Full wwPDB X-ray Structure Validation Report ⓘ

Apr 3, 2024 – 01:16 pm BST

PDB ID	:	8P9V
Title	:	Crystal Structure of Two-Domain Laccase mutant M199G/R240H/D268N from Streptomyces griseoflavus
Authors	:	Kolyadenko, I.A.; Tishchenko, S.V.; Gabdulkhakov, A.G.
Deposited on	:	2023-06-06
Resolution	:	2.20 Å(reported)

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

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

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

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

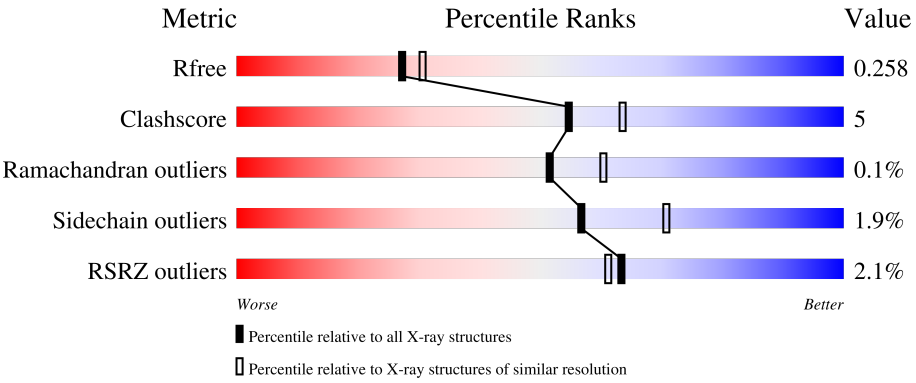
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	278	2% 90% 10%
1	B	278	2% 88% 12%
1	C	278	% 82% 16% ••
1	D	278	2% 78% 21% •
1	E	278	3% 88% 11% •

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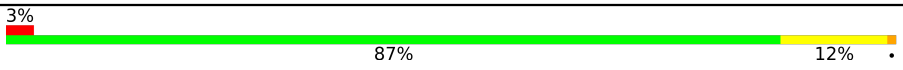
Mol	Chain	Length	Quality of chain
1	F	278	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12923 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Two-domain laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	2	3	0
			2146	1337	392	405	12			
1	B	277	Total	C	N	O	S	1	2	0
			2130	1329	389	400	12			
1	C	275	Total	C	N	O	S	0	2	0
			2115	1320	387	396	12			
1	D	277	Total	C	N	O	S	2	3	0
			2140	1334	391	402	13			
1	E	275	Total	C	N	O	S	1	1	0
			2111	1316	387	396	12			
1	F	277	Total	C	N	O	S	3	0	0
			2120	1322	388	399	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
A	240	HIS	ARG	engineered mutation	UNP A0A0M4FJ81
A	268	ASN	ASP	engineered mutation	UNP A0A0M4FJ81
B	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
B	240	HIS	ARG	engineered mutation	UNP A0A0M4FJ81
B	268	ASN	ASP	engineered mutation	UNP A0A0M4FJ81
C	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
C	240	HIS	ARG	engineered mutation	UNP A0A0M4FJ81
C	268	ASN	ASP	engineered mutation	UNP A0A0M4FJ81
D	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
D	240	HIS	ARG	engineered mutation	UNP A0A0M4FJ81
D	268	ASN	ASP	engineered mutation	UNP A0A0M4FJ81
E	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
E	240	HIS	ARG	engineered mutation	UNP A0A0M4FJ81
E	268	ASN	ASP	engineered mutation	UNP A0A0M4FJ81
F	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
F	240	HIS	ARG	engineered mutation	UNP A0A0M4FJ81

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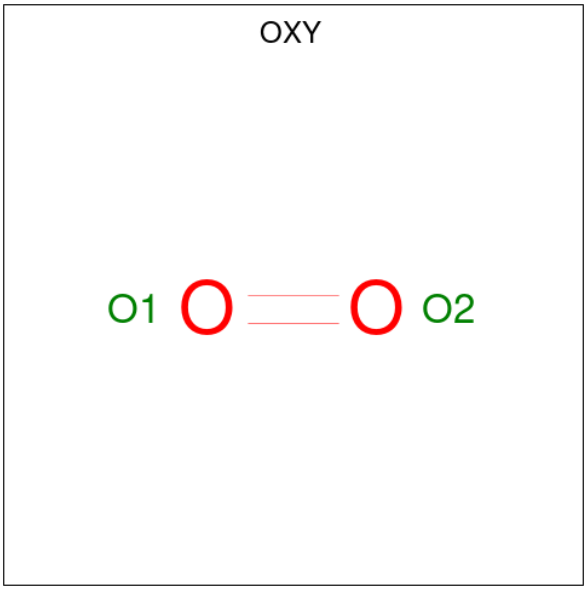
Chain	Residue	Modelled	Actual	Comment	Reference
F	268	ASN	ASP	engineered mutation	UNP A0A0M4FJ81

- Molecule 2 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 2 2	0	0
2	A	1	Total O 2 2	0	0
2	F	1	Total O 2 2	0	0
2	F	1	Total O 2 2	0	0

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Cu 4 4	0	0
3	B	5	Total Cu 5 5	0	0
3	C	3	Total Cu 3 3	0	0
3	D	5	Total Cu 5 5	0	0

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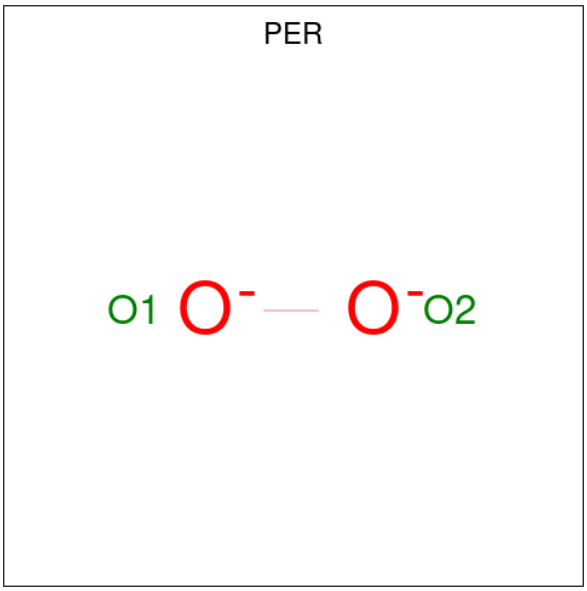
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	3	Total Cu 3 3	0	0
3	F	4	Total Cu 4 4	0	0

- Molecule 4 is PEROXIDE ION (three-letter code: PER) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O 2 2	0	0

- Molecule 5 is water.

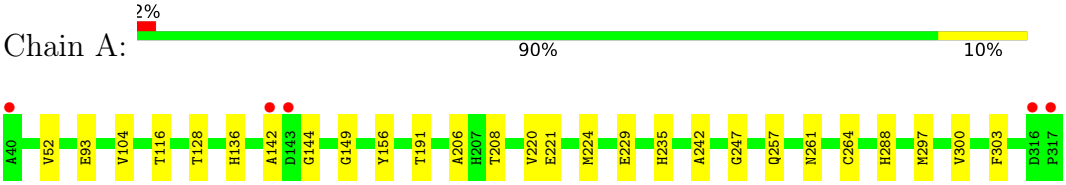
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	21	Total O 21 21	0	0
5	B	26	Total O 26 26	0	0
5	C	18	Total O 18 18	0	0
5	D	11	Total O 11 11	0	0
5	E	28	Total O 28 28	0	0
5	F	23	Total O 23 23	0	0

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.

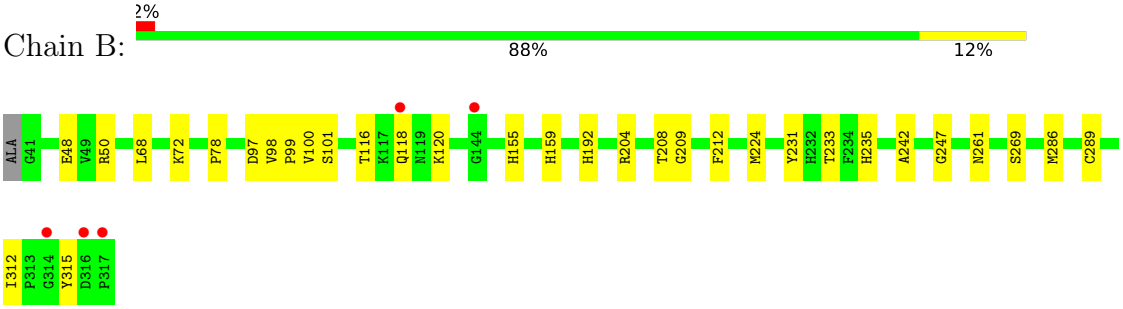
• Molecule 1: Two-domain laccase

Chain A:



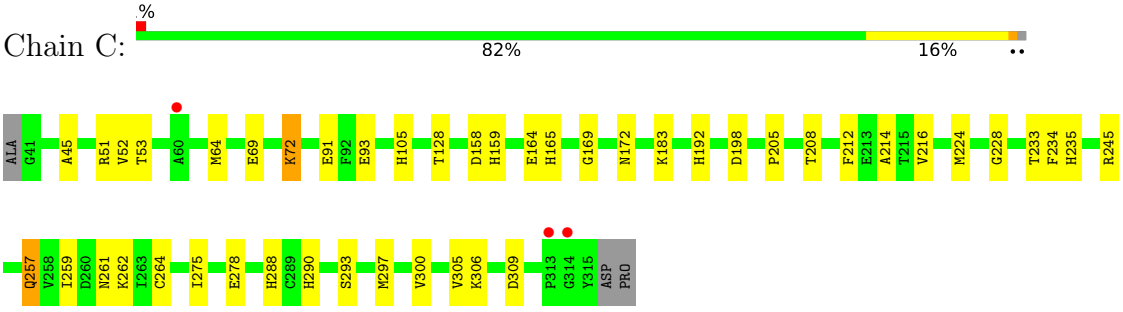
• Molecule 1: Two-domain laccase

Chain B:



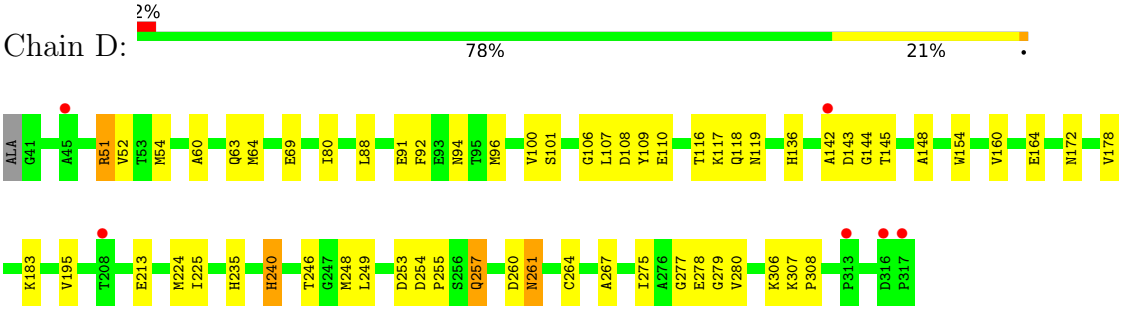
• Molecule 1: Two-domain laccase

Chain C:



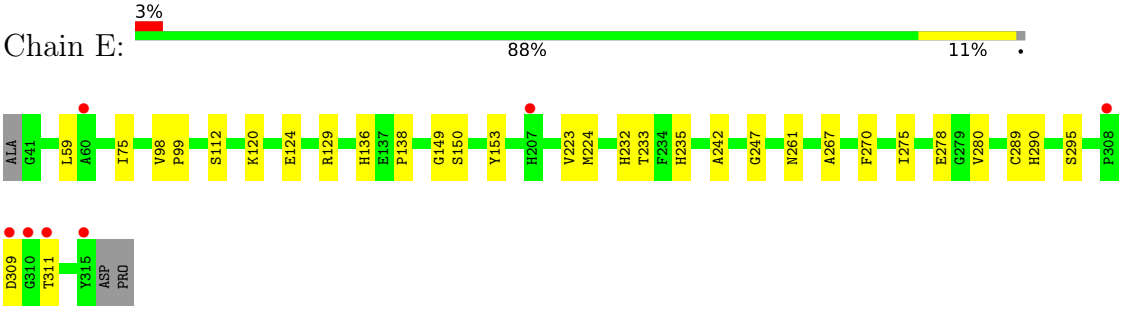
• Molecule 1: Two-domain laccase

Chain D:



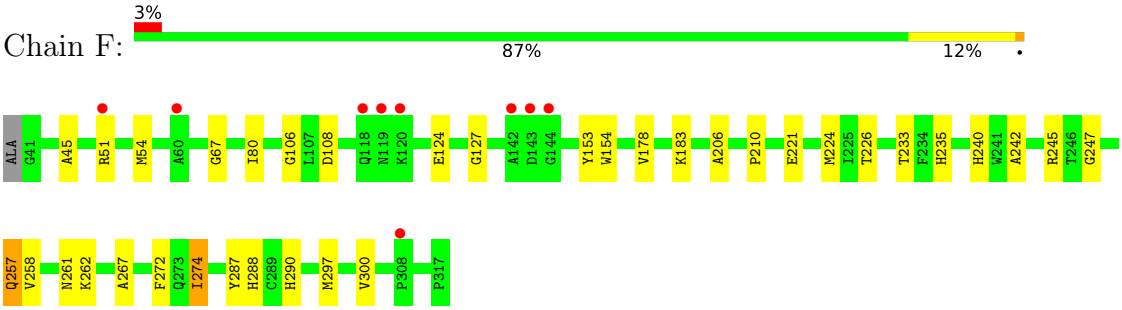
• Molecule 1: Two-domain laccase

Chain E:



• Molecule 1: Two-domain laccase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.37Å 93.92Å 119.59Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	23.76 – 2.20 23.76 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (23.76-2.20) 98.3 (23.76-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.19Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.215 , 0.258 0.215 , 0.258	Depositor DCC
R_{free} test set	4132 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12923	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PER, CU, OXY

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	0/2212	0.67	0/3007
1	B	0.48	0/2196	0.69	0/2985
1	C	0.46	0/2180	0.66	0/2962
1	D	0.44	0/2206	0.67	1/2997 (0.0%)
1	E	0.47	0/2173	0.67	0/2952
1	F	0.45	0/2183	0.66	0/2967
All	All	0.46	0/13150	0.67	1/17870 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	260	ASP	CB-CG-OD1	5.08	122.87	118.30

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	2146	0	2009	16	0
1	B	2130	0	1999	21	0
1	C	2115	0	1988	28	0
1	D	2140	0	2006	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2111	0	1979	21	0
1	F	2120	0	1986	19	0
2	A	4	0	0	0	0
2	F	4	0	0	0	0
3	A	4	0	0	0	0
3	B	5	0	0	0	0
3	C	3	0	0	0	0
3	D	5	0	0	0	0
3	E	3	0	0	0	0
3	F	4	0	0	0	0
4	D	2	0	0	0	0
5	A	21	0	0	0	0
5	B	26	0	0	1	0
5	C	18	0	0	0	0
5	D	11	0	0	1	0
5	E	28	0	0	0	0
5	F	23	0	0	0	0
All	All	12923	0	11967	128	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 5.

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:HIS:HB2	1:D:261:ASN:ND2	2.01	0.76
1:D:64:MET:HB2	1:D:172:ASN:HB3	1.76	0.68
1:B:99:PRO:HD2	1:E:98:VAL:HG12	1.74	0.68
1:E:235:HIS:HB2	1:E:261:ASN:HD22	1.59	0.67
1:C:288:HIS:HB3	1:C:300[A]:VAL:HG23	1.76	0.66
1:C:93:GLU:HG3	1:C:128:THR:HG22	1.78	0.65
1:F:235:HIS:HB2	1:F:261:ASN:ND2	2.13	0.64
1:C:257:GLN:HG2	1:C:259:ILE:HG23	1.78	0.64
1:D:52:VAL:HG22	1:D:88:LEU:HD11	1.79	0.64
1:F:45:ALA:HB2	1:F:183:LYS:HD2	1.78	0.64
1:D:213:GLU:OE1	1:D:306:LYS:HE2	1.98	0.63
1:E:124:GLU:CD	1:E:124:GLU:H	2.02	0.62
1:A:235:HIS:HB2	1:A:261:ASN:HD22	1.65	0.61
1:C:293:SER:O	1:C:297:MET:HG2	2.02	0.59
1:B:116:THR:HB	1:B:118:GLN:OE1	2.03	0.58
1:B:242:ALA:O	1:B:247:GLY:HA2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ILE:HB	1:D:178:VAL:HG13	1.85	0.57
1:A:288:HIS:HB3	1:A:300:VAL:HG13	1.87	0.57
1:C:64:MET:HG3	1:C:172:ASN:HB3	1.87	0.56
1:A:93:GLU:HG3	1:A:128:THR:HG22	1.87	0.56
1:C:205:PRO:HG2	1:C:208:THR:HG21	1.87	0.56
1:F:124:GLU:OE2	1:F:127:GLY:HA3	2.05	0.56
1:C:51:ARG:NH1	1:C:91:GLU:OE2	2.38	0.55
1:D:116:THR:HB	1:D:118:GLN:OE1	2.06	0.55
1:C:216:VAL:HG23	1:C:306:LYS:O	2.07	0.55
1:C:224:MET:HE1	1:C:264[A]:CYS:SG	2.48	0.54
1:C:257:GLN:HG2	1:C:259:ILE:CG2	2.37	0.54
1:E:242:ALA:O	1:E:247:GLY:HA2	2.09	0.53
1:D:275:ILE:HB	1:D:278:GLU:HB2	1.89	0.52
1:A:229:GLU:O	1:B:231:TYR:OH	2.26	0.52
1:E:235:HIS:HB2	1:E:261:ASN:ND2	2.22	0.52
1:A:235:HIS:HB2	1:A:261:ASN:ND2	2.25	0.52
1:C:214:ALA:O	1:C:306:LYS:HE2	2.09	0.52
1:B:204:ARG:NH2	1:B:208:THR:O	2.25	0.52
1:C:192:HIS:HB3	1:C:212:PHE:CE1	2.45	0.51
1:F:153:TYR:OH	1:F:221:GLU:OE2	2.28	0.51
1:D:307:LYS:HE2	1:D:308:PRO:HD3	1.93	0.51
1:E:233:THR:O	1:E:289:CYS:HA	2.11	0.50
1:D:249:LEU:HD22	1:D:254:ASP:HB3	1.93	0.50
1:B:233:THR:O	1:B:289:CYS:HA	2.12	0.49
1:D:94:ASN:OD1	1:D:96:MET:HB2	2.11	0.49
1:F:233:THR:HA	1:F:262:LYS:O	2.12	0.49
1:B:48:GLU:HB2	1:B:50:ARG:NH1	2.27	0.49
1:D:240:HIS:HD2	5:D:511:HOH:O	1.94	0.49
1:C:275:ILE:HB	1:C:278:GLU:HB2	1.95	0.49
1:B:98:VAL:HG12	1:E:99:PRO:HD2	1.93	0.49
1:D:108:ASP:OD2	1:D:136:HIS:HD2	1.96	0.49
1:D:307:LYS:HE2	1:D:307:LYS:HA	1.94	0.48
1:C:235:HIS:HB2	1:C:261:ASN:ND2	2.28	0.48
1:D:136:HIS:HE1	1:D:148:ALA:O	1.95	0.48
1:D:235:HIS:HB2	1:D:261:ASN:HD21	1.78	0.48
1:D:101:SER:HB3	1:D:160:VAL:HG22	1.94	0.48
1:B:209:GLY:N	5:B:503:HOH:O	2.47	0.48
1:C:159:HIS:CE1	1:C:165:HIS:HA	2.49	0.47
1:E:275:ILE:HB	1:E:278:GLU:HB2	1.97	0.47
1:B:101:SER:HG	1:B:159:HIS:H	1.61	0.47
1:E:224:MET:HE2	1:E:270:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257[A]:GLN:HG3	1:F:245:ARG:HA	1.97	0.47
1:F:272:PHE:HE1	1:F:274:ILE:HD13	1.80	0.47
1:F:124:GLU:H	1:F:124:GLU:CD	2.18	0.47
1:D:253:ASP:O	1:D:255:PRO:HD3	2.15	0.46
1:F:257:GLN:HG3	1:F:258:VAL:N	2.30	0.46
1:C:198:ASP:OD1	1:C:228:GLY:HA3	2.16	0.46
1:C:234:PHE:O	1:C:261:ASN:HA	2.15	0.46
1:B:101:SER:OG	1:B:159:HIS:N	2.41	0.46
1:C:53:THR:HG22	1:C:91:GLU:OE1	2.14	0.46
1:B:118:GLN:H	1:B:118:GLN:CD	2.16	0.46
1:A:191:THR:OG1	1:A:221:GLU:OE1	2.29	0.45
1:C:45:ALA:HB2	1:C:183:LYS:HD3	1.98	0.45
1:E:289:CYS:O	1:E:295:SER:HB3	2.17	0.45
1:A:220:VAL:HG21	1:A:303:PHE:HZ	1.82	0.45
1:E:112:SER:O	1:E:129:ARG:NH2	2.40	0.45
1:F:206:ALA:HB1	1:F:297:MET:O	2.17	0.45
1:B:155:HIS:CD2	1:B:269:SER:HB3	2.52	0.45
1:C:233:THR:HA	1:C:262:LYS:O	2.18	0.44
1:D:279:GLY:O	1:F:108:ASP:HB3	2.17	0.44
1:B:97:ASP:OD1	1:B:98:VAL:HG13	2.18	0.44
1:C:235:HIS:HB2	1:C:261:ASN:HD22	1.83	0.44
1:F:210:PRO:O	1:F:287:TYR:OH	2.27	0.44
1:F:242:ALA:O	1:F:247:GLY:HA2	2.17	0.44
1:D:143:ASP:OD1	1:D:145:THR:OG1	2.32	0.44
1:F:288:HIS:HB3	1:F:300:VAL:HG13	2.00	0.44
1:A:104:VAL:HG23	1:A:156:TYR:HB3	2.00	0.43
1:D:246:THR:HB	1:D:248:MET:HE3	1.99	0.43
1:F:106:GLY:HA3	1:F:154:TRP:CD2	2.53	0.43
1:C:290:HIS:O	1:C:290:HIS:ND1	2.49	0.43
1:A:235:HIS:CE1	1:C:105:HIS:CE1	3.07	0.43
1:D:195:VAL:HA	1:D:225:ILE:O	2.19	0.43
1:C:69:GLU:O	1:C:72:LYS:HB2	2.19	0.43
1:E:138:PRO:HD3	1:E:149:GLY:HA3	2.01	0.43
1:F:226:THR:O	1:F:267:ALA:N	2.45	0.43
1:B:192:HIS:HB3	1:B:212:PHE:CE1	2.54	0.43
1:D:109:TYR:H	1:E:280:VAL:HG12	1.84	0.43
1:A:116:THR:HG21	1:B:286:MET:CE	2.49	0.42
1:A:257[A]:GLN:HG3	1:C:245:ARG:HA	2.01	0.42
1:A:242:ALA:O	1:A:247:GLY:HA2	2.20	0.42
1:D:117:LYS:C	1:D:119:ASN:H	2.23	0.42
1:B:235:HIS:HB2	1:B:261:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:GLY:HA3	1:D:154:TRP:CD2	2.54	0.42
1:E:232:HIS:HB3	1:E:289:CYS:SG	2.60	0.42
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.81	0.41
1:D:100:VAL:HG22	1:D:101:SER:H	1.85	0.41
1:D:54:MET:O	1:D:92:PHE:HA	2.20	0.41
1:D:107:LEU:N	1:D:107:LEU:HD23	2.35	0.41
1:B:312:ILE:HD12	1:B:315:TYR:CD2	2.55	0.41
1:D:60:ALA:O	1:D:63:GLN:HG3	2.20	0.41
1:D:277:GLY:HA2	1:D:280:VAL:HG23	2.01	0.41
1:E:59:LEU:HD12	1:E:75:ILE:HD11	2.02	0.41
1:F:54:MET:HA	1:F:67:GLY:O	2.20	0.41
1:A:206:ALA:HB1	1:A:297:MET:O	2.19	0.41
1:D:51:ARG:NH1	1:D:91:GLU:OE2	2.53	0.41
1:D:142:ALA:C	1:D:144:GLY:H	2.23	0.41
1:D:267:ALA:HB2	1:E:290:HIS:CD2	2.56	0.41
1:E:136:HIS:CE1	1:E:150:SER:HG	2.37	0.41
1:F:80:ILE:HB	1:F:178:VAL:HG13	2.02	0.41
1:B:100:VAL:HG22	1:B:101:SER:H	1.85	0.41
1:A:136:HIS:CD2	1:A:149:GLY:HA2	2.56	0.41
1:C:159:HIS:ND1	1:C:165:HIS:HA	2.36	0.41
1:C:216:VAL:HG22	1:C:305:VAL:HG12	2.03	0.41
1:D:110:GLU:HA	1:E:280:VAL:O	2.21	0.41
1:D:195:VAL:HG22	1:D:225:ILE:HB	2.02	0.41
1:E:153:TYR:CD1	1:E:223:VAL:HG22	2.56	0.41
1:A:142:ALA:C	1:A:144:GLY:H	2.24	0.40
1:E:267:ALA:HB2	1:F:290:HIS:CE1	2.56	0.40
1:E:309:ASP:OD1	1:E:311:THR:HG23	2.21	0.40
1:A:206:ALA:O	1:A:208:THR:HG23	2.20	0.40
1:B:68:LEU:HG	1:B:78:PRO:HG3	2.04	0.40
1:C:158:ASP:OD2	1:C:169:GLY:HA3	2.22	0.40

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	279/278 (100%)	269 (96%)	10 (4%)	0	100 100
1	B	277/278 (100%)	272 (98%)	5 (2%)	0	100 100
1	C	275/278 (99%)	264 (96%)	10 (4%)	1 (0%)	34 37
1	D	278/278 (100%)	262 (94%)	16 (6%)	0	100 100
1	E	274/278 (99%)	268 (98%)	6 (2%)	0	100 100
1	F	275/278 (99%)	268 (98%)	7 (2%)	0	100 100
All	All	1658/1668 (99%)	1603 (97%)	54 (3%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	GLU

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	221/218 (101%)	217 (98%)	4 (2%)	59 72
1	B	220/218 (101%)	217 (99%)	3 (1%)	67 80
1	C	218/218 (100%)	214 (98%)	4 (2%)	59 72
1	D	221/218 (101%)	209 (95%)	12 (5%)	22 26
1	E	217/218 (100%)	216 (100%)	1 (0%)	88 94
1	F	218/218 (100%)	213 (98%)	5 (2%)	50 63
All	All	1315/1308 (100%)	1286 (98%)	29 (2%)	57 65

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL

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Mol	Chain	Res	Type
1	A	224	MET
1	A	264[A]	CYS
1	A	264[B]	CYS
1	B	72	LYS
1	B	120	LYS
1	B	224	MET
1	C	52	VAL
1	C	72	LYS
1	C	257	GLN
1	C	309	ASP
1	D	51	ARG
1	D	69	GLU
1	D	164	GLU
1	D	183	LYS
1	D	224[A]	MET
1	D	224[B]	MET
1	D	240	HIS
1	D	257[A]	GLN
1	D	257[B]	GLN
1	D	261	ASN
1	D	264[A]	CYS
1	D	264[B]	CYS
1	E	120	LYS
1	F	51	ARG
1	F	224	MET
1	F	240	HIS
1	F	257	GLN
1	F	274	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	ASN
1	A	268	ASN
1	B	261	ASN
1	B	268	ASN
1	C	261	ASN
1	C	268	ASN
1	D	136	HIS
1	D	240	HIS
1	D	261	ASN
1	D	268	ASN

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Mol	Chain	Res	Type
1	E	261	ASN
1	F	261	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 24 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
2	OXY	A	402	3	1,1,1	0.08	0	-		
2	OXY	F	401	3	1,1,1	0.14	0	-		
4	PER	D	401	3	0,1,1	-	-	-		
2	OXY	A	401	3	1,1,1	0.11	0	-		
2	OXY	F	402	3	1,1,1	0.20	0	-		

There are no bond length outliers.

There are no bond angle outliers.

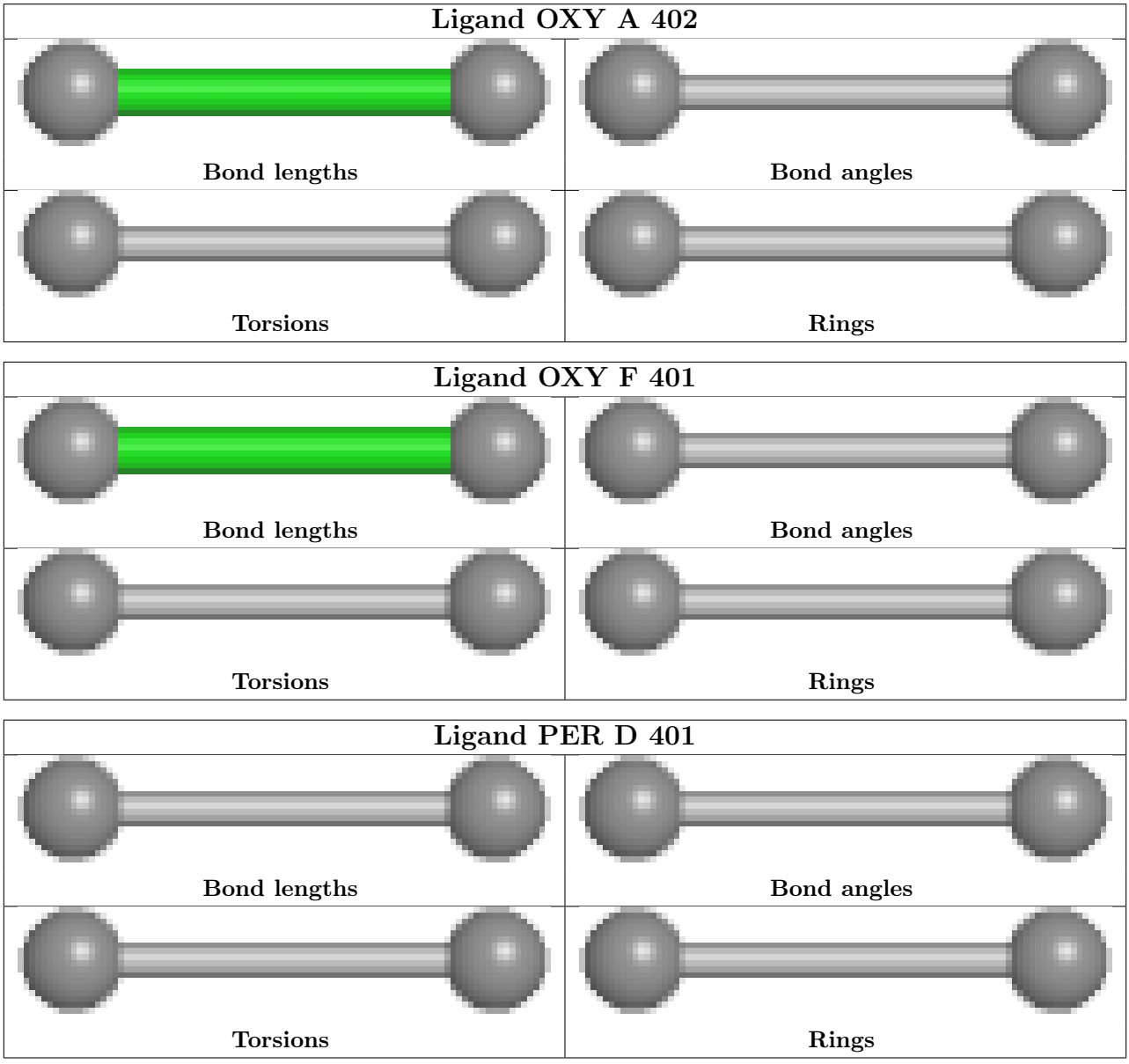
There are no chirality outliers.

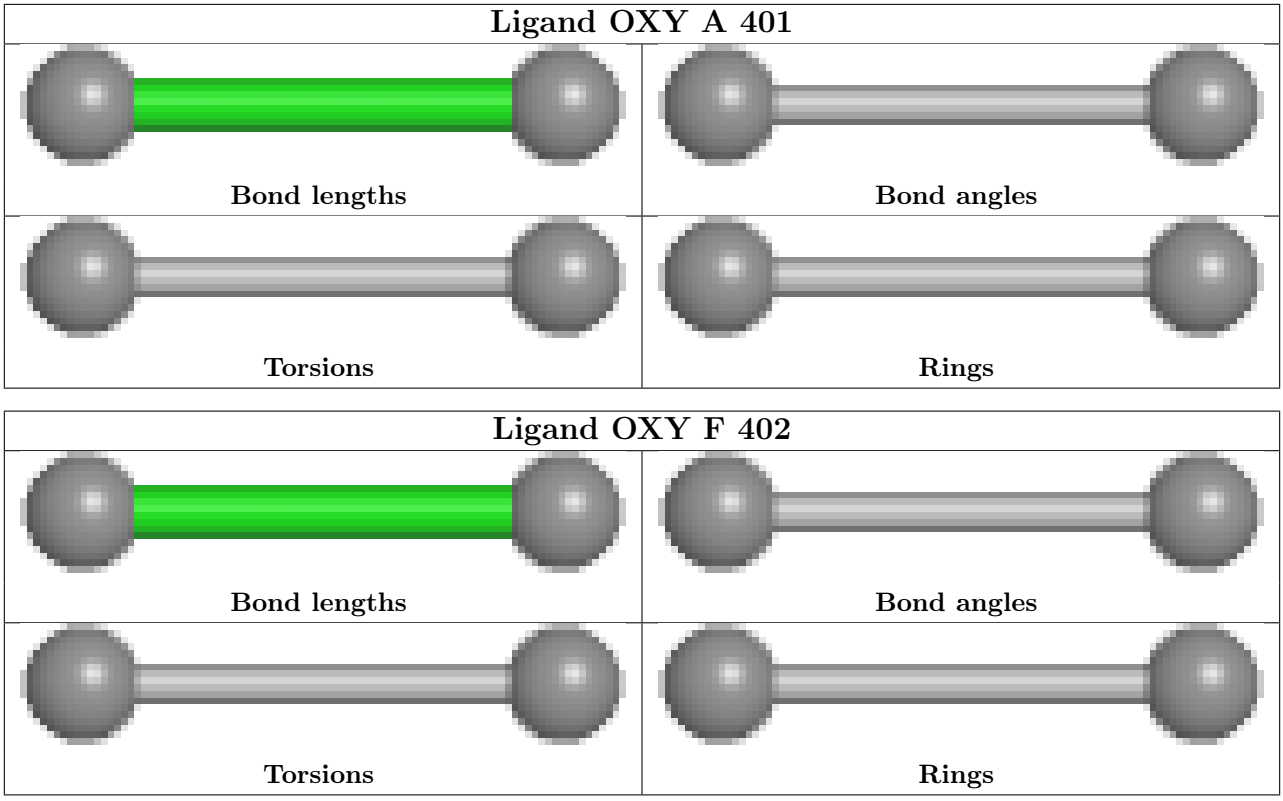
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.





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	278/278 (100%)	0.03	5 (1%)	68	66	9, 19, 32, 45	3 (1%)
1	B	277/278 (99%)	-0.11	5 (1%)	68	66	7, 15, 28, 61	2 (0%)
1	C	275/278 (98%)	0.03	3 (1%)	80	79	11, 20, 33, 42	2 (0%)
1	D	277/278 (99%)	0.26	6 (2%)	62	59	13, 25, 39, 76	4 (1%)
1	E	275/278 (98%)	-0.11	7 (2%)	57	55	6, 17, 31, 49	1 (0%)
1	F	277/278 (99%)	0.17	9 (3%)	47	45	8, 21, 34, 55	5 (1%)
All	All	1659/1668 (99%)	0.04	35 (2%)	63	61	6, 20, 34, 76	17 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	316	ASP	6.2
1	D	317	PRO	4.8
1	B	316	ASP	4.8
1	A	142	ALA	4.5
1	F	144	GLY	3.8
1	C	60	ALA	3.7
1	B	144	GLY	3.5
1	E	308	PRO	3.2
1	B	118	GLN	3.1
1	F	142	ALA	3.1
1	F	60	ALA	3.1
1	F	118	GLN	3.0
1	A	40	ALA	2.9
1	E	310	GLY	2.8
1	D	313	PRO	2.7
1	A	317	PRO	2.6
1	A	316	ASP	2.5
1	C	313	PRO	2.5
1	C	314	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	120	LYS	2.4
1	F	143	ASP	2.4
1	D	45	ALA	2.4
1	E	309	ASP	2.3
1	B	317	PRO	2.3
1	E	60	ALA	2.3
1	F	308	PRO	2.3
1	E	311	THR	2.3
1	E	207	HIS	2.2
1	F	119	ASN	2.2
1	B	314	GLY	2.2
1	E	315	TYR	2.1
1	F	51	ARG	2.1
1	D	208	THR	2.1
1	D	142	ALA	2.0
1	A	143	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	CU	D	405	1/1	0.88	0.23	22,22,22,22	1
3	CU	F	403	1/1	0.93	0.07	31,31,31,31	1
3	CU	D	402	1/1	0.94	0.06	35,35,35,35	1
3	CU	D	406	1/1	0.95	0.12	20,20,20,20	1
3	CU	D	403	1/1	0.96	0.17	27,27,27,27	1
2	OXY	F	401	2/2	0.96	0.11	21,21,21,24	0
3	CU	B	405	1/1	0.96	0.10	28,28,28,28	1

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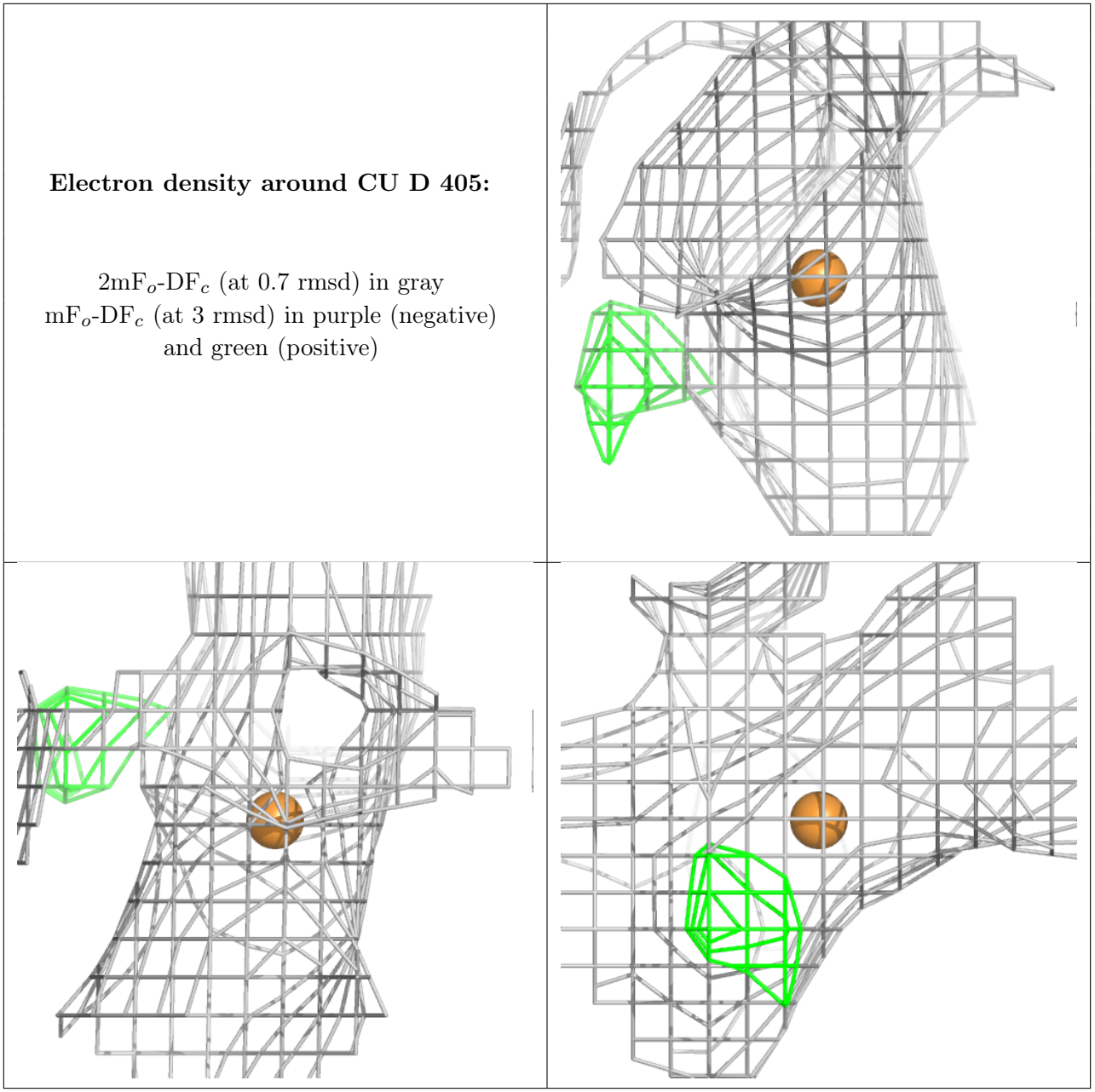
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OXY	A	402	2/2	0.96	0.15	22,22,22,24	2
3	CU	A	406	1/1	0.97	0.09	23,23,23,23	1
3	CU	E	402	1/1	0.97	0.05	25,25,25,25	1
3	CU	B	404	1/1	0.97	0.08	23,23,23,23	1
3	CU	B	403	1/1	0.98	0.17	21,21,21,21	1
3	CU	A	403	1/1	0.98	0.05	27,27,27,27	0
3	CU	A	405	1/1	0.98	0.23	24,24,24,24	1
3	CU	C	401	1/1	0.98	0.04	36,36,36,36	1
2	OXY	A	401	2/2	0.98	0.11	10,10,10,15	2
4	PER	D	401	2/2	0.98	0.10	13,13,13,22	2
2	OXY	F	402	2/2	0.99	0.13	15,15,15,15	2
3	CU	E	403	1/1	0.99	0.06	21,21,21,21	1
3	CU	A	404	1/1	0.99	0.05	29,29,29,29	1
3	CU	F	405	1/1	0.99	0.07	26,26,26,26	0
3	CU	F	406	1/1	0.99	0.18	14,14,14,14	1
3	CU	E	401	1/1	0.99	0.04	21,21,21,21	1
3	CU	D	404	1/1	1.00	0.03	17,17,17,17	1
3	CU	C	402	1/1	1.00	0.05	20,20,20,20	0
3	CU	F	404	1/1	1.00	0.03	22,22,22,22	0
3	CU	C	403	1/1	1.00	0.04	28,28,28,28	0
3	CU	B	401	1/1	1.00	0.03	18,18,18,18	0
3	CU	B	402	1/1	1.00	0.04	34,34,34,34	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.

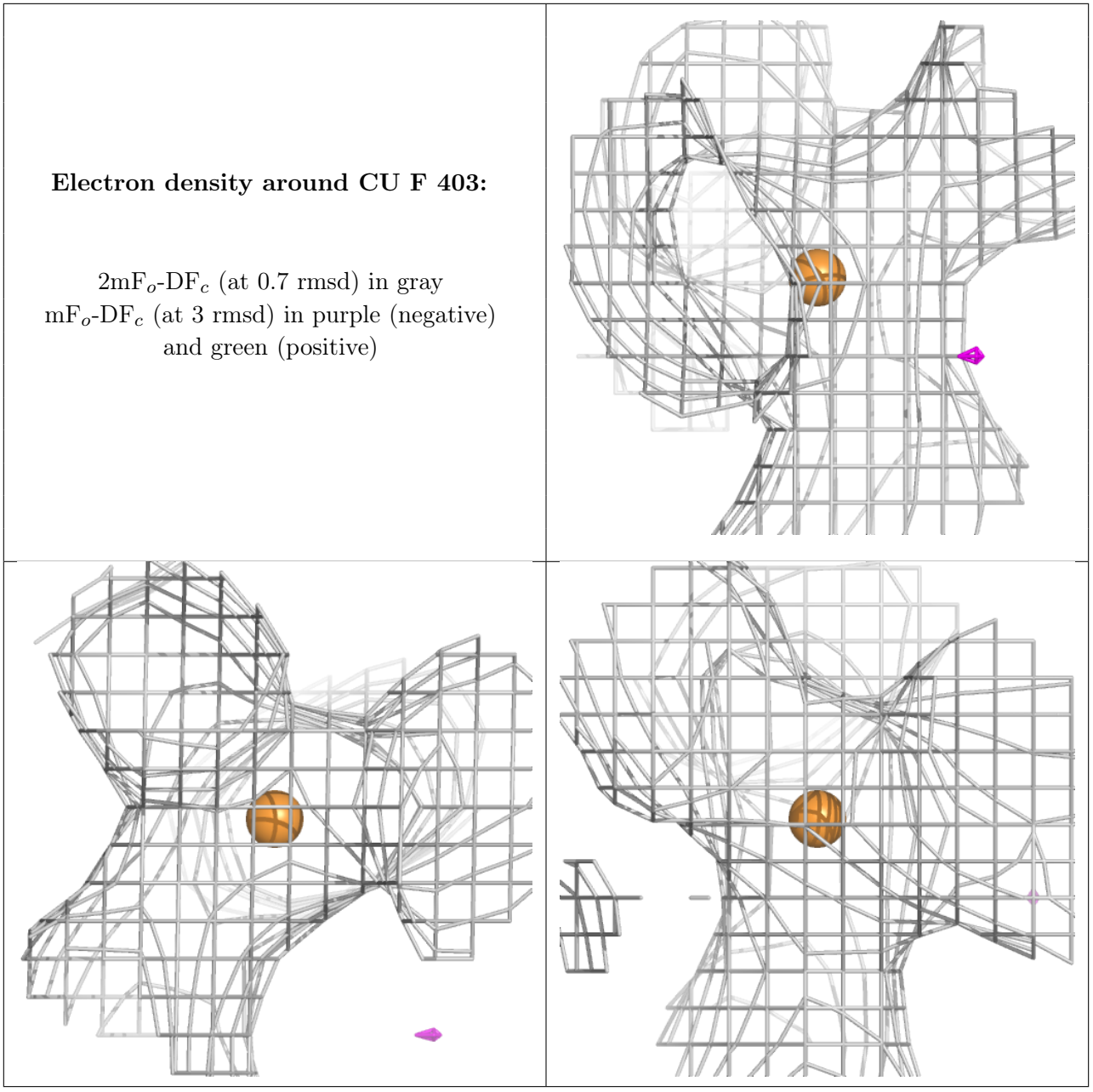
Electron density around CU D 405:

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



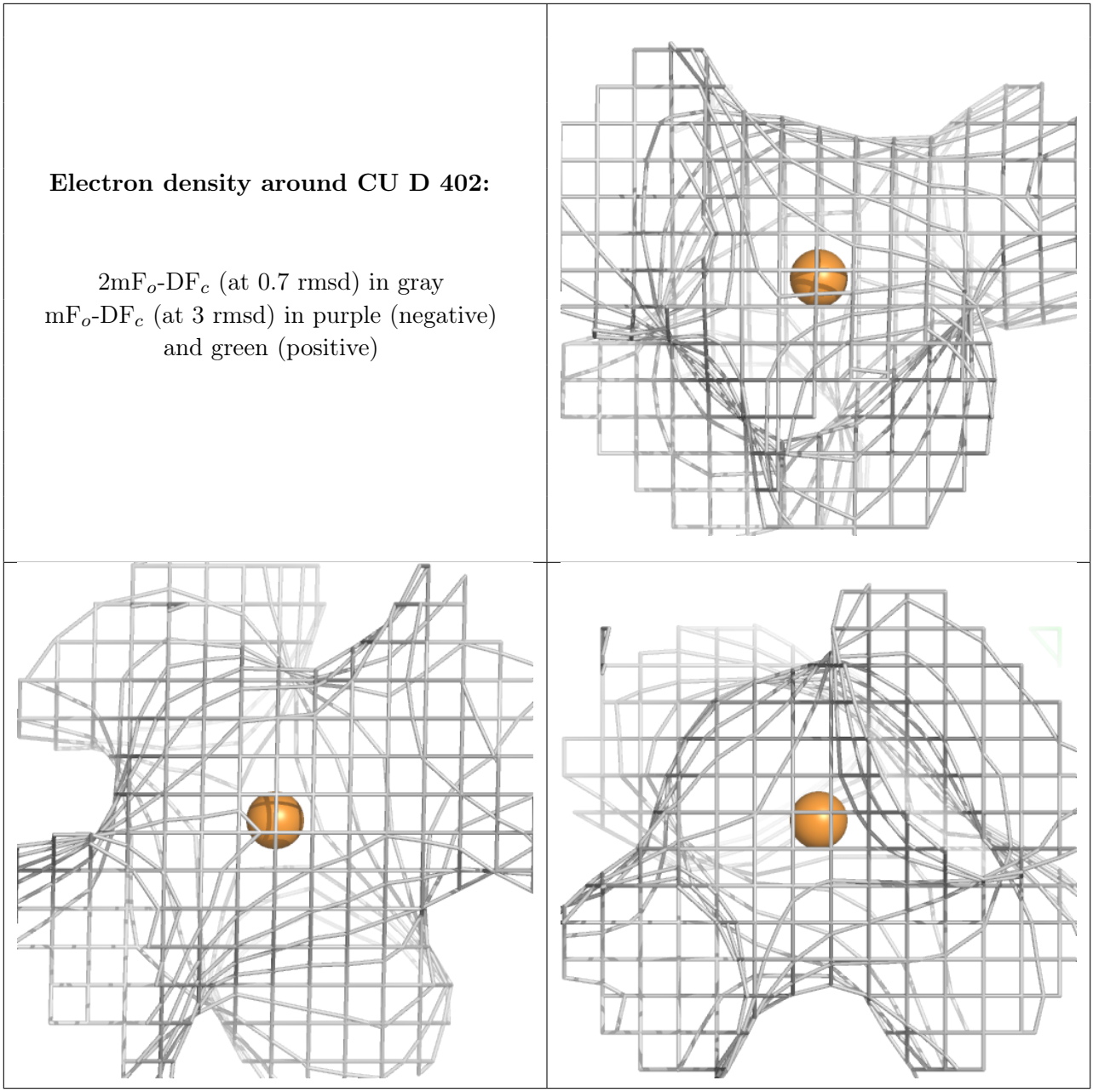
Electron density around CU F 403:

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



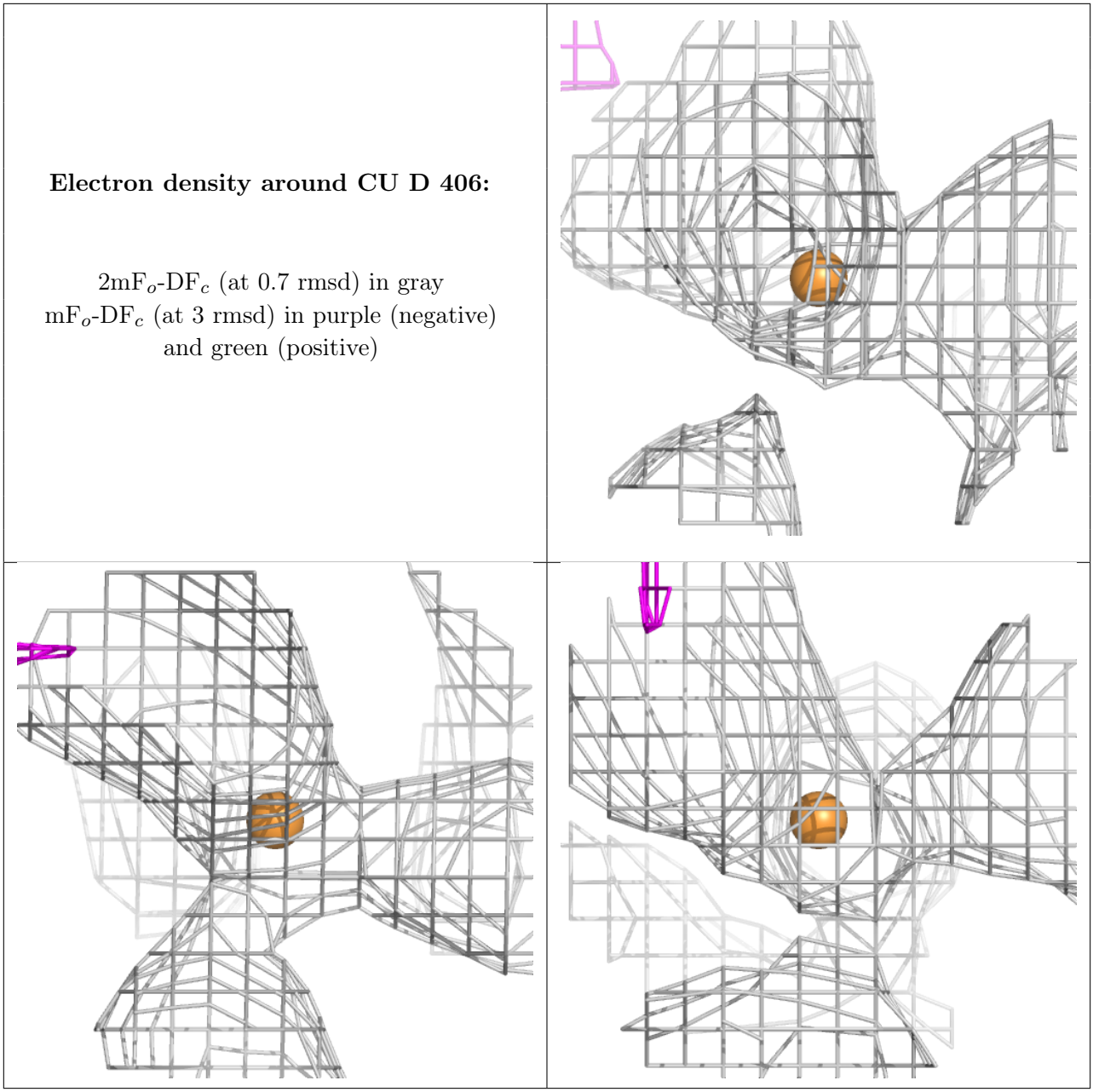
Electron density around CU D 402:

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



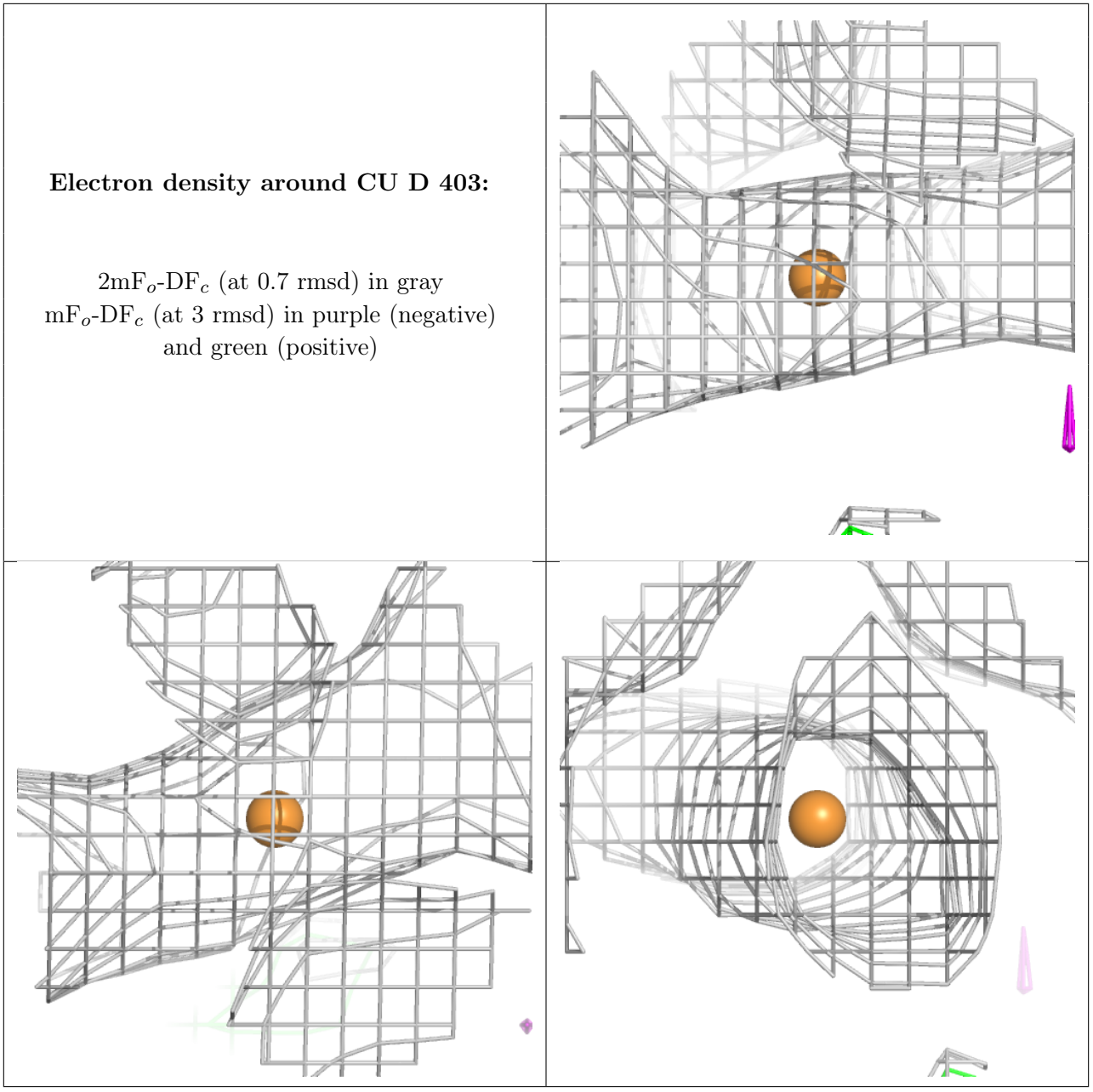
Electron density around CU D 406:

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



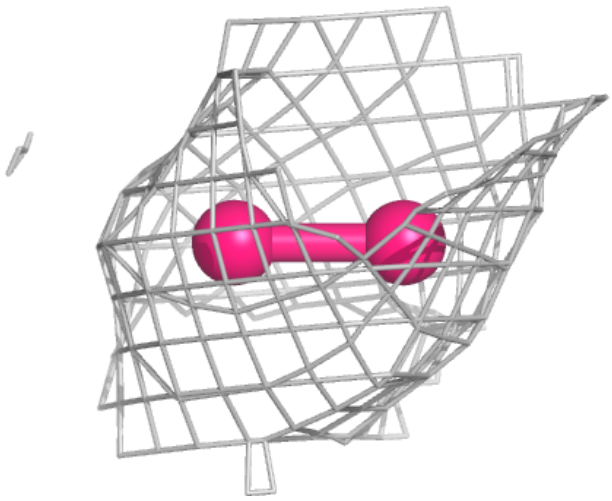
Electron density around CU D 403:

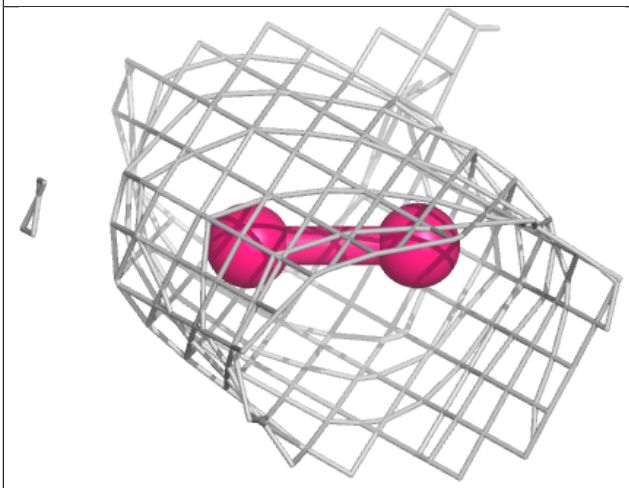
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

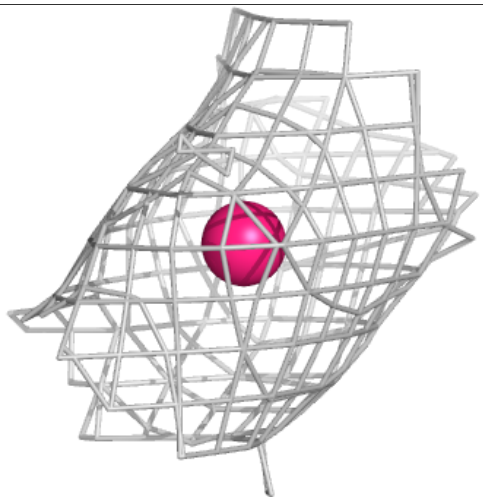


Electron density around OXY F 401:

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

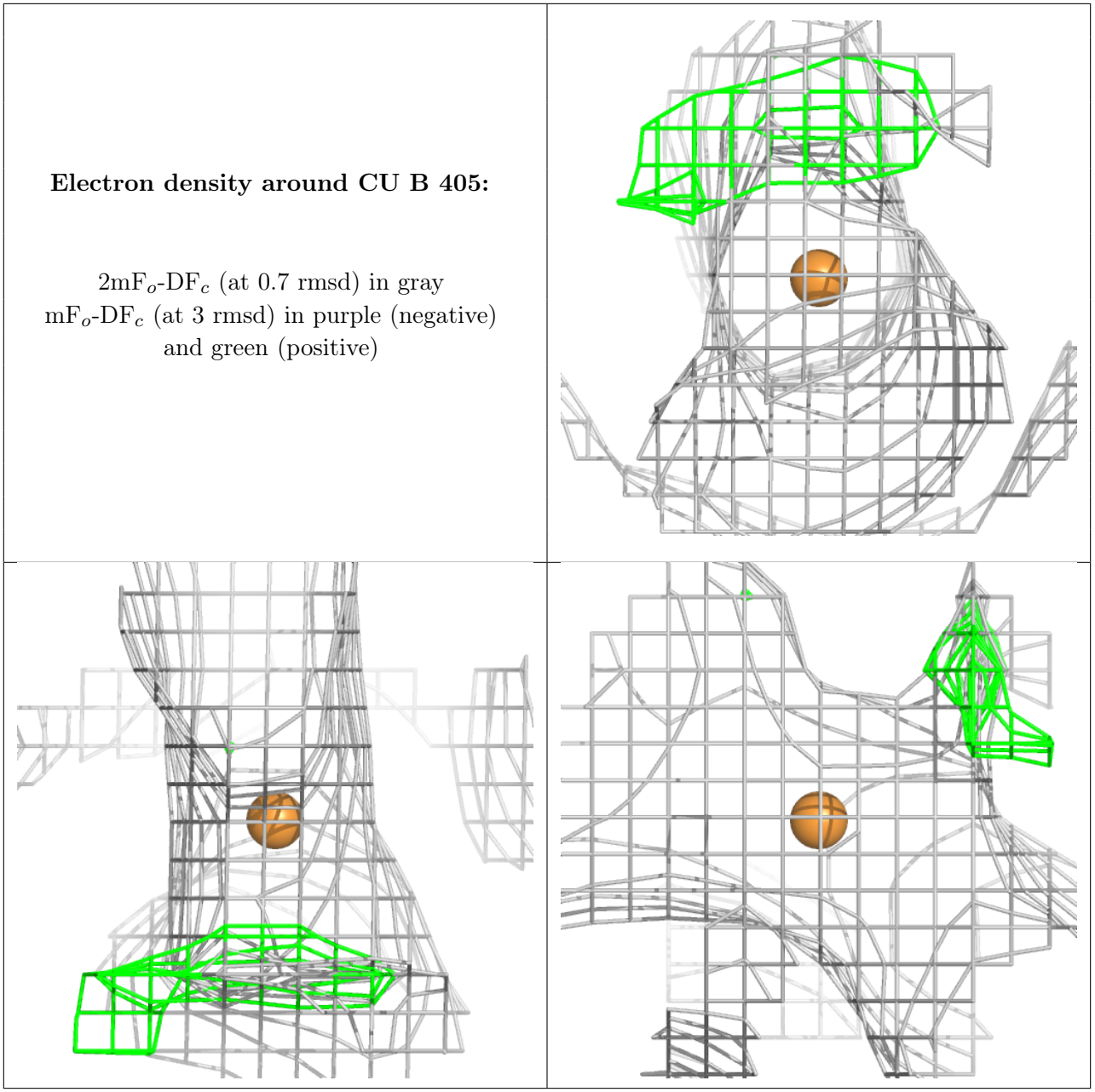






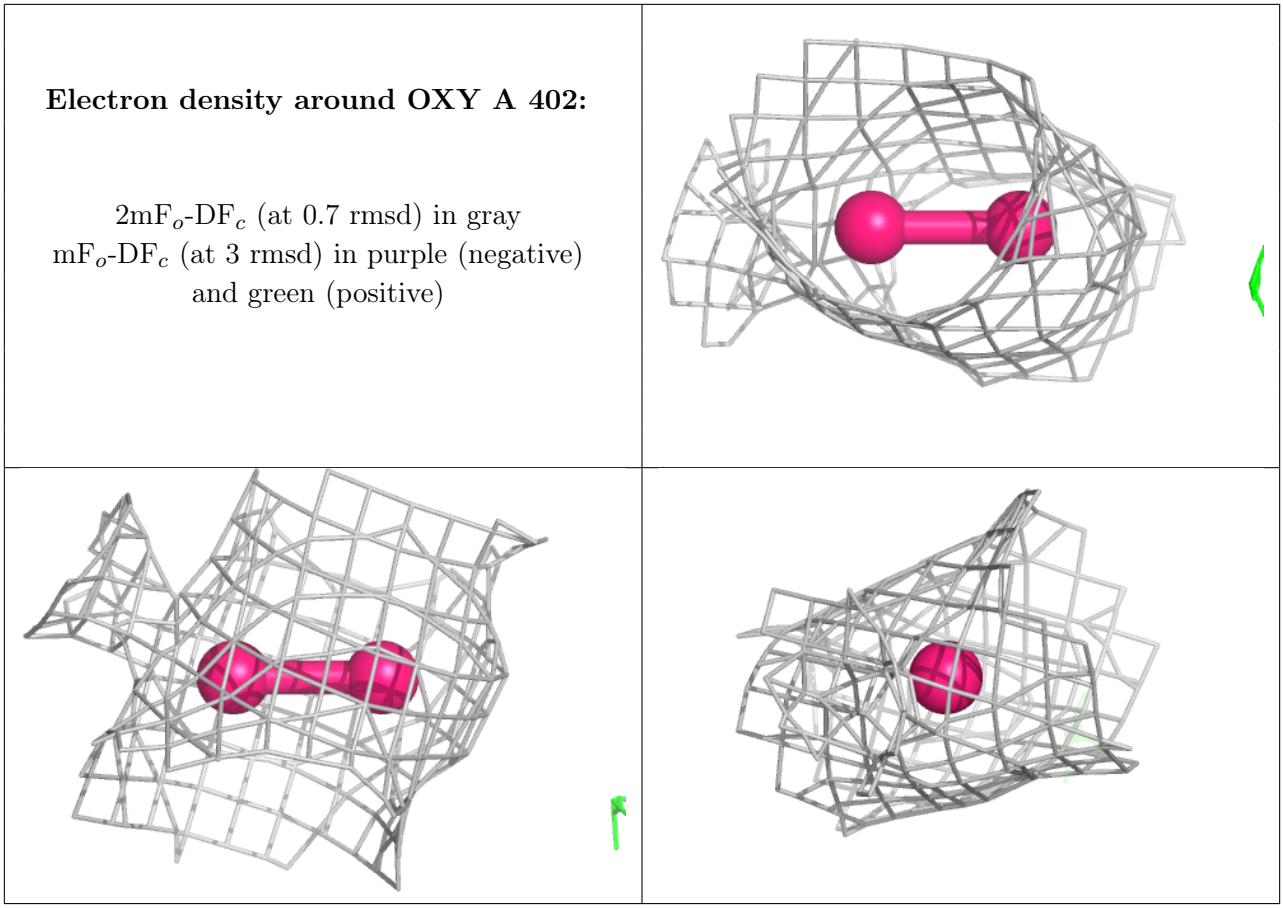
Electron density around CU B 405:

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



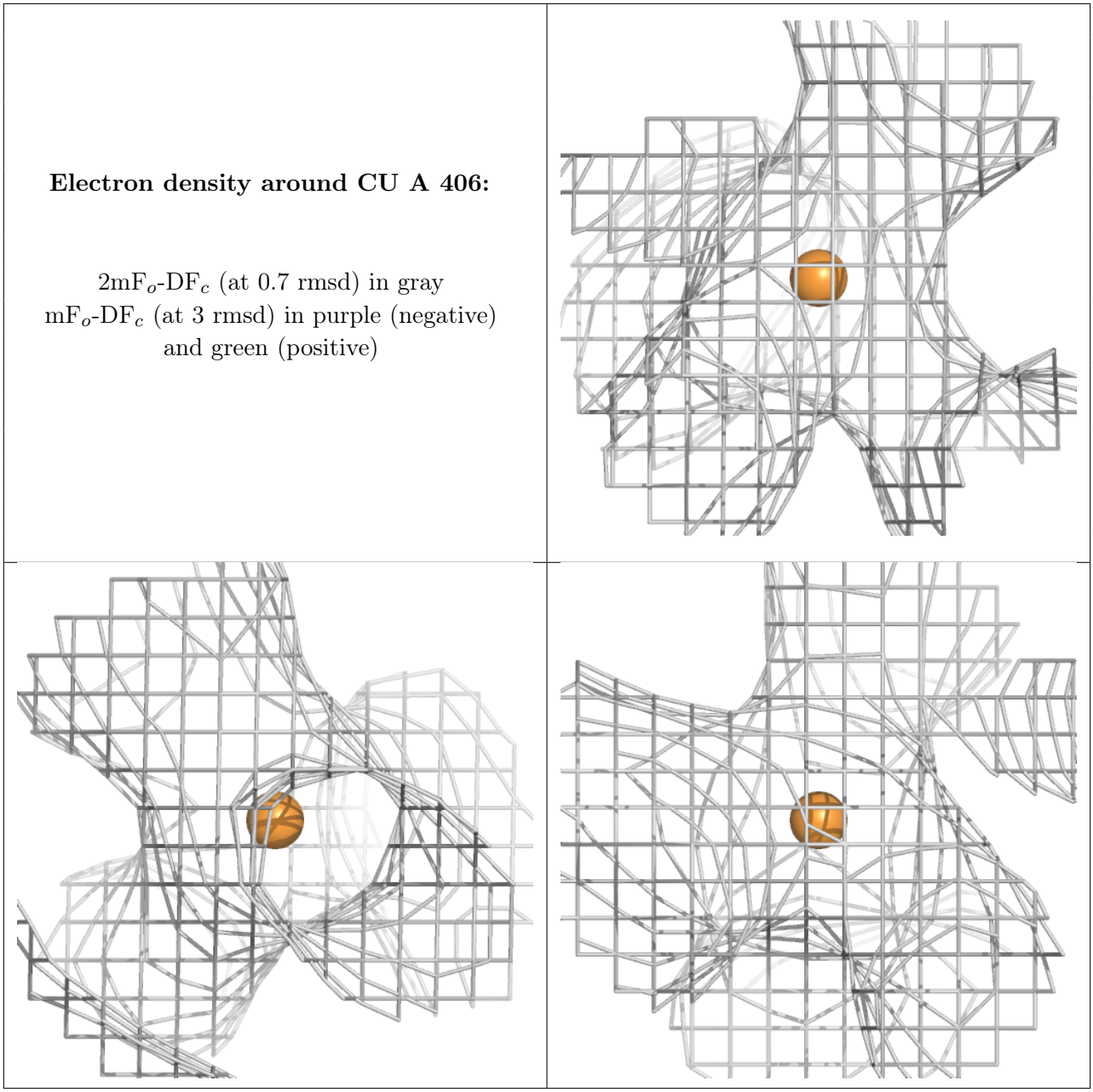
Electron density around OXY A 402:

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



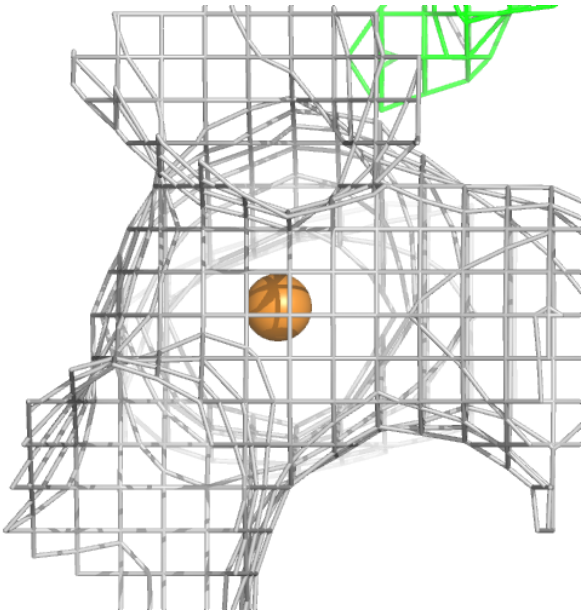
Electron density around CU A 406:

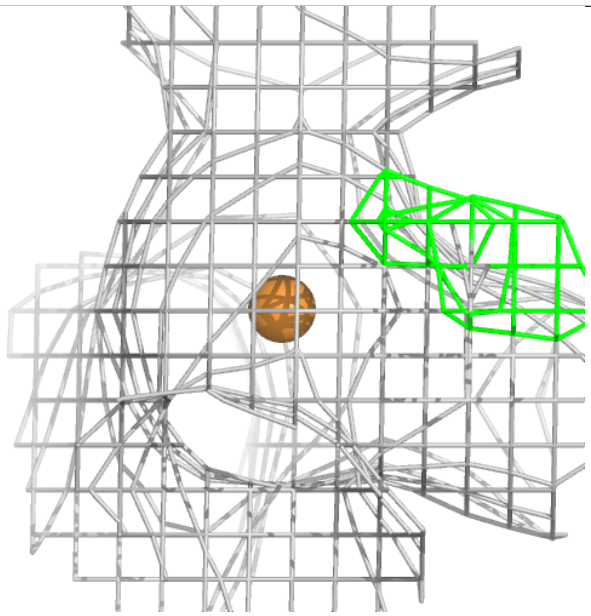
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

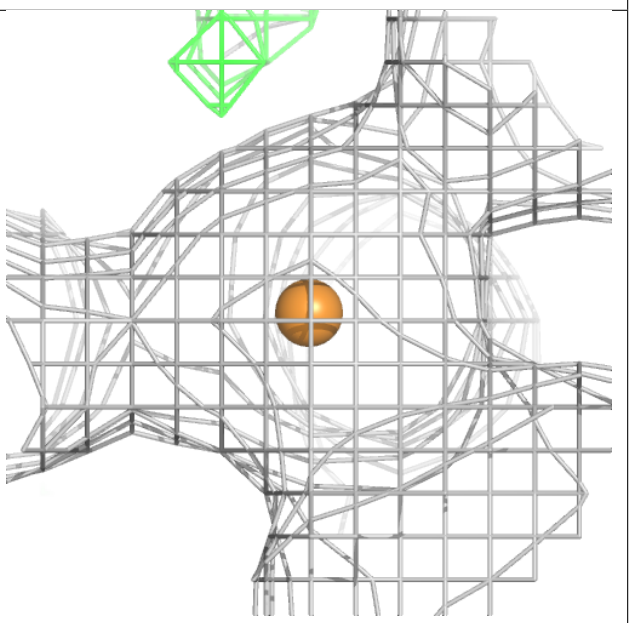


Electron density around CU E 402:

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

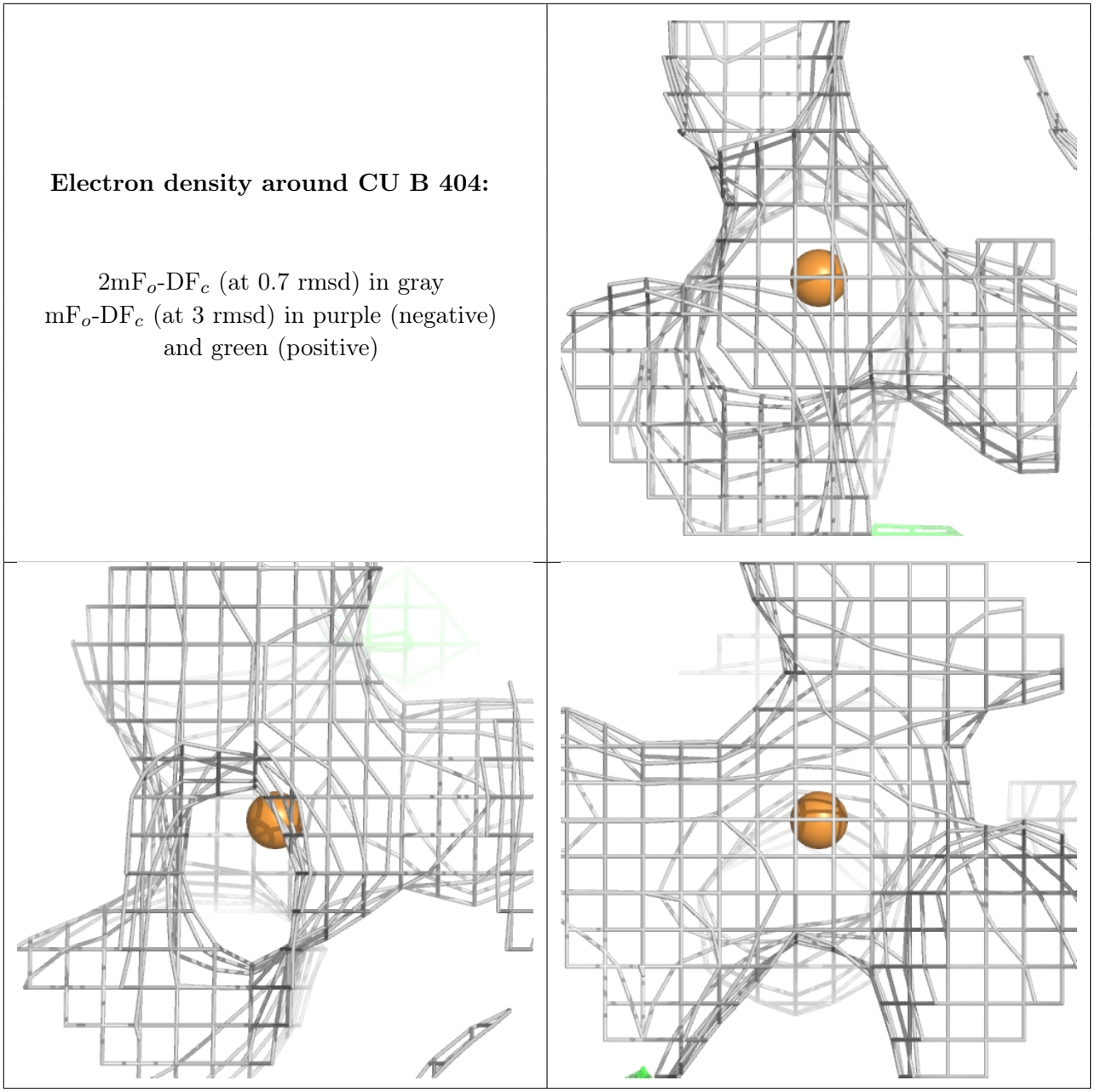






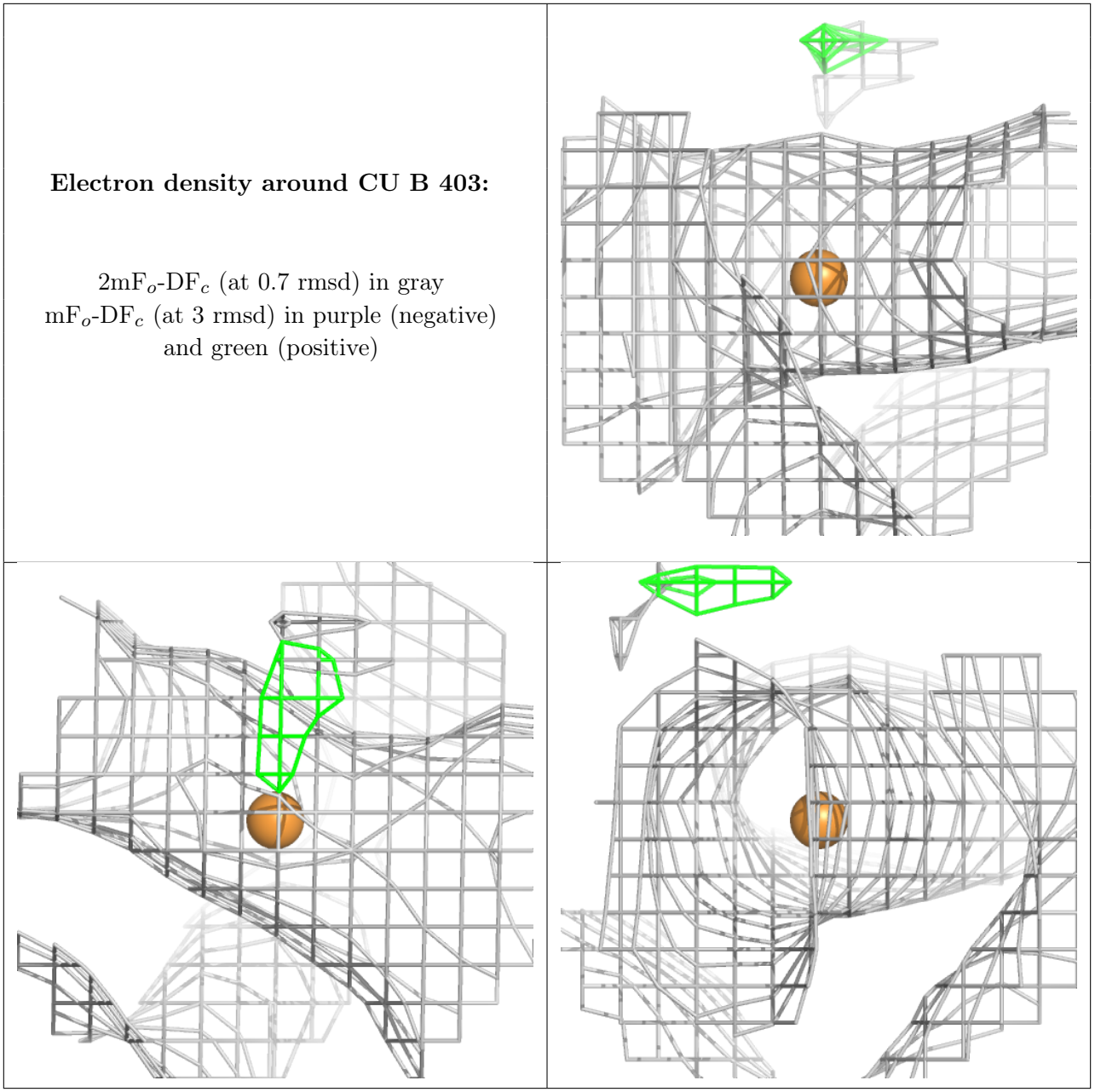
Electron density around CU B 404:

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



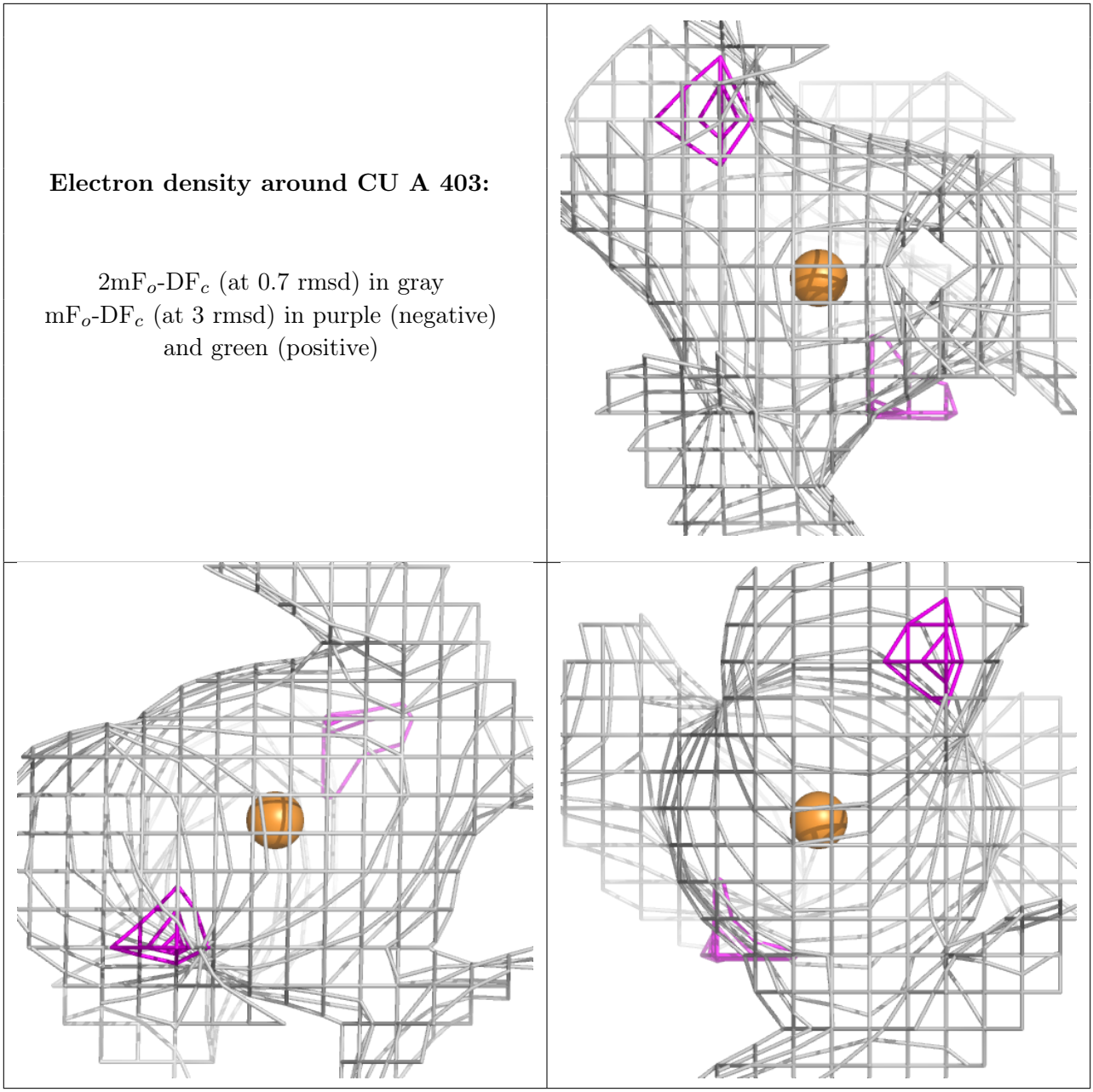
Electron density around CU B 403:

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



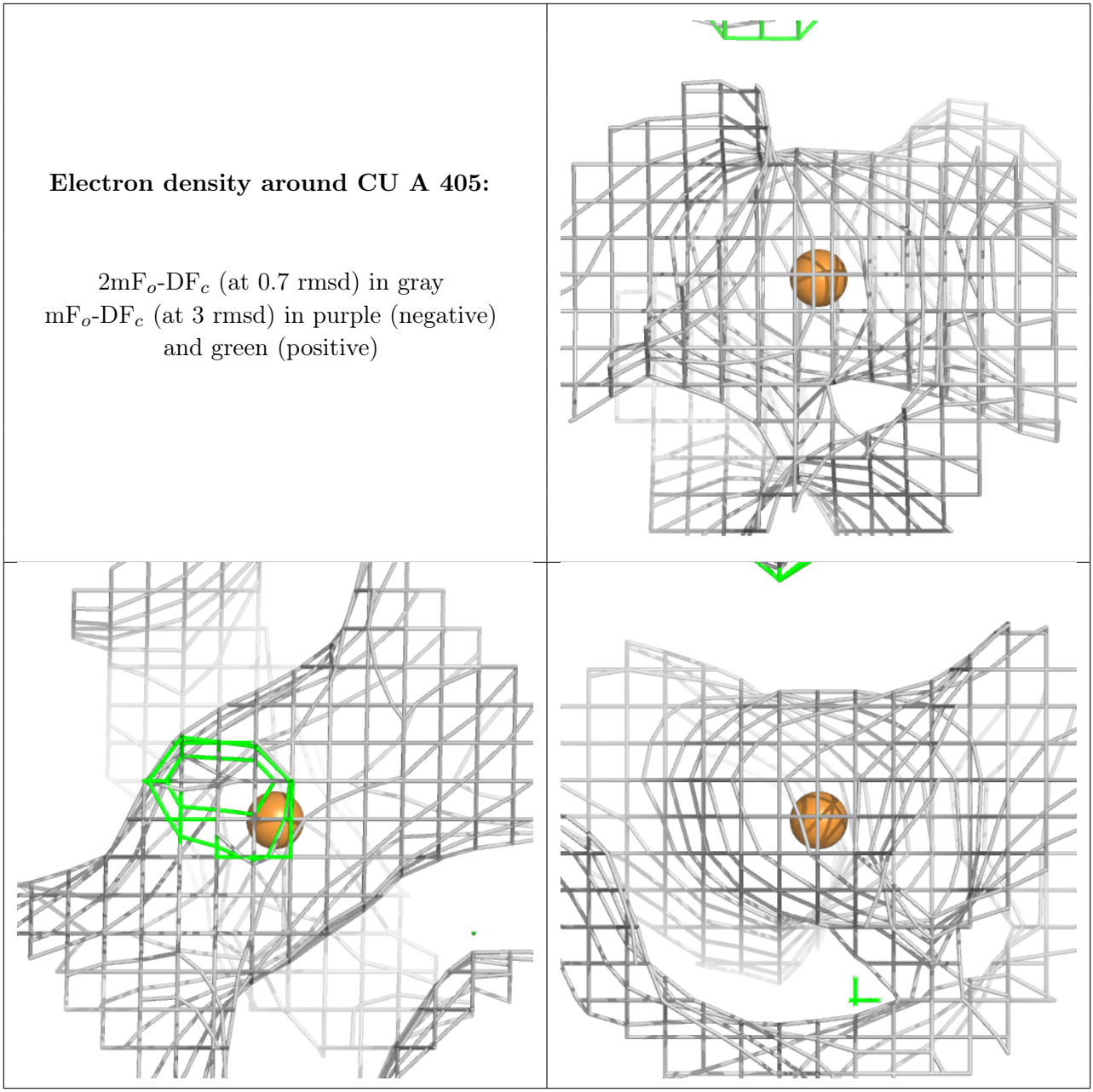
Electron density around CU A 403:

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



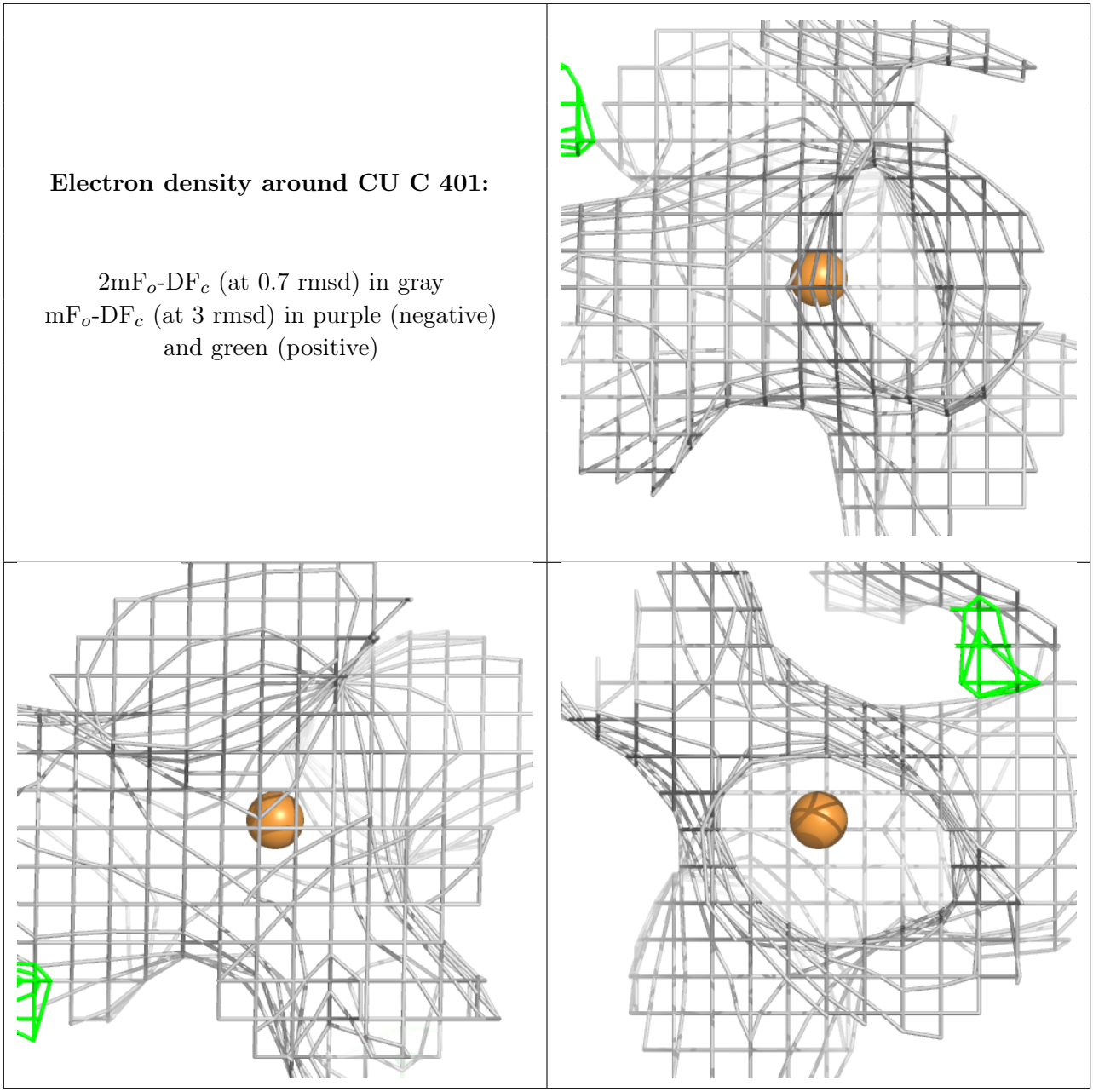
Electron density around CU A 405:

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



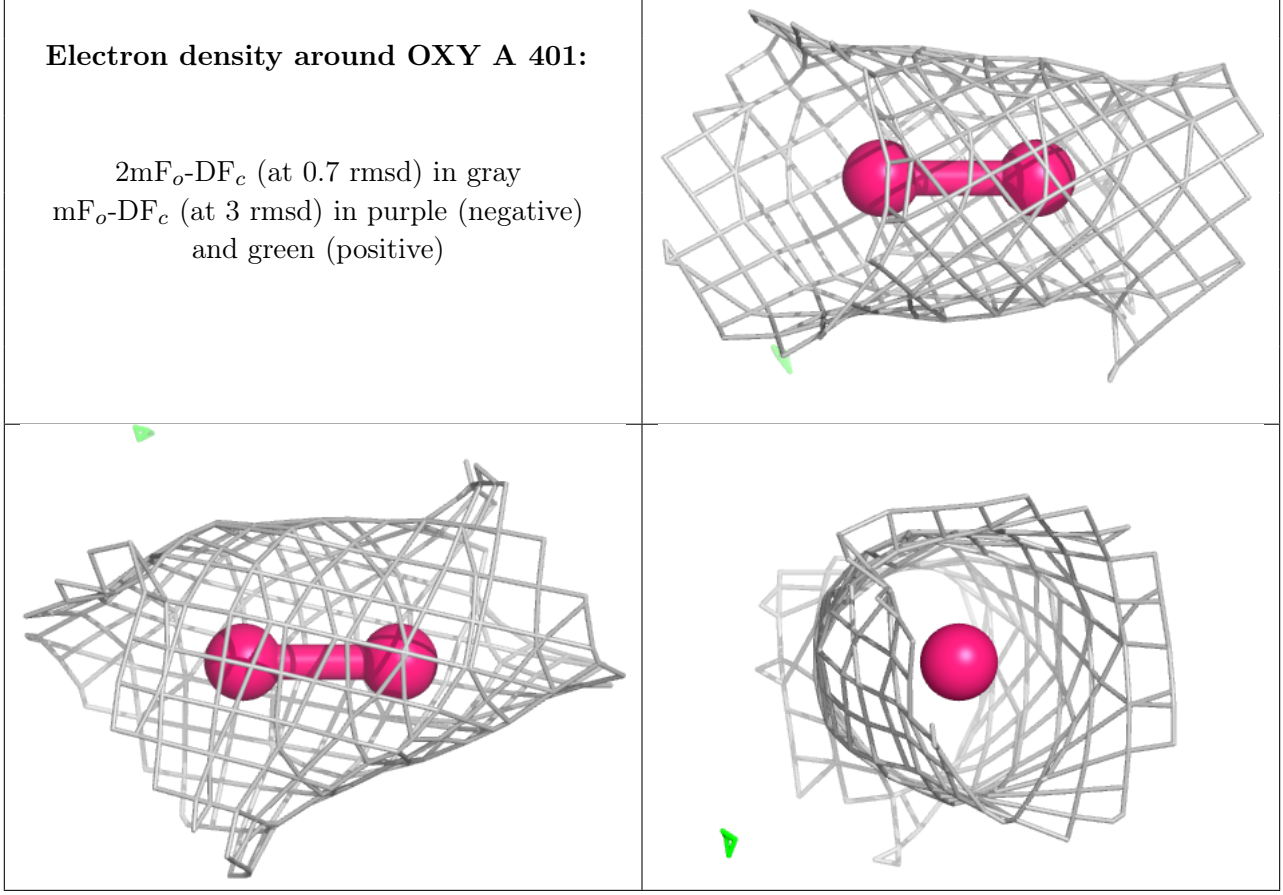
Electron density around CU C 401:

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



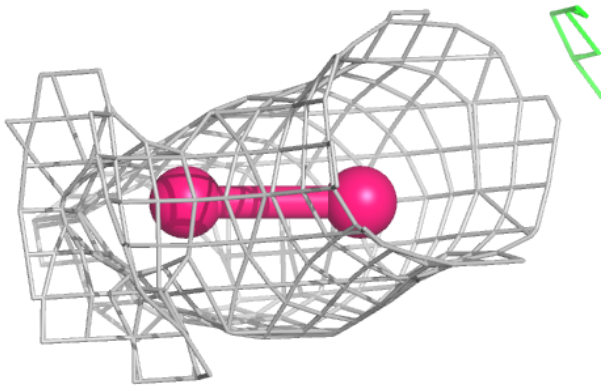
Electron density around OXY A 401:

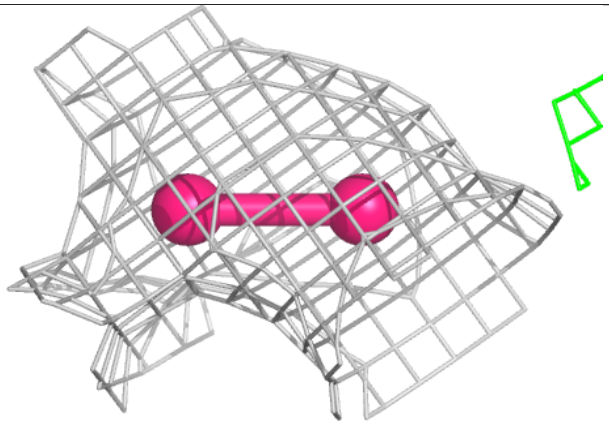
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

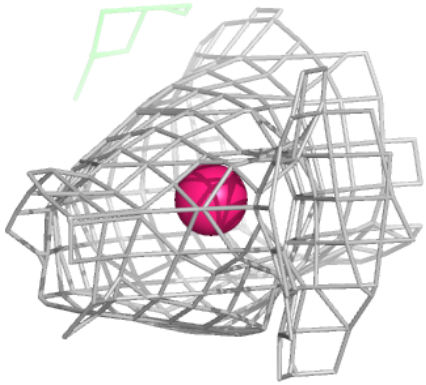


Electron density around PER D 401:

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

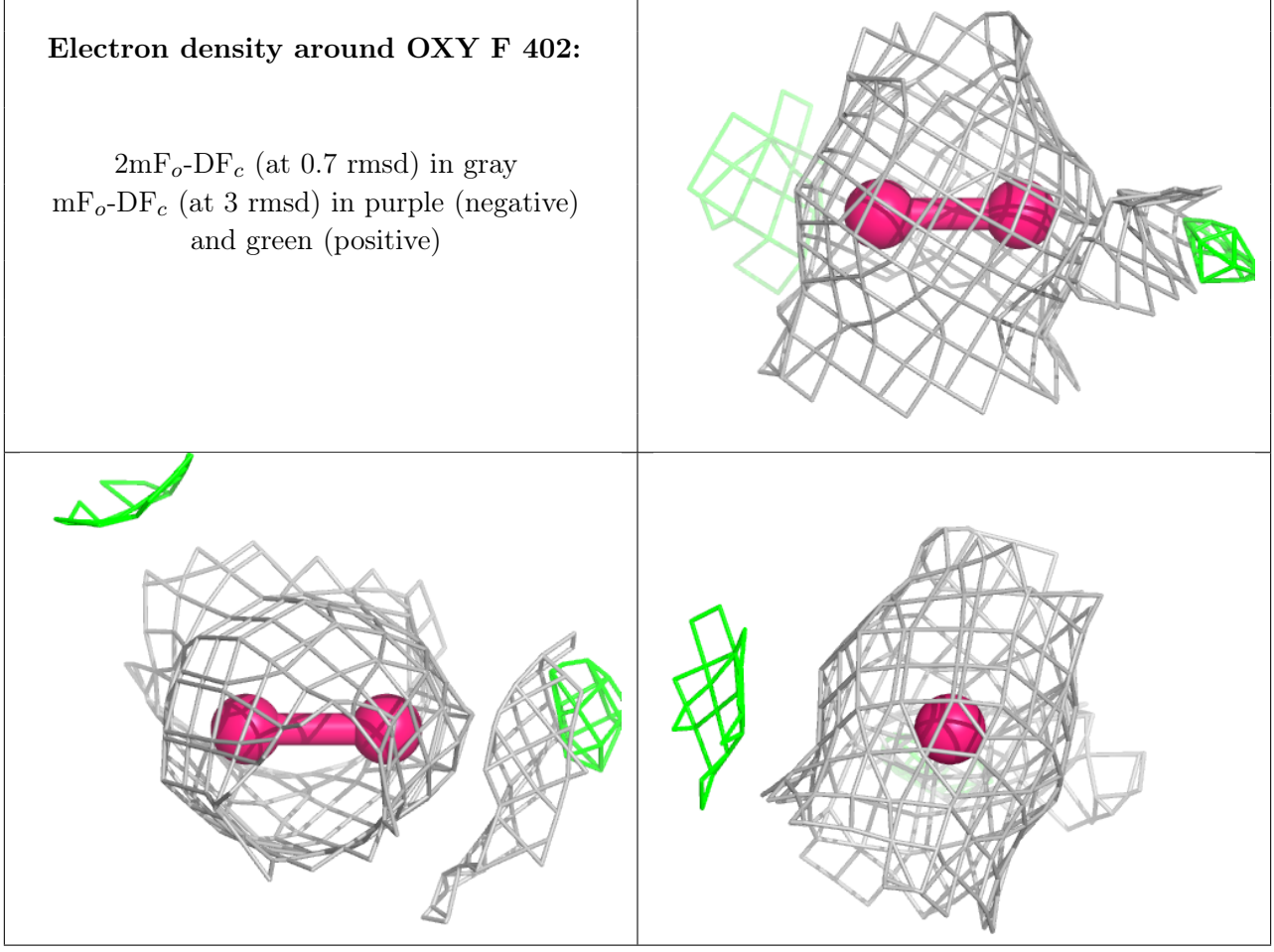






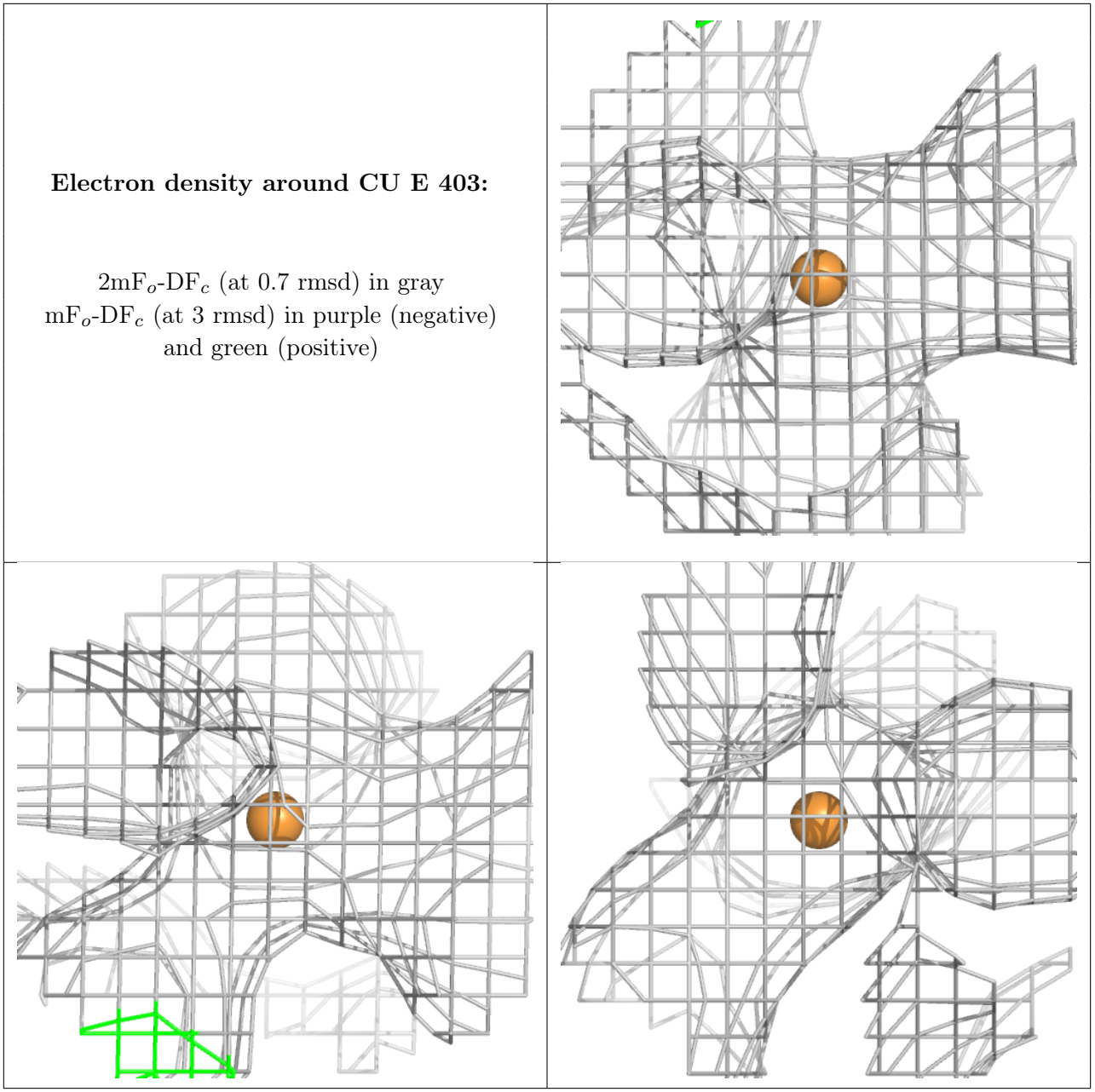
Electron density around OXY F 402:

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



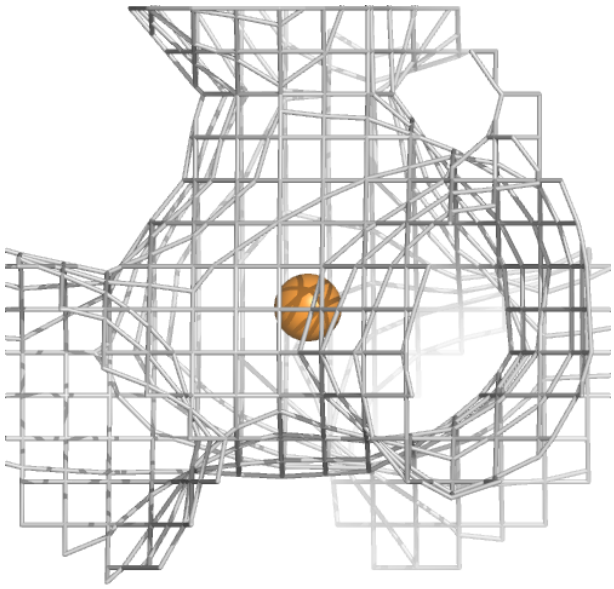
Electron density around CU E 403:

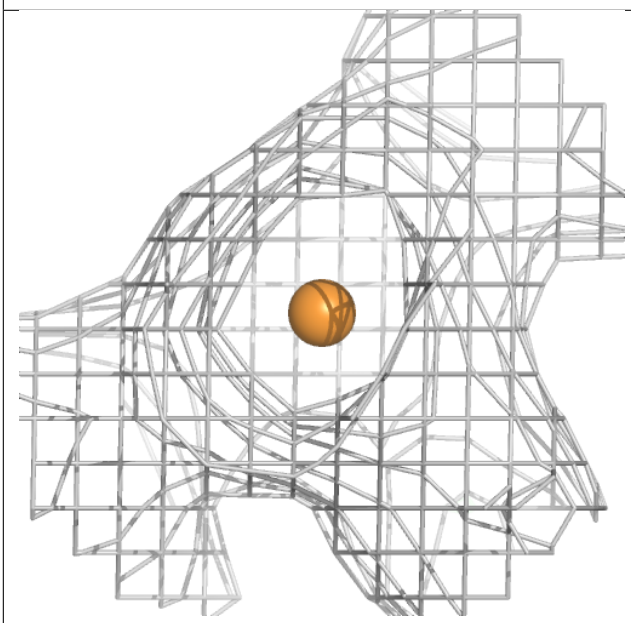
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

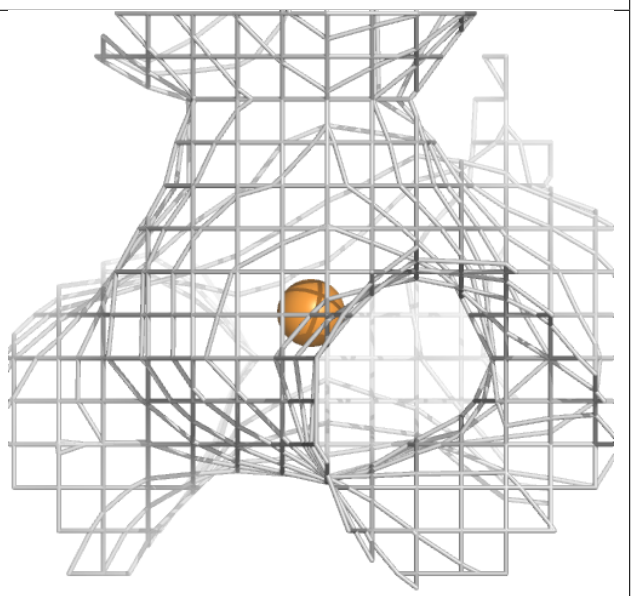


Electron density around CU A 404:

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

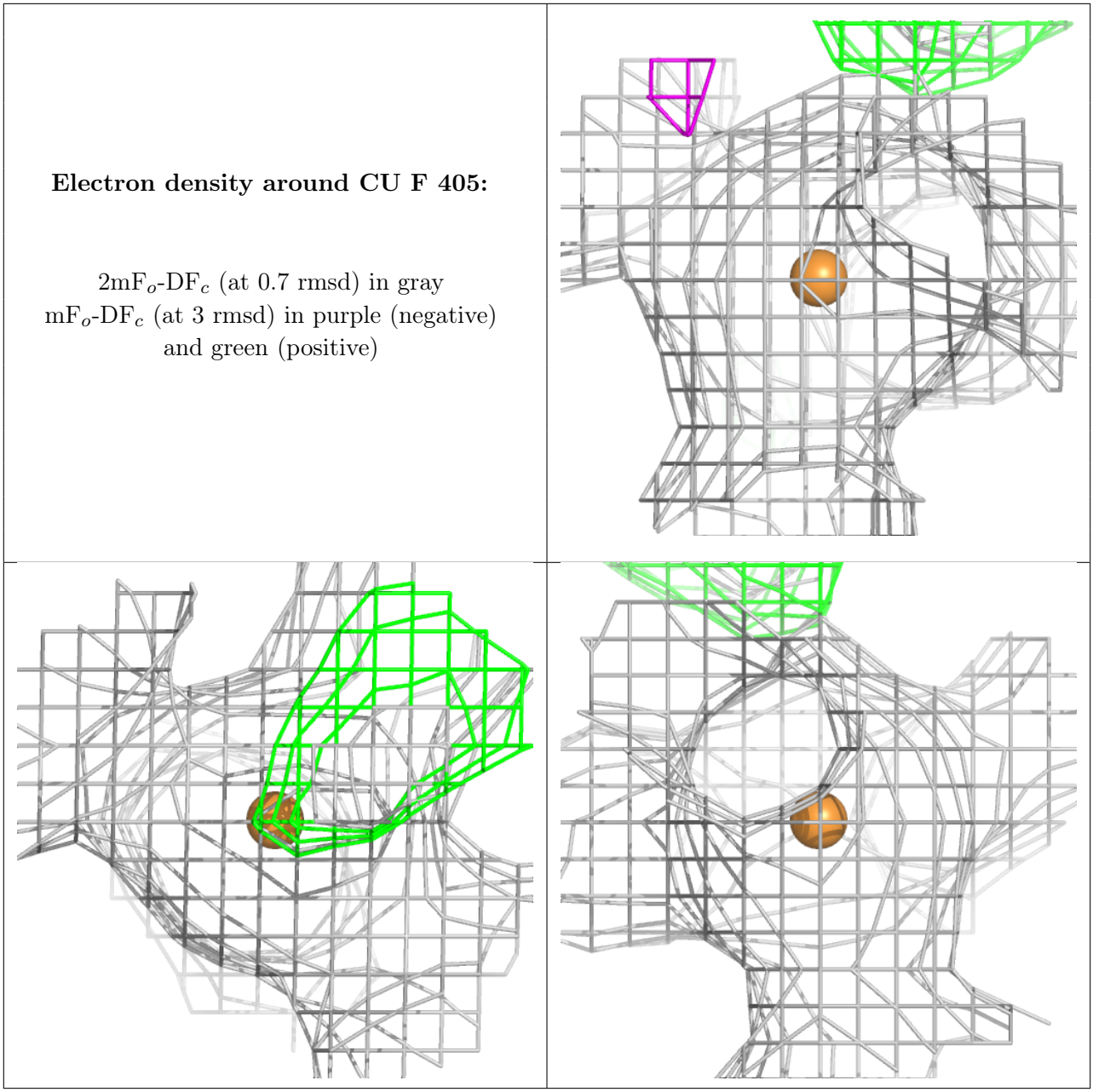






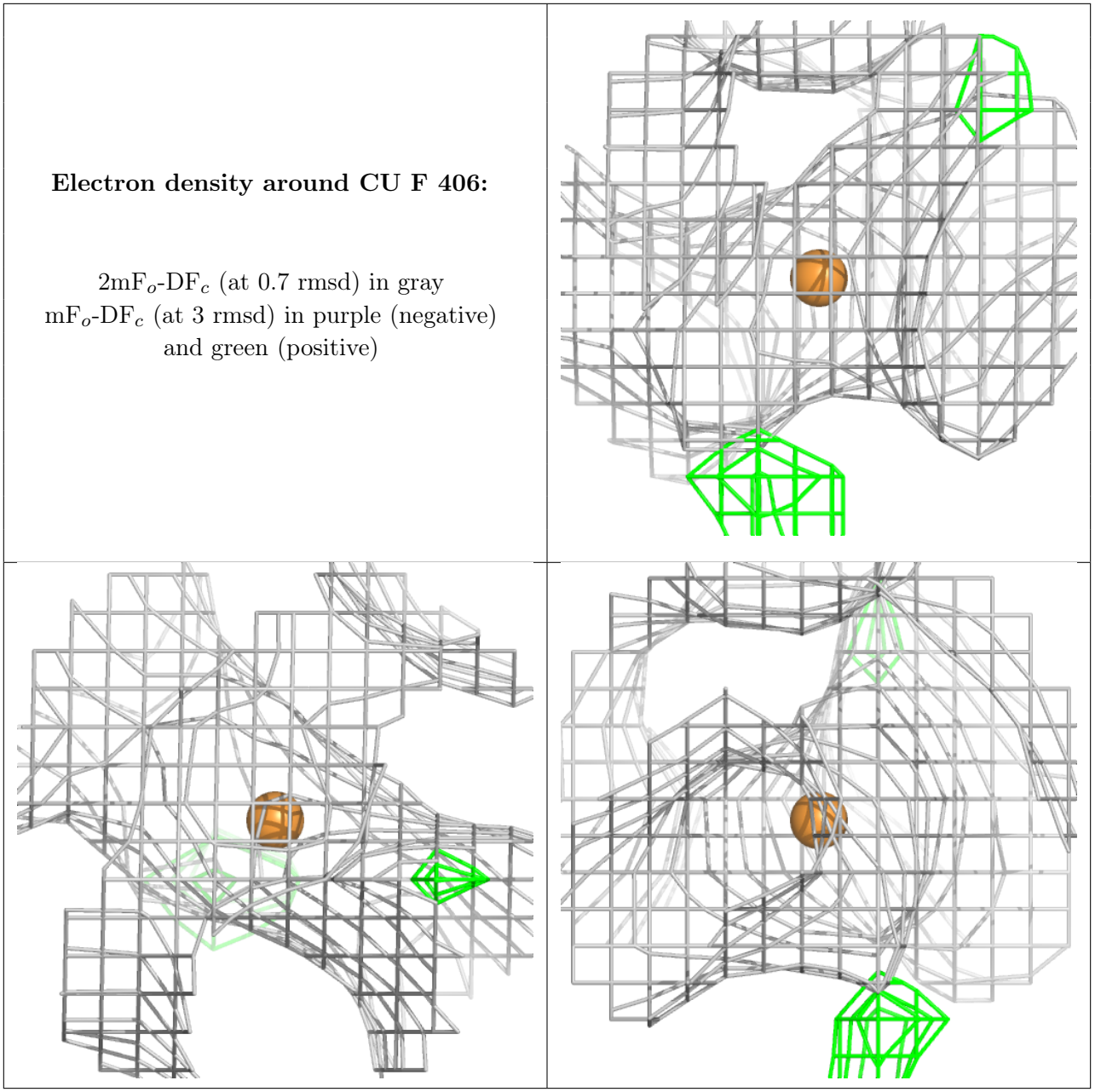
Electron density around CU F 405:

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



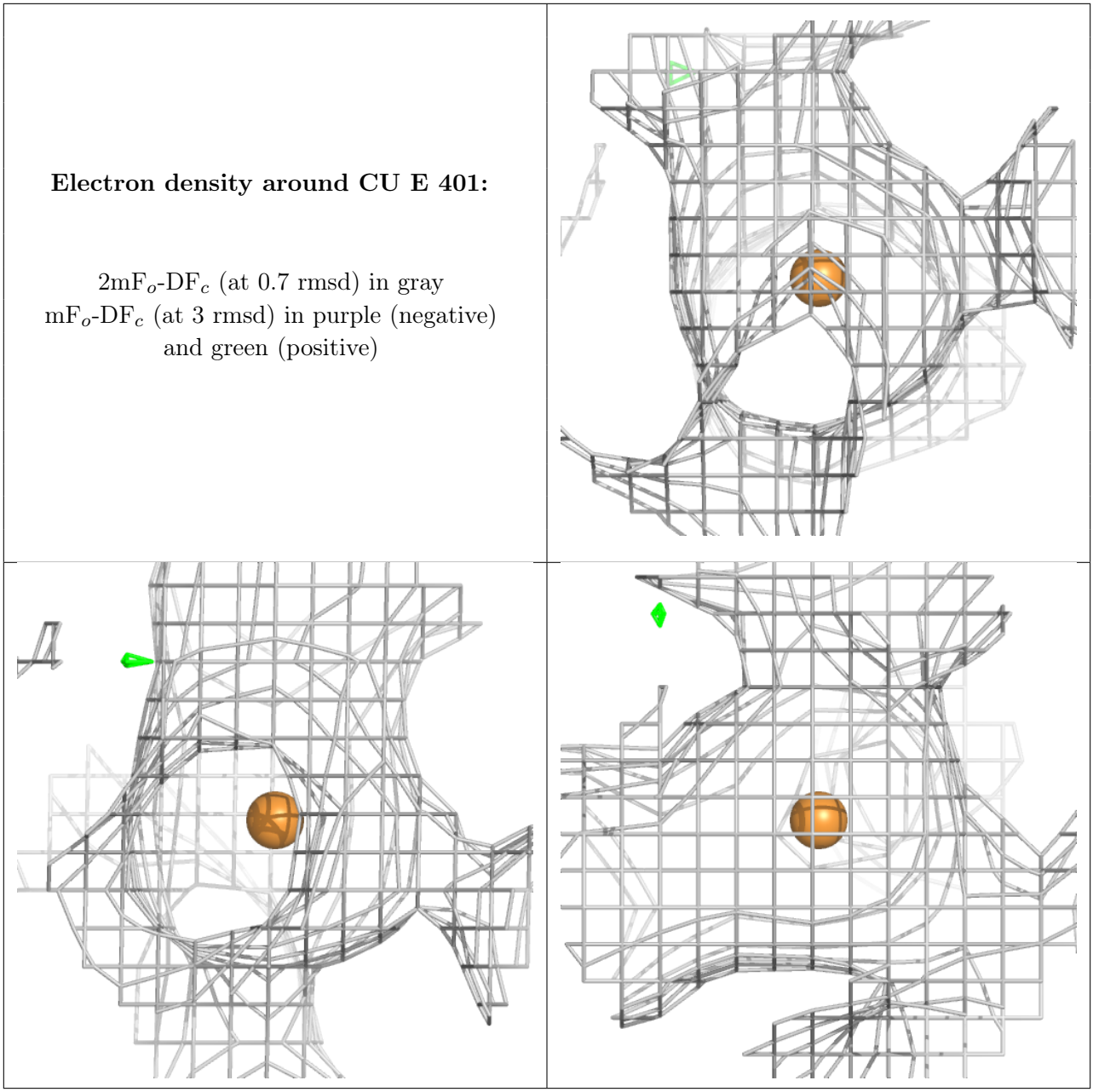
Electron density around CU F 406:

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



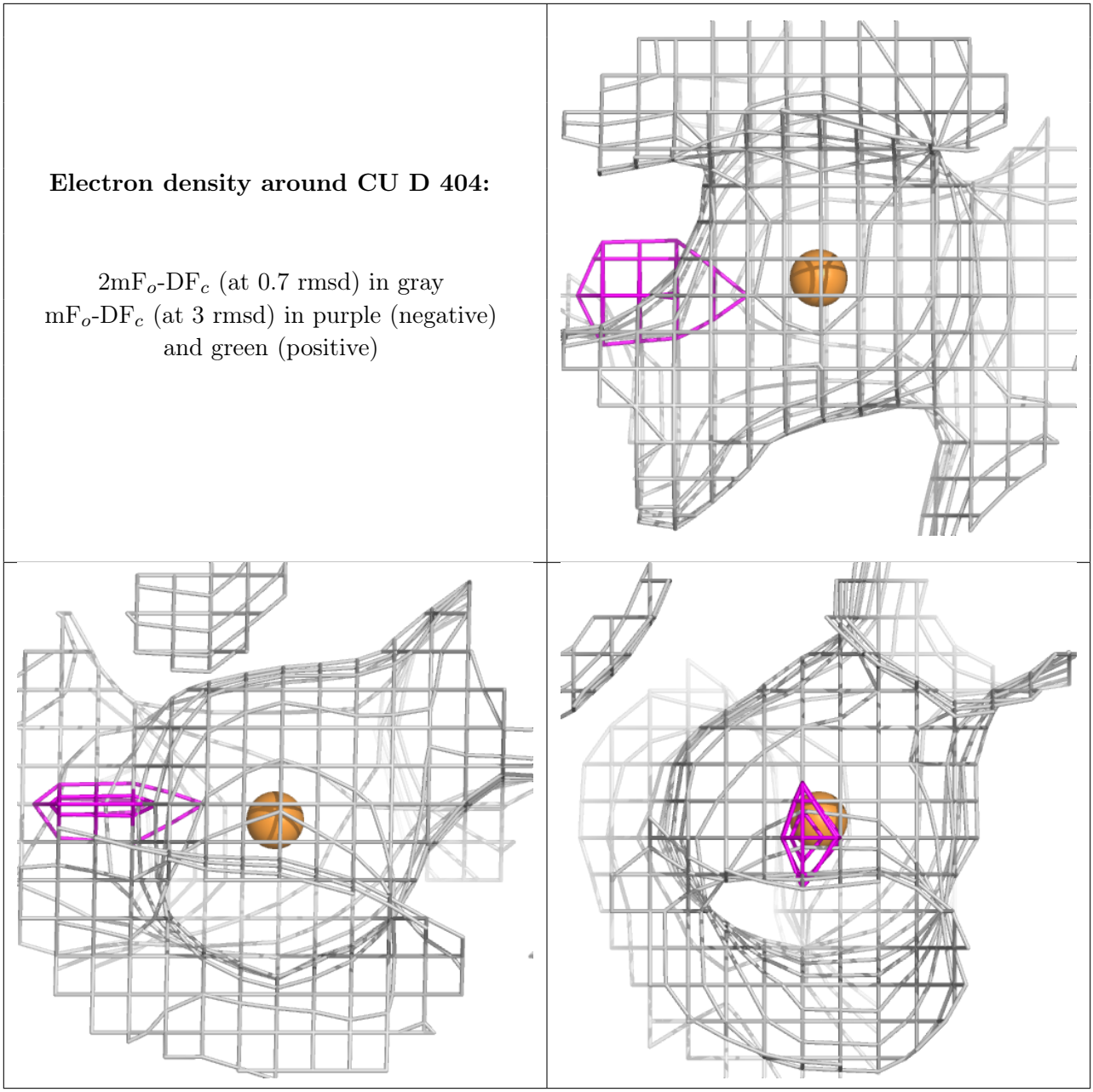
Electron density around CU E 401:

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



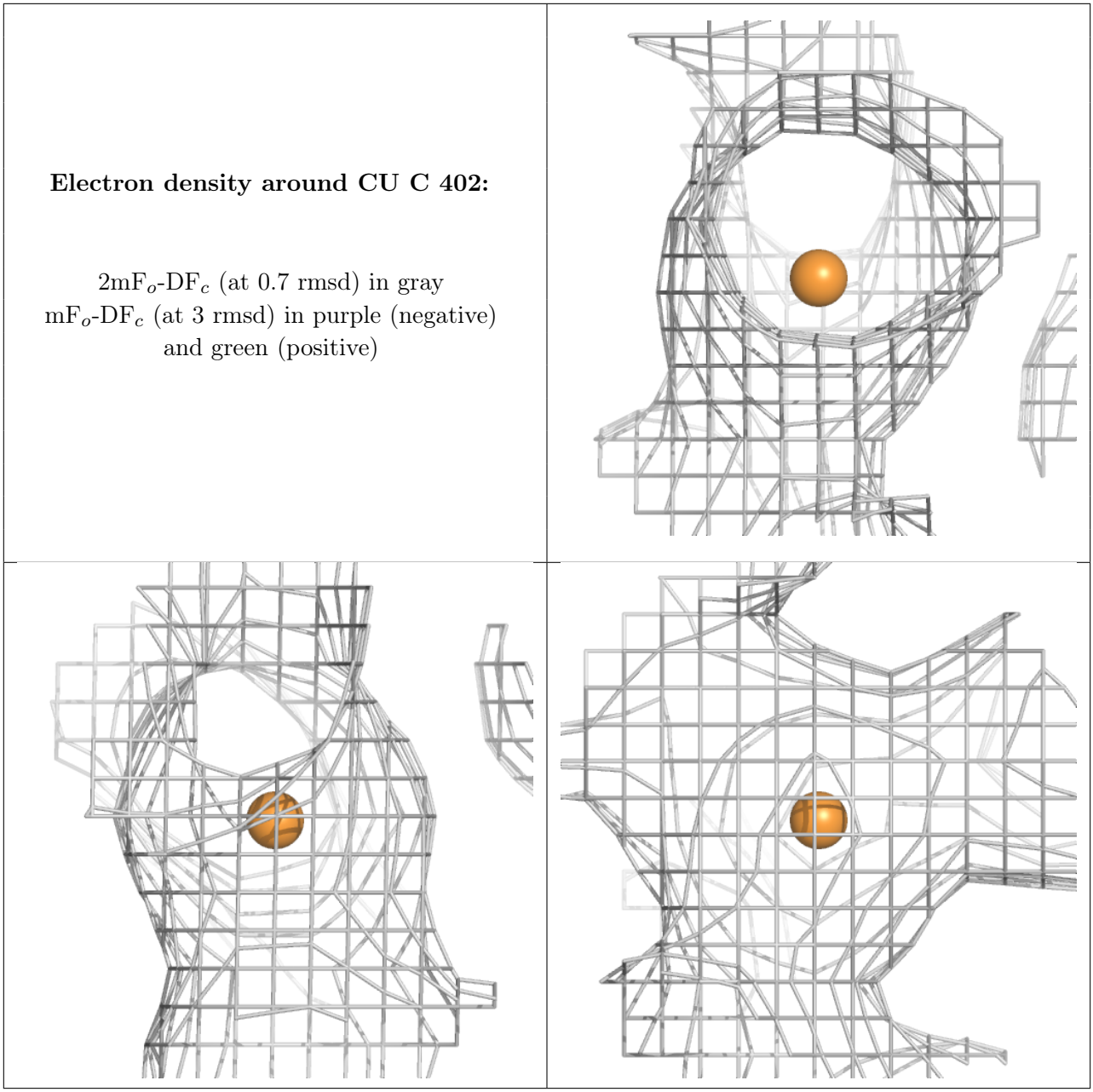
Electron density around CU D 404:

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



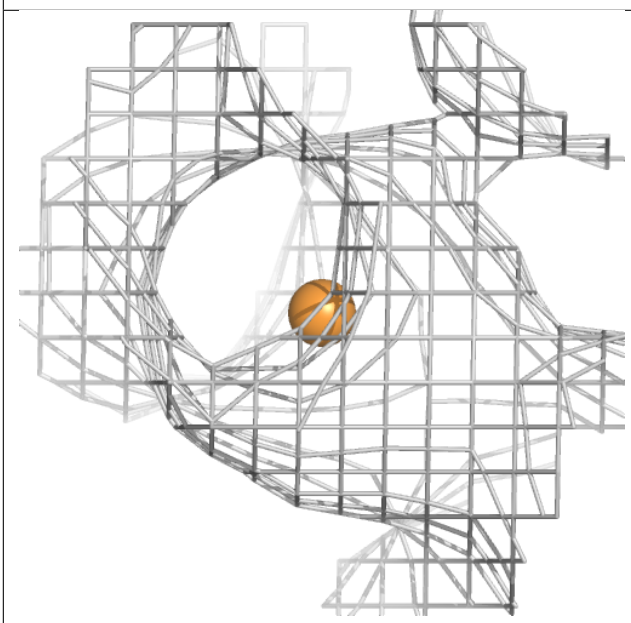
Electron density around CU C 402:

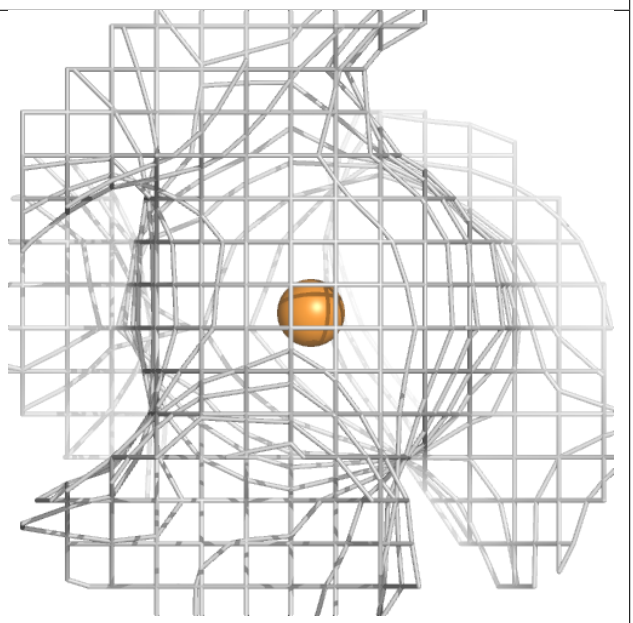
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CU F 404:

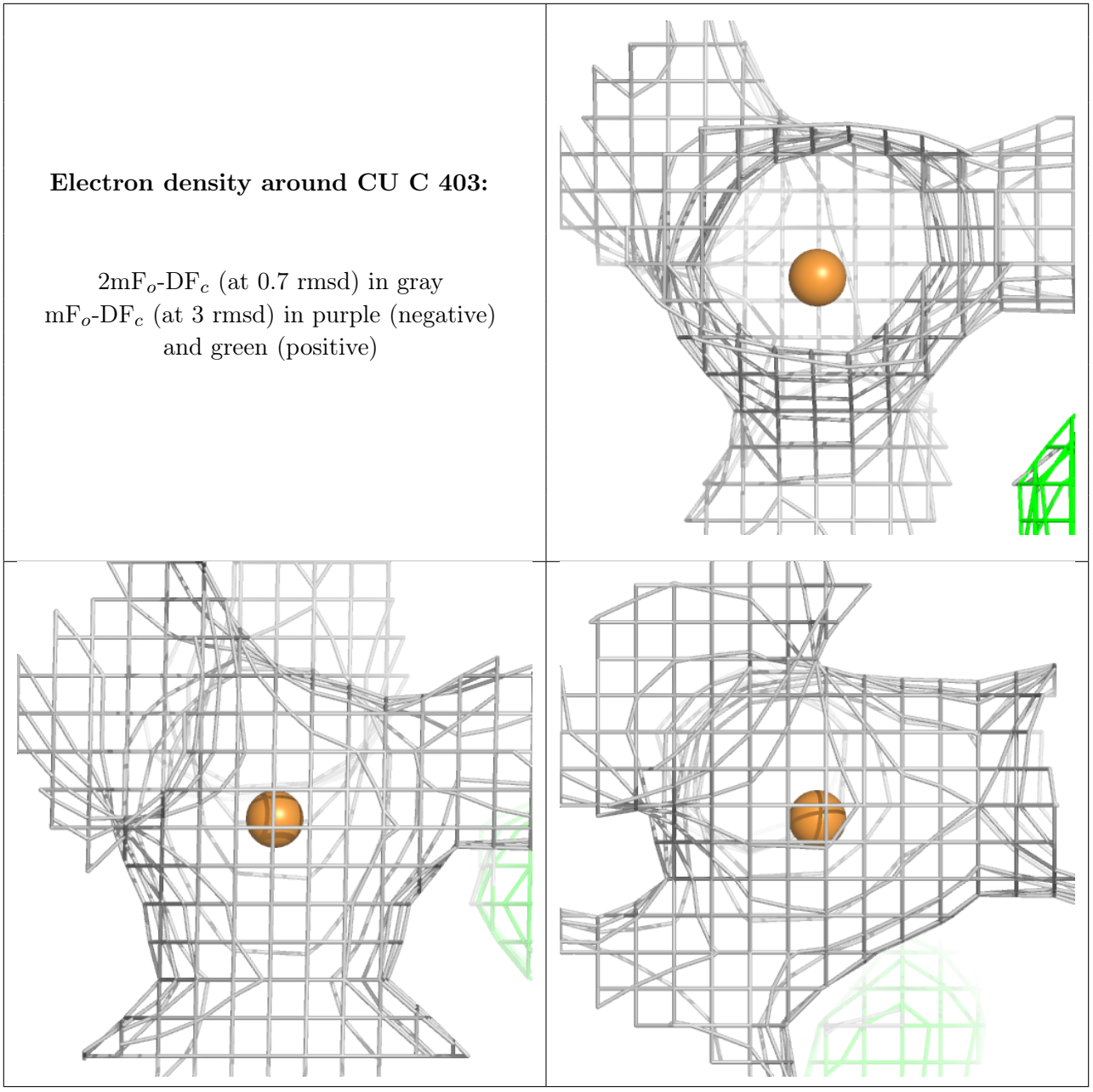
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





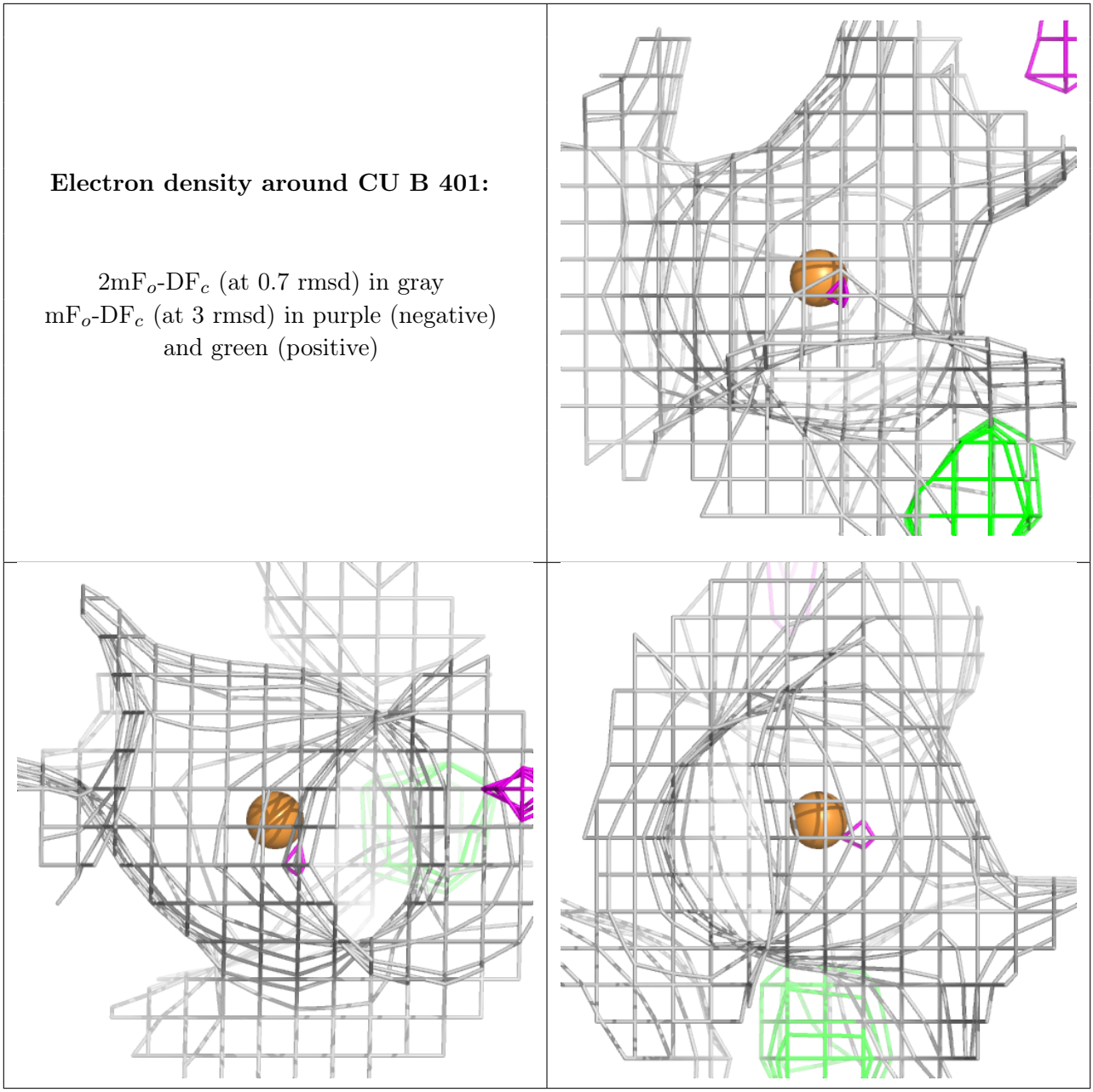
Electron density around CU C 403:

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



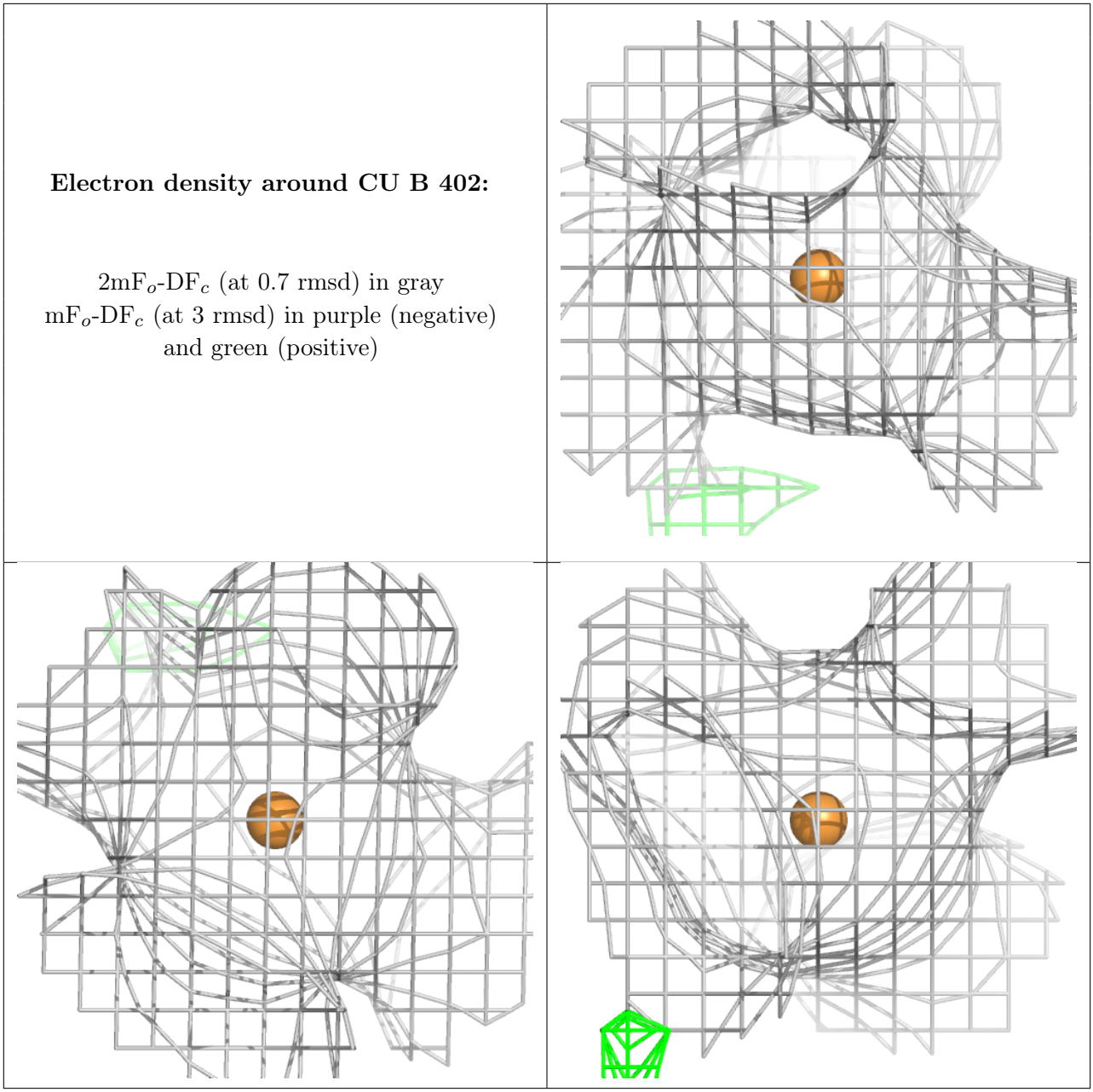
Electron density around CU B 401:

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



Electron density around CU 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)



6.5 Other polymers

There are no such residues in this entry.