wwPDB X-ray Structure Validation Summary Report (i)

Nov 9, 2020 – 07:29 PM GMT

PDB ID	:	6Y9D
Title	:	Crystal structure of the quaternary ammonium Rieske monooxygenase CntA in complex with substrate L-Carnitine
Authors	:	Quareshy, M.; Shanmugam, M.; Bugg, T.D.; Cameron, A.; Chen, Y.
Deposited on	:	2020-03-06
Resolution	:	1.97 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 following versions of software and data (see references (1)) were used in the production of this report:

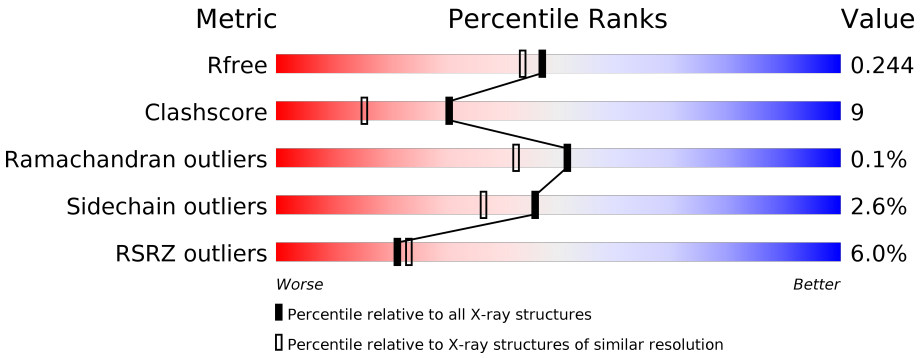
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 on 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	391	5% 75% 14% • 10%
1	B	391	9% 72% 18% • 10%
1	C	391	6% 74% 15% • 10%
1	D	391	4% 77% 13% 10%
1	E	391	3% 76% 13% • 10%
1	F	391	4% 77% 12% • 10%

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Mol	Chain	Length	Quality of chain
1	G	391	4% 71% 18% • 10%
1	H	391	5% 76% 13% • 10%
1	I	391	4% 73% 16% • 10%
1	J	391	10% 69% 20% • 10%
1	K	391	5% 72% 17% • 10%
1	L	391	5% 69% 20% • 10%

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
5	SCN	B	404	-	-	X	-
5	SCN	I	404	-	-	X	-
5	SCN	J	404	-	-	X	X
5	SCN	K	404	-	-	X	-
6	EPE	C	405	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35958 atoms, of which 204 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 Carnitine monooxygenase oxygenase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2862	1832	485	529	16			
1	B	352	Total	C	N	O	S	0	0	0
			2862	1832	485	529	16			
1	C	352	Total	C	N	O	S	0	0	0
			2862	1832	485	529	16			
1	D	352	Total	C	N	O	S	0	0	0
			2862	1832	485	529	16			
1	E	352	Total	C	N	O	S	0	0	0
			2862	1832	485	529	16			
1	F	352	Total	C	N	O	S	0	0	0
			2862	1832	485	529	16			
1	G	352	Total	C	N	O	S	0	0	0
			2862	1832	485	529	16			
1	H	352	Total	C	N	O	S	0	0	0
			2862	1832	485	529	16			
1	I	352	Total	C	N	O	S	0	0	0
			2862	1832	485	529	16			
1	J	352	Total	C	N	O	S	0	0	0
			2862	1832	485	529	16			
1	K	352	Total	C	N	O	S	0	0	0
			2862	1832	485	529	16			
1	L	352	Total	C	N	O	S	0	0	0
			2862	1832	485	529	16			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A059ZPP5
A	-18	GLY	-	expression tag	UNP A0A059ZPP5
A	-17	SER	-	expression tag	UNP A0A059ZPP5
A	-16	SER	-	expression tag	UNP A0A059ZPP5
A	-15	HIS	-	expression tag	UNP A0A059ZPP5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP A0A059ZPP5
A	-13	HIS	-	expression tag	UNP A0A059ZPP5
A	-12	HIS	-	expression tag	UNP A0A059ZPP5
A	-11	HIS	-	expression tag	UNP A0A059ZPP5
A	-10	HIS	-	expression tag	UNP A0A059ZPP5
A	-9	SER	-	expression tag	UNP A0A059ZPP5
A	-8	SER	-	expression tag	UNP A0A059ZPP5
A	-7	GLY	-	expression tag	UNP A0A059ZPP5
A	-6	LEU	-	expression tag	UNP A0A059ZPP5
A	-5	VAL	-	expression tag	UNP A0A059ZPP5
A	-4	PRO	-	expression tag	UNP A0A059ZPP5
A	-3	ARG	-	expression tag	UNP A0A059ZPP5
A	-2	GLY	-	expression tag	UNP A0A059ZPP5
A	-1	SER	-	expression tag	UNP A0A059ZPP5
A	0	HIS	-	expression tag	UNP A0A059ZPP5
B	-19	MET	-	initiating methionine	UNP A0A059ZPP5
B	-18	GLY	-	expression tag	UNP A0A059ZPP5
B	-17	SER	-	expression tag	UNP A0A059ZPP5
B	-16	SER	-	expression tag	UNP A0A059ZPP5
B	-15	HIS	-	expression tag	UNP A0A059ZPP5
B	-14	HIS	-	expression tag	UNP A0A059ZPP5
B	-13	HIS	-	expression tag	UNP A0A059ZPP5
B	-12	HIS	-	expression tag	UNP A0A059ZPP5
B	-11	HIS	-	expression tag	UNP A0A059ZPP5
B	-10	HIS	-	expression tag	UNP A0A059ZPP5
B	-9	SER	-	expression tag	UNP A0A059ZPP5
B	-8	SER	-	expression tag	UNP A0A059ZPP5
B	-7	GLY	-	expression tag	UNP A0A059ZPP5
B	-6	LEU	-	expression tag	UNP A0A059ZPP5
B	-5	VAL	-	expression tag	UNP A0A059ZPP5
B	-4	PRO	-	expression tag	UNP A0A059ZPP5
B	-3	ARG	-	expression tag	UNP A0A059ZPP5
B	-2	GLY	-	expression tag	UNP A0A059ZPP5
B	-1	SER	-	expression tag	UNP A0A059ZPP5
B	0	HIS	-	expression tag	UNP A0A059ZPP5
C	-19	MET	-	initiating methionine	UNP A0A059ZPP5
C	-18	GLY	-	expression tag	UNP A0A059ZPP5
C	-17	SER	-	expression tag	UNP A0A059ZPP5
C	-16	SER	-	expression tag	UNP A0A059ZPP5
C	-15	HIS	-	expression tag	UNP A0A059ZPP5
C	-14	HIS	-	expression tag	UNP A0A059ZPP5
C	-13	HIS	-	expression tag	UNP A0A059ZPP5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP A0A059ZPP5
C	-11	HIS	-	expression tag	UNP A0A059ZPP5
C	-10	HIS	-	expression tag	UNP A0A059ZPP5
C	-9	SER	-	expression tag	UNP A0A059ZPP5
C	-8	SER	-	expression tag	UNP A0A059ZPP5
C	-7	GLY	-	expression tag	UNP A0A059ZPP5
C	-6	LEU	-	expression tag	UNP A0A059ZPP5
C	-5	VAL	-	expression tag	UNP A0A059ZPP5
C	-4	PRO	-	expression tag	UNP A0A059ZPP5
C	-3	ARG	-	expression tag	UNP A0A059ZPP5
C	-2	GLY	-	expression tag	UNP A0A059ZPP5
C	-1	SER	-	expression tag	UNP A0A059ZPP5
C	0	HIS	-	expression tag	UNP A0A059ZPP5
D	-19	MET	-	initiating methionine	UNP A0A059ZPP5
D	-18	GLY	-	expression tag	UNP A0A059ZPP5
D	-17	SER	-	expression tag	UNP A0A059ZPP5
D	-16	SER	-	expression tag	UNP A0A059ZPP5
D	-15	HIS	-	expression tag	UNP A0A059ZPP5
D	-14	HIS	-	expression tag	UNP A0A059ZPP5
D	-13	HIS	-	expression tag	UNP A0A059ZPP5
D	-12	HIS	-	expression tag	UNP A0A059ZPP5
D	-11	HIS	-	expression tag	UNP A0A059ZPP5
D	-10	HIS	-	expression tag	UNP A0A059ZPP5
D	-9	SER	-	expression tag	UNP A0A059ZPP5
D	-8	SER	-	expression tag	UNP A0A059ZPP5
D	-7	GLY	-	expression tag	UNP A0A059ZPP5
D	-6	LEU	-	expression tag	UNP A0A059ZPP5
D	-5	VAL	-	expression tag	UNP A0A059ZPP5
D	-4	PRO	-	expression tag	UNP A0A059ZPP5
D	-3	ARG	-	expression tag	UNP A0A059ZPP5
D	-2	GLY	-	expression tag	UNP A0A059ZPP5
D	-1	SER	-	expression tag	UNP A0A059ZPP5
D	0	HIS	-	expression tag	UNP A0A059ZPP5
E	-19	MET	-	initiating methionine	UNP A0A059ZPP5
E	-18	GLY	-	expression tag	UNP A0A059ZPP5
E	-17	SER	-	expression tag	UNP A0A059ZPP5
E	-16	SER	-	expression tag	UNP A0A059ZPP5
E	-15	HIS	-	expression tag	UNP A0A059ZPP5
E	-14	HIS	-	expression tag	UNP A0A059ZPP5
E	-13	HIS	-	expression tag	UNP A0A059ZPP5
E	-12	HIS	-	expression tag	UNP A0A059ZPP5
E	-11	HIS	-	expression tag	UNP A0A059ZPP5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP A0A059ZPP5
E	-9	SER	-	expression tag	UNP A0A059ZPP5
E	-8	SER	-	expression tag	UNP A0A059ZPP5
E	-7	GLY	-	expression tag	UNP A0A059ZPP5
E	-6	LEU	-	expression tag	UNP A0A059ZPP5
E	-5	VAL	-	expression tag	UNP A0A059ZPP5
E	-4	PRO	-	expression tag	UNP A0A059ZPP5
E	-3	ARG	-	expression tag	UNP A0A059ZPP5
E	-2	GLY	-	expression tag	UNP A0A059ZPP5
E	-1	SER	-	expression tag	UNP A0A059ZPP5
E	0	HIS	-	expression tag	UNP A0A059ZPP5
F	-19	MET	-	initiating methionine	UNP A0A059ZPP5
F	-18	GLY	-	expression tag	UNP A0A059ZPP5
F	-17	SER	-	expression tag	UNP A0A059ZPP5
F	-16	SER	-	expression tag	UNP A0A059ZPP5
F	-15	HIS	-	expression tag	UNP A0A059ZPP5
F	-14	HIS	-	expression tag	UNP A0A059ZPP5
F	-13	HIS	-	expression tag	UNP A0A059ZPP5
F	-12	HIS	-	expression tag	UNP A0A059ZPP5
F	-11	HIS	-	expression tag	UNP A0A059ZPP5
F	-10	HIS	-	expression tag	UNP A0A059ZPP5
F	-9	SER	-	expression tag	UNP A0A059ZPP5
F	-8	SER	-	expression tag	UNP A0A059ZPP5
F	-7	GLY	-	expression tag	UNP A0A059ZPP5
F	-6	LEU	-	expression tag	UNP A0A059ZPP5
F	-5	VAL	-	expression tag	UNP A0A059ZPP5
F	-4	PRO	-	expression tag	UNP A0A059ZPP5
F	-3	ARG	-	expression tag	UNP A0A059ZPP5
F	-2	GLY	-	expression tag	UNP A0A059ZPP5
F	-1	SER	-	expression tag	UNP A0A059ZPP5
F	0	HIS	-	expression tag	UNP A0A059ZPP5
G	-19	MET	-	initiating methionine	UNP A0A059ZPP5
G	-18	GLY	-	expression tag	UNP A0A059ZPP5
G	-17	SER	-	expression tag	UNP A0A059ZPP5
G	-16	SER	-	expression tag	UNP A0A059ZPP5
G	-15	HIS	-	expression tag	UNP A0A059ZPP5
G	-14	HIS	-	expression tag	UNP A0A059ZPP5
G	-13	HIS	-	expression tag	UNP A0A059ZPP5
G	-12	HIS	-	expression tag	UNP A0A059ZPP5
G	-11	HIS	-	expression tag	UNP A0A059ZPP5
G	-10	HIS	-	expression tag	UNP A0A059ZPP5
G	-9	SER	-	expression tag	UNP A0A059ZPP5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	SER	-	expression tag	UNP A0A059ZPP5
G	-7	GLY	-	expression tag	UNP A0A059ZPP5
G	-6	LEU	-	expression tag	UNP A0A059ZPP5
G	-5	VAL	-	expression tag	UNP A0A059ZPP5
G	-4	PRO	-	expression tag	UNP A0A059ZPP5
G	-3	ARG	-	expression tag	UNP A0A059ZPP5
G	-2	GLY	-	expression tag	UNP A0A059ZPP5
G	-1	SER	-	expression tag	UNP A0A059ZPP5
G	0	HIS	-	expression tag	UNP A0A059ZPP5
H	-19	MET	-	initiating methionine	UNP A0A059ZPP5
H	-18	GLY	-	expression tag	UNP A0A059ZPP5
H	-17	SER	-	expression tag	UNP A0A059ZPP5
H	-16	SER	-	expression tag	UNP A0A059ZPP5
H	-15	HIS	-	expression tag	UNP A0A059ZPP5
H	-14	HIS	-	expression tag	UNP A0A059ZPP5
H	-13	HIS	-	expression tag	UNP A0A059ZPP5
H	-12	HIS	-	expression tag	UNP A0A059ZPP5
H	-11	HIS	-	expression tag	UNP A0A059ZPP5
H	-10	HIS	-	expression tag	UNP A0A059ZPP5
H	-9	SER	-	expression tag	UNP A0A059ZPP5
H	-8	SER	-	expression tag	UNP A0A059ZPP5
H	-7	GLY	-	expression tag	UNP A0A059ZPP5
H	-6	LEU	-	expression tag	UNP A0A059ZPP5
H	-5	VAL	-	expression tag	UNP A0A059ZPP5
H	-4	PRO	-	expression tag	UNP A0A059ZPP5
H	-3	ARG	-	expression tag	UNP A0A059ZPP5
H	-2	GLY	-	expression tag	UNP A0A059ZPP5
H	-1	SER	-	expression tag	UNP A0A059ZPP5
H	0	HIS	-	expression tag	UNP A0A059ZPP5
I	-19	MET	-	initiating methionine	UNP A0A059ZPP5
I	-18	GLY	-	expression tag	UNP A0A059ZPP5
I	-17	SER	-	expression tag	UNP A0A059ZPP5
I	-16	SER	-	expression tag	UNP A0A059ZPP5
I	-15	HIS	-	expression tag	UNP A0A059ZPP5
I	-14	HIS	-	expression tag	UNP A0A059ZPP5
I	-13	HIS	-	expression tag	UNP A0A059ZPP5
I	-12	HIS	-	expression tag	UNP A0A059ZPP5
I	-11	HIS	-	expression tag	UNP A0A059ZPP5
I	-10	HIS	-	expression tag	UNP A0A059ZPP5
I	-9	SER	-	expression tag	UNP A0A059ZPP5
I	-8	SER	-	expression tag	UNP A0A059ZPP5
I	-7	GLY	-	expression tag	UNP A0A059ZPP5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	expression tag	UNP A0A059ZPP5
I	-5	VAL	-	expression tag	UNP A0A059ZPP5
I	-4	PRO	-	expression tag	UNP A0A059ZPP5
I	-3	ARG	-	expression tag	UNP A0A059ZPP5
I	-2	GLY	-	expression tag	UNP A0A059ZPP5
I	-1	SER	-	expression tag	UNP A0A059ZPP5
I	0	HIS	-	expression tag	UNP A0A059ZPP5
J	-19	MET	-	initiating methionine	UNP A0A059ZPP5
J	-18	GLY	-	expression tag	UNP A0A059ZPP5
J	-17	SER	-	expression tag	UNP A0A059ZPP5
J	-16	SER	-	expression tag	UNP A0A059ZPP5
J	-15	HIS	-	expression tag	UNP A0A059ZPP5
J	-14	HIS	-	expression tag	UNP A0A059ZPP5
J	-13	HIS	-	expression tag	UNP A0A059ZPP5
J	-12	HIS	-	expression tag	UNP A0A059ZPP5
J	-11	HIS	-	expression tag	UNP A0A059ZPP5
J	-10	HIS	-	expression tag	UNP A0A059ZPP5
J	-9	SER	-	expression tag	UNP A0A059ZPP5
J	-8	SER	-	expression tag	UNP A0A059ZPP5
J	-7	GLY	-	expression tag	UNP A0A059ZPP5
J	-6	LEU	-	expression tag	UNP A0A059ZPP5
J	-5	VAL	-	expression tag	UNP A0A059ZPP5
J	-4	PRO	-	expression tag	UNP A0A059ZPP5
J	-3	ARG	-	expression tag	UNP A0A059ZPP5
J	-2	GLY	-	expression tag	UNP A0A059ZPP5
J	-1	SER	-	expression tag	UNP A0A059ZPP5
J	0	HIS	-	expression tag	UNP A0A059ZPP5
K	-19	MET	-	initiating methionine	UNP A0A059ZPP5
K	-18	GLY	-	expression tag	UNP A0A059ZPP5
K	-17	SER	-	expression tag	UNP A0A059ZPP5
K	-16	SER	-	expression tag	UNP A0A059ZPP5
K	-15	HIS	-	expression tag	UNP A0A059ZPP5
K	-14	HIS	-	expression tag	UNP A0A059ZPP5
K	-13	HIS	-	expression tag	UNP A0A059ZPP5
K	-12	HIS	-	expression tag	UNP A0A059ZPP5
K	-11	HIS	-	expression tag	UNP A0A059ZPP5
K	-10	HIS	-	expression tag	UNP A0A059ZPP5
K	-9	SER	-	expression tag	UNP A0A059ZPP5
K	-8	SER	-	expression tag	UNP A0A059ZPP5
K	-7	GLY	-	expression tag	UNP A0A059ZPP5
K	-6	LEU	-	expression tag	UNP A0A059ZPP5
K	-5	VAL	-	expression tag	UNP A0A059ZPP5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP A0A059ZPP5
K	-3	ARG	-	expression tag	UNP A0A059ZPP5
K	-2	GLY	-	expression tag	UNP A0A059ZPP5
K	-1	SER	-	expression tag	UNP A0A059ZPP5
K	0	HIS	-	expression tag	UNP A0A059ZPP5
L	-19	MET	-	initiating methionine	UNP A0A059ZPP5
L	-18	GLY	-	expression tag	UNP A0A059ZPP5
L	-17	SER	-	expression tag	UNP A0A059ZPP5
L	-16	SER	-	expression tag	UNP A0A059ZPP5
L	-15	HIS	-	expression tag	UNP A0A059ZPP5
L	-14	HIS	-	expression tag	UNP A0A059ZPP5
L	-13	HIS	-	expression tag	UNP A0A059ZPP5
L	-12	HIS	-	expression tag	UNP A0A059ZPP5
L	-11	HIS	-	expression tag	UNP A0A059ZPP5
L	-10	HIS	-	expression tag	UNP A0A059ZPP5
L	-9	SER	-	expression tag	UNP A0A059ZPP5
L	-8	SER	-	expression tag	UNP A0A059ZPP5
L	-7	GLY	-	expression tag	UNP A0A059ZPP5
L	-6	LEU	-	expression tag	UNP A0A059ZPP5
L	-5	VAL	-	expression tag	UNP A0A059ZPP5
L	-4	PRO	-	expression tag	UNP A0A059ZPP5
L	-3	ARG	-	expression tag	UNP A0A059ZPP5
L	-2	GLY	-	expression tag	UNP A0A059ZPP5
L	-1	SER	-	expression tag	UNP A0A059ZPP5
L	0	HIS	-	expression tag	UNP A0A059ZPP5

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Fe 1 1	0	0
2	J	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	K	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0

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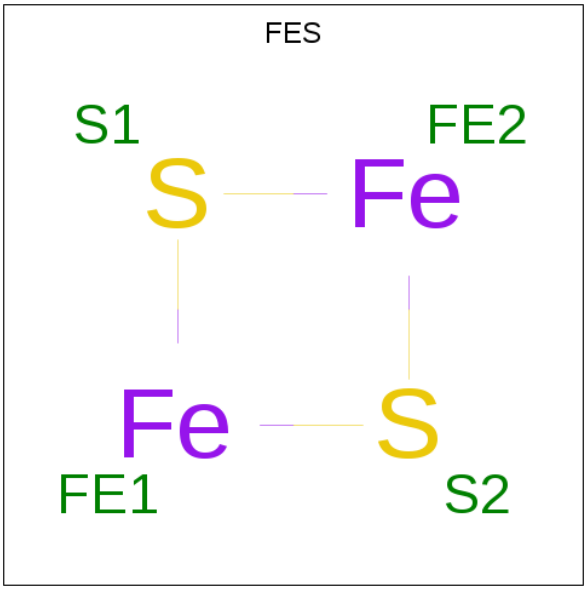
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0
3	C	1	Total Fe S 4 2 2	0	0
3	D	1	Total Fe S 4 2 2	0	0
3	E	1	Total Fe S 4 2 2	0	0

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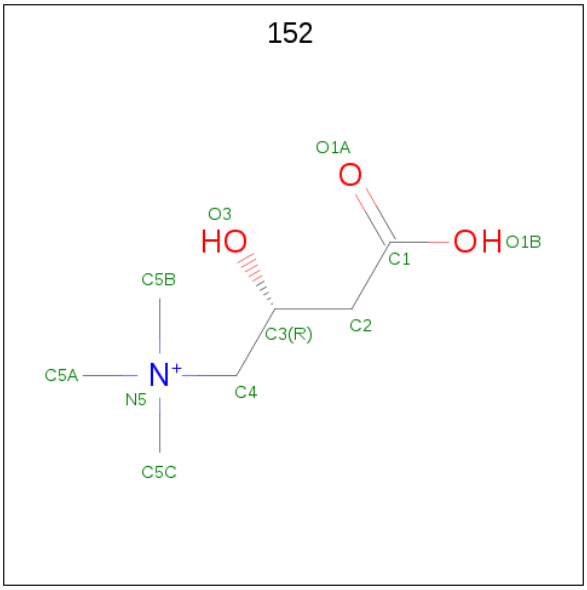
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total Fe S 4 2 2	0	0
3	G	1	Total Fe S 4 2 2	0	0
3	H	1	Total Fe S 4 2 2	0	0
3	I	1	Total Fe S 4 2 2	0	0
3	J	1	Total Fe S 4 2 2	0	0
3	K	1	Total Fe S 4 2 2	0	0
3	L	1	Total Fe S 4 2 2	0	0

- Molecule 4 is CARNITINE (three-letter code: 152) (formula: $C_7H_{16}NO_3$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 11 7 1 3	0	0
4	B	1	Total C N O 11 7 1 3	0	0
4	C	1	Total C N O 11 7 1 3	0	0
4	D	1	Total C N O 11 7 1 3	0	0

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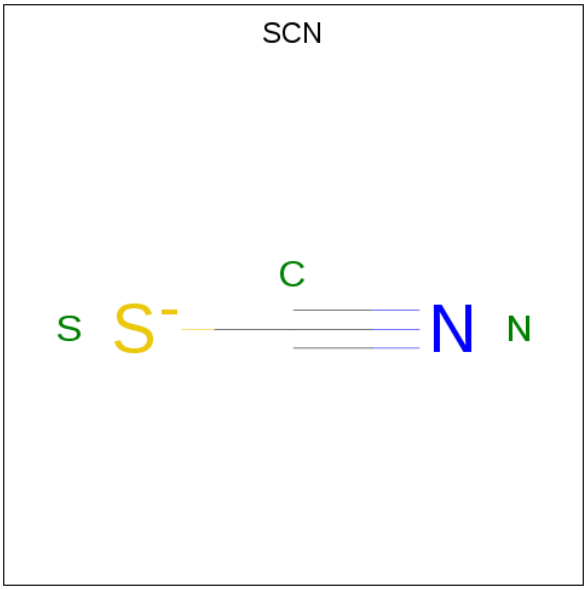
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C N O 11 7 1 3	0	0
4	F	1	Total C N O 11 7 1 3	0	0
4	G	1	Total C N O 11 7 1 3	0	0
4	H	1	Total C N O 11 7 1 3	0	0
4	I	1	Total C N O 11 7 1 3	0	0
4	J	1	Total C N O 11 7 1 3	0	0
4	K	1	Total C N O 11 7 1 3	0	0
4	L	1	Total C N O 11 7 1 3	0	0

- Molecule 5 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N S 3 1 1 1	0	0
5	B	1	Total C N S 3 1 1 1	0	0
5	C	1	Total C N S 3 1 1 1	0	0

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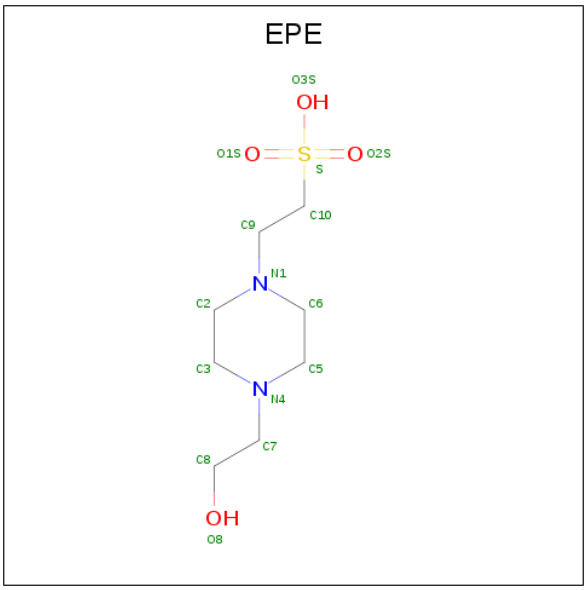
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C N S 3 1 1 1	0	0
5	E	1	Total C N S 3 1 1 1	0	0
5	F	1	Total C N S 3 1 1 1	0	0
5	G	1	Total C N S 3 1 1 1	0	0
5	H	1	Total C N S 3 1 1 1	0	0
5	I	1	Total C N S 3 1 1 1	0	0
5	J	1	Total C N S 3 1 1 1	0	0
5	K	1	Total C N S 3 1 1 1	0	0
5	L	1	Total C N S 3 1 1 1	0	0

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H N O S 32 8 17 2 4 1	0	0
6	B	1	Total C H N O S 32 8 17 2 4 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	D	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	E	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	F	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	G	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	H	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	I	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	J	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	K	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	L	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	94	Total	O	0	0
			94	94		
7	B	72	Total	O	0	0
			72	72		
7	C	69	Total	O	0	0
			69	69		
7	D	89	Total	O	0	0
			89	89		
7	E	105	Total	O	0	0
			105	105		
7	F	106	Total	O	0	0
			106	106		
7	G	96	Total	O	0	0
			96	96		
7	H	82	Total	O	0	0
			82	82		
7	I	89	Total	O	0	0
			89	89		

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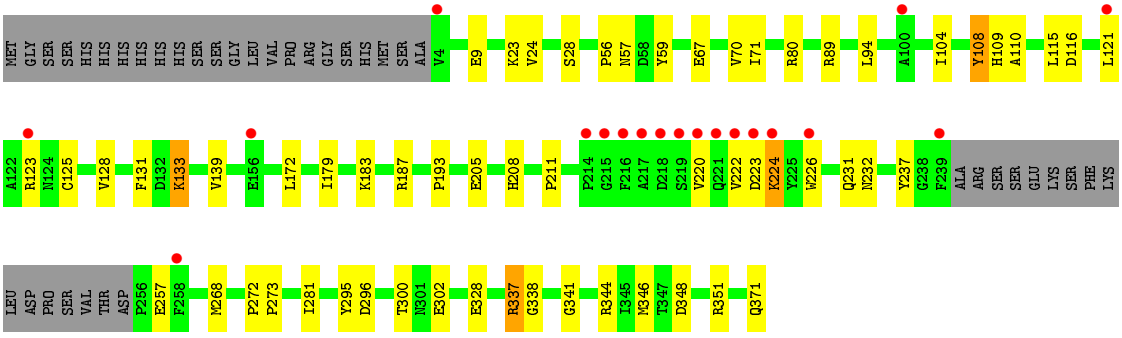
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	62	Total O 62 62	0	0
7	K	73	Total O 73 73	0	0
7	L	65	Total O 65 65	0	0

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.

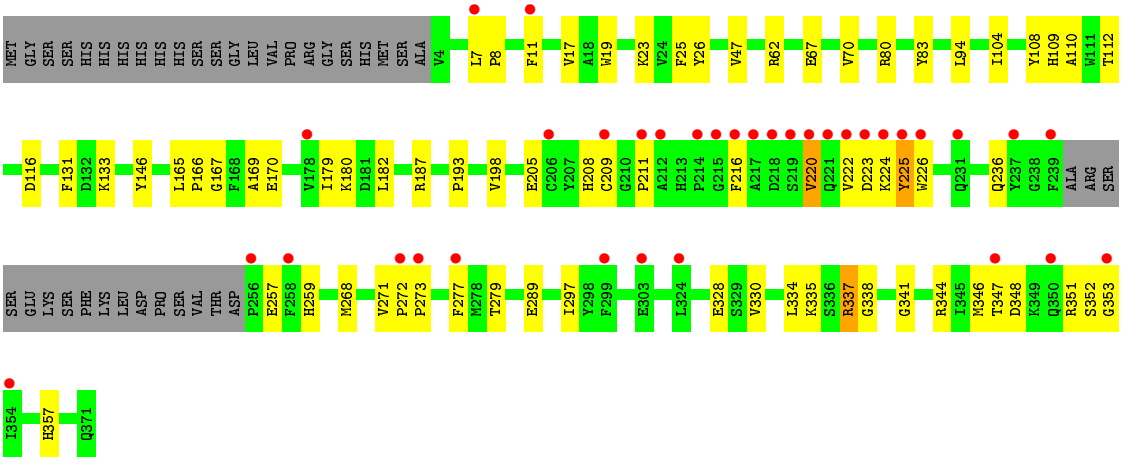
- Molecule 1: Carnitine monooxygenase oxygenase subunit

Chain A:



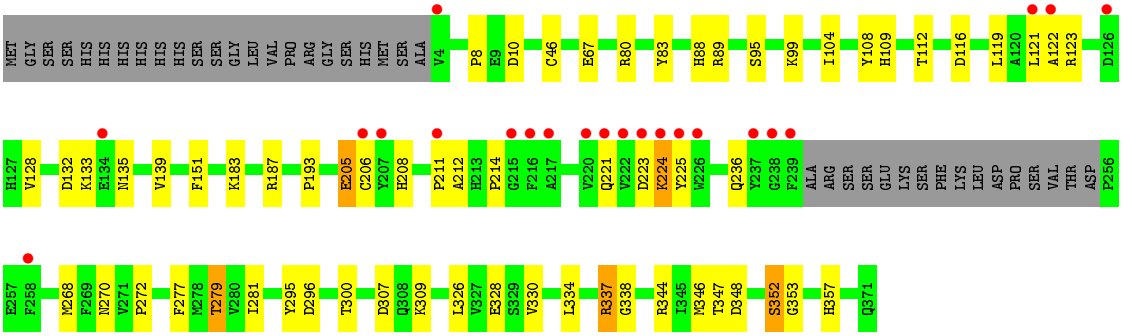
- Molecule 1: Carnitine monooxygenase oxygenase subunit

Chain B:

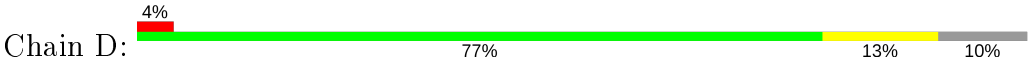


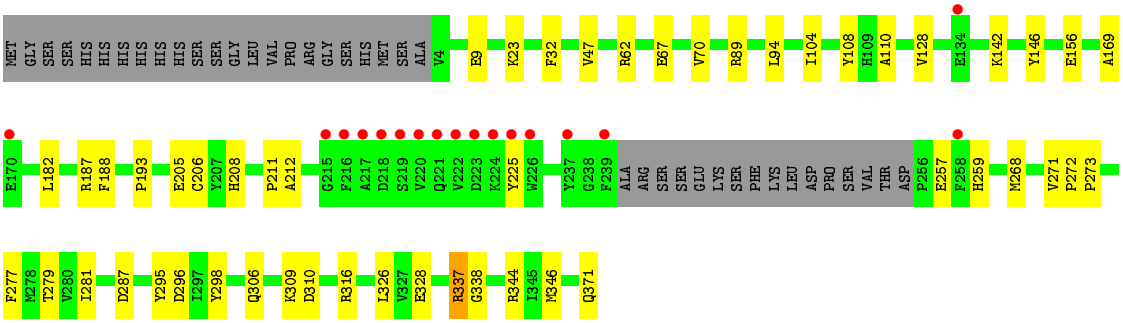
- Molecule 1: Carnitine monooxygenase oxygenase subunit

Chain C:

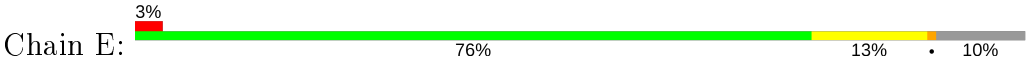


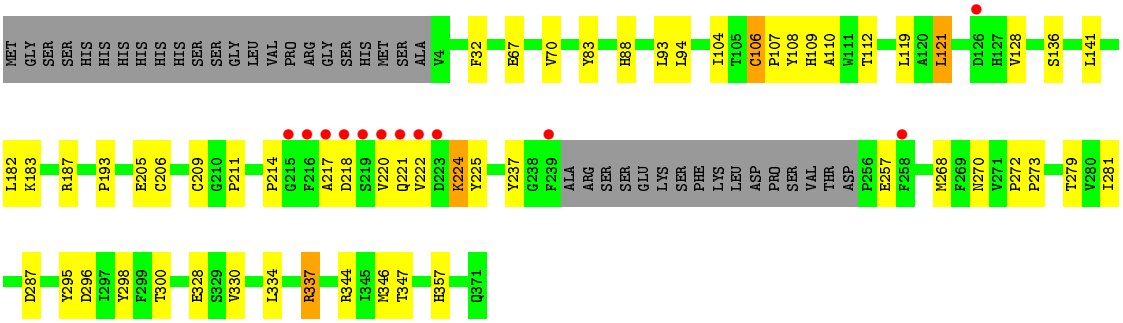
• Molecule 1: Carnitine monooxygenase oxygenase subunit



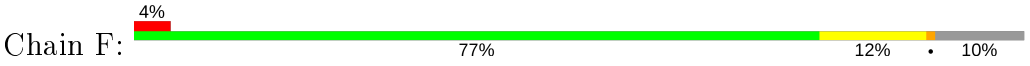


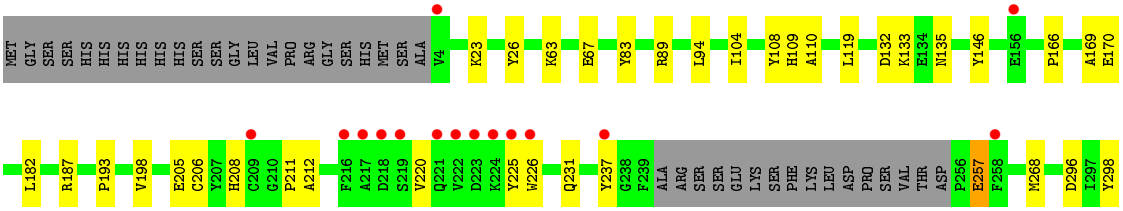
• Molecule 1: Carnitine monooxygenase oxygenase subunit





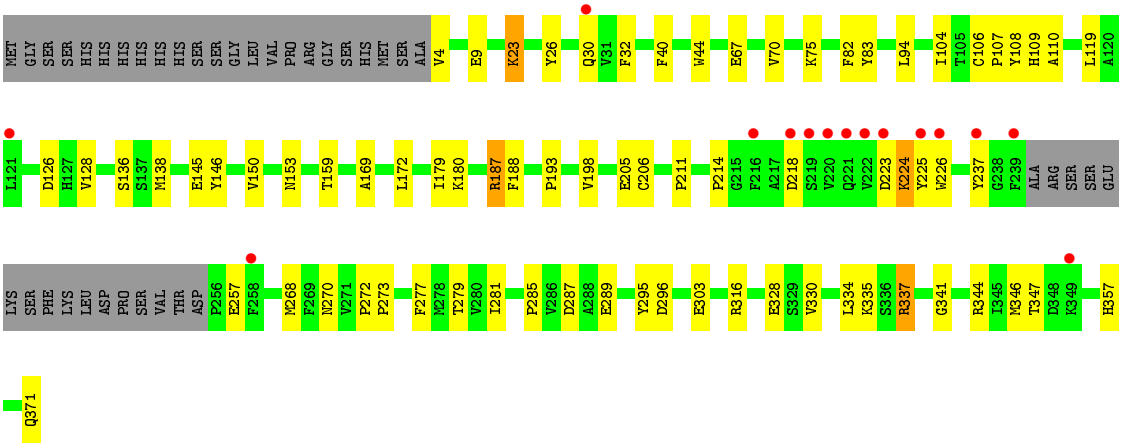
• Molecule 1: Carnitine monooxygenase oxygenase subunit





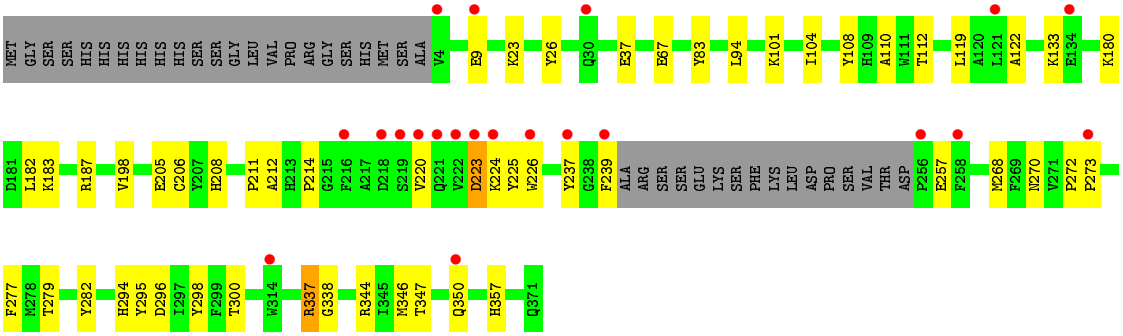
• Molecule 1: Carnitine monooxygenase oxygenase subunit

Chain G:



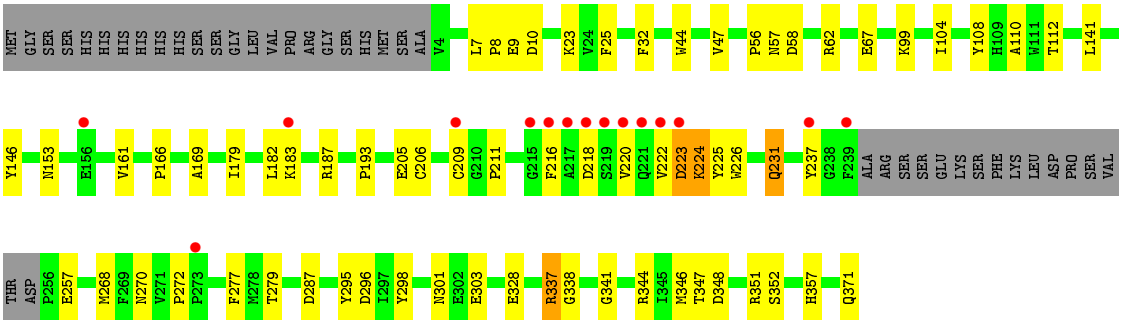
• Molecule 1: Carnitine monooxygenase oxygenase subunit

Chain H:



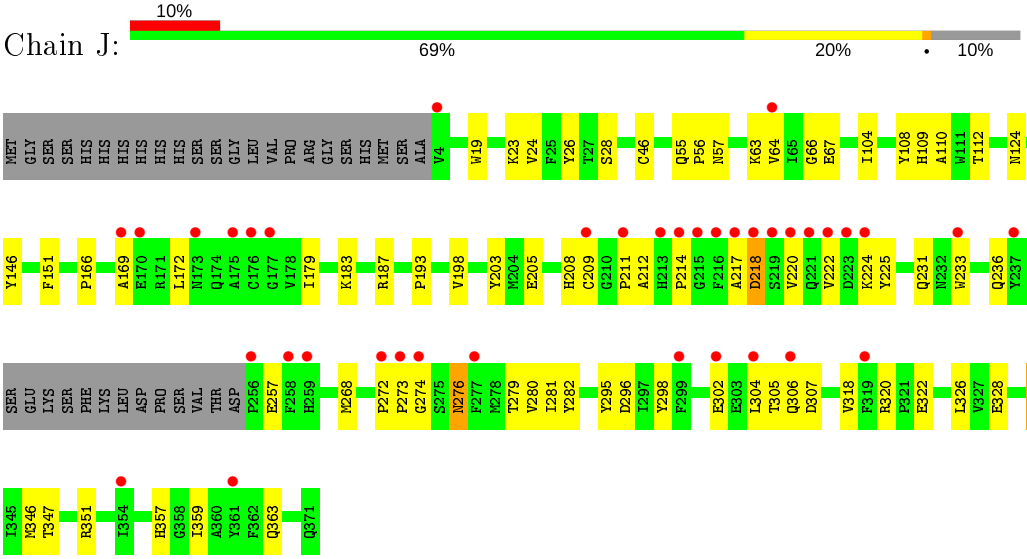
• Molecule 1: Carnitine monooxygenase oxygenase subunit

Chain I:



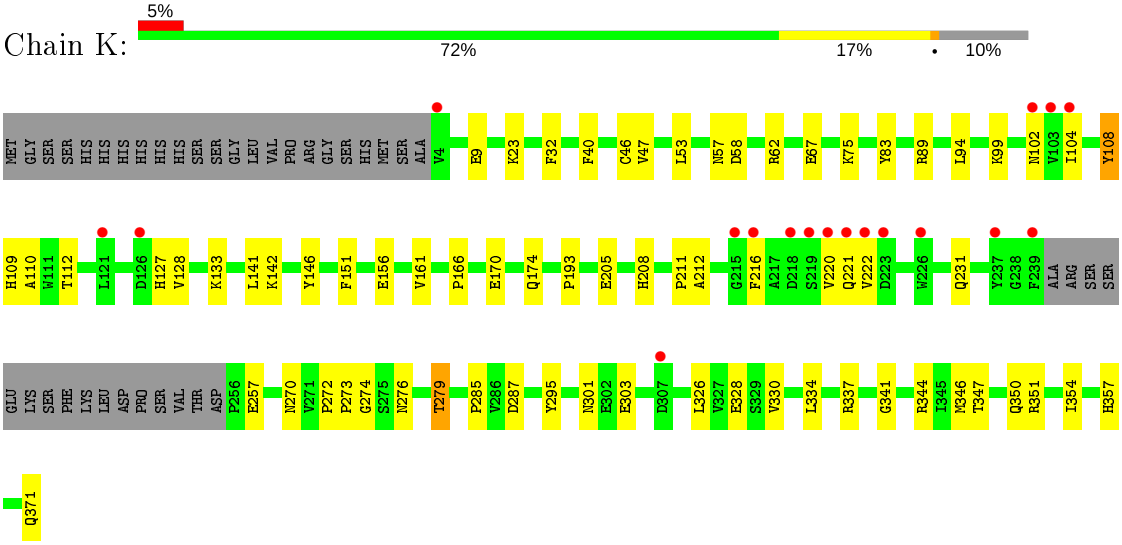
• Molecule 1: Carnitine monooxygenase oxygenase subunit

Chain J:



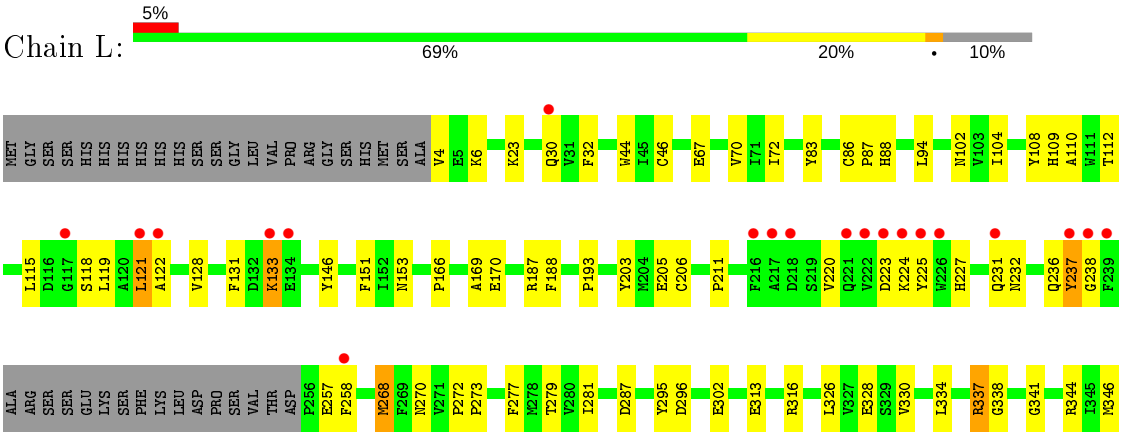
• Molecule 1: Carnitine monooxygenase oxygenase subunit

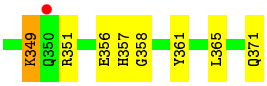
Chain K:



• Molecule 1: Carnitine monooxygenase oxygenase subunit

Chain L:




K349
Q350
R351
E356
H357
G358
Y361
L365
Q371

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.59Å 177.77Å 158.80Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	81.42 – 1.97 81.42 – 1.97	Depositor EDS
% Data completeness (in resolution range)	89.1 (81.42-1.97) 98.9 (81.42-1.97)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.210 , 0.247 0.208 , 0.244	Depositor DCC
R_{free} test set	17604 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.839	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	35958	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9432e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: EPE, 152, FE, SCN, FES

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	0.46	0/2948	0.64	0/4004
1	B	0.45	0/2948	0.62	0/4004
1	C	0.47	0/2948	0.61	0/4004
1	D	0.45	0/2948	0.65	0/4004
1	E	0.48	0/2948	0.63	0/4004
1	F	0.47	0/2948	0.65	0/4004
1	G	0.49	0/2948	0.66	0/4004
1	H	0.46	0/2948	0.61	0/4004
1	I	0.48	0/2948	0.63	0/4004
1	J	0.44	0/2948	0.60	0/4004
1	K	0.44	0/2948	0.62	0/4004
1	L	0.49	0/2948	0.63	0/4004
All	All	0.46	0/35376	0.63	0/48048

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2862	0	2707	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2862	0	2707	57	0
1	C	2862	0	2707	55	0
1	D	2862	0	2707	44	0
1	E	2862	0	2708	50	0
1	F	2862	0	2707	42	0
1	G	2862	0	2707	57	0
1	H	2862	0	2707	44	0
1	I	2862	0	2707	56	0
1	J	2862	0	2707	77	0
1	K	2862	0	2707	61	0
1	L	2862	0	2707	80	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	1	0
3	C	4	0	0	1	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	1	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	1	0
3	K	4	0	0	1	0
3	L	4	0	0	0	0
4	A	11	0	15	2	0
4	B	11	0	15	3	0
4	C	11	0	15	2	0
4	D	11	0	15	2	0
4	E	11	0	15	1	0
4	F	11	0	15	2	0
4	G	11	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	11	0	15	1	0
4	I	11	0	15	1	0
4	J	11	0	15	4	0
4	K	11	0	15	0	0
4	L	11	0	15	3	0
5	A	3	0	0	1	0
5	B	3	0	0	2	0
5	C	3	0	0	1	0
5	D	3	0	0	0	0
5	E	3	0	0	1	0
5	F	3	0	0	0	0
5	G	3	0	0	0	0
5	H	3	0	0	1	0
5	I	3	0	0	2	0
5	J	3	0	0	2	0
5	K	3	0	0	2	0
5	L	3	0	0	1	0
6	A	15	17	17	0	0
6	B	15	17	17	0	0
6	C	15	17	17	0	0
6	D	15	17	17	0	0
6	E	15	17	17	0	0
6	F	15	17	17	0	0
6	G	15	17	18	0	0
6	H	15	17	17	0	0
6	I	15	17	17	0	0
6	J	15	17	18	3	0
6	K	15	17	17	0	0
6	L	15	17	17	0	0
7	A	94	0	0	0	0
7	B	72	0	0	0	0
7	C	69	0	0	1	0
7	D	89	0	0	1	0
7	E	105	0	0	0	0
7	F	106	0	0	1	0
7	G	96	0	0	2	0
7	H	82	0	0	1	0
7	I	89	0	0	1	0
7	J	62	0	0	1	0
7	K	73	0	0	1	0
7	L	65	0	0	3	0
All	All	35754	204	32871	619	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 9.

The worst 5 of 619 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:L:4:VAL:HG22	1:L:30:GLN:HE22	1.13	1.12
1:K:270:ASN:HD22	1:K:279:THR:HG22	1.16	1.11
1:F:119:LEU:HD23	1:F:133:LYS:HD2	1.12	1.07
1:B:216:PHE:O	1:B:220:VAL:HG23	1.53	1.06
1:J:214:PRO:O	1:J:218:ASP:HB2	1.58	1.02

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	348/391 (89%)	332 (95%)	15 (4%)	1 (0%)	41 29
1	B	348/391 (89%)	332 (95%)	16 (5%)	0	100 100
1	C	348/391 (89%)	332 (95%)	15 (4%)	1 (0%)	41 29
1	D	348/391 (89%)	334 (96%)	14 (4%)	0	100 100
1	E	348/391 (89%)	333 (96%)	15 (4%)	0	100 100
1	F	348/391 (89%)	333 (96%)	15 (4%)	0	100 100
1	G	348/391 (89%)	333 (96%)	14 (4%)	1 (0%)	41 29
1	H	348/391 (89%)	331 (95%)	17 (5%)	0	100 100
1	I	348/391 (89%)	328 (94%)	17 (5%)	3 (1%)	17 8
1	J	348/391 (89%)	332 (95%)	16 (5%)	0	100 100
1	K	348/391 (89%)	332 (95%)	16 (5%)	0	100 100
1	L	348/391 (89%)	330 (95%)	18 (5%)	0	100 100
All	All	4176/4692 (89%)	3982 (95%)	188 (4%)	6 (0%)	51 42

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LYS
1	I	223	ASP
1	C	224	LYS
1	G	224	LYS
1	I	222	VAL

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	308/342 (90%)	302 (98%)	6 (2%)	57	50
1	B	308/342 (90%)	299 (97%)	9 (3%)	42	31
1	C	308/342 (90%)	298 (97%)	10 (3%)	39	28
1	D	308/342 (90%)	303 (98%)	5 (2%)	62	56
1	E	308/342 (90%)	299 (97%)	9 (3%)	42	31
1	F	308/342 (90%)	300 (97%)	8 (3%)	46	37
1	G	308/342 (90%)	301 (98%)	7 (2%)	50	44
1	H	308/342 (90%)	299 (97%)	9 (3%)	42	31
1	I	308/342 (90%)	300 (97%)	8 (3%)	46	37
1	J	308/342 (90%)	301 (98%)	7 (2%)	50	44
1	K	308/342 (90%)	301 (98%)	7 (2%)	50	44
1	L	308/342 (90%)	297 (96%)	11 (4%)	35	23
All	All	3696/4104 (90%)	3600 (97%)	96 (3%)	46	37

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	257	GLU
1	G	337	ARG
1	L	121	LEU
1	F	268	MET

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Mol	Chain	Res	Type
1	G	108	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	221	GLN
1	I	135	ASN
1	K	350	GLN
1	H	157	ASN
1	L	30	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 60 ligands modelled in this entry, 12 are monoatomic - leaving 48 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FES	C	402	1	0,4,4	0.00	-	-		
6	EPE	B	405	-	15,15,15	0.98	1 (6%)	18,20,20	1.94	7 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EPE	H	405	-	15,15,15	1.06	1 (6%)	18,20,20	1.82	8 (44%)
4	152	B	403	-	7,10,10	1.45	1 (14%)	10,14,14	1.37	1 (10%)
4	152	A	403	-	7,10,10	1.40	1 (14%)	10,14,14	1.26	1 (10%)
6	EPE	D	405	-	15,15,15	0.96	1 (6%)	18,20,20	2.10	8 (44%)
6	EPE	C	405	-	15,15,15	1.13	1 (6%)	18,20,20	1.79	7 (38%)
4	152	C	403	-	7,10,10	1.46	1 (14%)	10,14,14	0.84	1 (10%)
4	152	I	403	-	7,10,10	1.38	1 (14%)	10,14,14	1.32	1 (10%)
3	FES	D	402	1	0,4,4	0.00	-	-		
5	SCN	I	404	2	1,2,2	0.75	0	0,1,1	0.00	-
6	EPE	J	405	-	15,15,15	2.08	1 (6%)	18,20,20	1.37	1 (5%)
3	FES	L	402	1	0,4,4	0.00	-	-		
5	SCN	F	404	2	1,2,2	0.64	0	0,1,1	0.00	-
3	FES	G	402	1	0,4,4	0.00	-	-		
3	FES	I	402	1	0,4,4	0.00	-	-		
5	SCN	J	404	2	1,2,2	0.40	0	0,1,1	0.00	-
3	FES	K	402	1	0,4,4	0.00	-	-		
5	SCN	D	404	2	1,2,2	0.46	0	0,1,1	0.00	-
5	SCN	H	404	2	1,2,2	0.47	0	0,1,1	0.00	-
5	SCN	E	404	2	1,2,2	0.55	0	0,1,1	0.00	-
6	EPE	G	405	-	15,15,15	1.06	1 (6%)	18,20,20	1.84	5 (27%)
6	EPE	A	405	-	15,15,15	2.23	1 (6%)	18,20,20	1.54	4 (22%)
5	SCN	K	404	2	1,2,2	0.67	0	0,1,1	0.00	-
3	FES	H	402	1	0,4,4	0.00	-	-		
3	FES	A	402	1	0,4,4	0.00	-	-		
3	FES	E	402	1	0,4,4	0.00	-	-		
3	FES	J	402	1	0,4,4	0.00	-	-		
4	152	E	403	-	7,10,10	1.42	1 (14%)	10,14,14	0.71	0
6	EPE	I	405	-	15,15,15	1.04	1 (6%)	18,20,20	1.99	7 (38%)
4	152	L	403	-	7,10,10	1.38	1 (14%)	10,14,14	1.23	1 (10%)
5	SCN	L	404	2	1,2,2	0.67	0	0,1,1	0.00	-
4	152	J	403	-	7,10,10	1.42	1 (14%)	10,14,14	1.16	1 (10%)
4	152	K	403	-	7,10,10	1.48	1 (14%)	10,14,14	1.31	1 (10%)
6	EPE	F	405	-	15,15,15	1.06	1 (6%)	18,20,20	1.86	5 (27%)
3	FES	B	402	1	0,4,4	0.00	-	-		
5	SCN	C	404	2	1,2,2	0.41	0	0,1,1	0.00	-
4	152	F	403	-	7,10,10	1.33	1 (14%)	10,14,14	1.25	1 (10%)
4	152	D	403	-	7,10,10	1.26	1 (14%)	10,14,14	1.14	1 (10%)
6	EPE	K	405	-	15,15,15	0.97	1 (6%)	18,20,20	1.89	7 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	152	G	403	-	7,10,10	1.35	1 (14%)	10,14,14	0.75	1 (10%)
5	SCN	A	404	2	1,2,2	0.60	0	0,1,1	0.00	-
3	FES	F	402	1	0,4,4	0.00	-	-		
5	SCN	G	404	2	1,2,2	0.83	0	0,1,1	0.00	-
4	152	H	403	-	7,10,10	1.34	1 (14%)	10,14,14	0.82	1 (10%)
6	EPE	E	405	-	15,15,15	1.03	1 (6%)	18,20,20	1.92	8 (44%)
6	EPE	L	405	-	15,15,15	0.96	1 (6%)	18,20,20	1.95	9 (50%)
5	SCN	B	404	2	1,2,2	0.46	0	0,1,1	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EPE	B	405	-	-	2/9/19/19	0/1/1/1
3	FES	C	402	1	-	-	0/1/1/1
4	152	B	403	-	-	5/7/9/9	-
4	152	A	403	-	-	3/7/9/9	-
3	FES	E	402	1	-	-	0/1/1/1
6	EPE	C	405	-	-	4/9/19/19	0/1/1/1
4	152	C	403	-	-	3/7/9/9	-
4	152	I	403	-	-	3/7/9/9	-
3	FES	D	402	1	-	-	0/1/1/1
6	EPE	H	405	-	-	3/9/19/19	0/1/1/1
6	EPE	J	405	-	-	0/9/19/19	0/1/1/1
3	FES	L	402	1	-	-	0/1/1/1
6	EPE	F	405	-	-	3/9/19/19	0/1/1/1
4	152	F	403	-	-	3/7/9/9	-
6	EPE	K	405	-	-	3/9/19/19	0/1/1/1
3	FES	K	402	1	-	-	0/1/1/1
6	EPE	E	405	-	-	3/9/19/19	0/1/1/1
6	EPE	G	405	-	-	3/9/19/19	0/1/1/1
6	EPE	A	405	-	-	1/9/19/19	0/1/1/1
4	152	K	403	-	-	3/7/9/9	-
3	FES	A	402	1	-	-	0/1/1/1
6	EPE	D	405	-	-	4/9/19/19	0/1/1/1
3	FES	J	402	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	152	E	403	-	-	4/7/9/9	-
6	EPE	I	405	-	-	3/9/19/19	0/1/1/1
4	152	L	403	-	-	5/7/9/9	-
4	152	J	403	-	-	5/7/9/9	-
3	FES	H	402	1	-	-	0/1/1/1
3	FES	G	402	1	-	-	0/1/1/1
3	FES	B	402	1	-	-	0/1/1/1
3	FES	I	402	1	-	-	0/1/1/1
4	152	D	403	-	-	5/7/9/9	-
4	152	G	403	-	-	3/7/9/9	-
3	FES	F	402	1	-	-	0/1/1/1
4	152	H	403	-	-	4/7/9/9	-
6	EPE	L	405	-	-	3/9/19/19	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	405	EPE	C10-S	-8.50	1.65	1.77
6	J	405	EPE	C10-S	-7.90	1.66	1.77
6	C	405	EPE	C10-S	3.88	1.83	1.77
6	G	405	EPE	C10-S	3.63	1.82	1.77
6	H	405	EPE	C10-S	3.63	1.82	1.77

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	405	EPE	C9-N1-C2	-4.56	99.56	111.23
6	I	405	EPE	C9-N1-C2	-4.30	100.25	111.23
4	K	403	152	C3-C4-N5	-4.01	109.98	116.83
4	B	403	152	C3-C4-N5	-3.99	110.01	116.83
4	I	403	152	C3-C4-N5	-3.95	110.07	116.83

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	152	C1-C2-C3-O3
4	B	403	152	C1-C2-C3-C4
6	C	405	EPE	C8-C7-N4-C5
6	C	405	EPE	S-C10-C9-N1

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Mol	Chain	Res	Type	Atoms
6	A	405	EPE	C10-C9-N1-C2

There are no ring outliers.

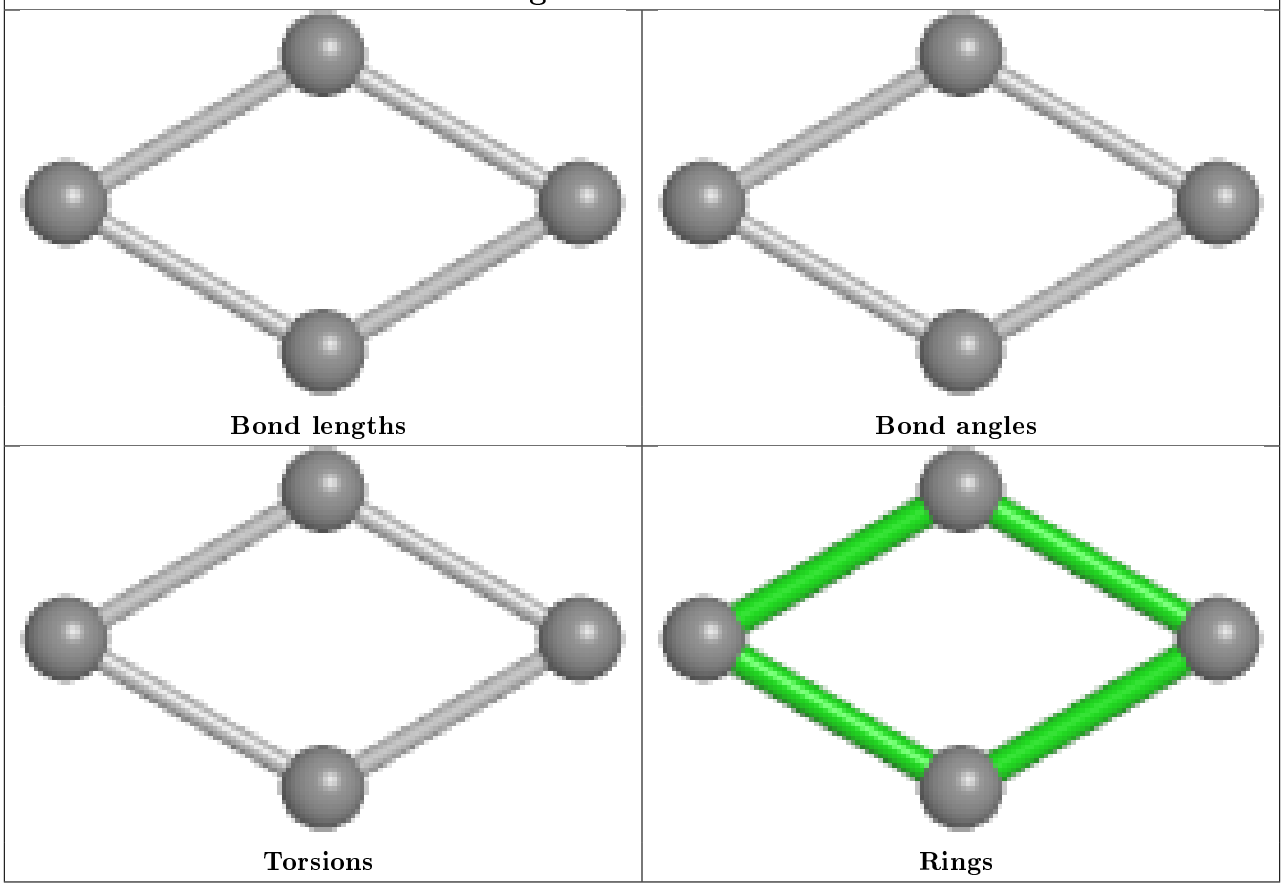
26 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	FES	1	0
4	B	403	152	3	0
4	A	403	152	2	0
4	C	403	152	2	0
4	I	403	152	1	0
5	I	404	SCN	2	0
6	J	405	EPE	3	0
5	J	404	SCN	2	0
3	K	402	FES	1	0
5	H	404	SCN	1	0
5	E	404	SCN	1	0
5	K	404	SCN	2	0
3	J	402	FES	1	0
4	E	403	152	1	0
4	L	403	152	3	0
5	L	404	SCN	1	0
4	J	403	152	4	0
3	B	402	FES	1	0
5	C	404	SCN	1	0
4	F	403	152	2	0
4	D	403	152	2	0
4	G	403	152	1	0
5	A	404	SCN	1	0
3	F	402	FES	1	0
4	H	403	152	1	0
5	B	404	SCN	2	0

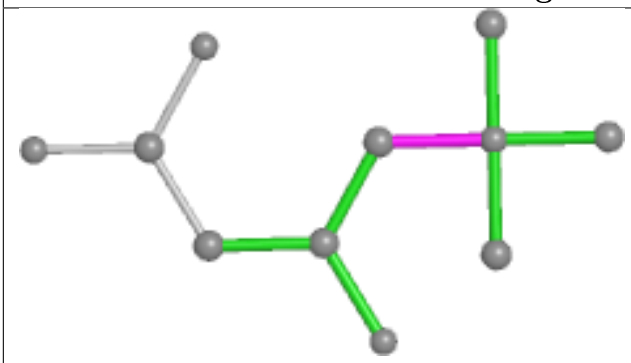
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

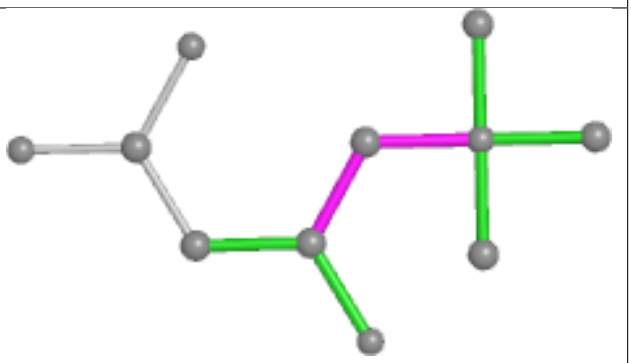
Ligand FES C 402



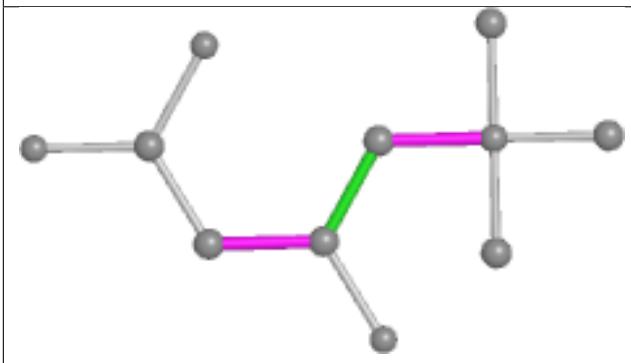
Ligand 152 B 403



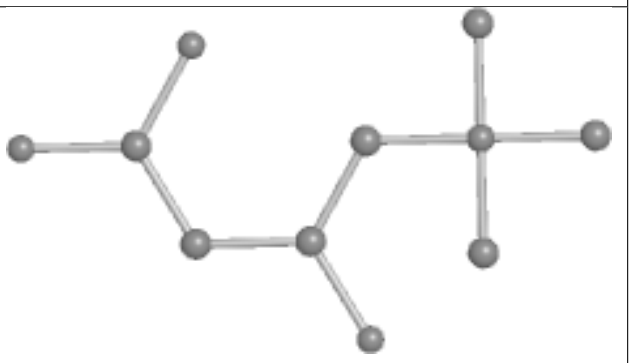
Bond lengths



Bond angles

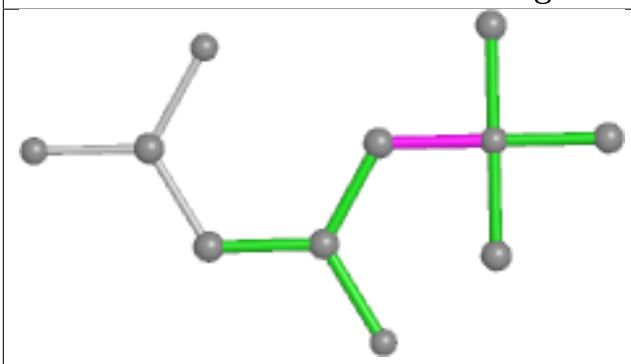


Torsions

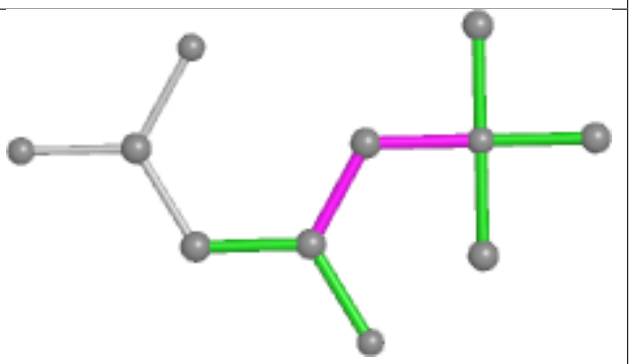


Rings

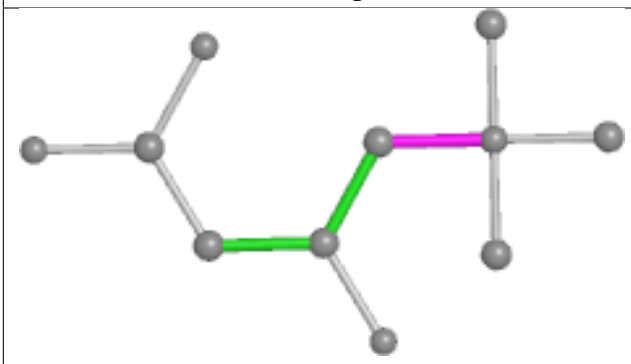
Ligand 152 A 403



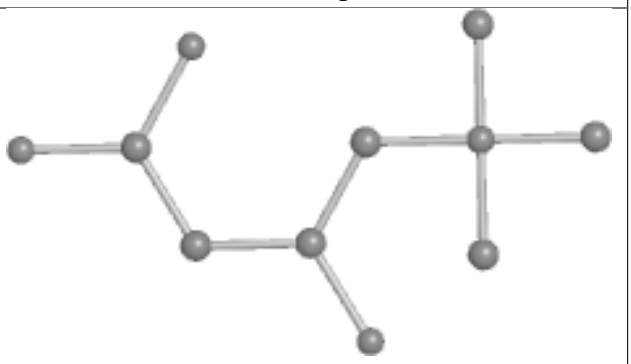
Bond lengths



Bond angles

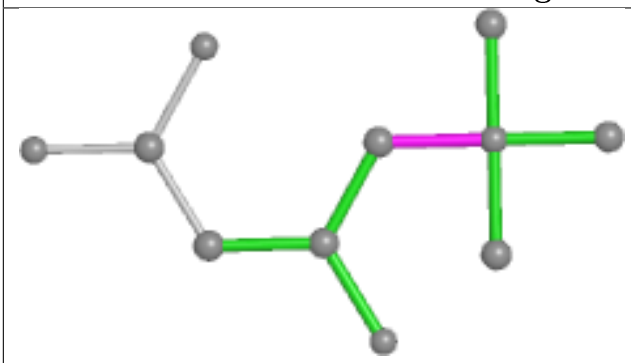


Torsions

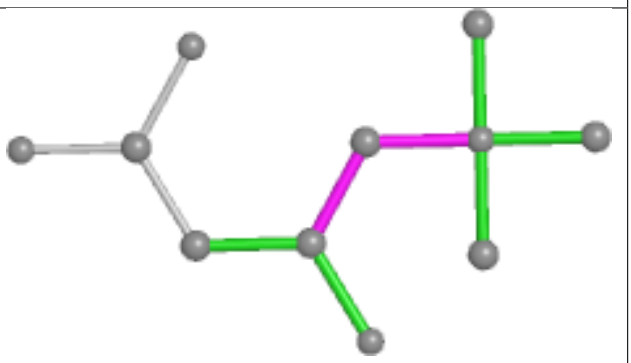


Rings

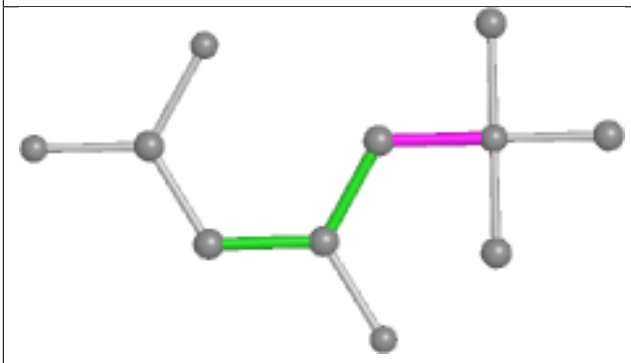
Ligand 152 C 403



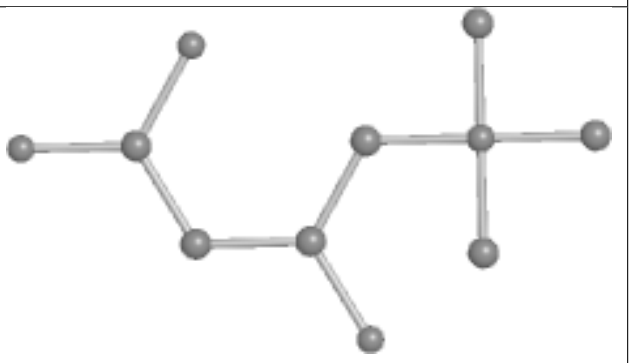
Bond lengths



Bond angles

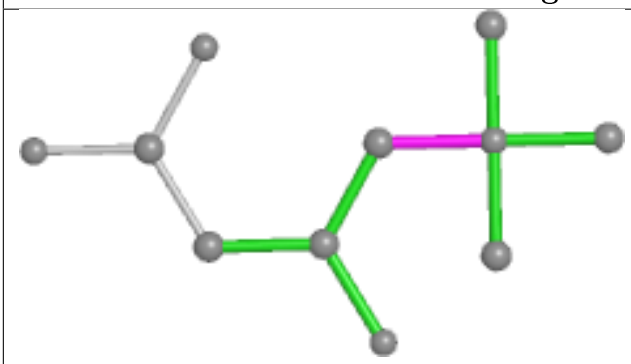


Torsions

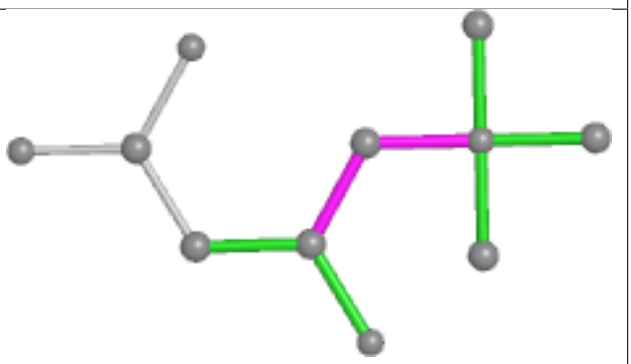


Rings

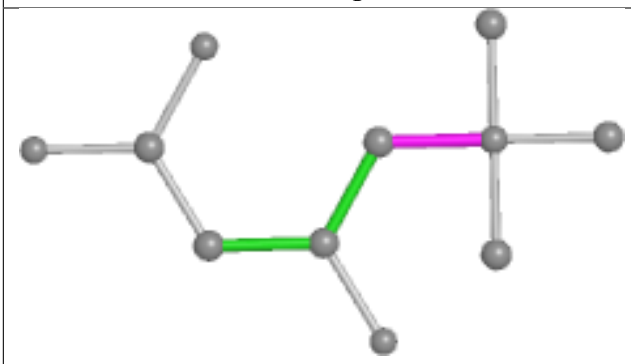
Ligand 152 I 403



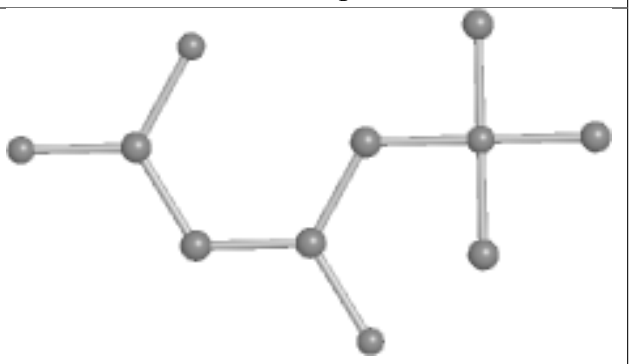
Bond lengths



Bond angles

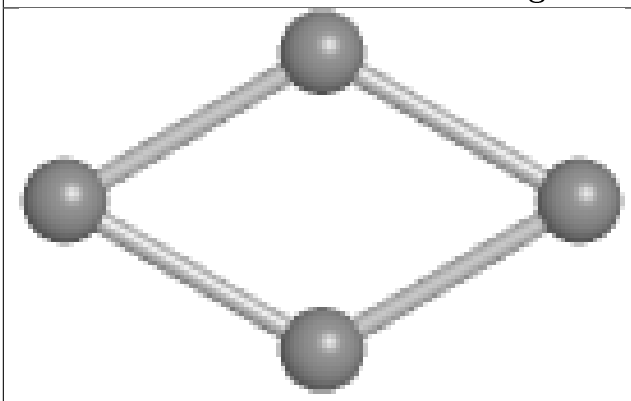


Torsions

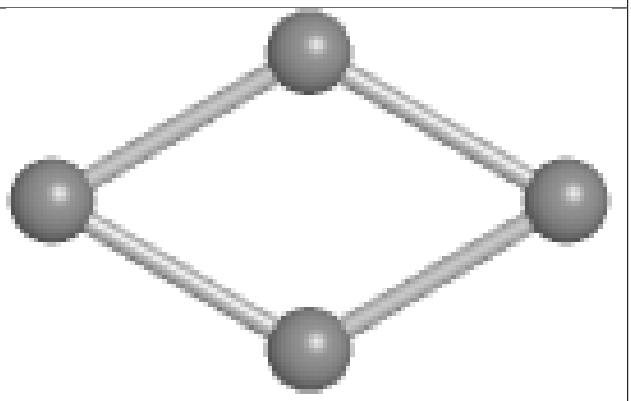


Rings

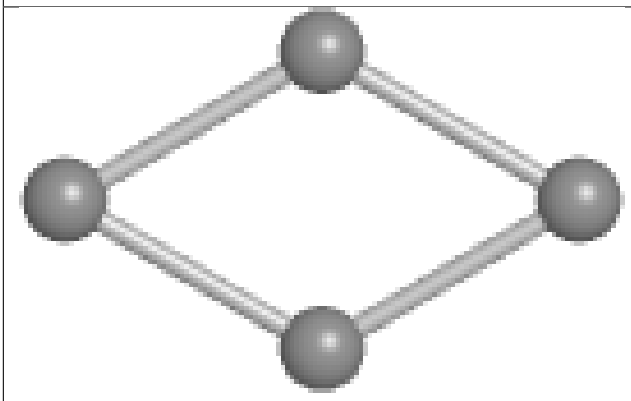
Ligand FES D 402



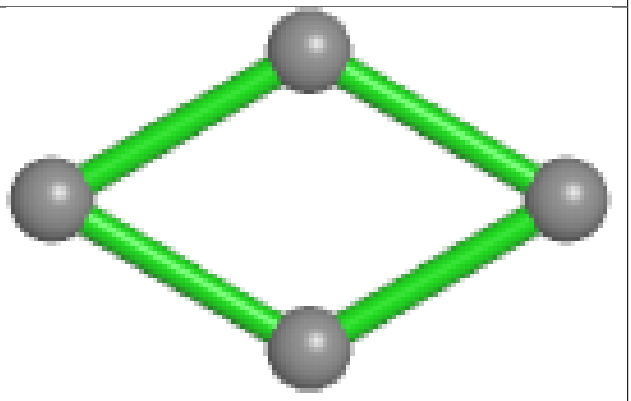
Bond lengths



Bond angles

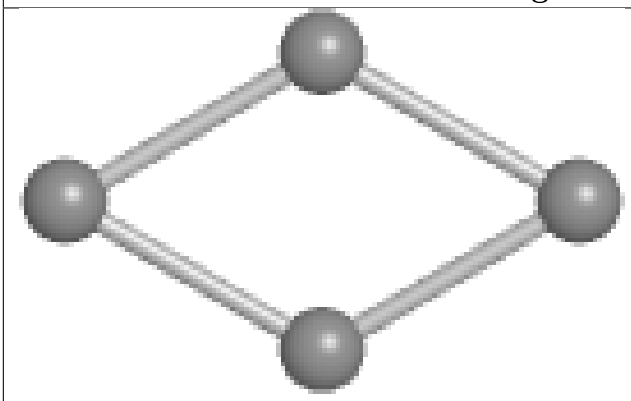


Torsions

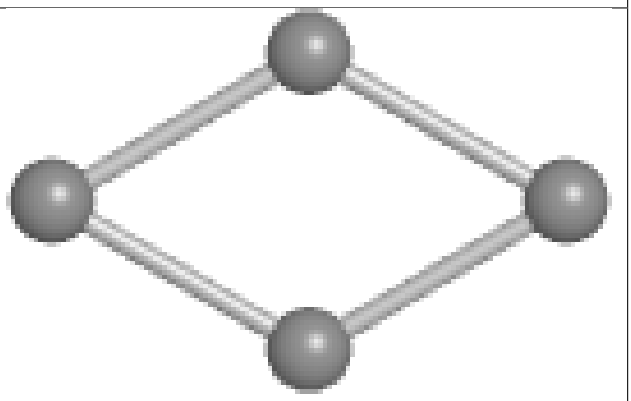


Rings

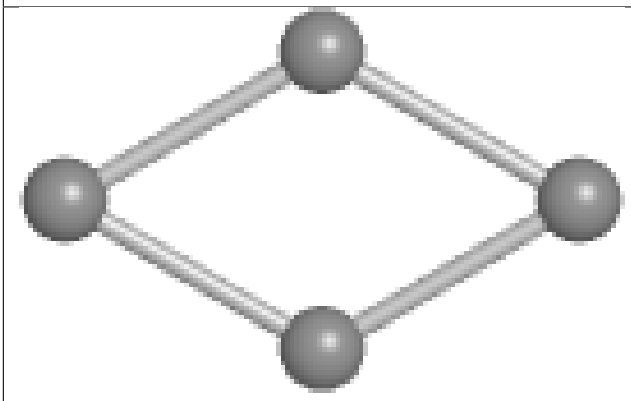
Ligand FES L 402



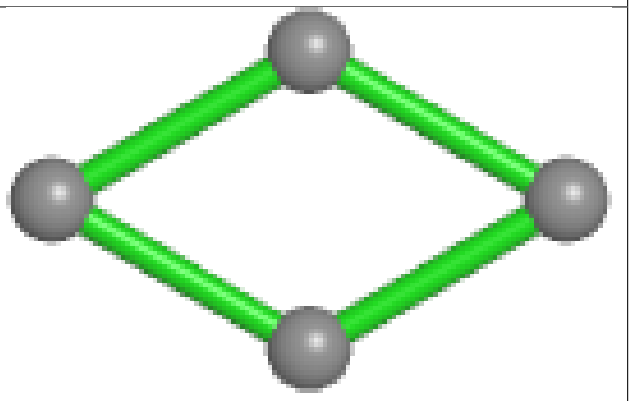
Bond lengths



Bond angles

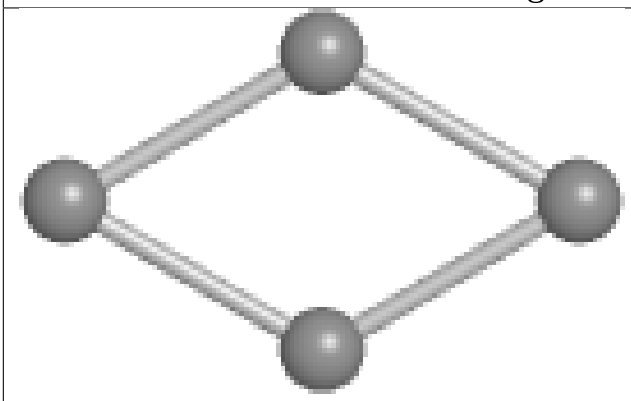


Torsions



Rings

Ligand FES G 402



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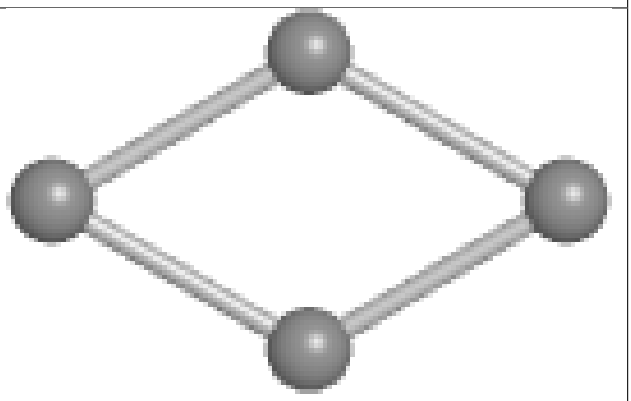
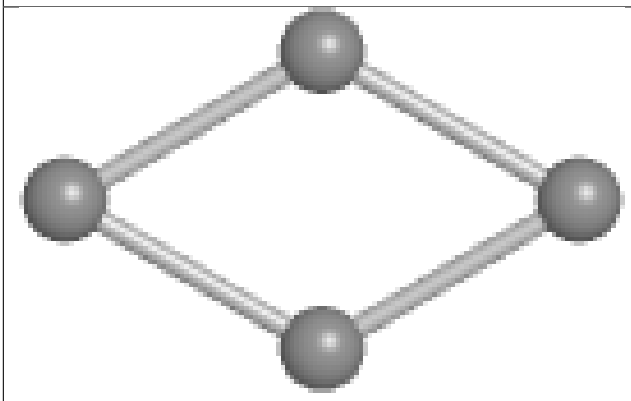


Bond angles



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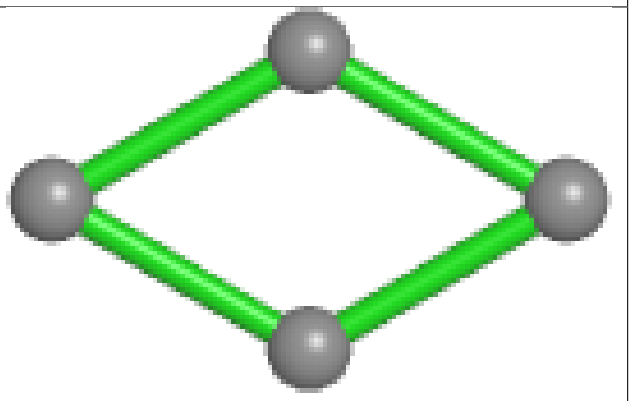
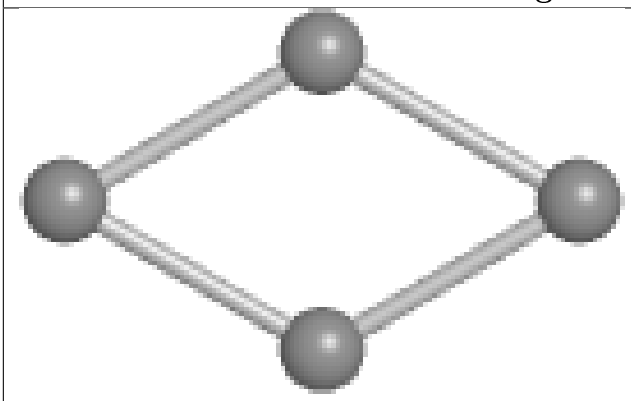


Rings

Ligand FES I 402



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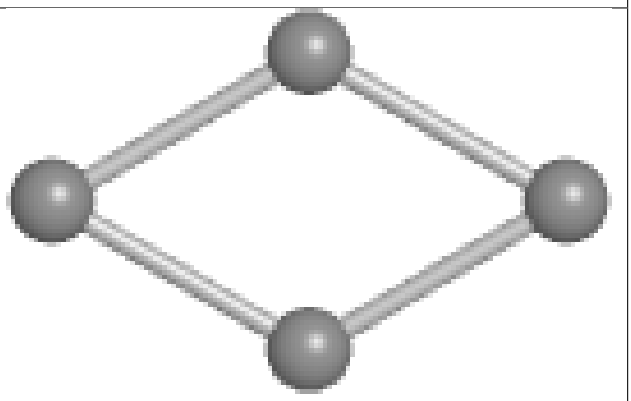

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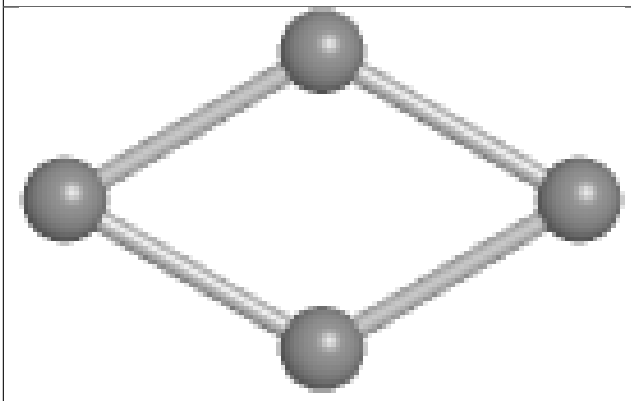

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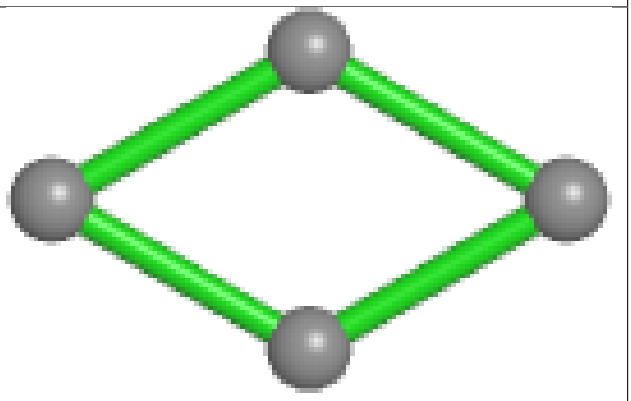
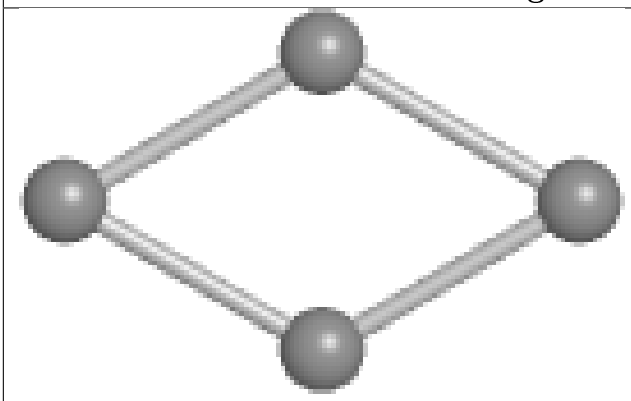


Rings

Ligand FES K 402



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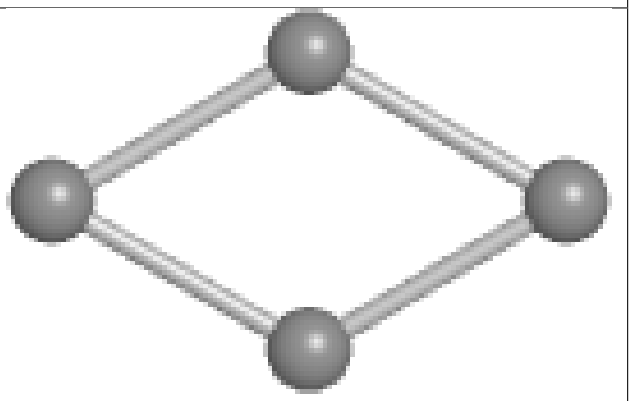

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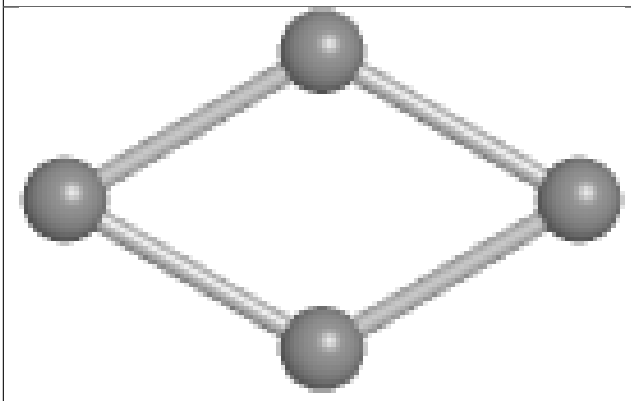

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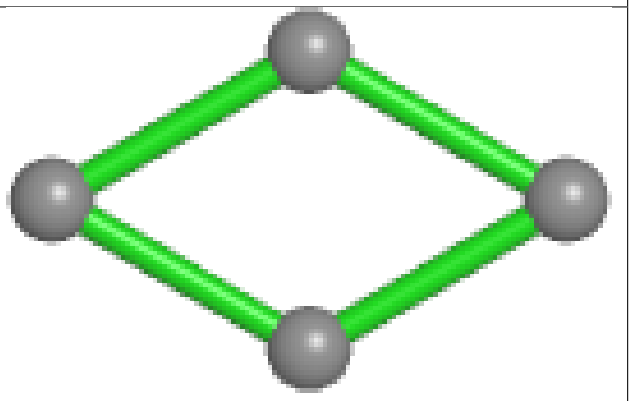
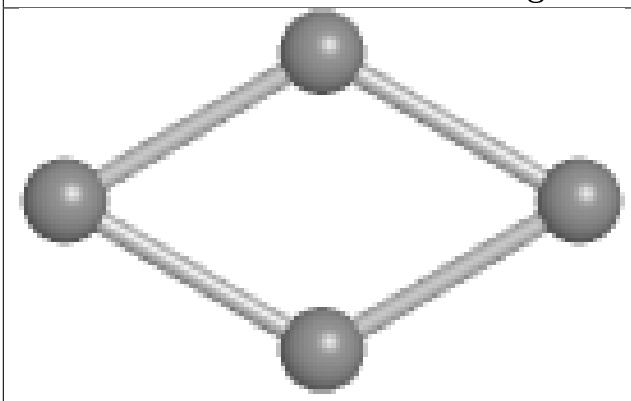


Rings

Ligand FES H 402



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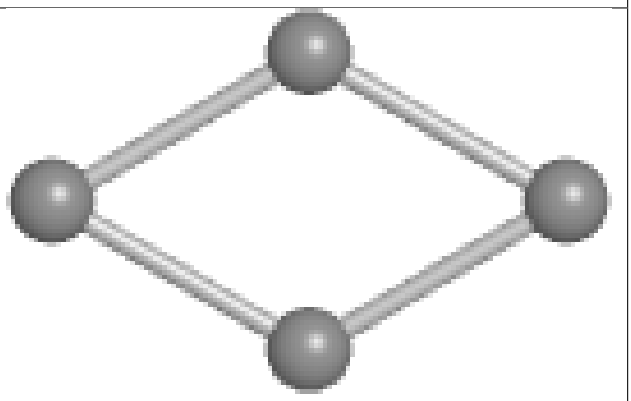

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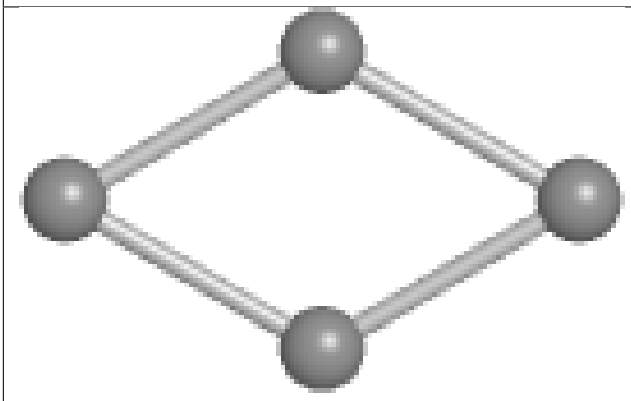

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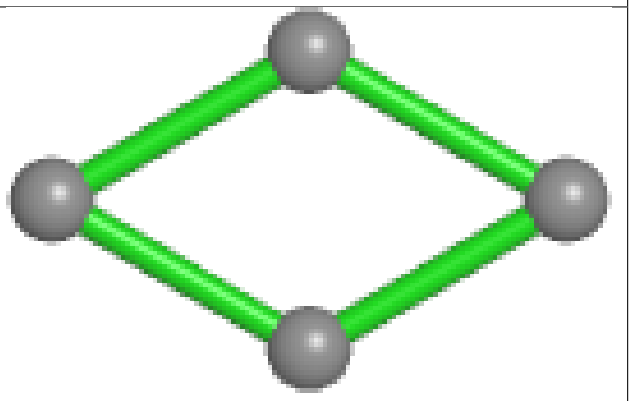
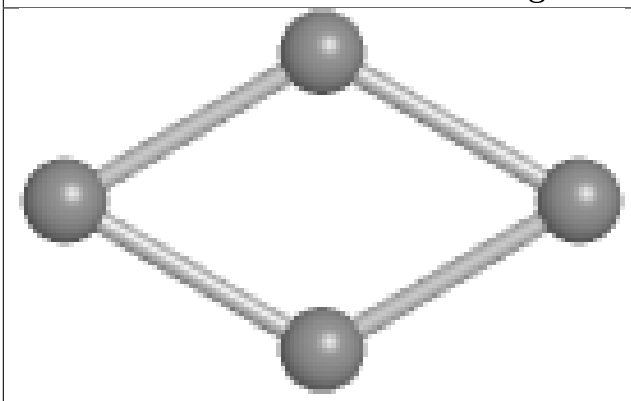


Rings

Ligand FES A 402



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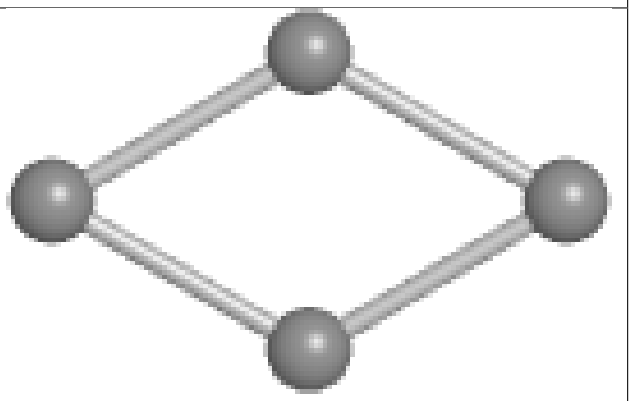
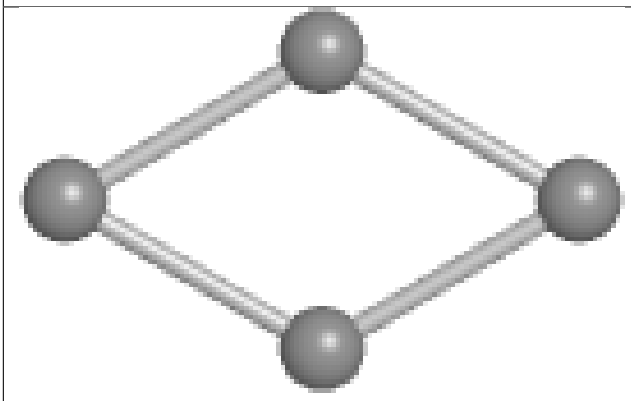


Bond angles



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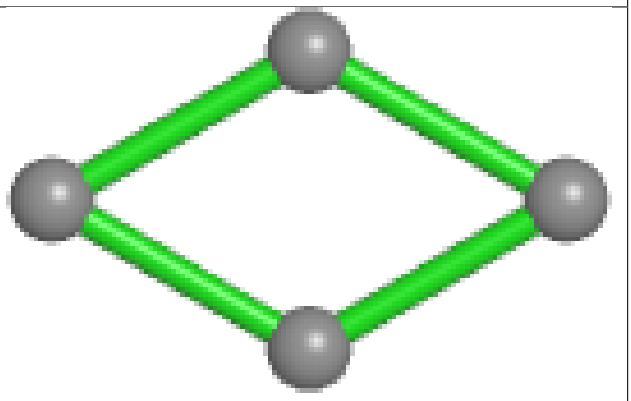

Rings

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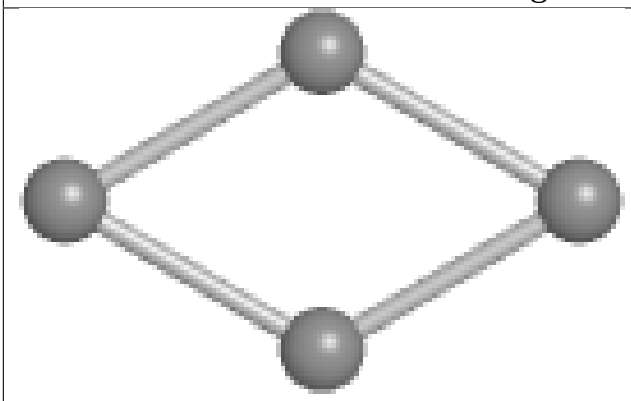

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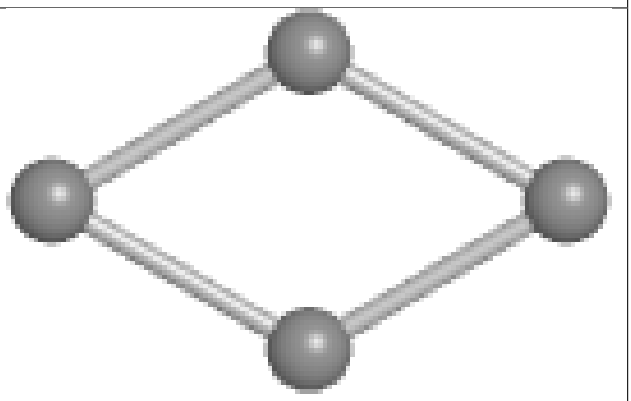
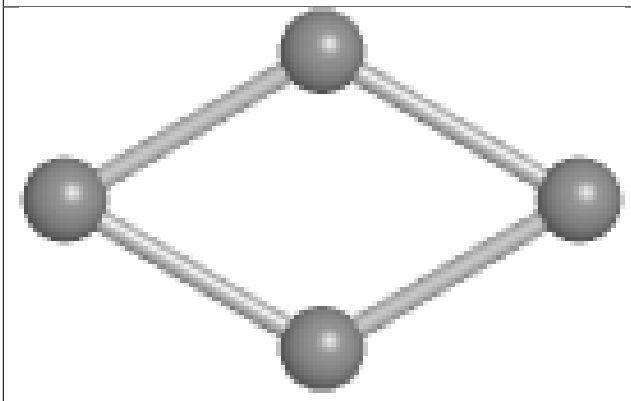


Bond angles



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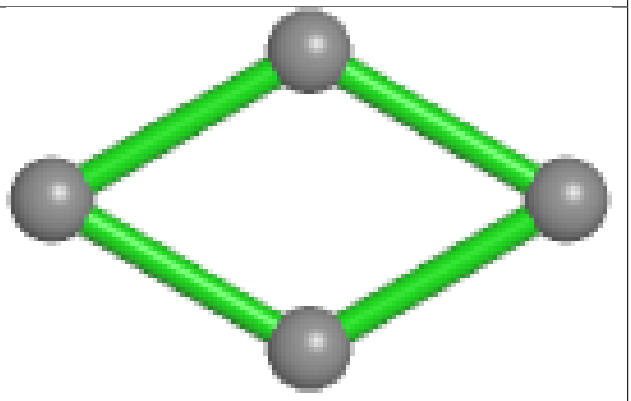
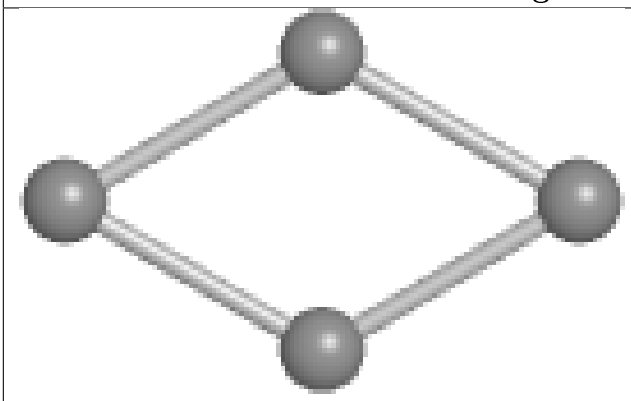


Rings

Ligand FES J 402



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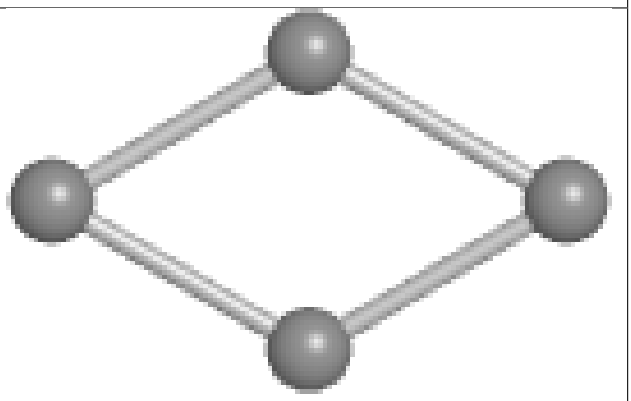
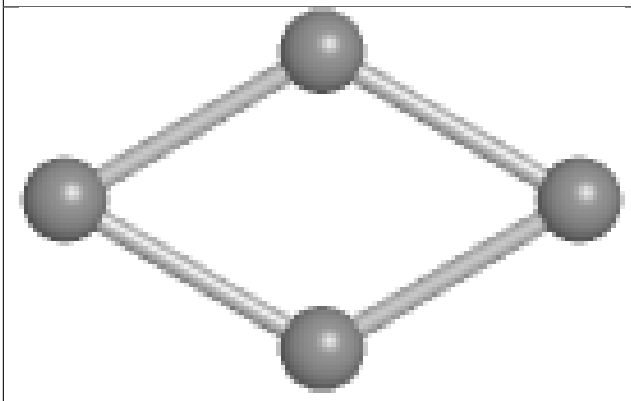


Bond angles



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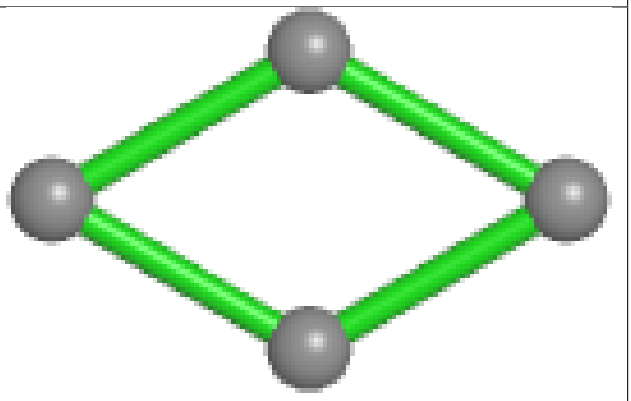
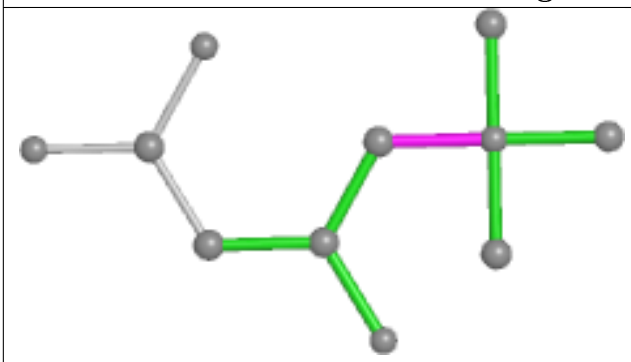


Rings

Ligand 152 E 403



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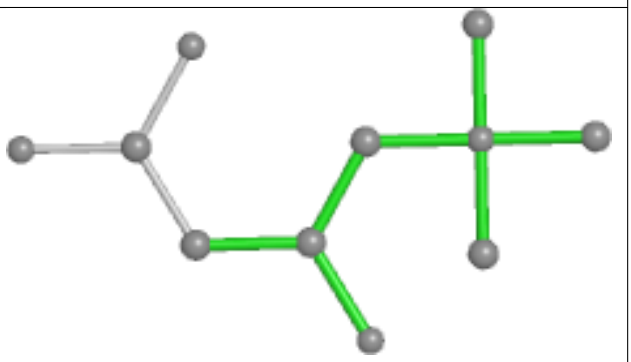

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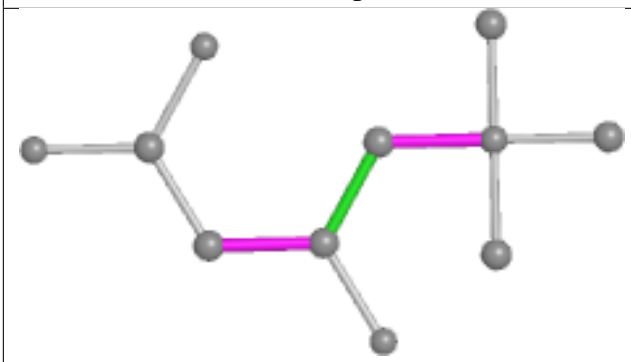

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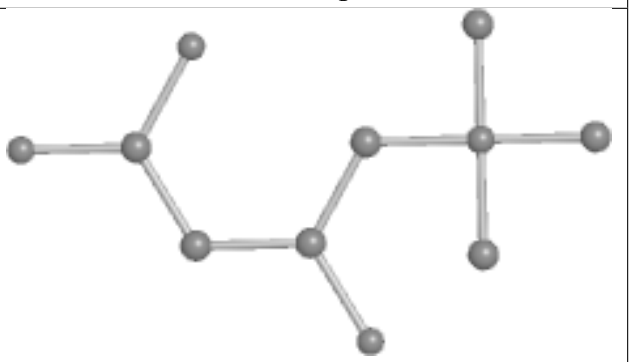
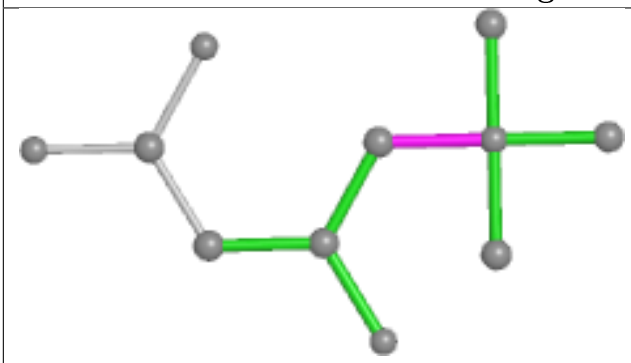


Rings

Ligand 152 L 403



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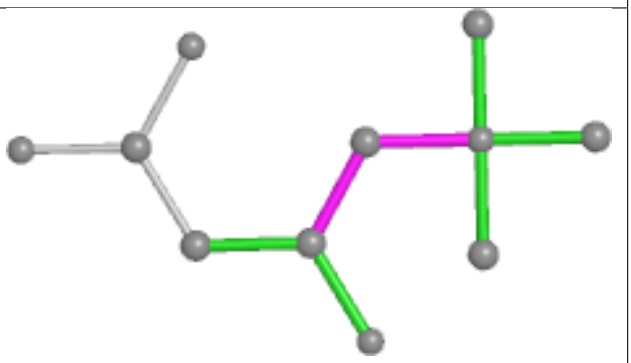

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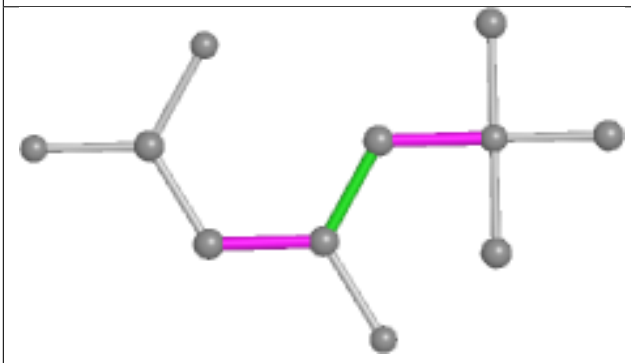

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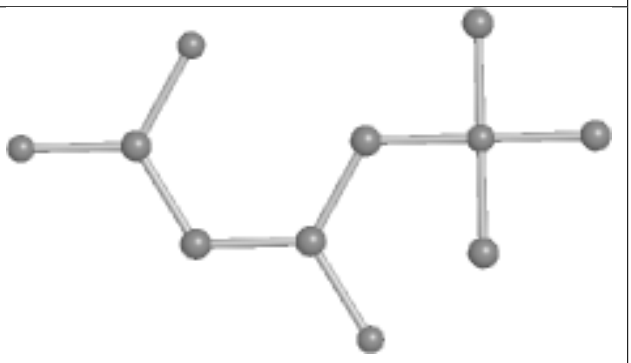
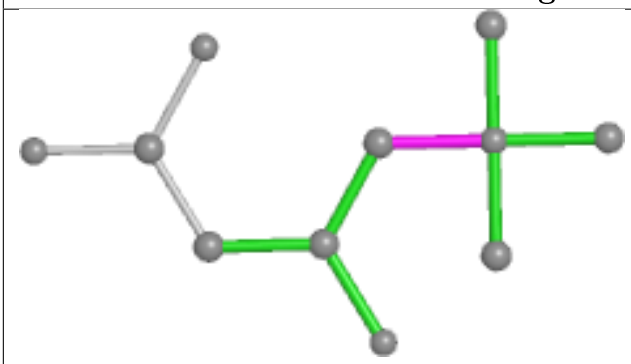


Rings

Ligand 152 J 403



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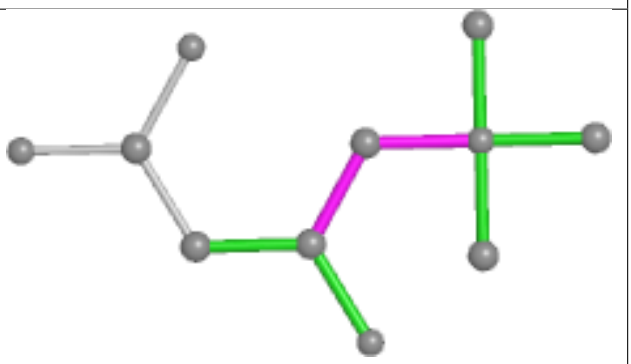

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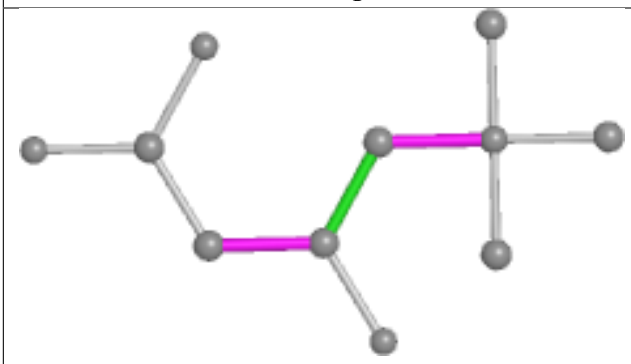

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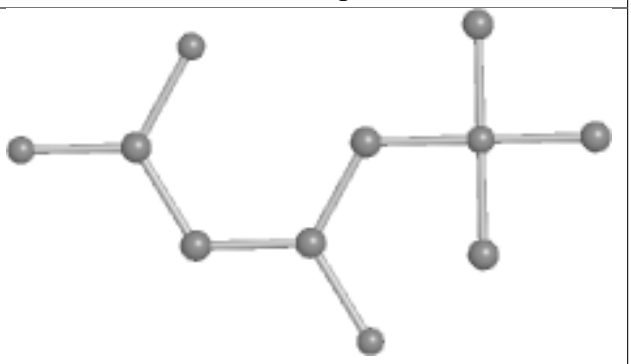
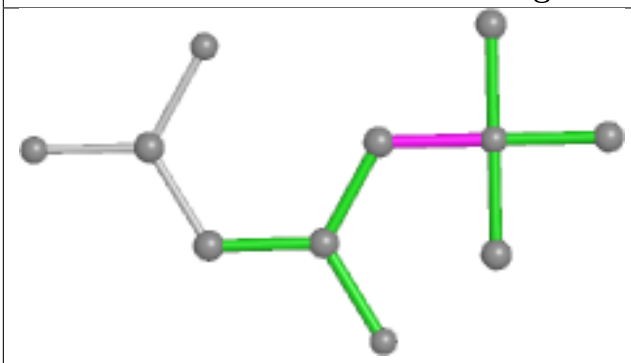


Rings

Ligand 152 K 403



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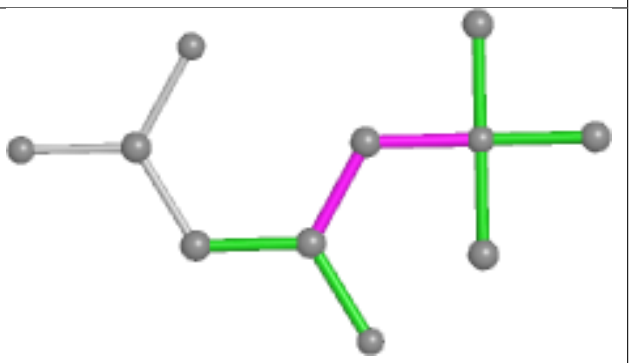

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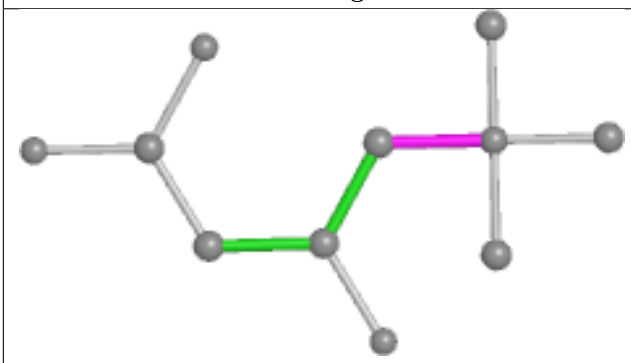

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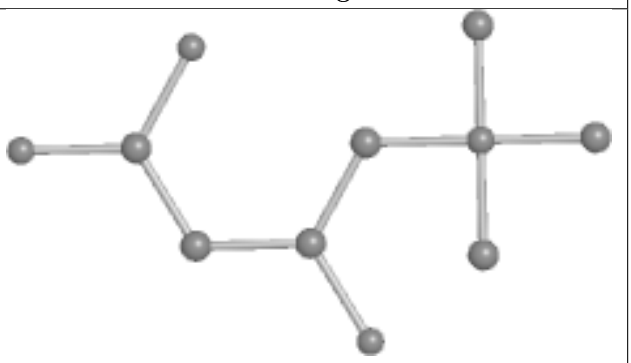
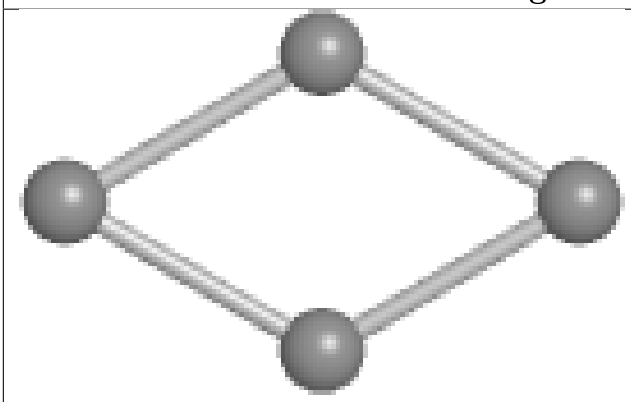


Rings

Ligand FES B 402



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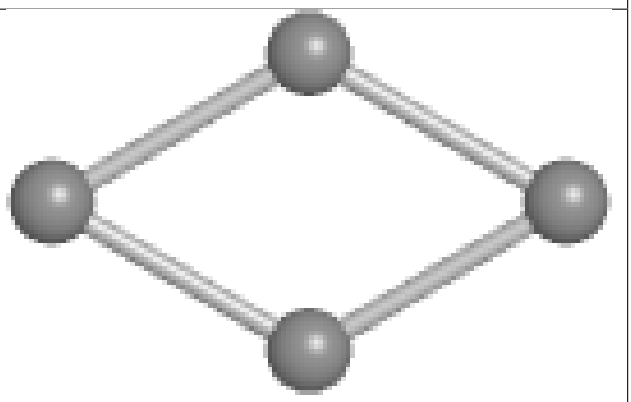
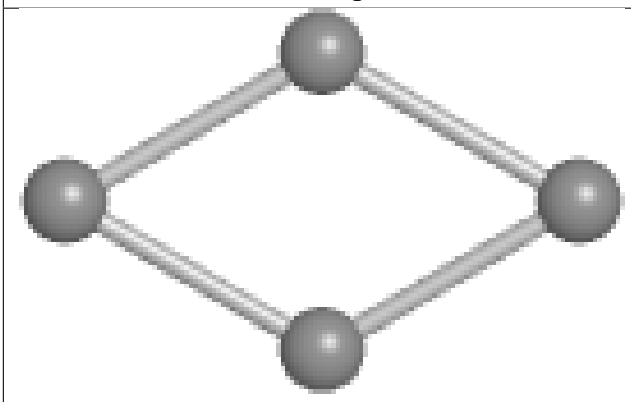


Bond angles



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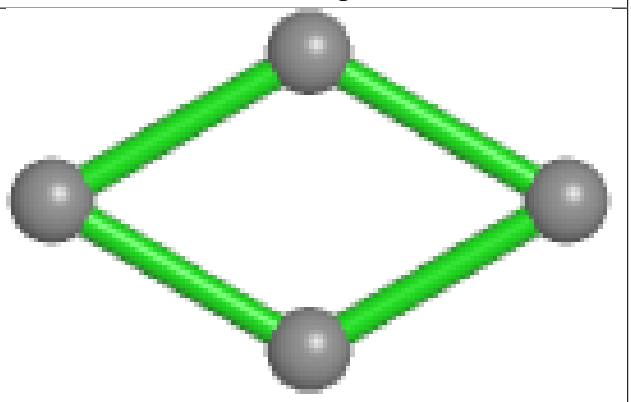
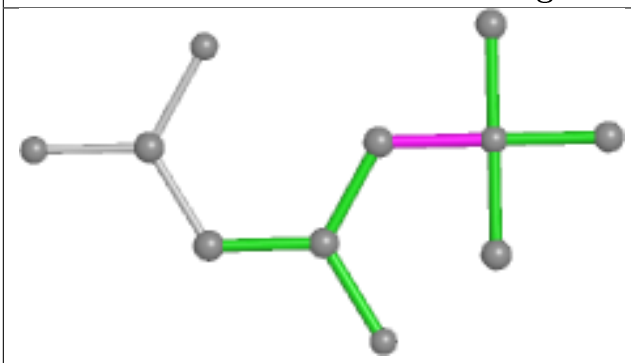


Rings

Ligand 152 F 403



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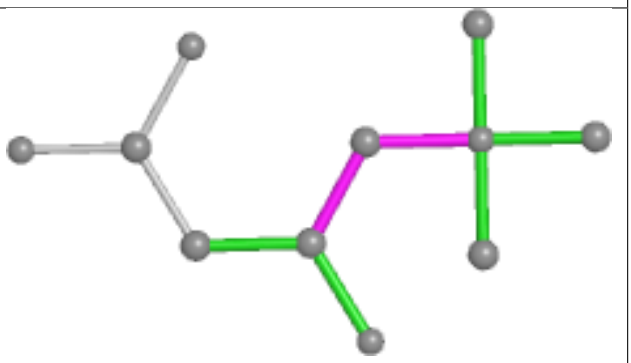
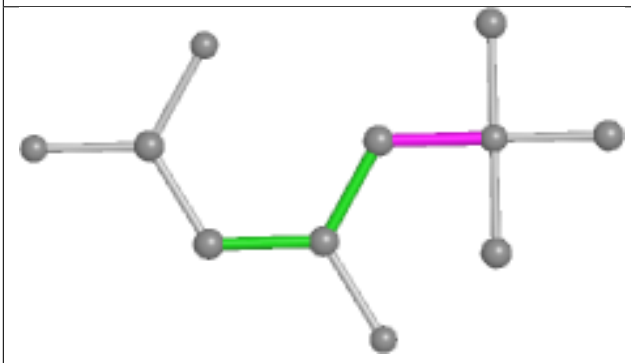


Bond angles



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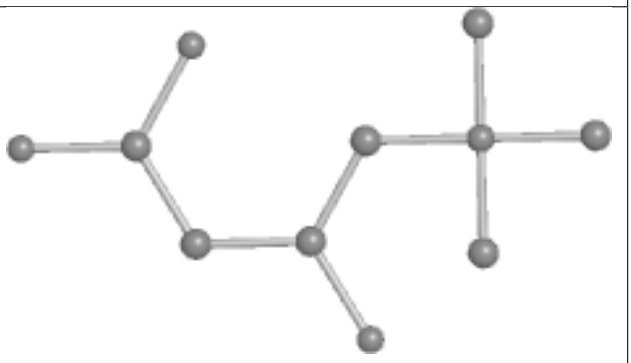
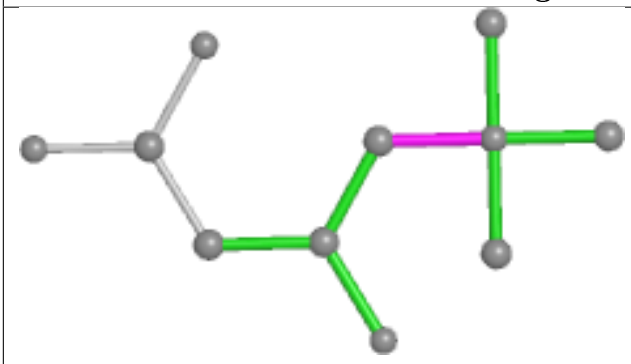
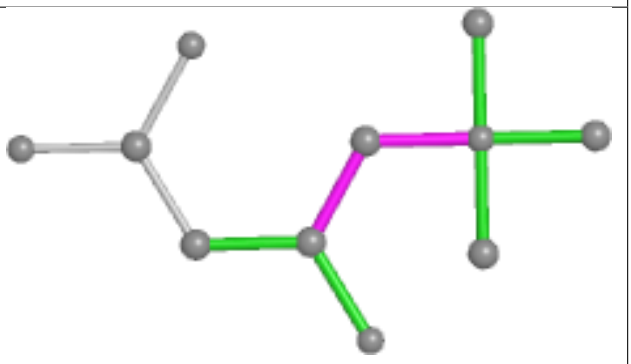


Rings

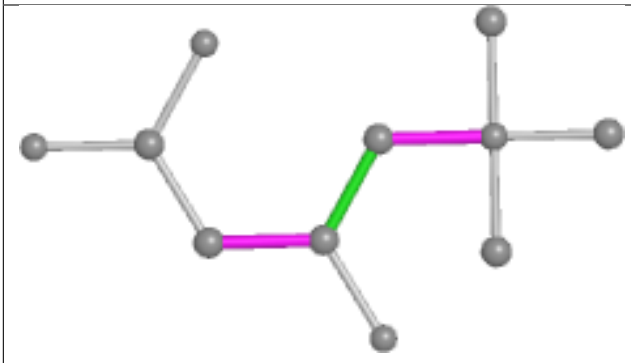
Ligand 152 D 403



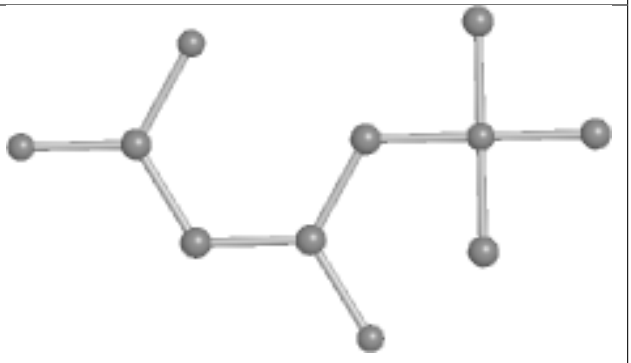
Bond lengths



Bond angles

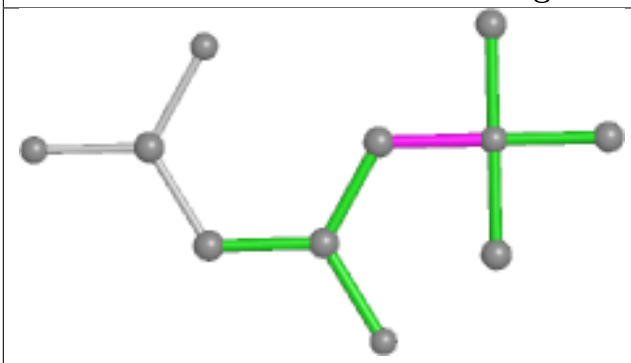


Torsions

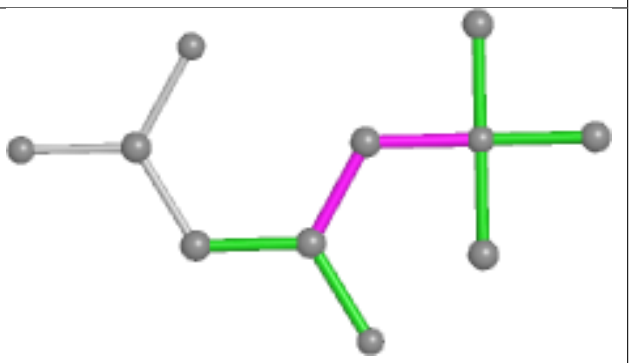


Rings

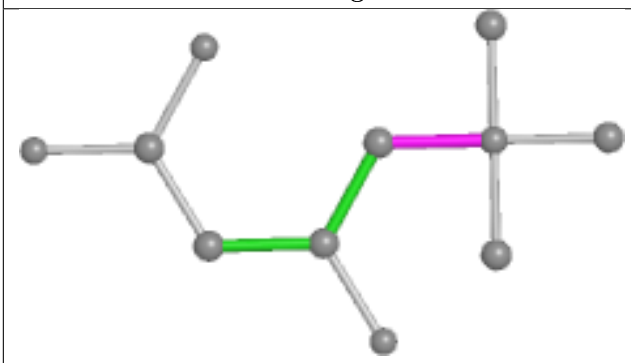
Ligand 152 G 403



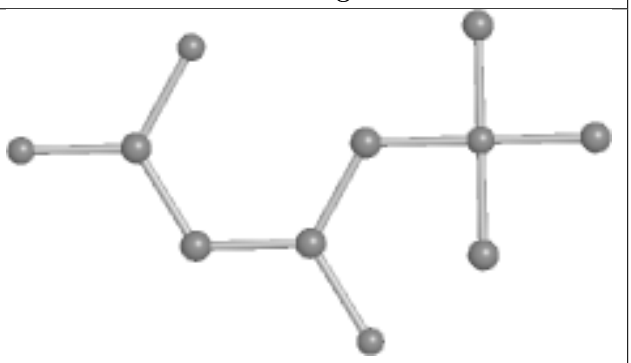
Bond lengths



Bond angles

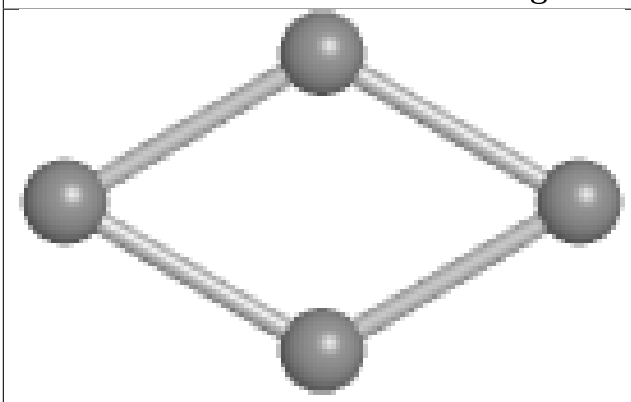


Torsions

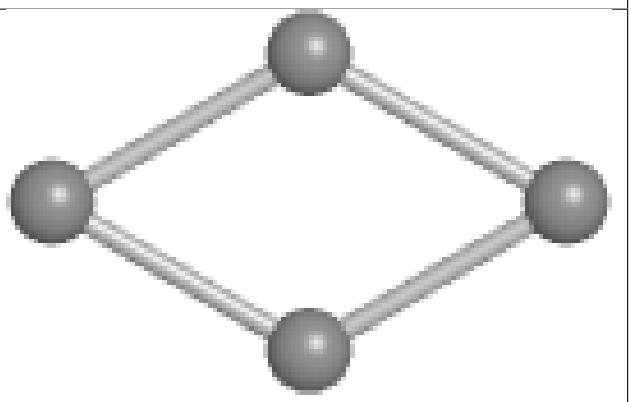


Rings

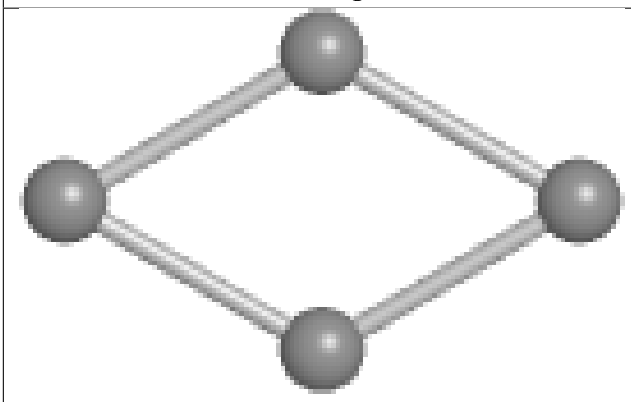
Ligand FES F 402



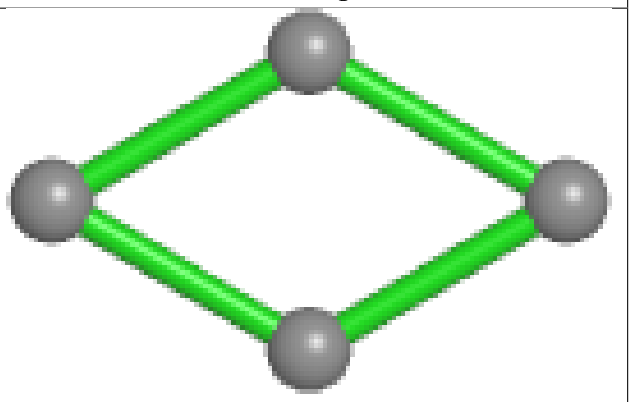
Bond lengths



Bond angles

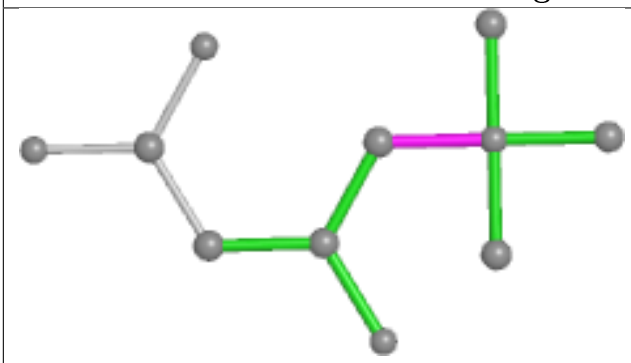


Torsions

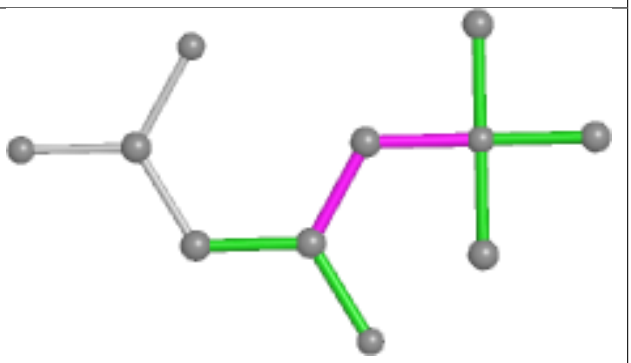


Rings

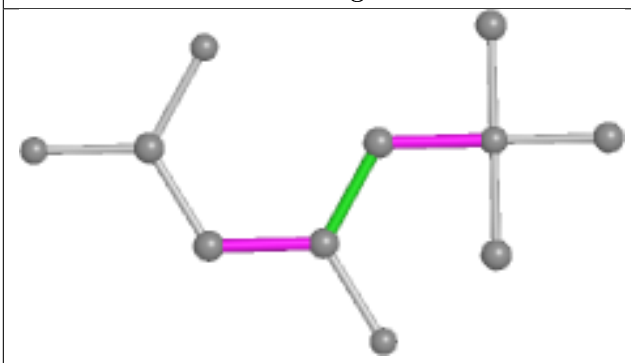
Ligand 152 H 403



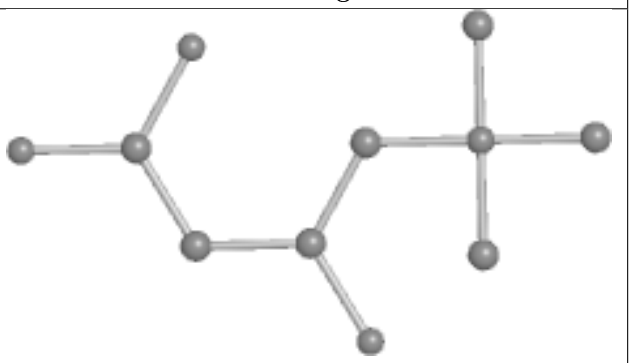
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	352/391 (90%)	0.55	19 (5%)	25	28	23, 39, 78, 131	0
1	B	352/391 (90%)	0.90	35 (9%)	7	8	24, 46, 91, 153	0
1	C	352/391 (90%)	0.58	22 (6%)	20	22	24, 40, 79, 154	0
1	D	352/391 (90%)	0.53	17 (4%)	30	32	22, 38, 75, 157	0
1	E	352/391 (90%)	0.52	12 (3%)	45	48	21, 36, 69, 159	0
1	F	352/391 (90%)	0.49	16 (4%)	33	35	23, 37, 70, 129	0
1	G	352/391 (90%)	0.50	15 (4%)	35	37	22, 36, 68, 140	0
1	H	352/391 (90%)	0.59	21 (5%)	21	23	26, 39, 74, 152	0
1	I	352/391 (90%)	0.53	15 (4%)	35	37	22, 39, 70, 150	0
1	J	352/391 (90%)	0.99	41 (11%)	4	5	29, 50, 100, 165	0
1	K	352/391 (90%)	0.58	18 (5%)	28	30	24, 44, 78, 139	0
1	L	352/391 (90%)	0.57	21 (5%)	21	23	24, 42, 81, 133	0
All	All	4224/4692 (90%)	0.61	252 (5%)	21	23	21, 40, 80, 165	0

The worst 5 of 252 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	216	PHE	14.5
1	I	222	VAL	13.4
1	B	216	PHE	12.1
1	J	221	GLN	12.0
1	J	218	ASP	11.9

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
3	FES	E	402	4/4	0.42	0.24	16,19,50,68	0
6	EPE	G	405	15/15	0.48	0.33	61,89,102,115	0
6	EPE	E	405	15/15	0.49	0.34	66,89,103,115	0
6	EPE	K	405	15/15	0.53	0.29	58,87,101,114	0
6	EPE	B	405	15/15	0.58	0.30	60,87,99,112	0
6	EPE	D	405	15/15	0.59	0.30	53,85,102,112	0
6	EPE	C	405	15/15	0.59	0.41	64,91,99,111	0
6	EPE	F	405	15/15	0.59	0.38	63,89,100,112	0
6	EPE	J	405	15/15	0.60	0.24	60,87,108,111	0
6	EPE	I	405	15/15	0.61	0.26	47,84,97,109	0
6	EPE	H	405	15/15	0.62	0.31	55,86,102,115	0
6	EPE	A	405	15/15	0.63	0.26	53,82,100,112	0
5	SCN	J	404	3/3	0.65	0.58	93,93,94,94	0
6	EPE	L	405	15/15	0.68	0.34	60,87,99,111	0
5	SCN	B	404	3/3	0.78	0.31	82,82,83,84	0
3	FES	G	402	4/4	0.80	0.26	66,70,75,97	0
4	152	B	403	11/11	0.82	0.30	64,65,70,71	0
2	FE	J	401	1/1	0.82	0.11	91,91,91,91	0
5	SCN	E	404	3/3	0.84	0.12	58,58,62,67	0
5	SCN	G	404	3/3	0.84	0.16	45,45,50,59	0
5	SCN	H	404	3/3	0.85	0.43	76,76,78,79	0
4	152	J	403	11/11	0.87	0.35	67,69,70,70	0
3	FES	L	402	4/4	0.88	0.14	43,48,53,67	0
5	SCN	C	404	3/3	0.89	0.25	64,64,65,66	0
5	SCN	F	404	3/3	0.89	0.27	51,51,56,59	0
4	152	D	403	11/11	0.89	0.17	46,49,55,56	0
3	FES	I	402	4/4	0.89	0.16	29,40,41,55	0
4	152	C	403	11/11	0.89	0.14	48,51,54,55	0
5	SCN	D	404	3/3	0.89	0.23	69,69,72,74	0
3	FES	D	402	4/4	0.89	0.18	28,48,50,54	0
2	FE	L	401	1/1	0.90	0.10	42,42,42,42	0
4	152	H	403	11/11	0.90	0.16	48,50,52,52	0

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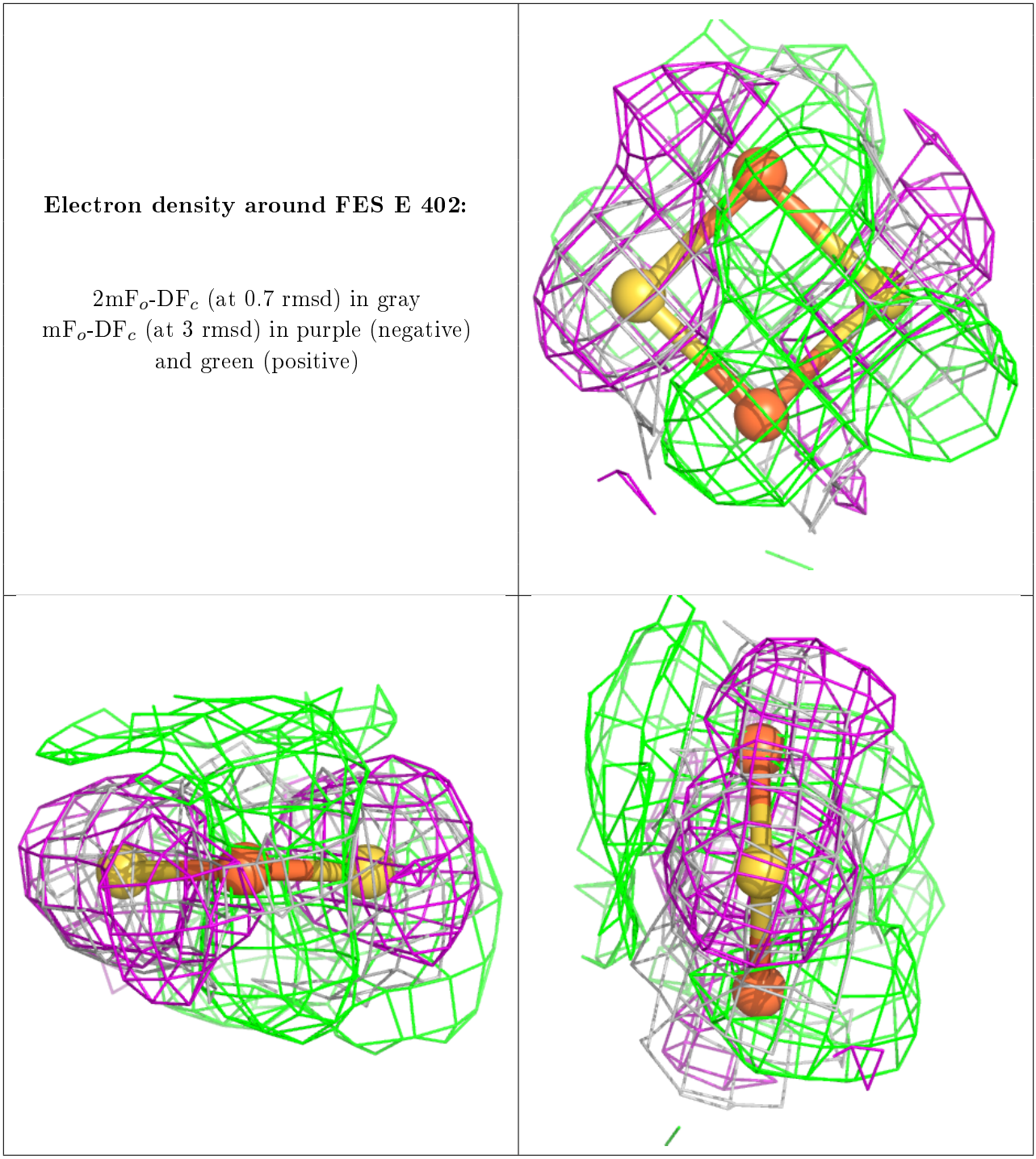
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	152	I	403	11/11	0.91	0.15	46,48,54,54	0
5	SCN	A	404	3/3	0.91	0.19	62,62,64,64	0
5	SCN	L	404	3/3	0.92	0.18	54,54,56,61	0
2	FE	B	401	1/1	0.92	0.05	50,50,50,50	0
4	152	K	403	11/11	0.93	0.12	44,47,51,51	0
3	FES	F	402	4/4	0.93	0.17	27,28,30,31	0
4	152	G	403	11/11	0.93	0.16	35,40,47,47	0
3	FES	J	402	4/4	0.94	0.11	29,29,30,34	0
4	152	E	403	11/11	0.94	0.13	37,39,43,44	0
5	SCN	I	404	3/3	0.94	0.11	52,52,55,58	0
3	FES	H	402	4/4	0.94	0.14	28,30,31,34	0
4	152	A	403	11/11	0.94	0.16	43,47,50,50	0
4	152	F	403	11/11	0.95	0.14	35,39,47,47	0
5	SCN	K	404	3/3	0.95	0.15	53,53,56,59	0
3	FES	A	402	4/4	0.95	0.12	30,32,35,49	0
4	152	L	403	11/11	0.95	0.14	48,49,50,51	0
2	FE	G	401	1/1	0.96	0.08	40,40,40,40	0
3	FES	K	402	4/4	0.96	0.09	36,37,37,38	0
3	FES	B	402	4/4	0.97	0.15	28,28,28,35	0
3	FES	C	402	4/4	0.97	0.11	41,43,46,64	0
2	FE	A	401	1/1	0.97	0.08	42,42,42,42	0
2	FE	H	401	1/1	0.98	0.04	48,48,48,48	0
2	FE	D	401	1/1	0.98	0.06	46,46,46,46	0
2	FE	C	401	1/1	0.98	0.09	49,49,49,49	0
2	FE	I	401	1/1	0.98	0.06	48,48,48,48	0
2	FE	K	401	1/1	0.99	0.08	44,44,44,44	0
2	FE	F	401	1/1	0.99	0.07	45,45,45,45	0
2	FE	E	401	1/1	0.99	0.06	42,42,42,42	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.

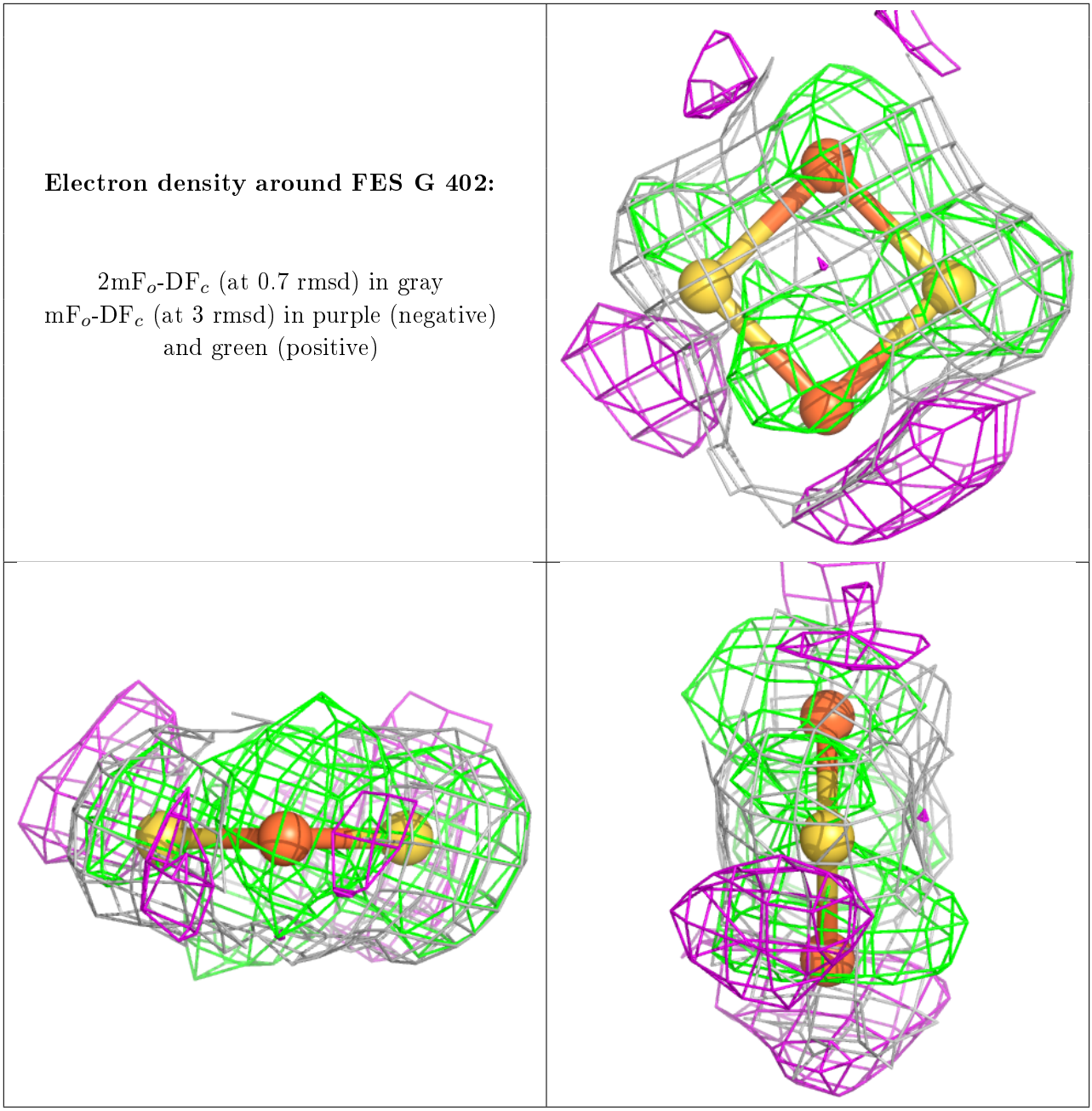
Electron density around FES E 402:

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



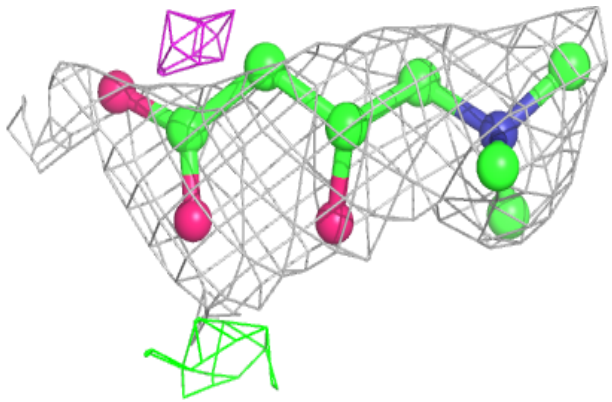
Electron density around FES G 402:

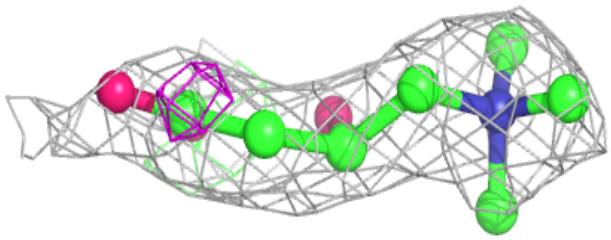
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

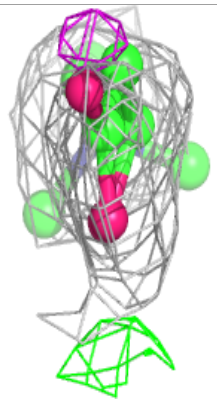


Electron density around 152 B 403:

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

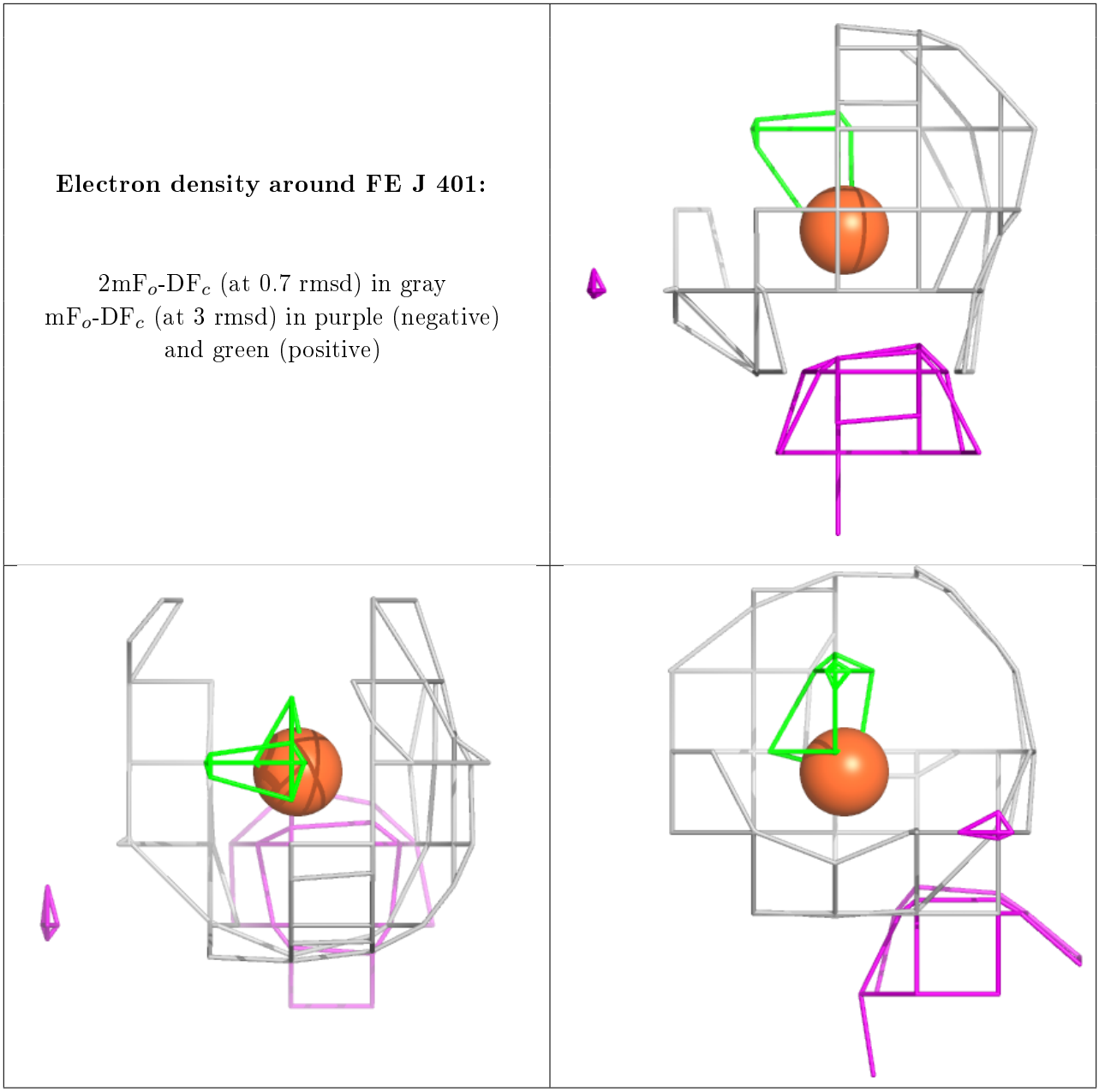






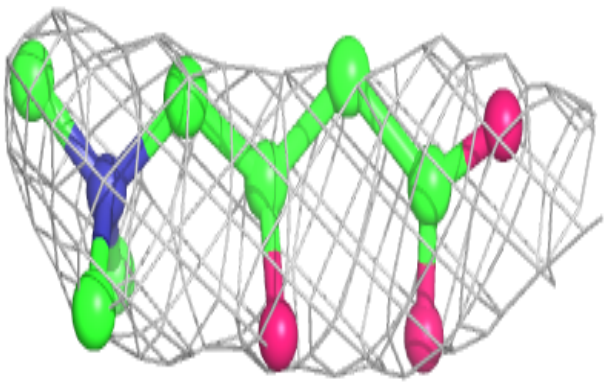
Electron density around FE J 401:

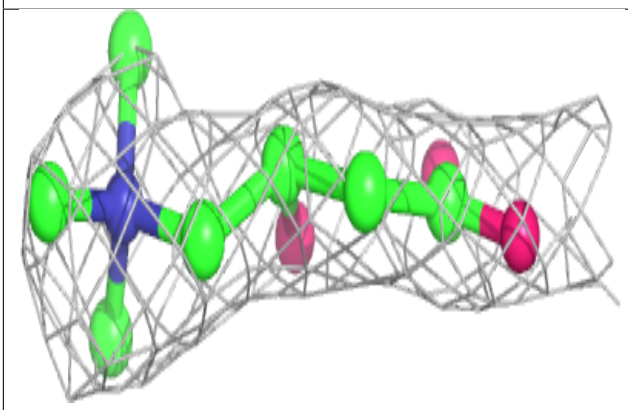
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

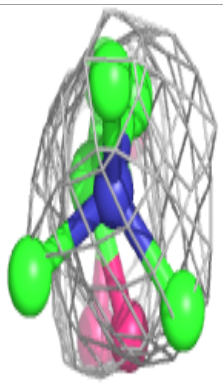


Electron density around 152 J 403:

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

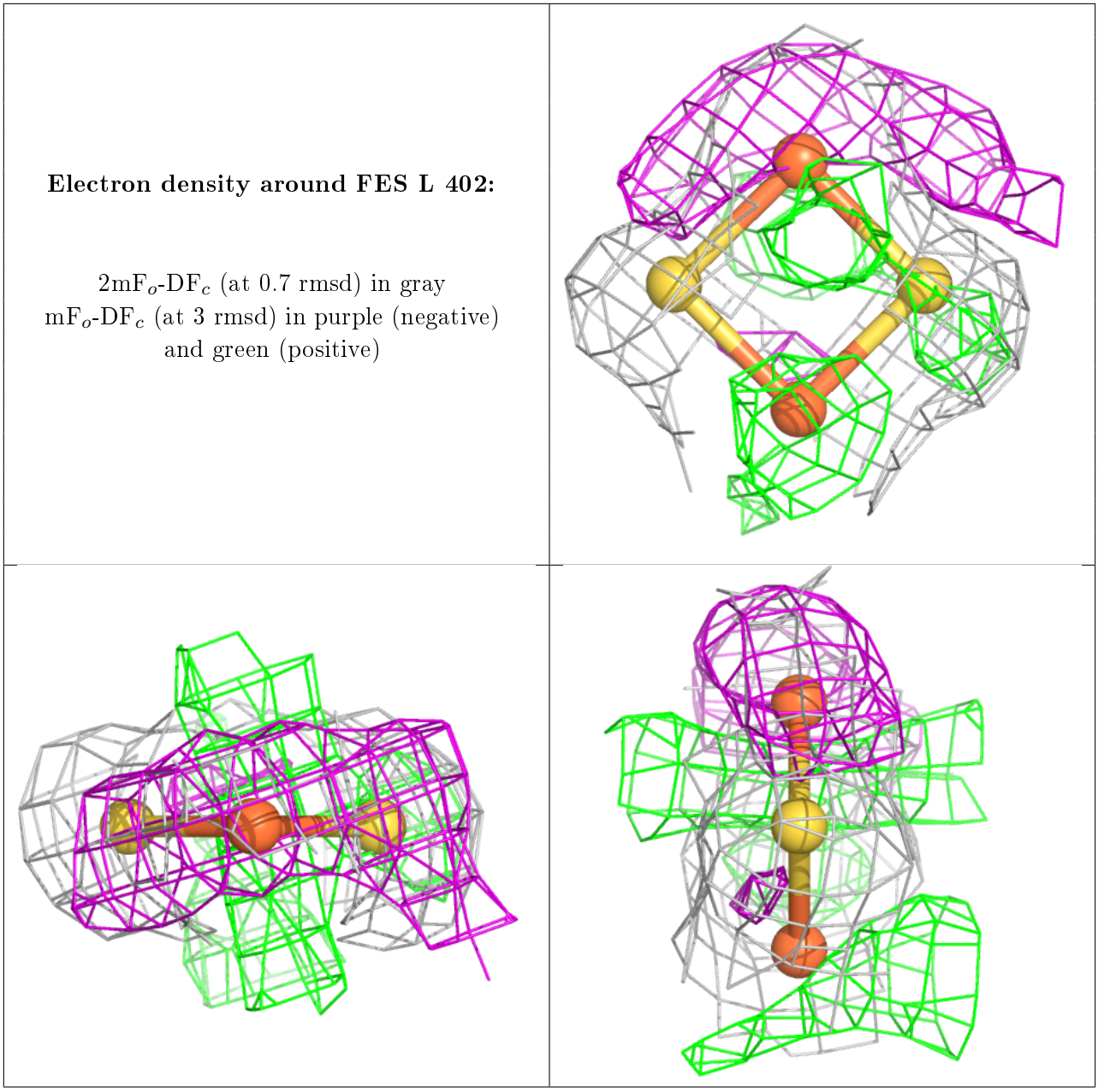






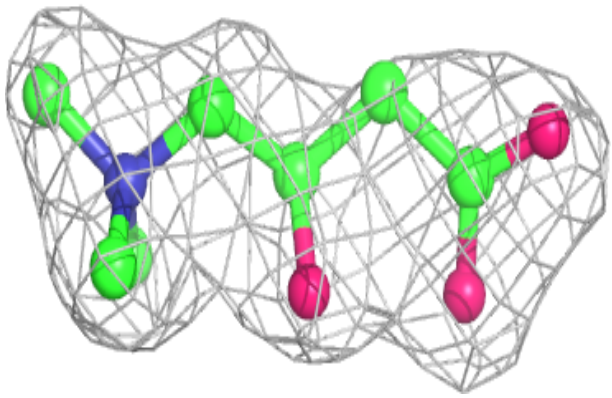
Electron density around FES L 402:

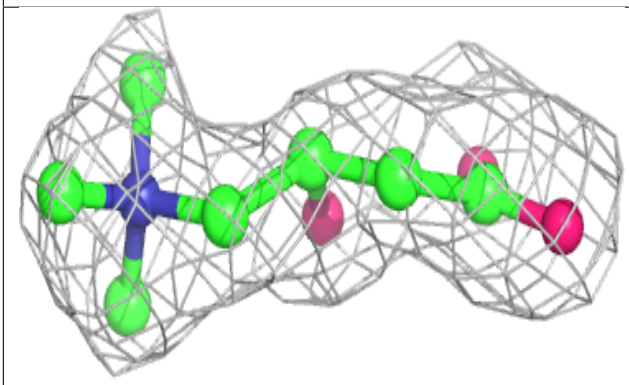
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

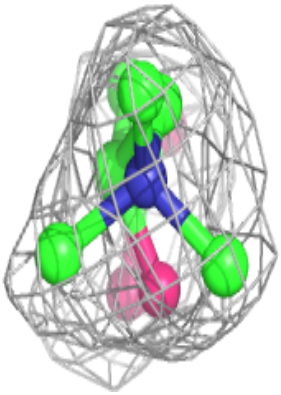


Electron density around 152 D 403:

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

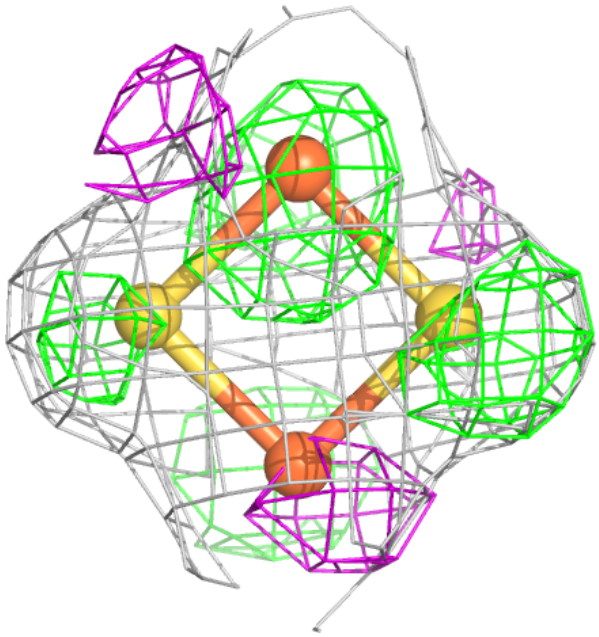


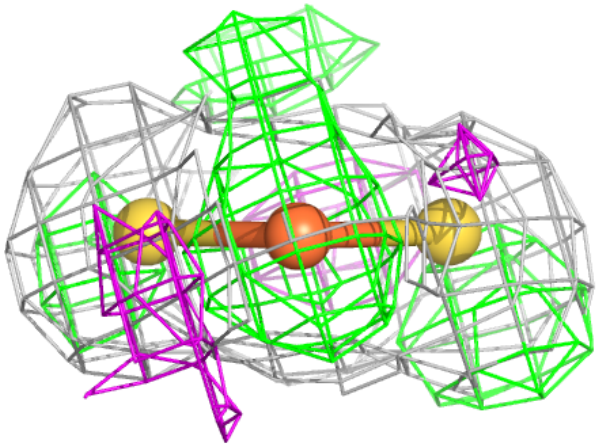


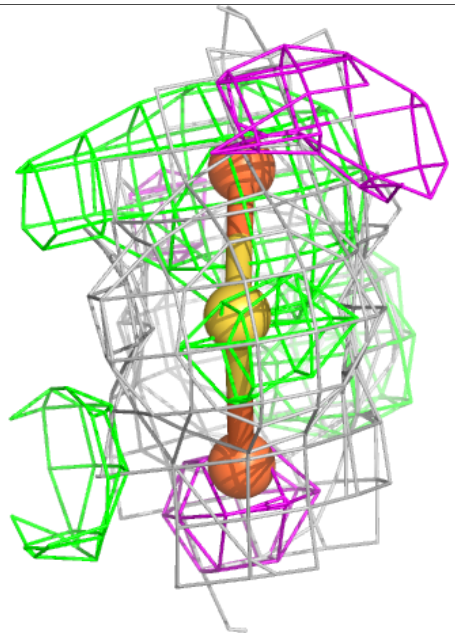


Electron density around FES I 402:

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

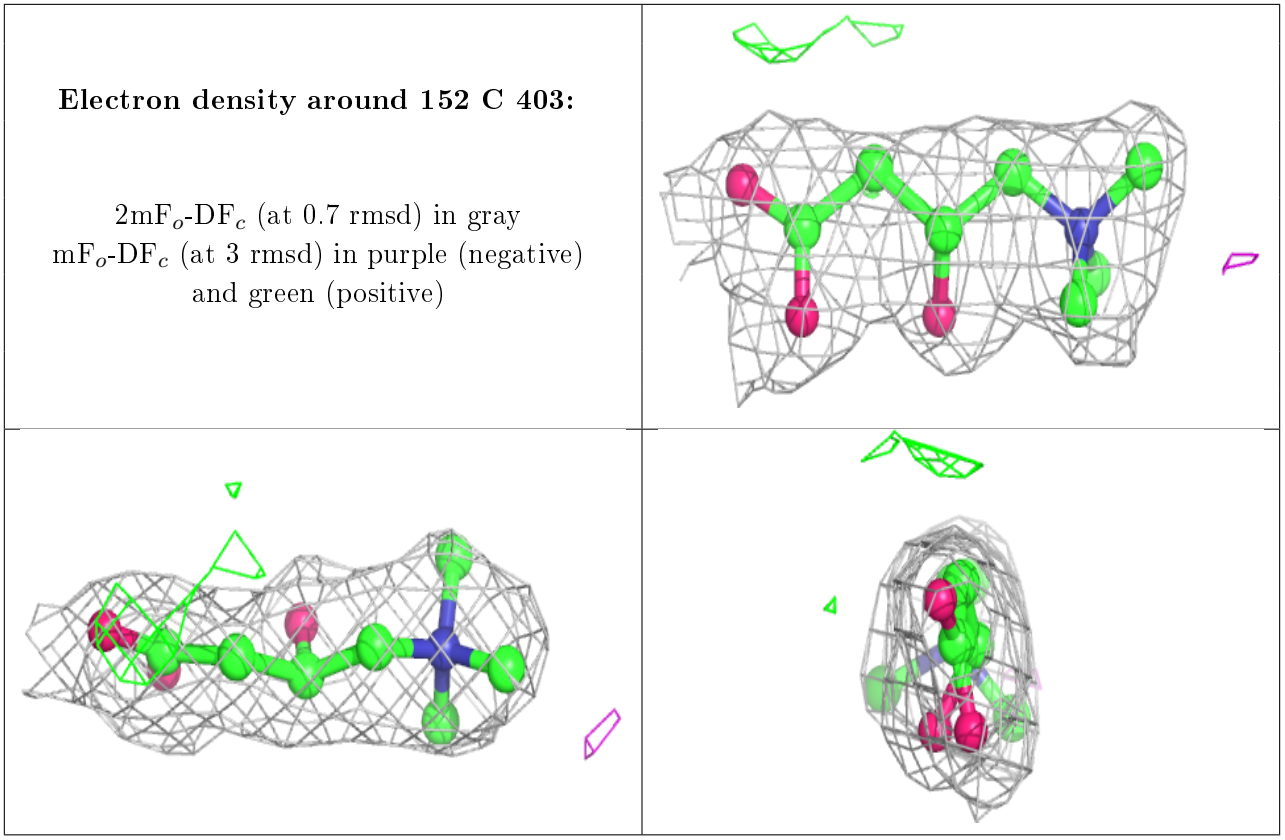






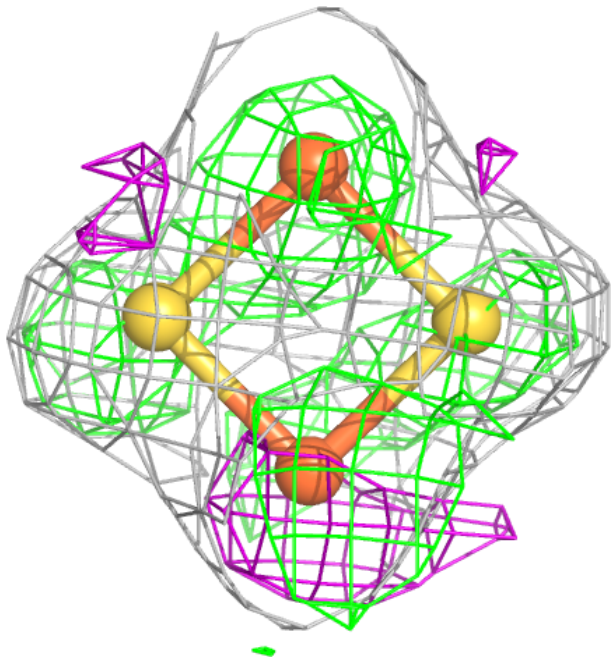
Electron density around 152 C 403:

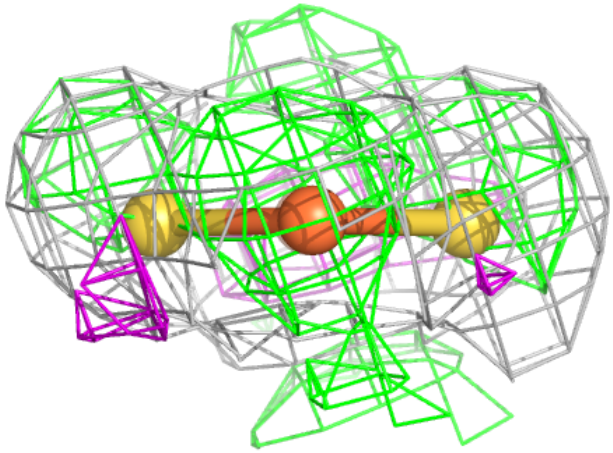
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

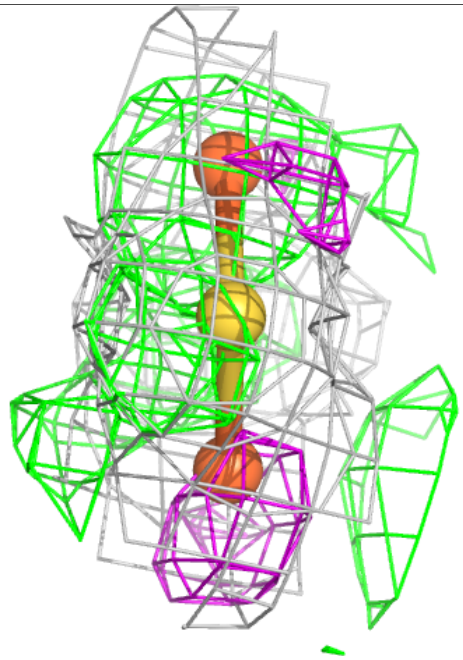


Electron density around FES D 402:

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

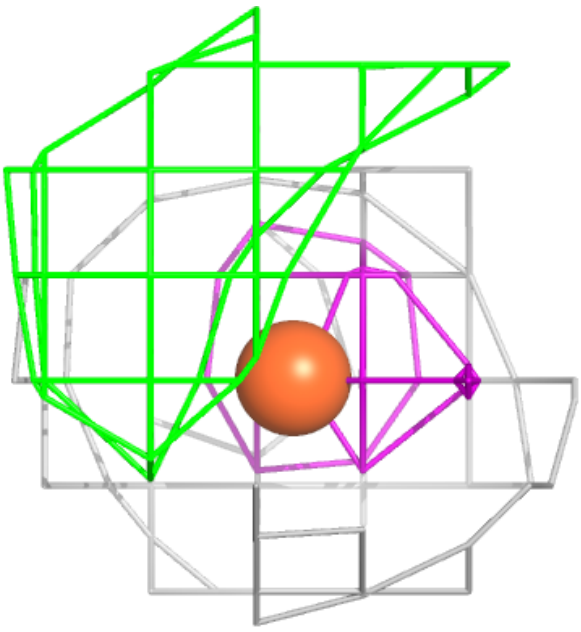


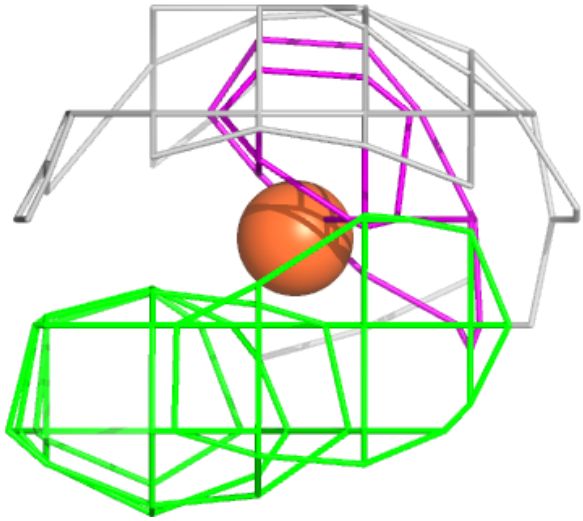


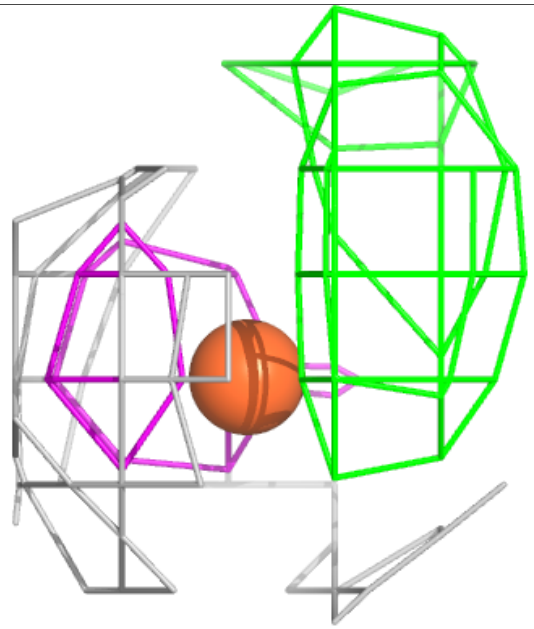


Electron density around FE L 401:

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

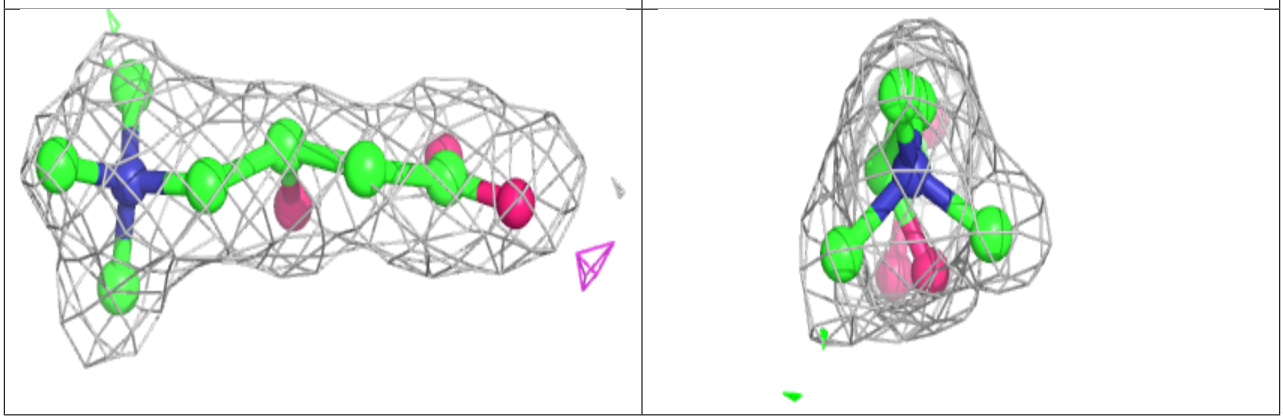






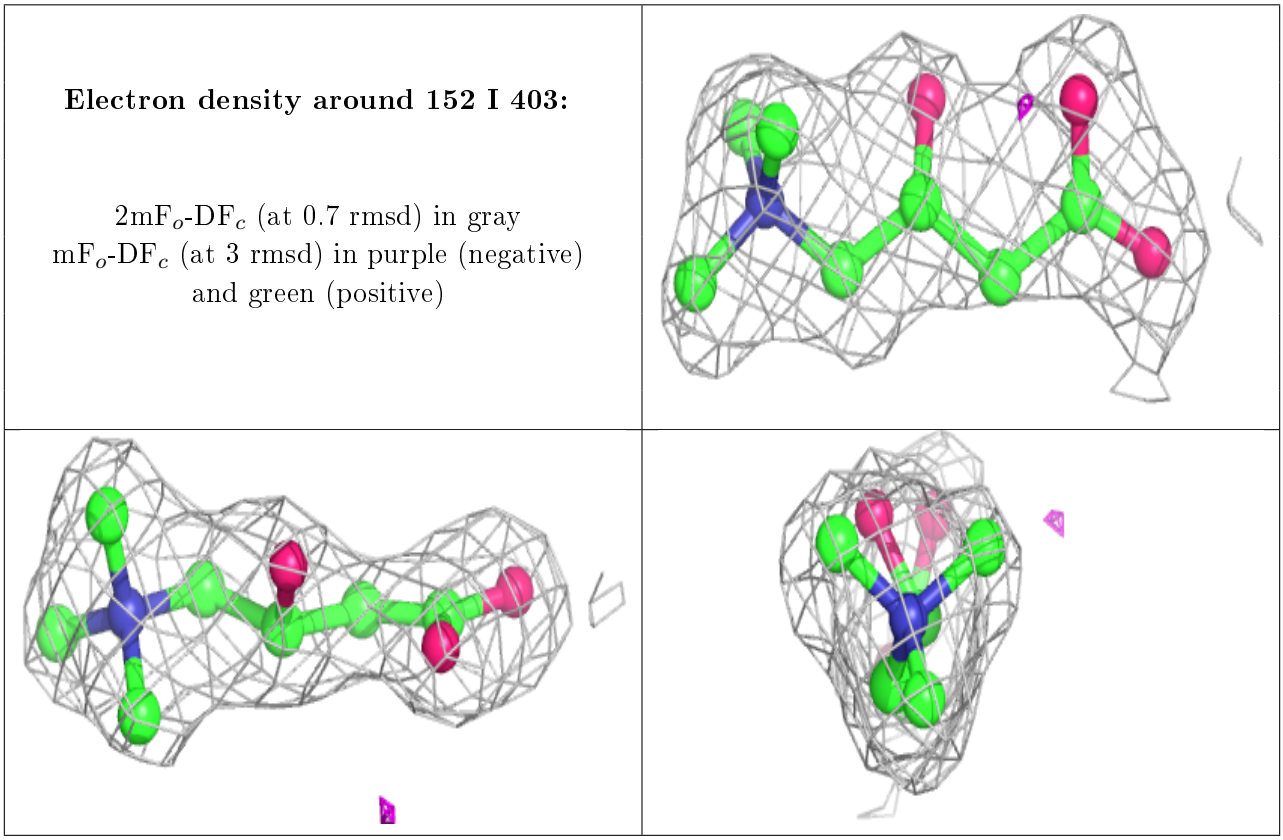
Electron density around 152 H 403:

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



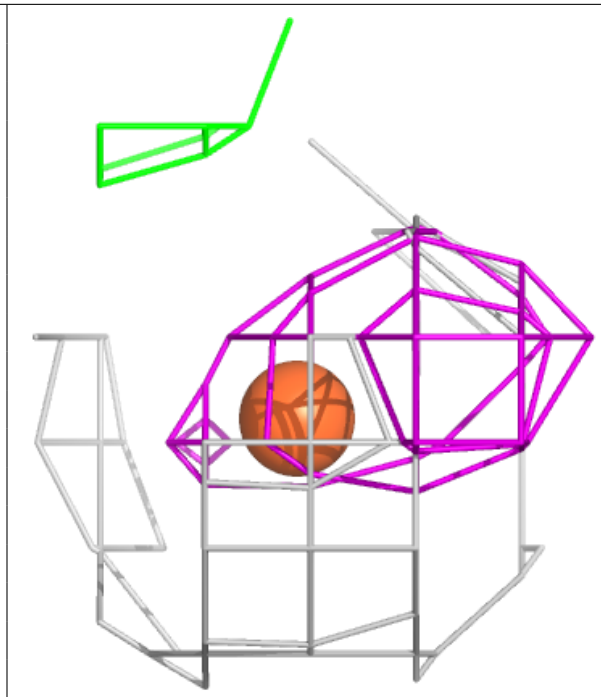
Electron density around 152 I 403:

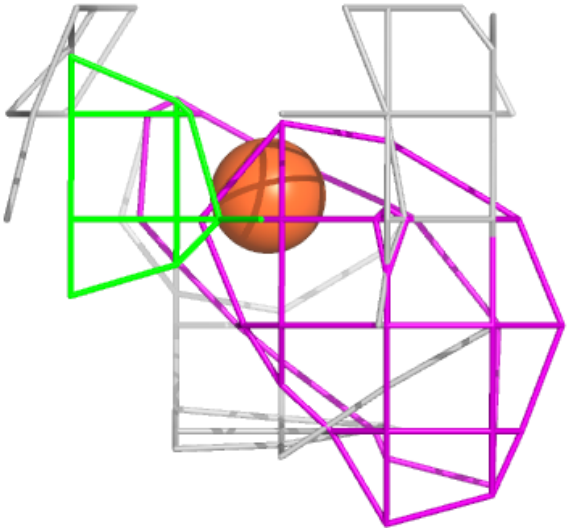
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

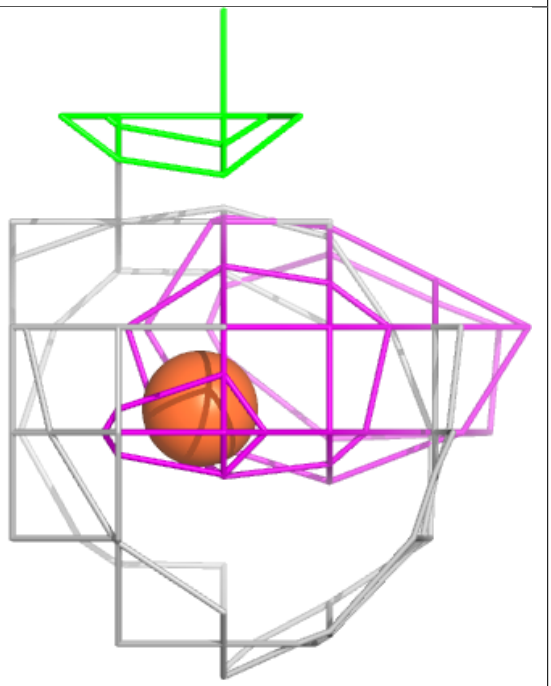


Electron density around FE B 401:

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

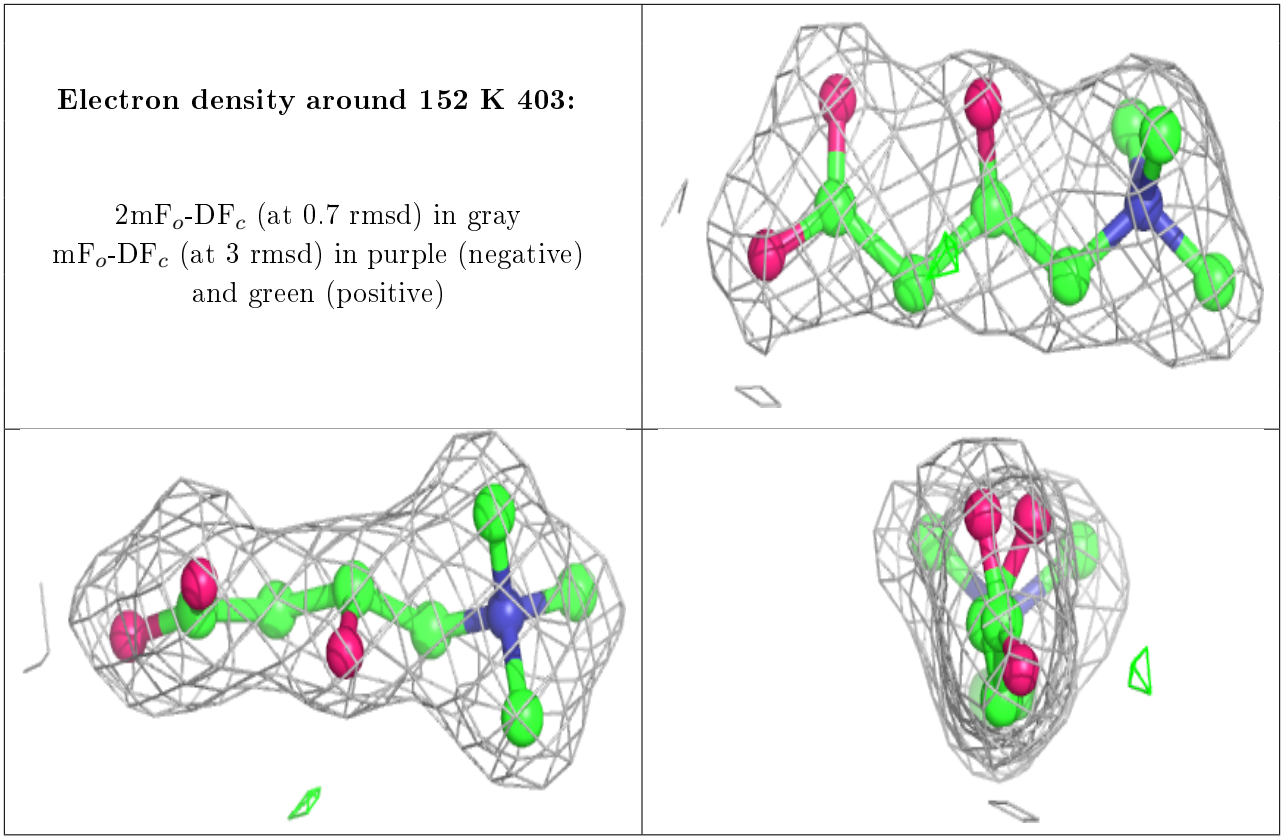






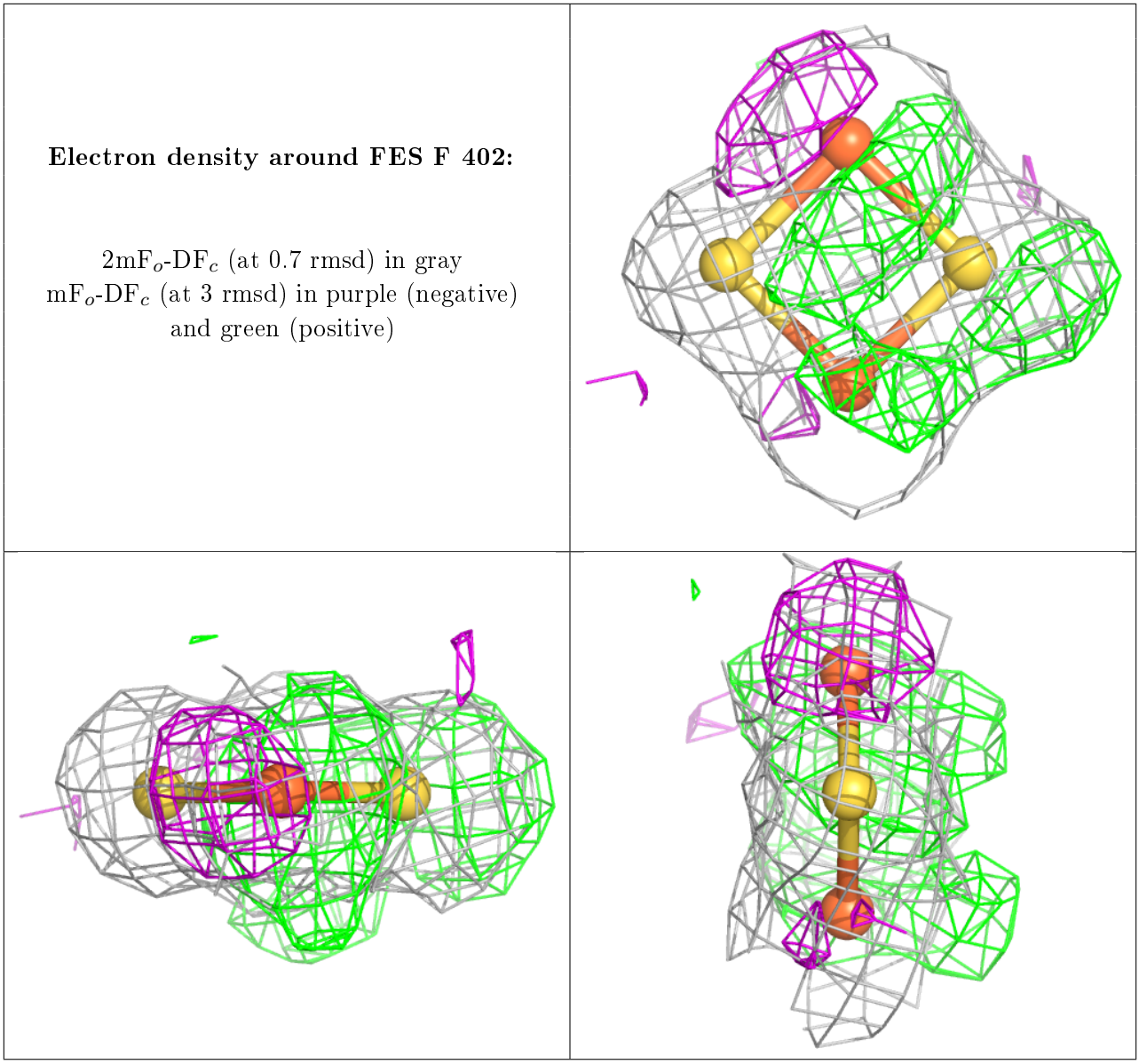
Electron density around 152 K 403:

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



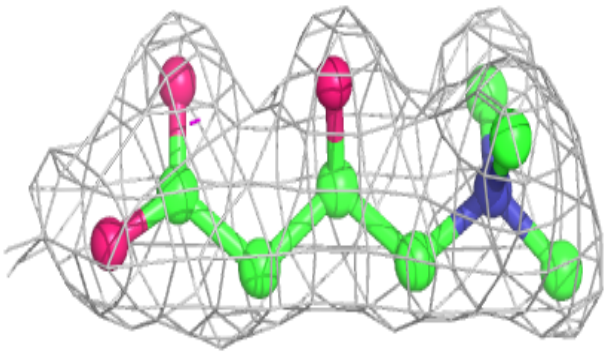
Electron density around FES F 402:

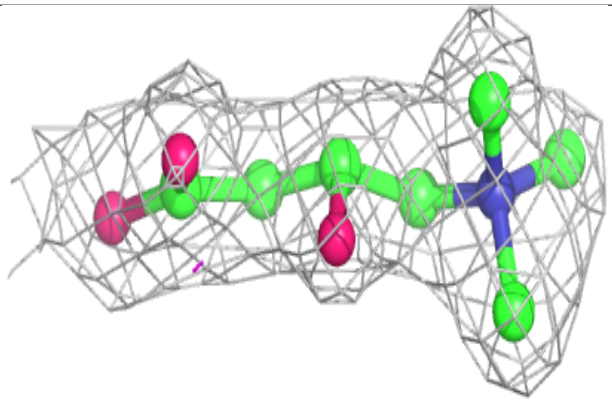
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

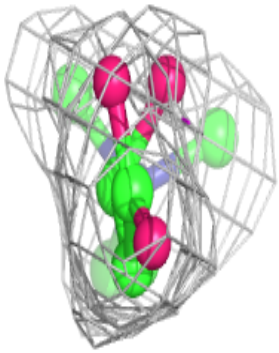


Electron density around 152 G 403:

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

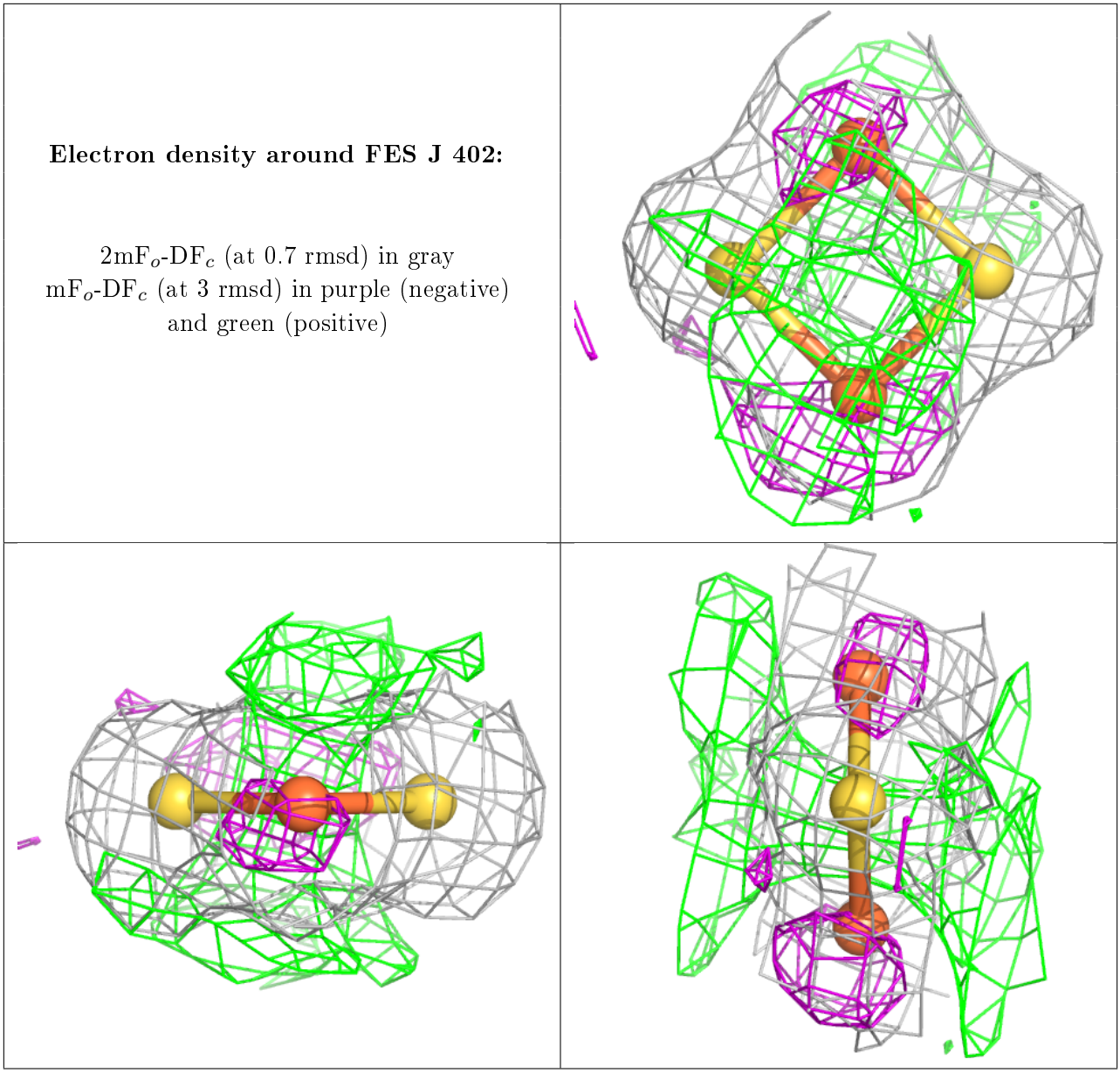






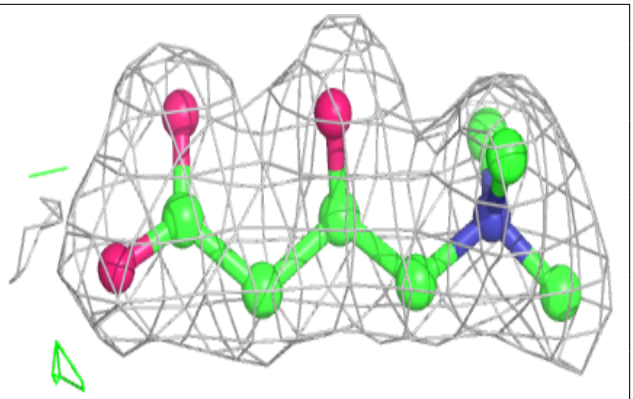
Electron density around FES J 402:

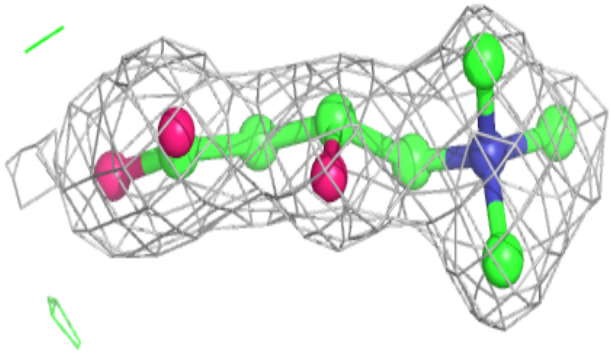
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

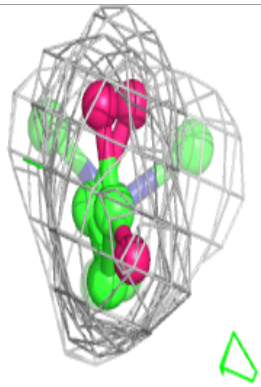


Electron density around 152 E 403:

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

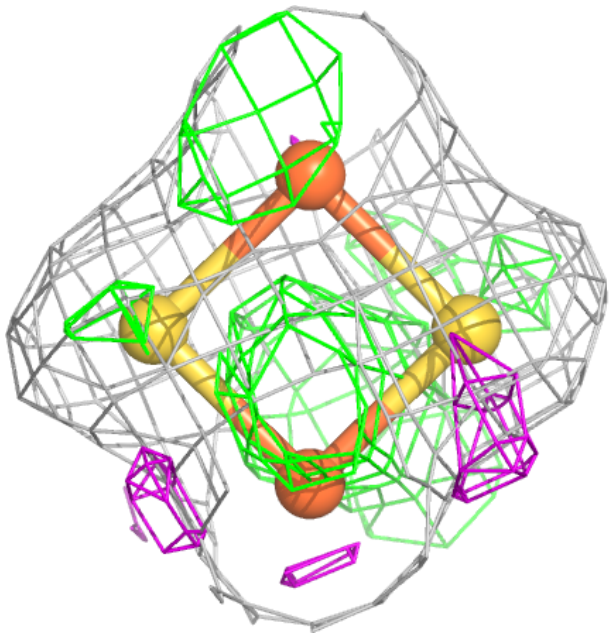


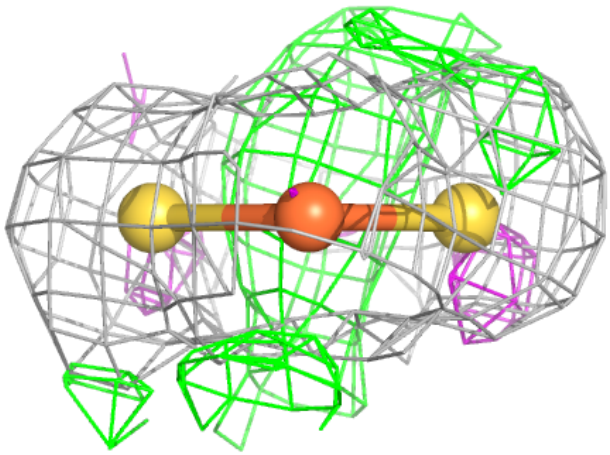


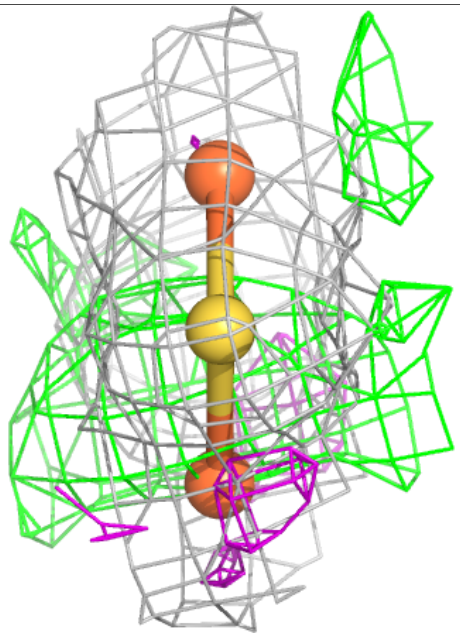


Electron density around FES H 402:

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

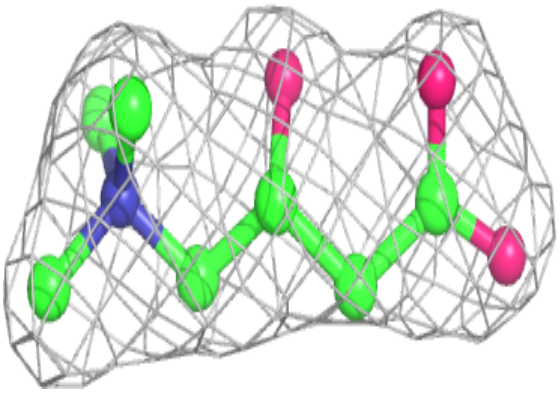


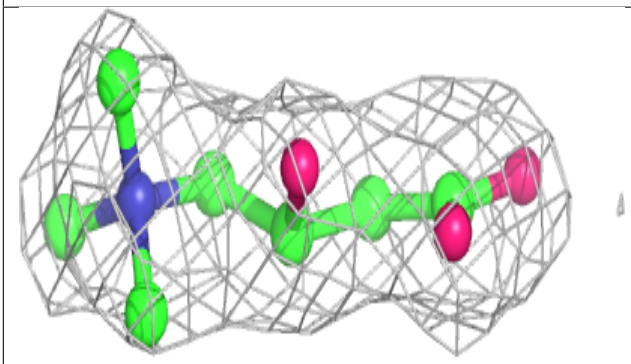


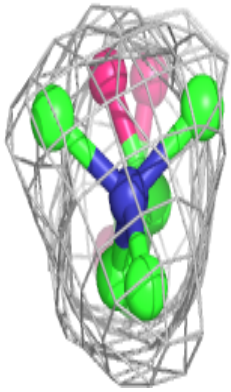


Electron density around 152 A 403:

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

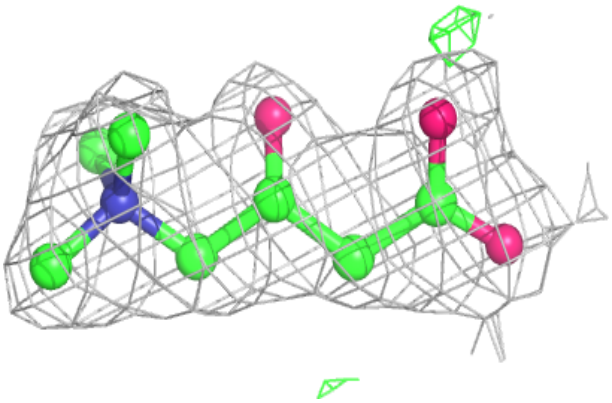


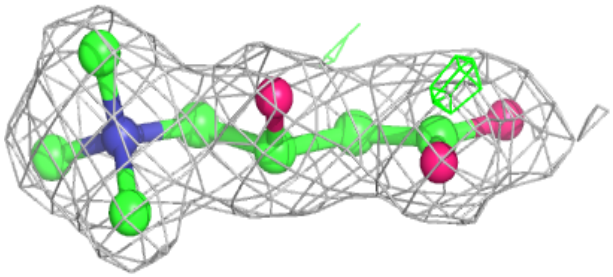


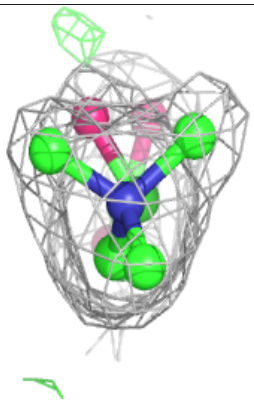


Electron density around 152 F 403:

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

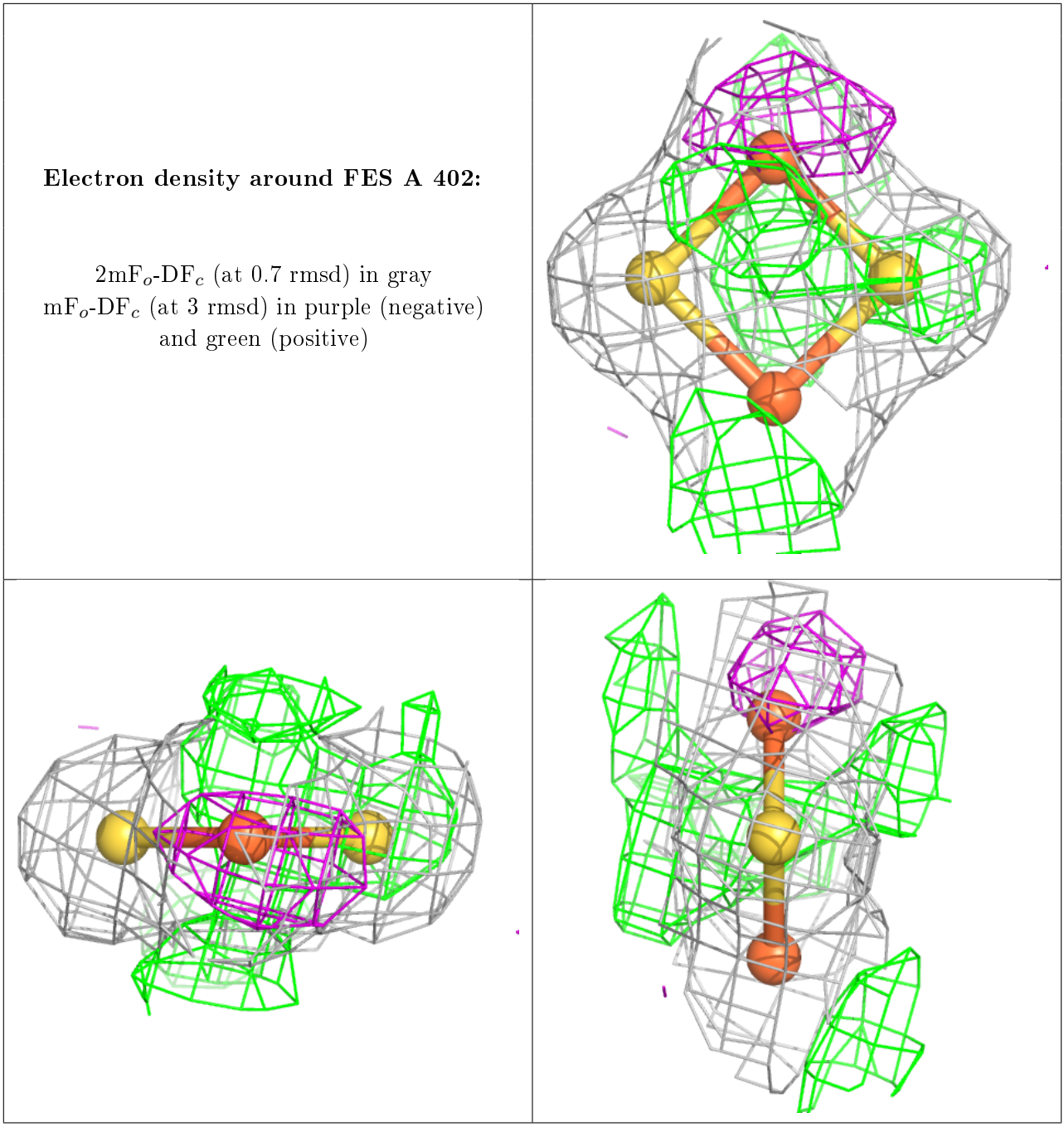






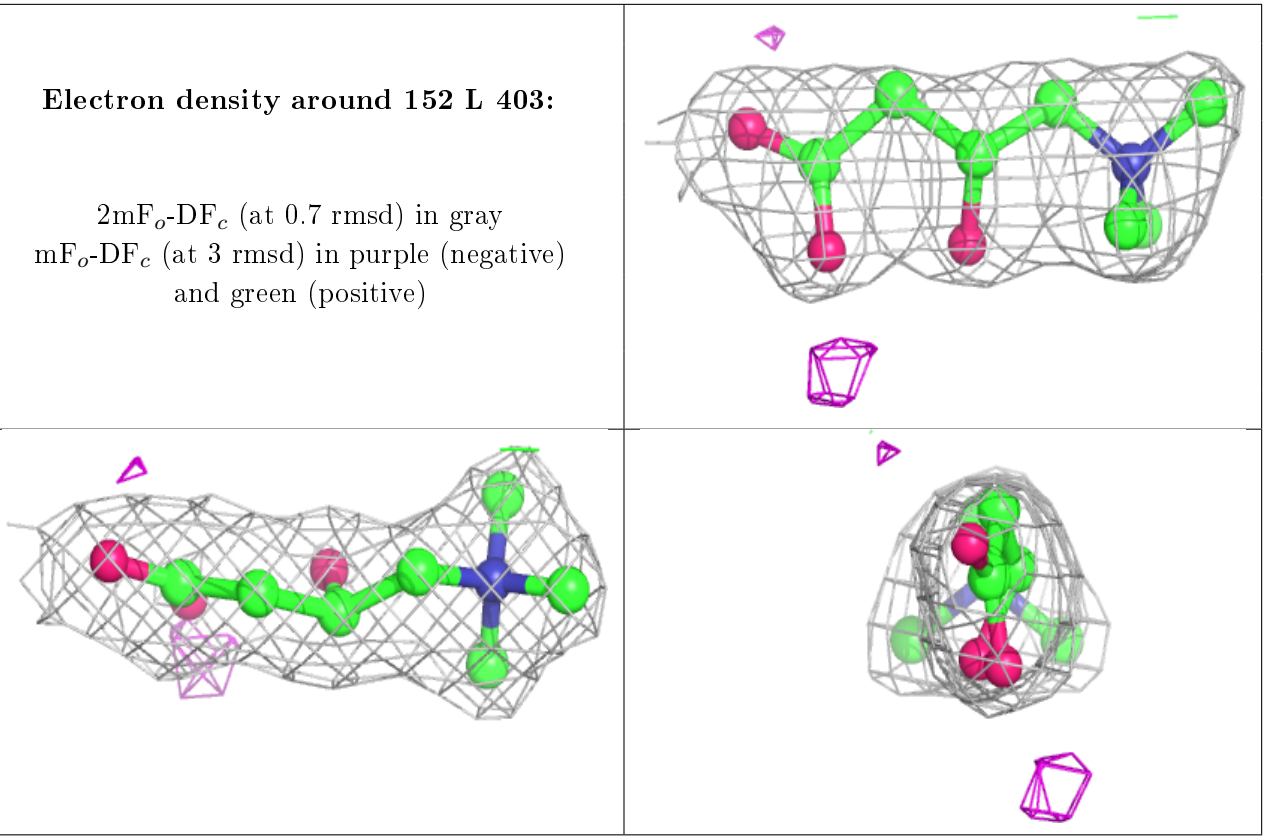
Electron density around FES A 402:

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



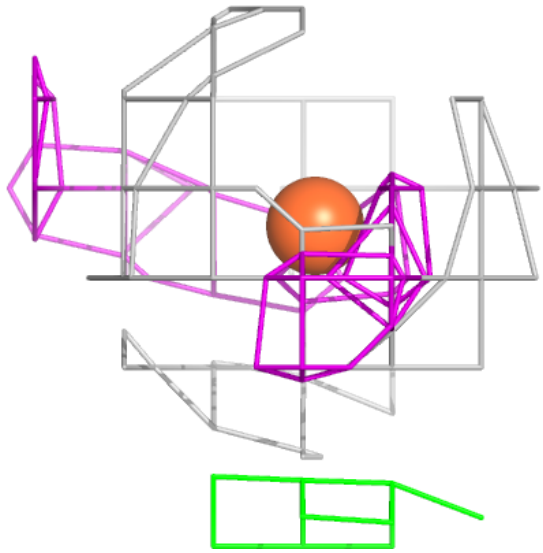
Electron density around 152 L 403:

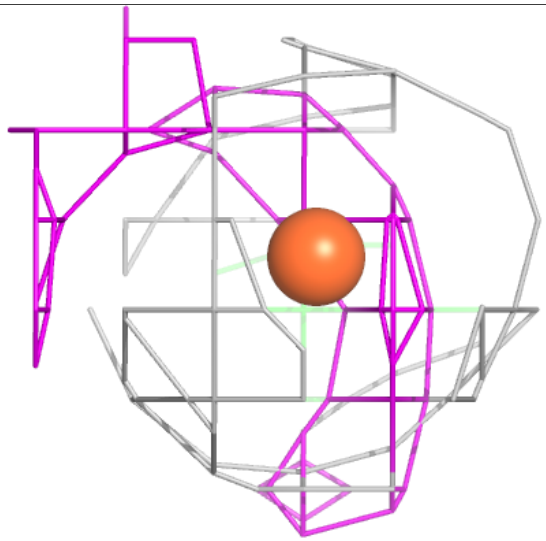
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

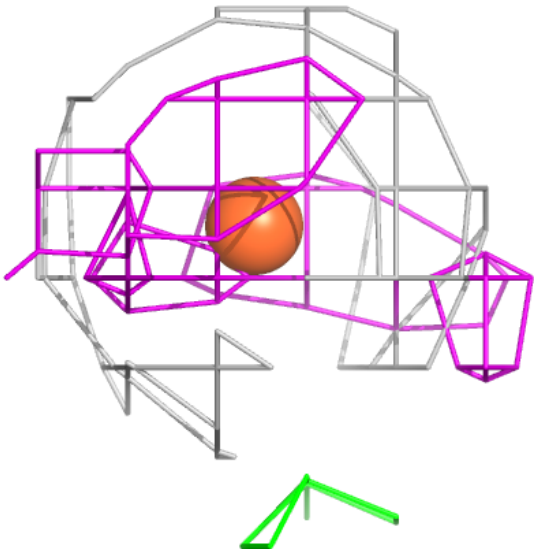


Electron density around FE G 401:

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

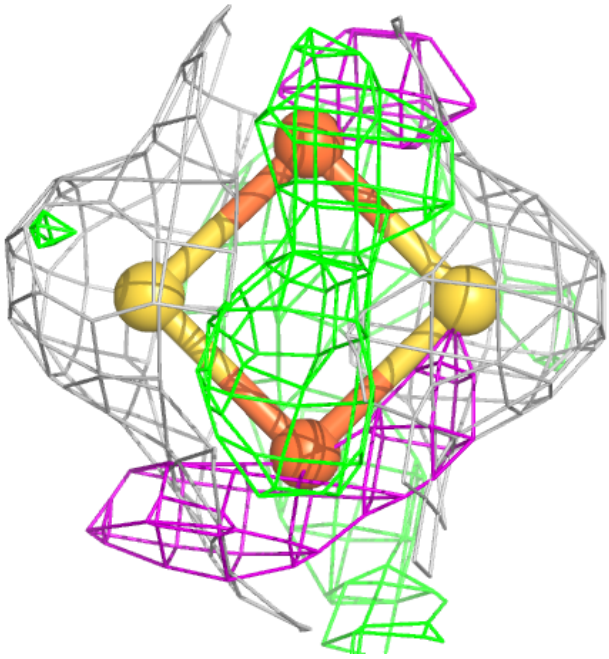


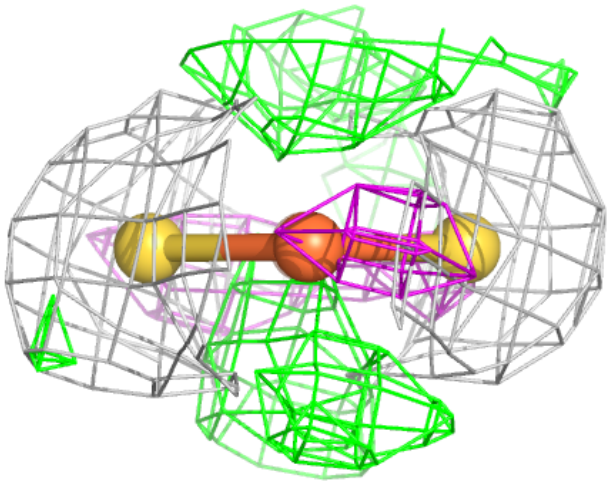


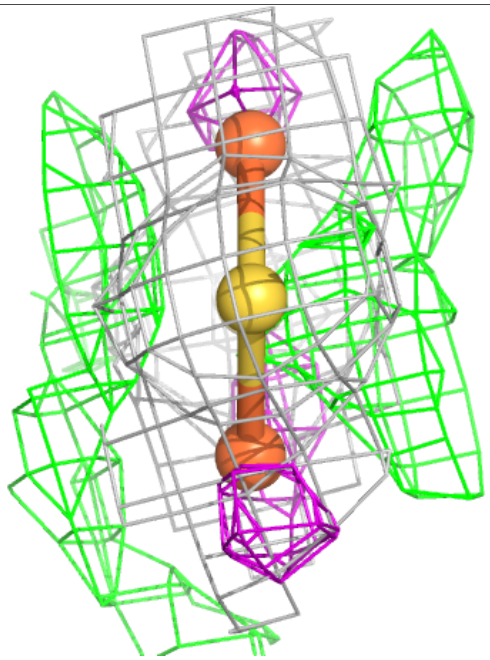


Electron density around FES K 402:

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

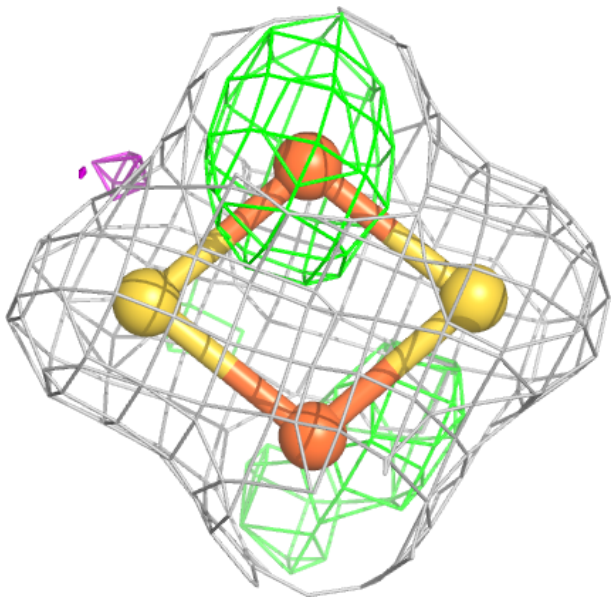


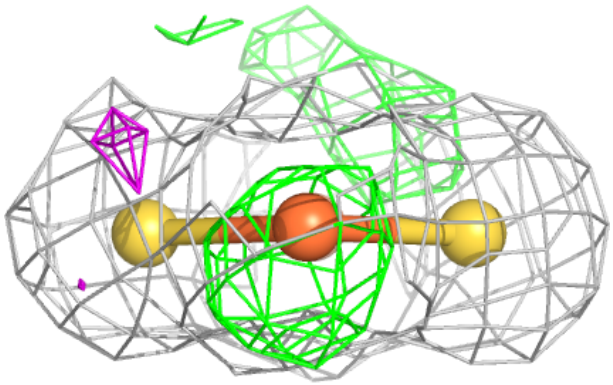


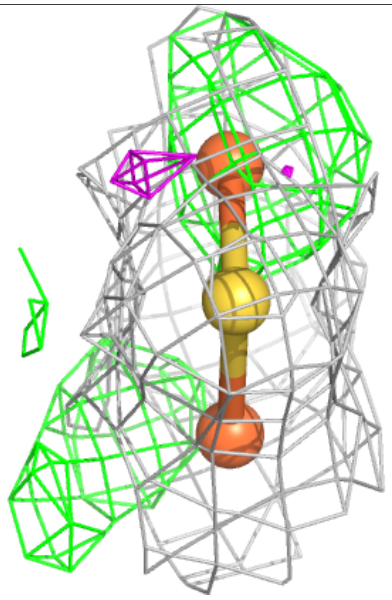


Electron density around FES B 402:

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

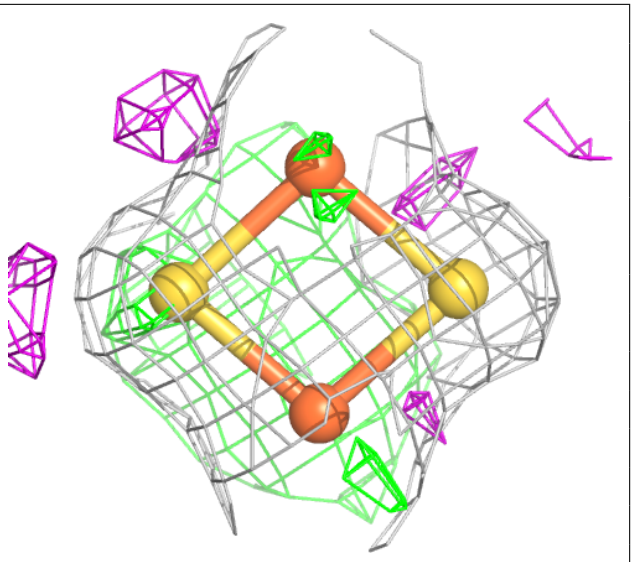


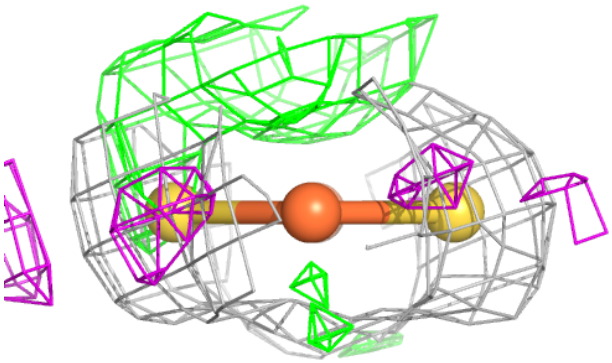


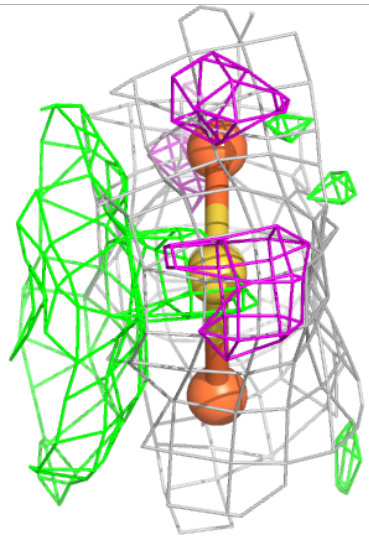


Electron density around FES C 402:

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

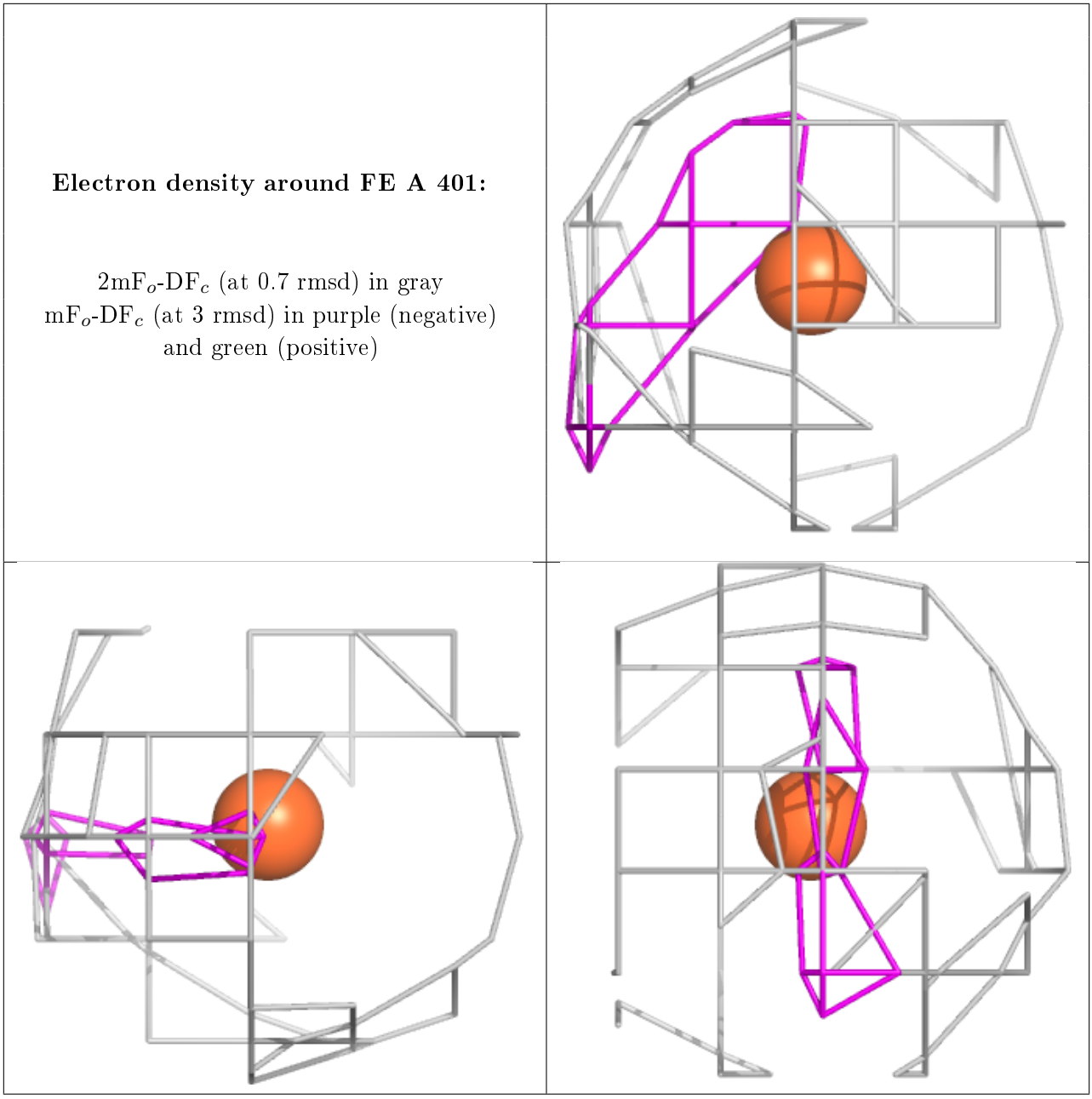






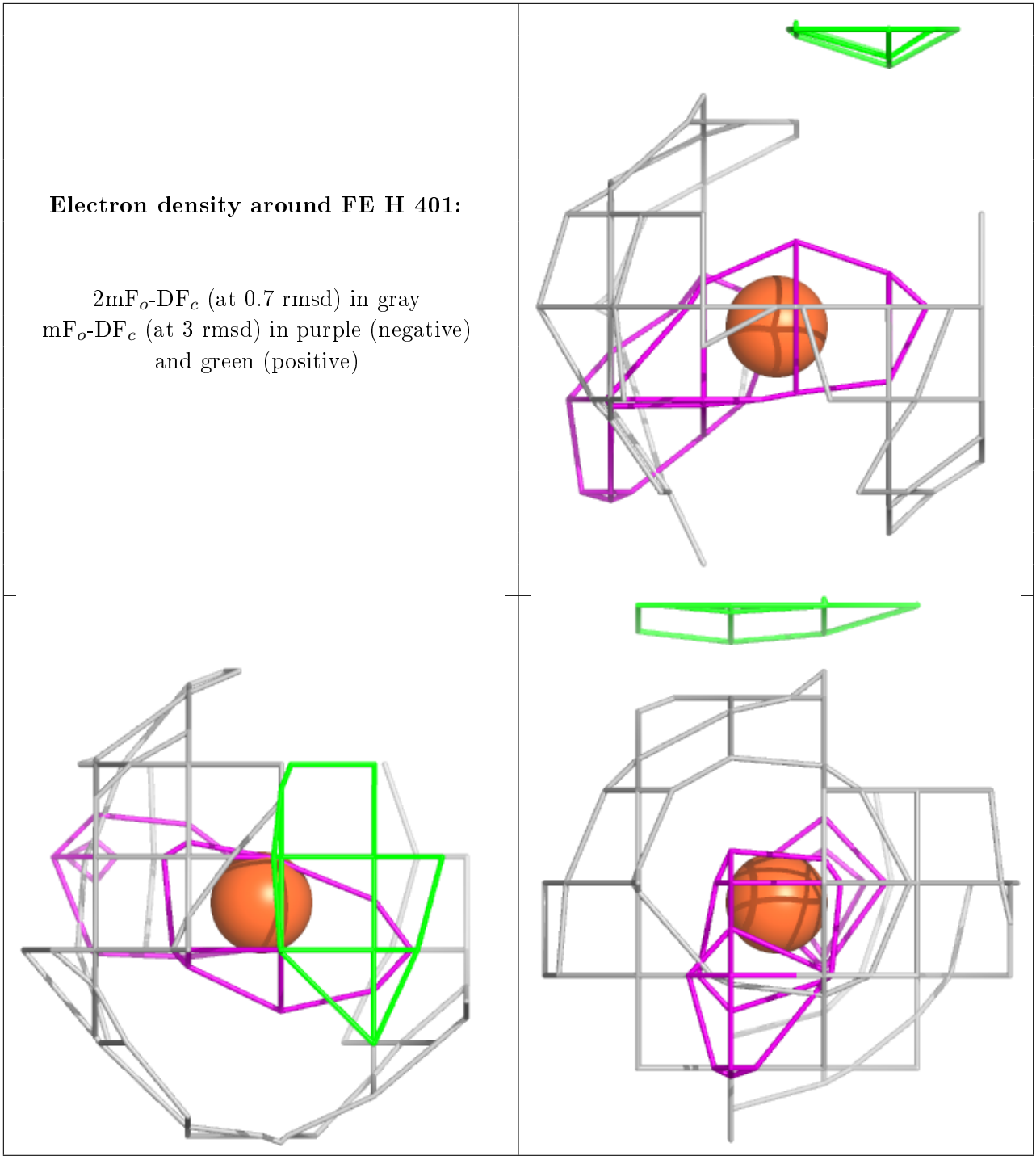
Electron density around FE A 401:

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



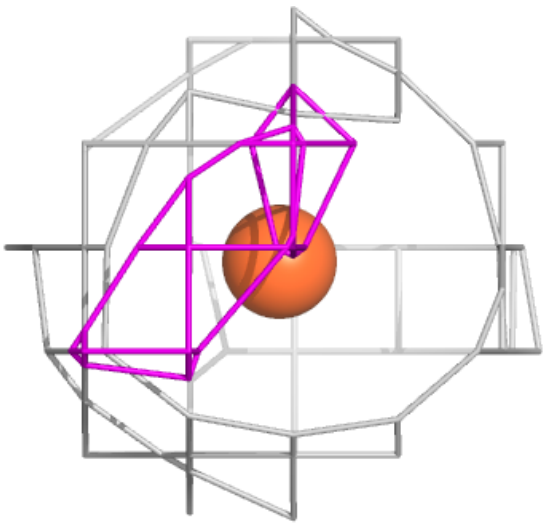
Electron density around FE H 401:

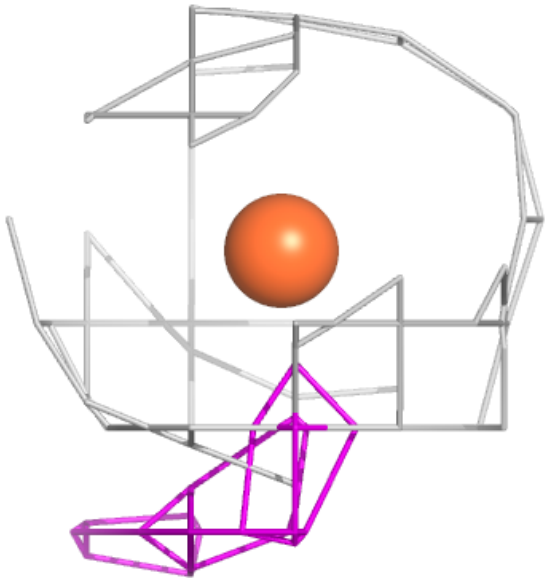
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

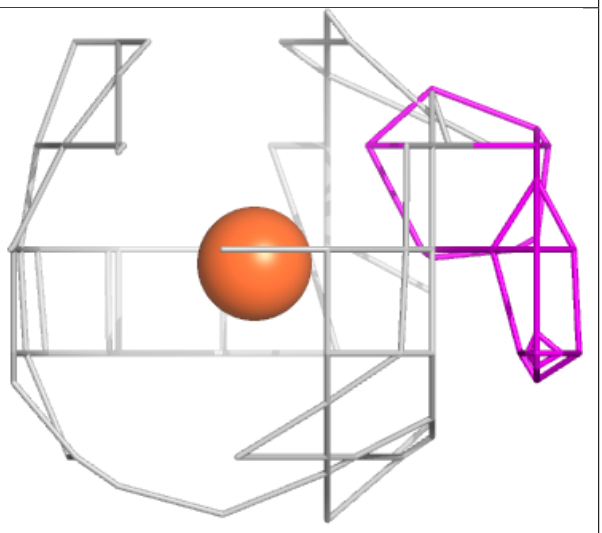


Electron density around FE D 401:

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

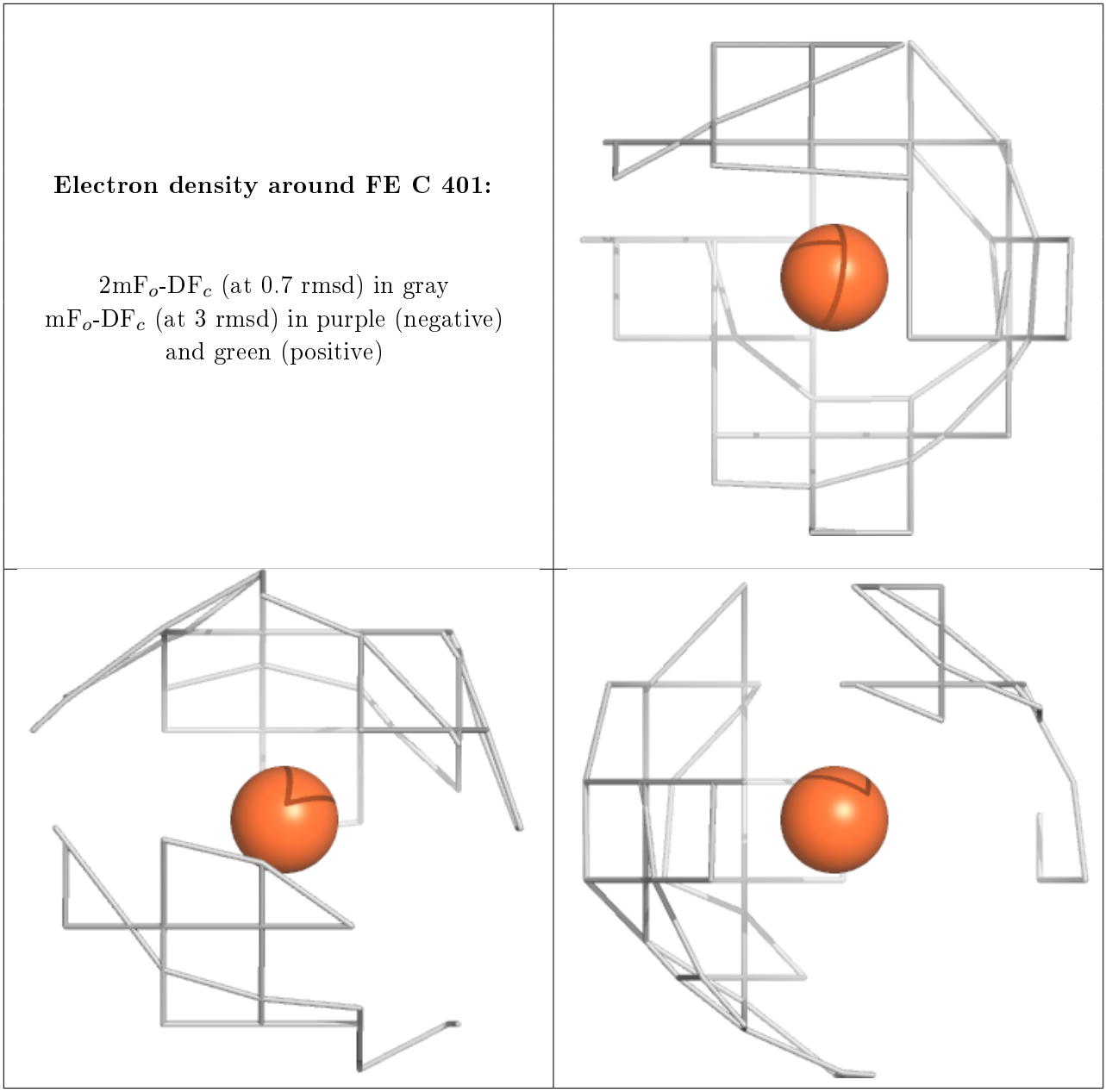






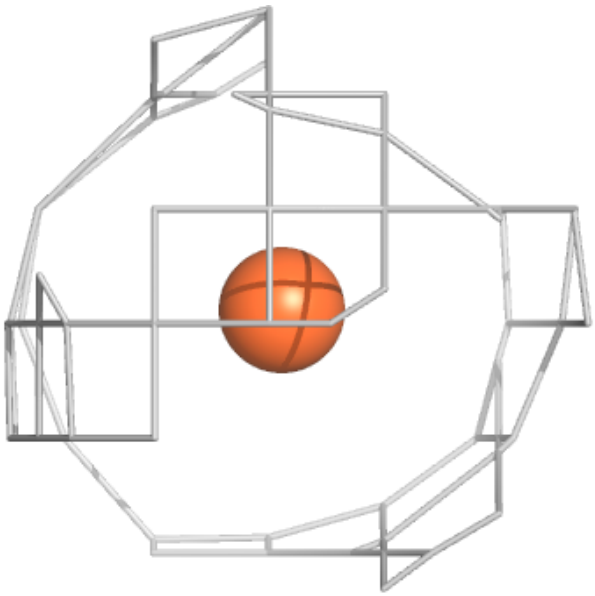
Electron density around FE C 401:

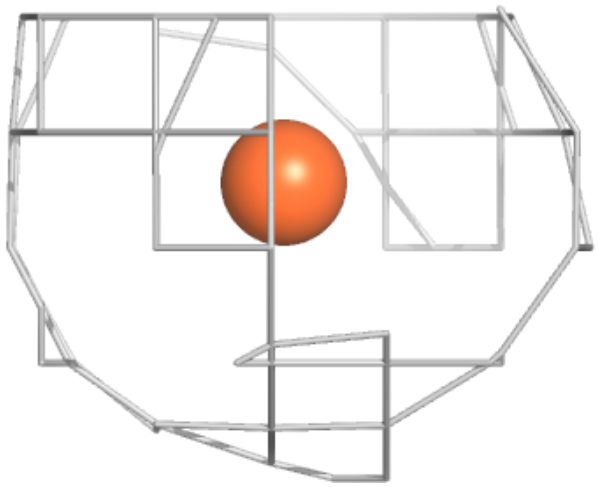
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

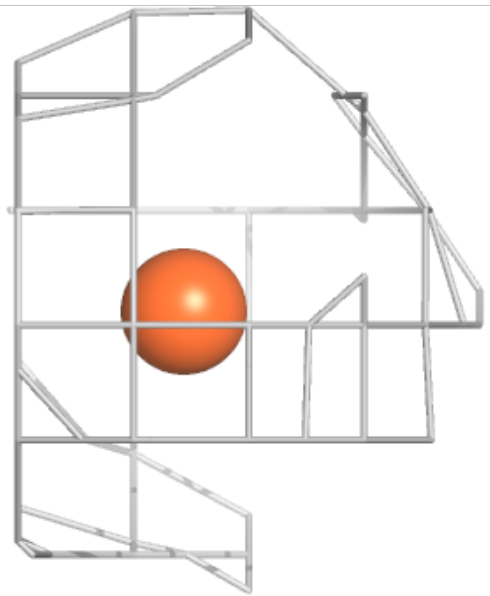


Electron density around FE I 401:

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

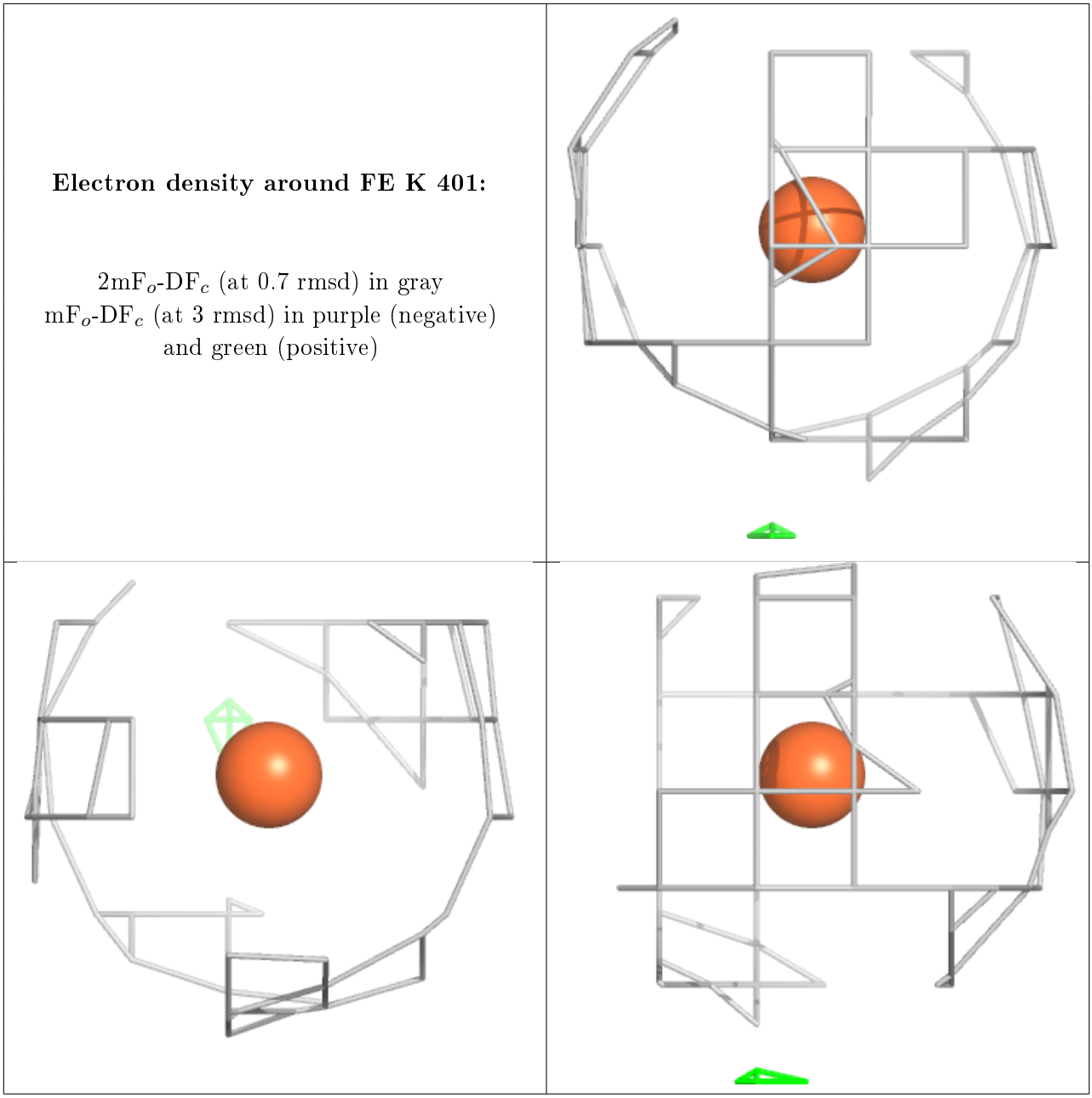






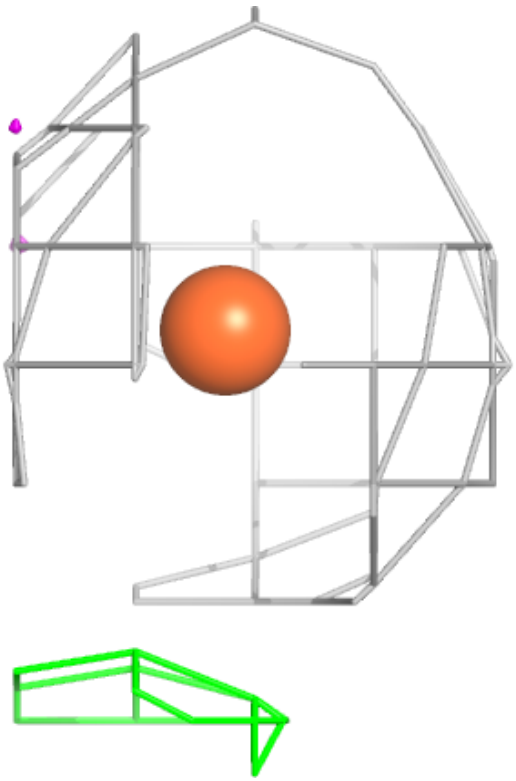
Electron density around FE K 401:

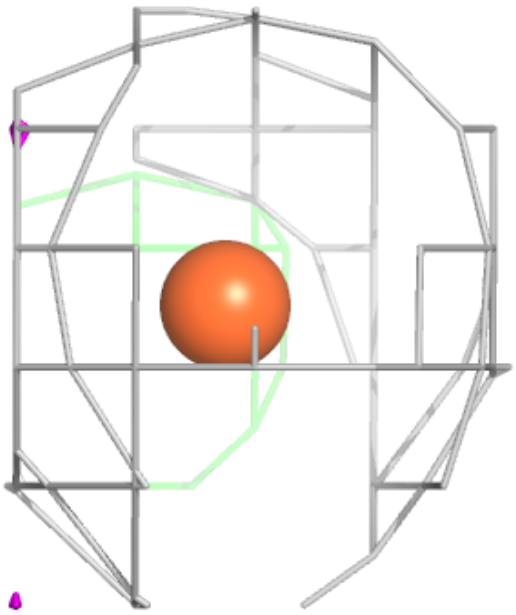
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

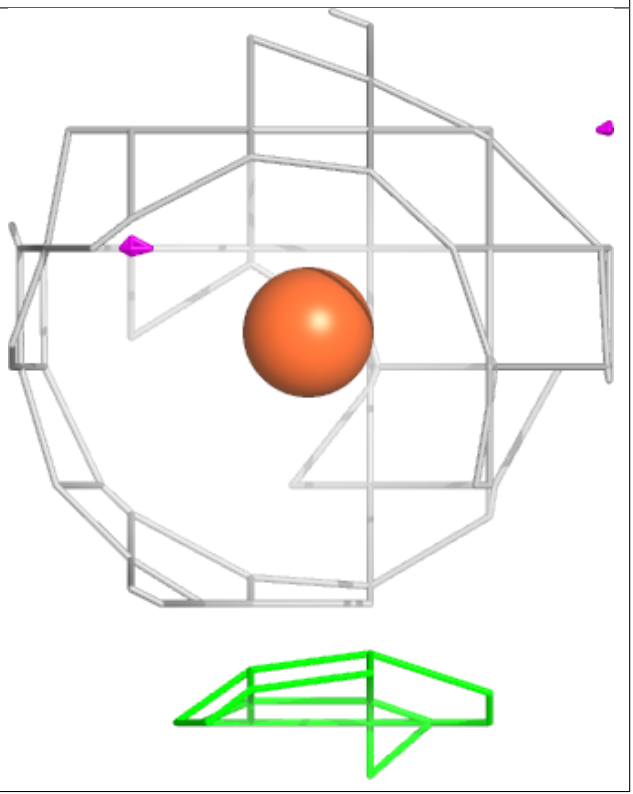


Electron density around FE F 401:

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

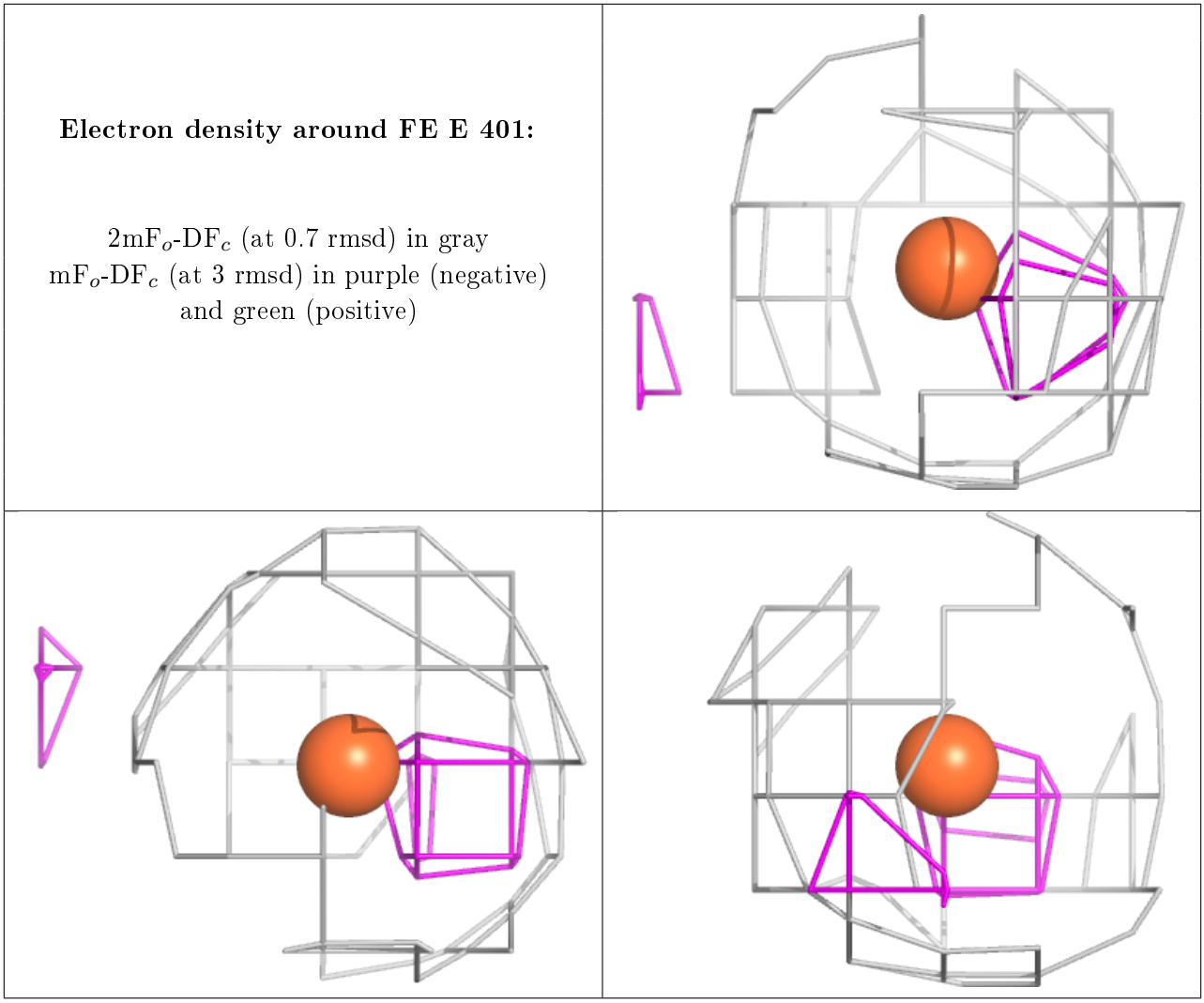






Electron density around FE E 401:

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



6.5 Other polymers

There are no such residues in this entry.