wwPDB X-ray Structure Validation Summary Report (i)

Nov 28, 2023 – 08:11 PM JST

PDB ID	:	8HMG
Title	:	The open state of RGLG2-VWA
Authors	:	Wang, Q.
Deposited on	:	2022-12-03
Resolution	:	2.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

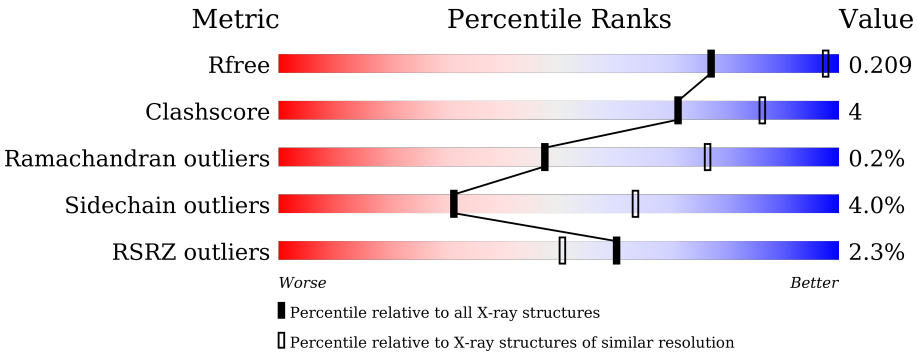
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.81 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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (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 <=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	2% 85% 8% 7%
1	B	307	% 86% 8% 6%
1	C	307	3% 85% 9% • 6%
1	D	307	% 86% 8% • 6%
1	E	307	3% 81% 12% 7%
1	F	307	3% 87% 7% • 6%

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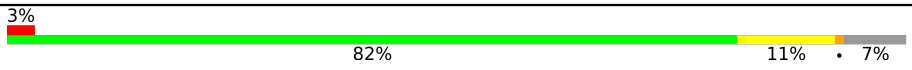
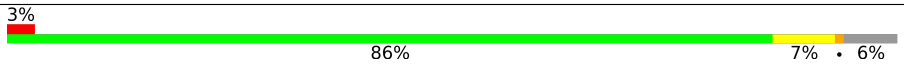
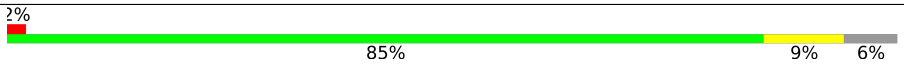
Mol	Chain	Length	Quality of chain
1	G	307	
1	H	307	
1	I	307	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	C	407	-	-	-	X
4	SO4	I	407	-	-	-	X

2 Entry composition (i)

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

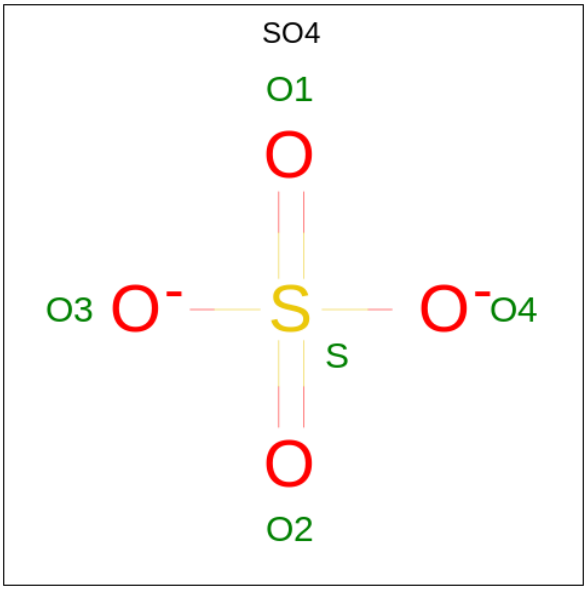
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	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 (three-letter code: SO4) (formula: O_4S) (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 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

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

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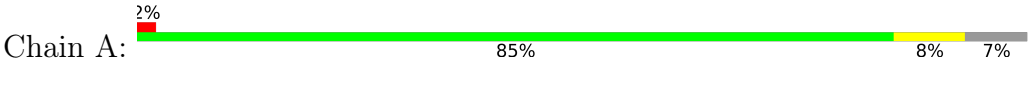
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	66	Total O 66 66	0	0
5	C	58	Total O 58 58	0	0
5	D	68	Total O 68 68	0	0
5	E	45	Total O 45 45	0	0
5	F	44	Total O 44 44	0	0
5	G	46	Total O 46 46	0	0
5	H	41	Total O 41 41	0	0
5	I	44	Total O 44 44	0	0

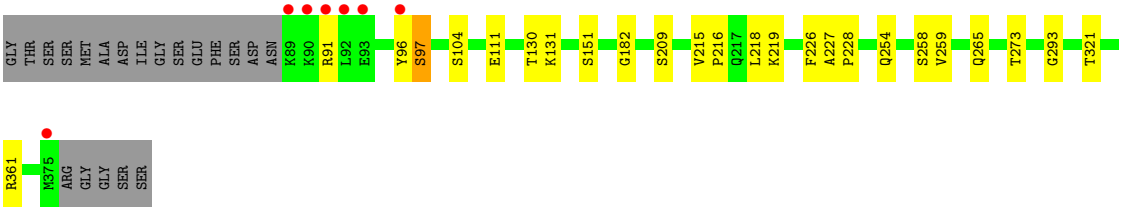
3 Residue-property plots (i)

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

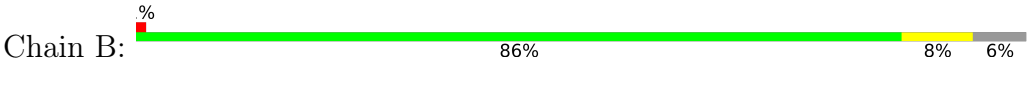
Chain A:

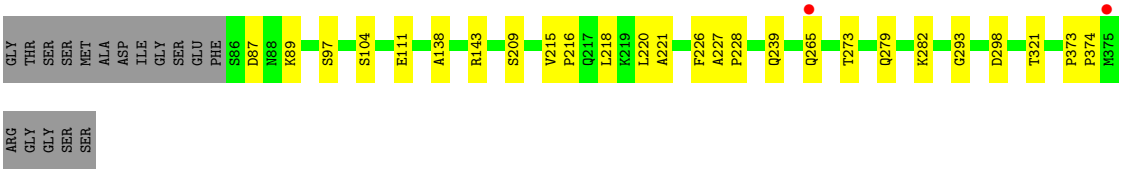




• Molecule 1: E3 ubiquitin-protein ligase RGLG2

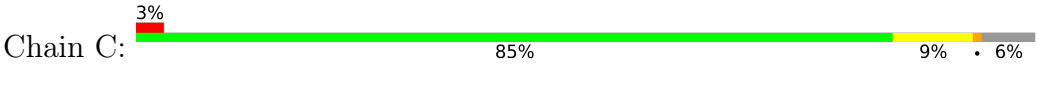
Chain B:

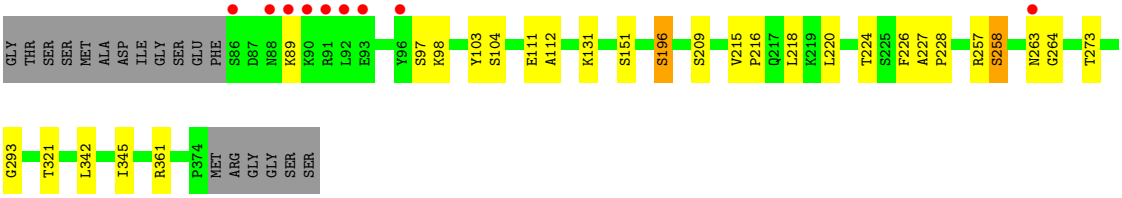




• Molecule 1: E3 ubiquitin-protein ligase RGLG2

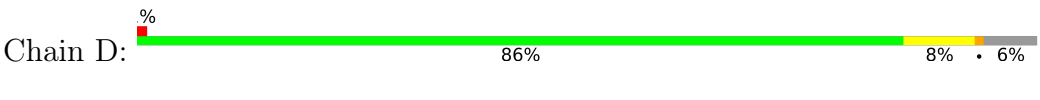
Chain C:

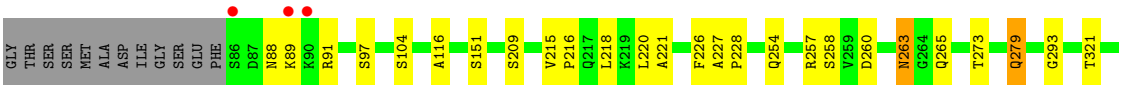


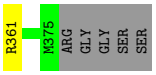


• Molecule 1: E3 ubiquitin-protein ligase RGLG2

Chain D:

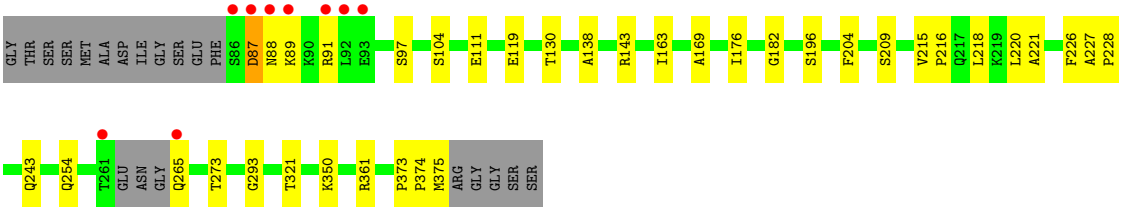






• Molecule 1: E3 ubiquitin-protein ligase RGLG2

Chain E:

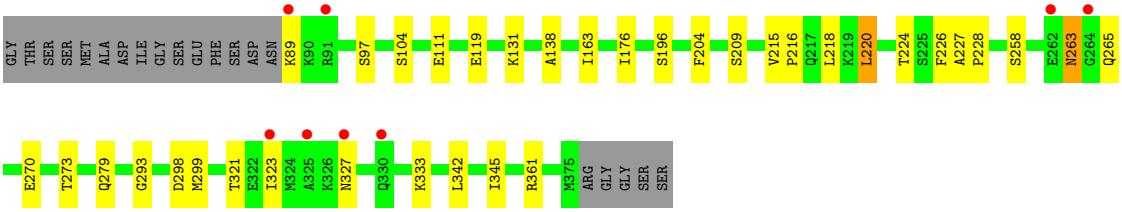


• Molecule 1: E3 ubiquitin-protein ligase RGLG2

Chain F:

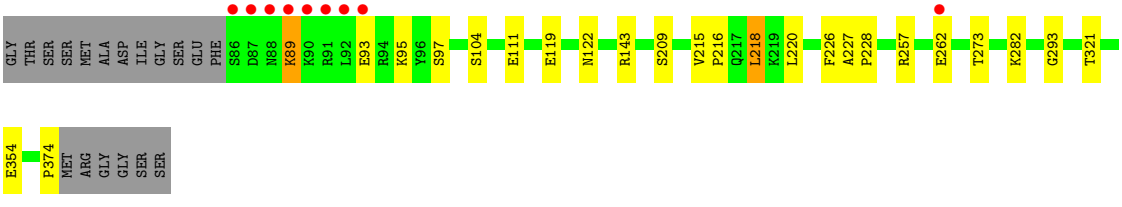
• Molecule 1: E3 ubiquitin-protein ligase RGLG2

Chain G:



• Molecule 1: E3 ubiquitin-protein ligase RGLG2

Chain H:



• Molecule 1: E3 ubiquitin-protein ligase RGLG2

Chain I:

GLY
THR
SER
SER
MET
ALA
ASP
ILE
GLY
SER
GLU
PHE
S86
D87
N88
K89
K90
R91
L92
E93
R94
S97
S104
E111
E119
N122
A138
R143
S151
S196
S209
V215
P216
Q217
L218
F226
A227
P228
D252
D260
T261
E262
N263
G264
Q265
E270
T273
G293
M299
T321
A329
L355
M375
ARG
GLY
GLY
SER
SER

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.44 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.183 , 0.208 0.191 , 0.209	Depositor DCC
R_{free} test set	5114 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)	0.30 , 31.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SO4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.67	0/2305	0.80	0/3121
1	B	0.67	0/2327	0.81	0/3151
1	C	0.66	0/2319	0.81	0/3141
1	D	0.69	0/2327	0.82	0/3151
1	E	0.67	0/2305	0.80	0/3120
1	F	0.67	0/2321	0.81	0/3143
1	G	0.66	0/2305	0.80	0/3121
1	H	0.68	0/2319	0.80	0/3141
1	I	0.66	0/2327	0.80	0/3151
All	All	0.67	0/20855	0.80	0/28240

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

There are no bond length outliers.

There are no bond angle outliers.

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	16	0
1	B	2280	0	2228	12	0
1	C	2272	0	2219	16	0
1	D	2280	0	2228	21	0
1	E	2259	0	2212	19	0
1	F	2274	0	2223	17	0
1	G	2258	0	2213	21	0
1	H	2272	0	2220	16	0
1	I	2280	0	2228	19	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	142	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.

The worst 5 of 142 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: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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	285/307 (93%)	268 (94%)	17 (6%)	0	100 100
1	B	288/307 (94%)	272 (94%)	15 (5%)	1 (0%)	41 70
1	C	287/307 (94%)	269 (94%)	18 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	288/307 (94%)	271 (94%)	17 (6%)	0	100	100
1	E	283/307 (92%)	271 (96%)	11 (4%)	1 (0%)	34	64
1	F	287/307 (94%)	269 (94%)	17 (6%)	1 (0%)	41	70
1	G	285/307 (93%)	269 (94%)	15 (5%)	1 (0%)	34	64
1	H	287/307 (94%)	271 (94%)	16 (6%)	0	100	100
1	I	288/307 (94%)	271 (94%)	16 (6%)	1 (0%)	41	70
All	All	2578/2763 (93%)	2431 (94%)	142 (6%)	5 (0%)	47	76

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/263 (94%)	239 (96%)	9 (4%)	35	67
1	B	251/263 (95%)	240 (96%)	11 (4%)	28	60
1	C	250/263 (95%)	240 (96%)	10 (4%)	31	64
1	D	251/263 (95%)	241 (96%)	10 (4%)	31	64
1	E	249/263 (95%)	238 (96%)	11 (4%)	28	60
1	F	250/263 (95%)	242 (97%)	8 (3%)	39	71
1	G	248/263 (94%)	237 (96%)	11 (4%)	28	60
1	H	250/263 (95%)	241 (96%)	9 (4%)	35	67
1	I	251/263 (95%)	241 (96%)	10 (4%)	31	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2248/2367 (95%)	2159 (96%)	89 (4%)	31 64

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	265	GLN
1	H	97	SER
1	G	97	SER
1	G	258	SER
1	H	209	SER

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

Mol	Chain	Res	Type
1	G	254	GLN
1	H	254	GLN
1	I	263	ASN
1	I	187	HIS
1	H	187	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	D	405	-	4,4,4	0.35	0	6,6,6	0.17	0
4	SO4	D	407	-	4,4,4	0.32	0	6,6,6	0.20	0
4	SO4	E	406	-	4,4,4	0.34	0	6,6,6	0.24	0
4	SO4	C	406	-	4,4,4	0.32	0	6,6,6	0.17	0
4	SO4	F	405	-	4,4,4	0.39	0	6,6,6	0.11	0
4	SO4	I	405	-	4,4,4	0.30	0	6,6,6	0.36	0
4	SO4	E	405	-	4,4,4	0.33	0	6,6,6	0.21	0
4	SO4	C	405	-	4,4,4	0.29	0	6,6,6	0.20	0
4	SO4	B	405	-	4,4,4	0.31	0	6,6,6	0.12	0
4	SO4	A	406	-	4,4,4	0.35	0	6,6,6	0.15	0
4	SO4	A	405	-	4,4,4	0.33	0	6,6,6	0.33	0
4	SO4	H	406	-	4,4,4	0.31	0	6,6,6	0.12	0
4	SO4	H	405	-	4,4,4	0.32	0	6,6,6	0.09	0
4	SO4	I	406	-	4,4,4	0.29	0	6,6,6	0.17	0
4	SO4	C	408	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	I	407	-	4,4,4	0.35	0	6,6,6	0.13	0
4	SO4	D	406	-	4,4,4	0.29	0	6,6,6	0.14	0
4	SO4	C	407	-	4,4,4	0.34	0	6,6,6	0.10	0
4	SO4	B	406	-	4,4,4	0.32	0	6,6,6	0.23	0
4	SO4	G	405	-	4,4,4	0.32	0	6,6,6	0.09	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.

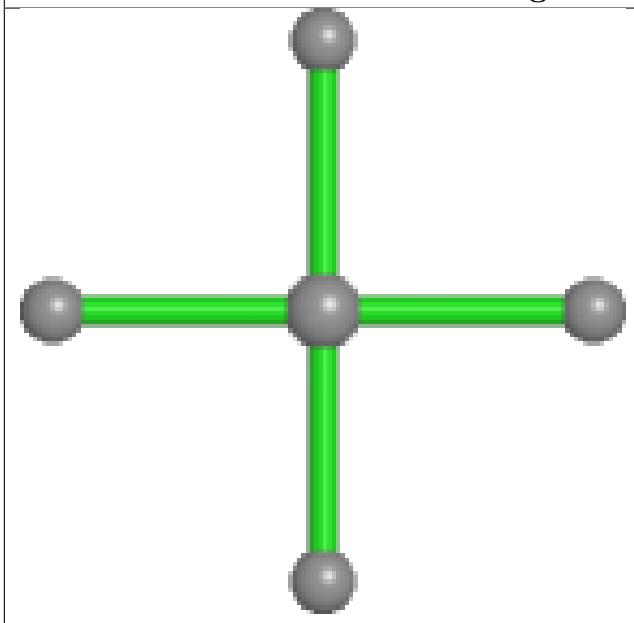
1 monomer is involved in 1 short contact:

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

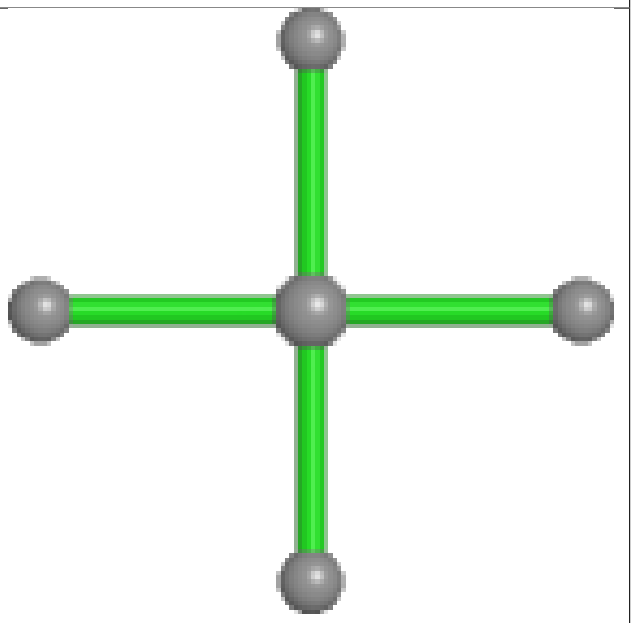
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

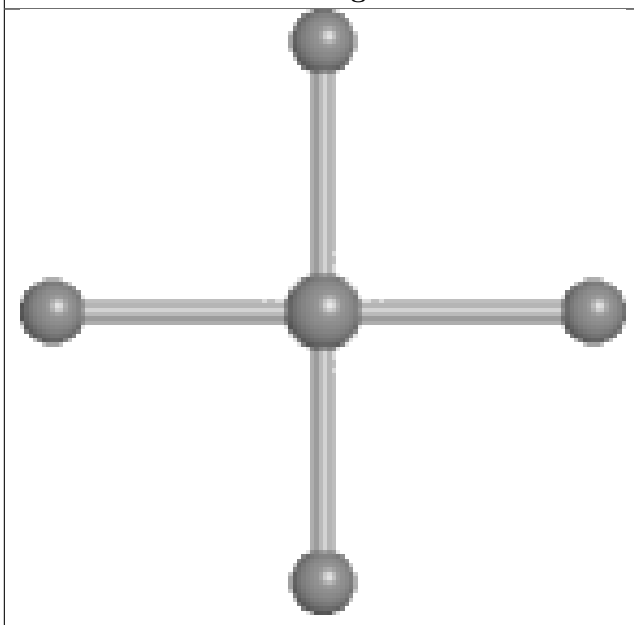
Ligand SO4 D 405



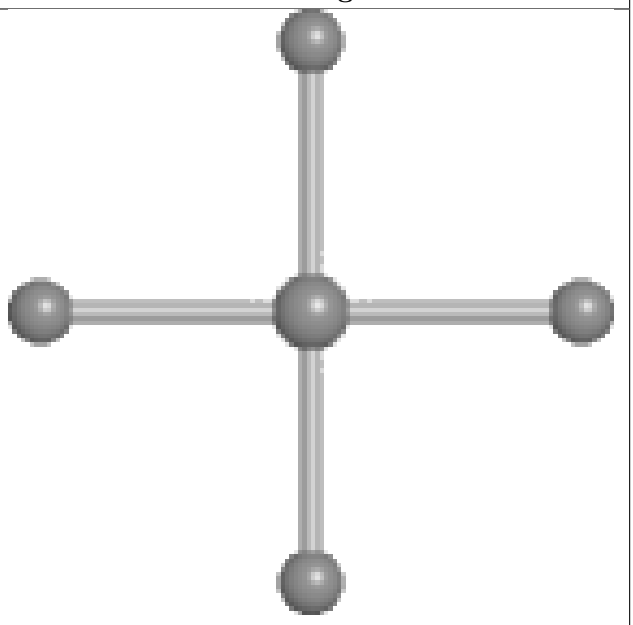
Bond lengths



Bond angles

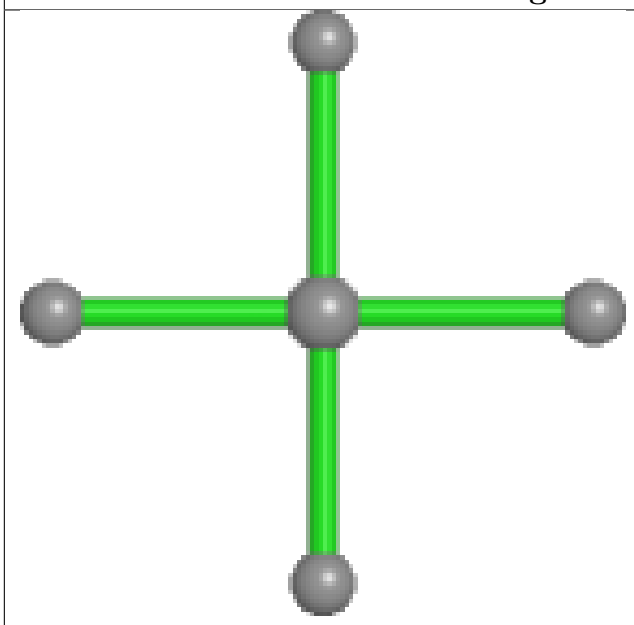


Torsions



Rings

Ligand SO4 D 407



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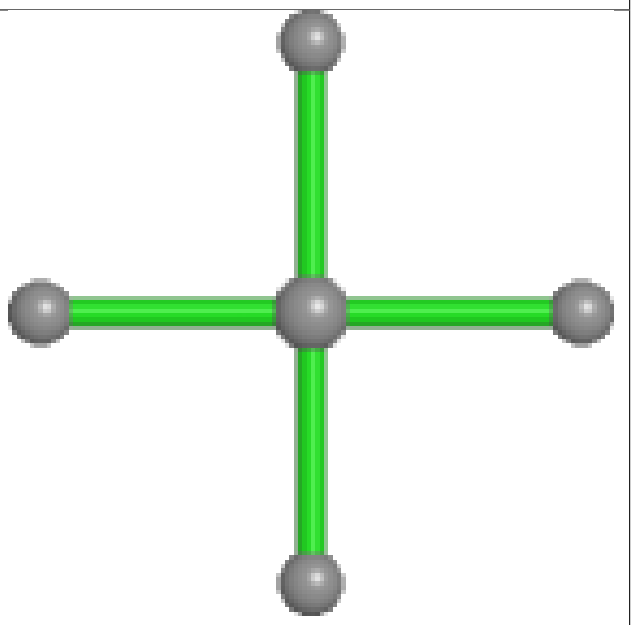

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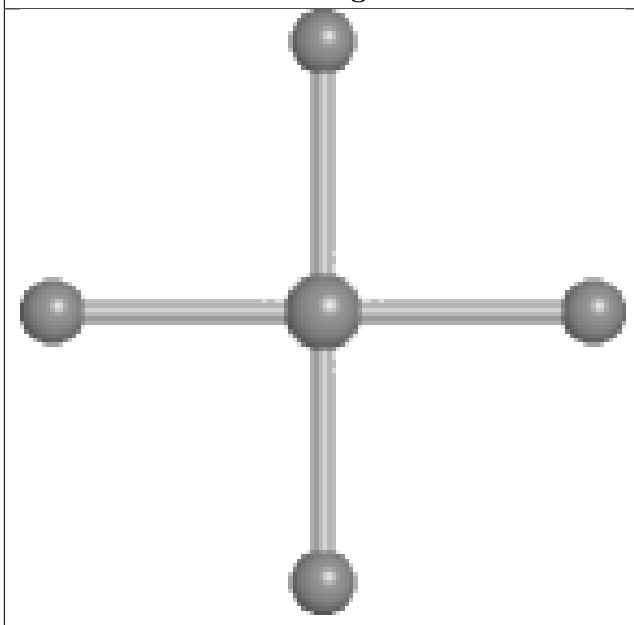

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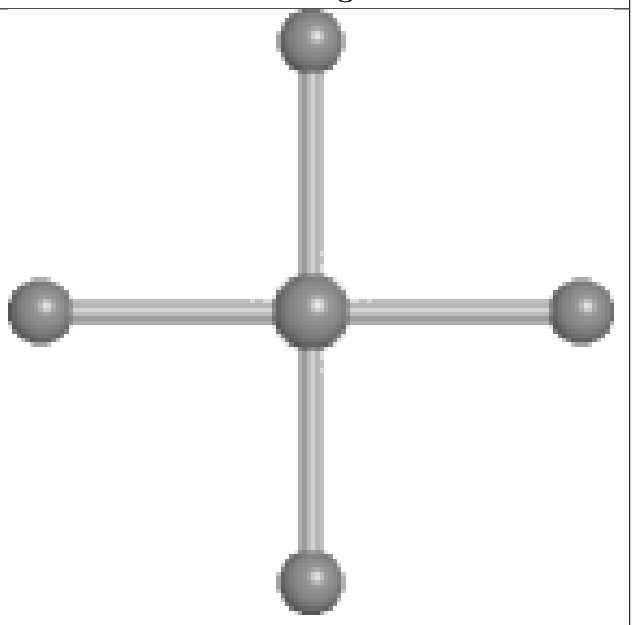
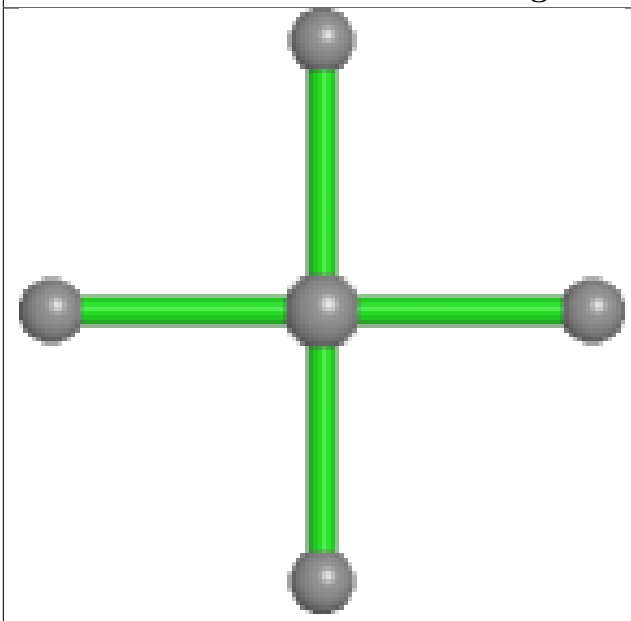


Rings

Ligand SO4 E 406



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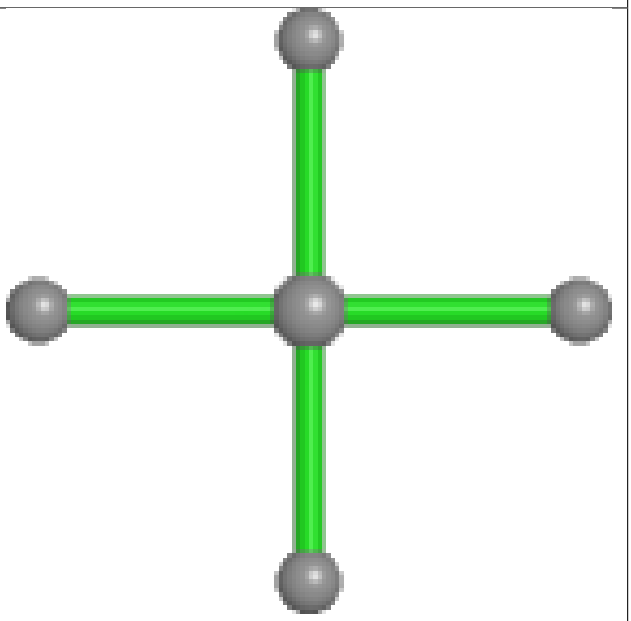

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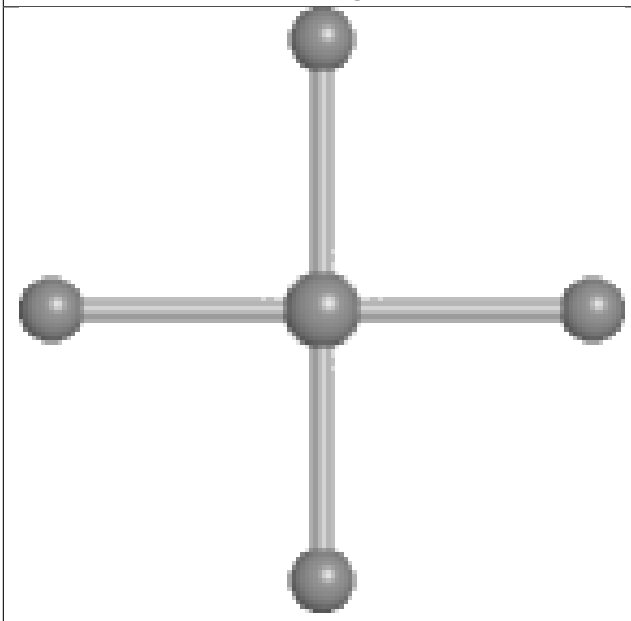

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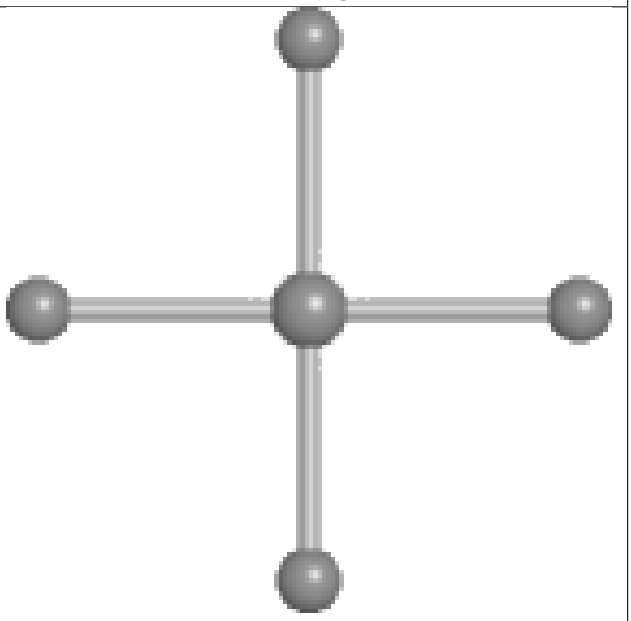
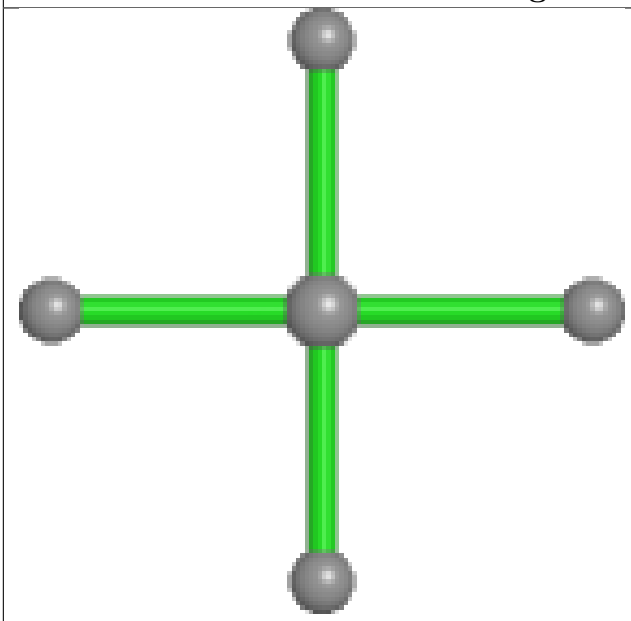


Rings

Ligand SO4 C 406



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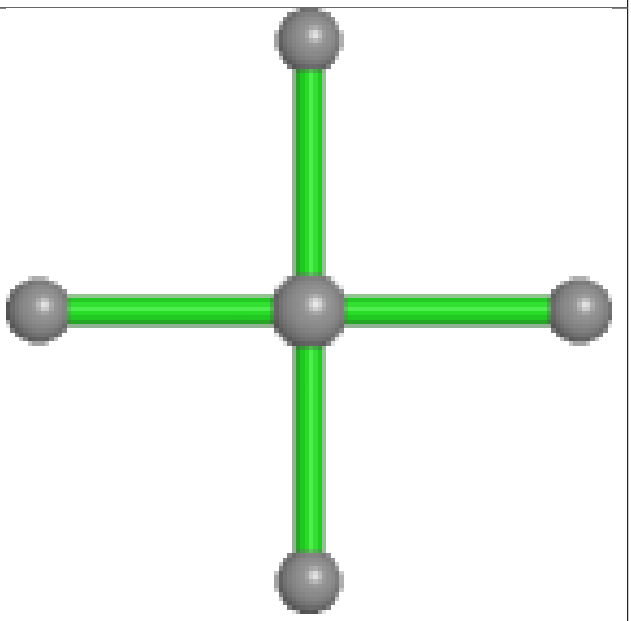

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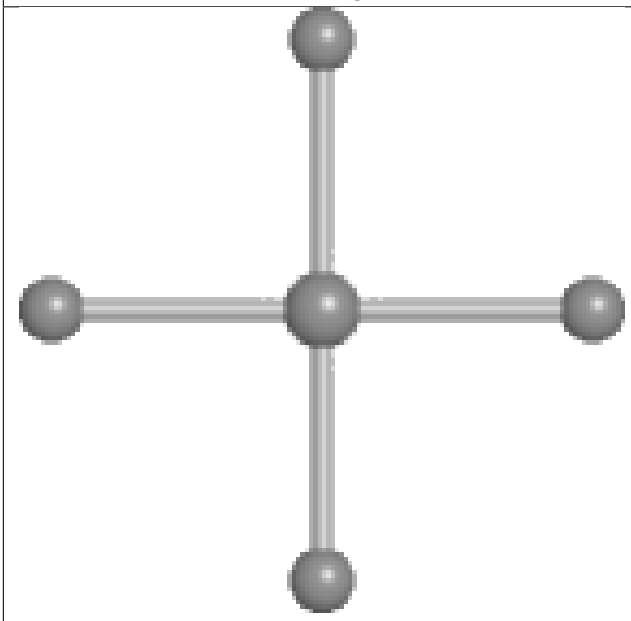

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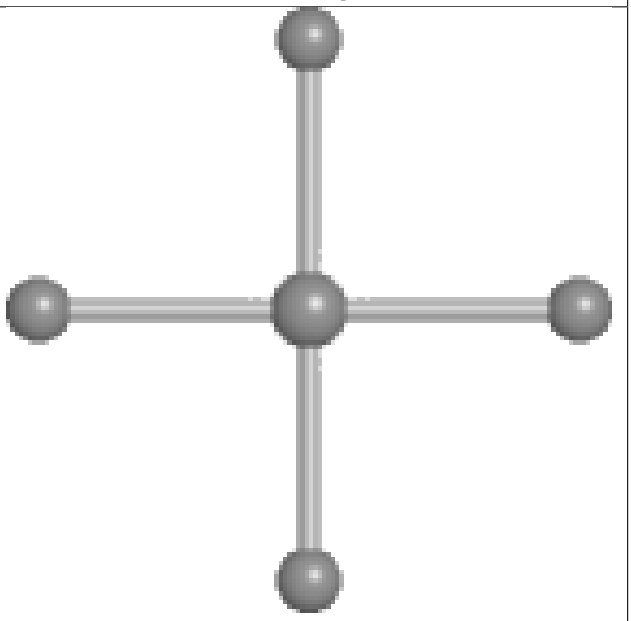
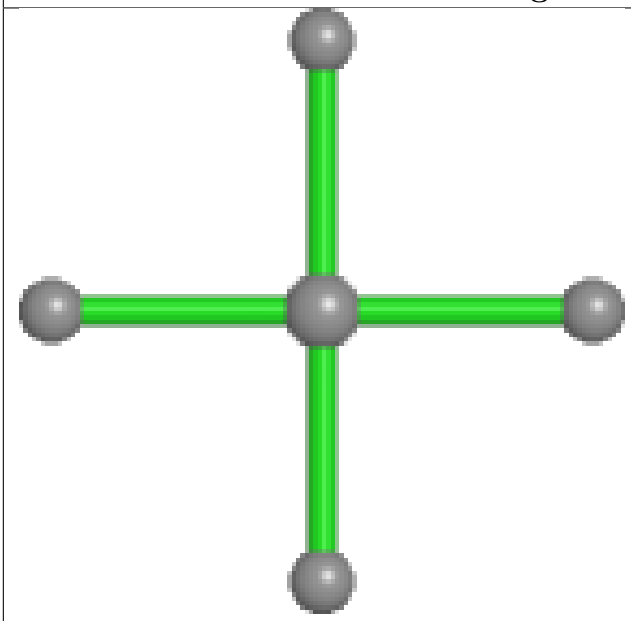


Rings

Ligand SO4 F 405



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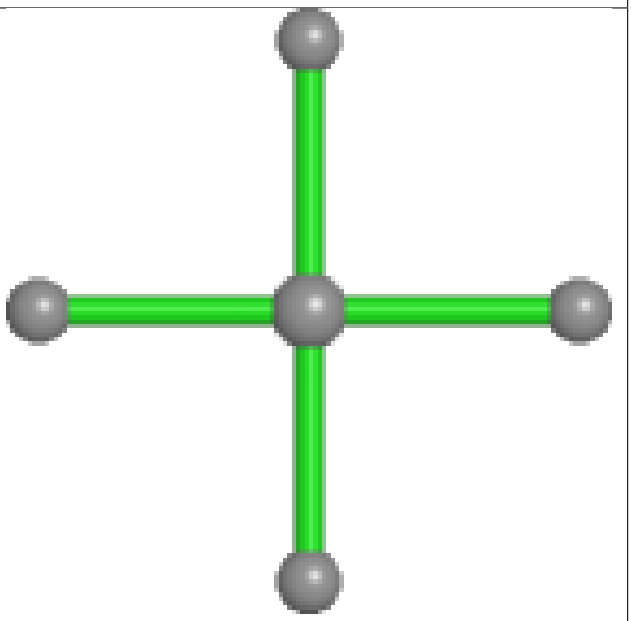
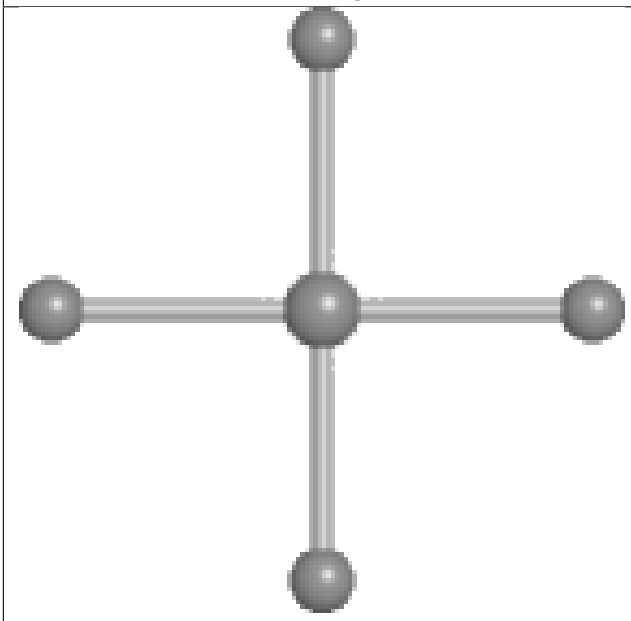


Bond angles



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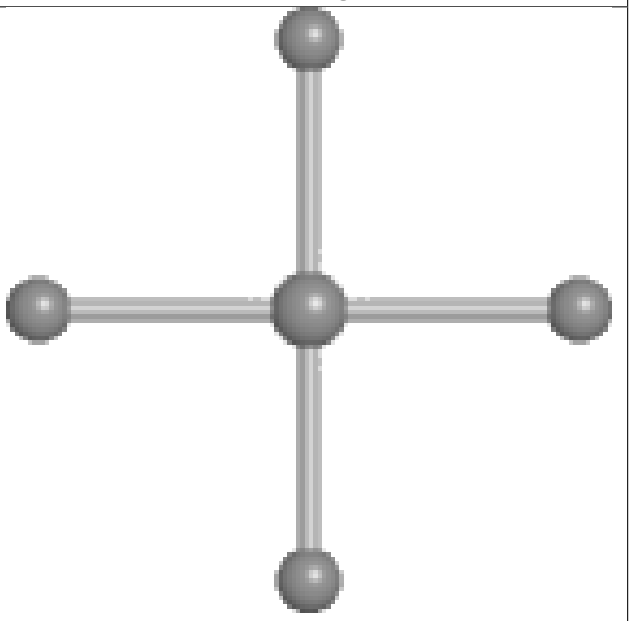
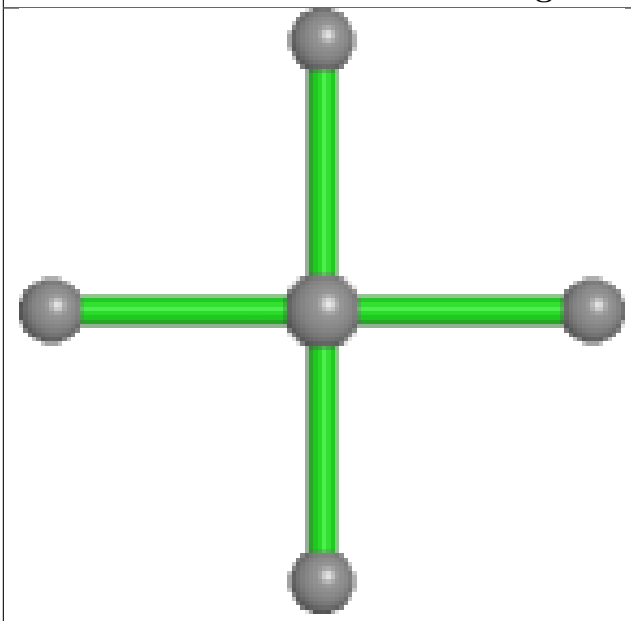
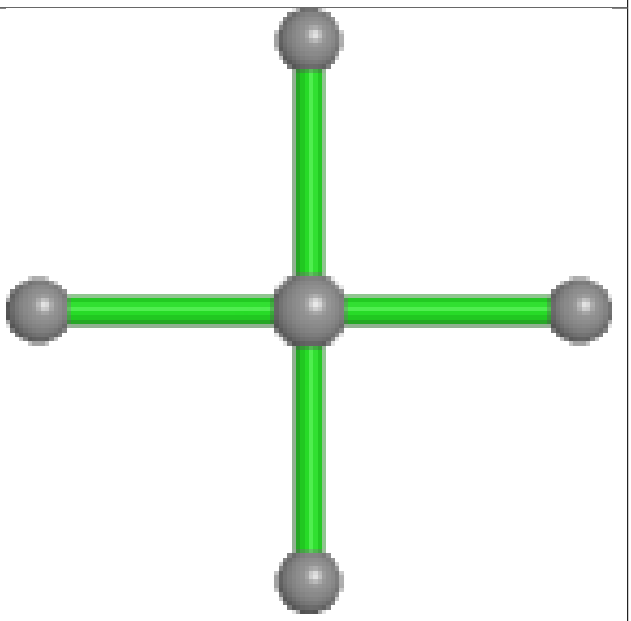


Rings

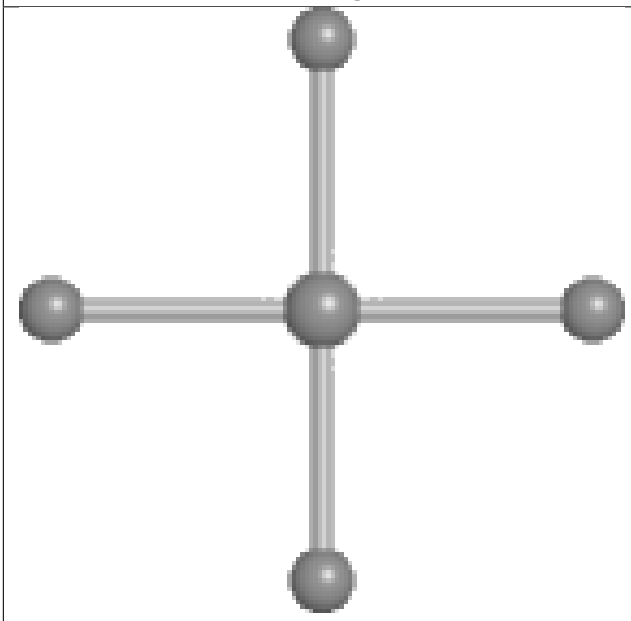
Ligand SO4 I 405



Bond lengths



Bond angles



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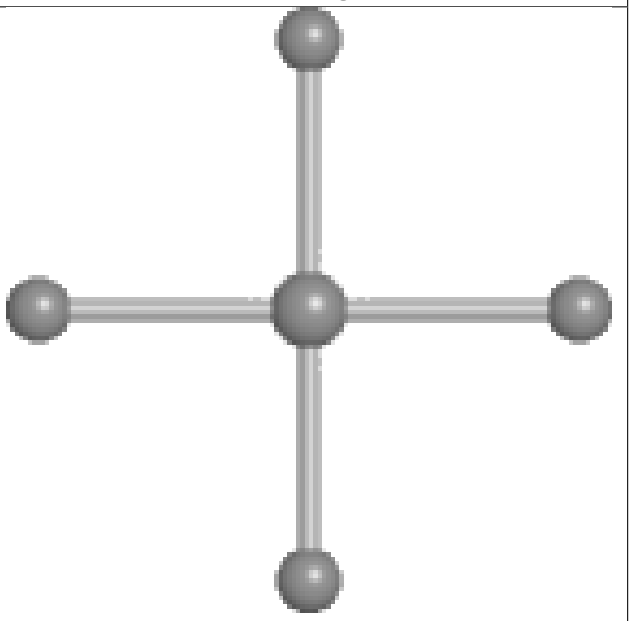
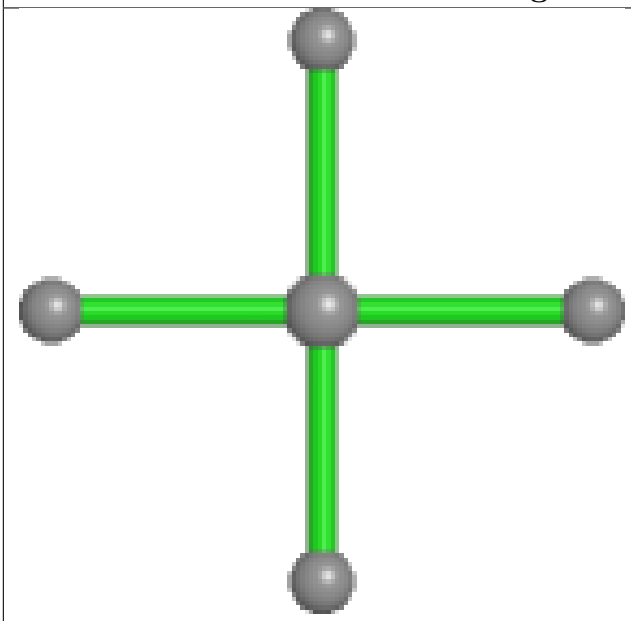
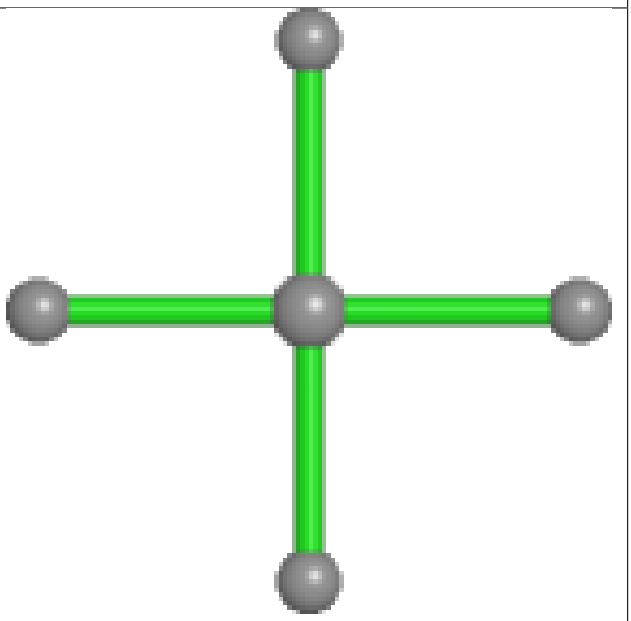


Rings

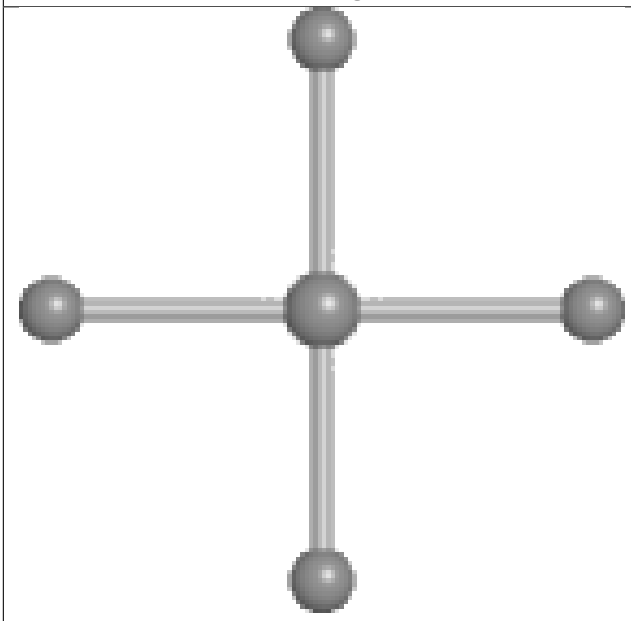
Ligand SO4 E 405



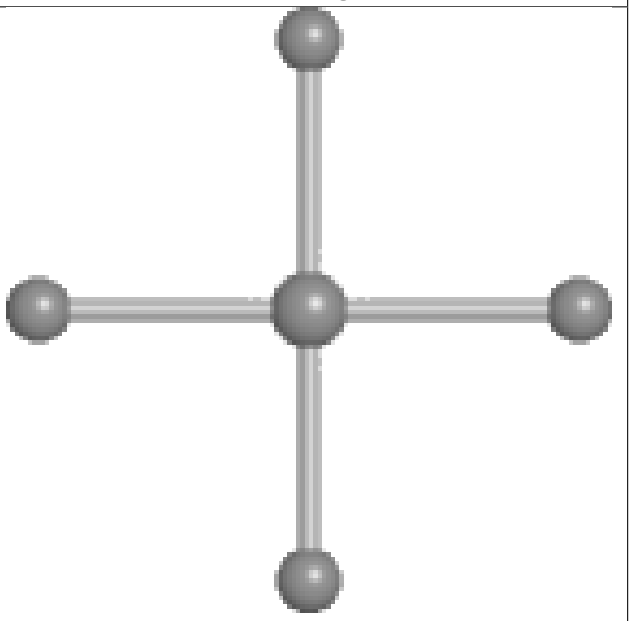
Bond lengths



Bond angles

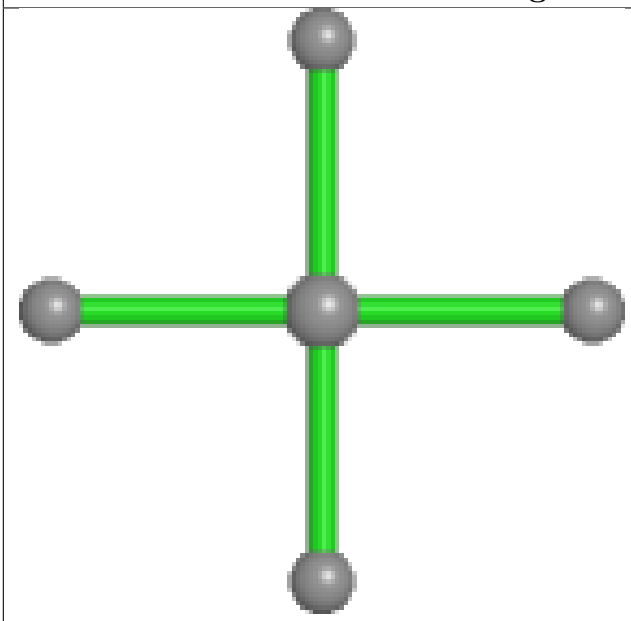


Torsions



Rings

Ligand SO4 C 405



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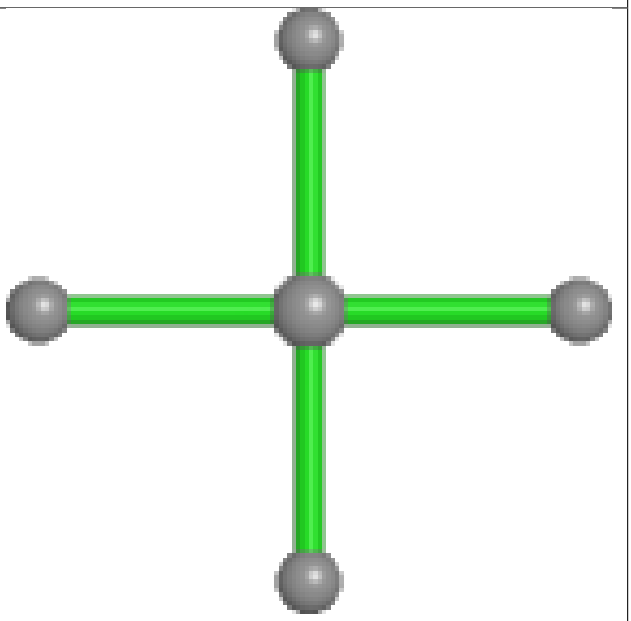
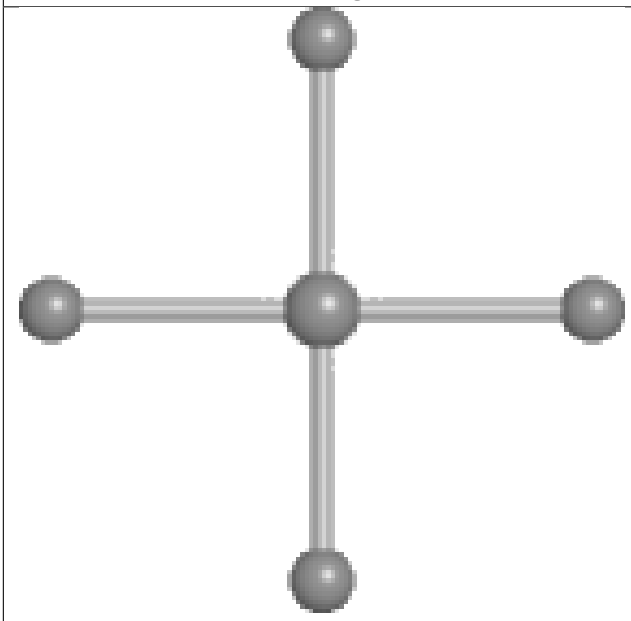


Bond angles



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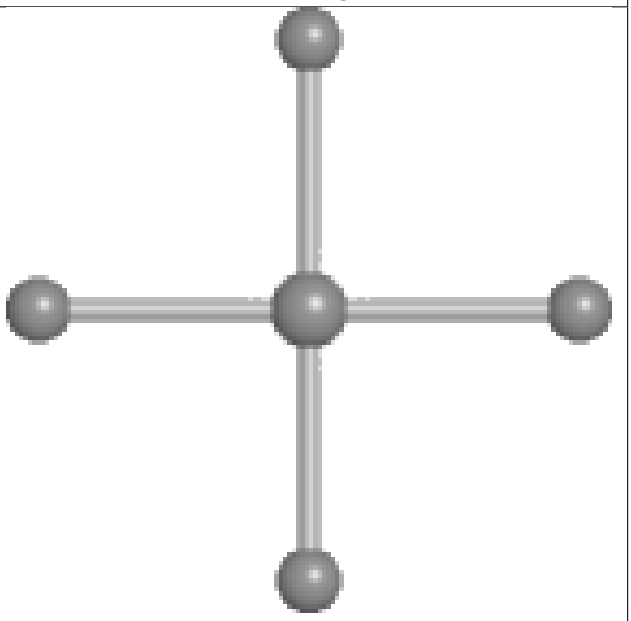
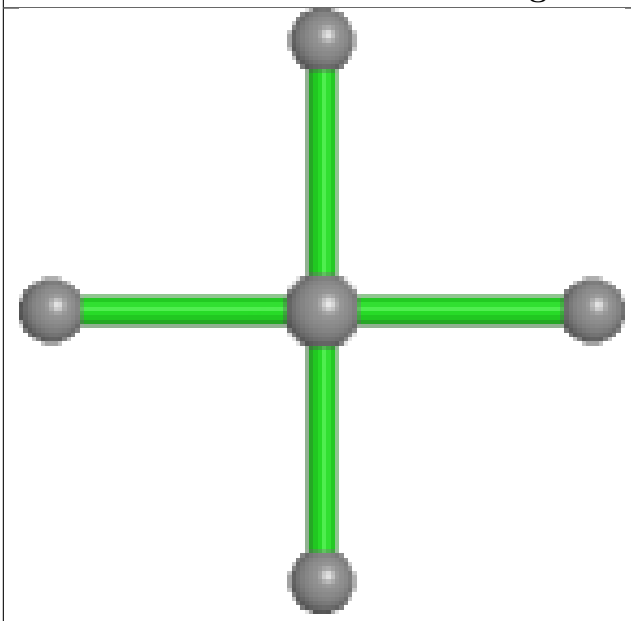


Rings

Ligand SO4 B 405



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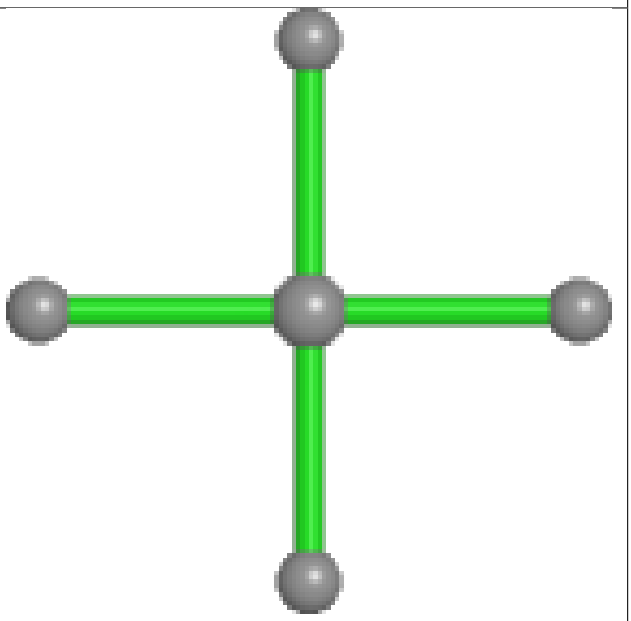
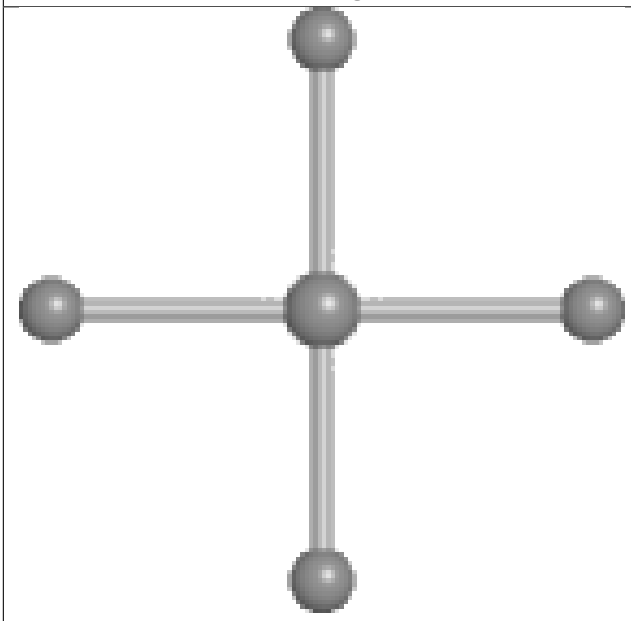


Bond angles



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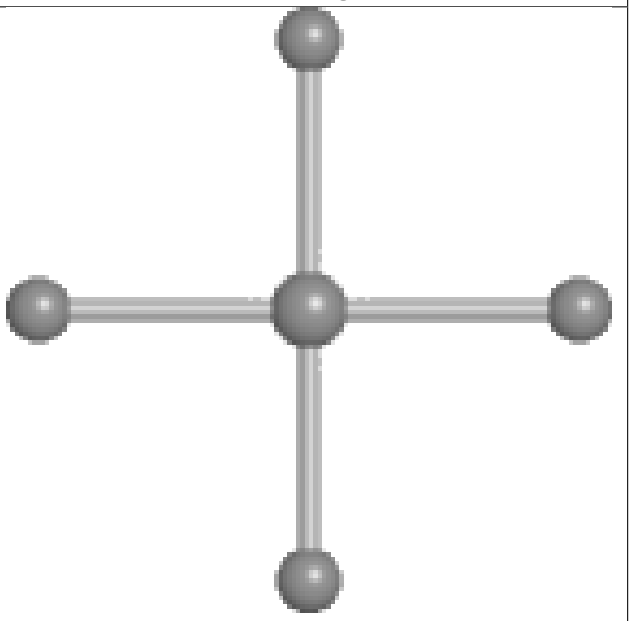
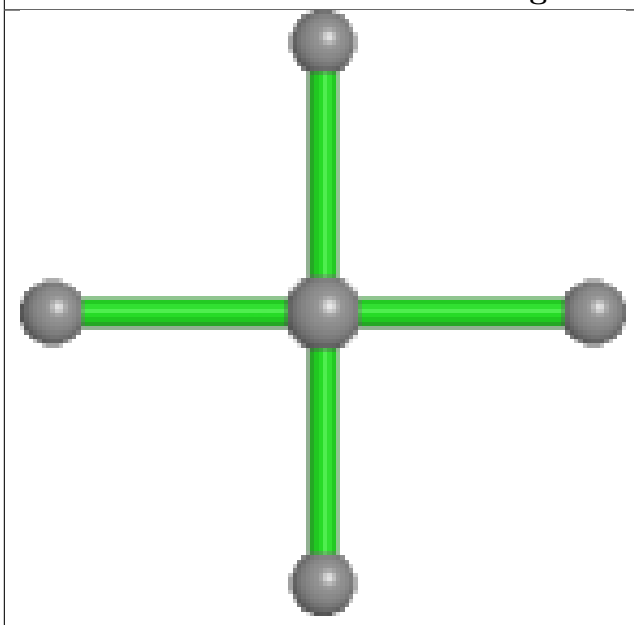


Rings

Ligand SO4 A 406



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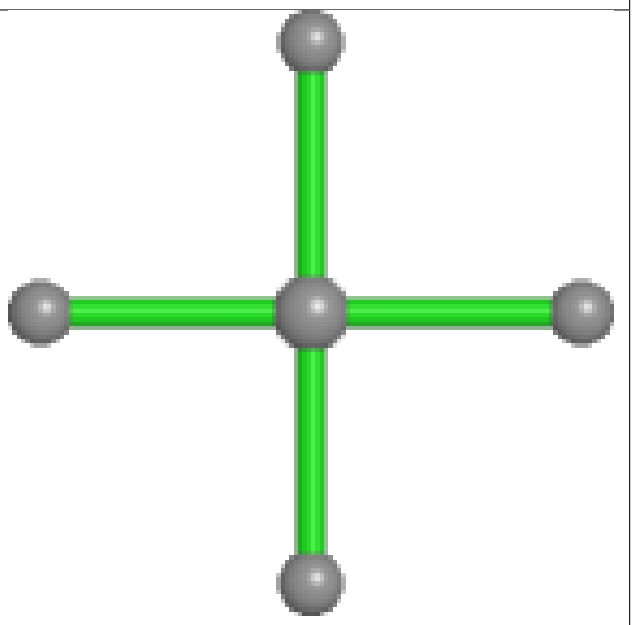

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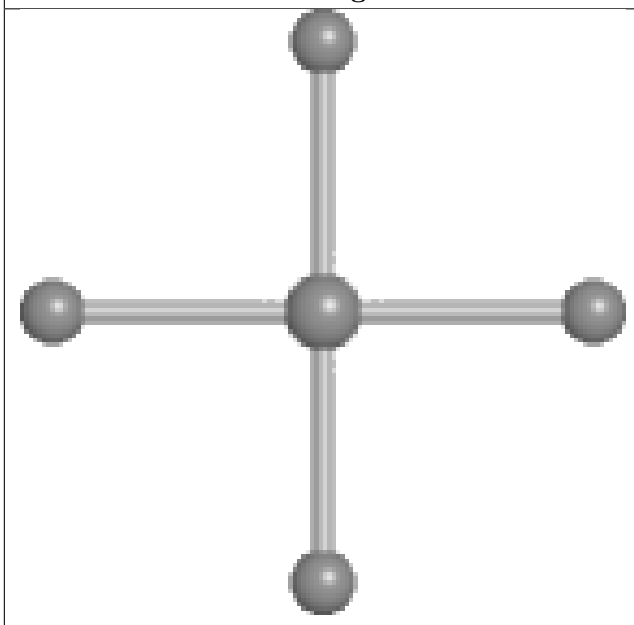

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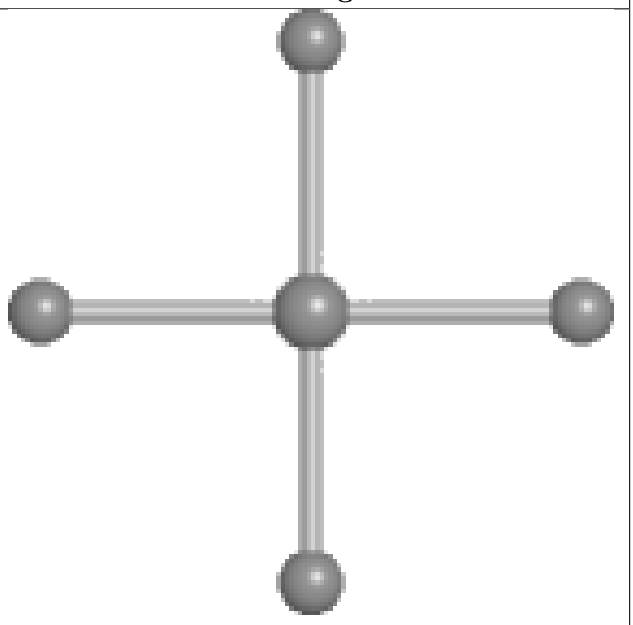
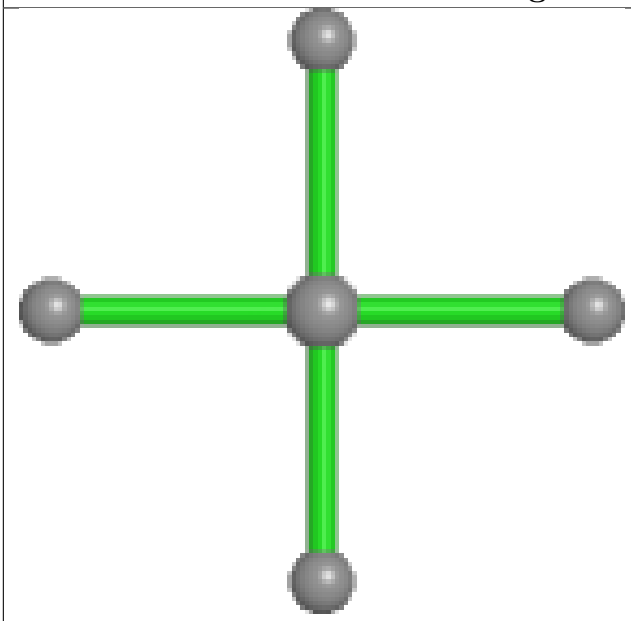


Rings

Ligand SO4 A 405



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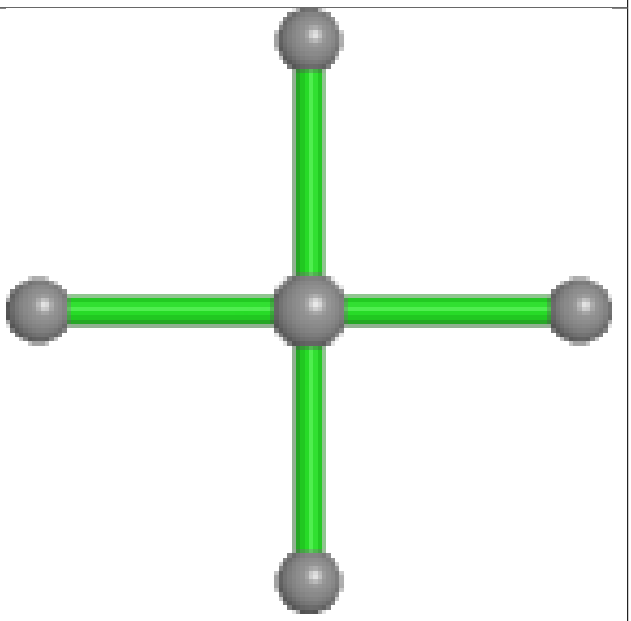
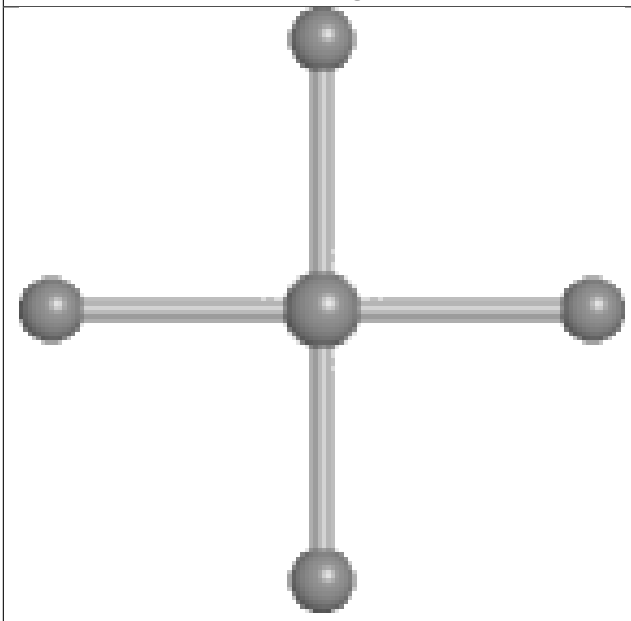


Bond angles



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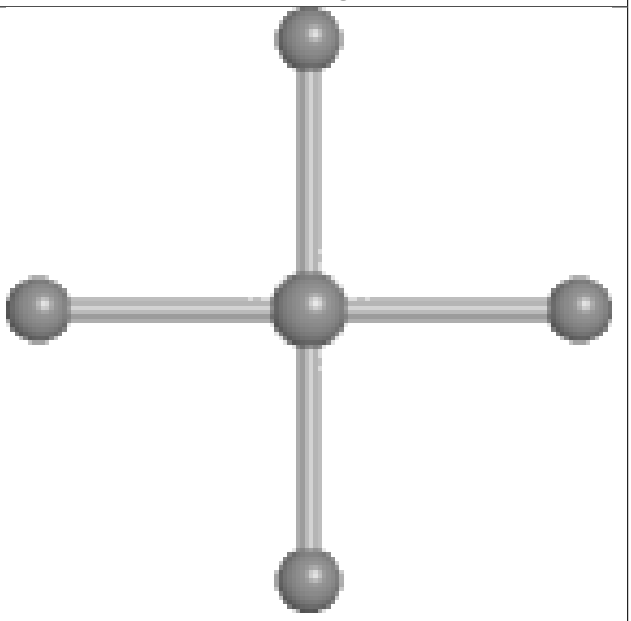
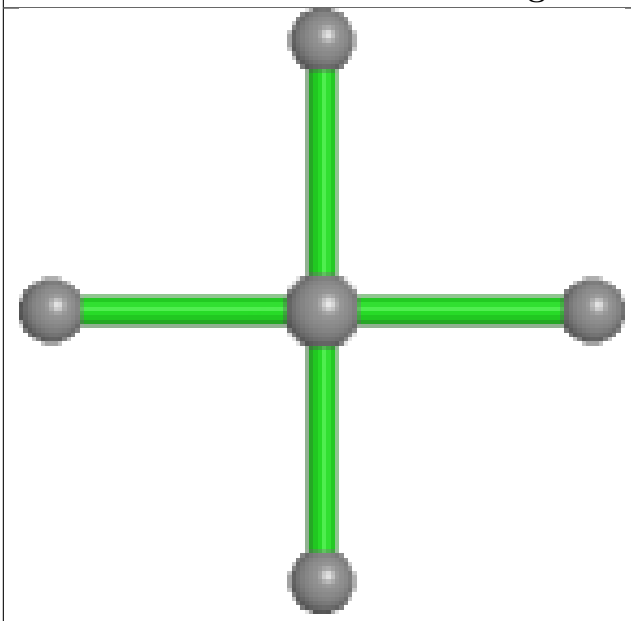


Rings

Ligand SO4 H 406



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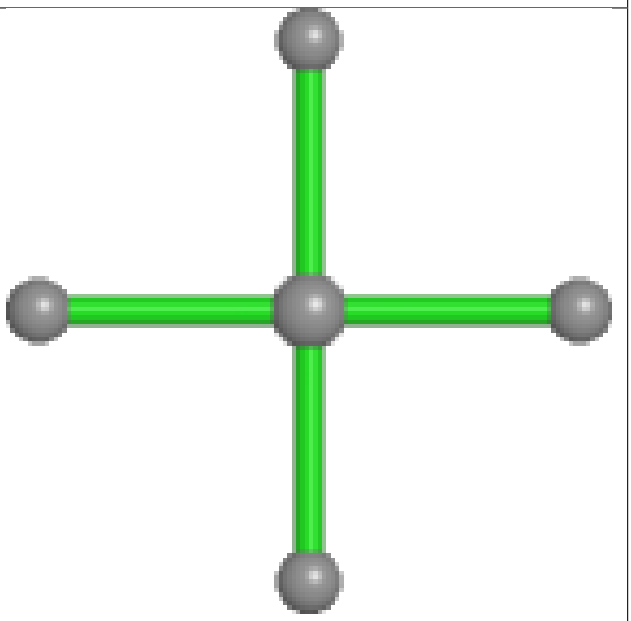

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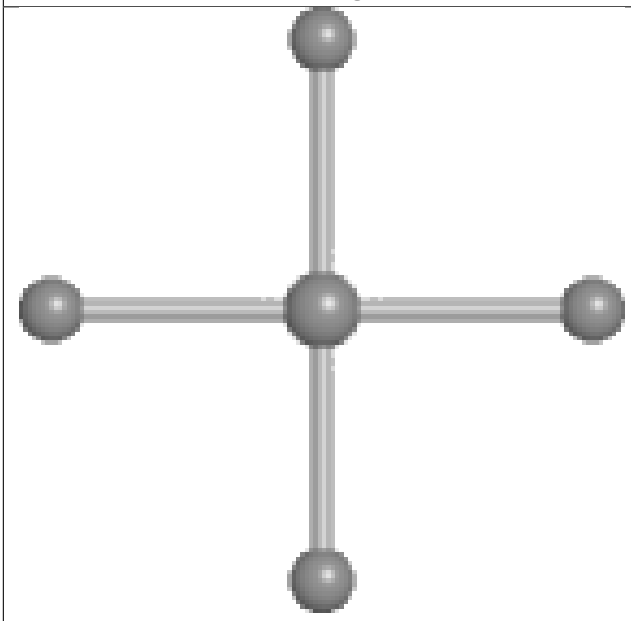
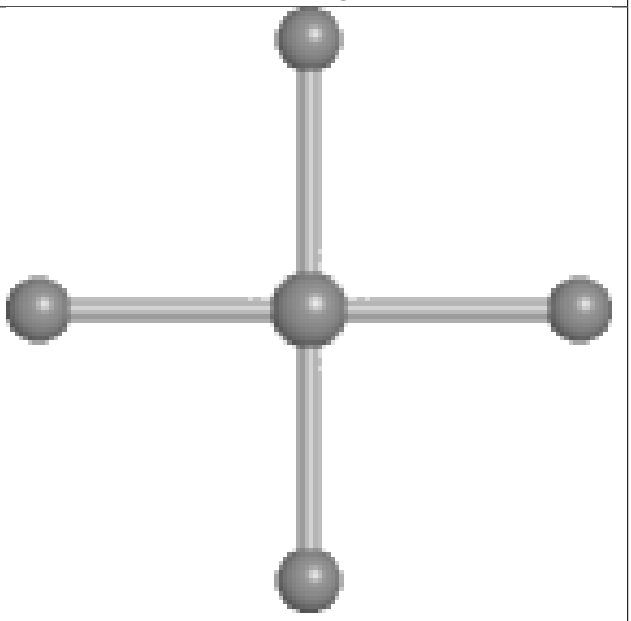
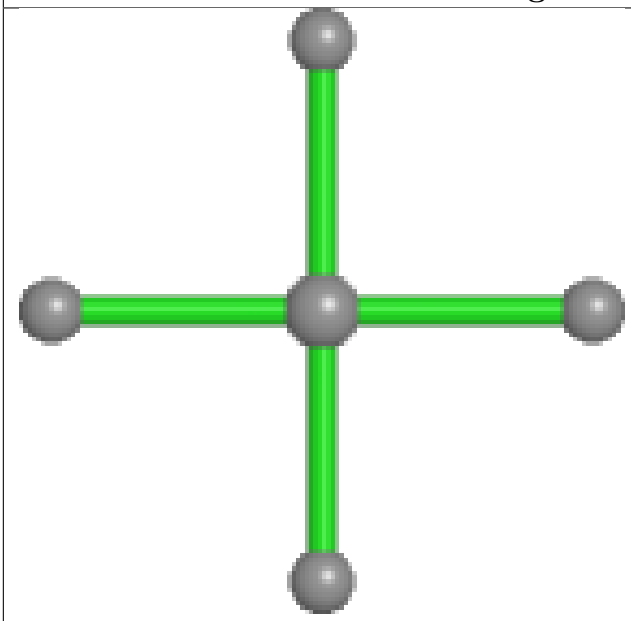


Torsions



Rings

Ligand SO4 H 405



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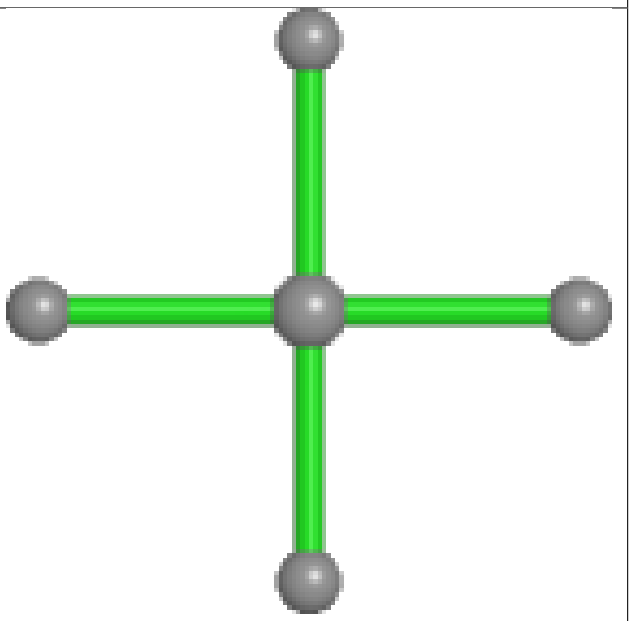

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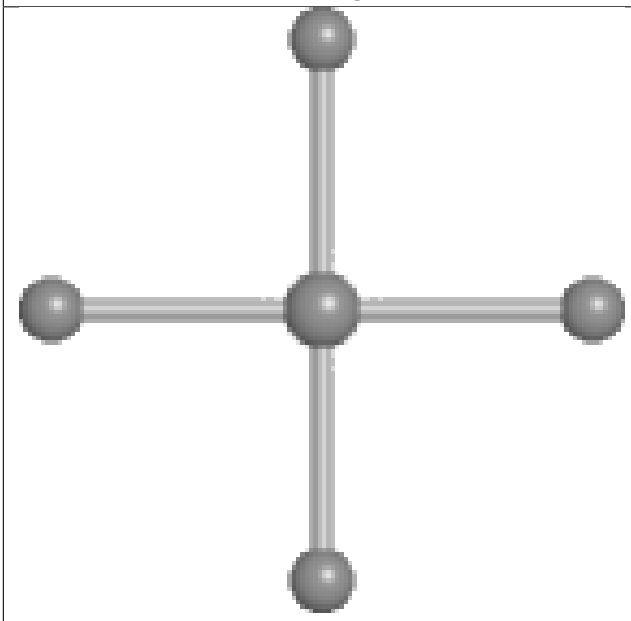

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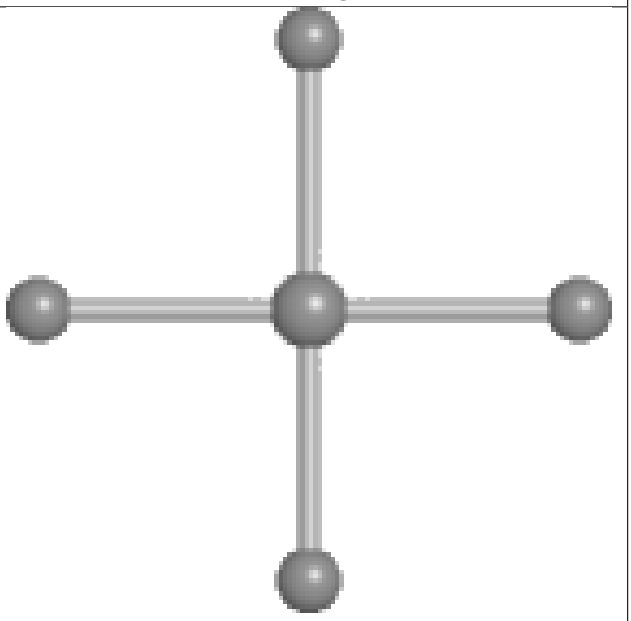
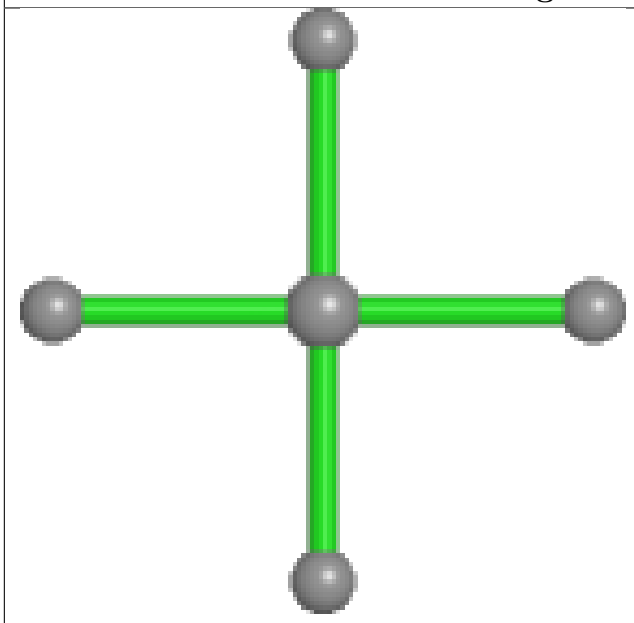


Rings

Ligand SO4 I 406



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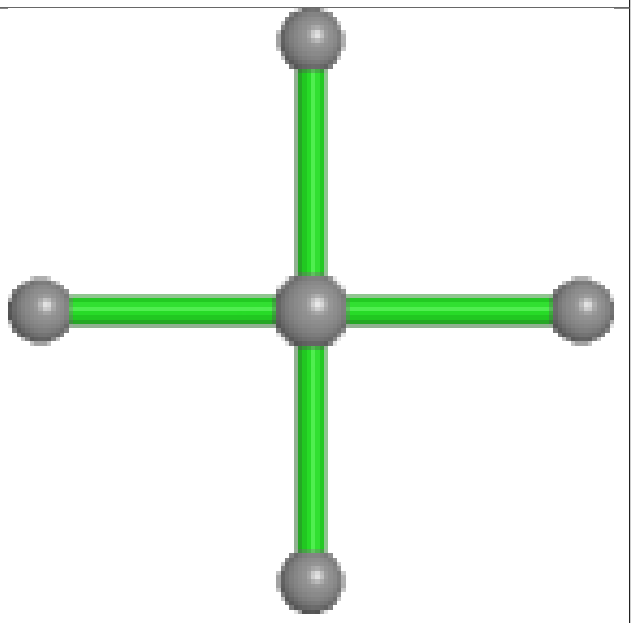
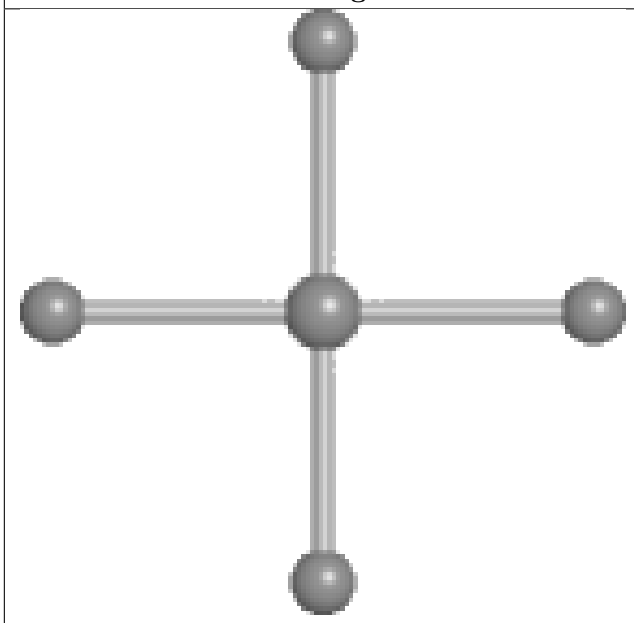


Bond angles



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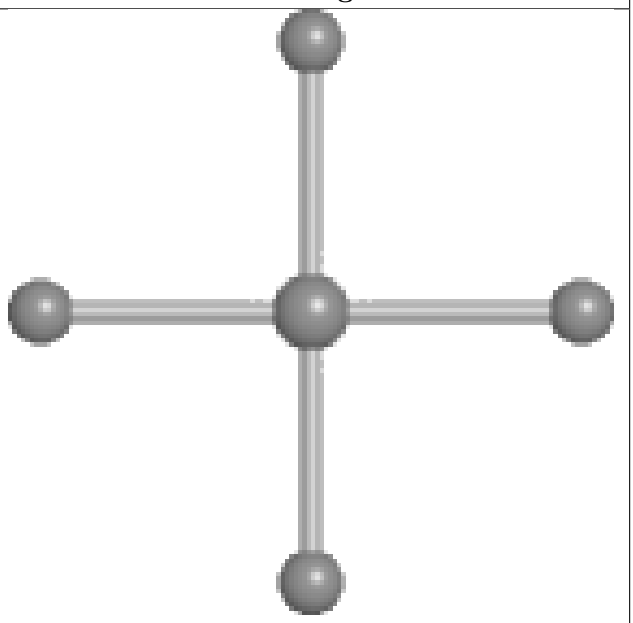
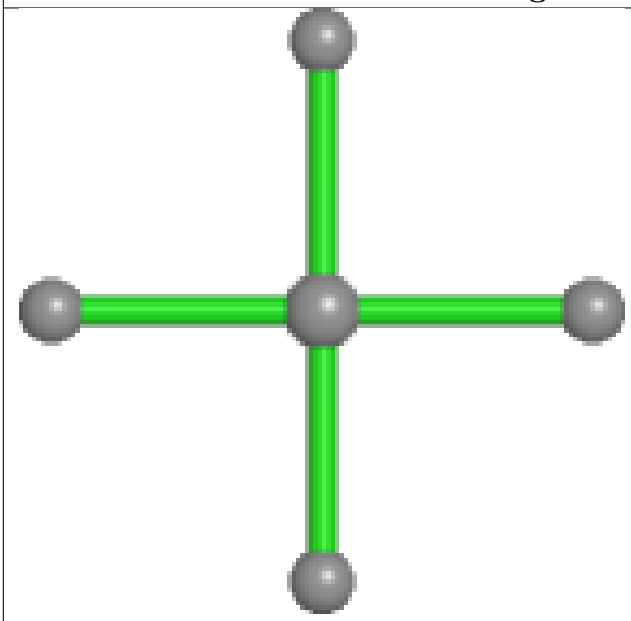


Rings

Ligand SO4 C 408



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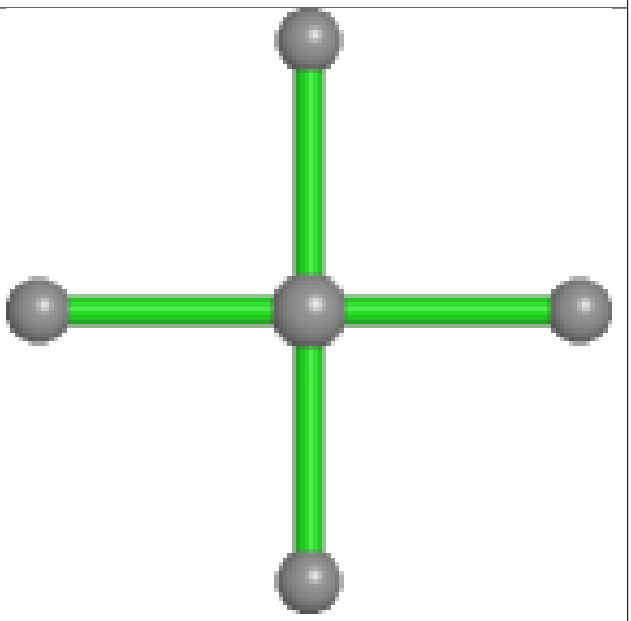
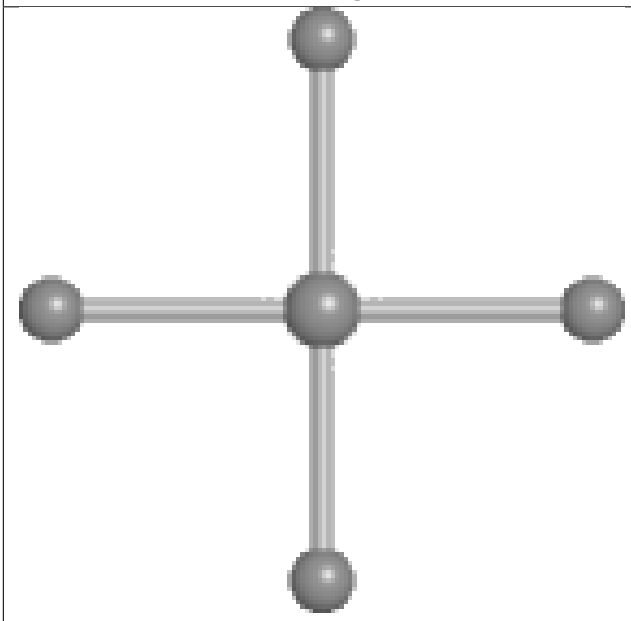


Bond angles



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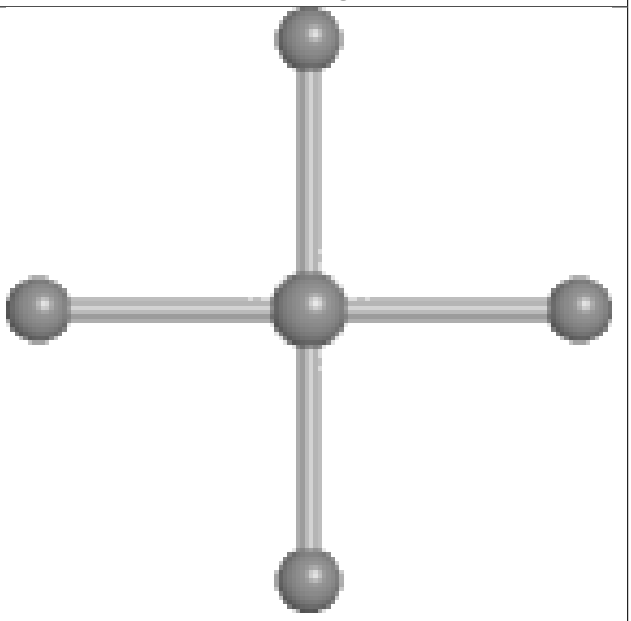
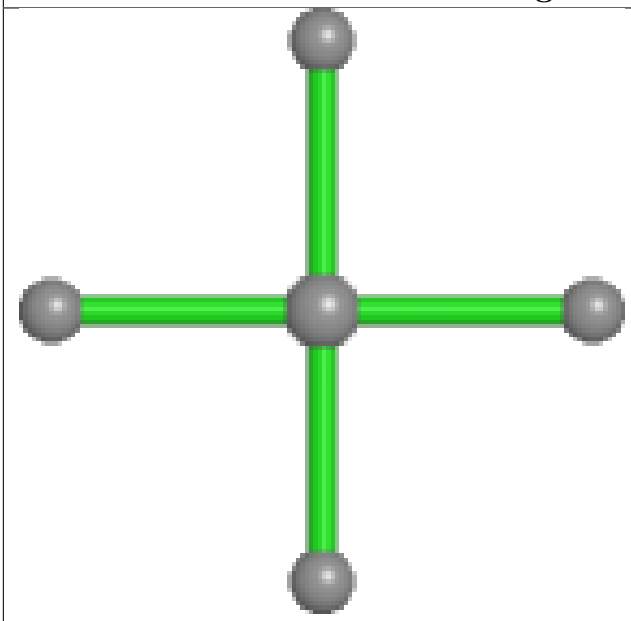


Rings

Ligand SO4 I 407



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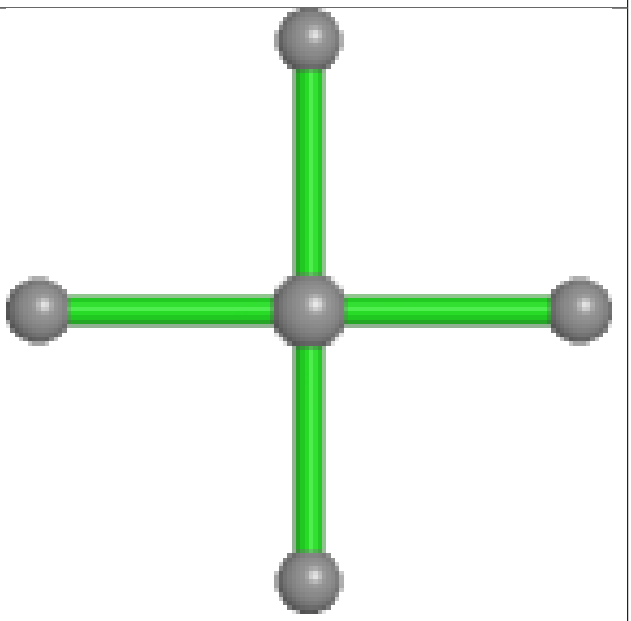
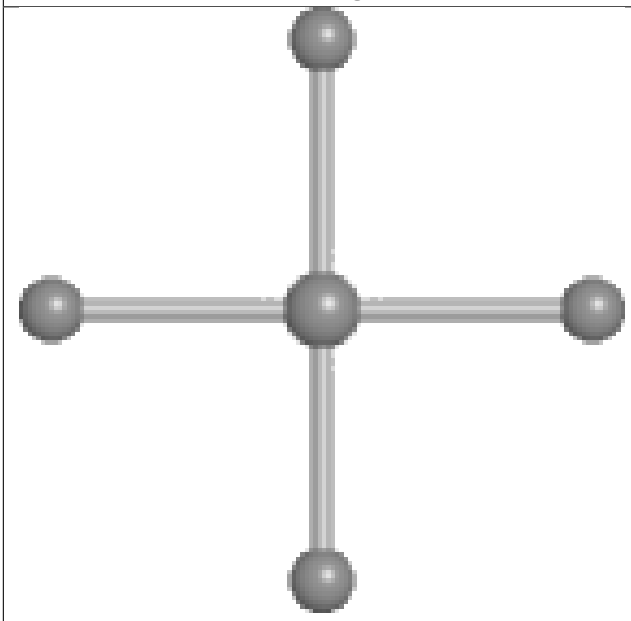


Bond angles



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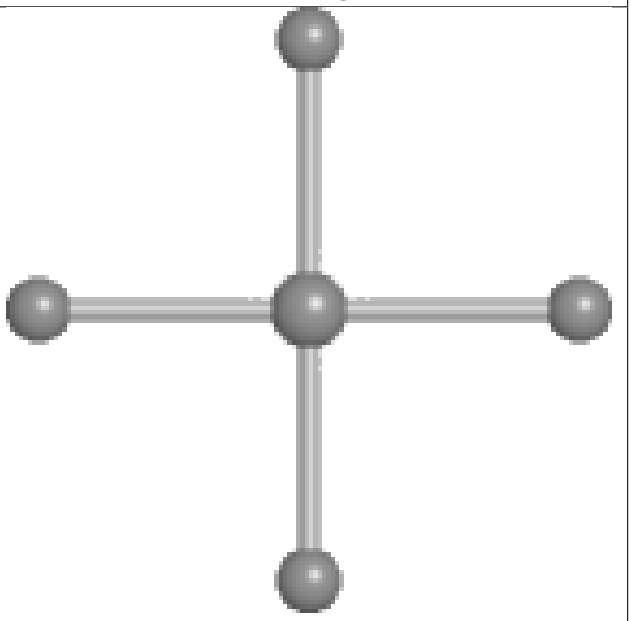
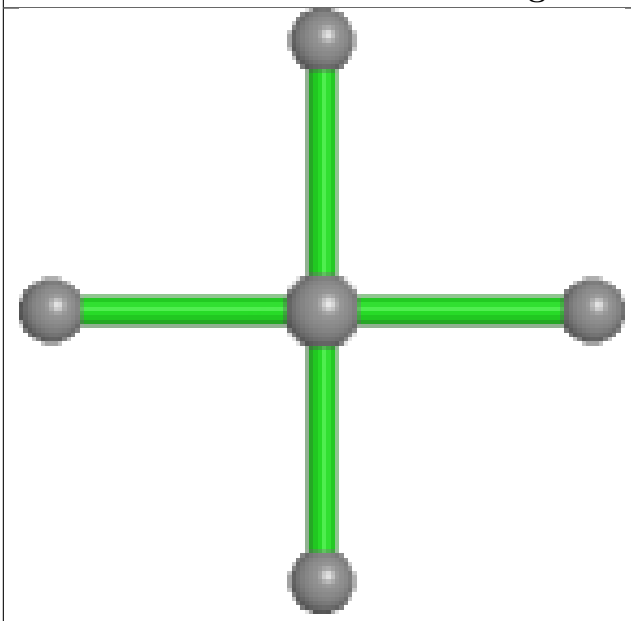


Rings

Ligand SO4 D 406



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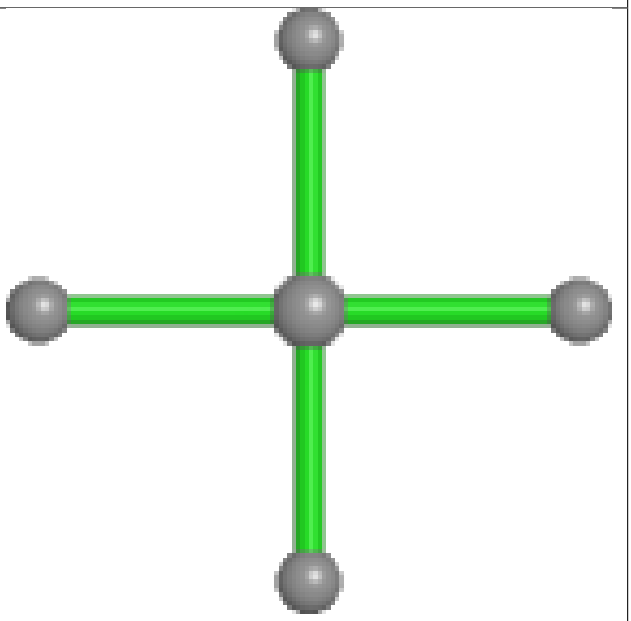
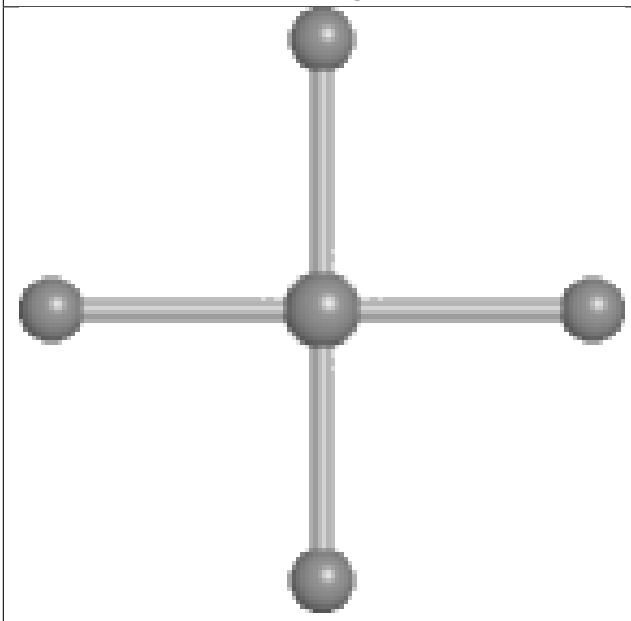
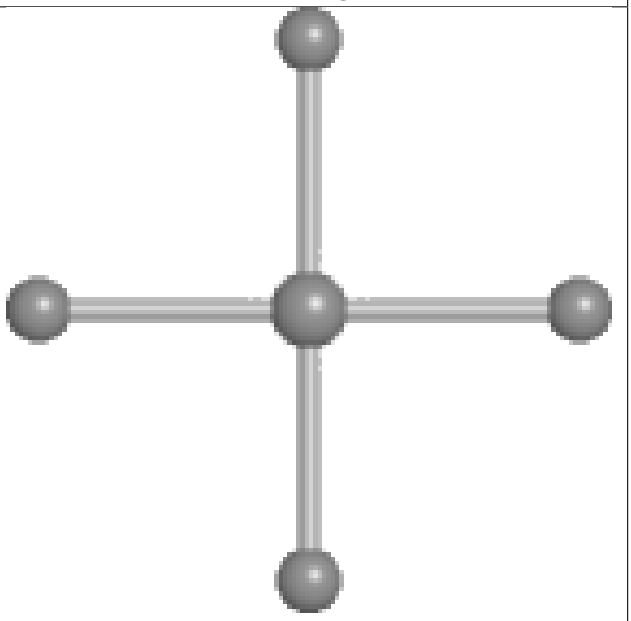


Bond angles

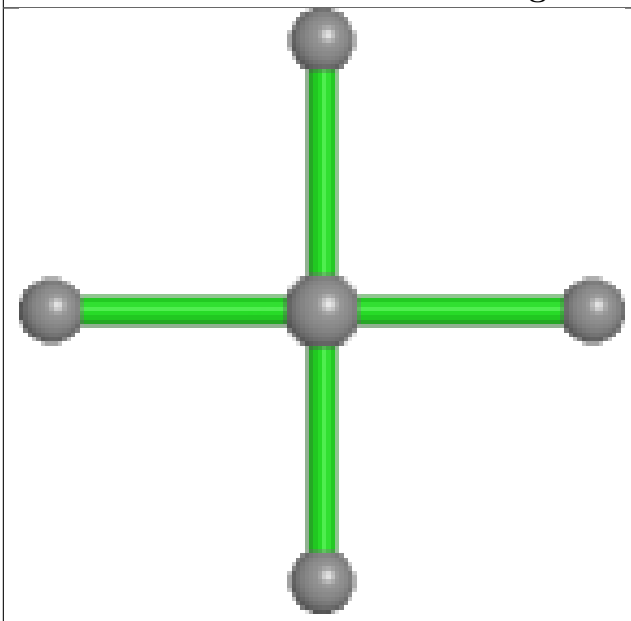


Torsions



Rings

Ligand SO4 C 407



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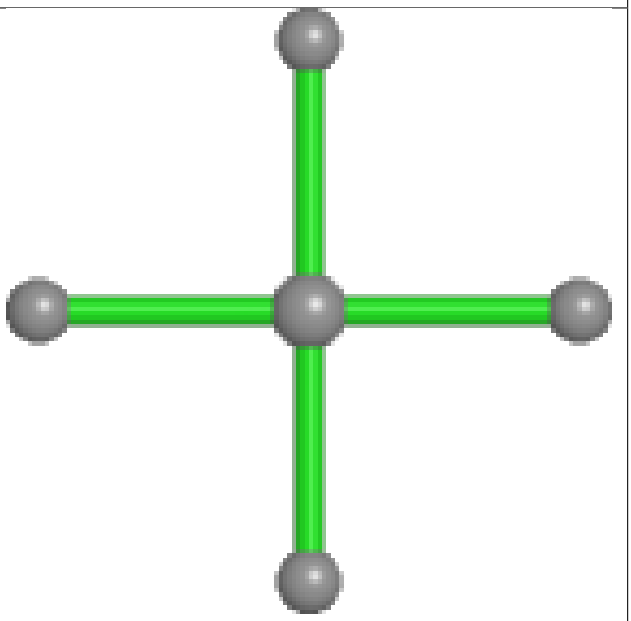
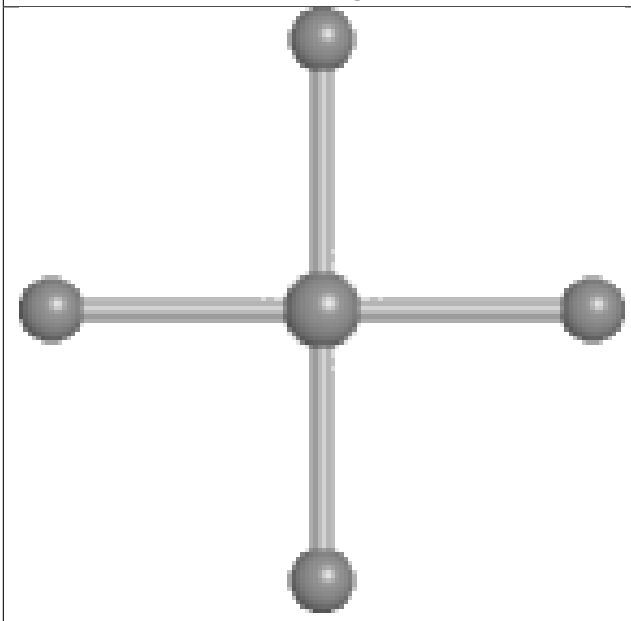
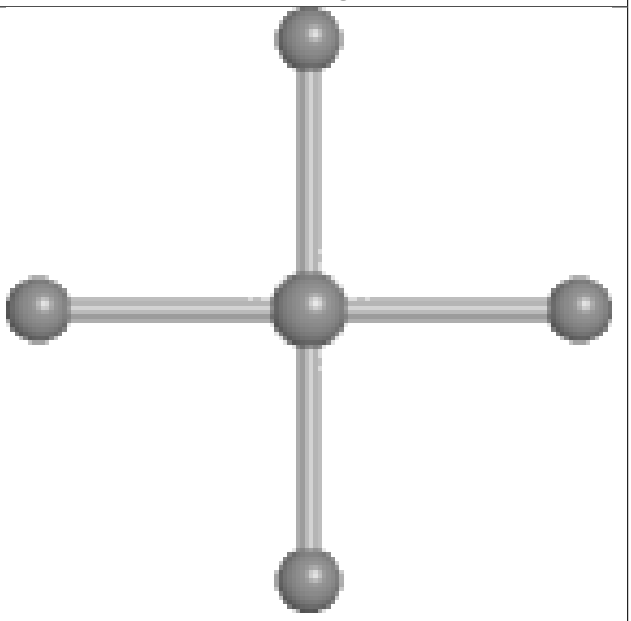


Bond angles

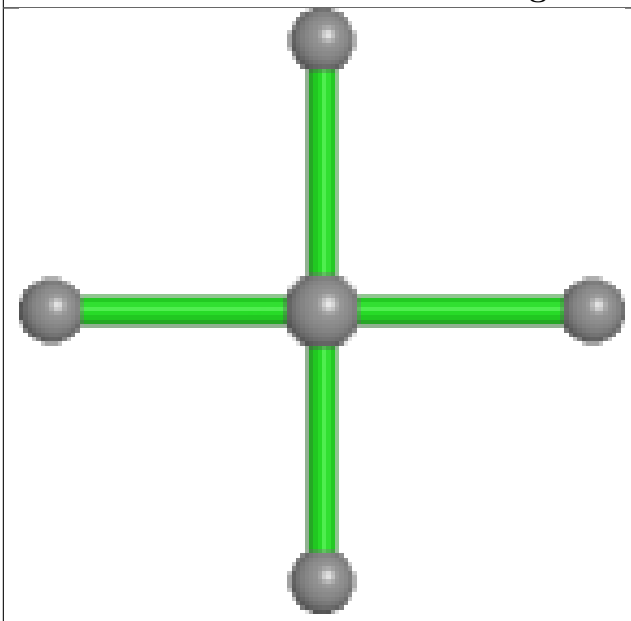


Torsions

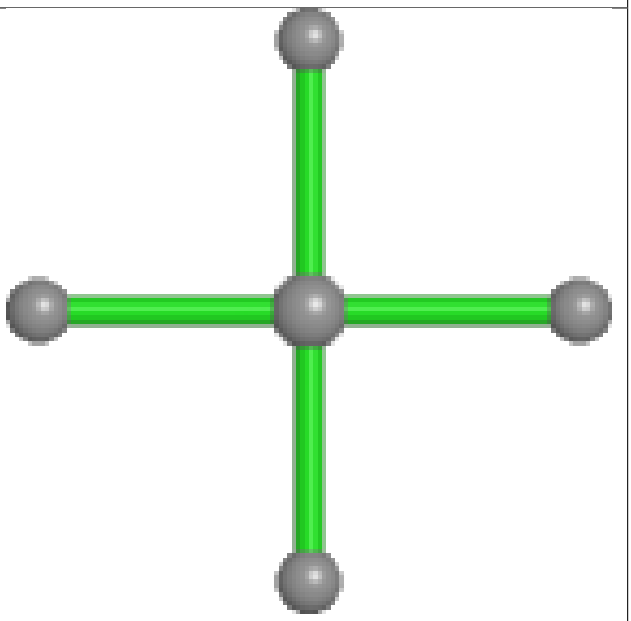


Rings

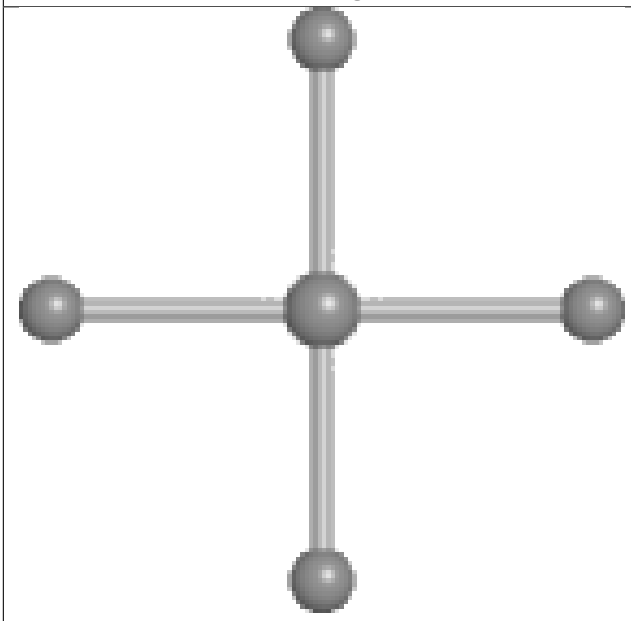
Ligand SO4 B 406



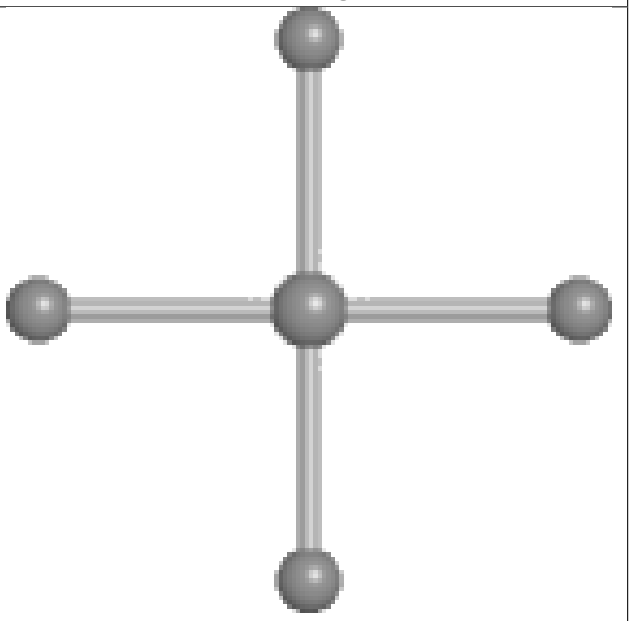
Bond lengths



Bond angles

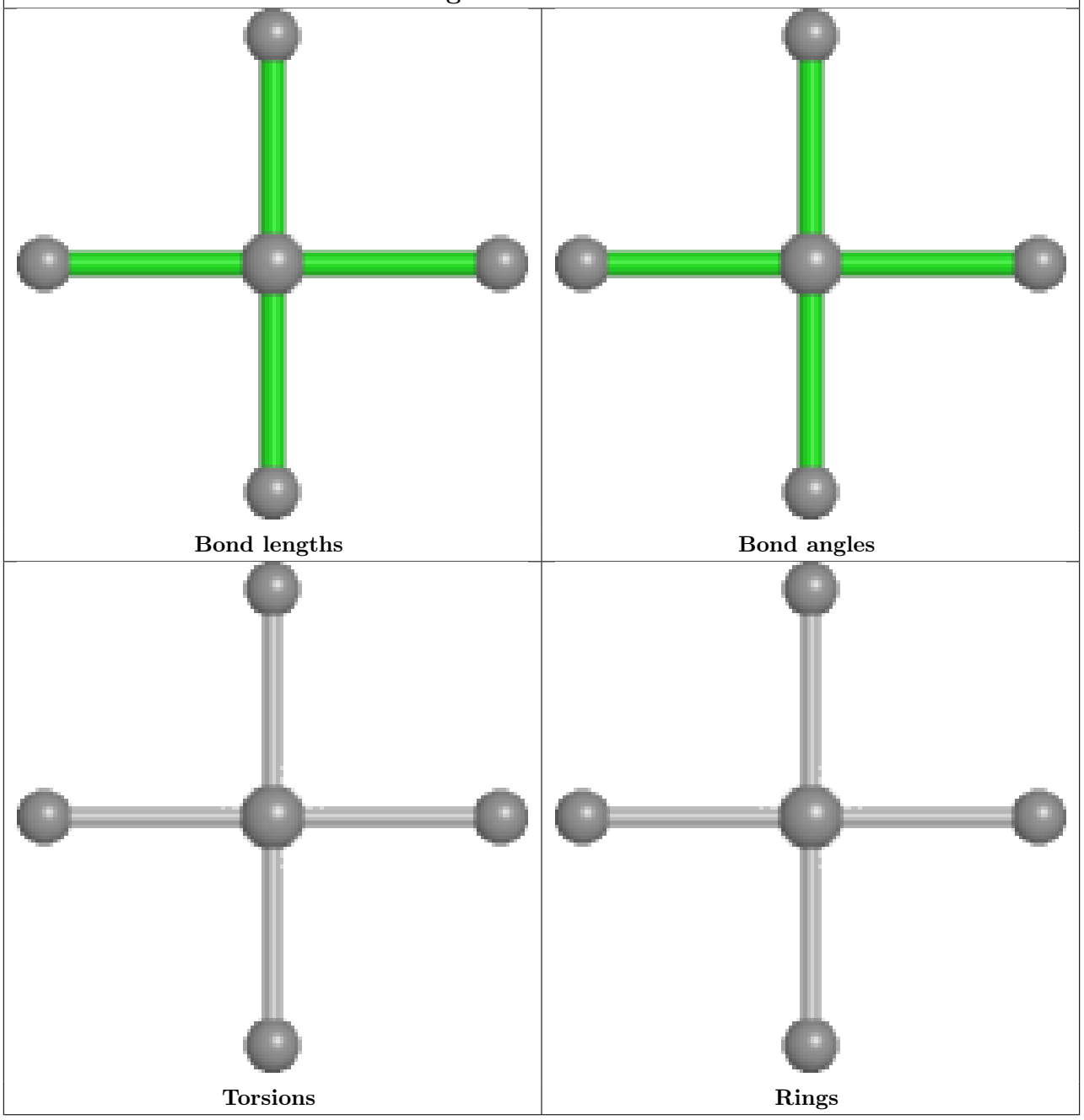


Torsions



Rings

Ligand SO4 G 405



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	287/307 (93%)	-0.40	7 (2%)	59	49	40, 54, 107, 195	0
1	B	290/307 (94%)	-0.46	2 (0%)	87	84	41, 58, 107, 152	0
1	C	289/307 (94%)	-0.32	9 (3%)	49	39	38, 61, 106, 162	0
1	D	290/307 (94%)	-0.40	3 (1%)	82	77	42, 60, 112, 164	0
1	E	287/307 (93%)	-0.26	9 (3%)	49	39	46, 68, 122, 163	0
1	F	289/307 (94%)	-0.27	8 (2%)	53	43	46, 66, 125, 167	0
1	G	287/307 (93%)	-0.14	8 (2%)	53	43	50, 77, 128, 165	0
1	H	289/307 (94%)	-0.27	9 (3%)	49	39	47, 66, 131, 211	0
1	I	290/307 (94%)	-0.32	6 (2%)	63	54	44, 64, 115, 158	0
All	All	2598/2763 (94%)	-0.32	61 (2%)	60	50	38, 64, 122, 211	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	88	ASN	5.6
1	A	92	LEU	5.3
1	H	86	SER	5.1
1	D	86	SER	4.9
1	E	86	SER	4.6

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	I	407	5/5	0.58	0.47	142,165,185,193	0
4	SO4	C	407	5/5	0.77	0.51	141,141,158,164	0
4	SO4	C	408	5/5	0.78	0.20	145,150,156,157	0
4	SO4	D	406	5/5	0.86	0.26	114,115,130,133	0
4	SO4	D	407	5/5	0.87	0.40	91,123,132,144	0
4	SO4	H	406	5/5	0.88	0.20	97,100,109,124	0
3	MG	D	404	1/1	0.90	0.07	73,73,73,73	0
4	SO4	B	406	5/5	0.91	0.15	86,91,120,130	0
4	SO4	E	405	5/5	0.93	0.10	84,96,106,117	0
4	SO4	E	406	5/5	0.93	0.12	97,101,110,110	0
4	SO4	C	406	5/5	0.94	0.12	92,94,106,108	0
3	MG	B	404	1/1	0.94	0.06	64,64,64,64	0
2	CA	G	402	1/1	0.94	0.05	74,74,74,74	0
4	SO4	H	405	5/5	0.94	0.12	90,96,106,113	0
4	SO4	D	405	5/5	0.94	0.15	83,87,88,97	0
2	CA	G	403	1/1	0.94	0.05	74,74,74,74	0
4	SO4	G	405	5/5	0.95	0.14	99,101,105,113	0
2	CA	A	402	1/1	0.95	0.08	47,47,47,47	0
3	MG	E	404	1/1	0.95	0.03	67,67,67,67	0
4	SO4	I	406	5/5	0.95	0.13	101,102,112,121	0
4	SO4	B	405	5/5	0.95	0.14	72,85,88,114	0
4	SO4	A	406	5/5	0.96	0.13	73,86,89,100	0
3	MG	C	404	1/1	0.96	0.07	50,50,50,50	0
3	MG	A	404	1/1	0.96	0.04	57,57,57,57	0
4	SO4	F	405	5/5	0.96	0.14	79,95,104,113	0
2	CA	E	403	1/1	0.96	0.04	62,62,62,62	0
3	MG	F	404	1/1	0.96	0.09	60,60,60,60	0
3	MG	G	404	1/1	0.96	0.07	80,80,80,80	0
4	SO4	I	405	5/5	0.96	0.13	60,65,73,81	0
3	MG	H	404	1/1	0.96	0.12	67,67,67,67	0
3	MG	I	404	1/1	0.96	0.07	64,64,64,64	0
4	SO4	A	405	5/5	0.97	0.13	47,52,65,78	0
2	CA	F	402	1/1	0.97	0.09	59,59,59,59	0
2	CA	D	401	1/1	0.97	0.08	56,56,56,56	0
2	CA	B	401	1/1	0.97	0.08	49,49,49,49	0
4	SO4	C	405	5/5	0.97	0.13	77,85,89,103	0
2	CA	F	401	1/1	0.98	0.10	54,54,54,54	0

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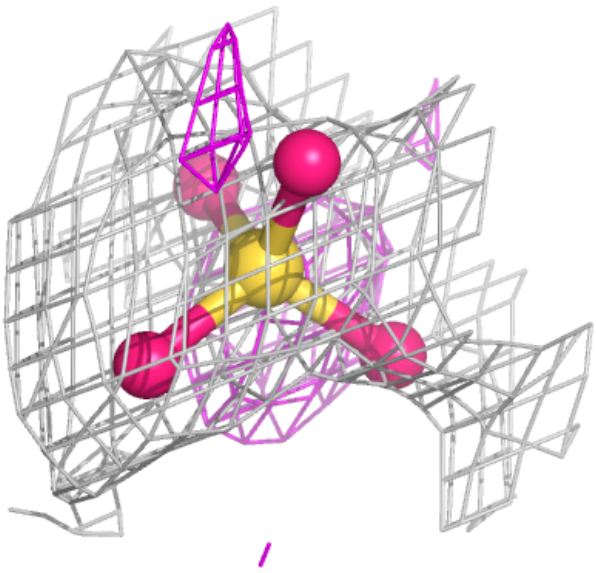
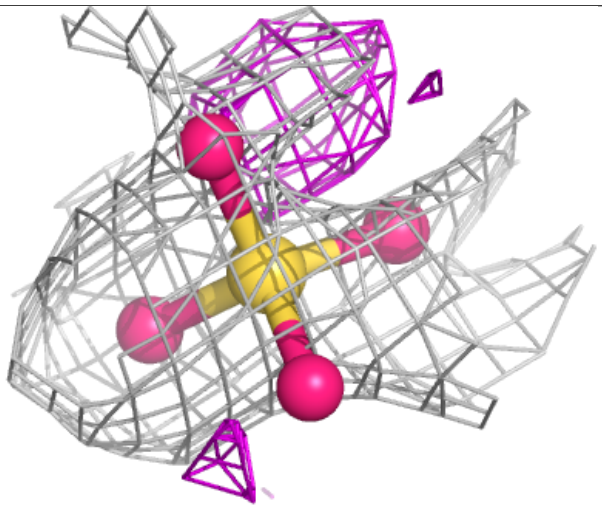
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	A	401	1/1	0.98	0.10	54,54,54,54	0
2	CA	I	402	1/1	0.98	0.08	51,51,51,51	0
2	CA	G	401	1/1	0.98	0.05	70,70,70,70	0
2	CA	F	403	1/1	0.99	0.09	58,58,58,58	0
2	CA	A	403	1/1	0.99	0.11	48,48,48,48	0
2	CA	D	402	1/1	0.99	0.07	58,58,58,58	0
2	CA	D	403	1/1	0.99	0.09	49,49,49,49	0
2	CA	H	401	1/1	0.99	0.04	62,62,62,62	0
2	CA	H	402	1/1	0.99	0.05	60,60,60,60	0
2	CA	H	403	1/1	0.99	0.10	60,60,60,60	0
2	CA	I	401	1/1	0.99	0.11	61,61,61,61	0
2	CA	E	401	1/1	0.99	0.07	63,63,63,63	0
2	CA	I	403	1/1	0.99	0.11	52,52,52,52	0
2	CA	B	402	1/1	0.99	0.07	56,56,56,56	0
2	CA	B	403	1/1	0.99	0.08	52,52,52,52	0
2	CA	C	402	1/1	0.99	0.07	54,54,54,54	0
2	CA	C	401	1/1	1.00	0.08	52,52,52,52	0
2	CA	C	403	1/1	1.00	0.05	55,55,55,55	0
2	CA	E	402	1/1	1.00	0.07	64,64,64,64	0

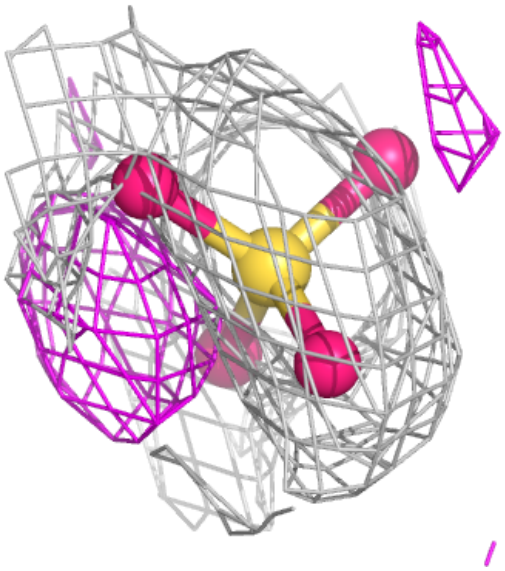
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

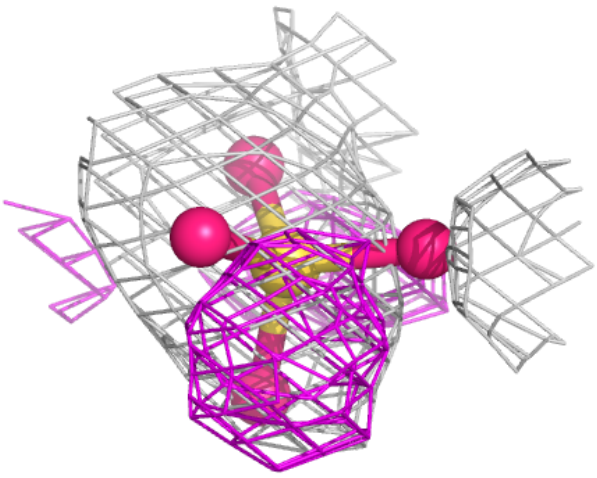


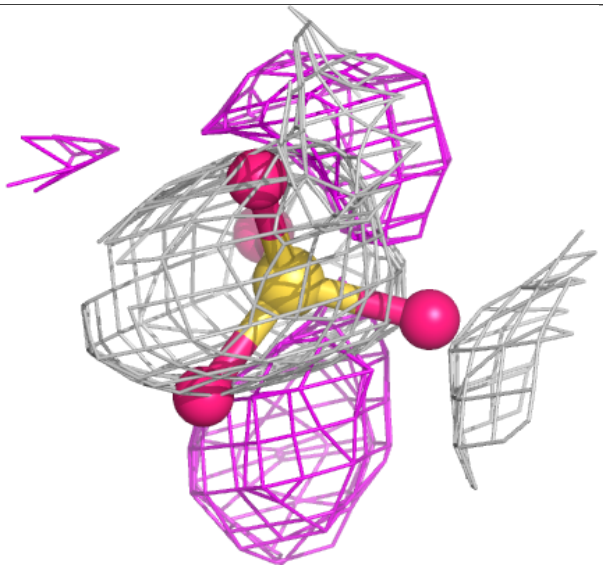


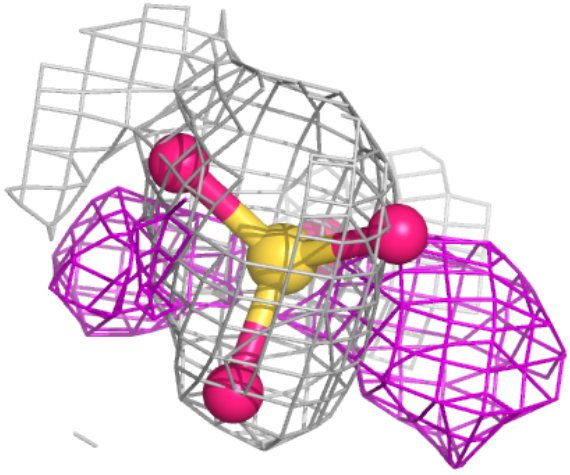


Electron density around SO4 C 407:

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

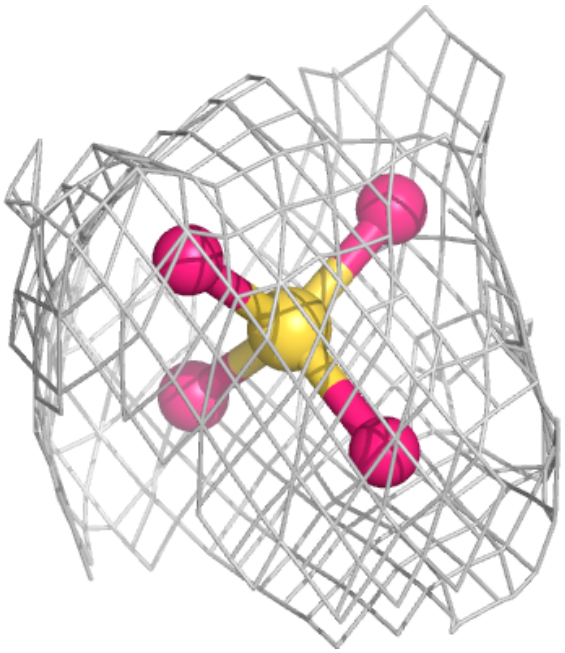


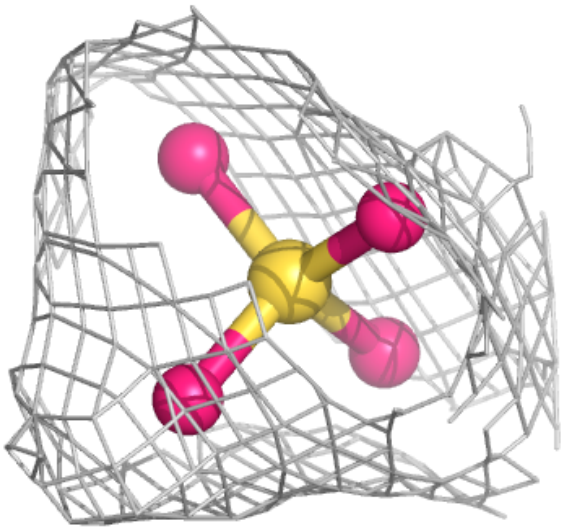


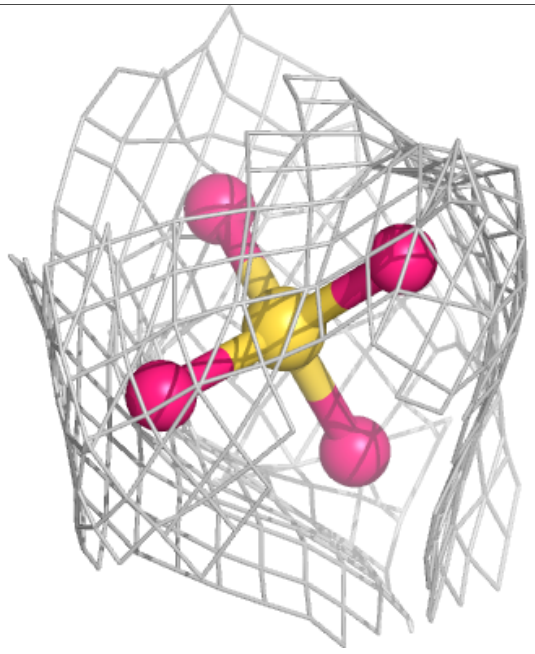


Electron density around SO4 C 408:

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

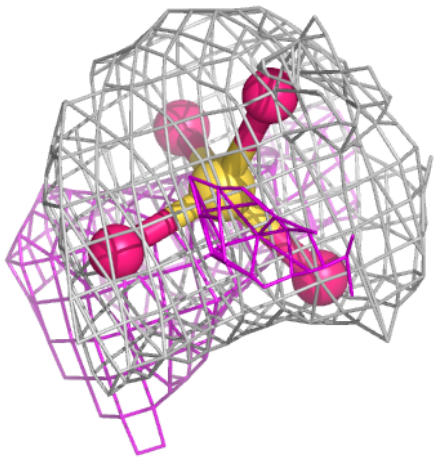


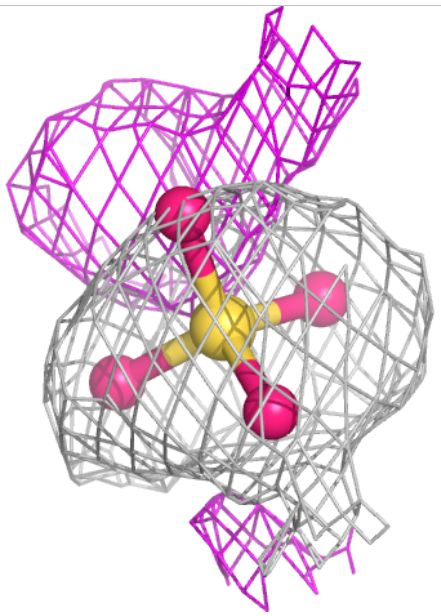


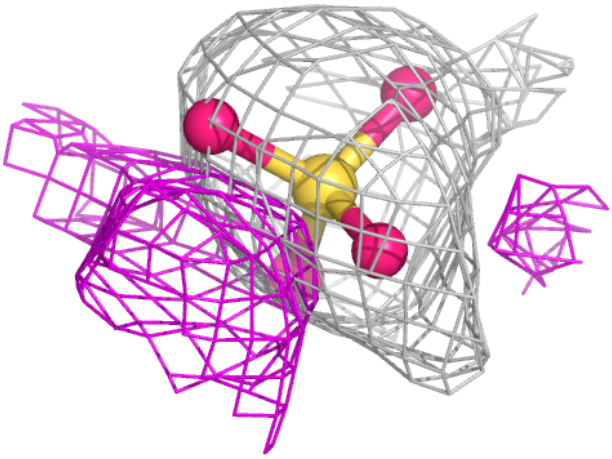


Electron density around SO4 D 406:

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

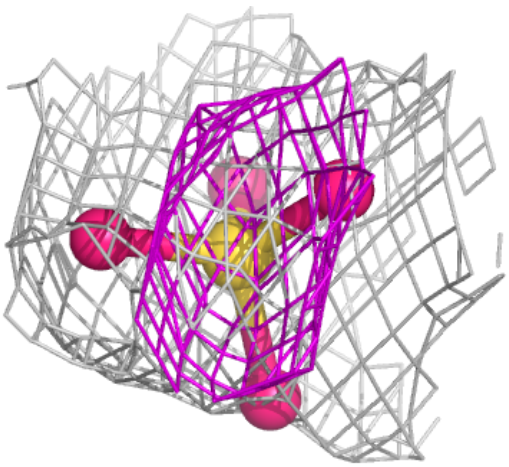


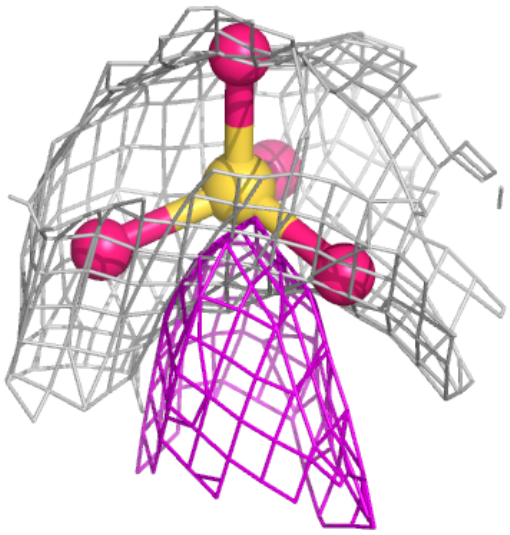


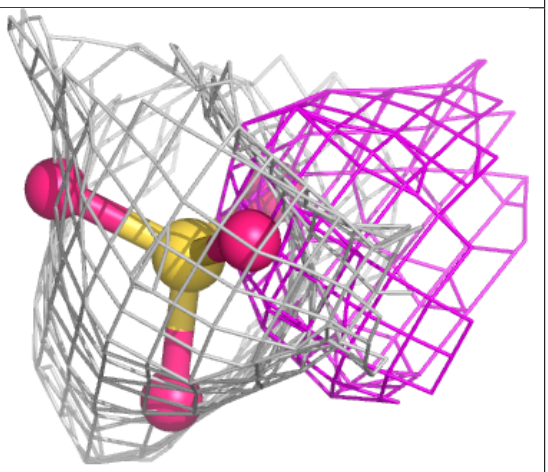


Electron density around SO4 D 407:

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

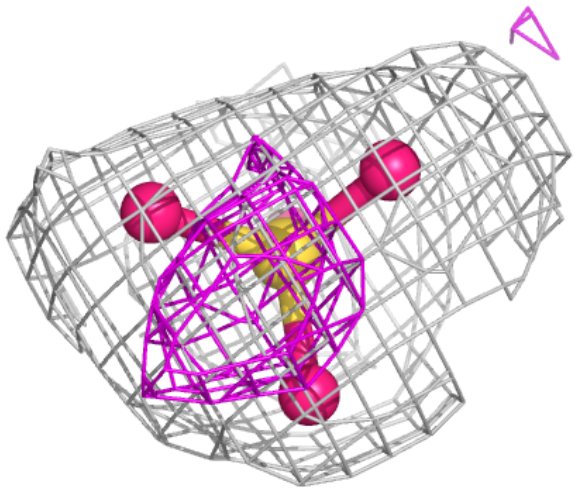


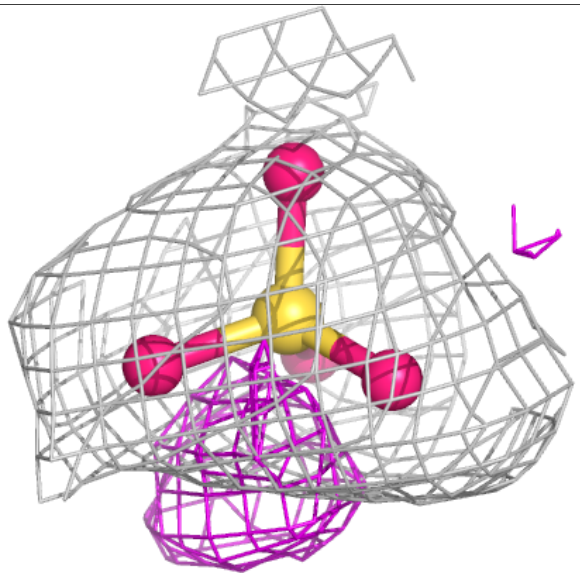


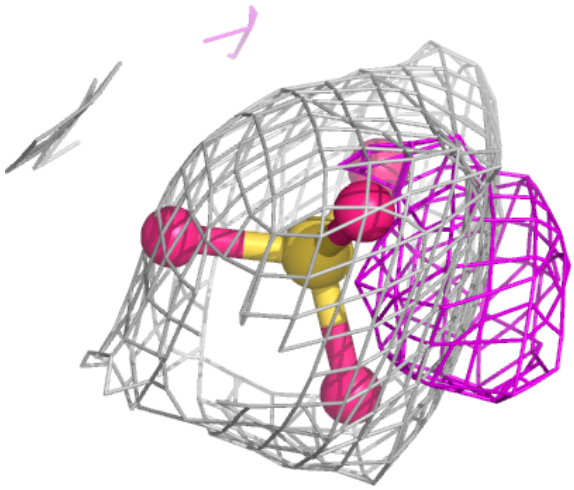


Electron density around SO4 H 406:

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

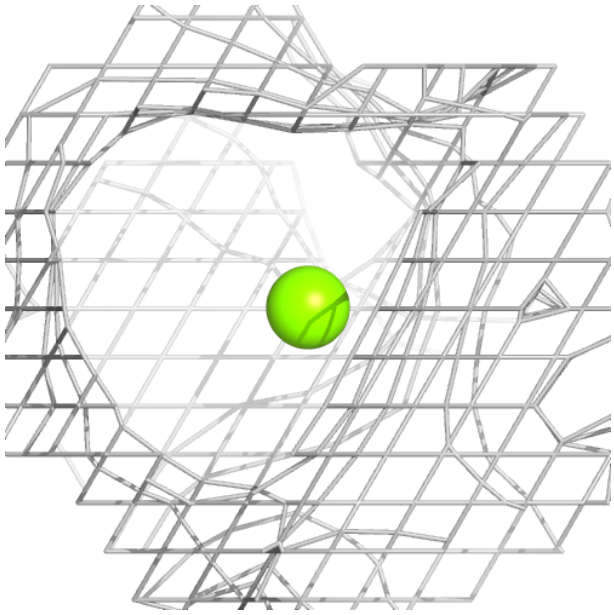


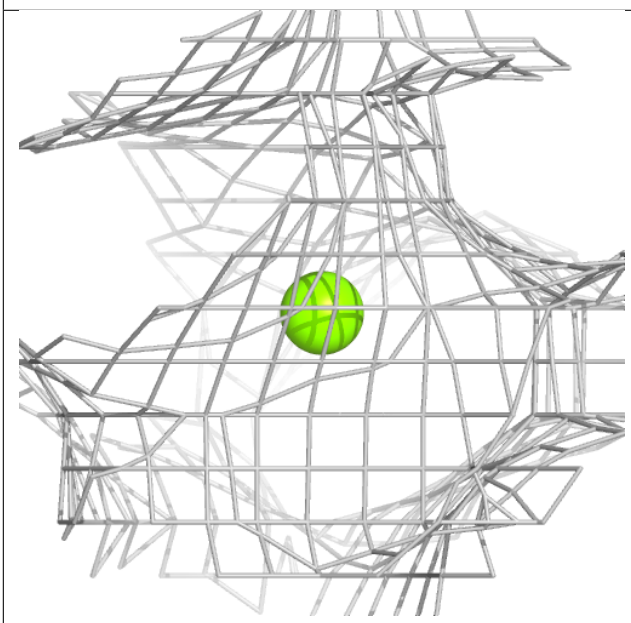


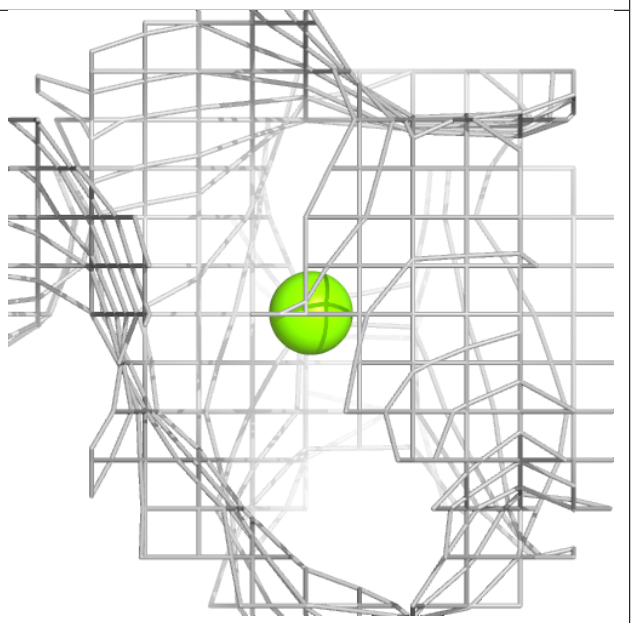


Electron density around MG D 404:

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

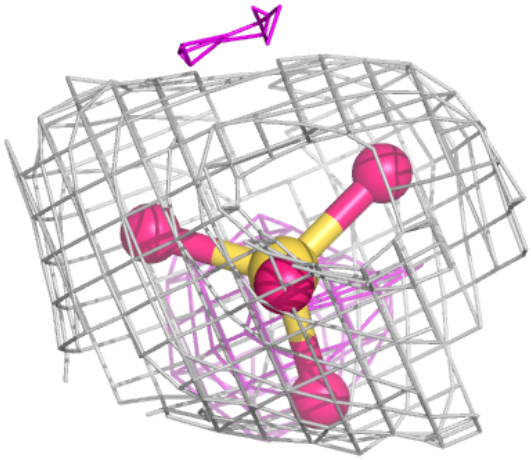


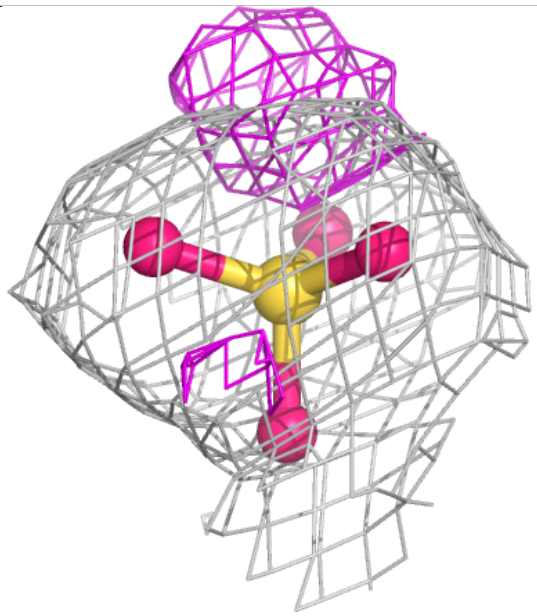


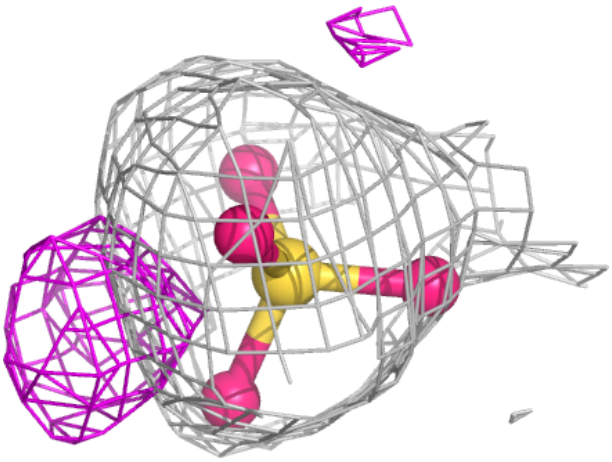


Electron density around SO4 B 406:

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

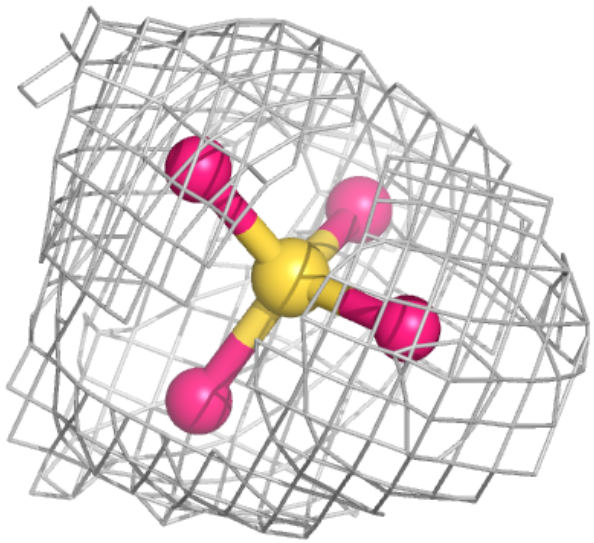


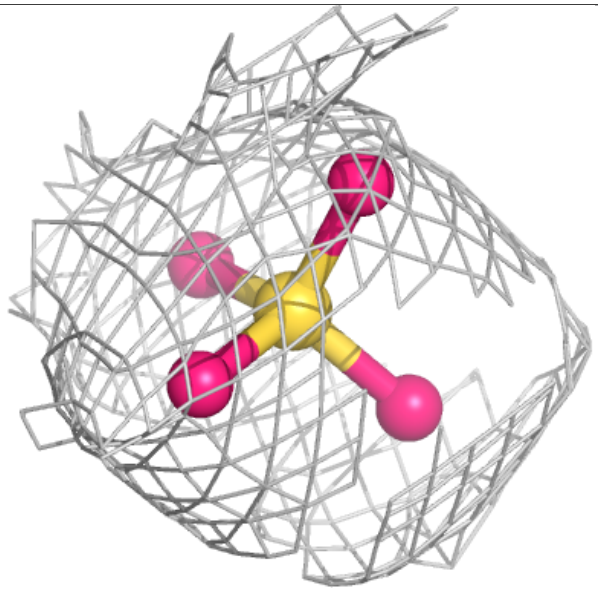


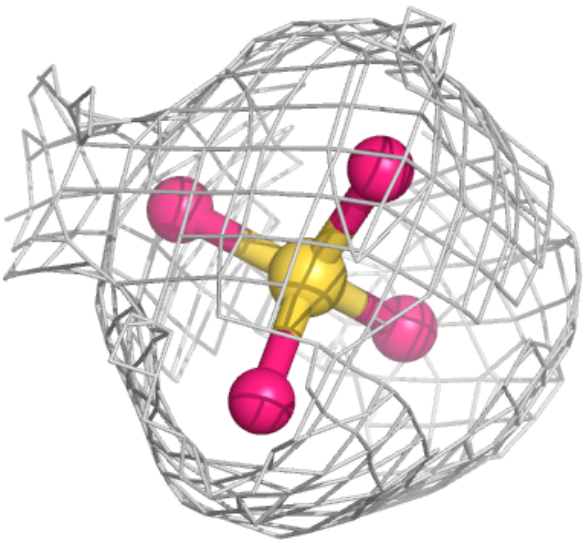


Electron density around SO4 E 405:

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

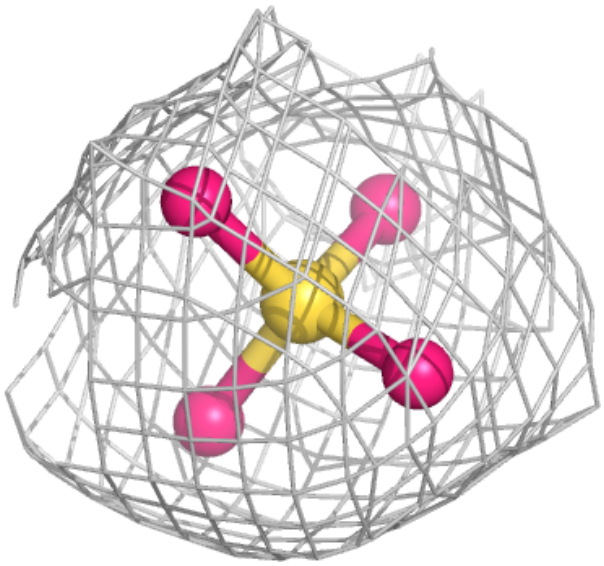


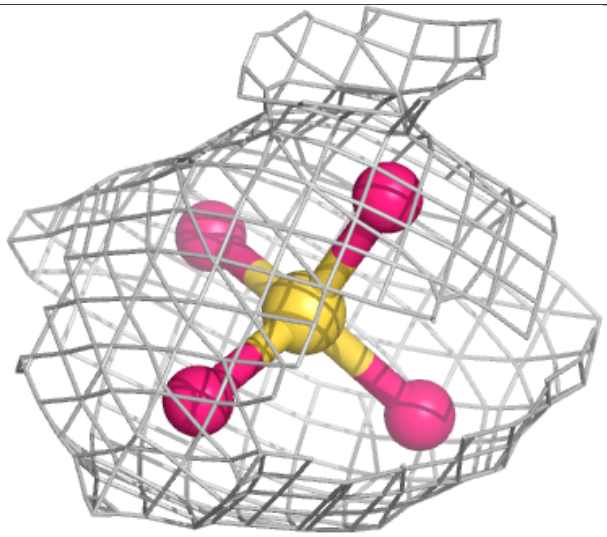


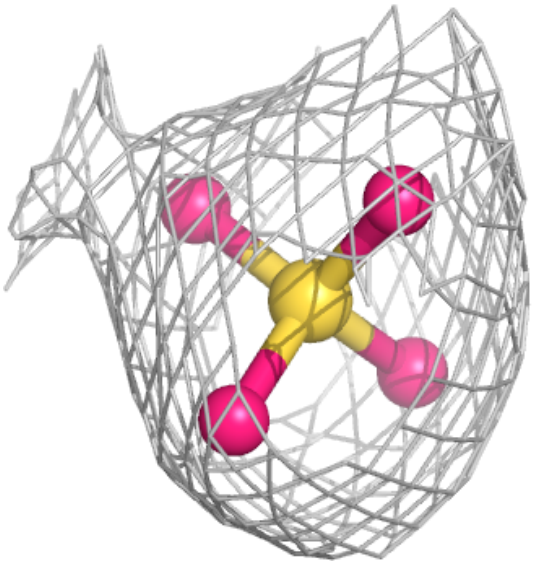


Electron density around SO4 E 406:

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

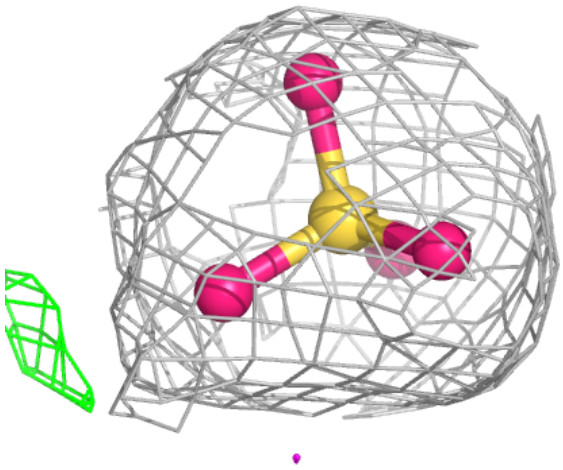


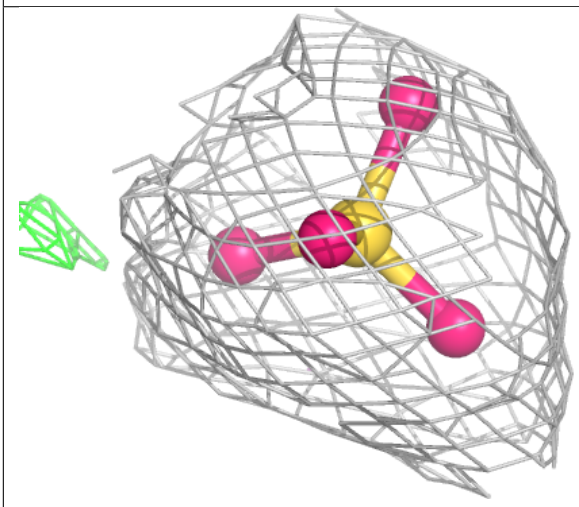


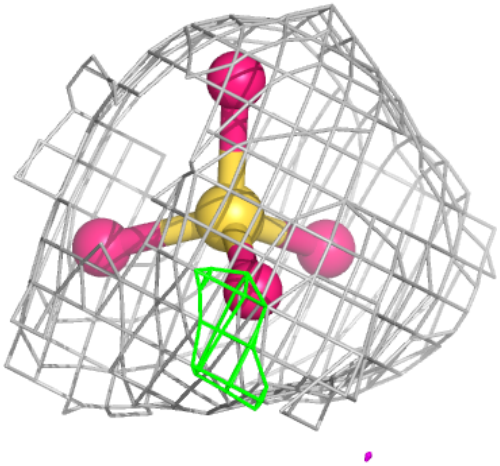


Electron density around SO4 C 406:

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







Electron density around MG B 404:

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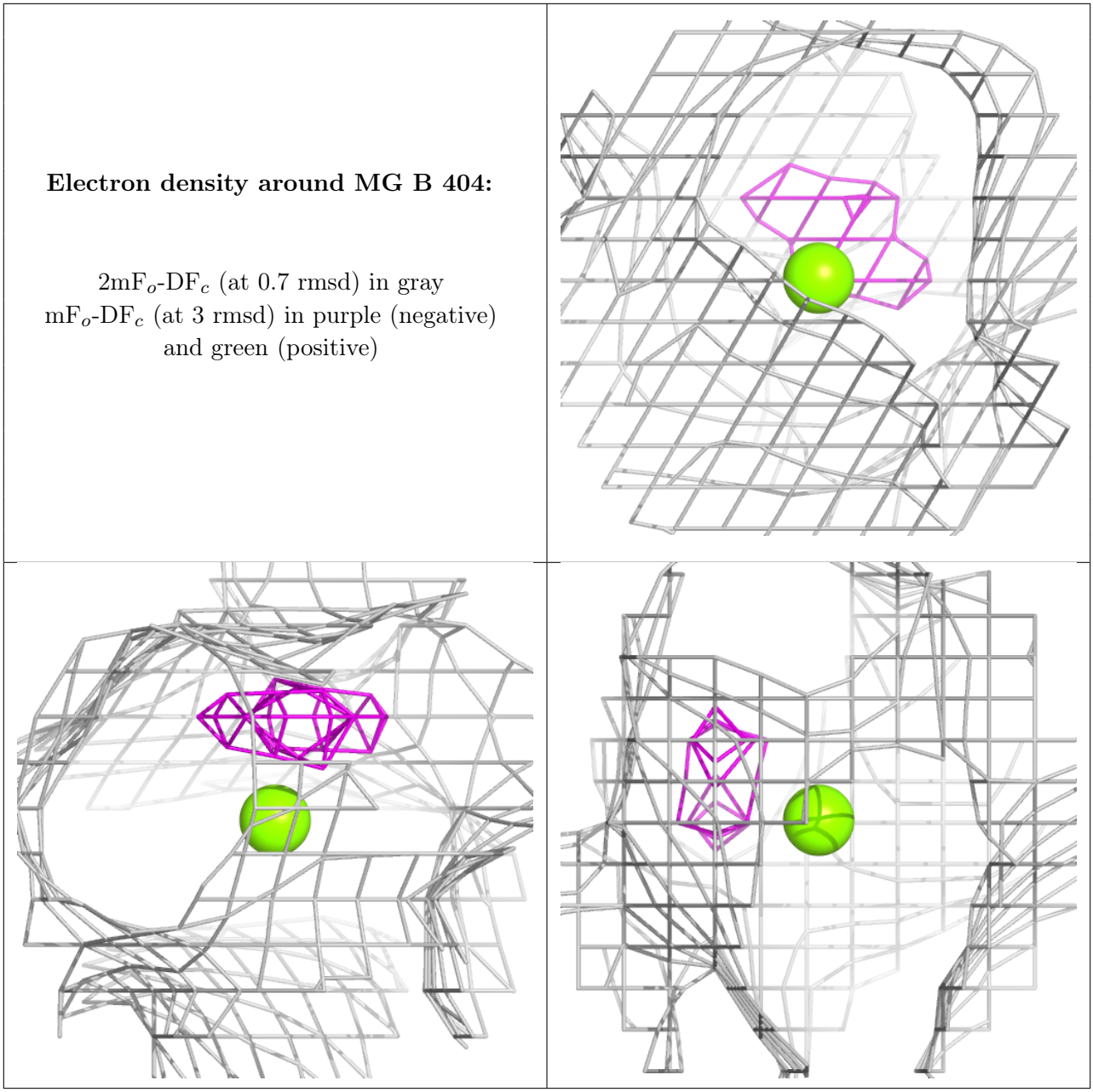
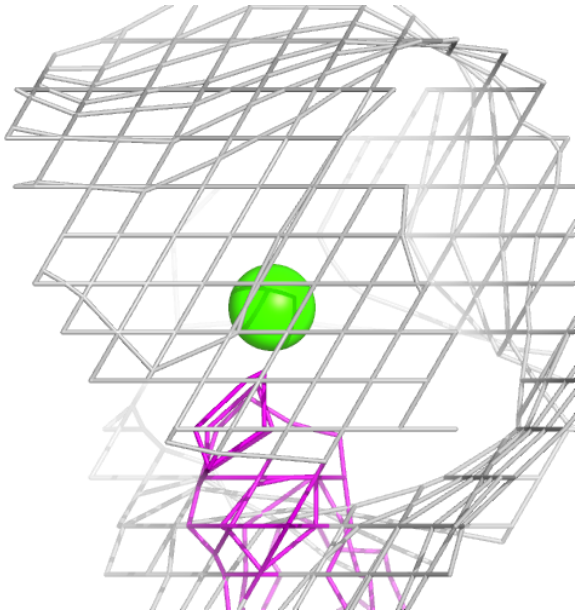
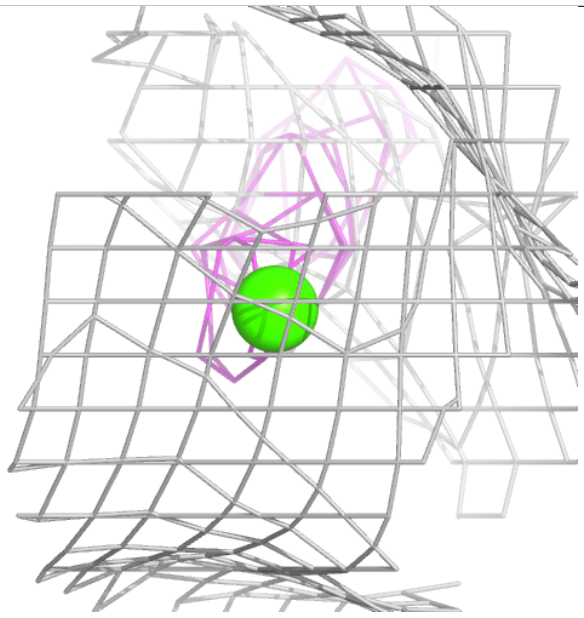
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

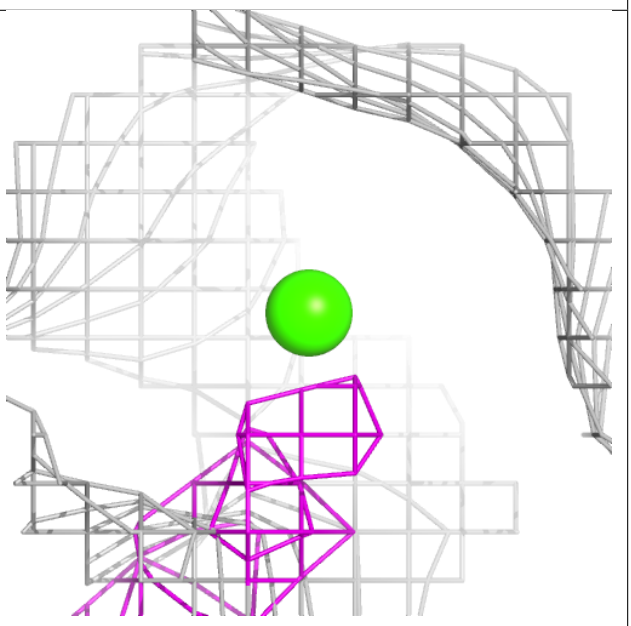


Electron density around CA G 402:

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

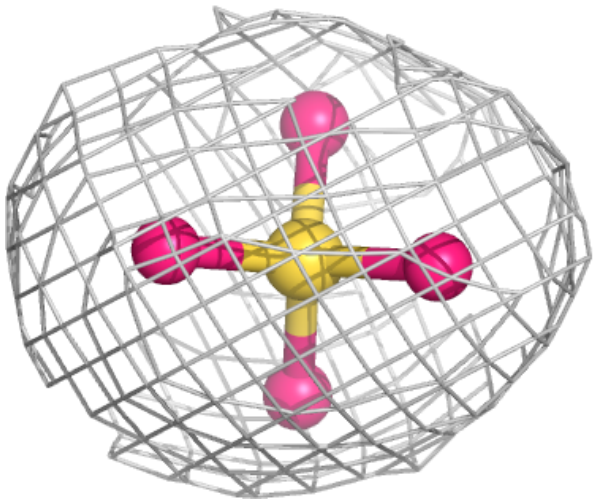


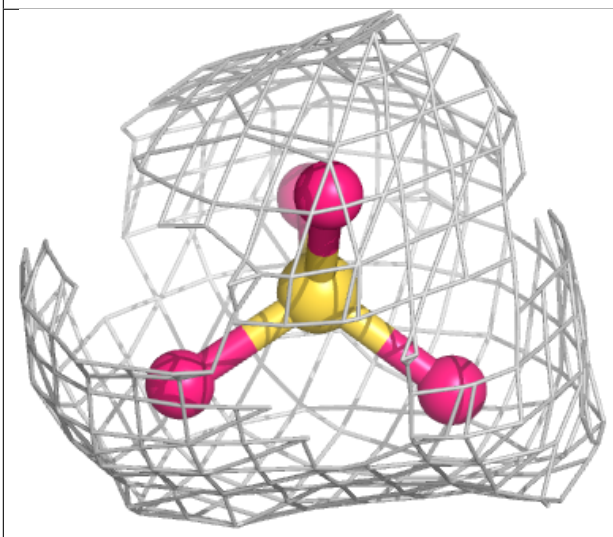


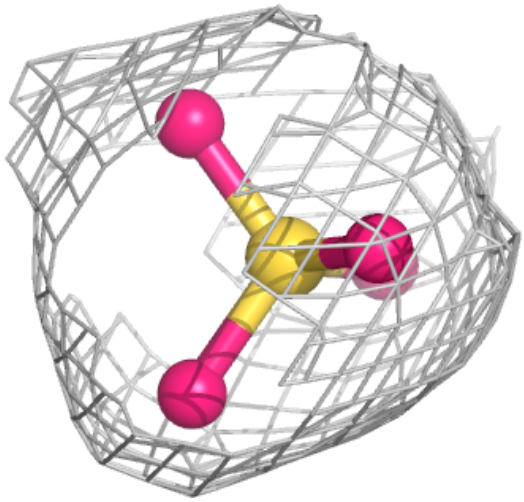


Electron density around SO4 H 405:

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

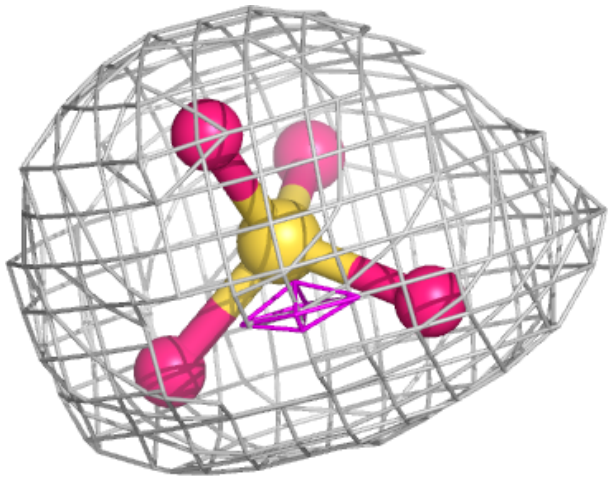


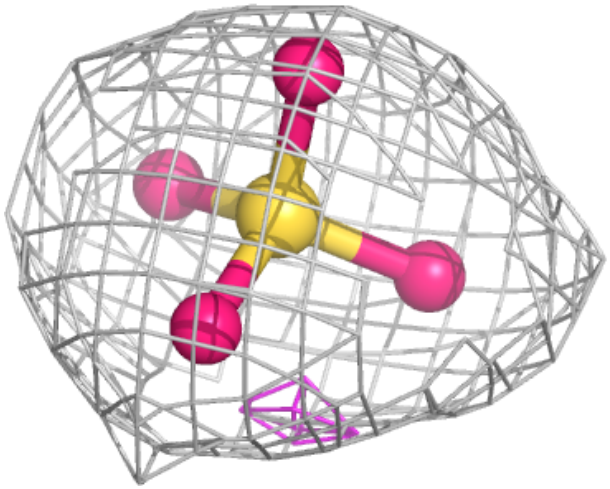


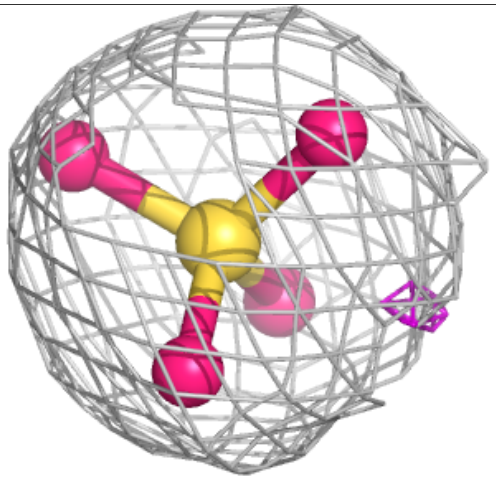


Electron density around SO4 D 405:

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

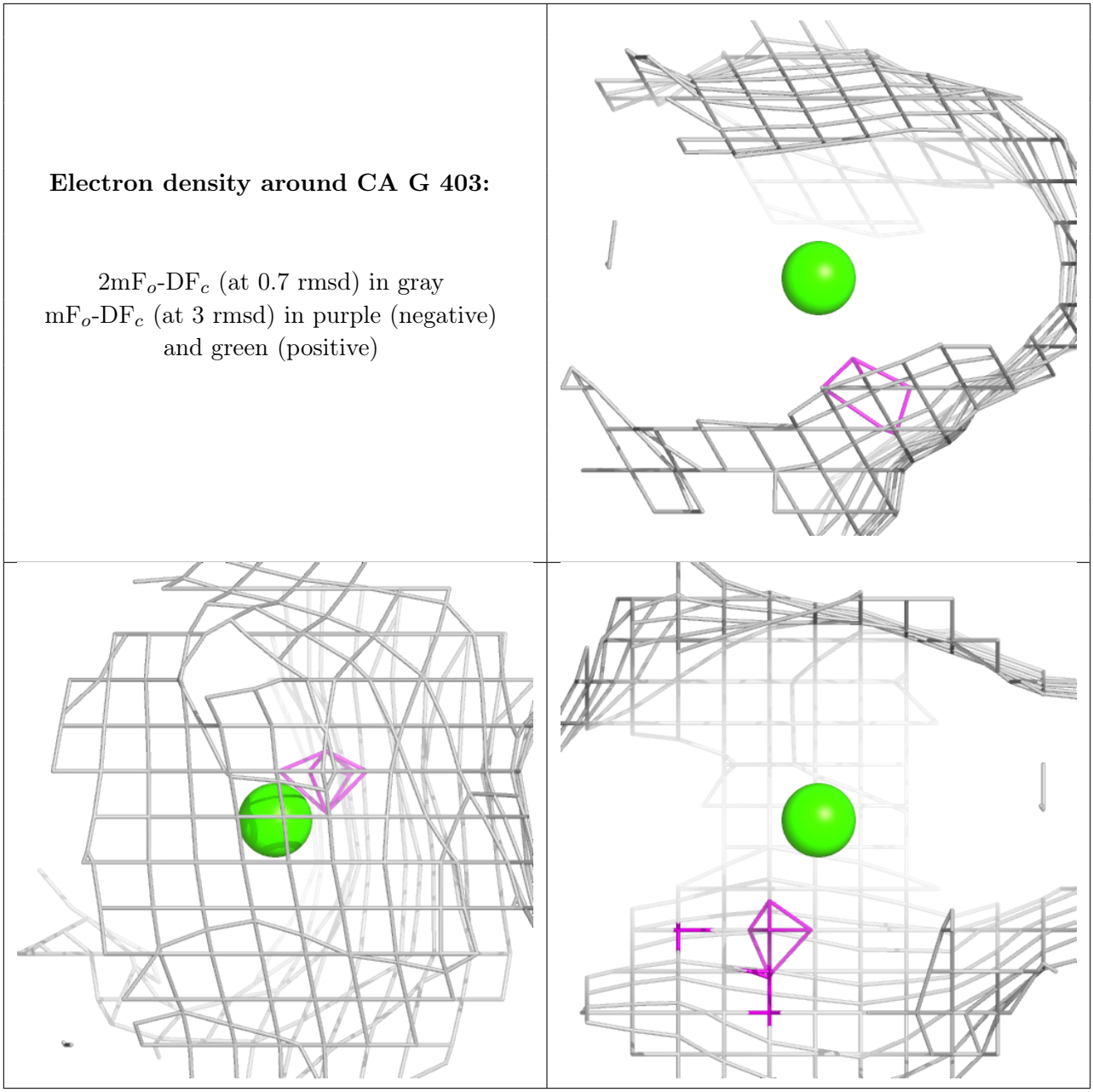






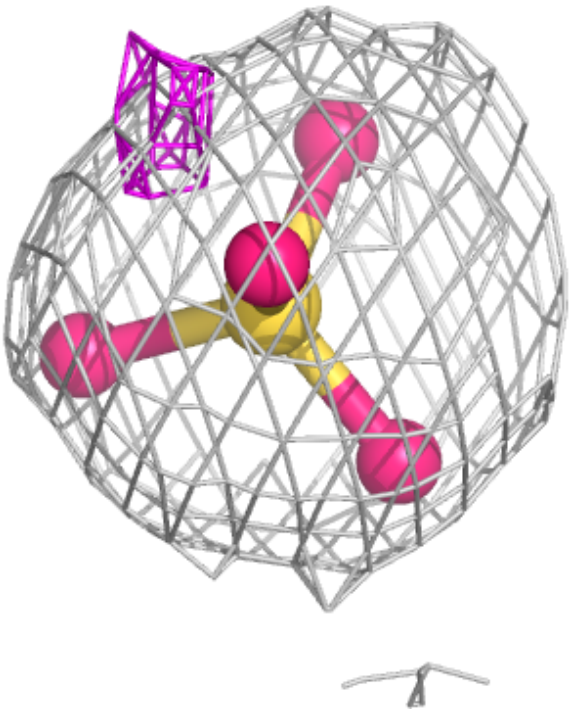
Electron density around CA G 403:

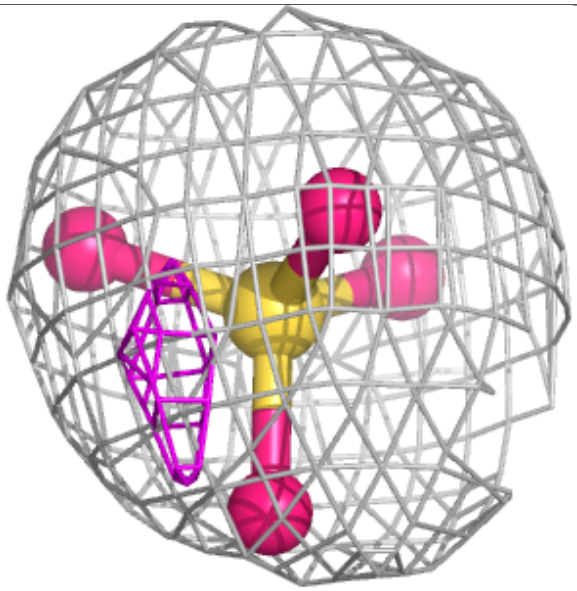
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

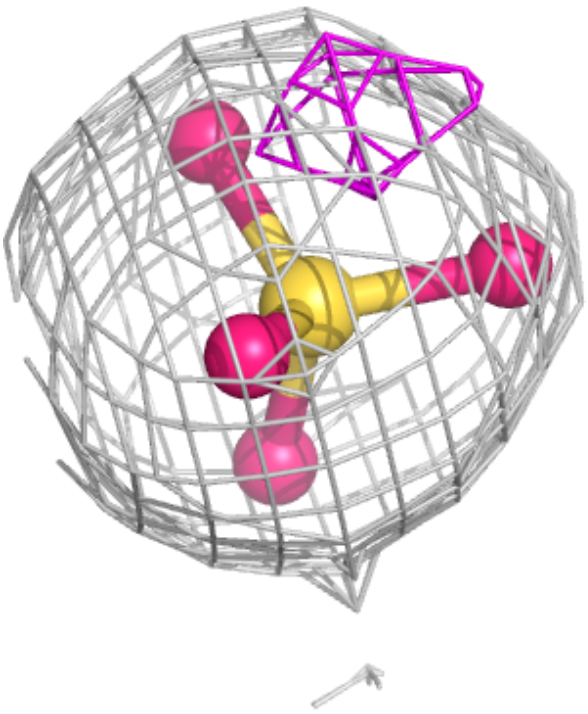


Electron density around SO4 G 405:

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

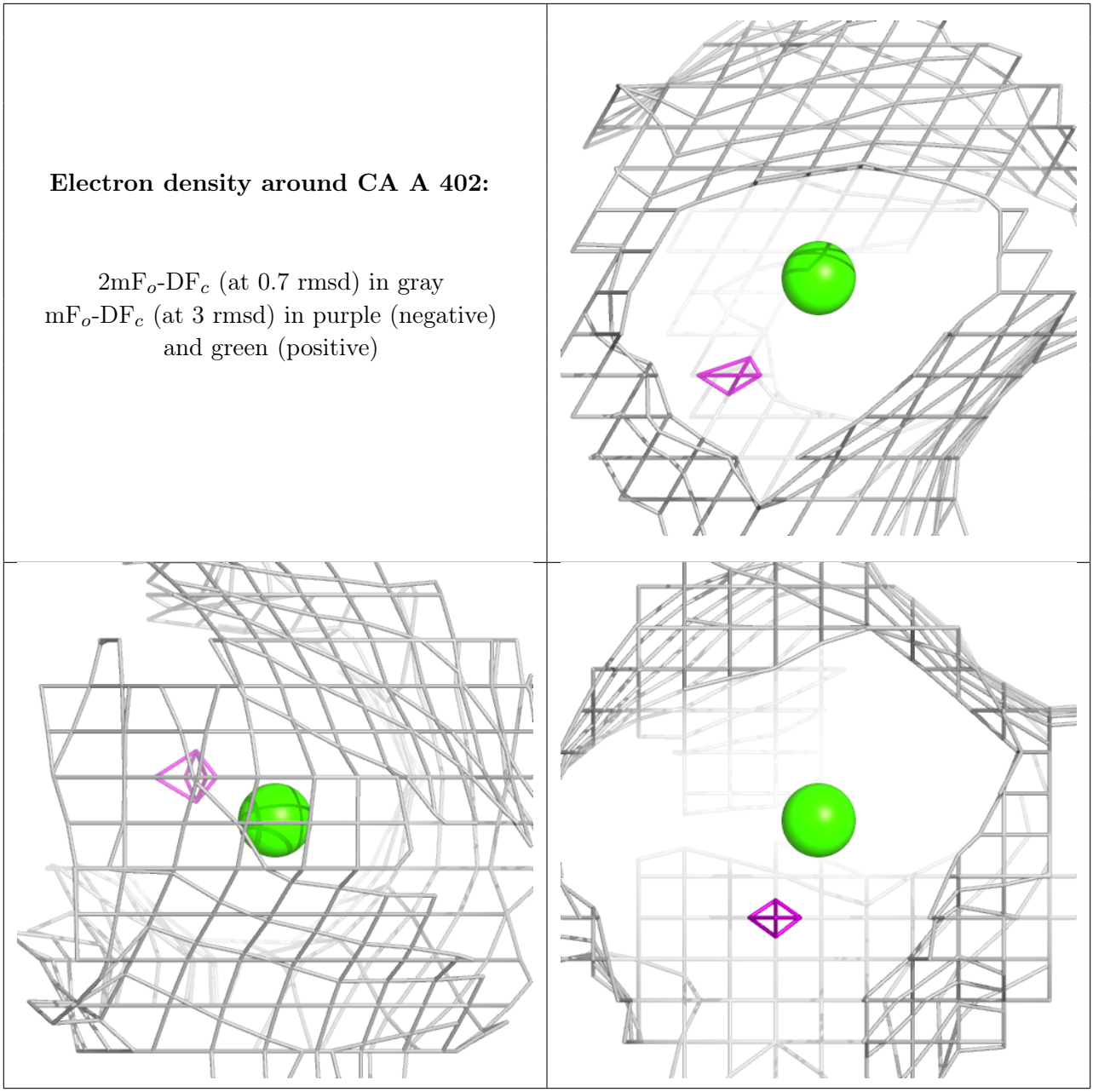






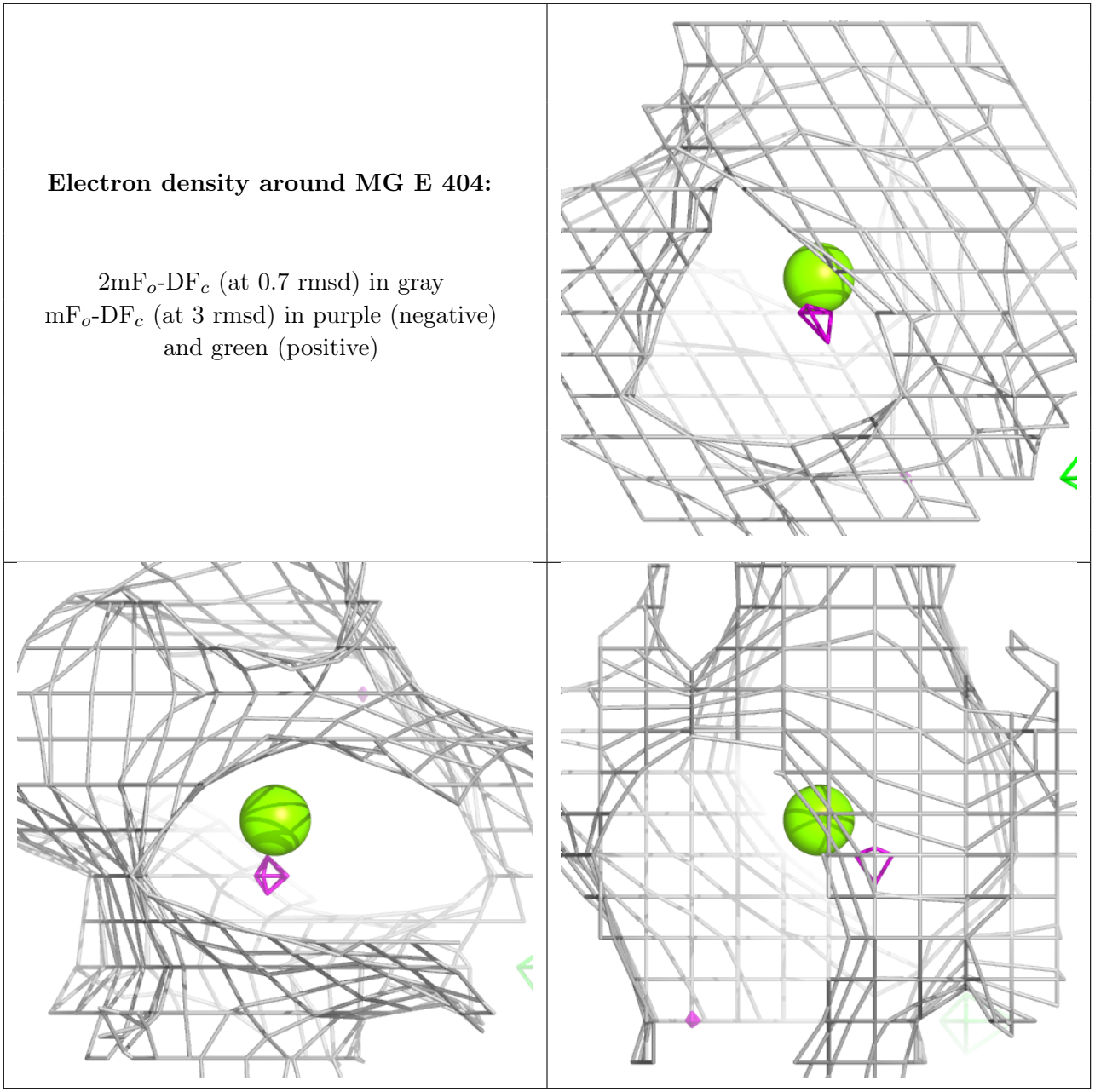
Electron density around CA A 402:

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



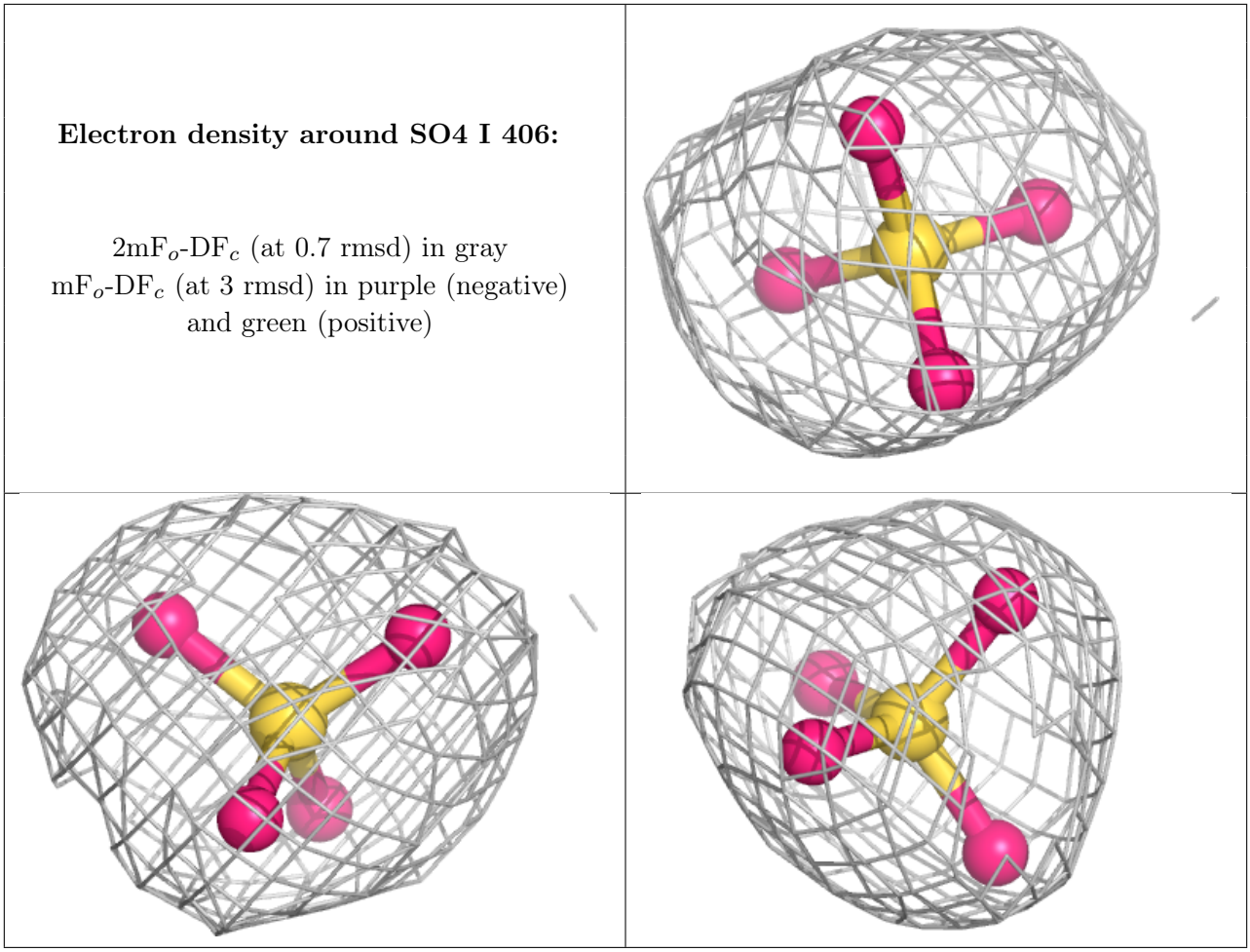
Electron density around MG E 404:

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



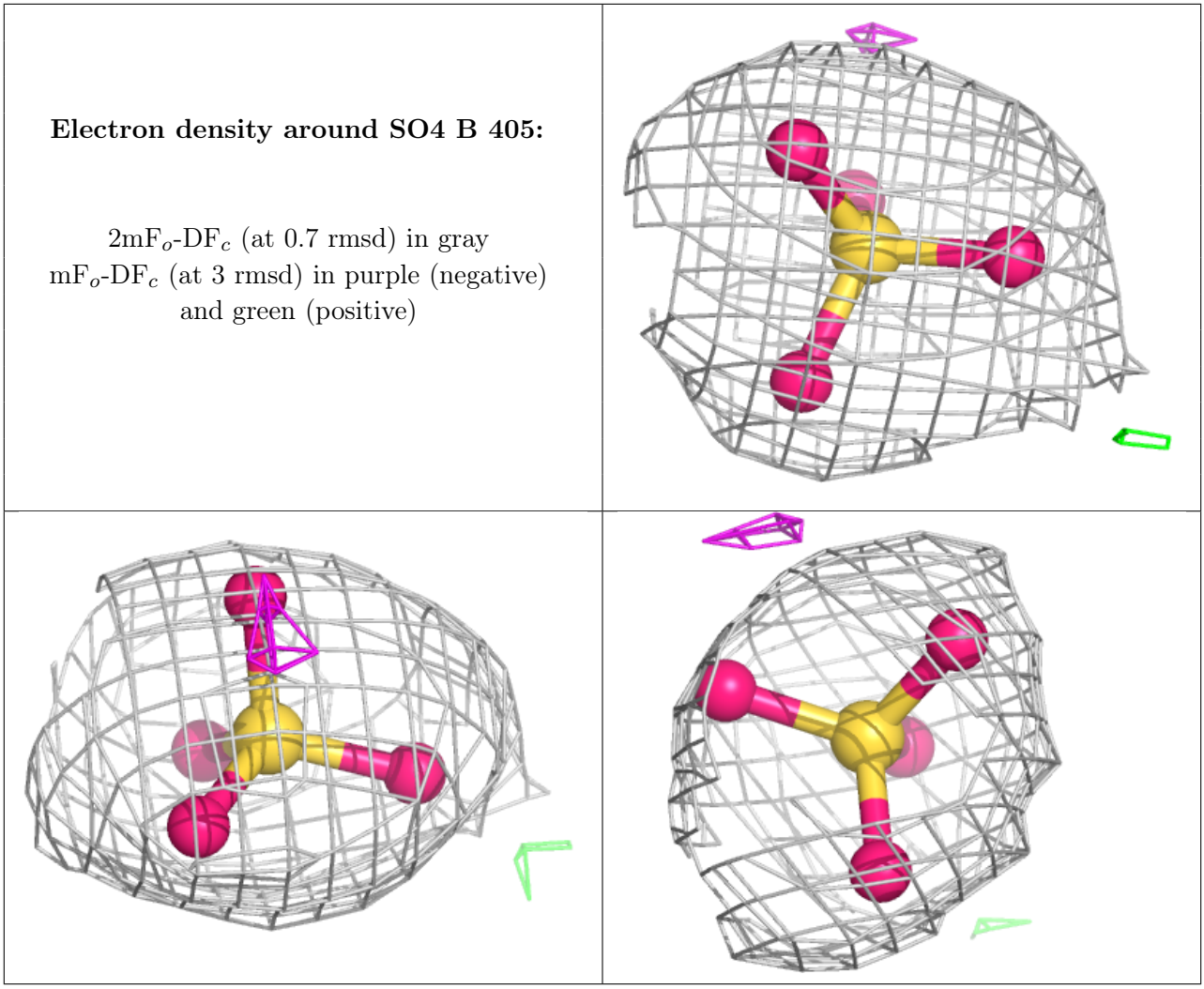
Electron density around SO4 I 406:

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



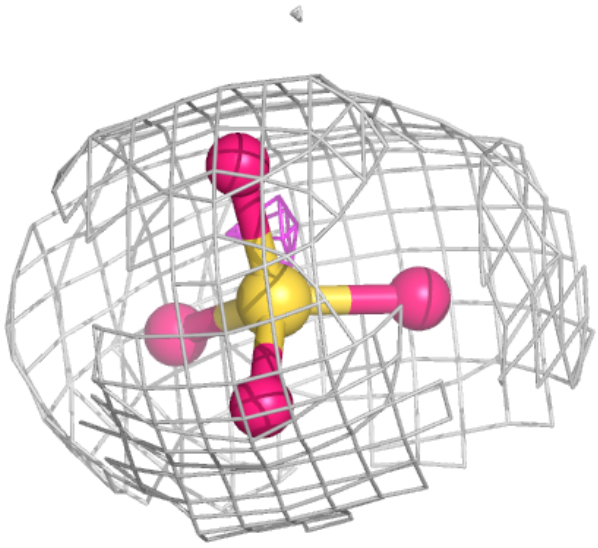
Electron density around SO4 B 405:

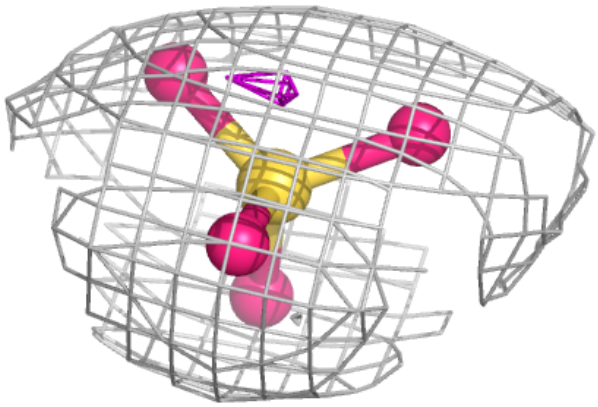
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

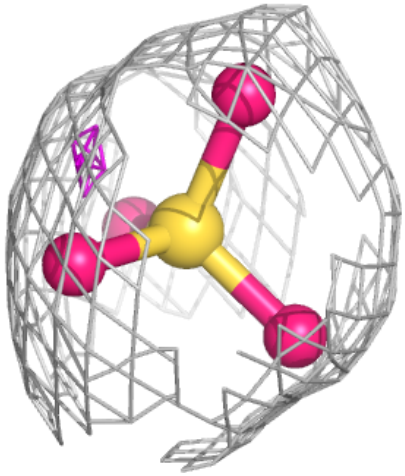


Electron density around SO4 A 406:

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

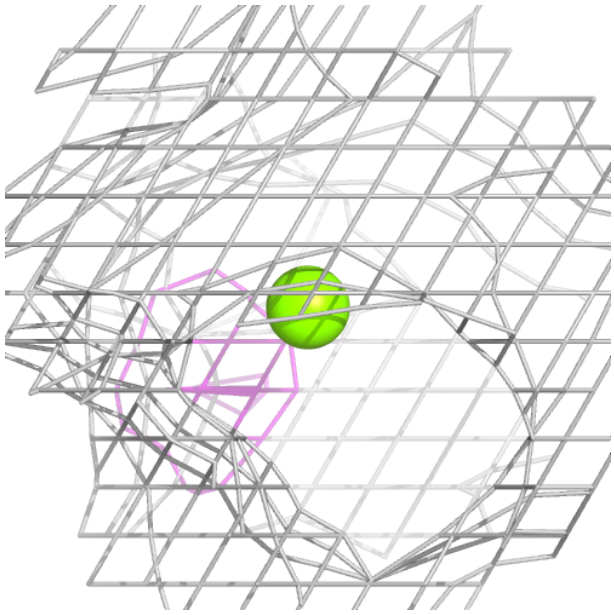


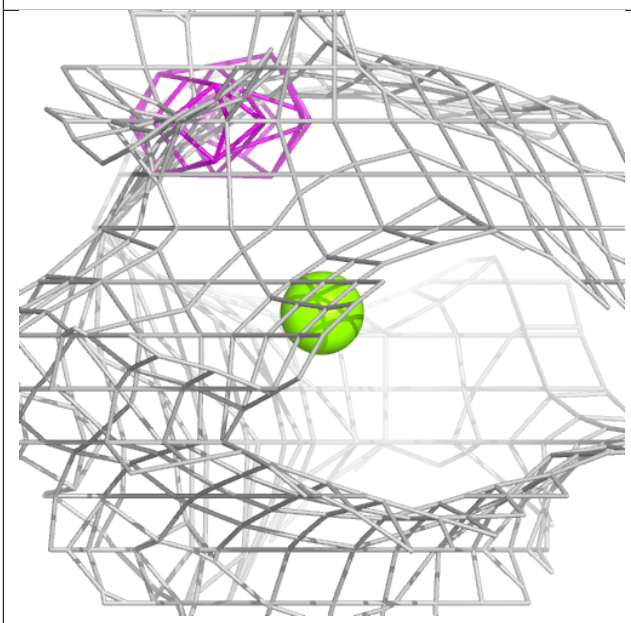


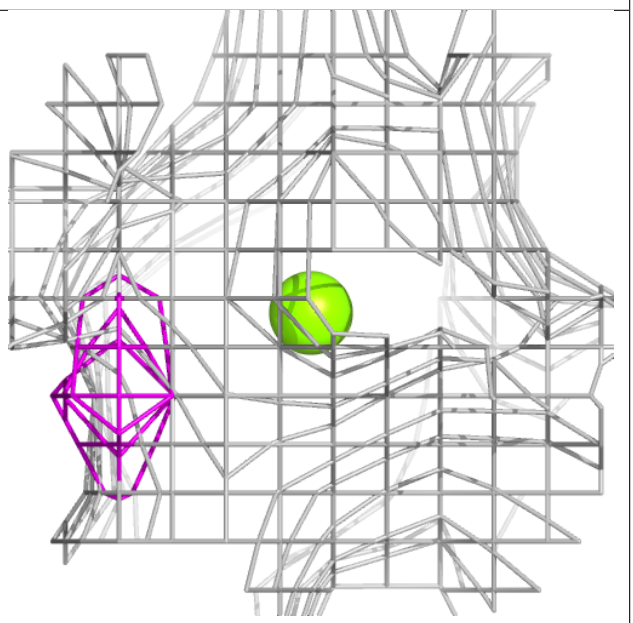


Electron density around MG C 404:

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

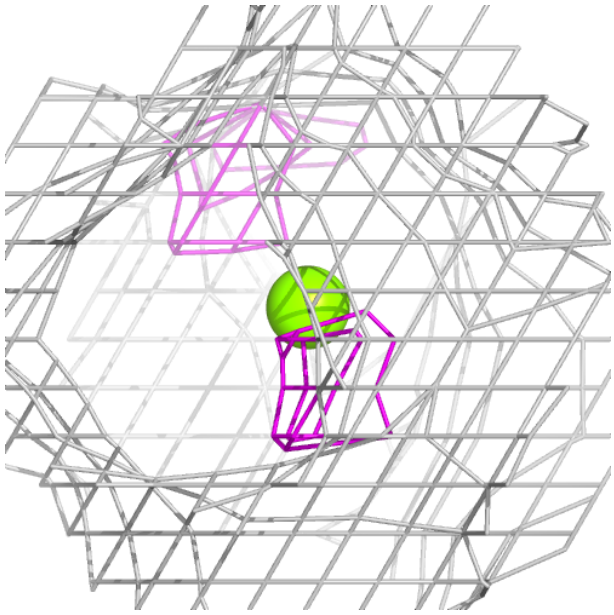


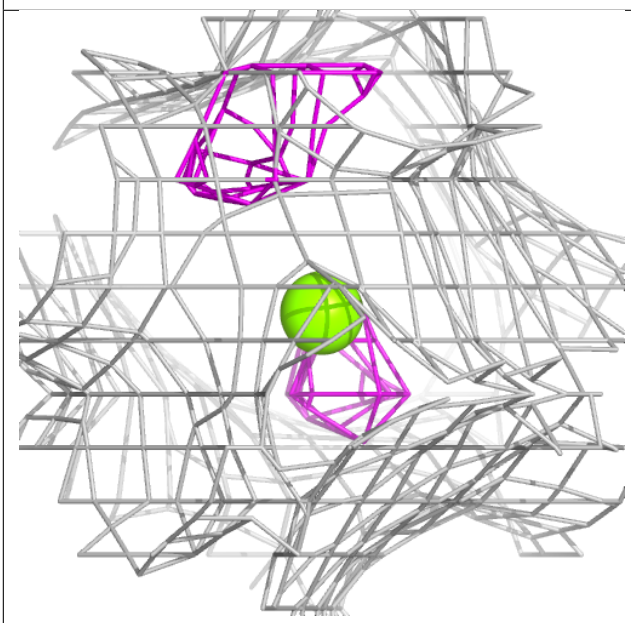


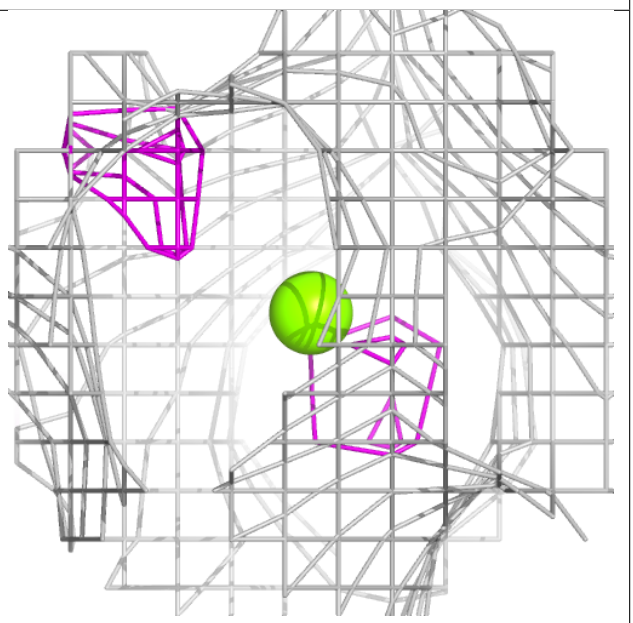


Electron density around MG A 404:

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

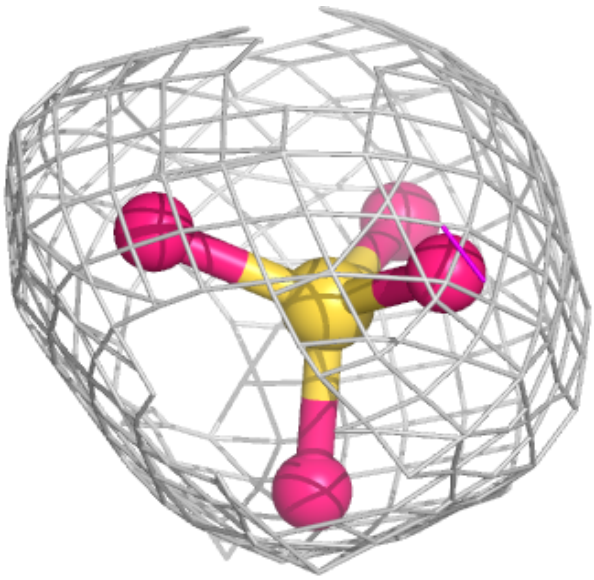


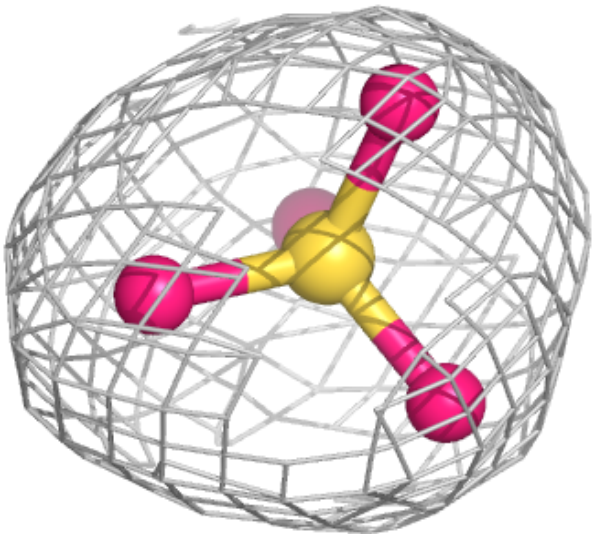


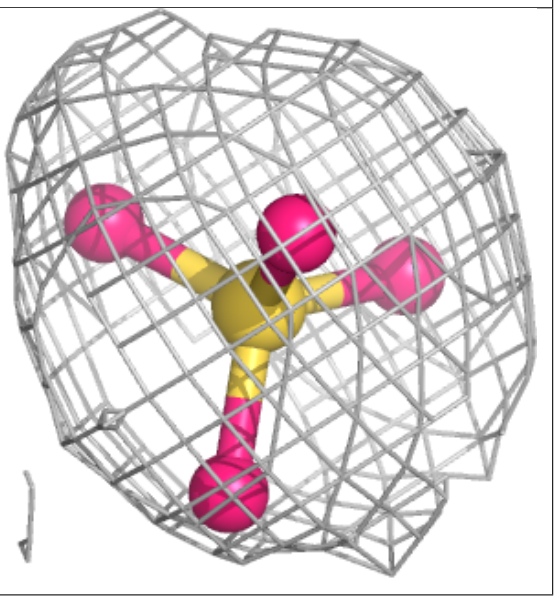


Electron density around SO4 F 405:

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

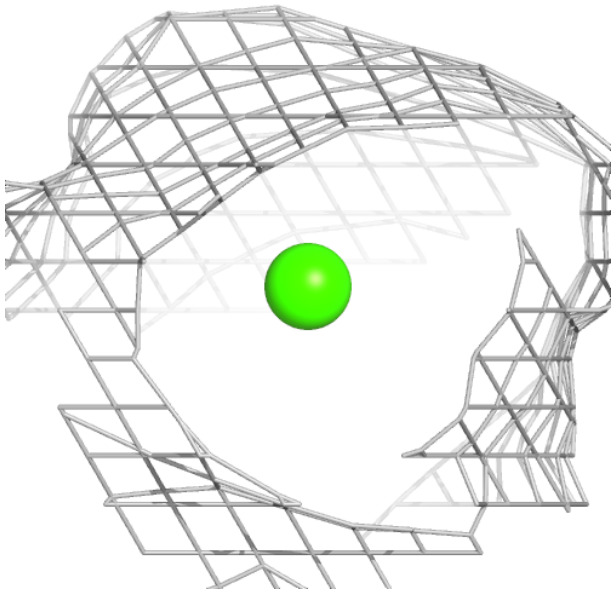


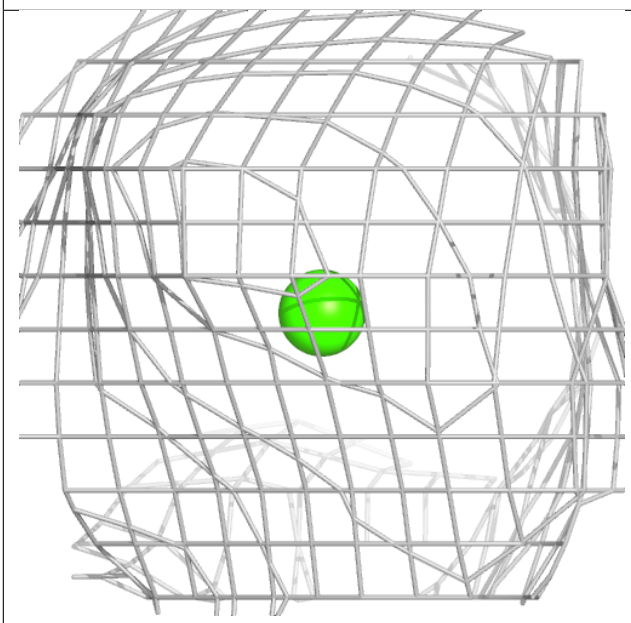


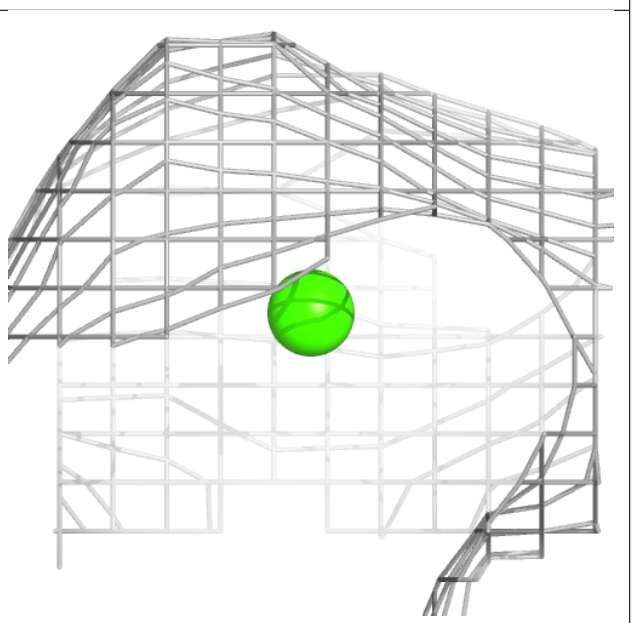


Electron density around CA E 403:

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

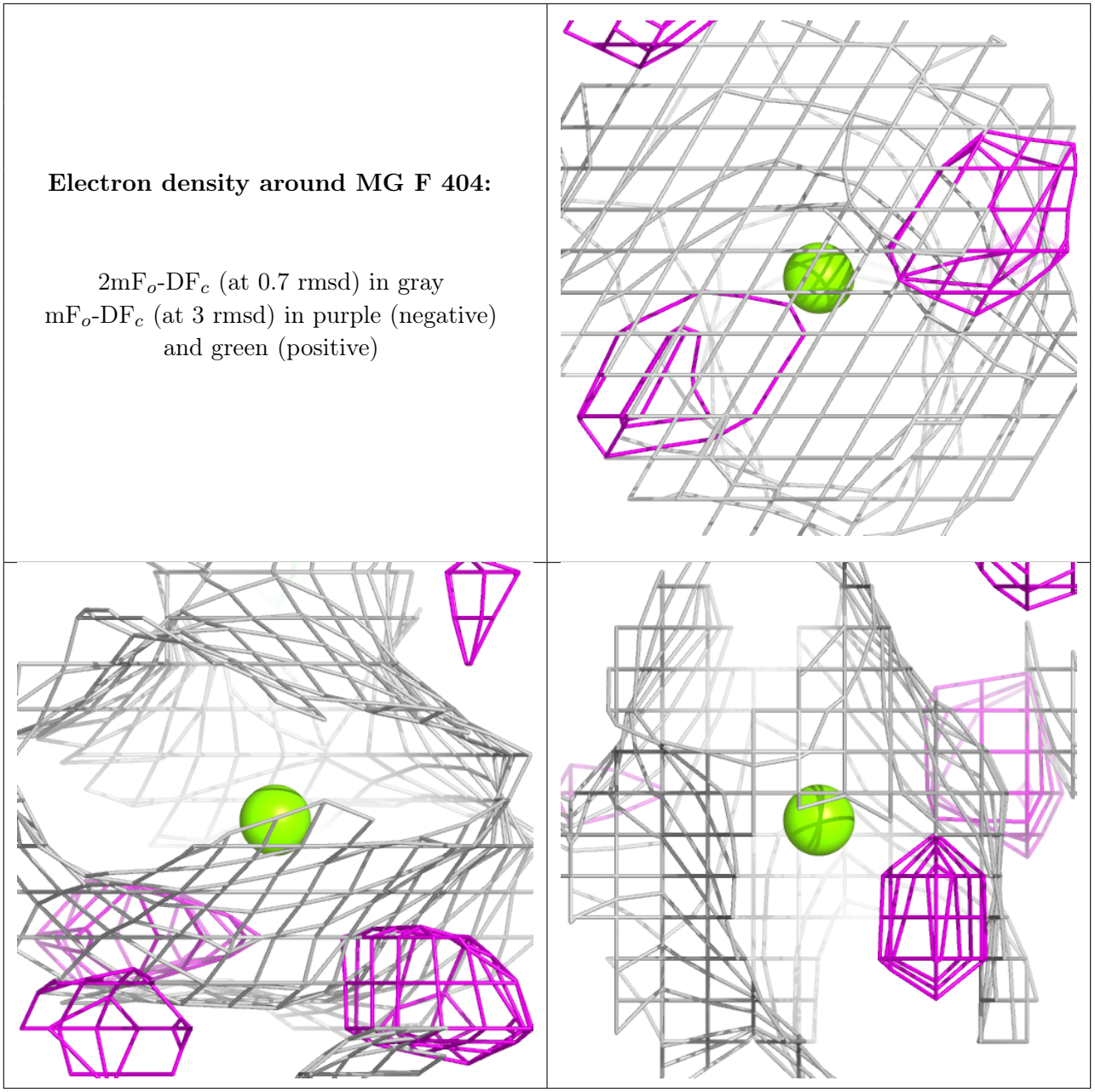






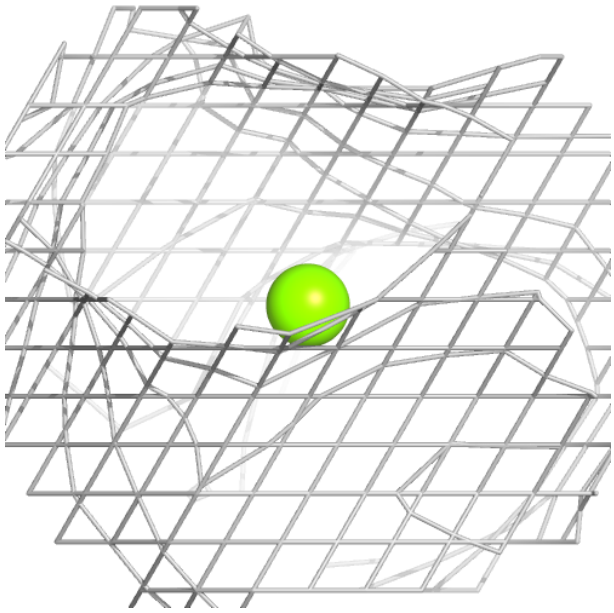
Electron density around MG F 404:

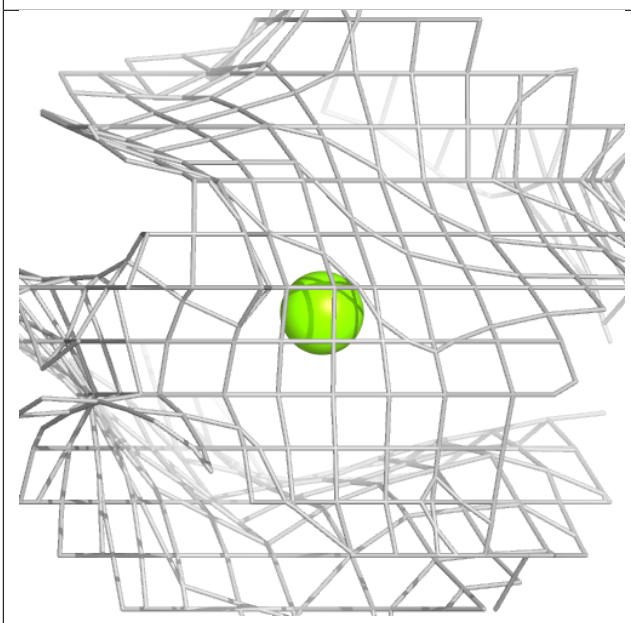
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

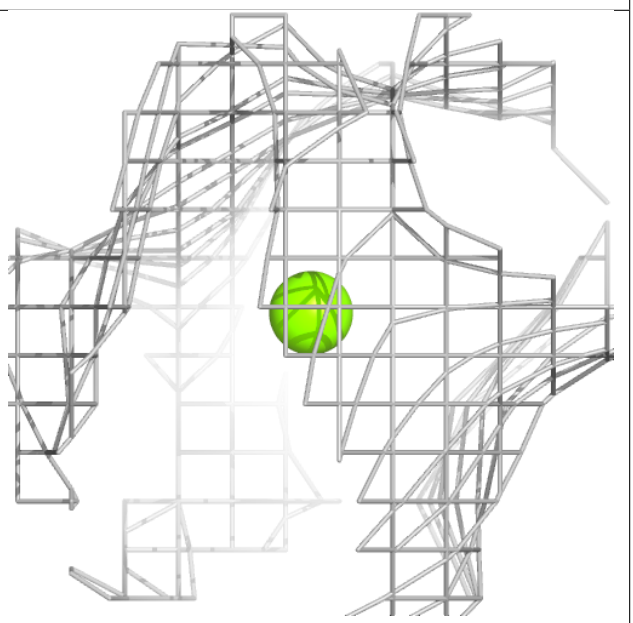


Electron density around MG G 404:

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

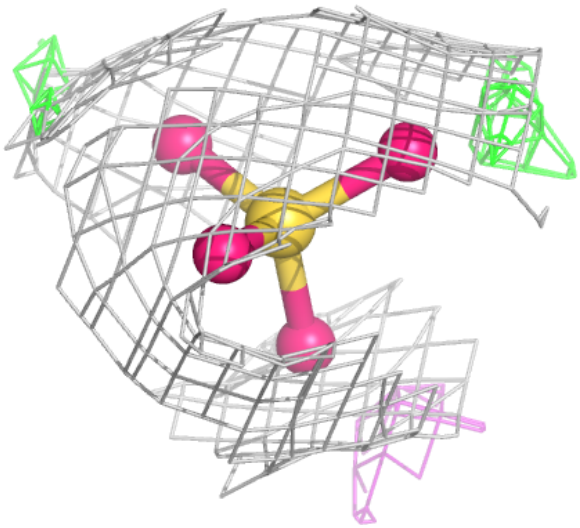


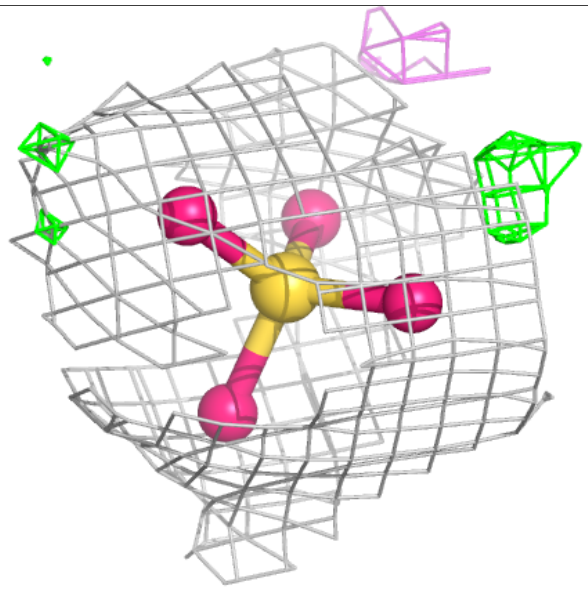


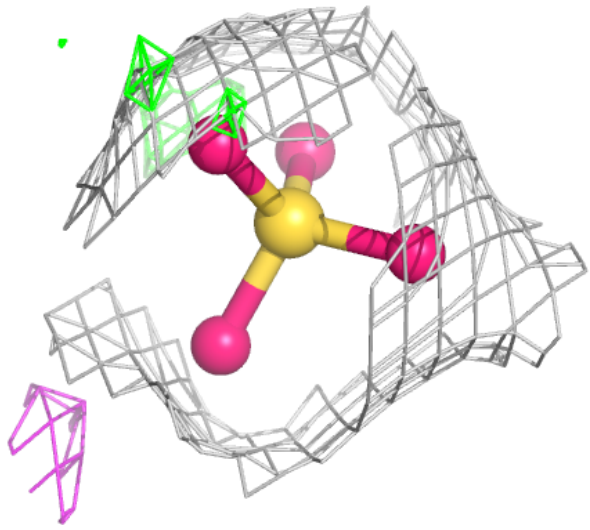


Electron density around SO4 I 405:

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

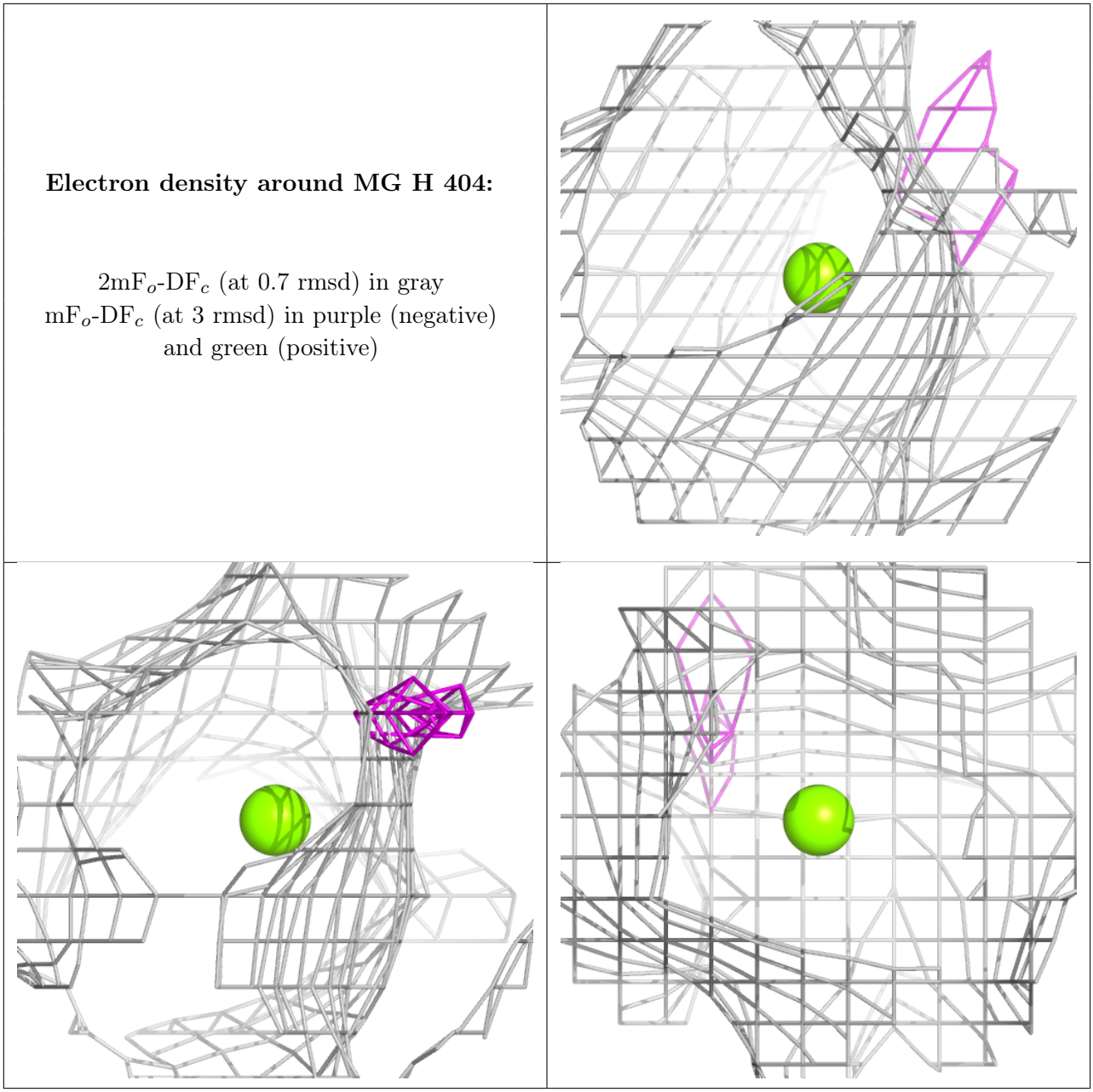






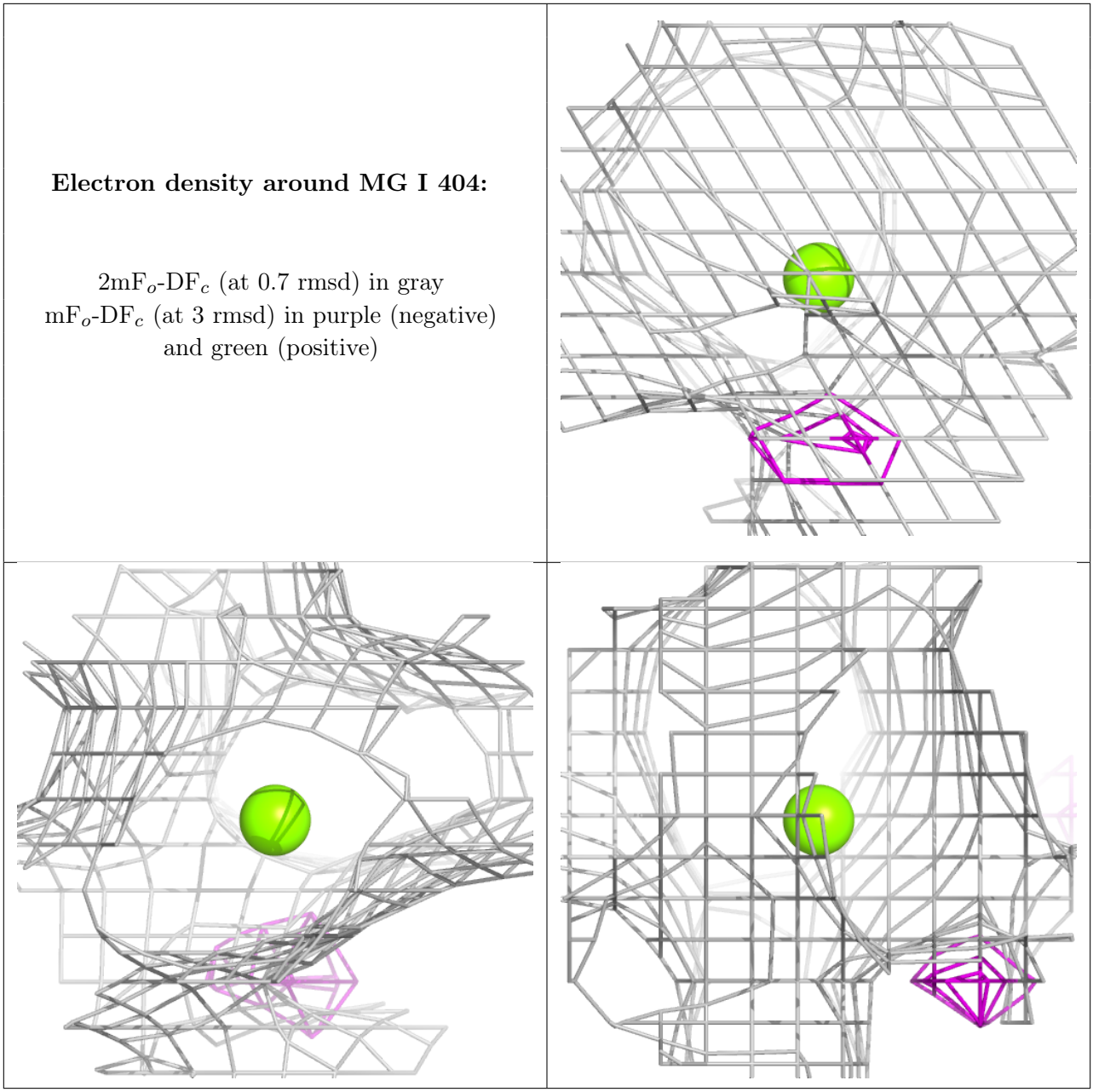
Electron density around MG H 404:

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



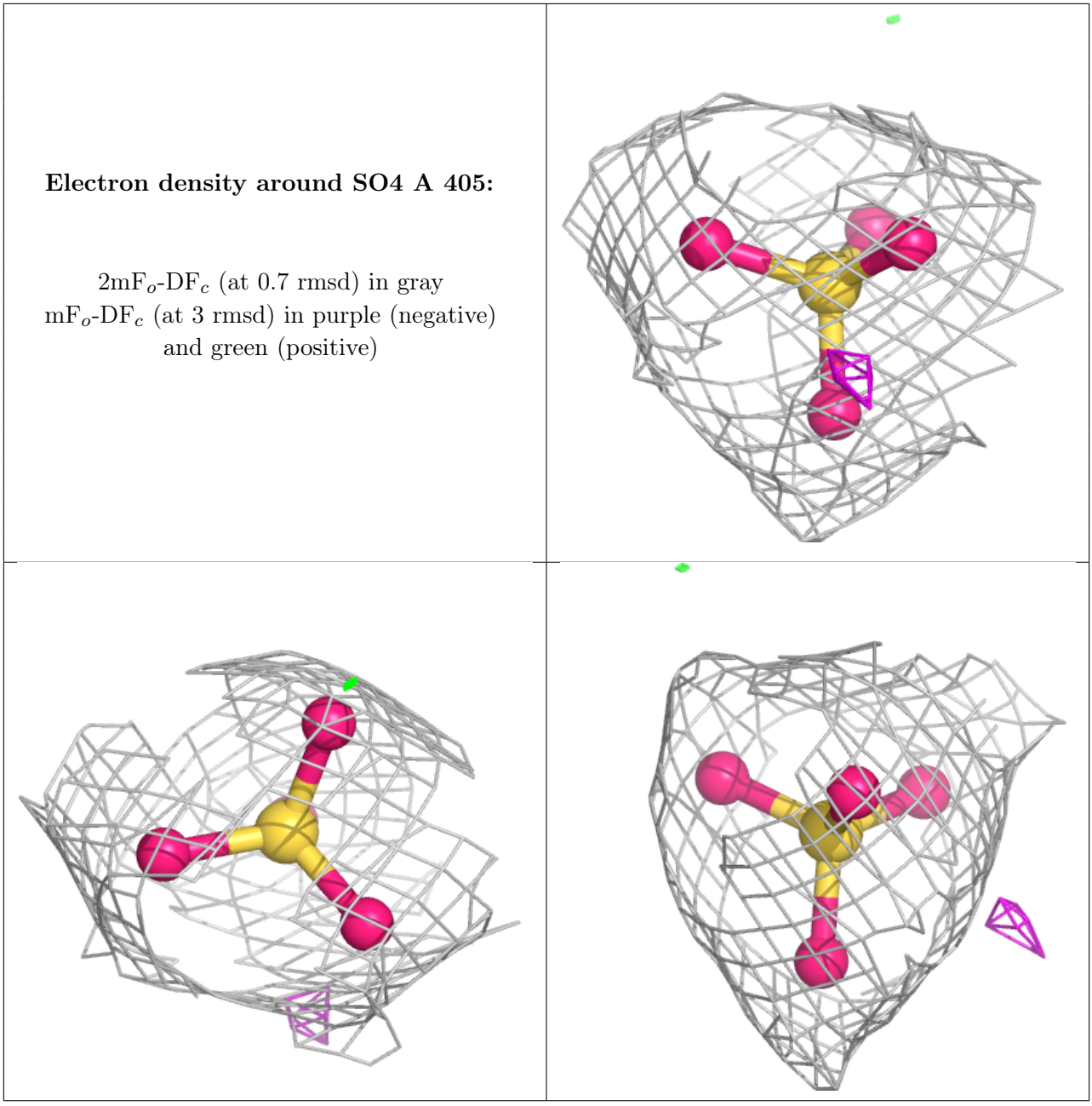
Electron density around MG I 404:

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



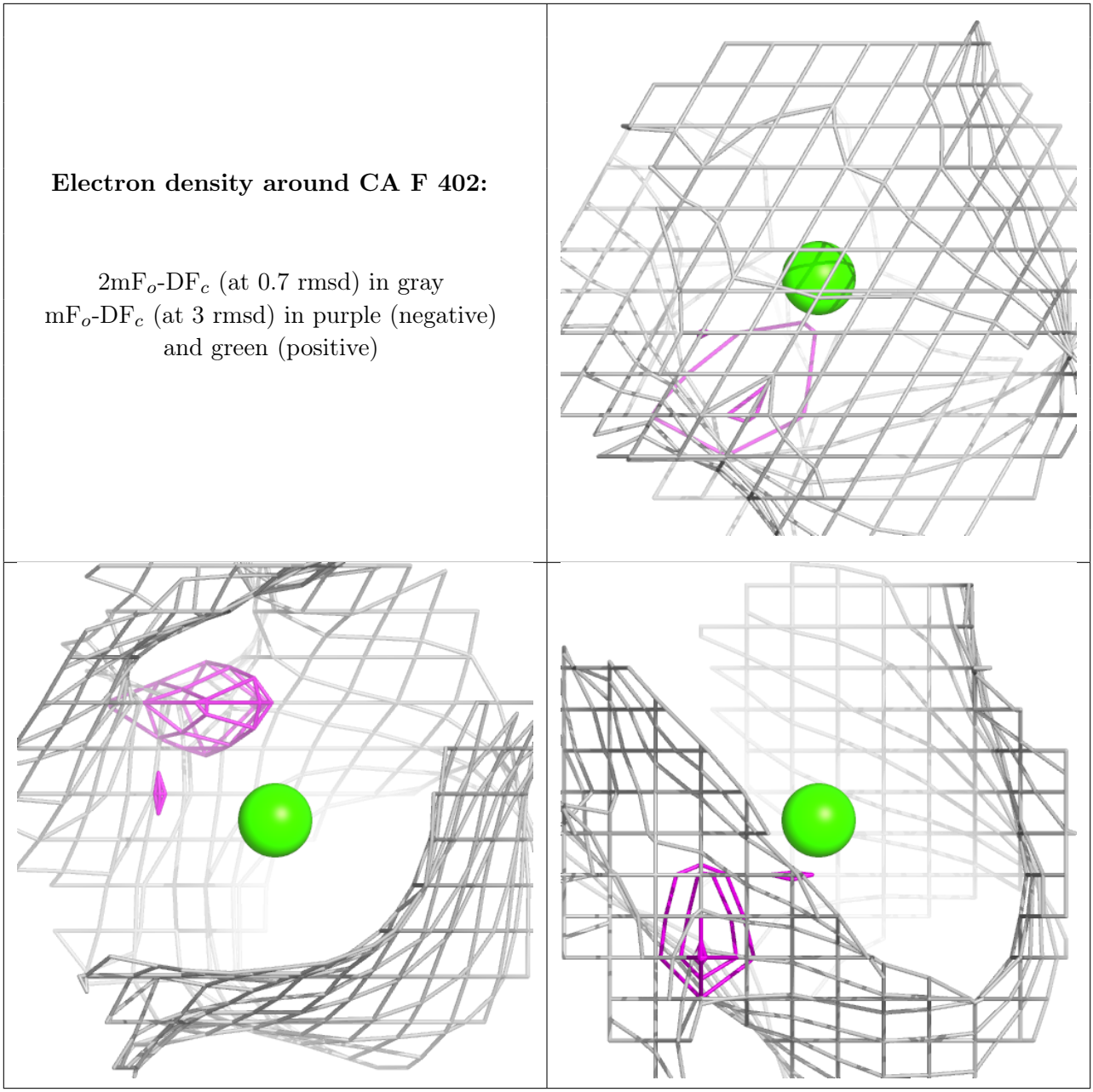
Electron density around SO4 A 405:

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



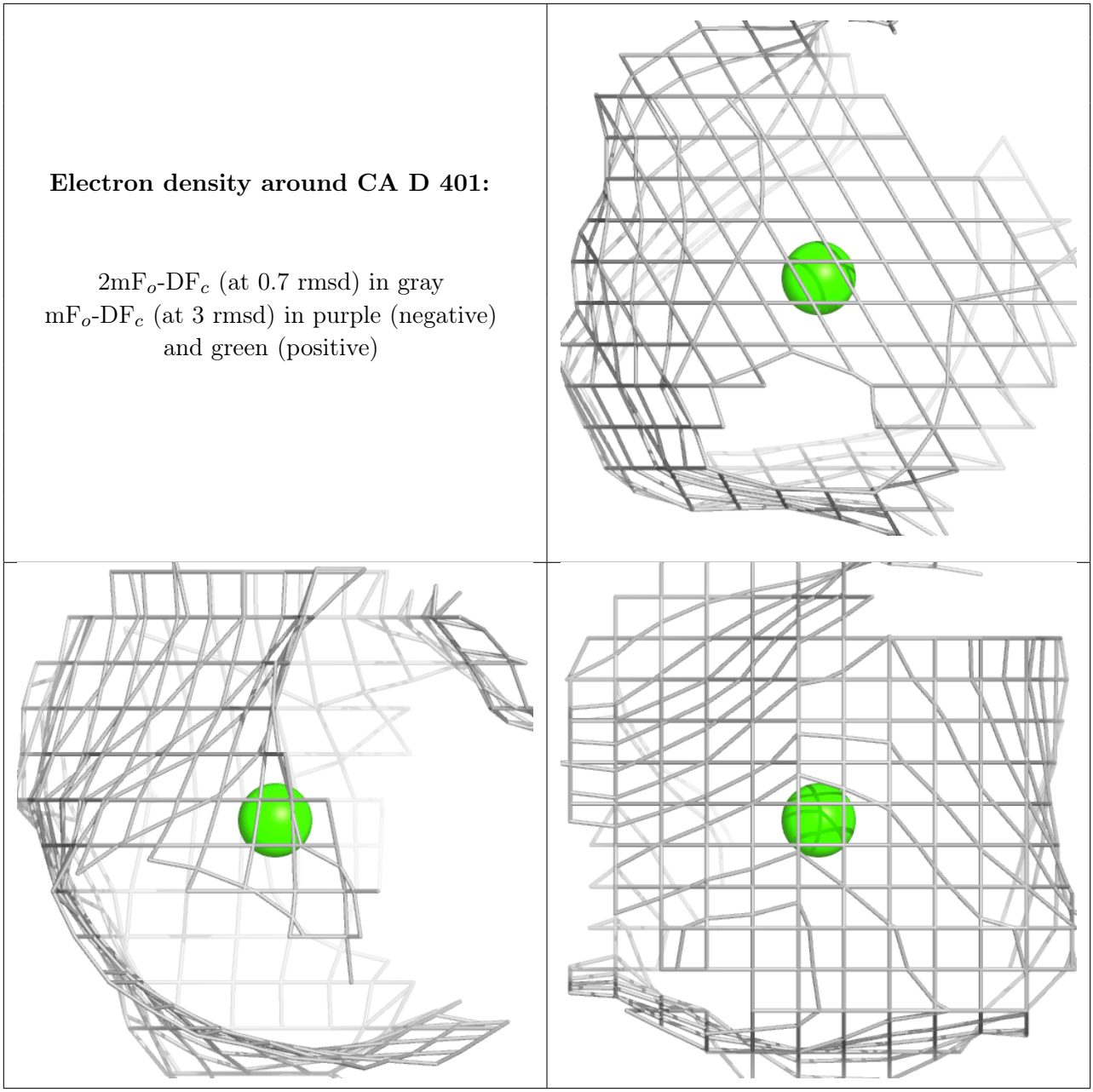
Electron density around CA F 402:

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



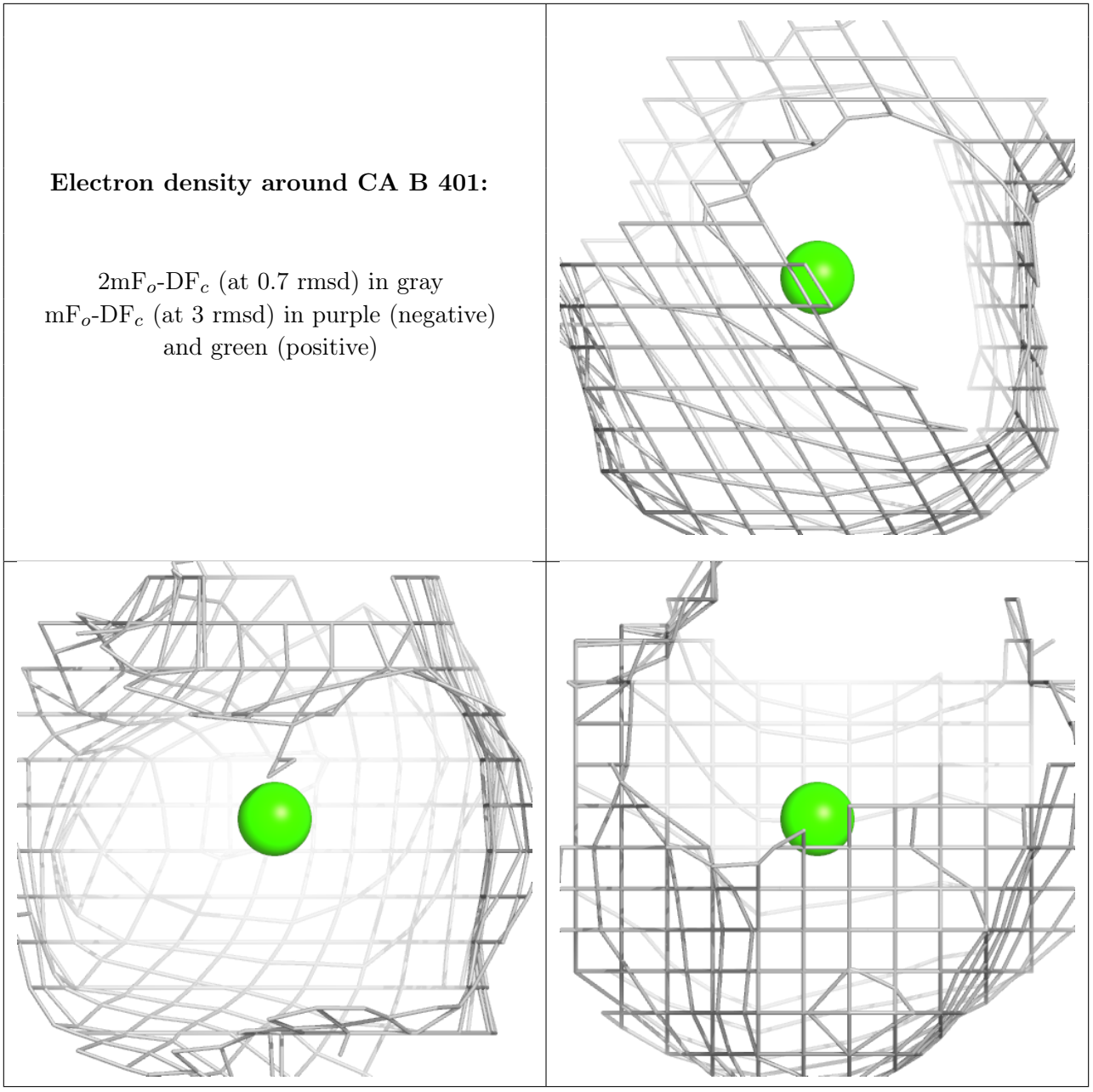
Electron density around CA D 401:

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



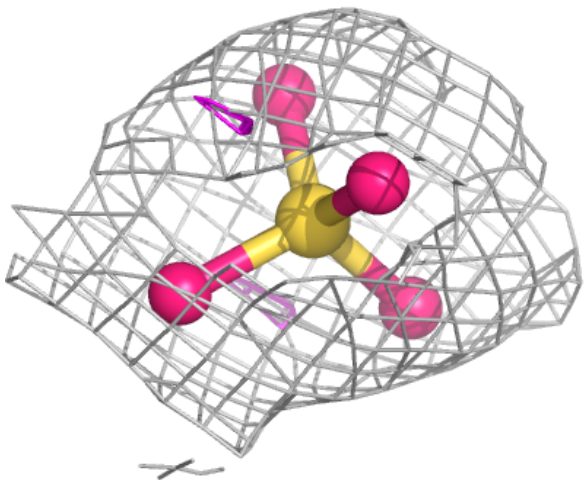
Electron density around CA B 401:

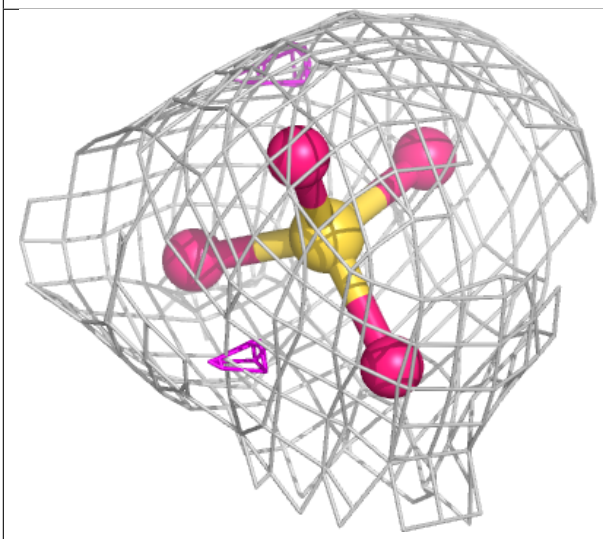
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

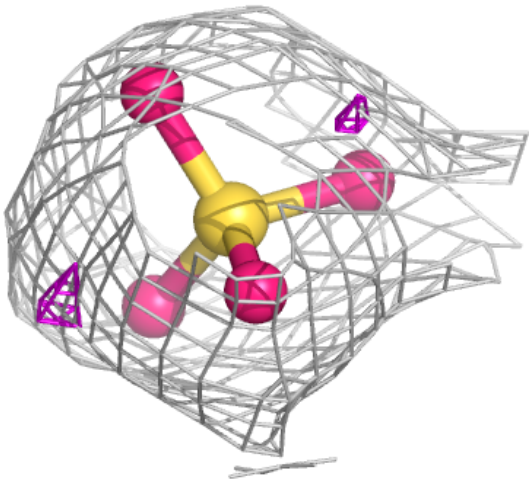


Electron density around SO4 C 405:

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

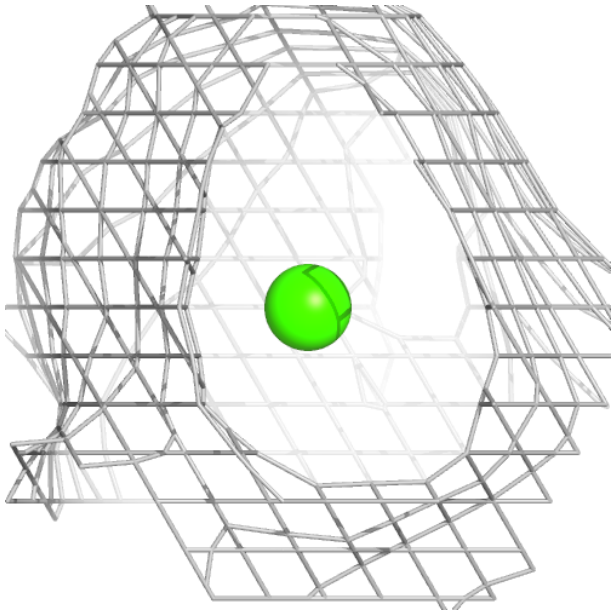


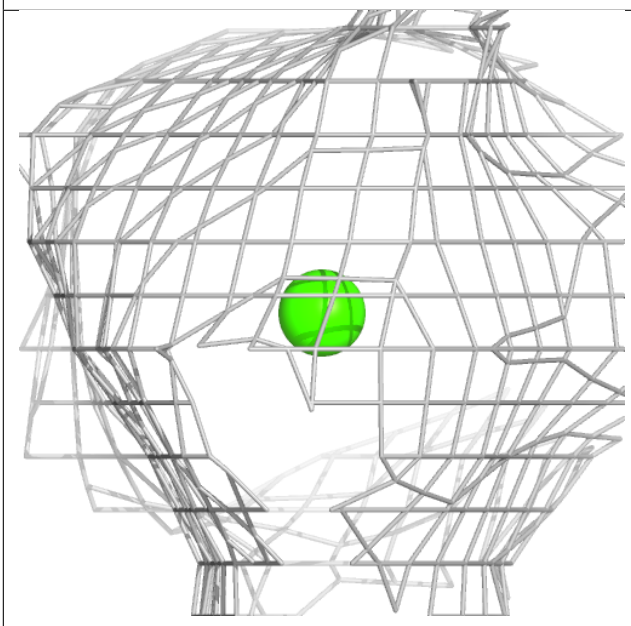


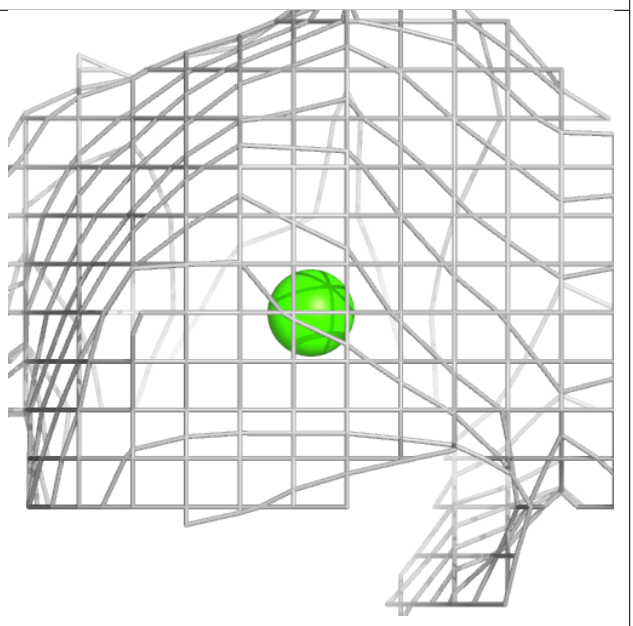


Electron density around CA F 401:

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

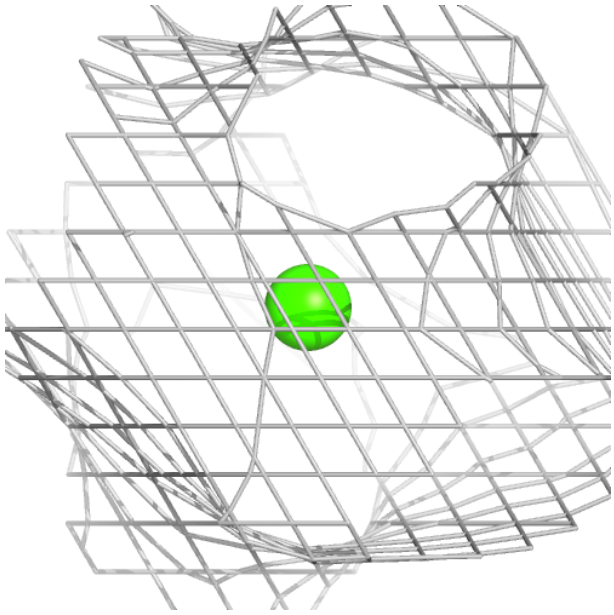


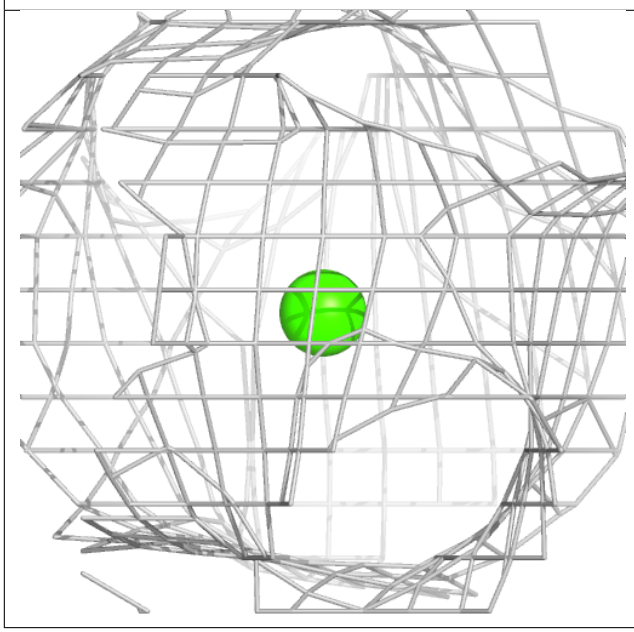


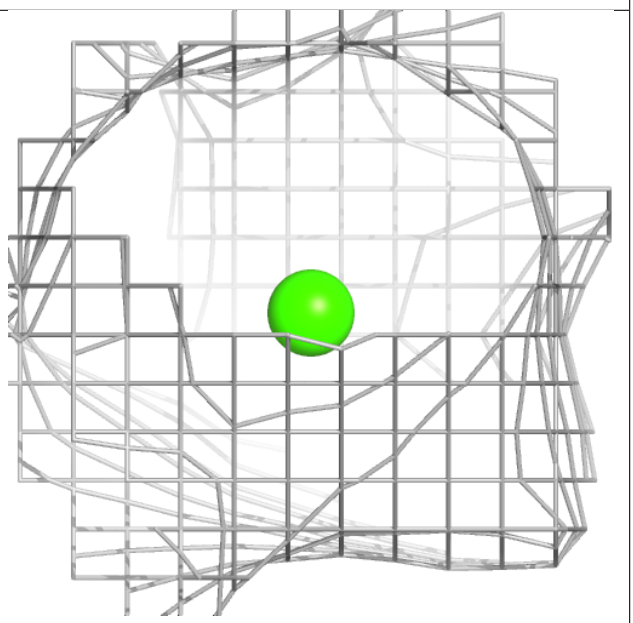


Electron density around CA A 401:

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

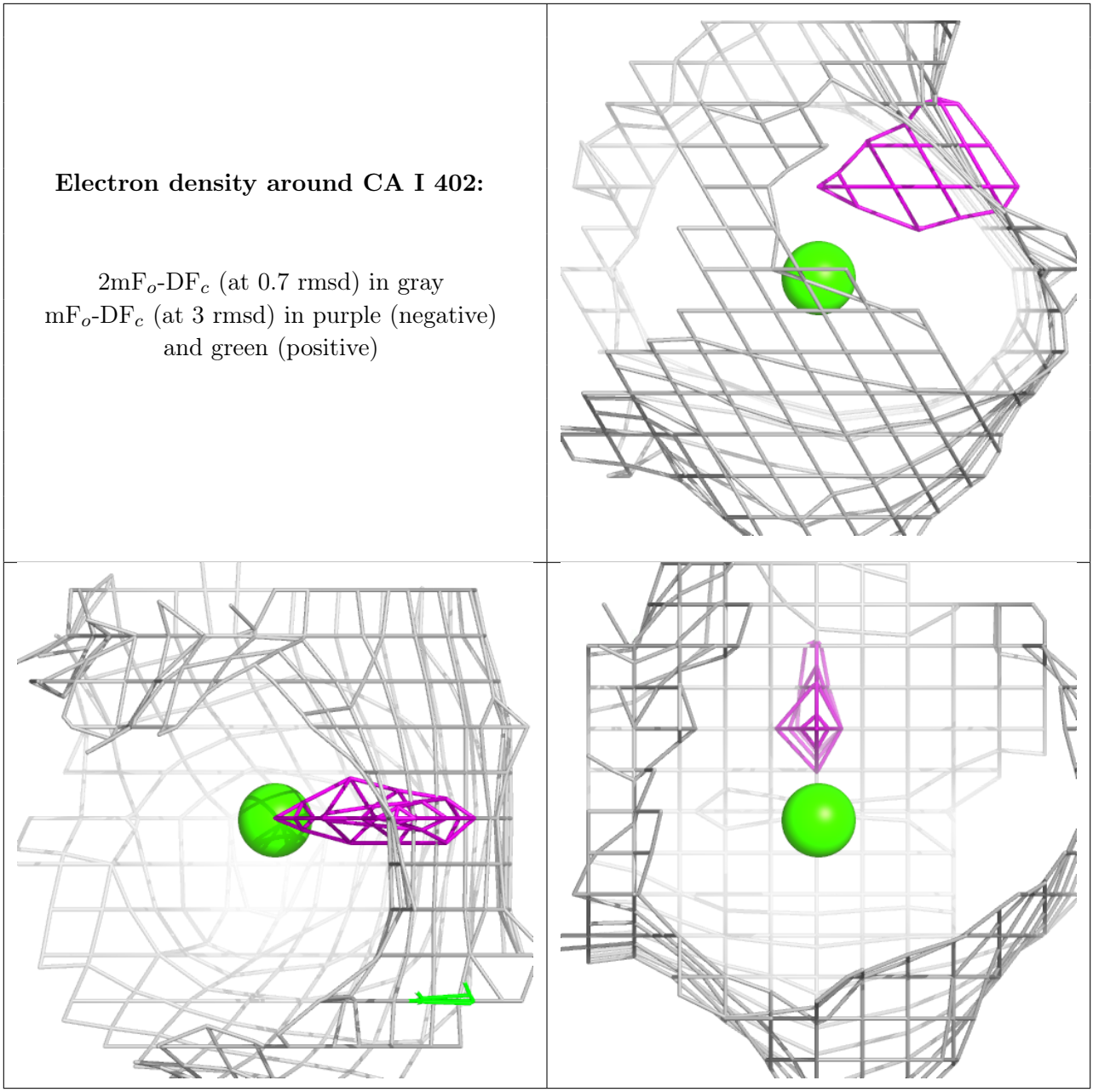






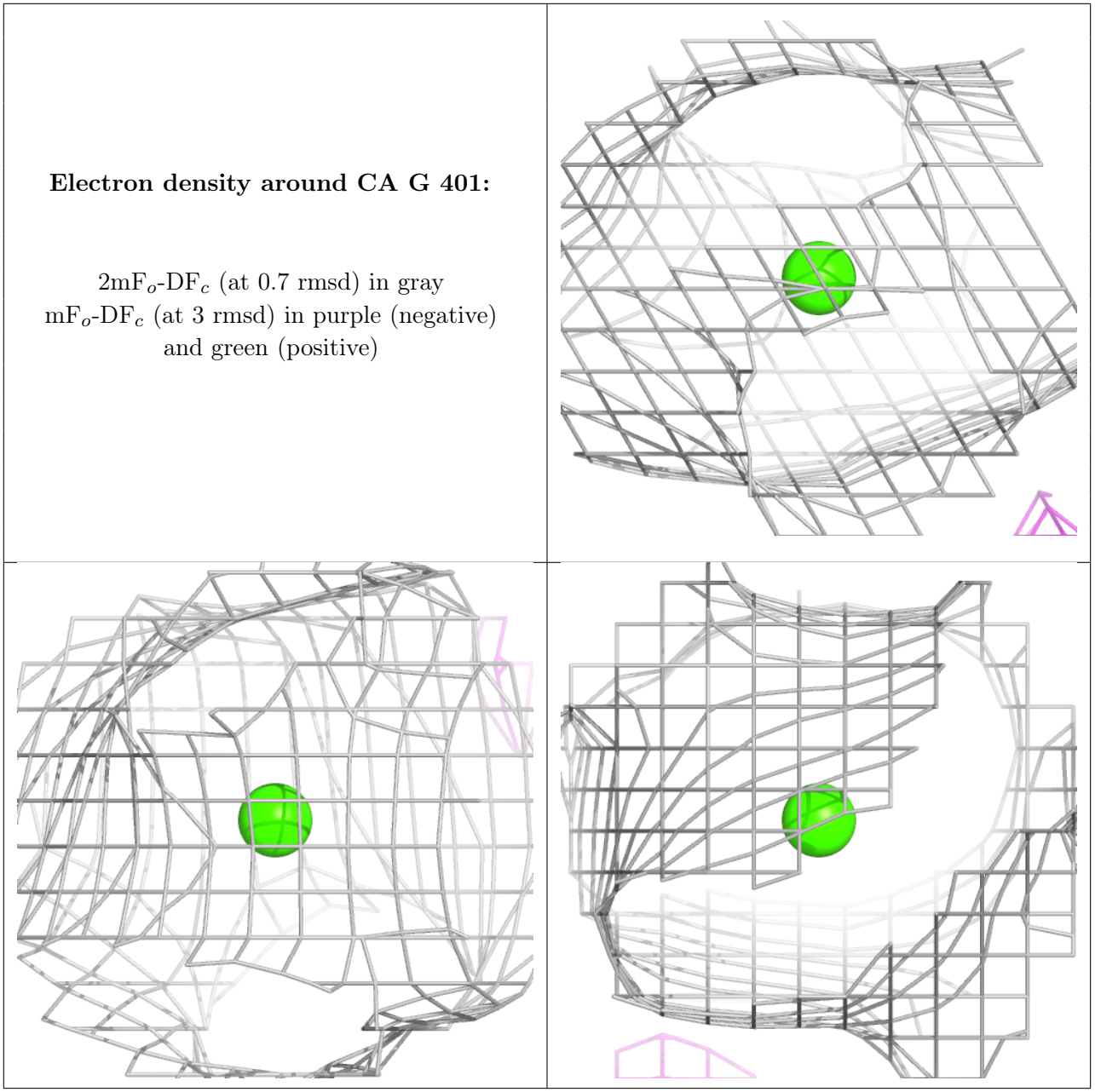
Electron density around CA I 402:

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



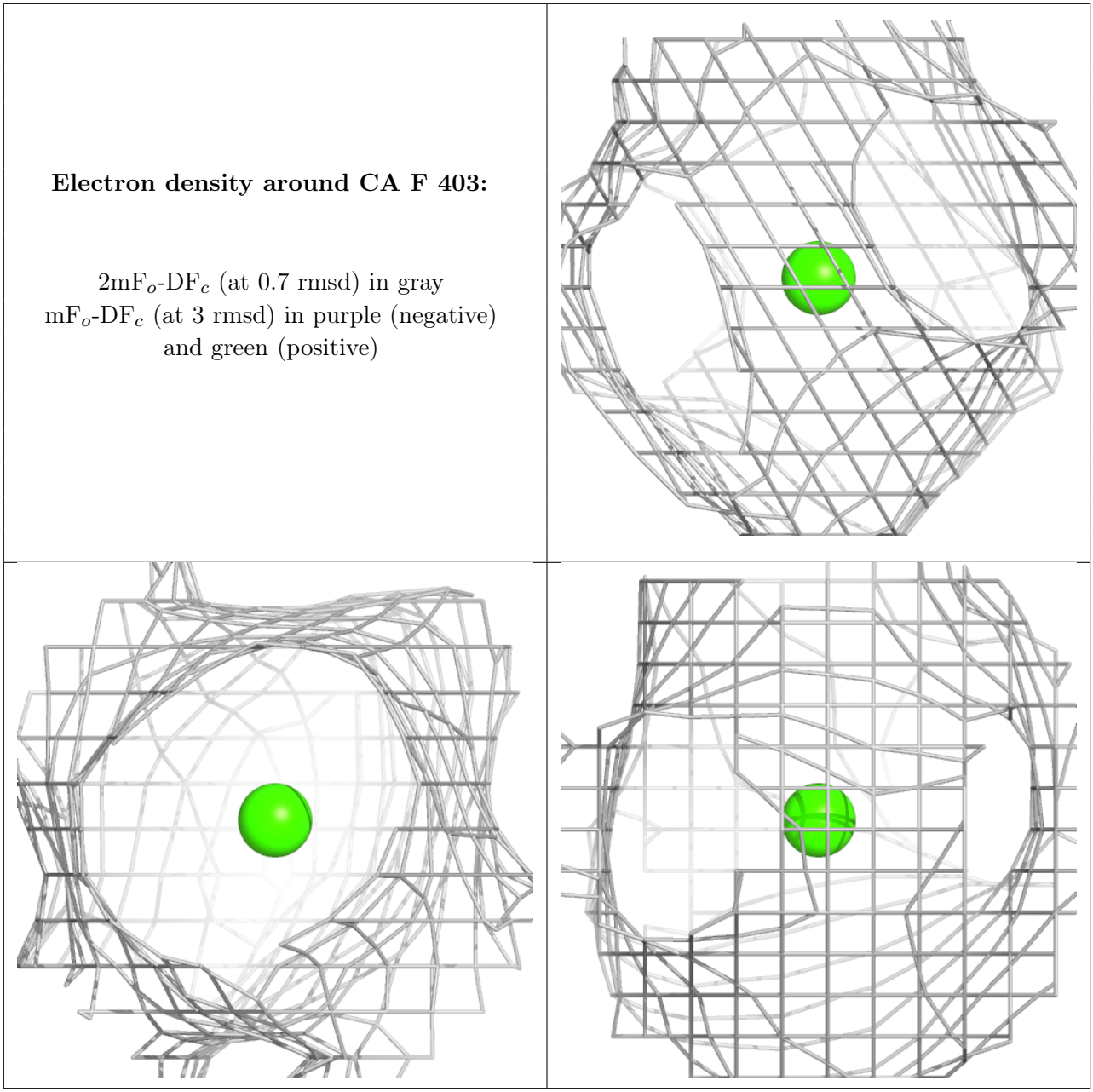
Electron density around CA G 401:

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



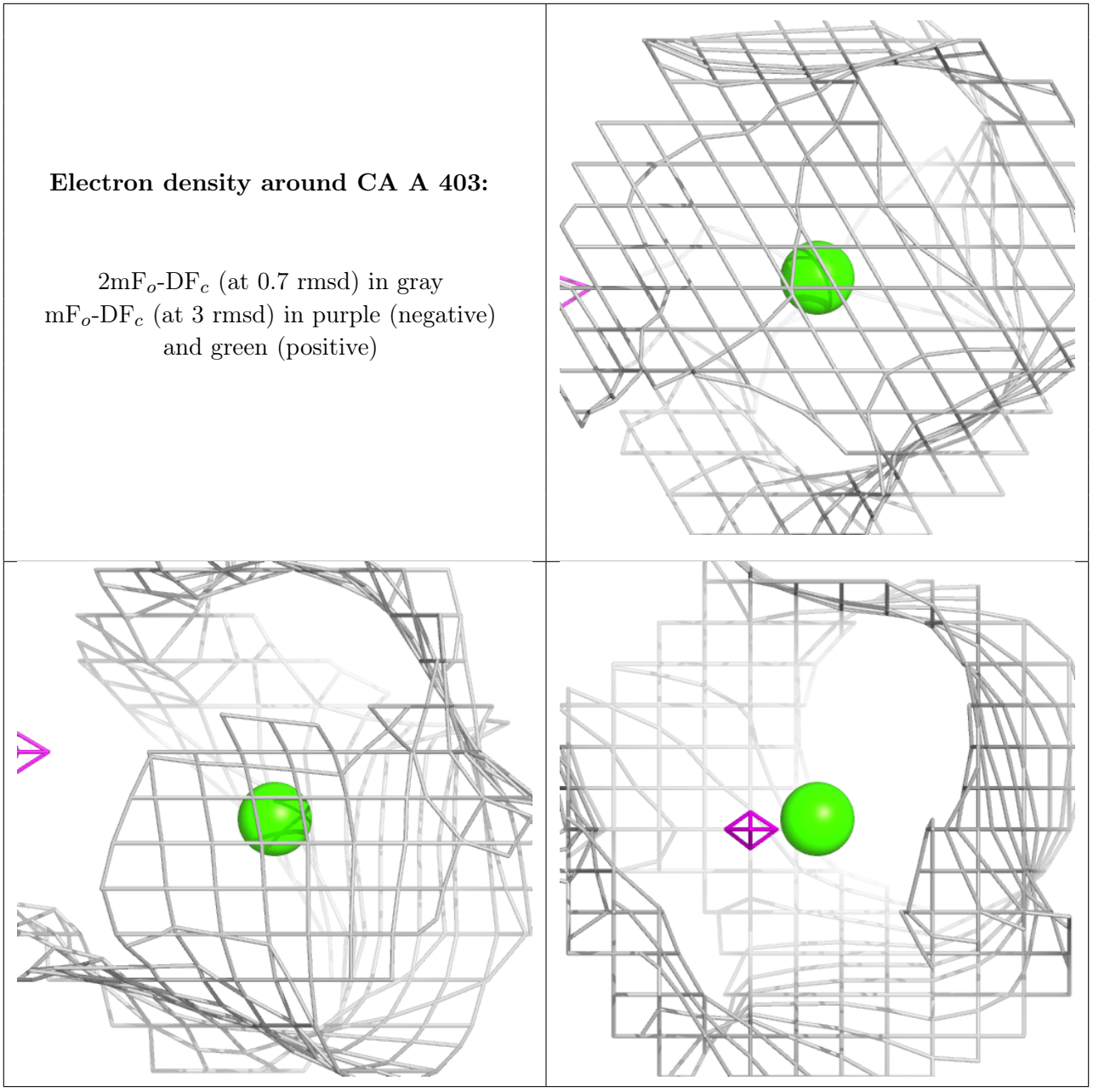
Electron density around CA F 403:

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



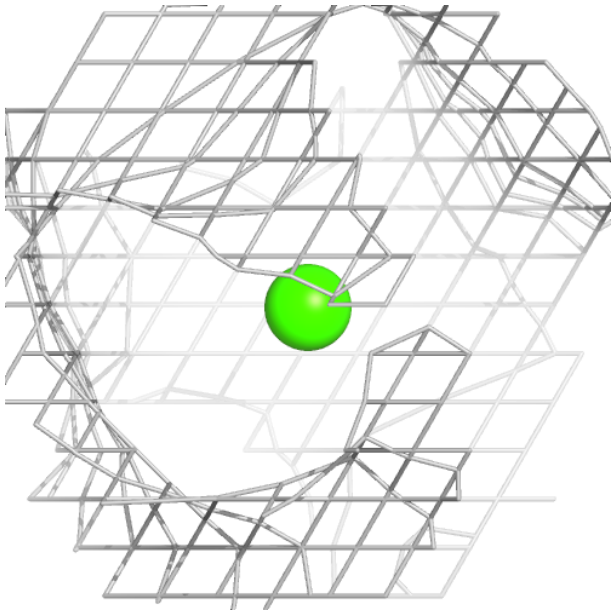
Electron density around CA A 403:

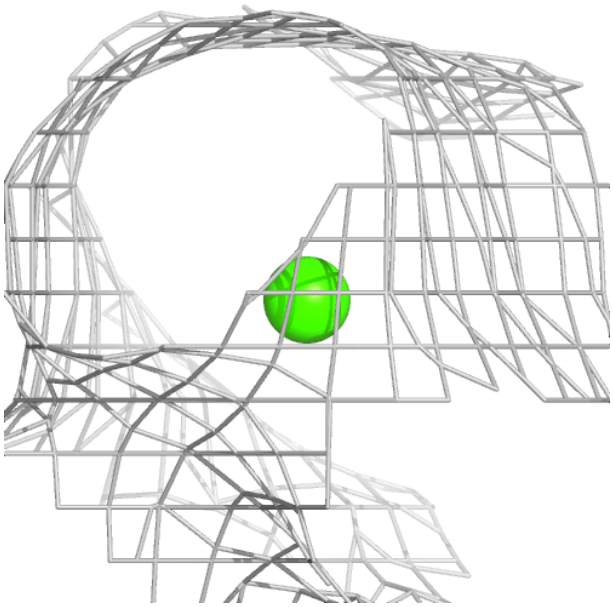
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

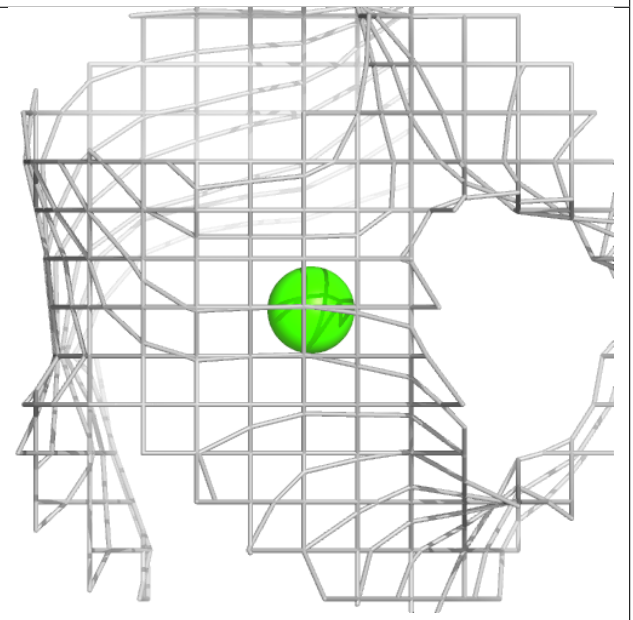


Electron density around CA D 402:

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

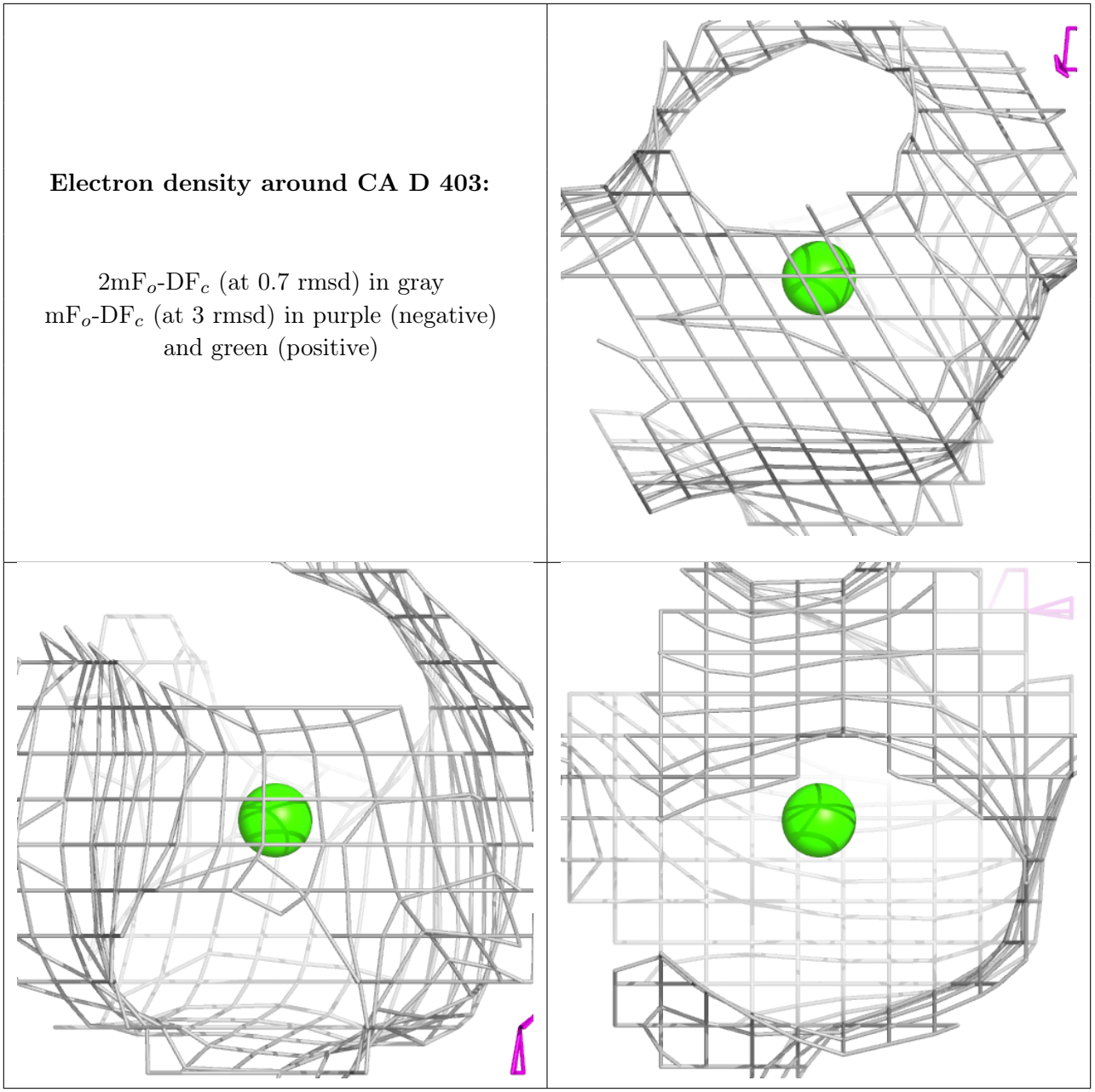






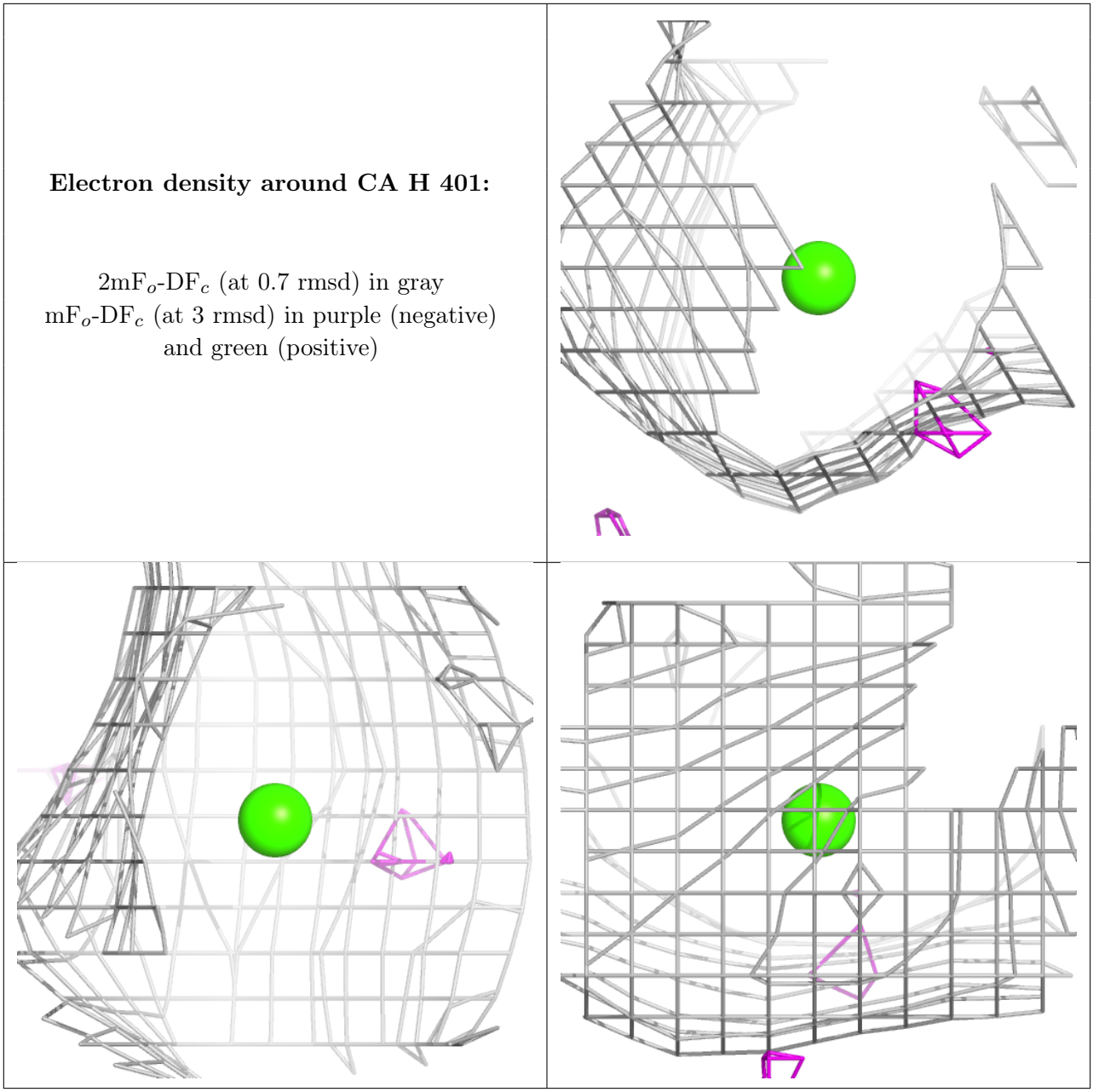
Electron density around CA D 403:

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



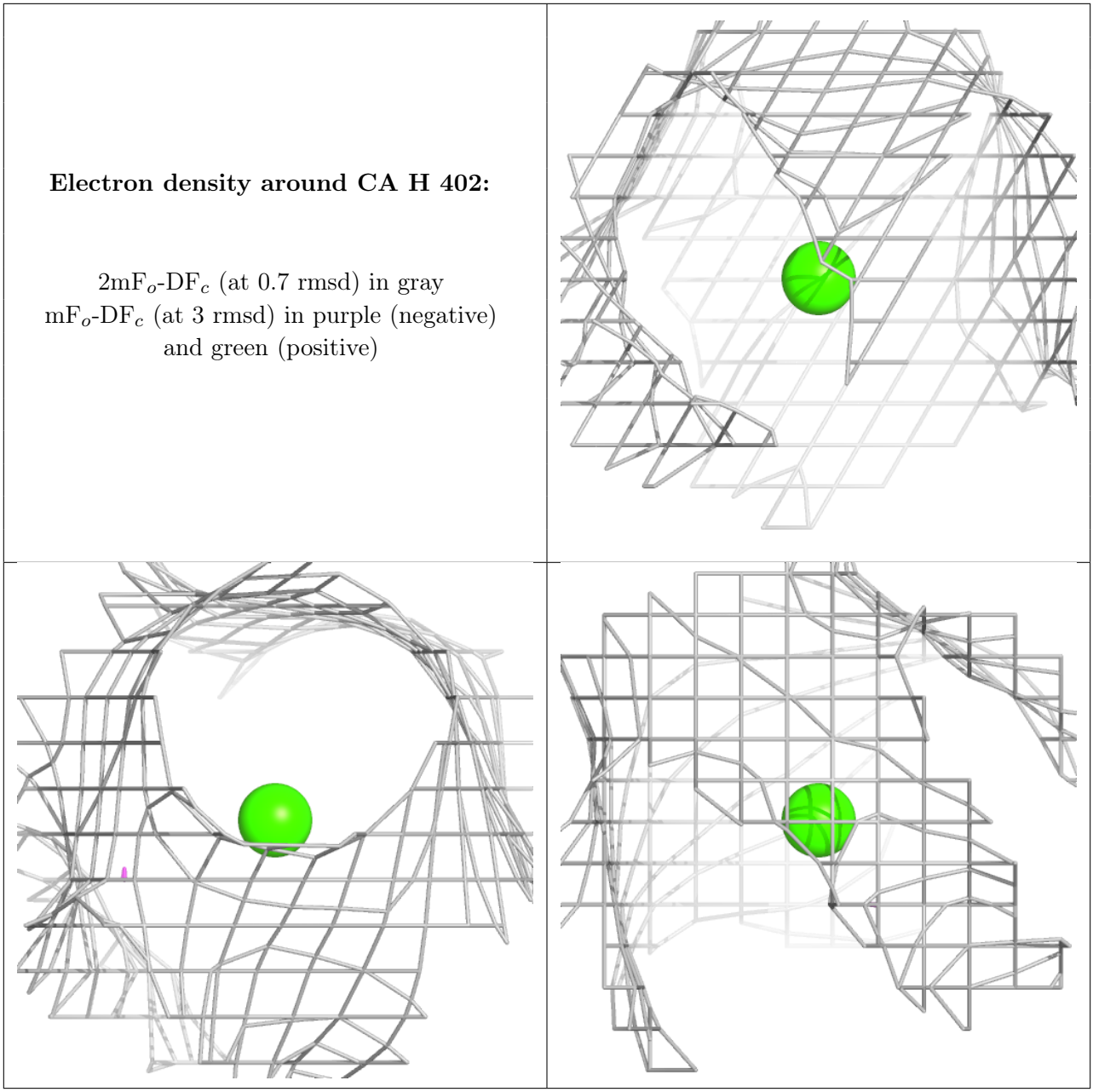
Electron density around CA H 401:

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



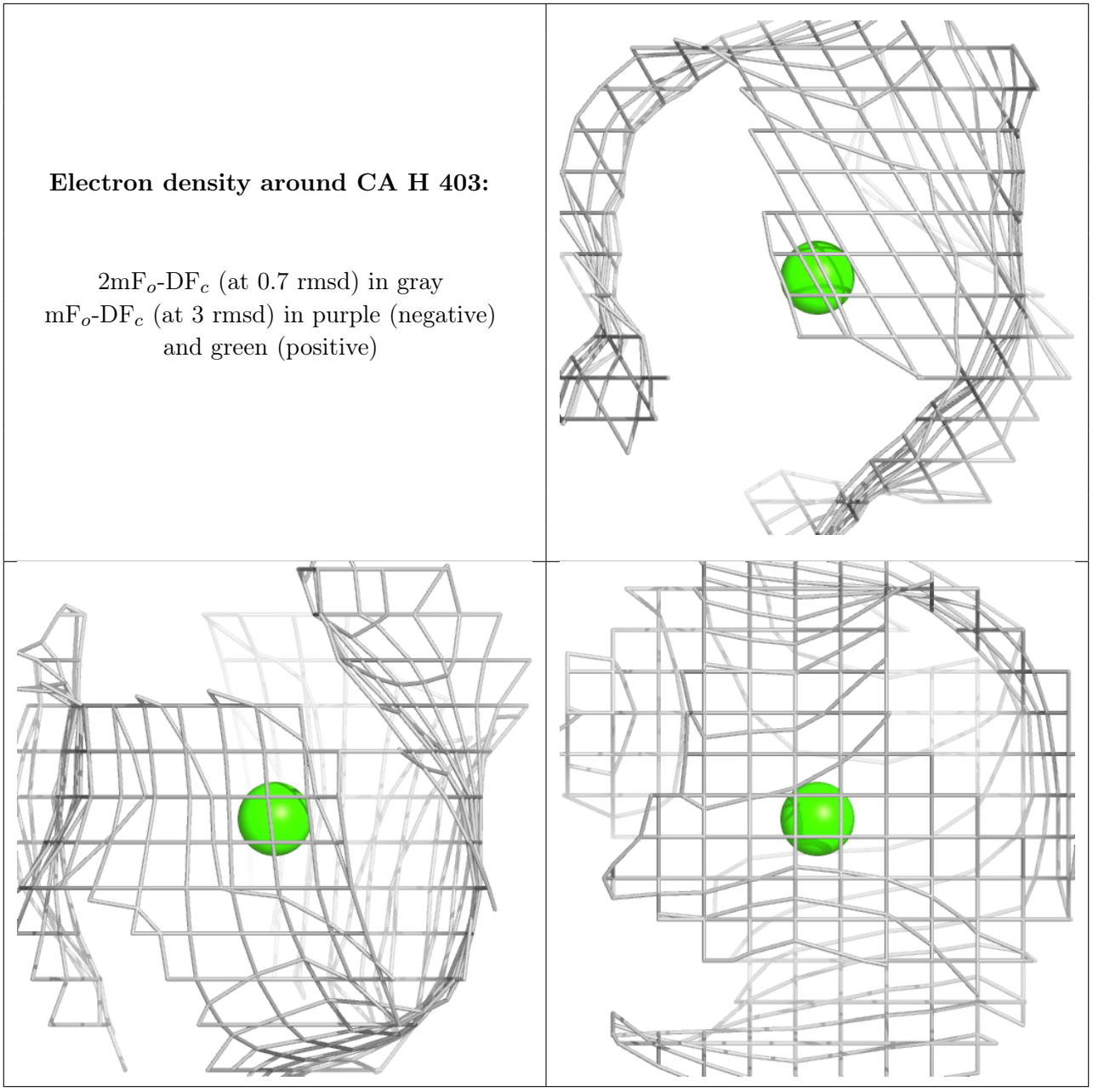
Electron density around CA H 402:

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



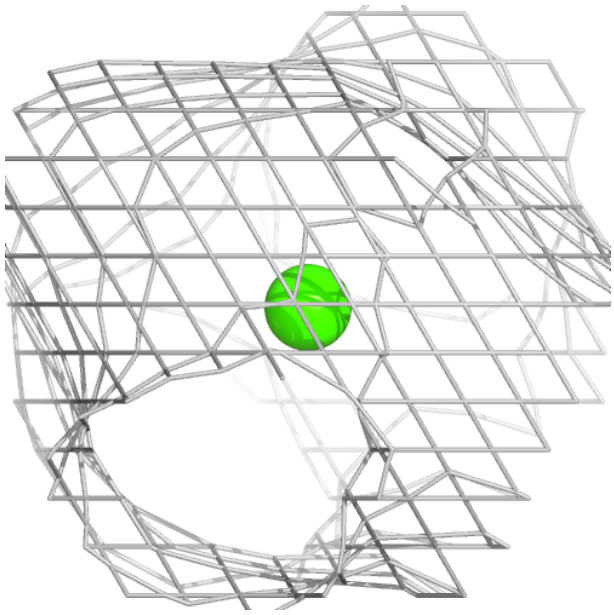
Electron density around CA H 403:

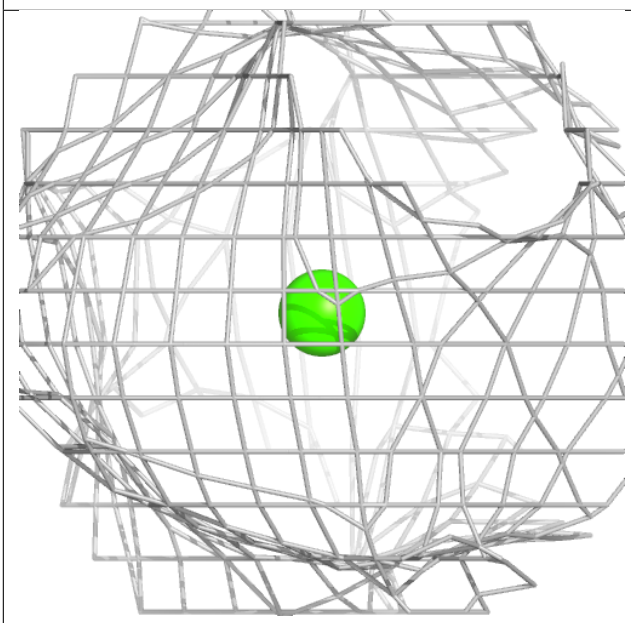
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

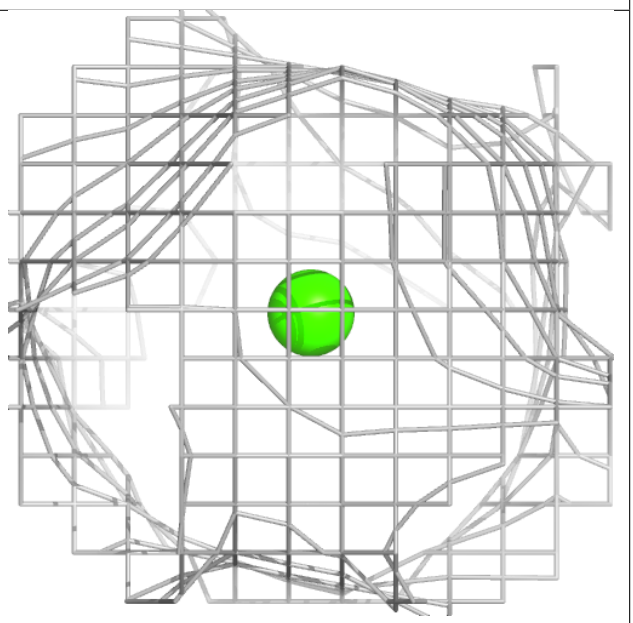


Electron density around CA I 401:

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

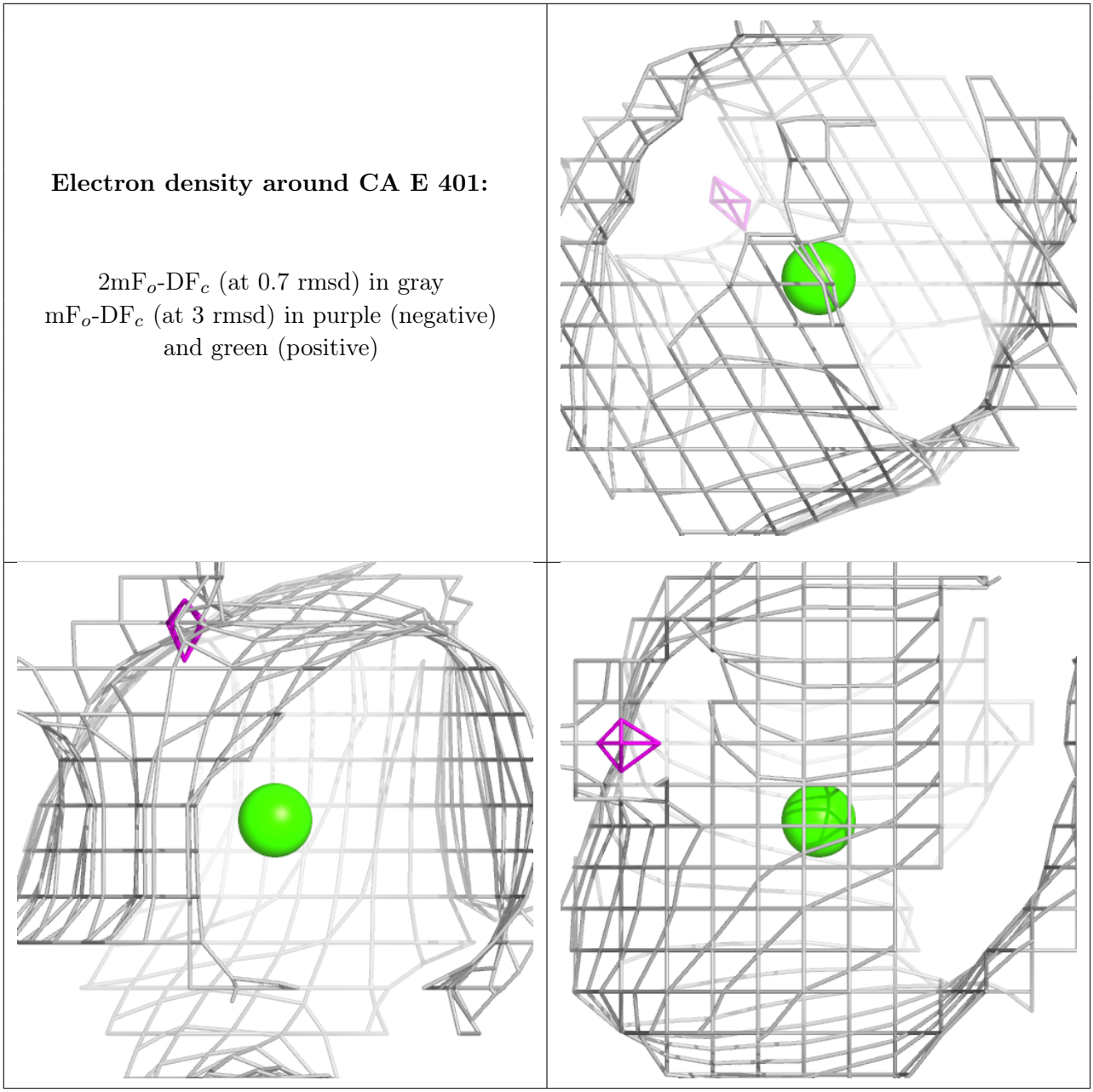






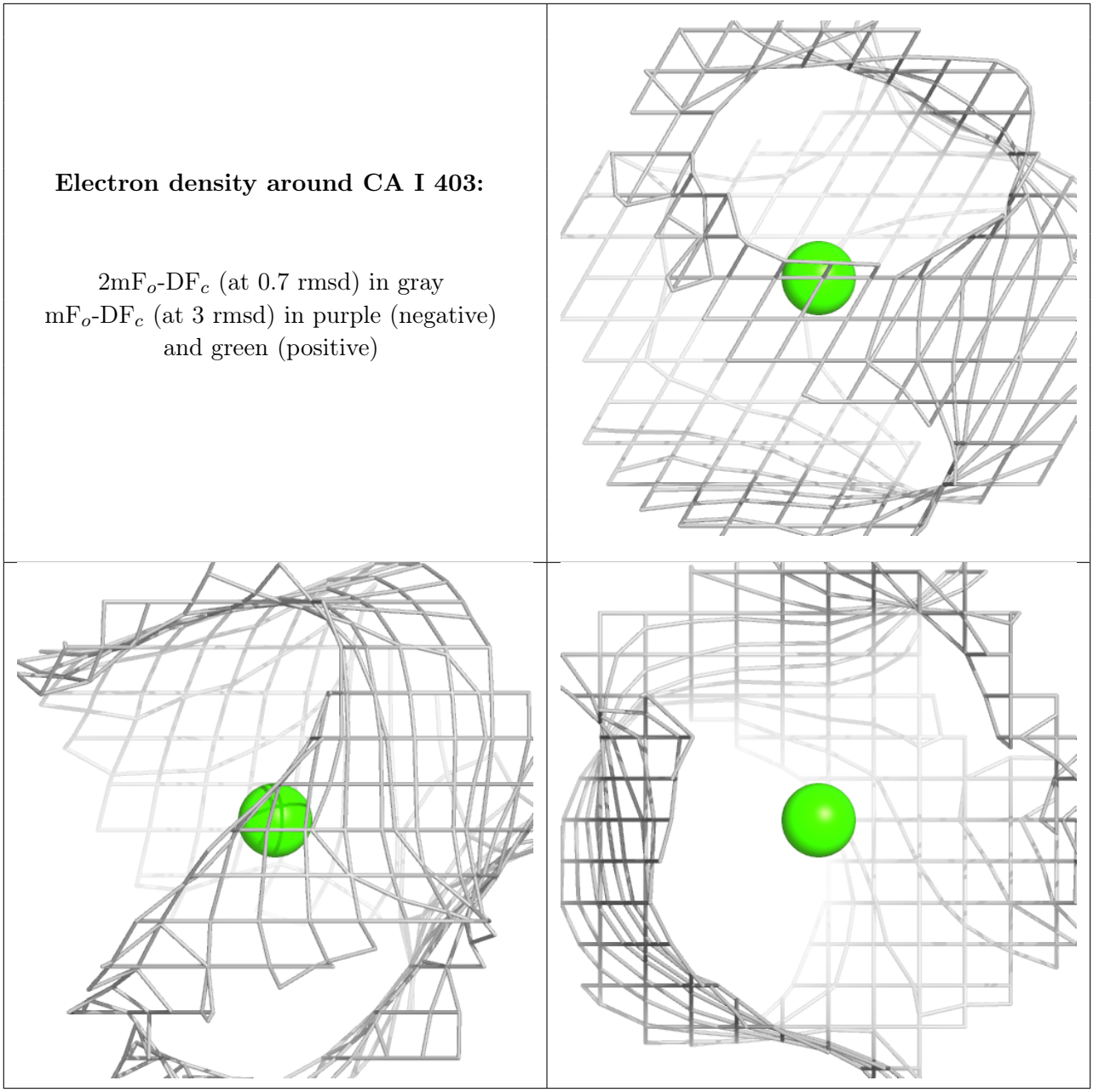
Electron density around CA E 401:

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



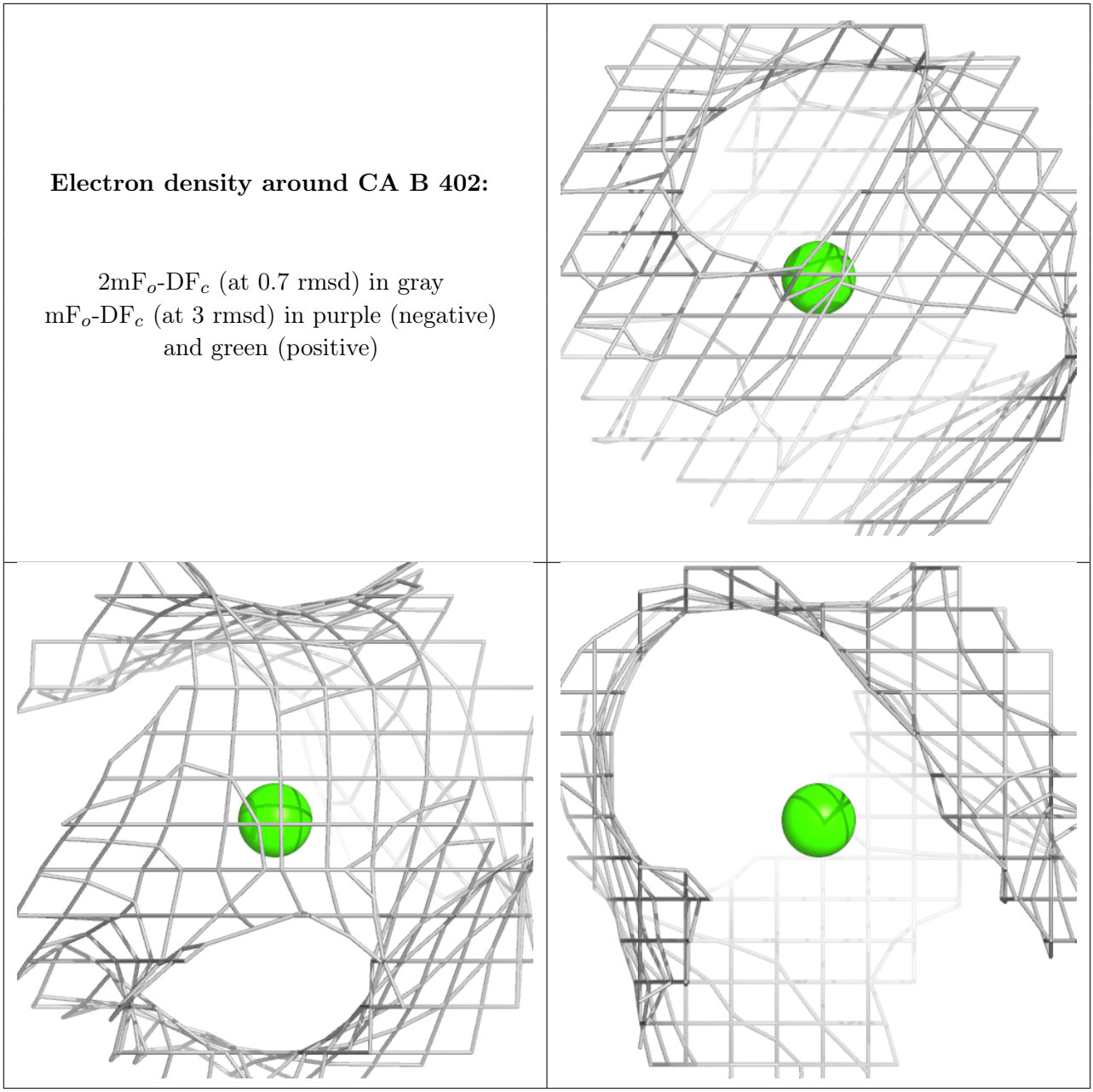
Electron density around CA I 403:

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



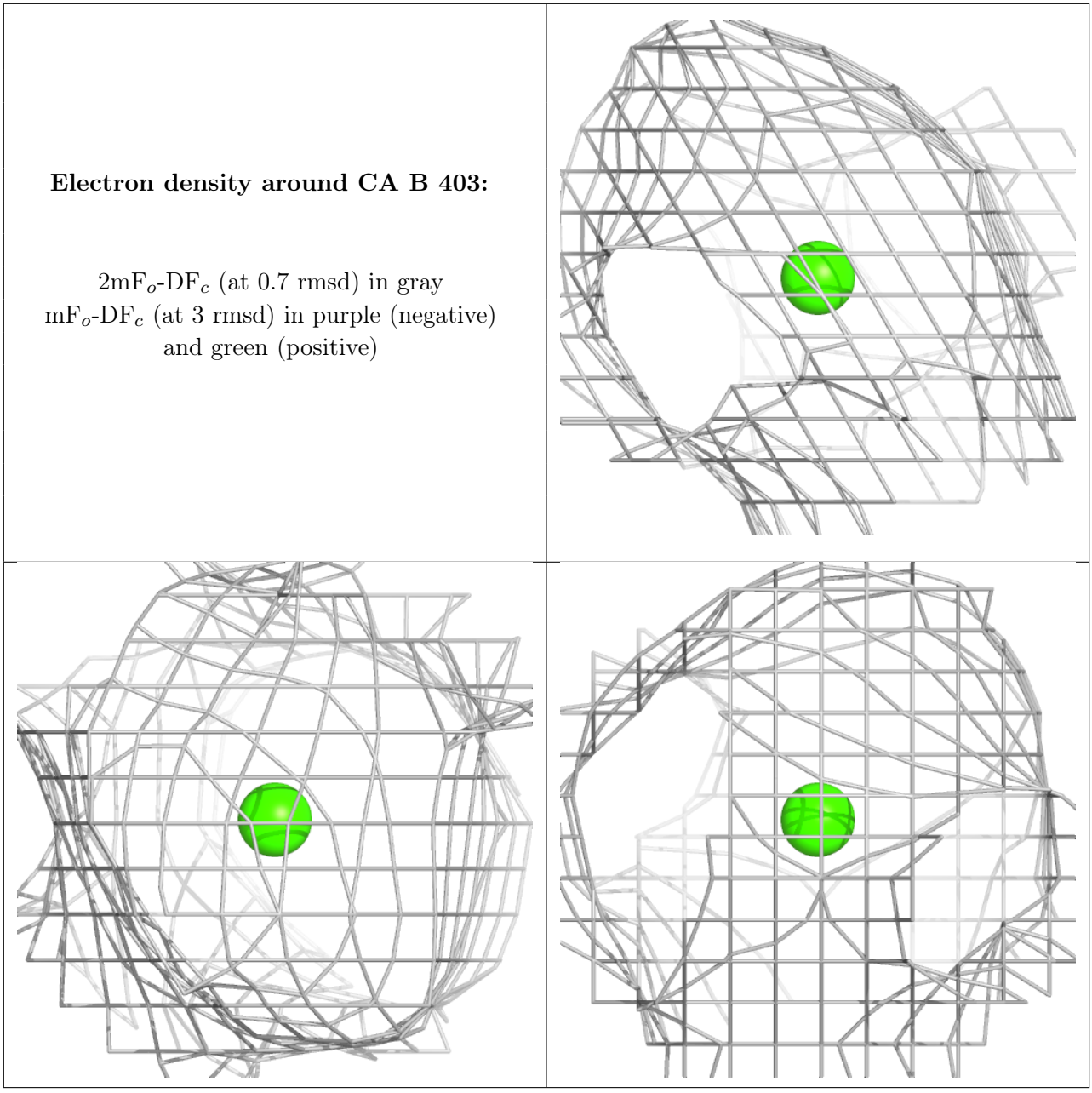
Electron density around CA B 402:

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



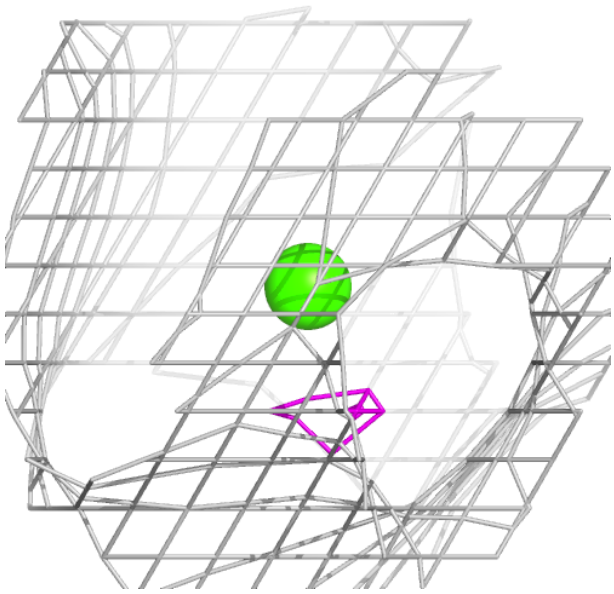
Electron density around CA B 403:

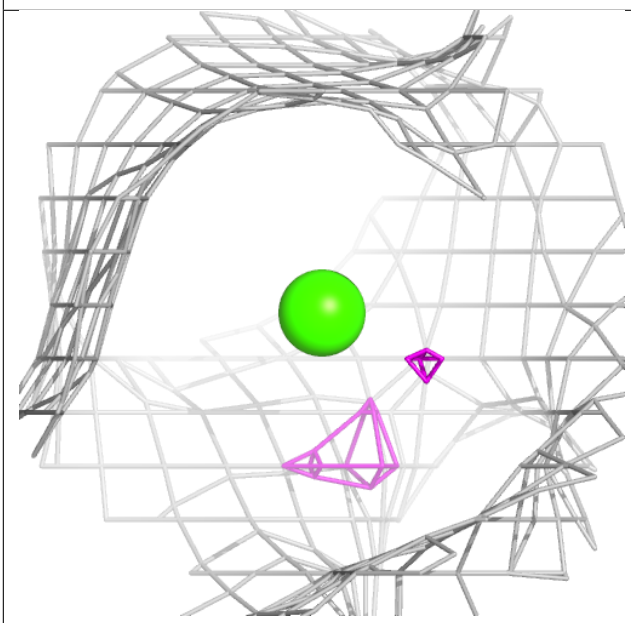
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

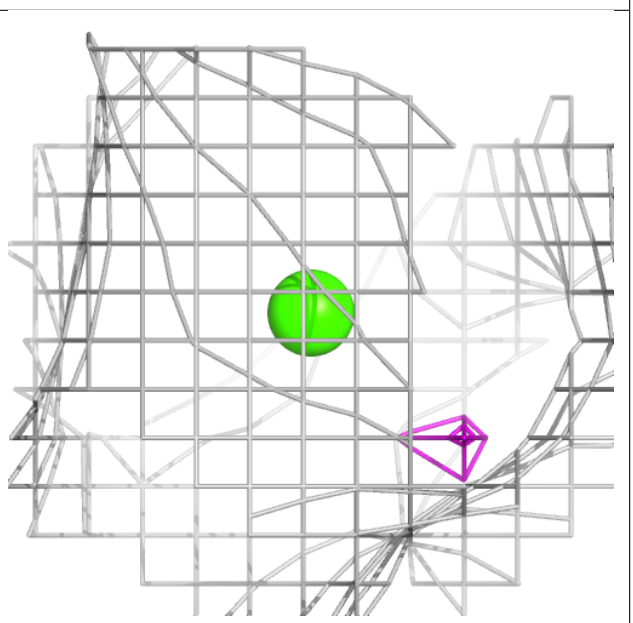


Electron density around CA C 402:

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

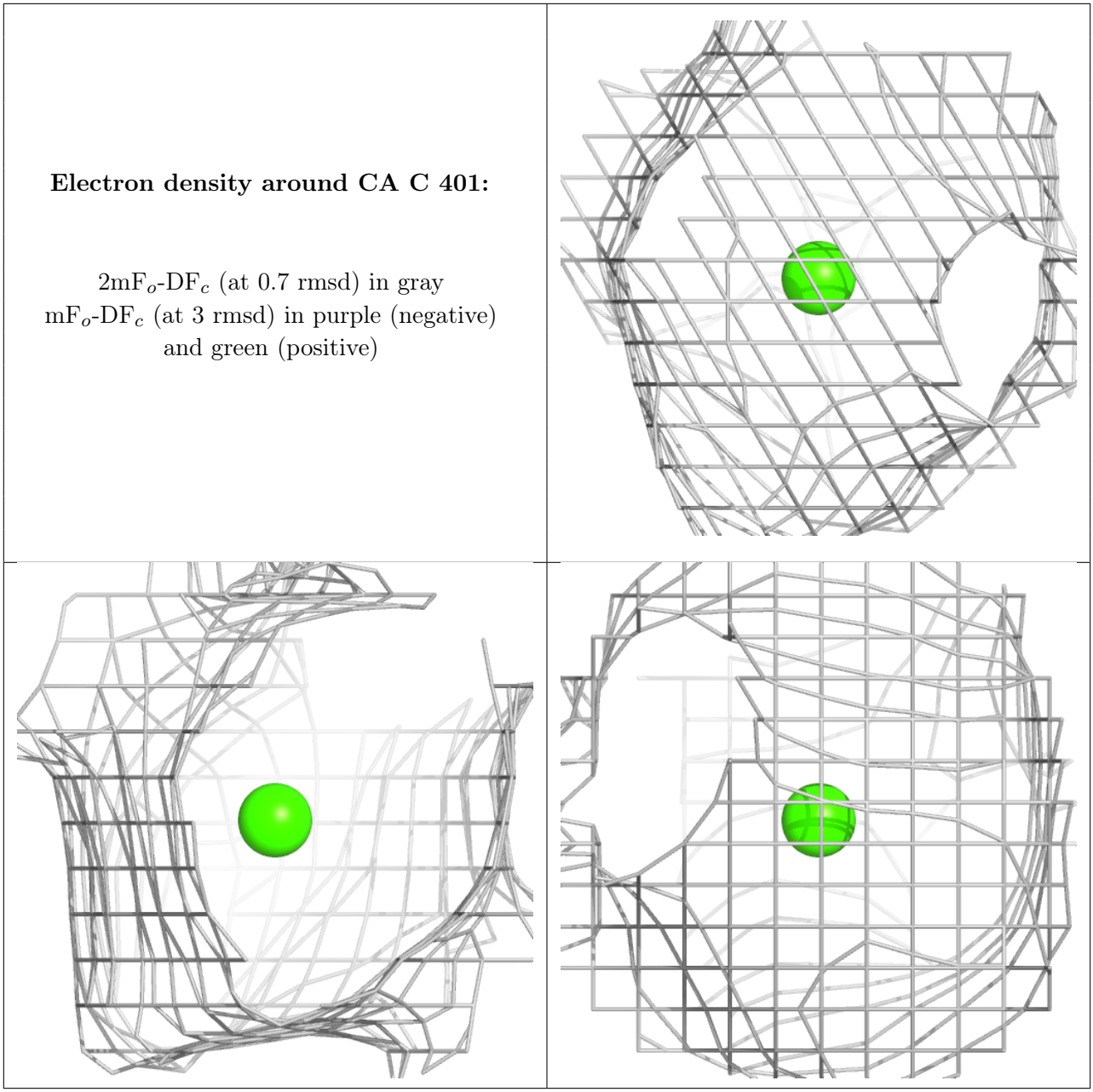






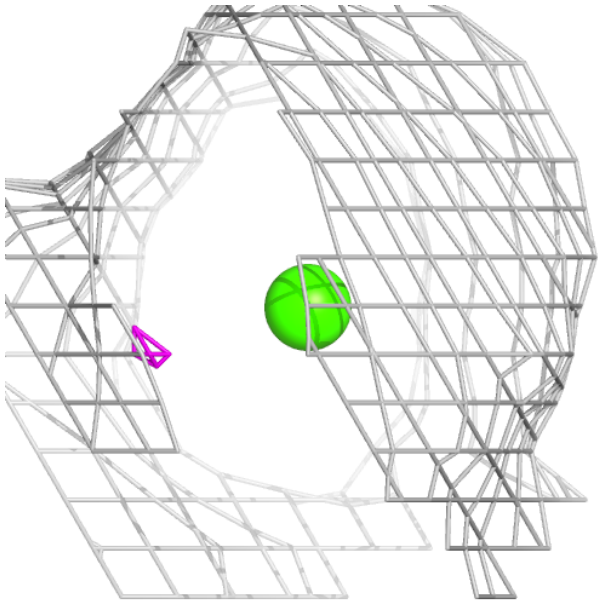
Electron density around CA C 401:

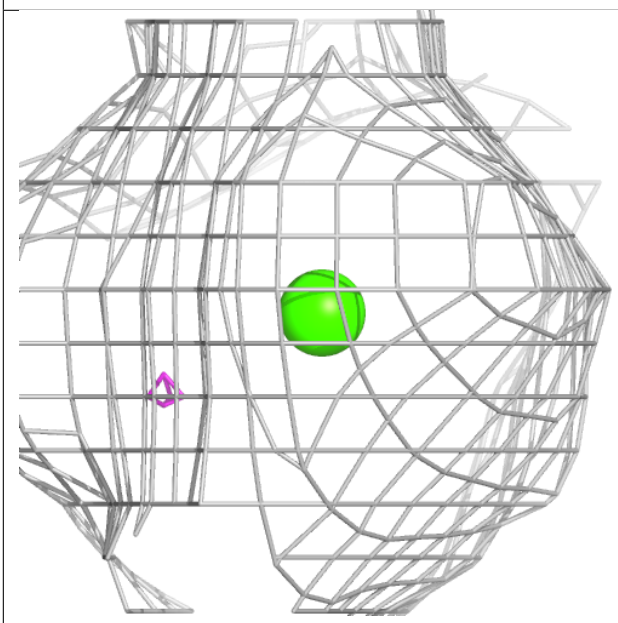
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

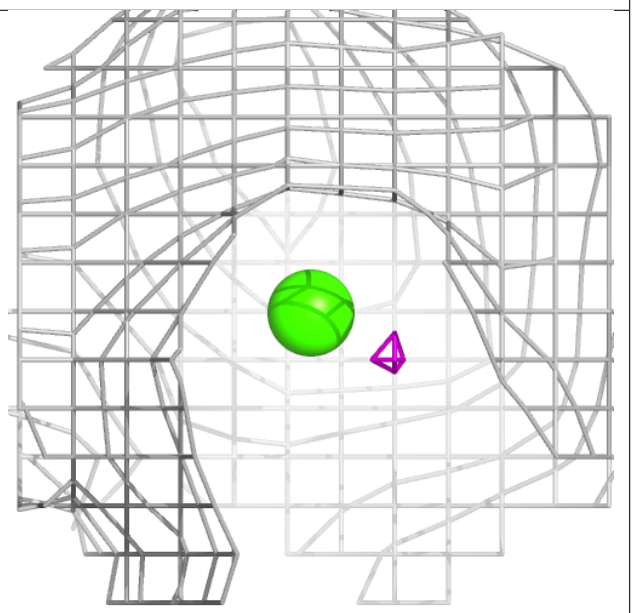


Electron density around CA C 403:

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

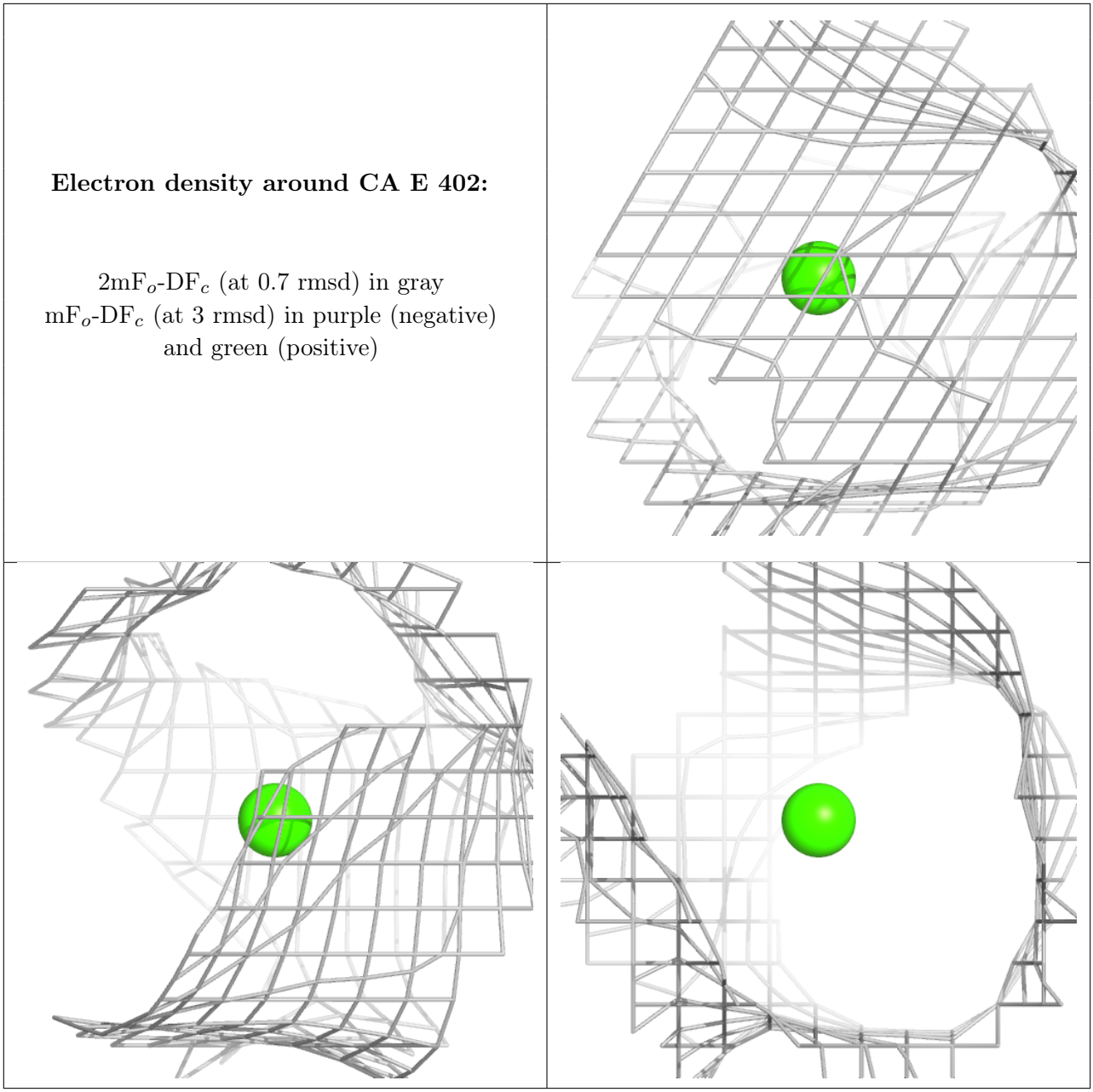






Electron density around CA E 402:

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



6.5 Other polymers (i)

There are no such residues in this entry.