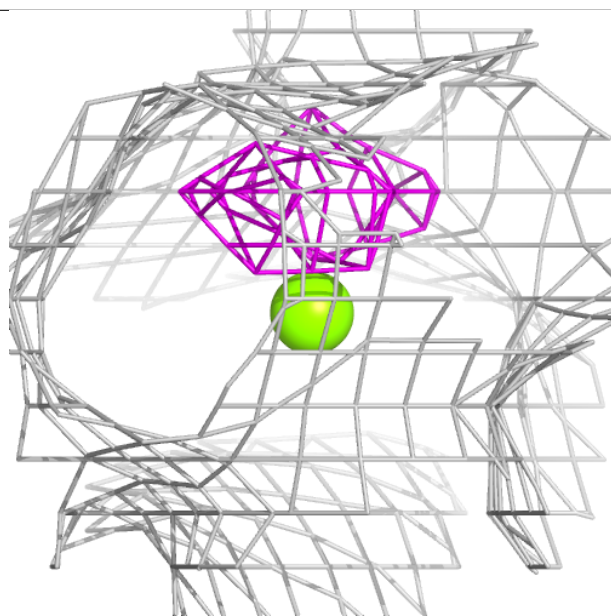
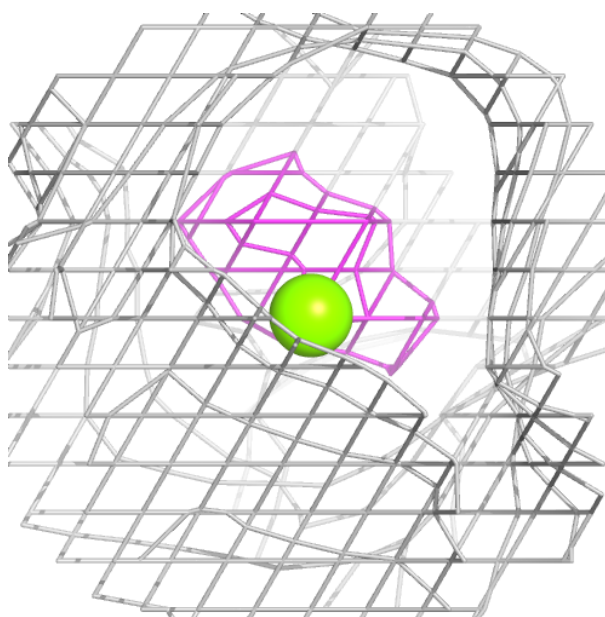
Electron density around MG G 404:

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



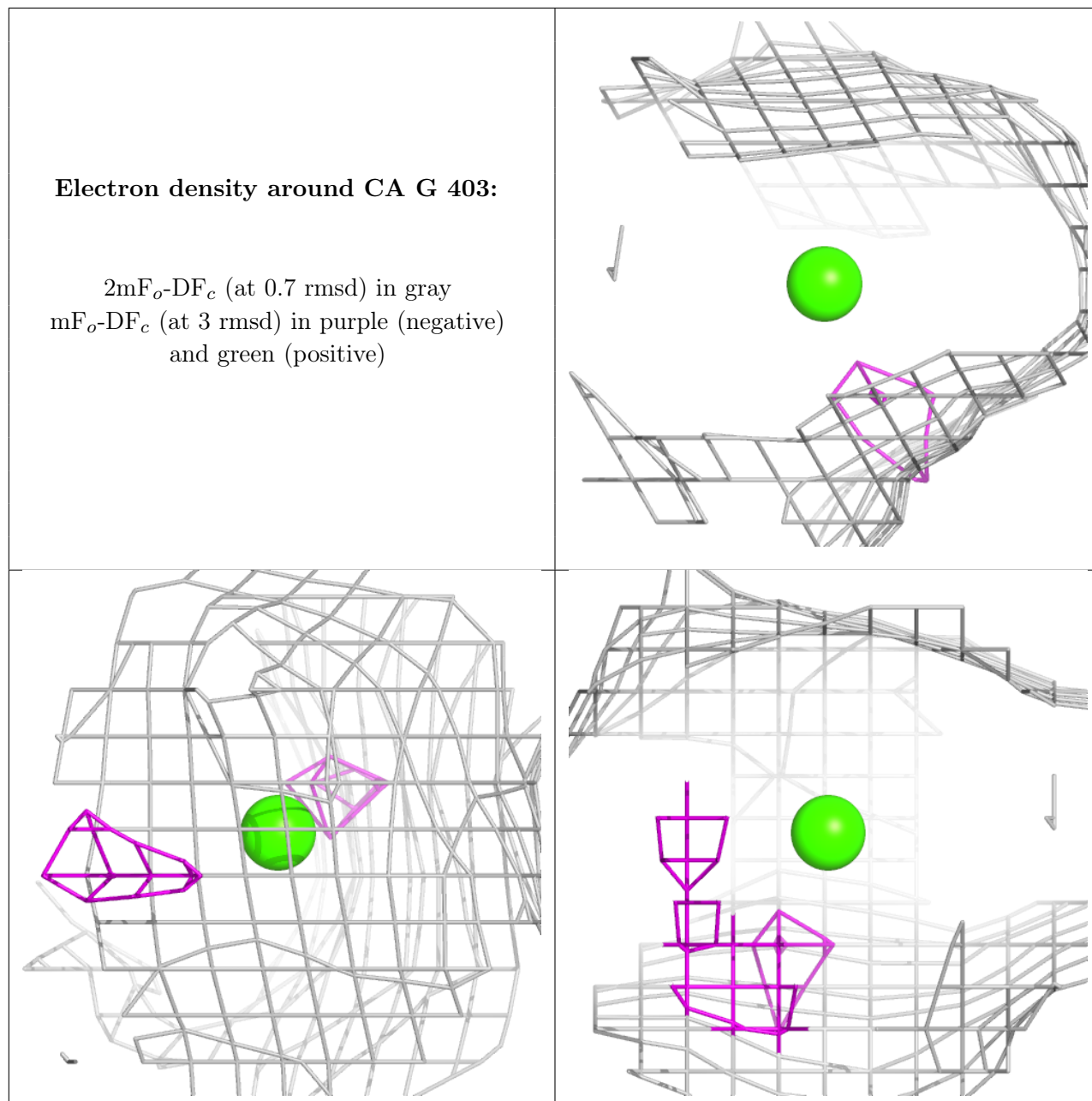
Electron density around MG B 404:

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



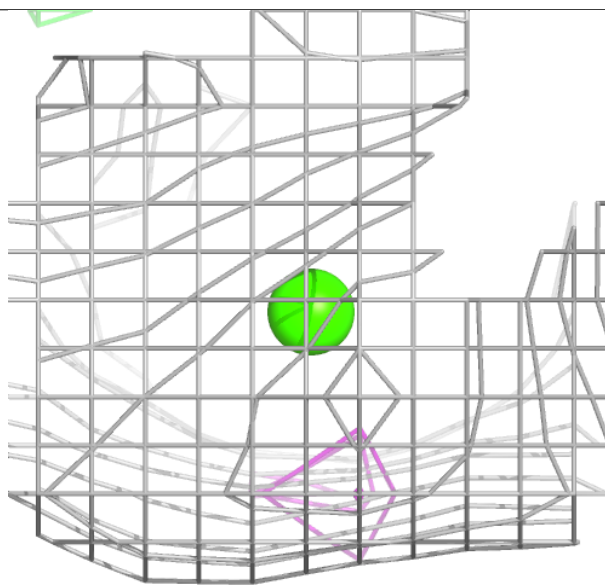
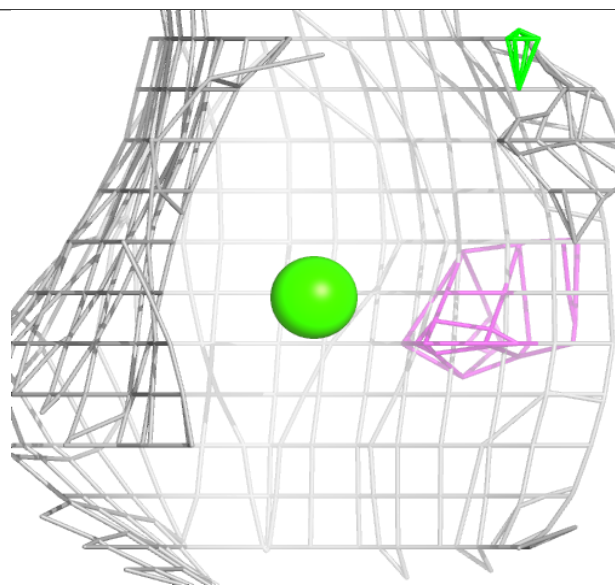
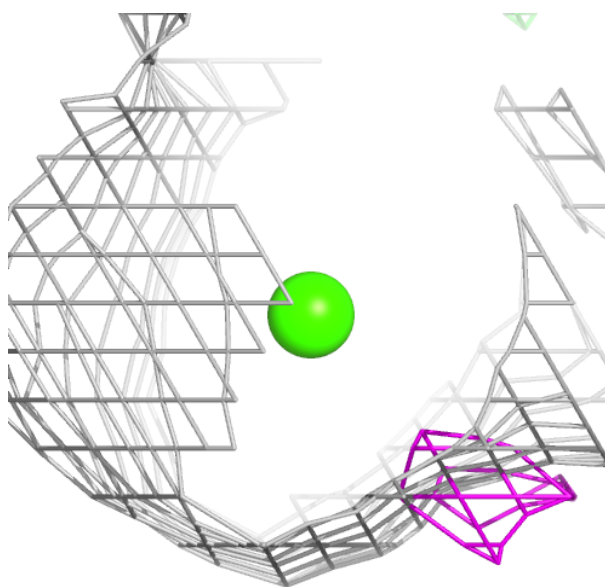
Electron density around CA G 403:

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



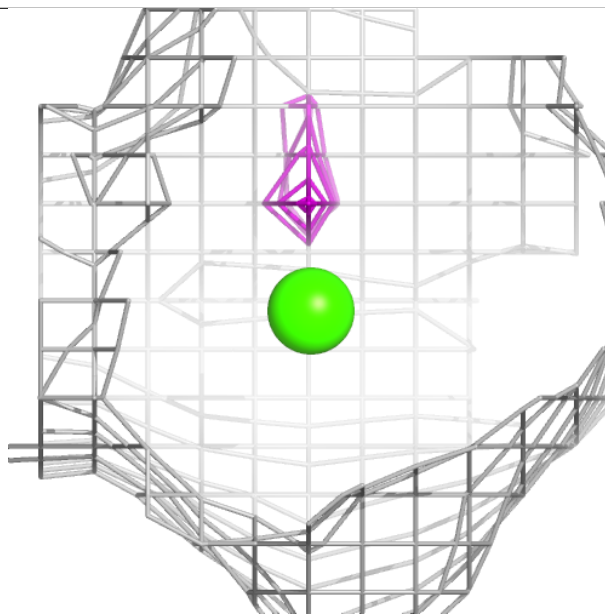
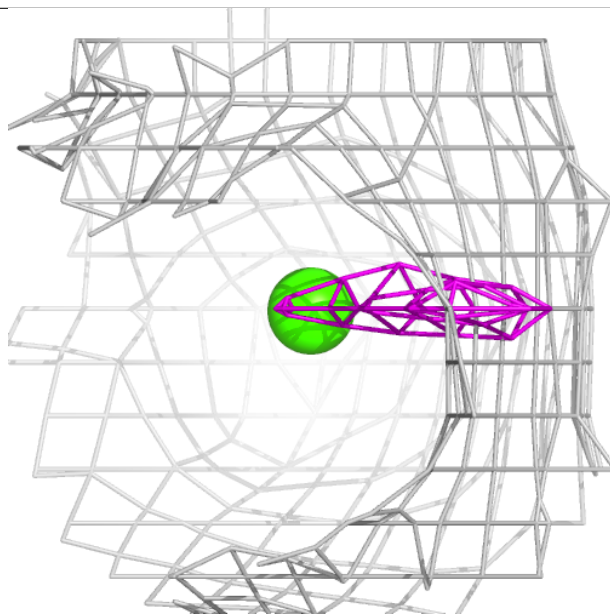
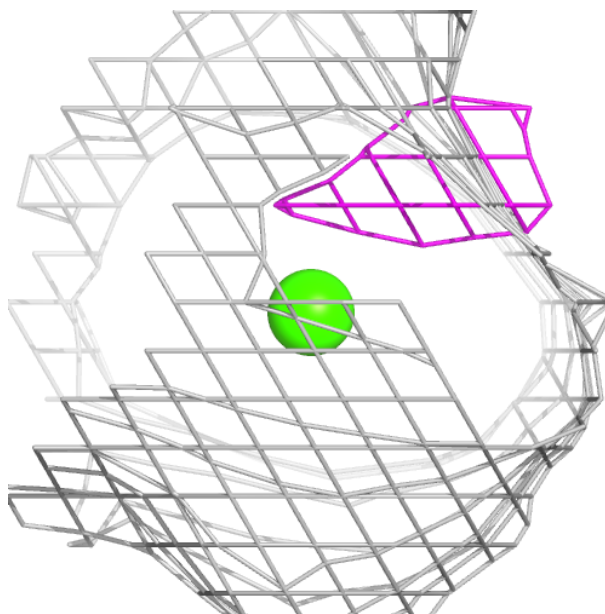
Electron density around CA H 401:

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



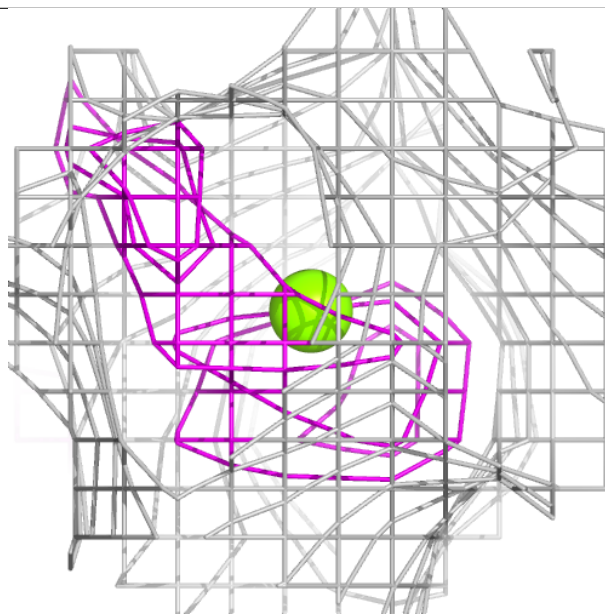
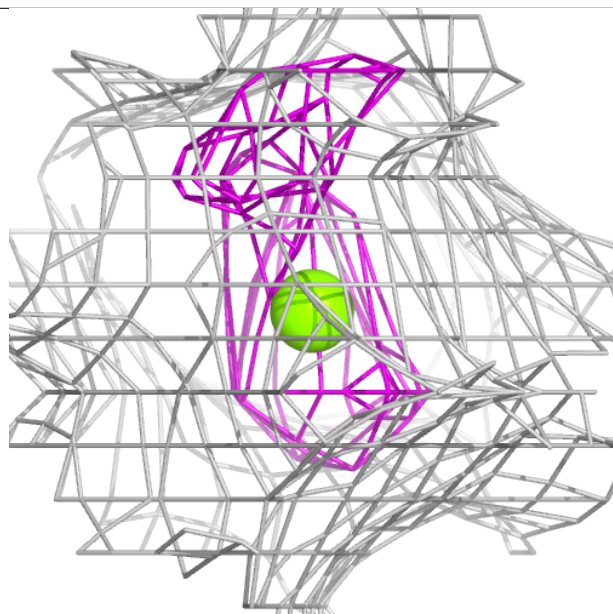
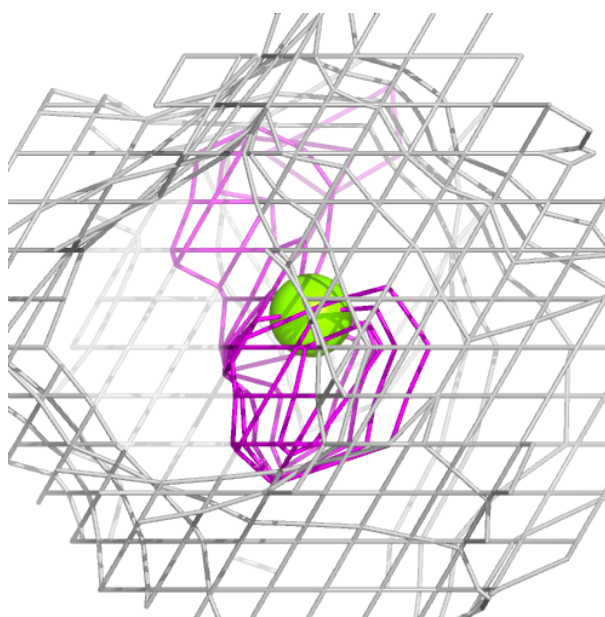
Electron density around CA I 402:

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



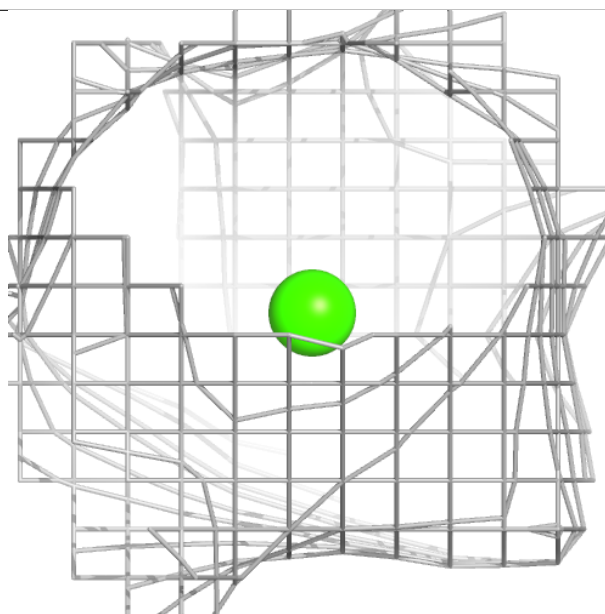
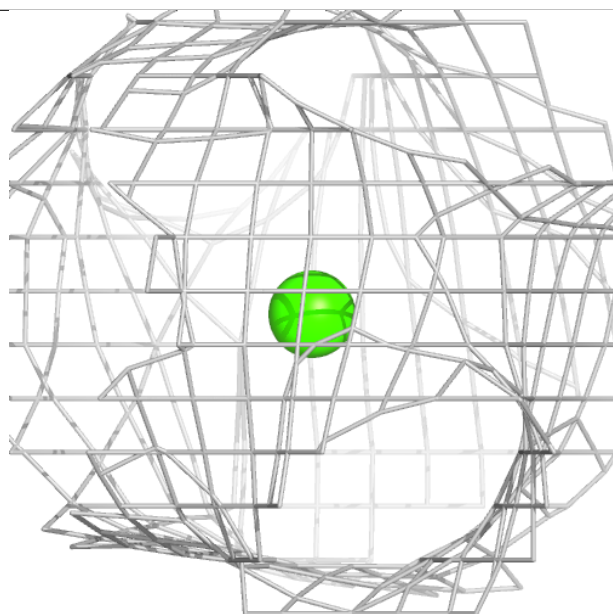
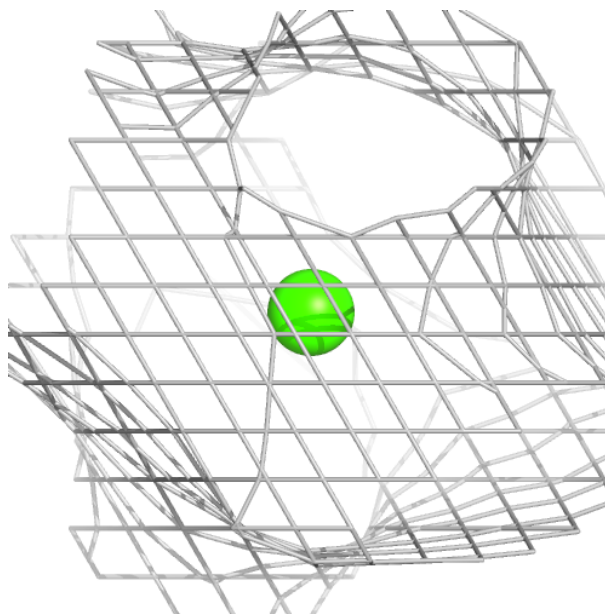
Electron density around MG A 404:

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



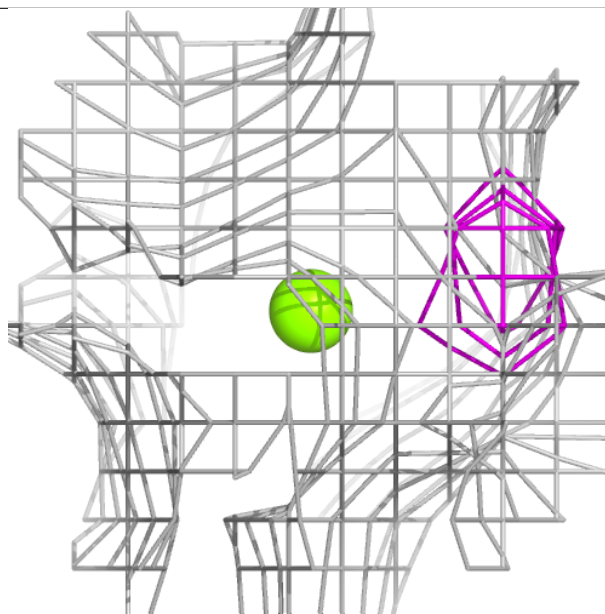
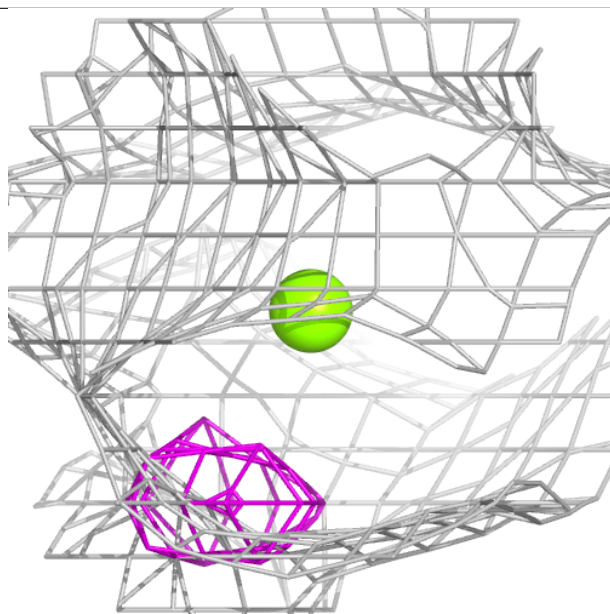
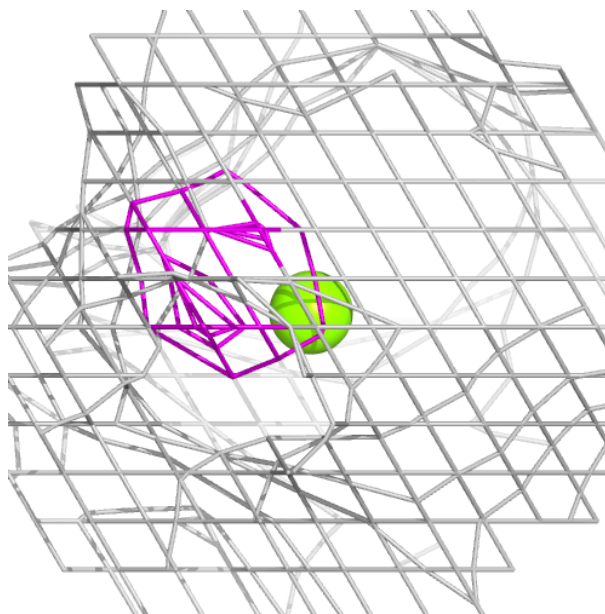
Electron density around CA A 401:

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



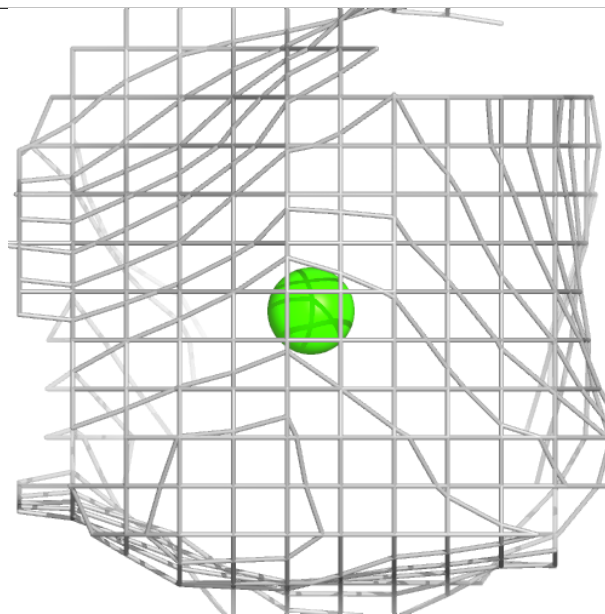
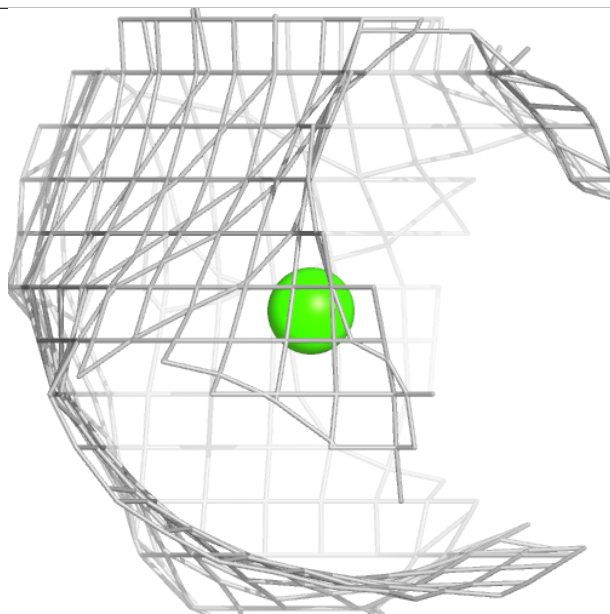
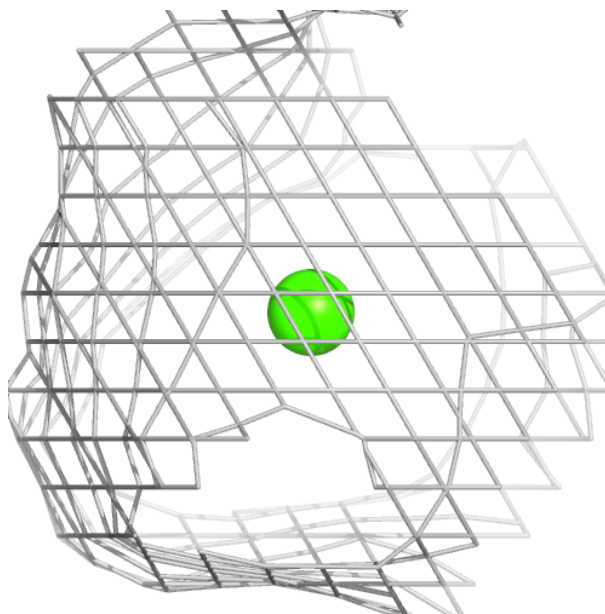
Electron density around MG C 404:

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



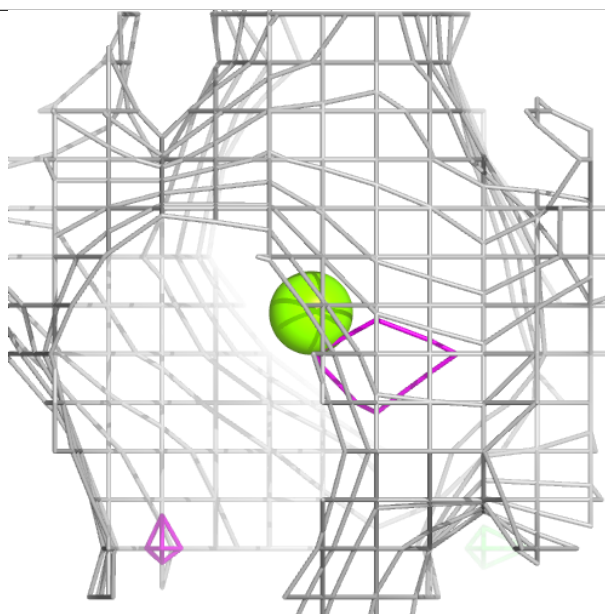
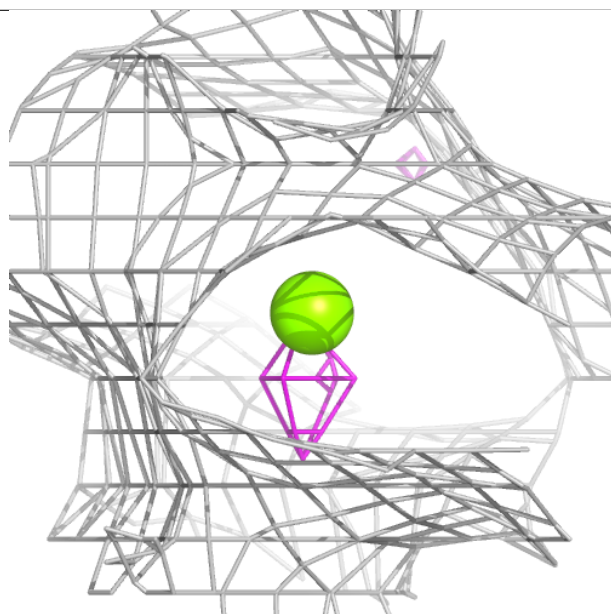
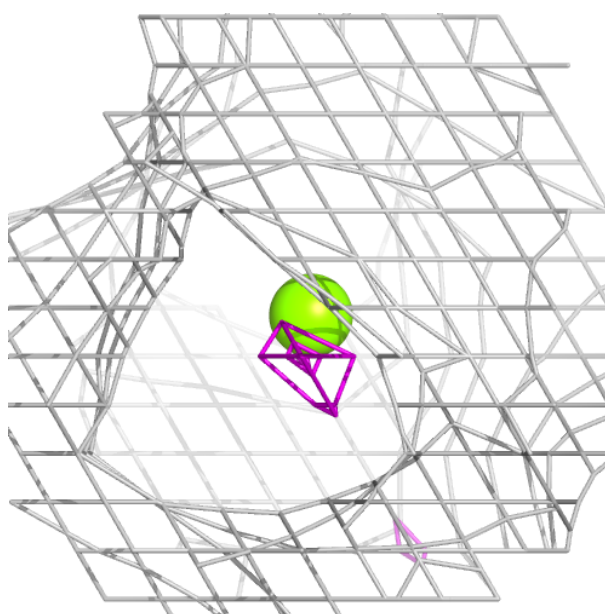
Electron density around CA D 401:

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



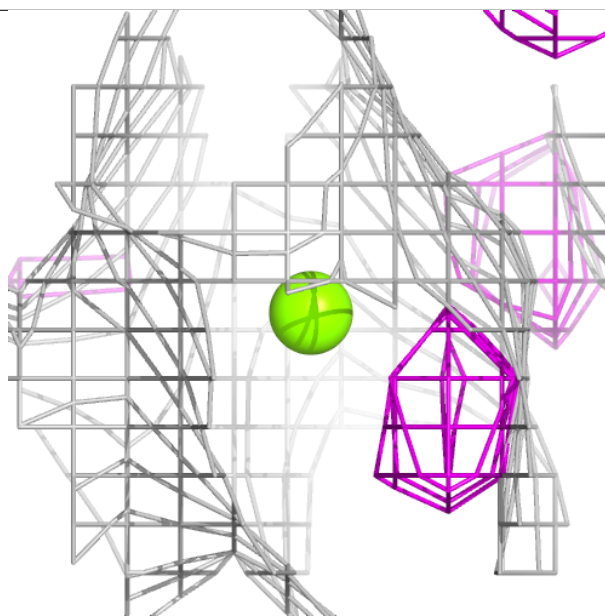
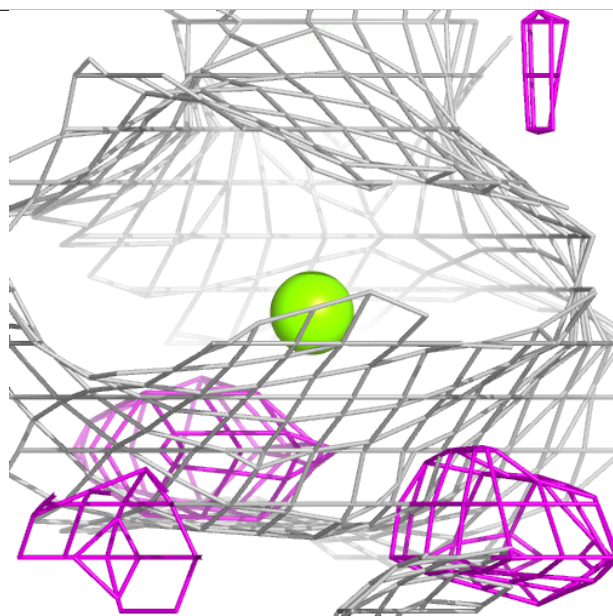
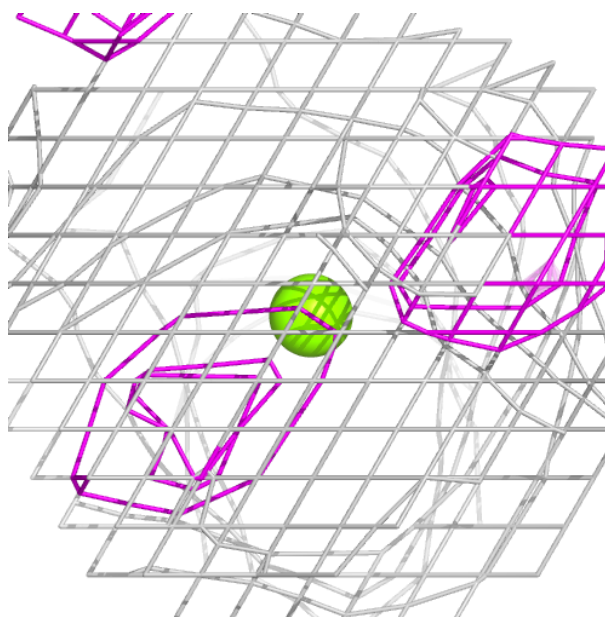
Electron density around MG E 404:

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



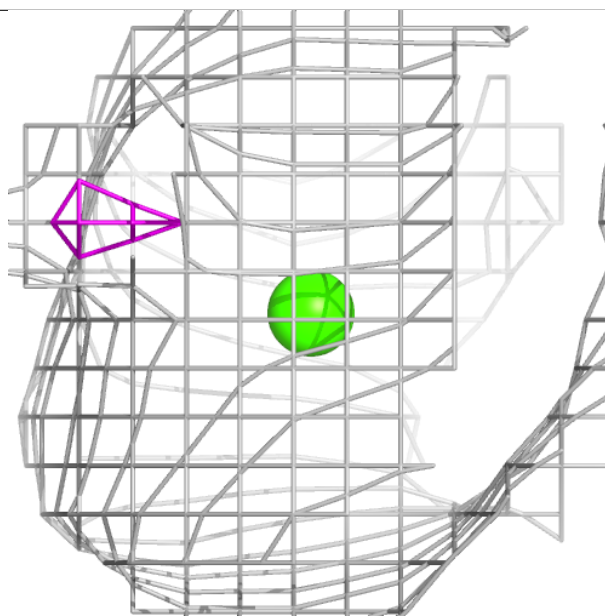
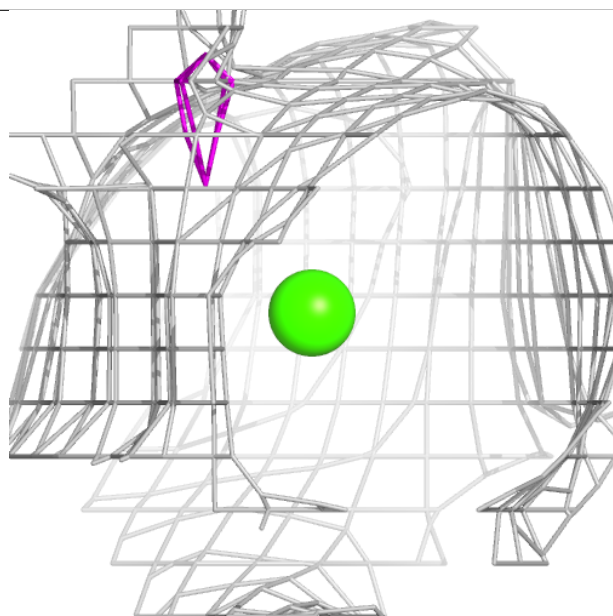
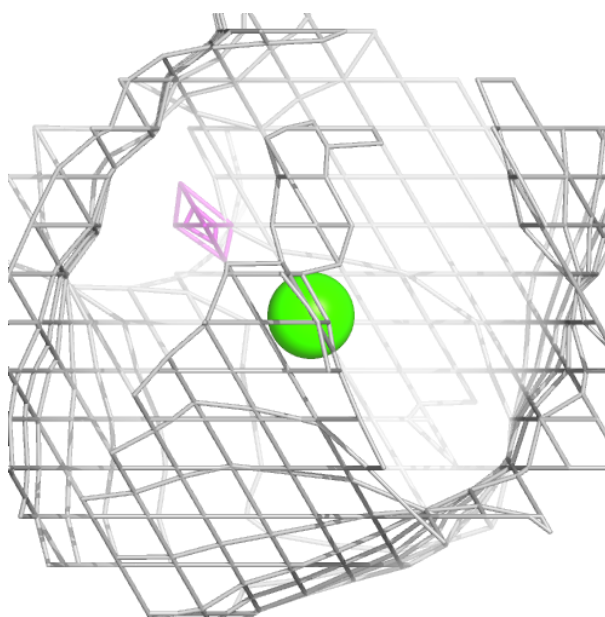
Electron density around MG F 404:

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



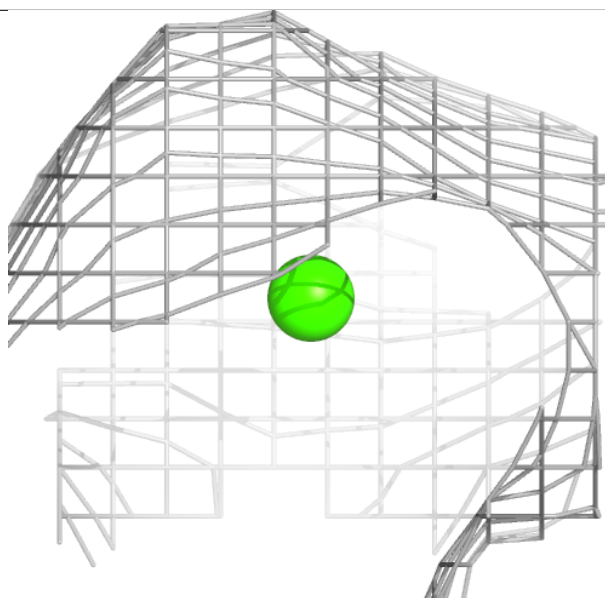
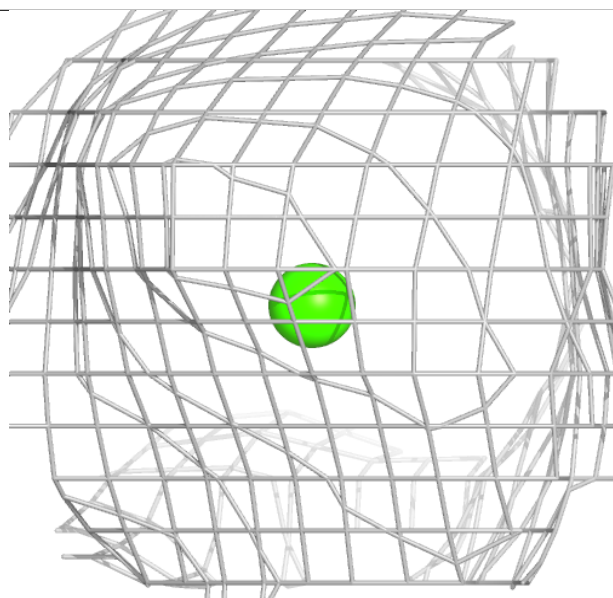
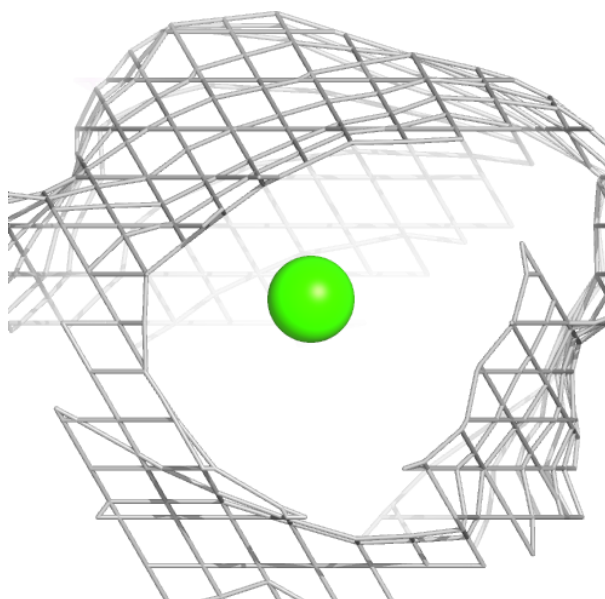
Electron density around CA E 401:

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



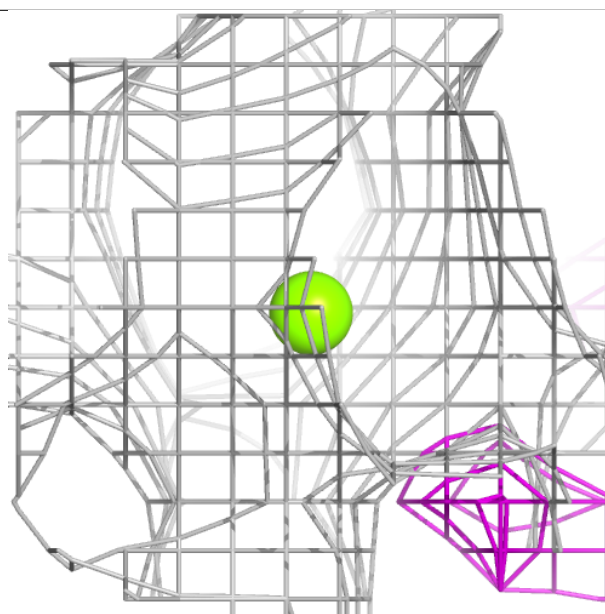
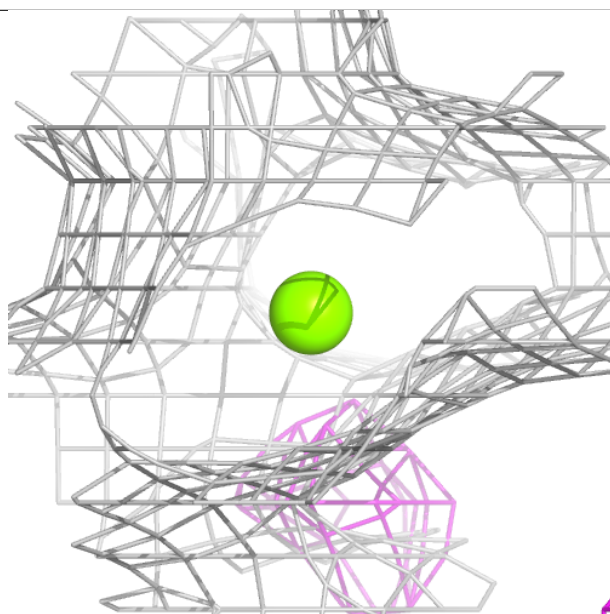
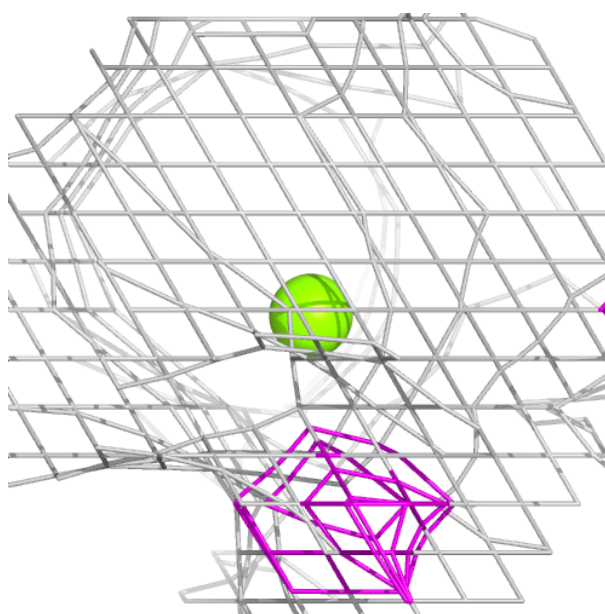
Electron density around CA E 403:

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



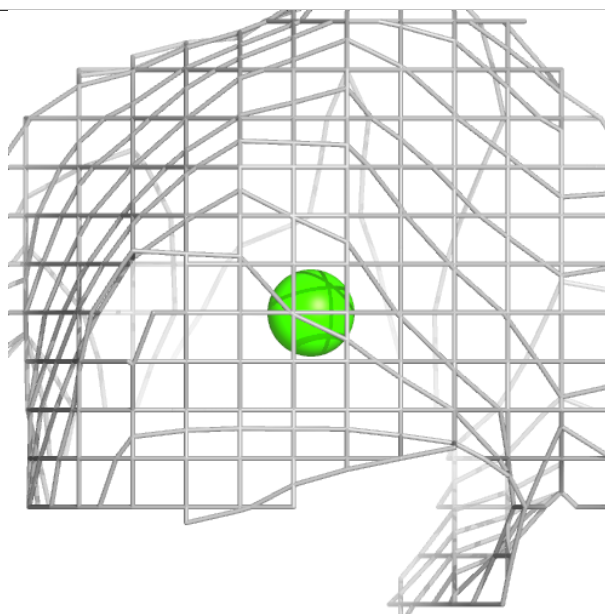
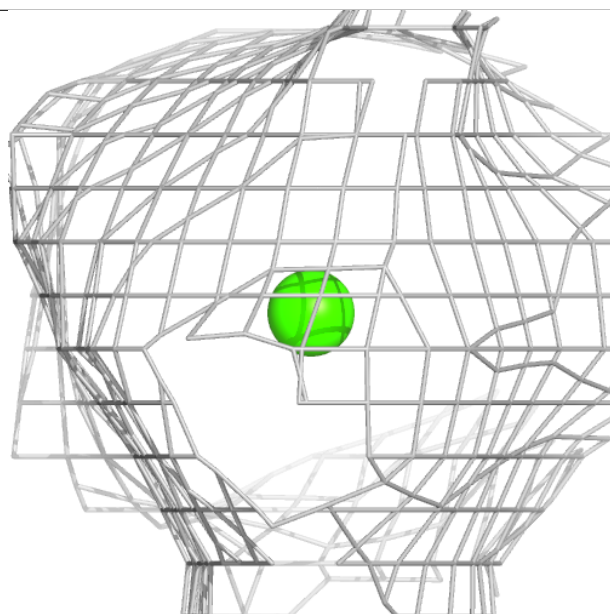
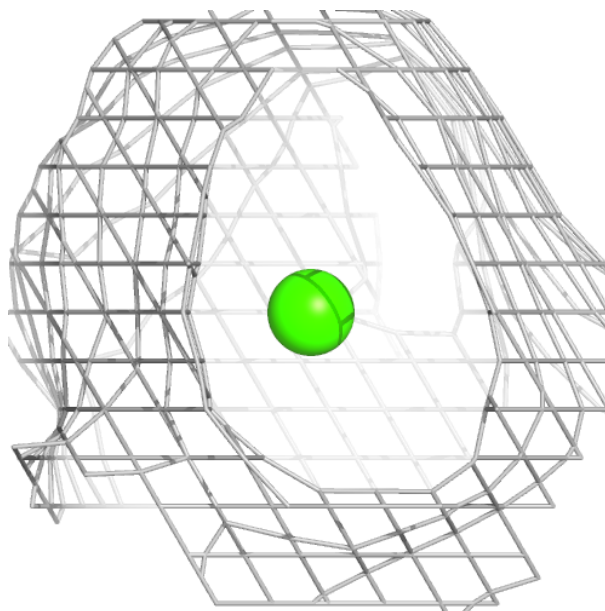
Electron density around MG I 404:

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



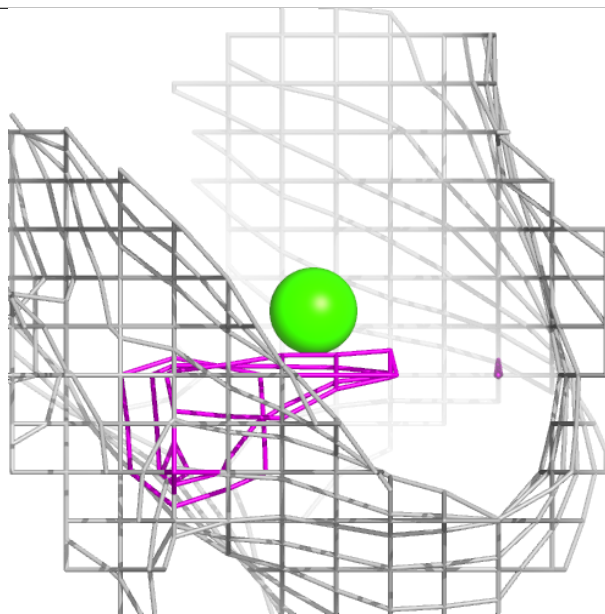
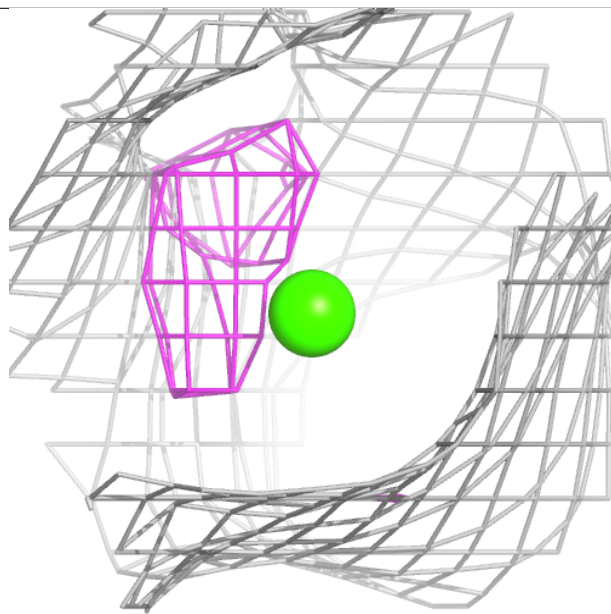
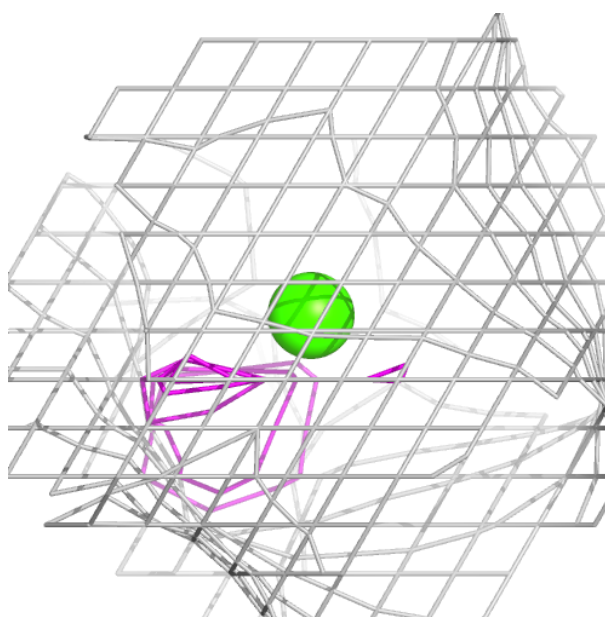
Electron density around CA F 401:

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



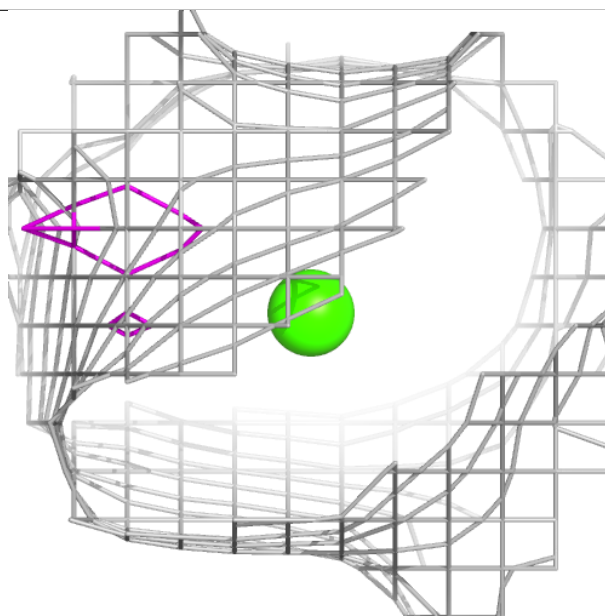
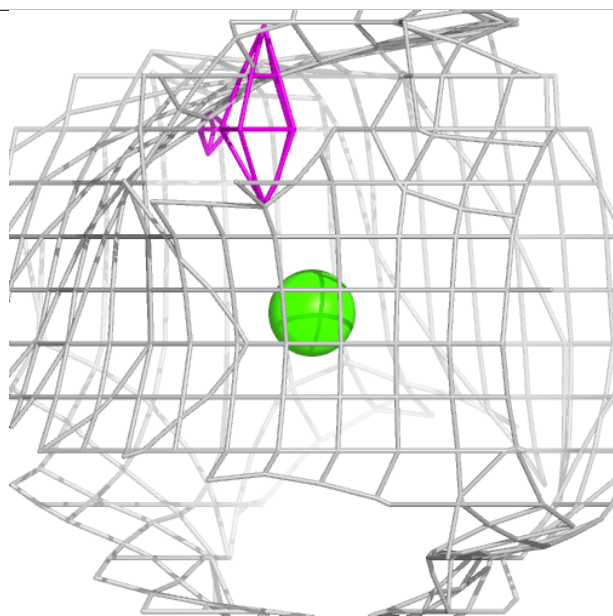
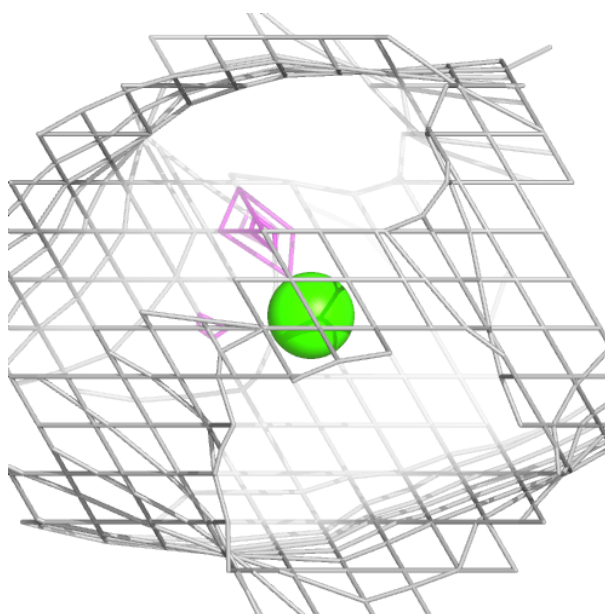
Electron density around CA F 402:

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



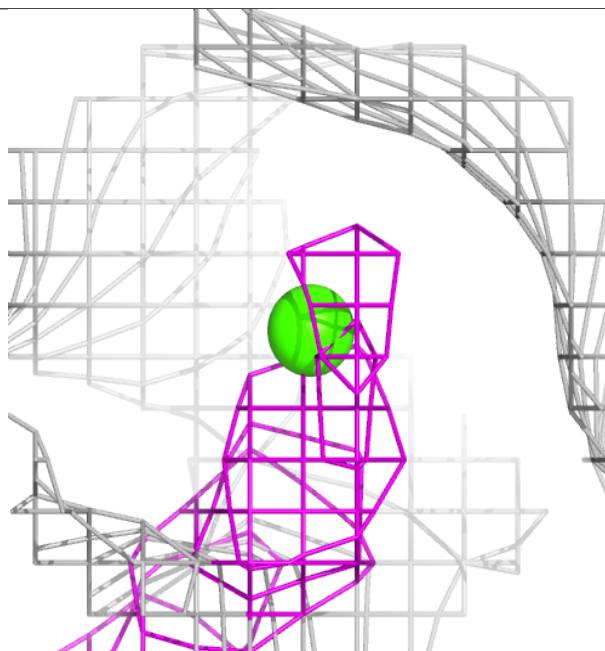
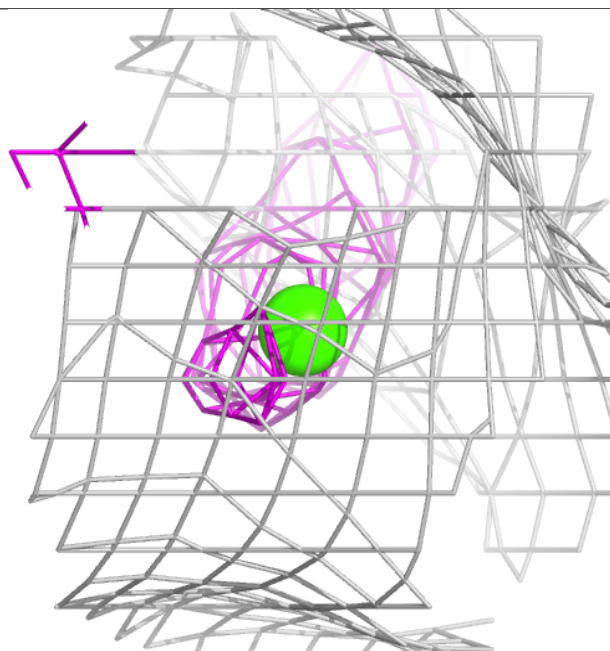
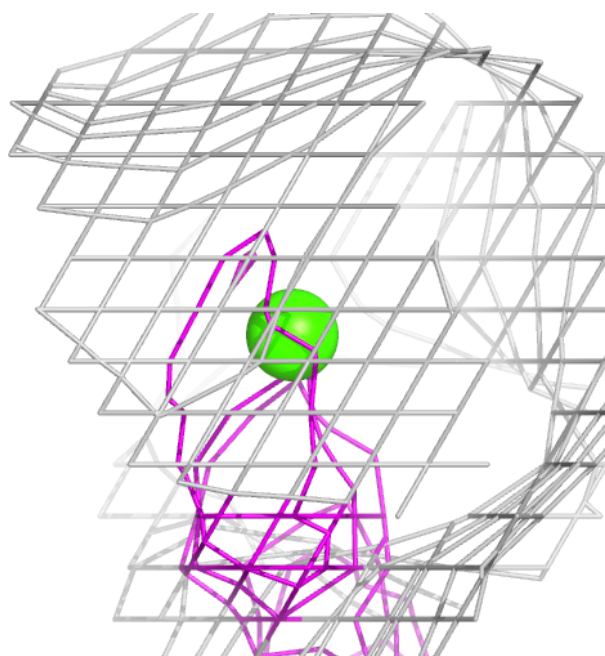
Electron density around CA G 401:

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



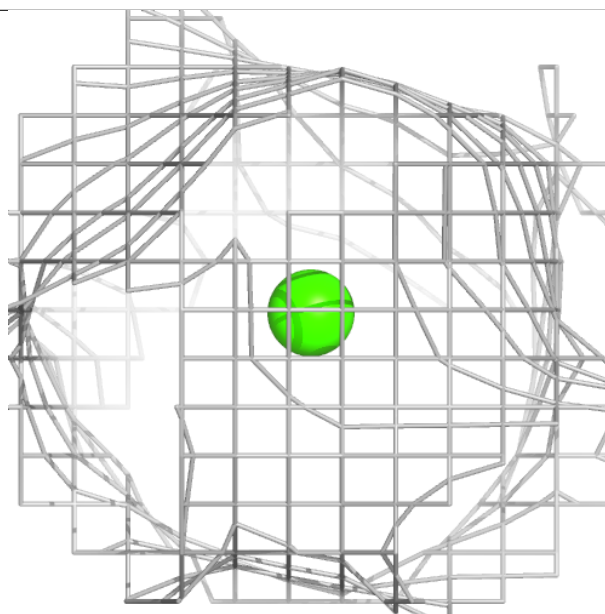
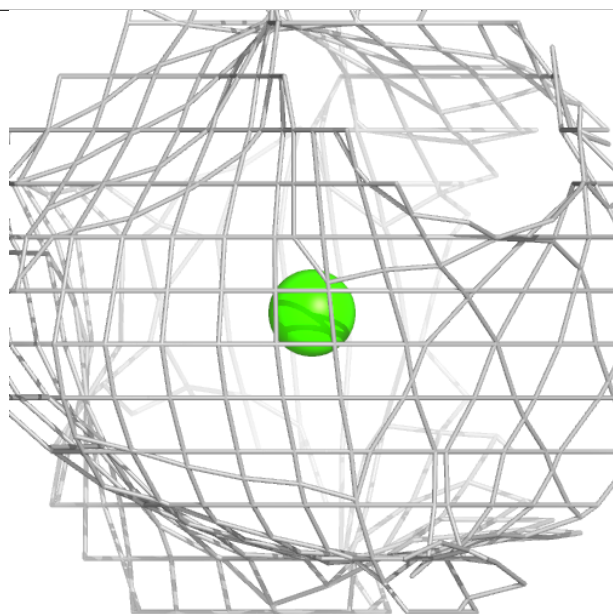
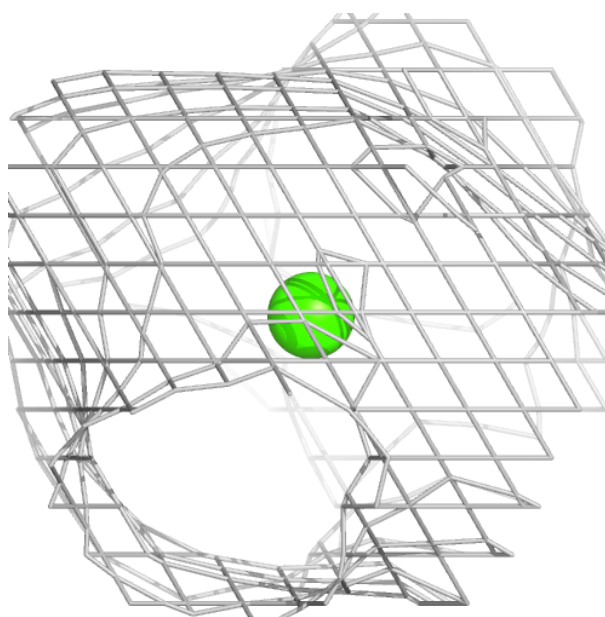
Electron density around CA G 402:

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



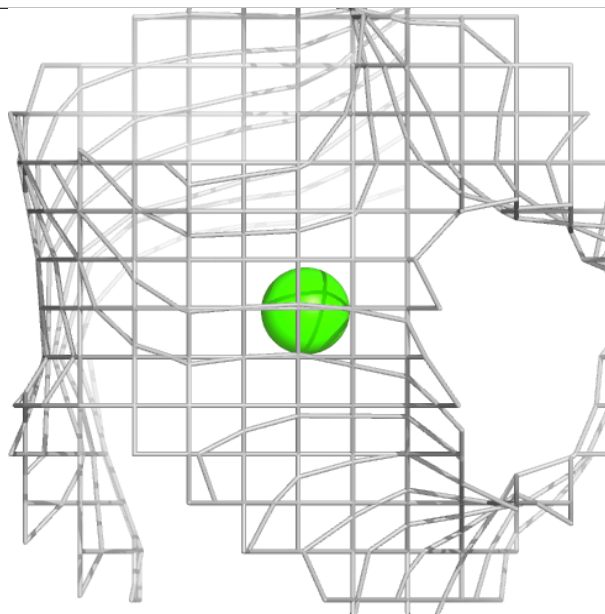
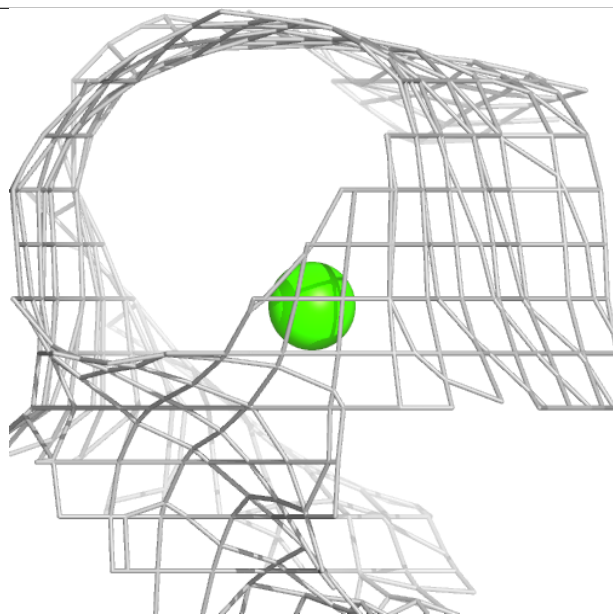
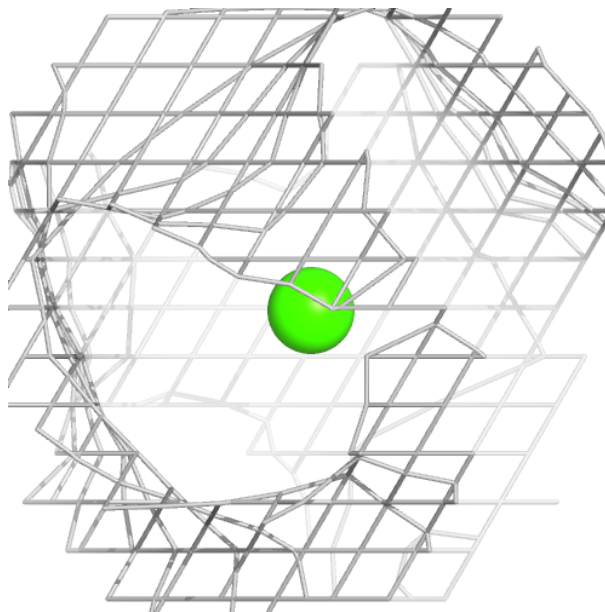
Electron density around CA I 401:

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



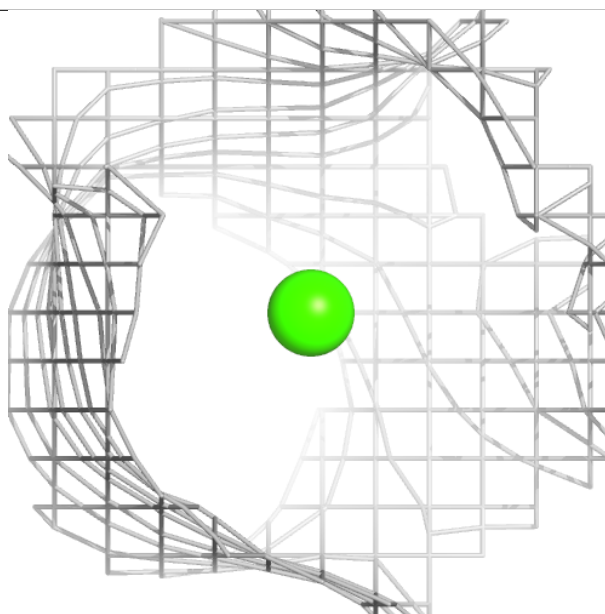
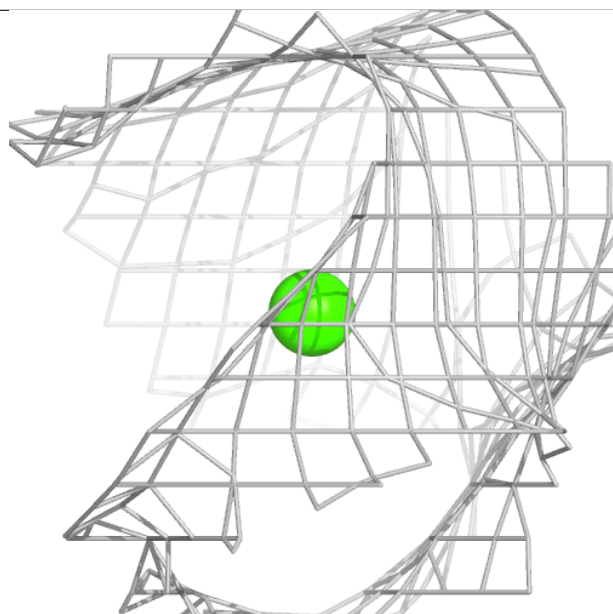
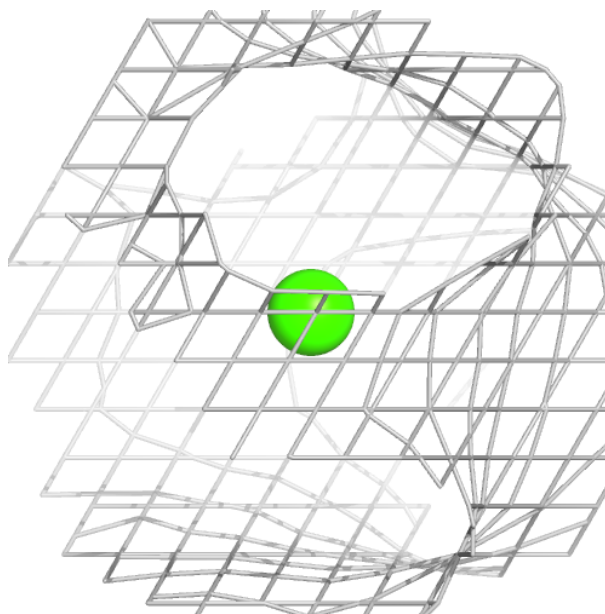
Electron density around CA D 402:

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



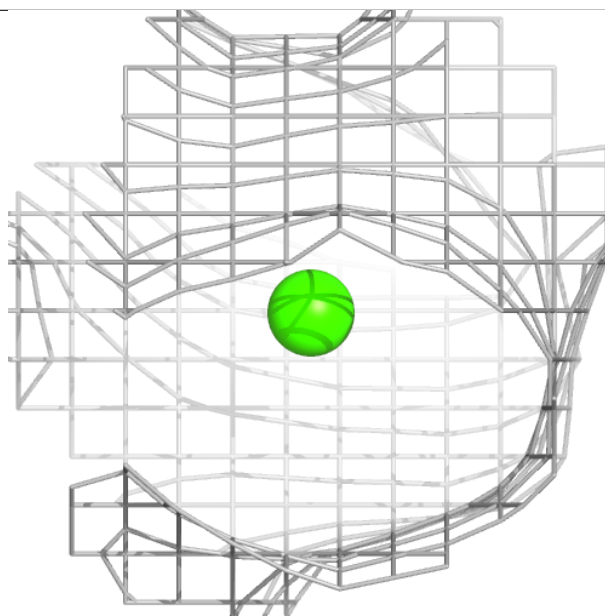
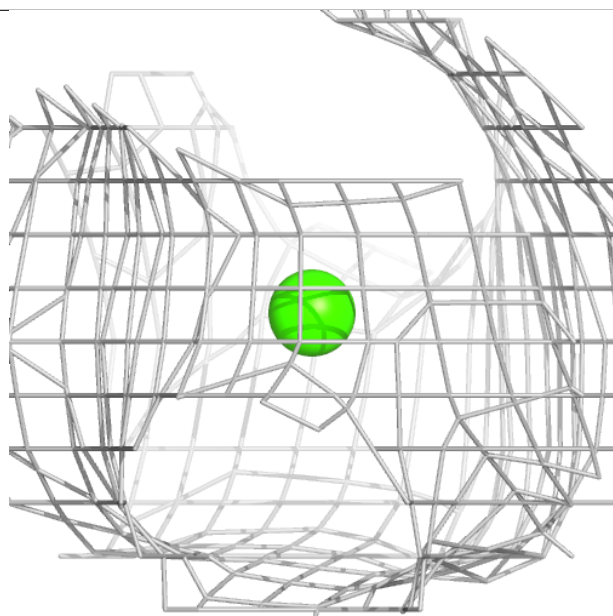
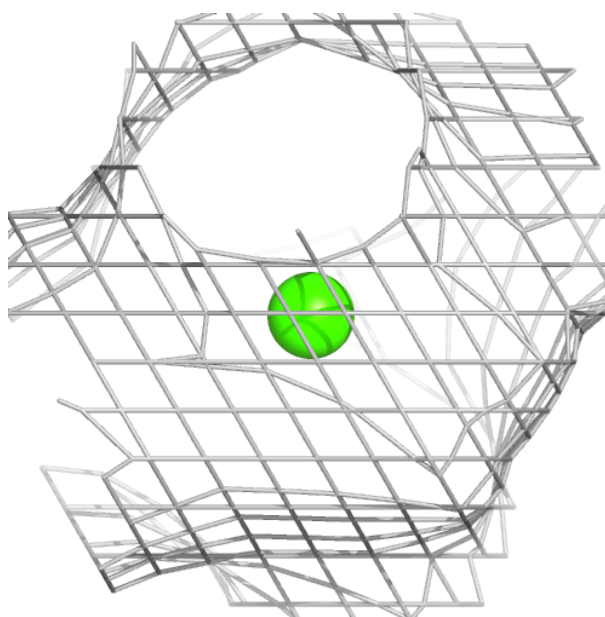
Electron density around CA I 403:

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



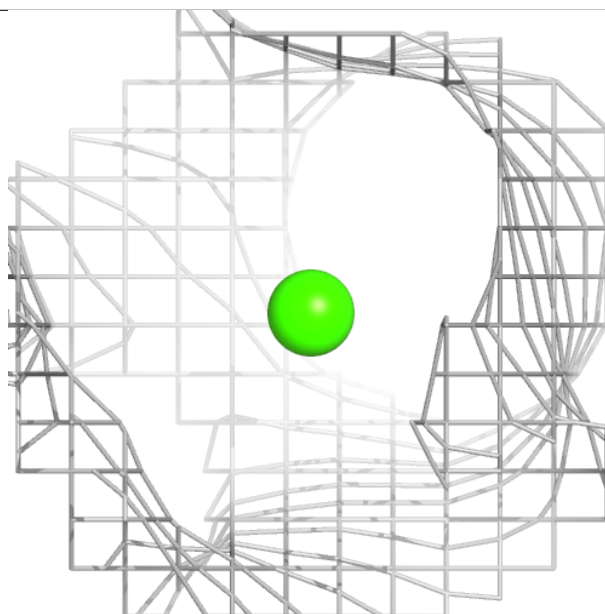
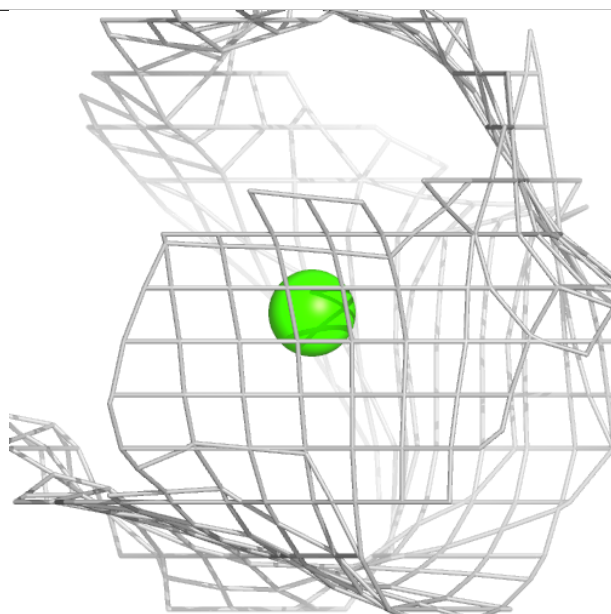
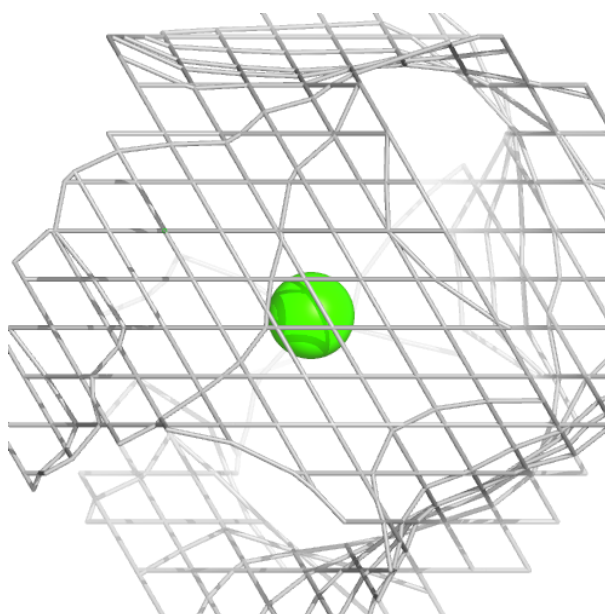
Electron density around CA D 403:

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



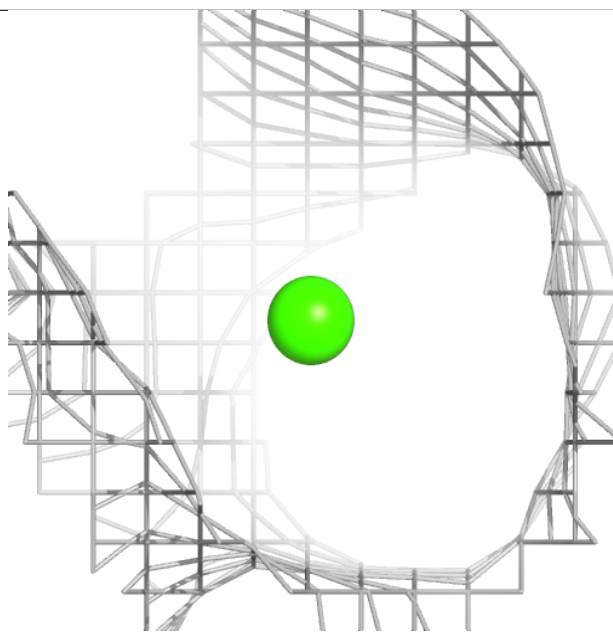
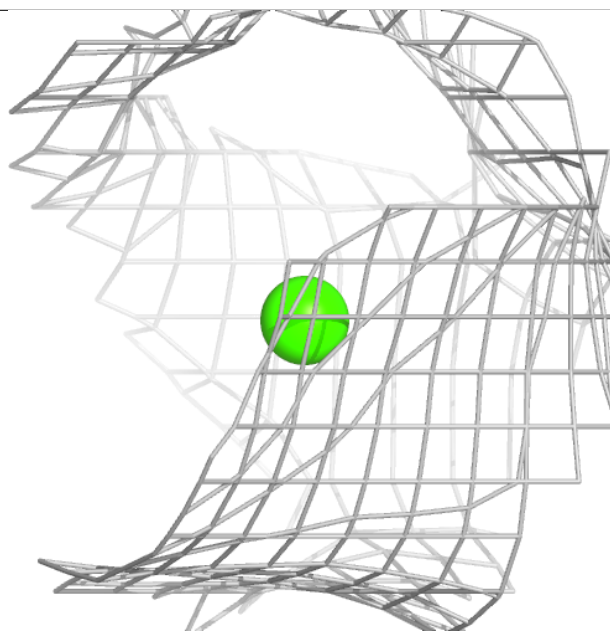
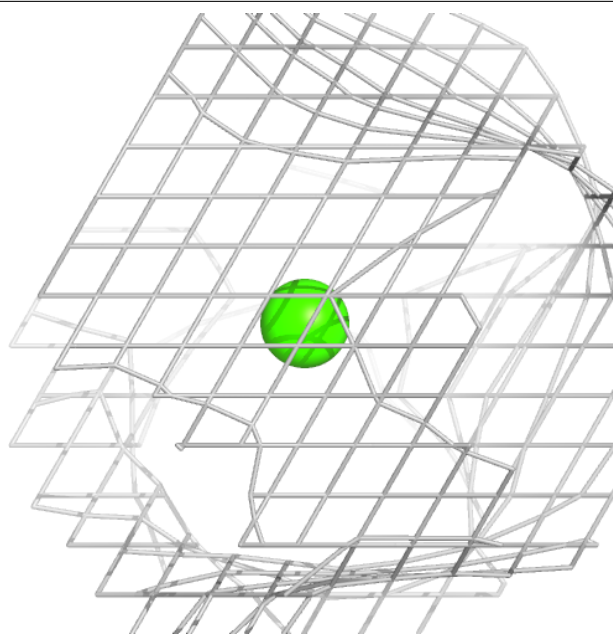
Electron density around CA A 403:

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



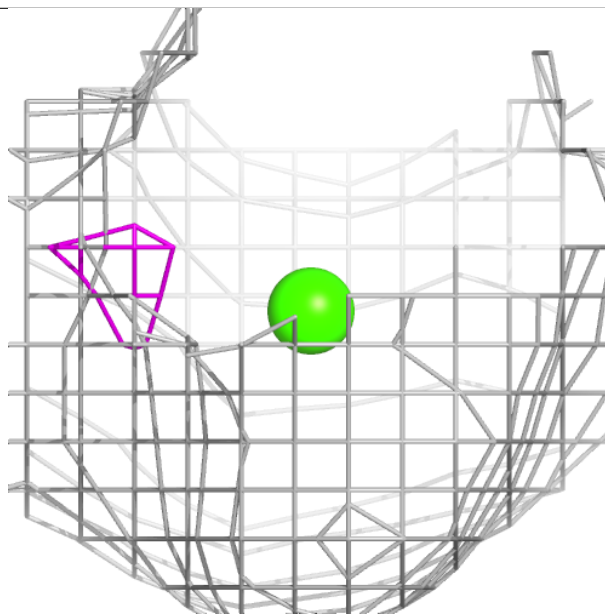
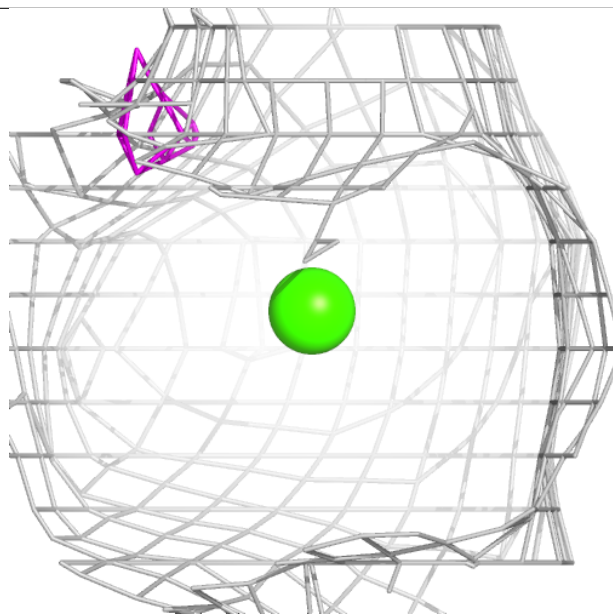
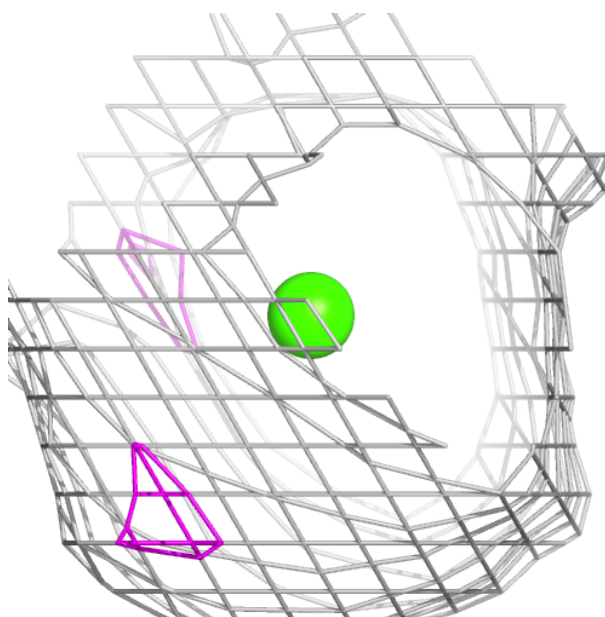
Electron density around CA E 402:

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



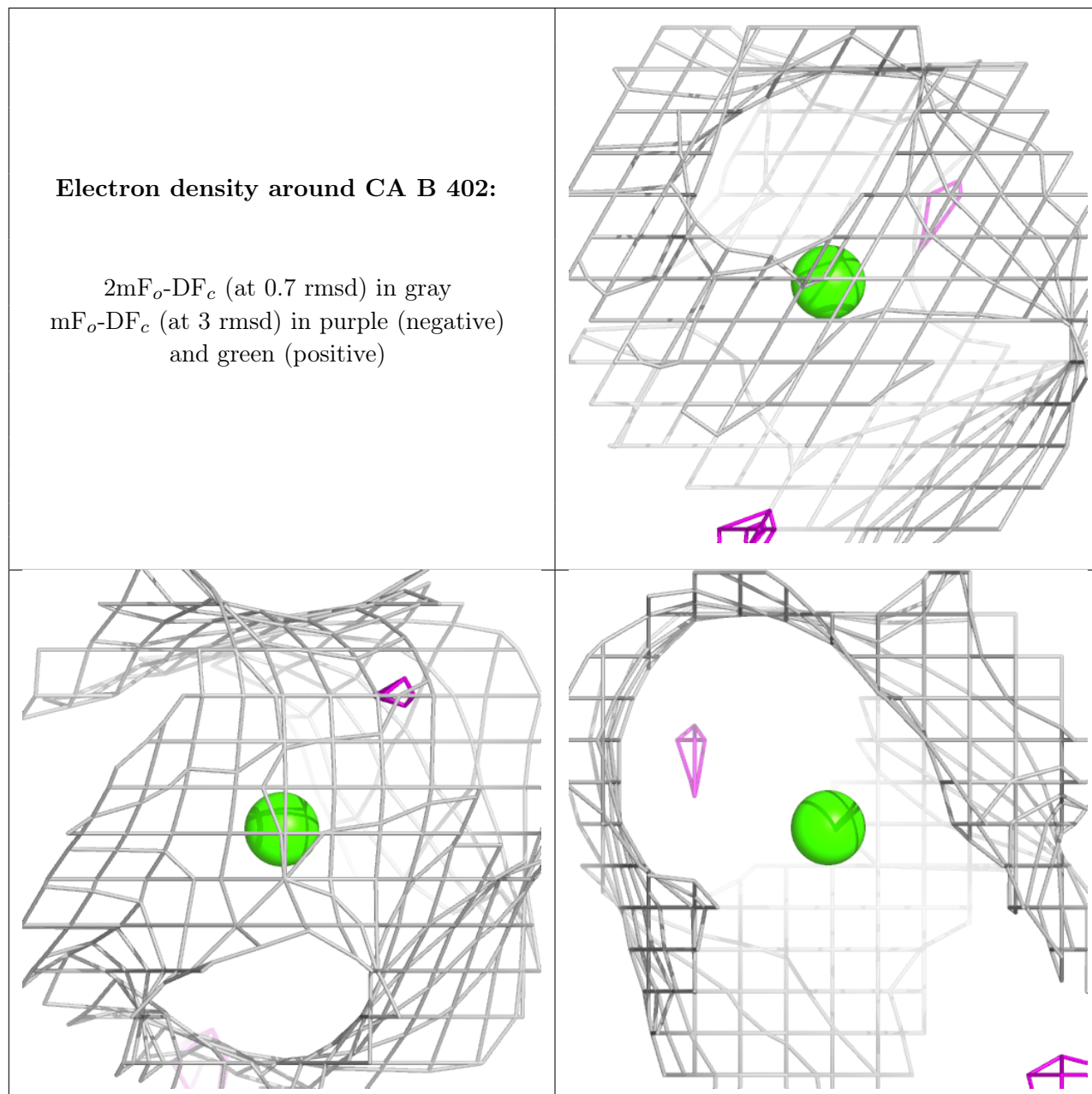
Electron density around CA B 401:

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



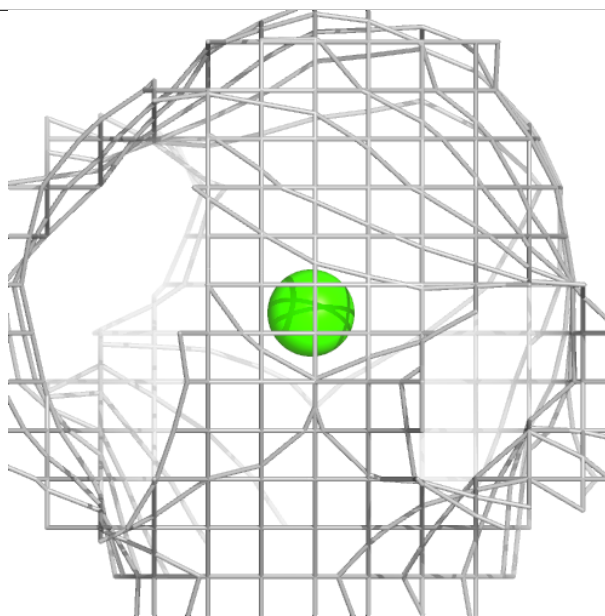
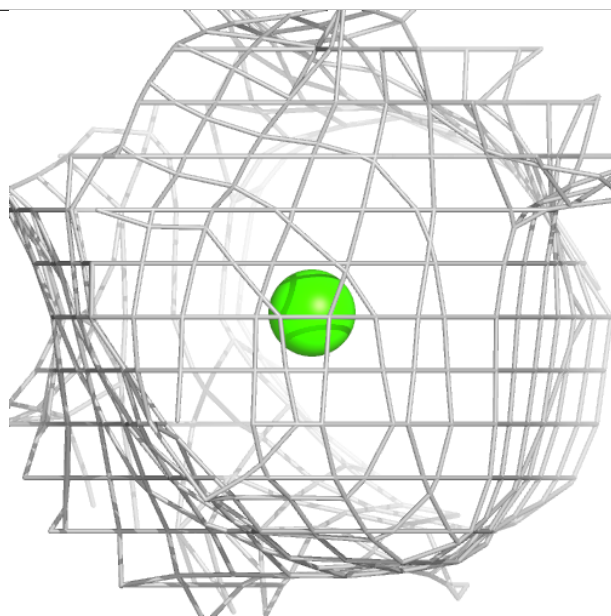
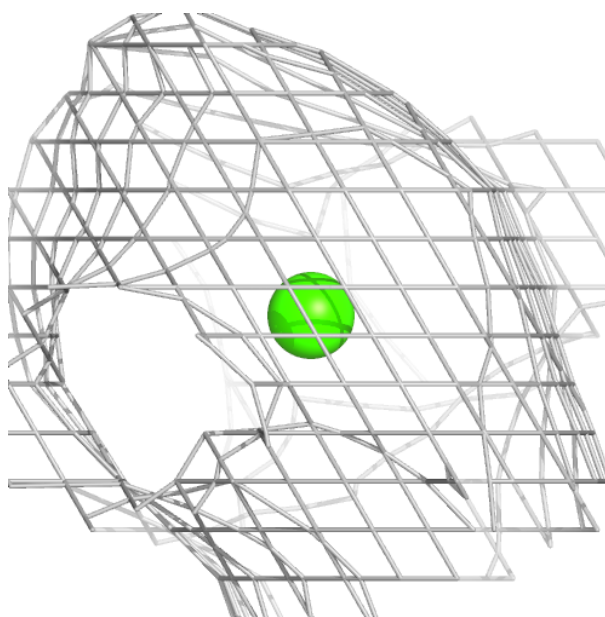
Electron density around CA B 402:

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



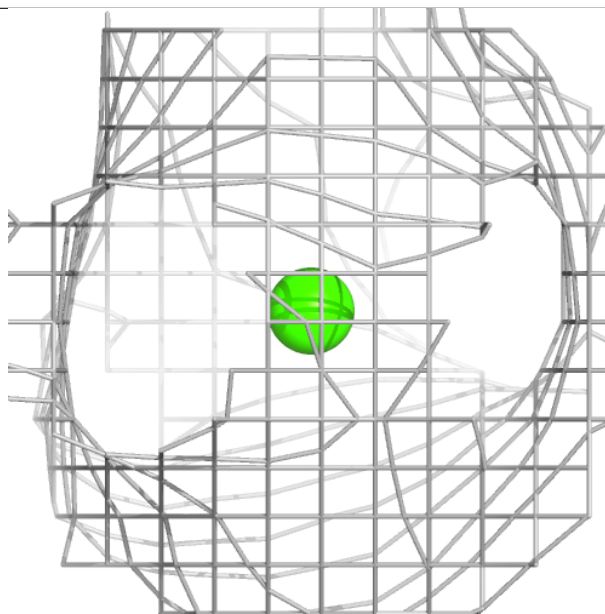
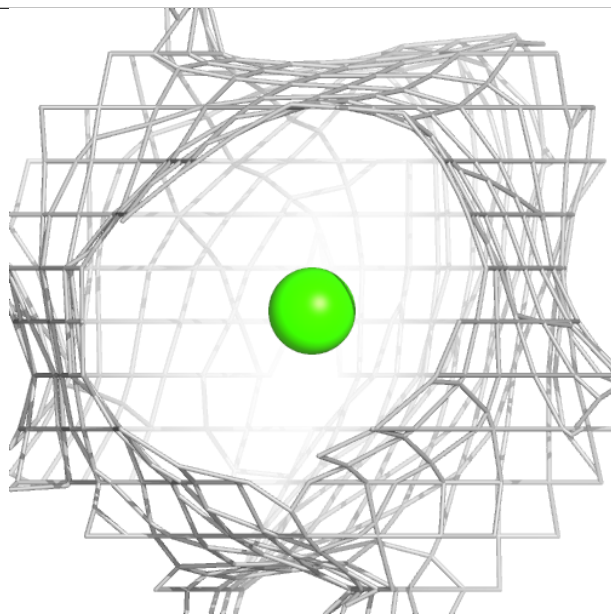
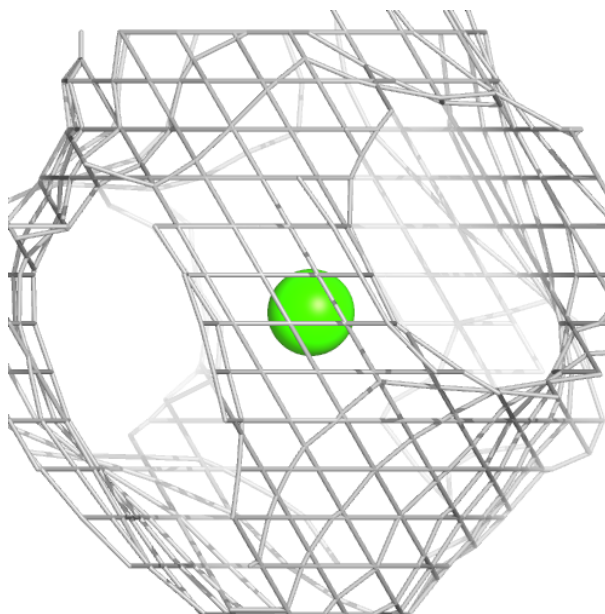
Electron density around CA B 403:

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



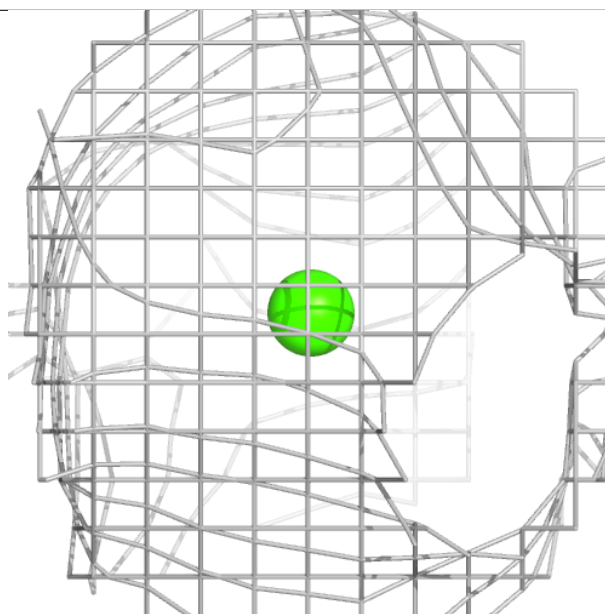
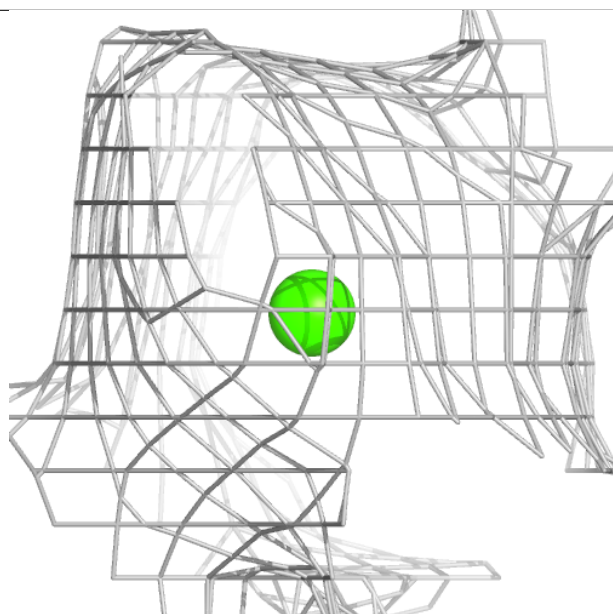
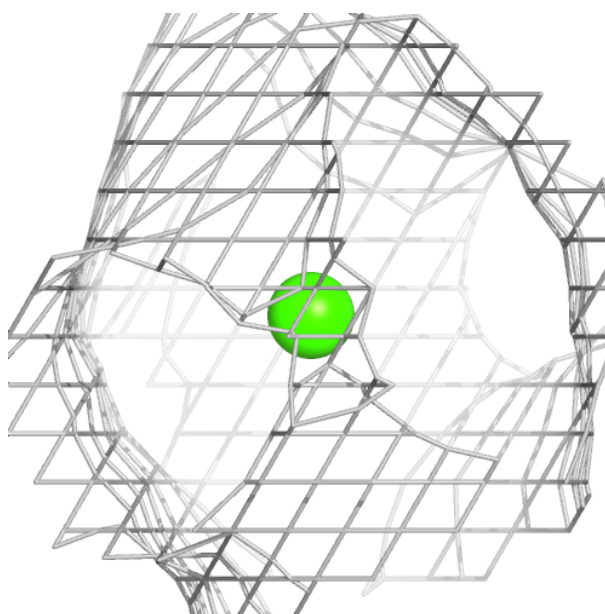
Electron density around CA F 403:

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



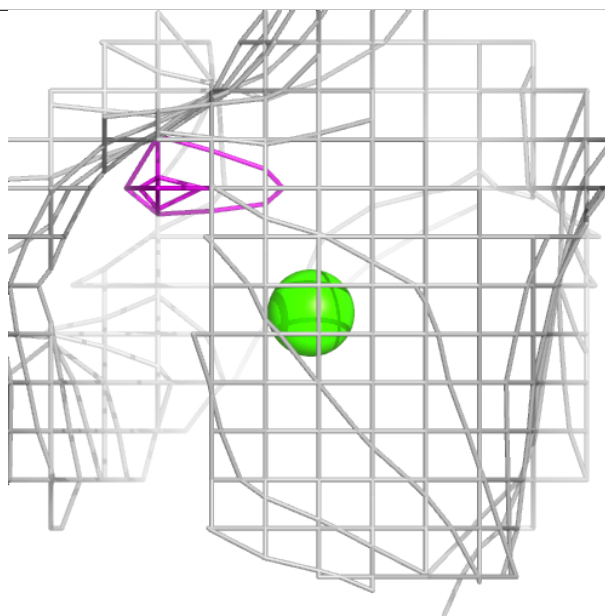
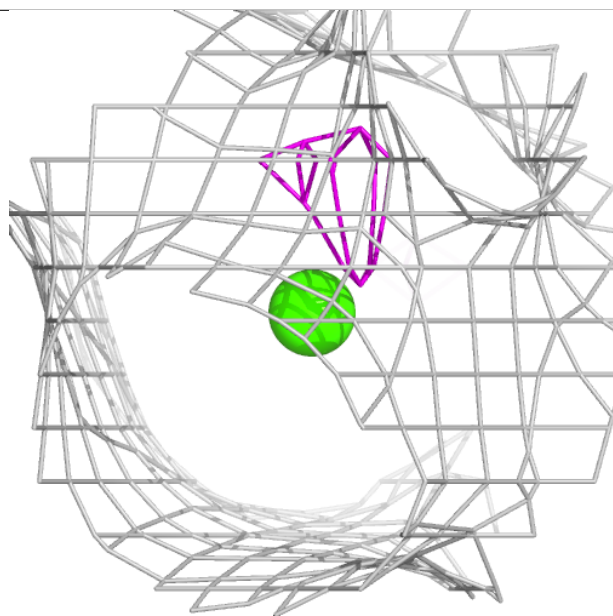
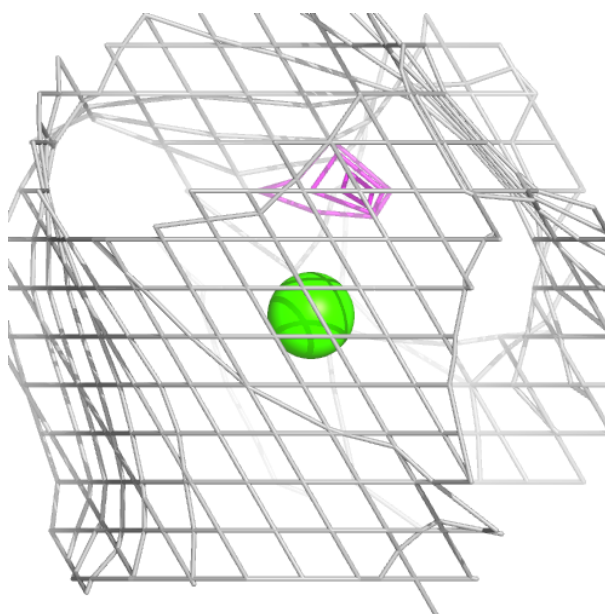
Electron density around CA C 401:

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



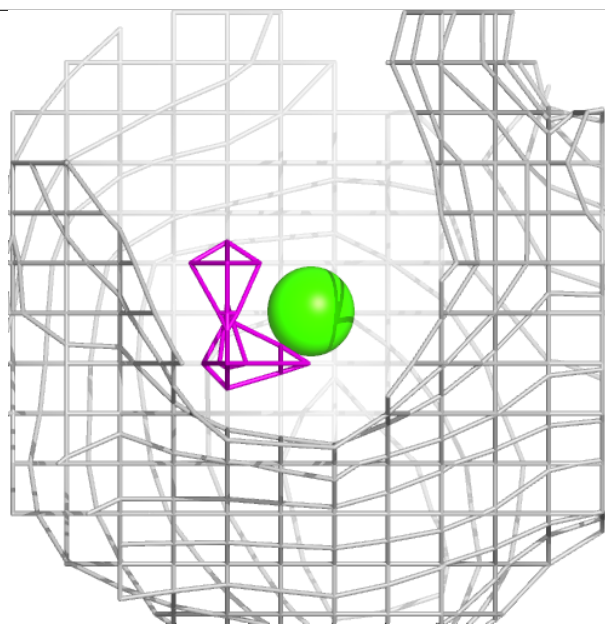
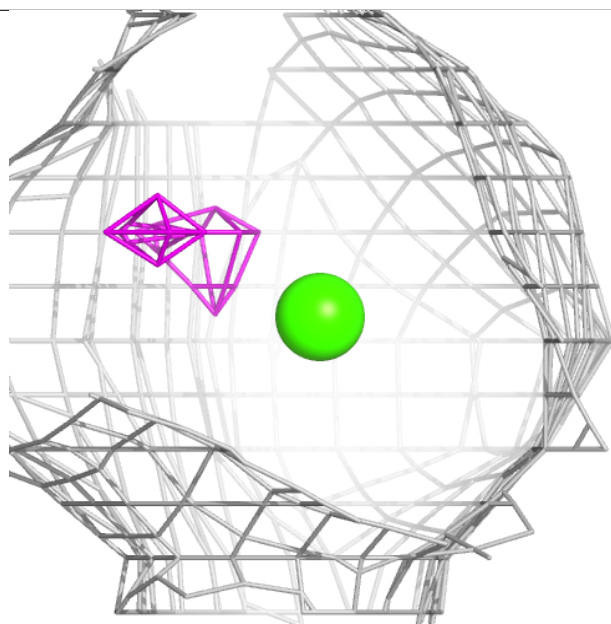
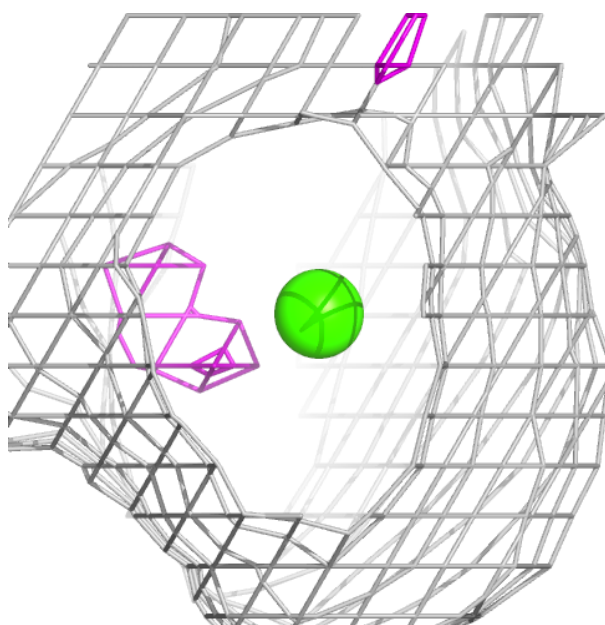
Electron density around CA C 402:

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



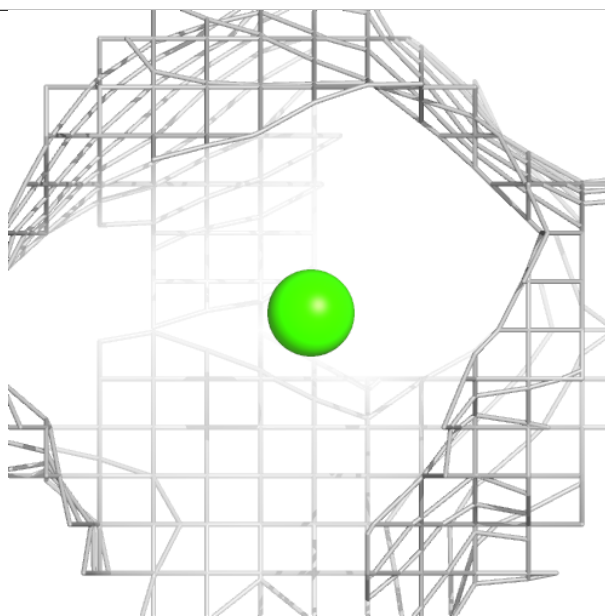
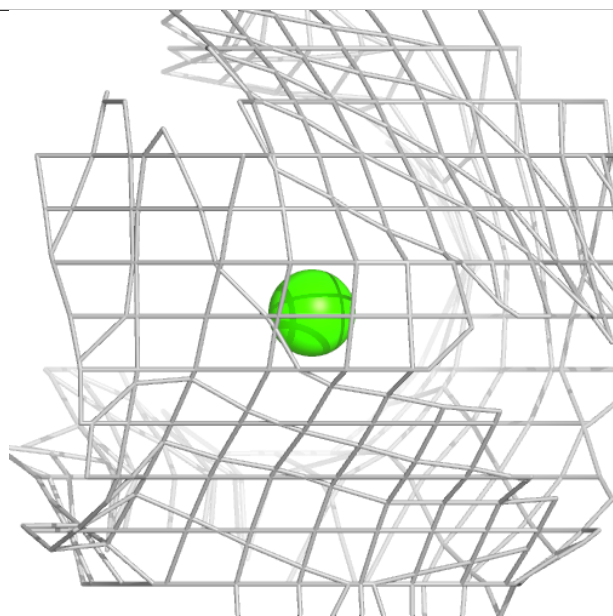
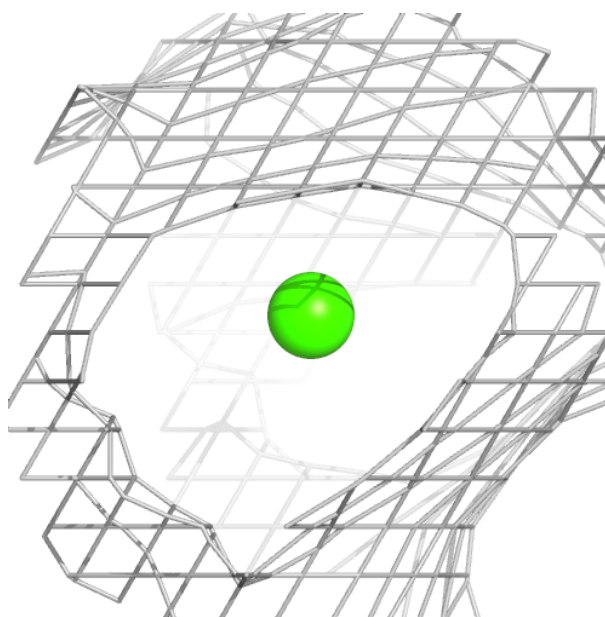
Electron density around CA C 403:

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



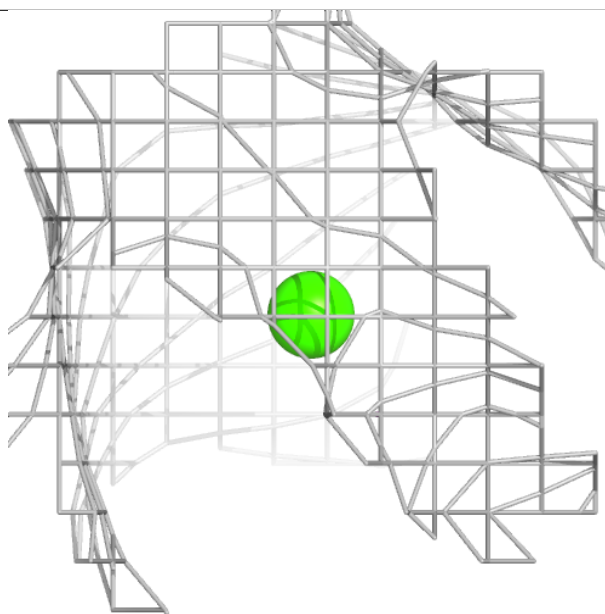
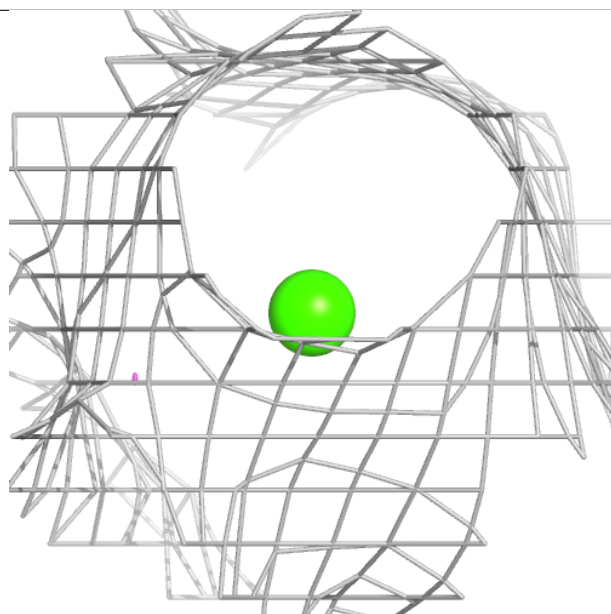
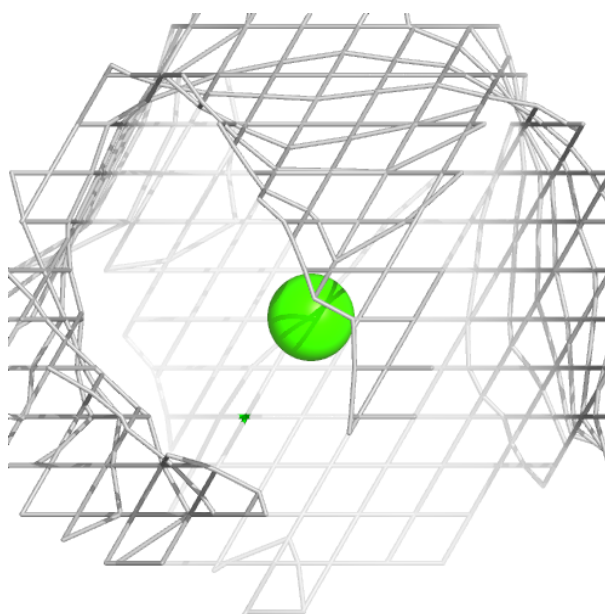
Electron density around CA A 402:

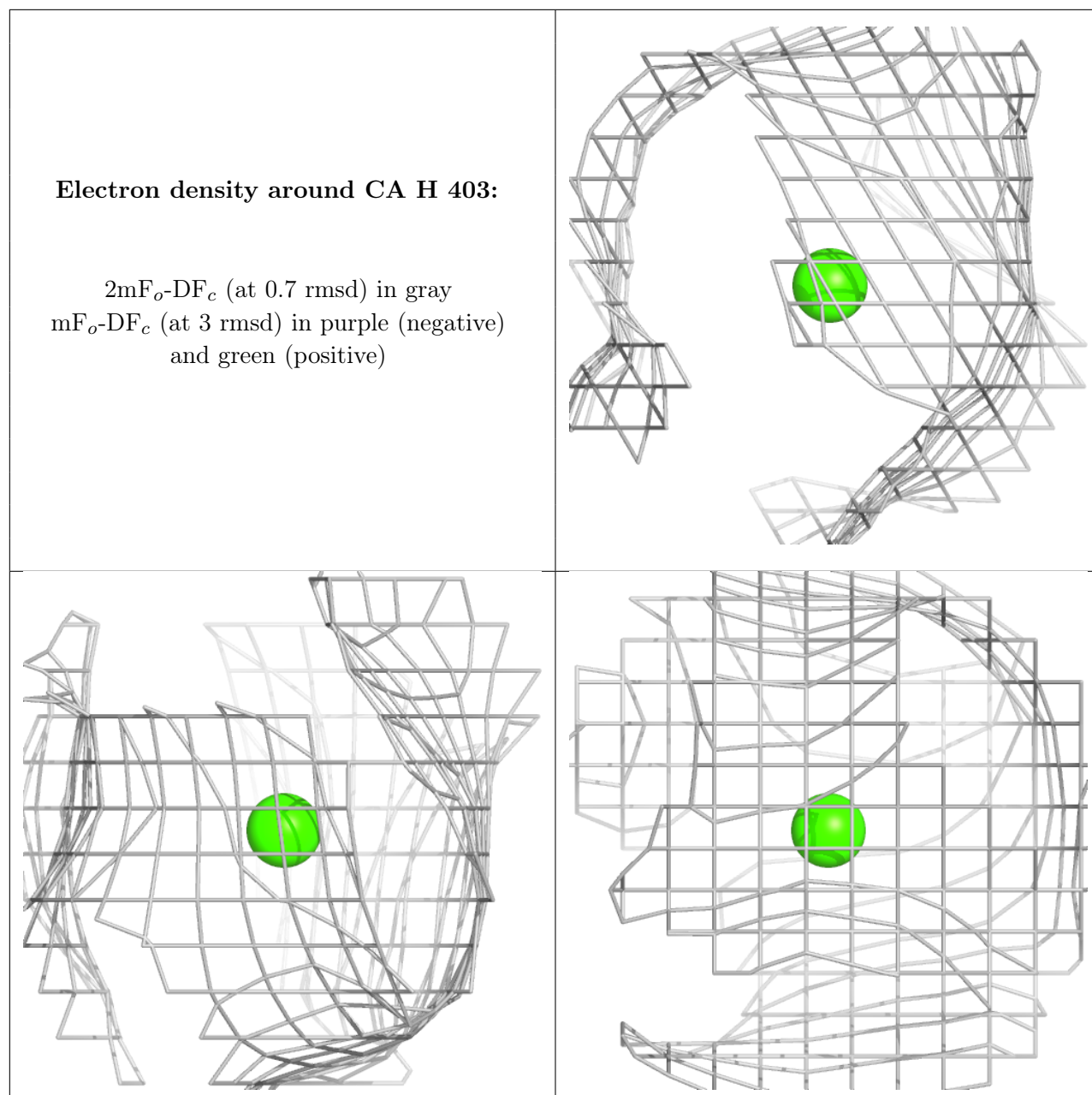
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA H 402:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.