wwPDB X-ray Structure Validation Summary Report (i)

Apr 30, 2024 – 02:32 PM JST

PDB ID	:	8Z76
Title	:	The structure of thiocyanate dehydrogenase from Pelomicrobium methylotrophicum (pmTcDH), activated by crystals soaking with 1 mM CuCl2 during 6 months
Authors	:	Varfolomeeva, L.A.; Solovieva, A.Y.; Shipkov, N.S.; Dergousova, N.I.; Boyko, K.M.; Tikhonova, T.V.; Popov, V.O.
Deposited on	:	2024-04-19
Resolution	:	1.80 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

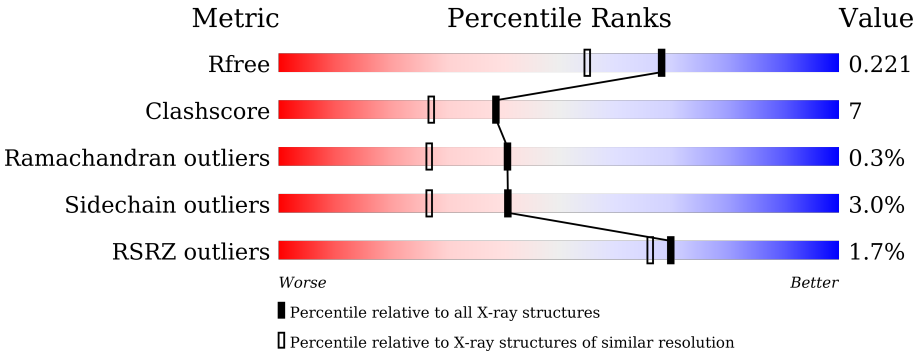
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	489	2% 80% 13% • 5%
1	B	489	% 83% 10% • 5%
1	C	489	2% 77% 15% • 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11754 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 Twin-arginine translocation signal domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	55	7	0
			3632	2334	613	671	14			
1	B	463	Total	C	N	O	S	23	4	0
			3609	2320	609	666	14			
1	C	463	Total	C	N	O	S	35	14	0
			3678	2364	622	678	14			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP A0A5C7ETD9
A	26	GLY	-	expression tag	UNP A0A5C7ETD9
A	27	SER	-	expression tag	UNP A0A5C7ETD9
A	28	ASP	-	expression tag	UNP A0A5C7ETD9
A	29	LYS	-	expression tag	UNP A0A5C7ETD9
A	30	ILE	-	expression tag	UNP A0A5C7ETD9
A	31	HIS	-	expression tag	UNP A0A5C7ETD9
A	32	HIS	-	expression tag	UNP A0A5C7ETD9
A	33	HIS	-	expression tag	UNP A0A5C7ETD9
A	34	HIS	-	expression tag	UNP A0A5C7ETD9
A	35	HIS	-	expression tag	UNP A0A5C7ETD9
A	36	HIS	-	expression tag	UNP A0A5C7ETD9
A	37	GLU	-	expression tag	UNP A0A5C7ETD9
A	38	ASN	-	expression tag	UNP A0A5C7ETD9
A	39	LEU	-	expression tag	UNP A0A5C7ETD9
A	40	TYR	-	expression tag	UNP A0A5C7ETD9
A	41	PHE	-	expression tag	UNP A0A5C7ETD9
A	42	GLN	-	expression tag	UNP A0A5C7ETD9
A	43	GLY	-	expression tag	UNP A0A5C7ETD9
A	44	HIS	-	expression tag	UNP A0A5C7ETD9
A	45	MET	-	expression tag	UNP A0A5C7ETD9
B	25	MET	-	initiating methionine	UNP A0A5C7ETD9
B	26	GLY	-	expression tag	UNP A0A5C7ETD9

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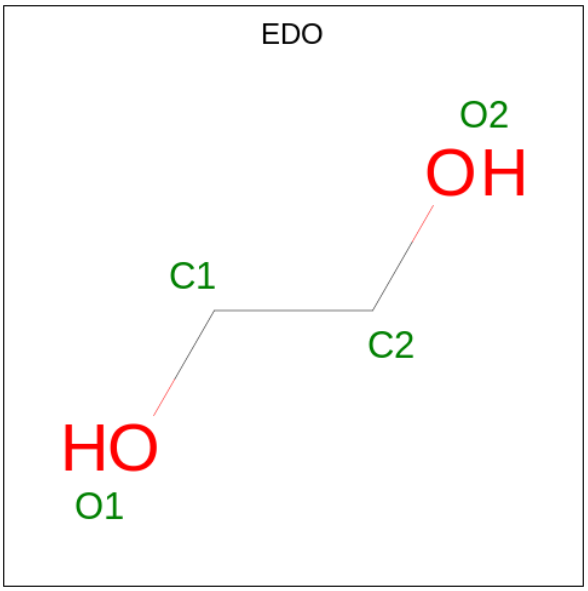
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	SER	-	expression tag	UNP A0A5C7ETD9
B	28	ASP	-	expression tag	UNP A0A5C7ETD9
B	29	LYS	-	expression tag	UNP A0A5C7ETD9
B	30	ILE	-	expression tag	UNP A0A5C7ETD9
B	31	HIS	-	expression tag	UNP A0A5C7ETD9
B	32	HIS	-	expression tag	UNP A0A5C7ETD9
B	33	HIS	-	expression tag	UNP A0A5C7ETD9
B	34	HIS	-	expression tag	UNP A0A5C7ETD9
B	35	HIS	-	expression tag	UNP A0A5C7ETD9
B	36	HIS	-	expression tag	UNP A0A5C7ETD9
B	37	GLU	-	expression tag	UNP A0A5C7ETD9
B	38	ASN	-	expression tag	UNP A0A5C7ETD9
B	39	LEU	-	expression tag	UNP A0A5C7ETD9
B	40	TYR	-	expression tag	UNP A0A5C7ETD9
B	41	PHE	-	expression tag	UNP A0A5C7ETD9
B	42	GLN	-	expression tag	UNP A0A5C7ETD9
B	43	GLY	-	expression tag	UNP A0A5C7ETD9
B	44	HIS	-	expression tag	UNP A0A5C7ETD9
B	45	MET	-	expression tag	UNP A0A5C7ETD9
C	25	MET	-	initiating methionine	UNP A0A5C7ETD9
C	26	GLY	-	expression tag	UNP A0A5C7ETD9
C	27	SER	-	expression tag	UNP A0A5C7ETD9
C	28	ASP	-	expression tag	UNP A0A5C7ETD9
C	29	LYS	-	expression tag	UNP A0A5C7ETD9
C	30	ILE	-	expression tag	UNP A0A5C7ETD9
C	31	HIS	-	expression tag	UNP A0A5C7ETD9
C	32	HIS	-	expression tag	UNP A0A5C7ETD9
C	33	HIS	-	expression tag	UNP A0A5C7ETD9
C	34	HIS	-	expression tag	UNP A0A5C7ETD9
C	35	HIS	-	expression tag	UNP A0A5C7ETD9
C	36	HIS	-	expression tag	UNP A0A5C7ETD9
C	37	GLU	-	expression tag	UNP A0A5C7ETD9
C	38	ASN	-	expression tag	UNP A0A5C7ETD9
C	39	LEU	-	expression tag	UNP A0A5C7ETD9
C	40	TYR	-	expression tag	UNP A0A5C7ETD9
C	41	PHE	-	expression tag	UNP A0A5C7ETD9
C	42	GLN	-	expression tag	UNP A0A5C7ETD9
C	43	GLY	-	expression tag	UNP A0A5C7ETD9
C	44	HIS	-	expression tag	UNP A0A5C7ETD9
C	45	MET	-	expression tag	UNP A0A5C7ETD9

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 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 5 5	0	1
3	B	3	Total Cu 4 4	0	1
3	C	3	Total Cu 4 4	0	1

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

- Molecule 5 is water.

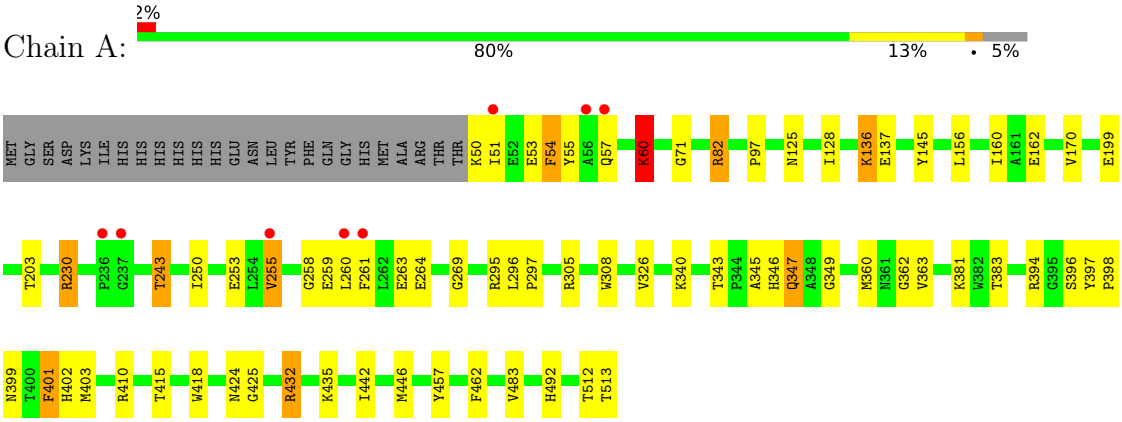
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	290	Total O 290 290	0	0
5	B	286	Total O 286 286	0	0
5	C	225	Total O 225 225	0	0

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.

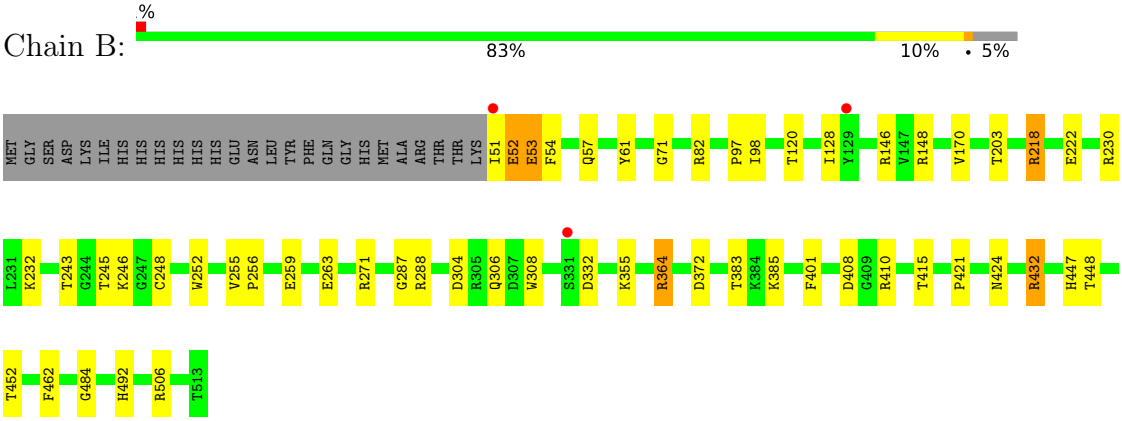
• Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain A:



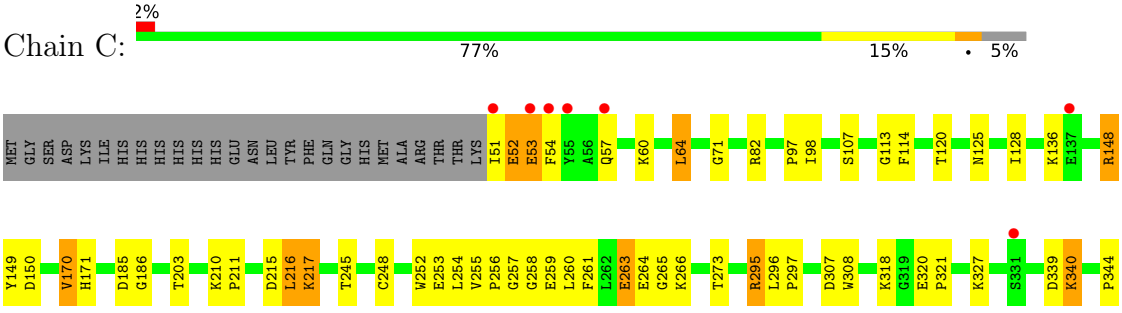
• Molecule 1: Twin-arginine translocation signal domain-containing protein

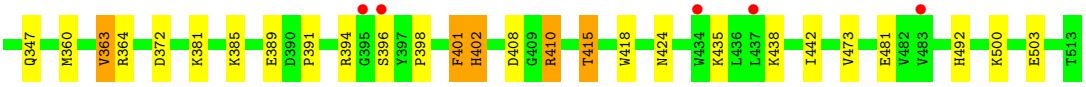
Chain B:



• Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain C:




Q347
M360
V363
R364
D372
K381
K385
E389
D390
P391
R394
G395
S396
Y397
P398
F401
H402
D408
G409
R410
T415
W418
N424
W434
K435
L436
L437
K438
I442
V473
E481
V482
V483
H492
K500
E503
T513

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	97.80Å 101.75Å 276.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.79 – 1.80 47.74 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.79-1.80) 98.8 (47.74-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.217 0.172 , 0.221	Depositor DCC
R_{free} test set	6278 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11754	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: CU, NA, EDO

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	0.94	8/3768 (0.2%)	1.30	18/5128 (0.4%)
1	B	0.74	2/3729 (0.1%)	1.16	14/5079 (0.3%)
1	C	1.10	6/3815 (0.2%)	1.18	18/5193 (0.3%)
All	All	0.94	16/11312 (0.1%)	1.22	50/15400 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	2
All	All	0	5

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	52	GLU	CA-CB	39.15	2.40	1.53
1	C	136	LYS	CE-NZ	-27.19	0.81	1.49
1	A	60	LYS	CD-CE	-26.08	0.86	1.51
1	C	60	LYS	CE-NZ	-24.92	0.86	1.49
1	A	137	GLU	CG-CD	17.96	1.78	1.51

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	LYS	CD-CE-NZ	18.06	153.24	111.70
1	C	52	GLU	N-CA-CB	-17.43	79.23	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	LYS	CG-CD-CE	17.29	163.76	111.90
1	A	136	LYS	CB-CG-CD	13.19	145.90	111.60
1	A	432	ARG	CB-CG-CD	12.85	145.01	111.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	462	PHE	Peptide
1	A	483	VAL	Peptide
1	B	462	PHE	Peptide
1	C	254	LEU	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3632	0	3571	49	0
1	B	3609	0	3550	33	0
1	C	3678	0	3614	83	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
2	C	4	0	6	0	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
4	A	1	0	0	0	0
5	A	290	0	0	5	0
5	B	286	0	0	2	0
5	C	225	0	0	8	0
All	All	11754	0	10765	160	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 7.

The worst 5 of 160 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260[B]:LEU:HB3	1:C:264:GLU:OE2	1.21	1.29
1:C:261[B]:PHE:CD1	1:C:266:LYS:HE2	1.69	1.27
1:C:261[B]:PHE:CD1	1:C:266:LYS:CE	2.29	1.16
1:C:260[B]:LEU:O	1:C:264:GLU:HG3	1.41	1.16
1:A:253[B]:GLU:OE2	5:A:701:HOH:O	1.72	1.08

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	469/489 (96%)	443 (94%)	25 (5%)	1 (0%)	47	33
1	B	465/489 (95%)	441 (95%)	23 (5%)	1 (0%)	47	33
1	C	475/489 (97%)	450 (95%)	23 (5%)	2 (0%)	34	21
All	All	1409/1467 (96%)	1334 (95%)	71 (5%)	4 (0%)	41	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	VAL
1	B	170	VAL
1	C	170	VAL
1	C	402	HIS

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	391/406 (96%)	377 (96%)	14 (4%)	35	20
1	B	387/406 (95%)	380 (98%)	7 (2%)	59	48
1	C	395/406 (97%)	382 (97%)	13 (3%)	38	23
All	All	1173/1218 (96%)	1139 (97%)	34 (3%)	41	29

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	363	VAL
1	C	396	SER
1	C	424	ASN
1	A	435	LYS
1	A	432	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	347	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 14 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	EDO	B	601	-	3,3,3	0.70	0	2,2,2	0.52	0
2	EDO	B	602	-	3,3,3	0.32	0	2,2,2	0.66	0
2	EDO	C	601	-	3,3,3	0.33	0	2,2,2	0.92	0
2	EDO	A	602	-	3,3,3	0.58	0	2,2,2	1.26	0
2	EDO	A	601	-	3,3,3	0.63	0	2,2,2	0.34	0

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
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	B	602	-	-	0/1/1/1	-
2	EDO	C	601	-	-	0/1/1/1	-
2	EDO	A	602	-	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-

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.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	464/489 (94%)	-0.23	8 (1%)	70	66	18, 26, 40, 68	16 (3%)
1	B	463/489 (94%)	-0.20	3 (0%)	89	87	19, 27, 43, 61	10 (2%)
1	C	463/489 (94%)	-0.07	12 (2%)	56	51	19, 30, 46, 82	17 (3%)
All	All	1390/1467 (94%)	-0.17	23 (1%)	70	66	18, 27, 44, 82	43 (3%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	54	PHE	4.7
1	A	51	ILE	3.5
1	C	51	ILE	3.4
1	C	53	GLU	3.3
1	C	331	SER	3.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

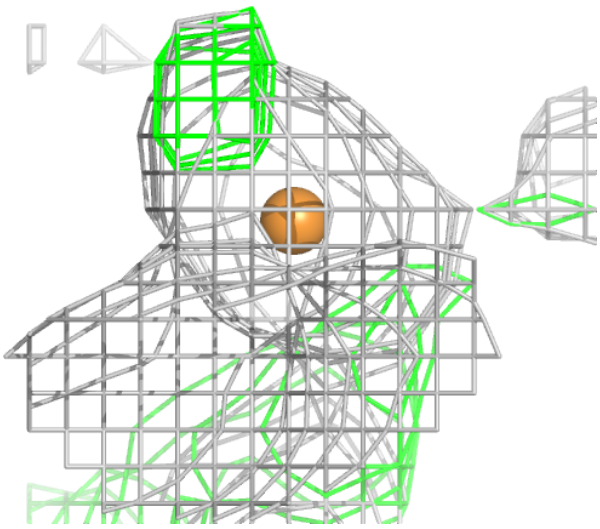
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

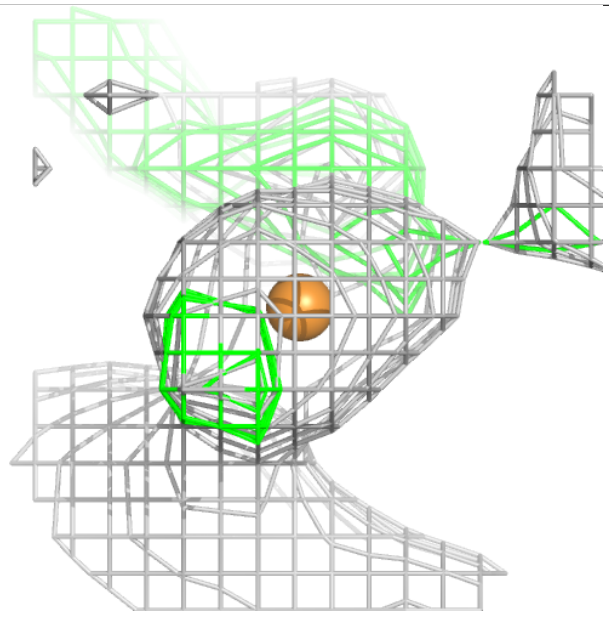
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	A	607	1/1	0.80	0.46	25,25,25,25	1
3	CU	A	606	1/1	0.86	0.32	35,35,35,35	1
2	EDO	B	602	4/4	0.90	0.13	20,21,22,24	4
2	EDO	A	602	4/4	0.91	0.24	17,19,22,29	4
2	EDO	A	601	4/4	0.95	0.13	29,30,30,33	0
2	EDO	C	601	4/4	0.95	0.11	27,31,34,35	0
2	EDO	B	601	4/4	0.98	0.06	30,32,35,38	0
3	CU	A	604[B]	1/1	1.00	0.07	27,27,27,27	1
3	CU	A	605	1/1	1.00	0.06	30,30,30,30	0
3	CU	A	603	1/1	1.00	0.07	26,26,26,26	0
3	CU	B	603	1/1	1.00	0.09	25,25,25,25	0
3	CU	B	604[A]	1/1	1.00	0.09	27,27,27,27	1
3	CU	B	604[B]	1/1	1.00	0.09	23,23,23,23	1
3	CU	B	605	1/1	1.00	0.09	25,25,25,25	0
3	CU	C	602	1/1	1.00	0.08	28,28,28,28	0
3	CU	C	603[A]	1/1	1.00	0.08	27,27,27,27	1
3	CU	C	603[B]	1/1	1.00	0.08	28,28,28,28	1
3	CU	C	604	1/1	1.00	0.06	30,30,30,30	0
3	CU	A	604[A]	1/1	1.00	0.07	24,24,24,24	1

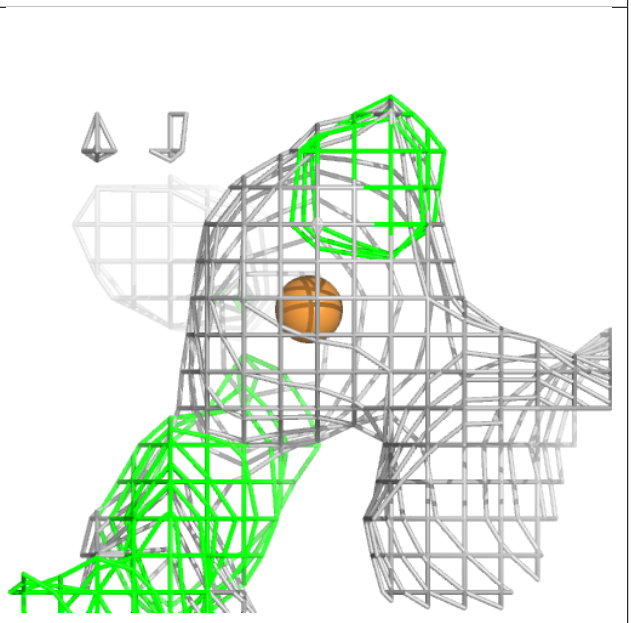
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CU A 606:

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

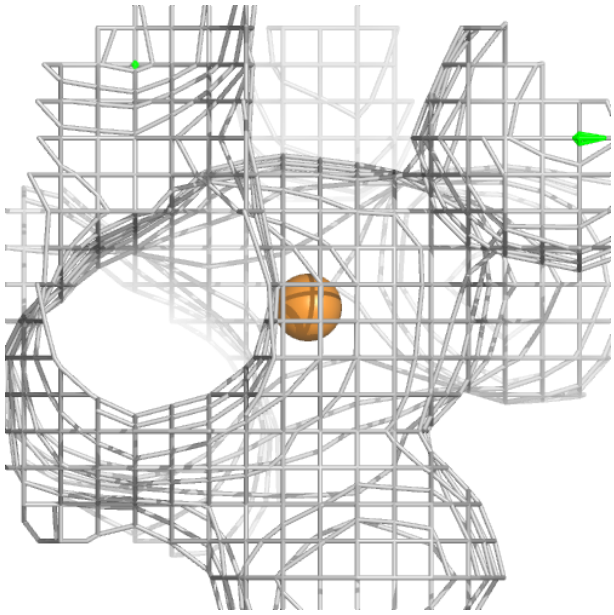


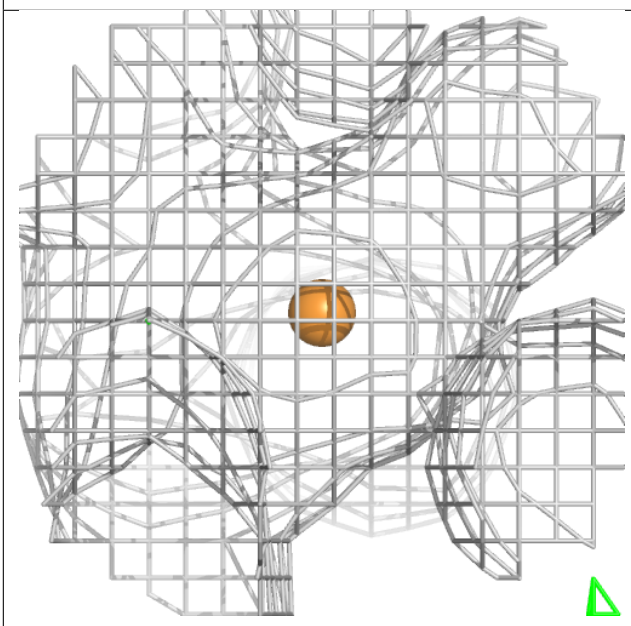


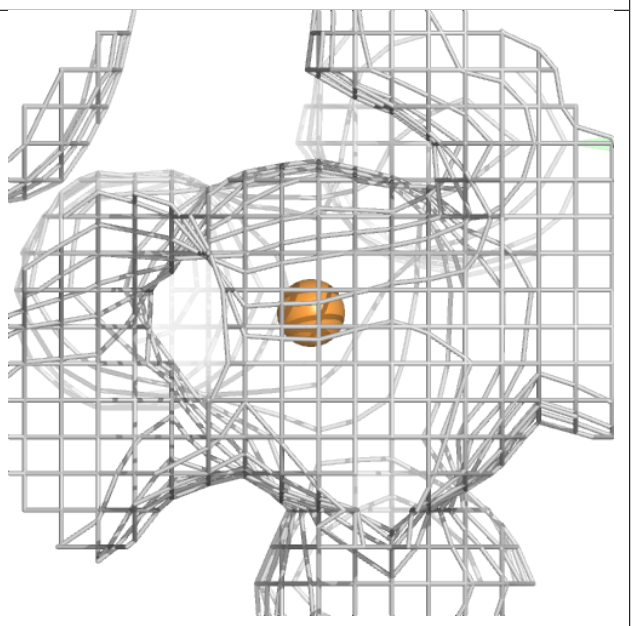


Electron density around CU A 604 (B):

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

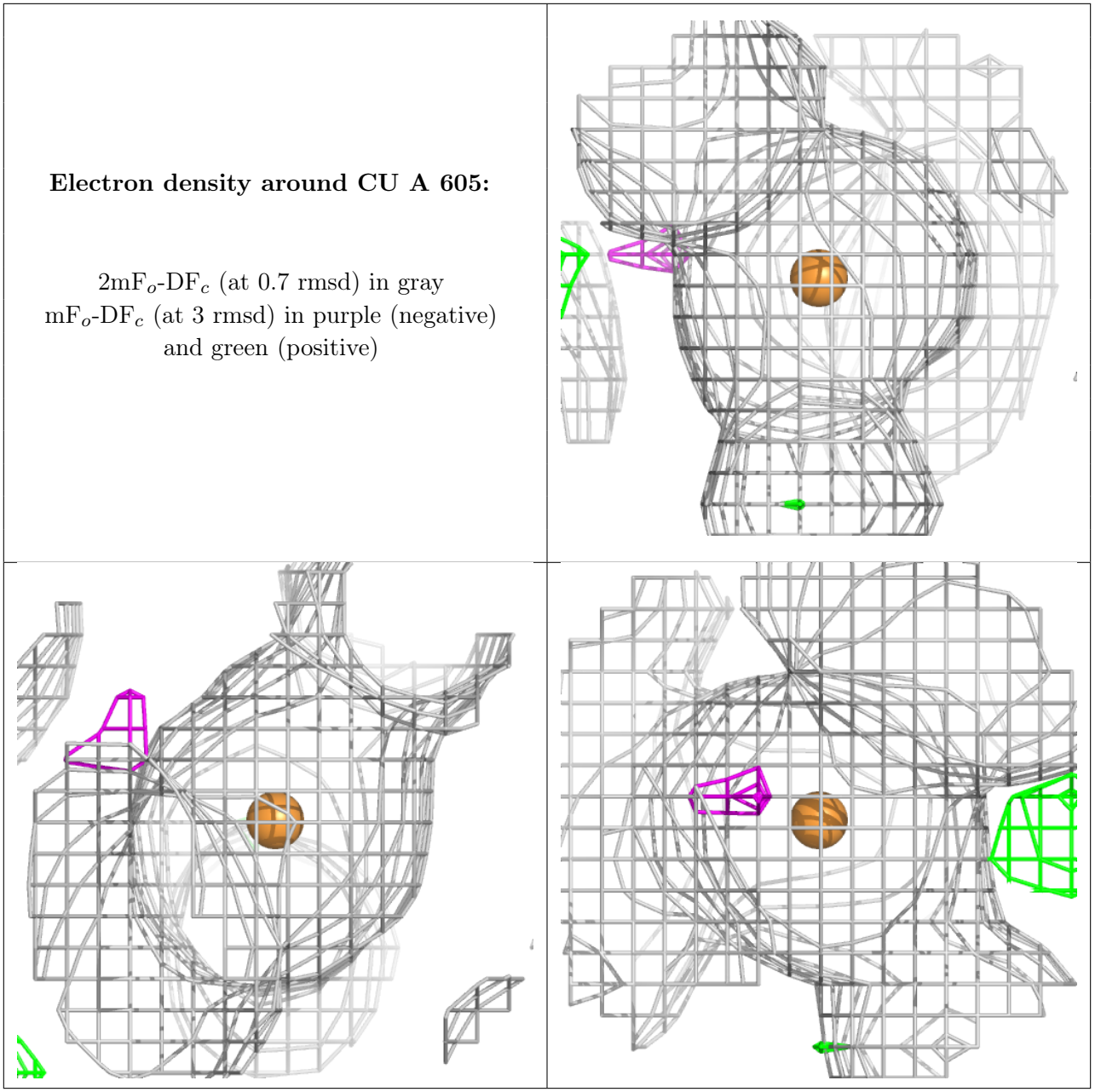






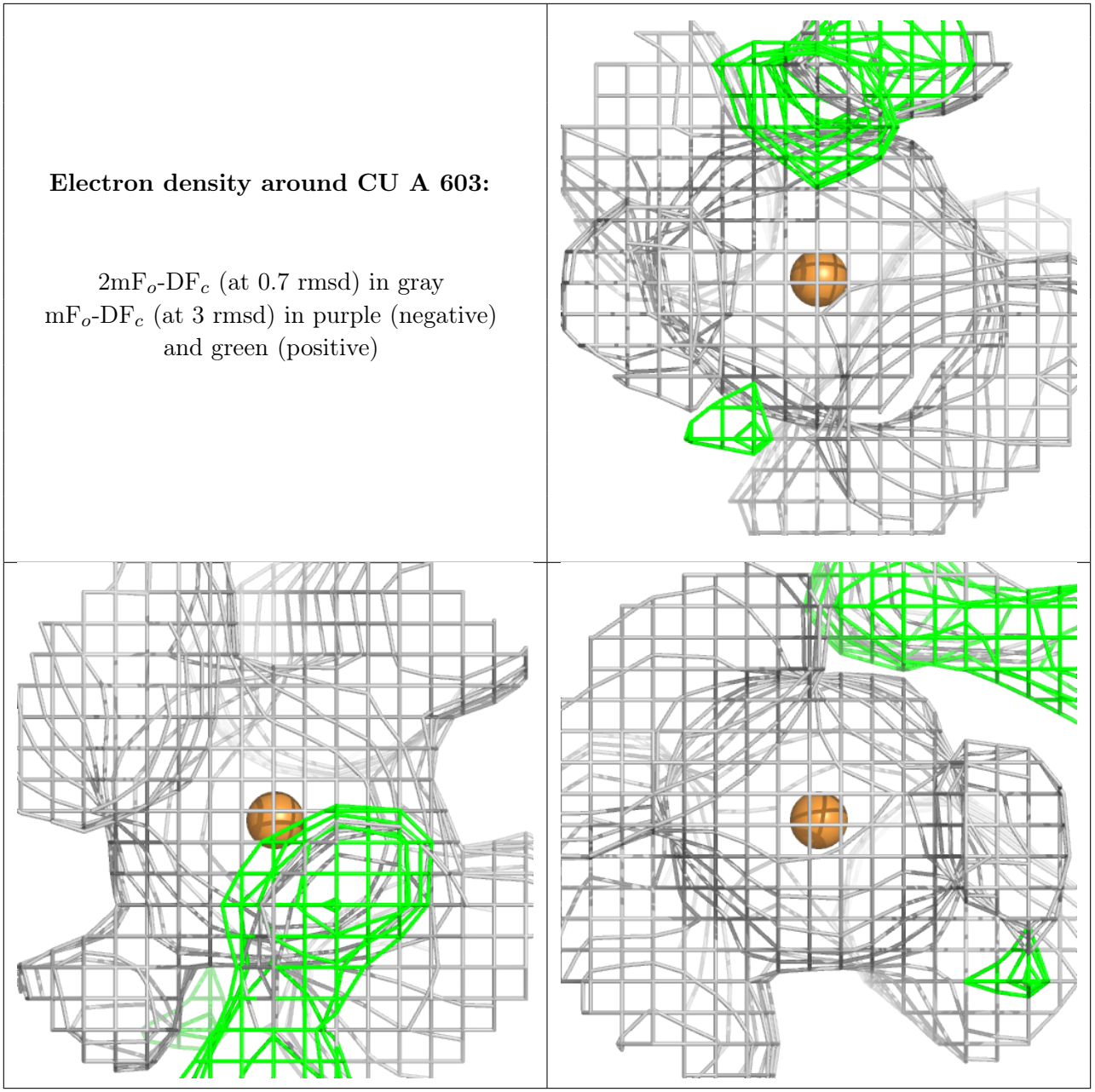
Electron density around CU A 605:

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



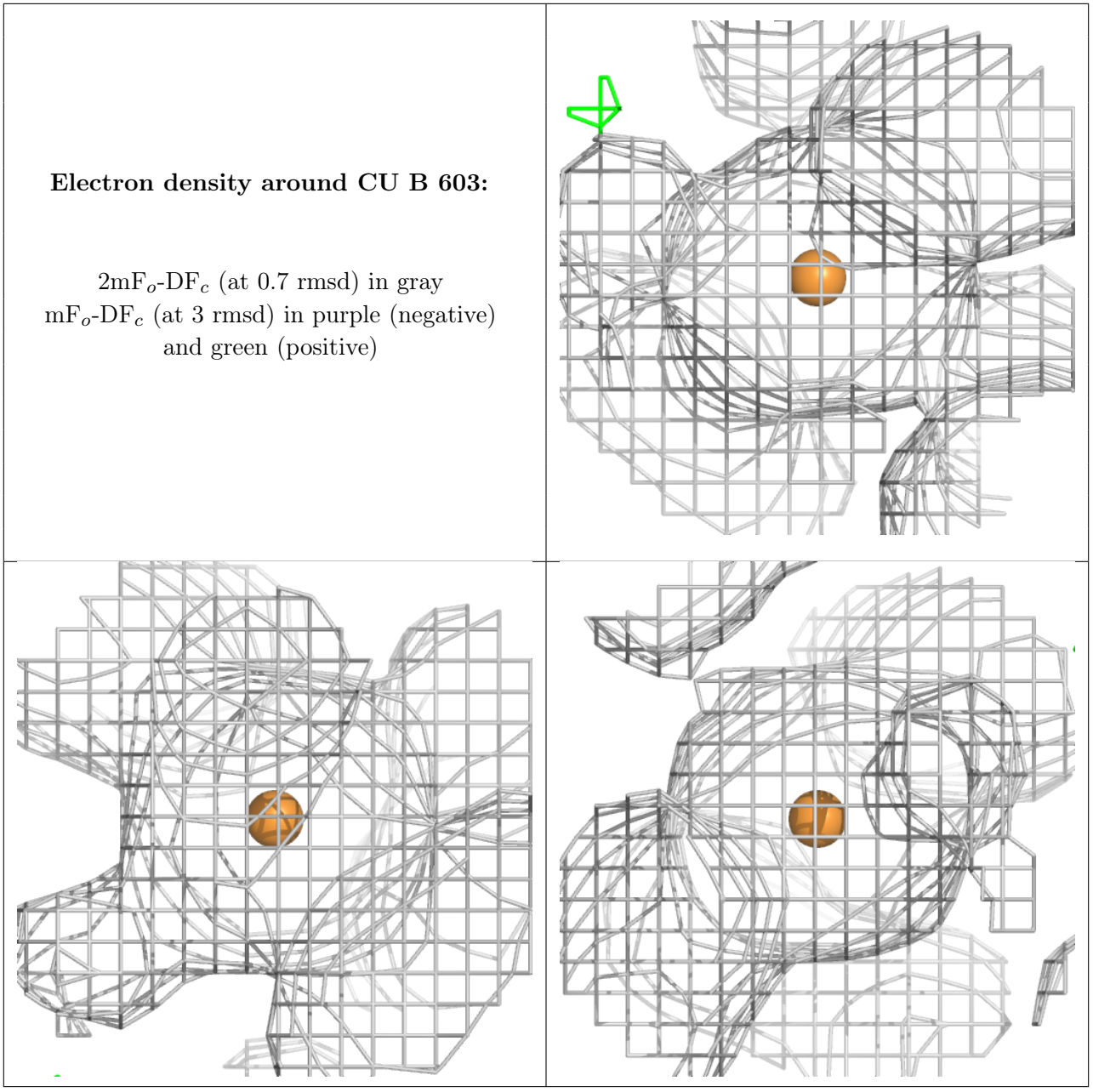
Electron density around CU A 603:

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



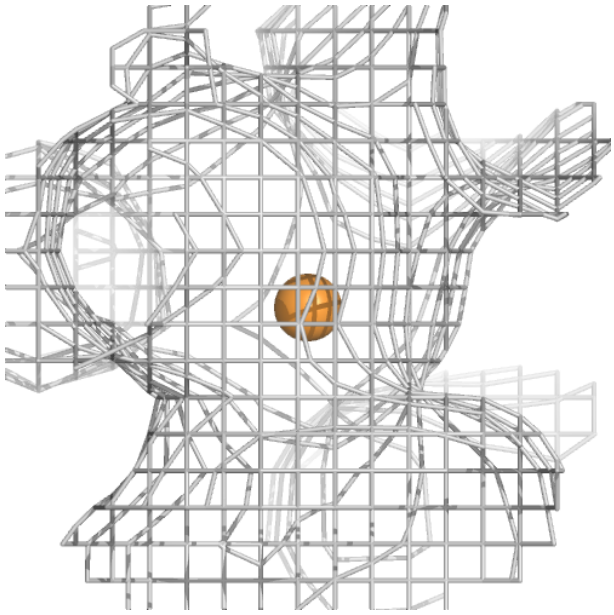
Electron density around CU B 603:

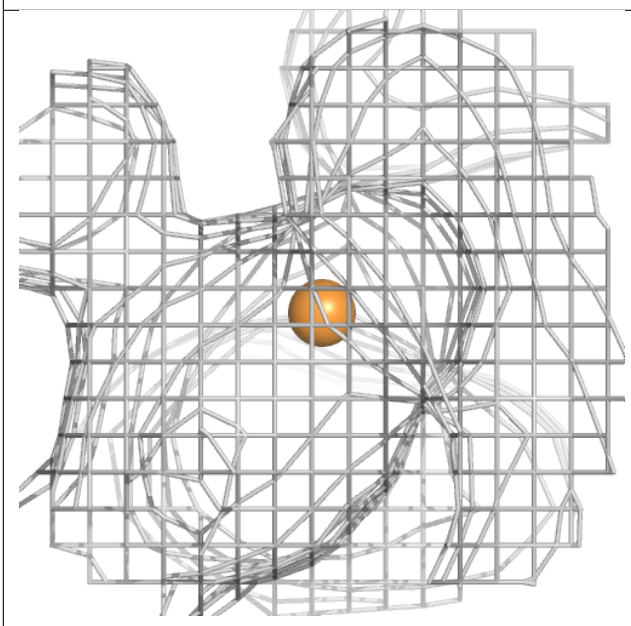
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CU B 604 (A):

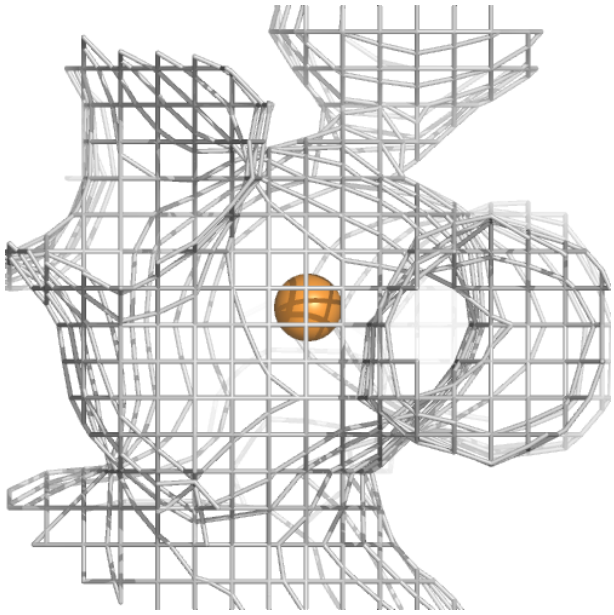
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

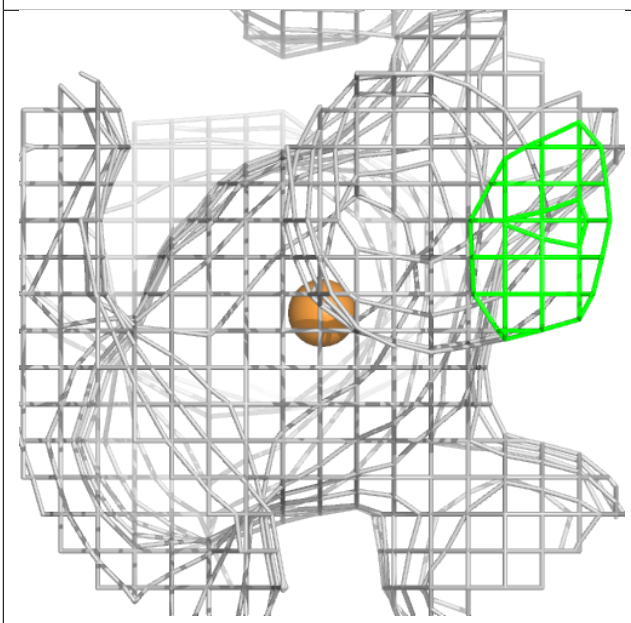


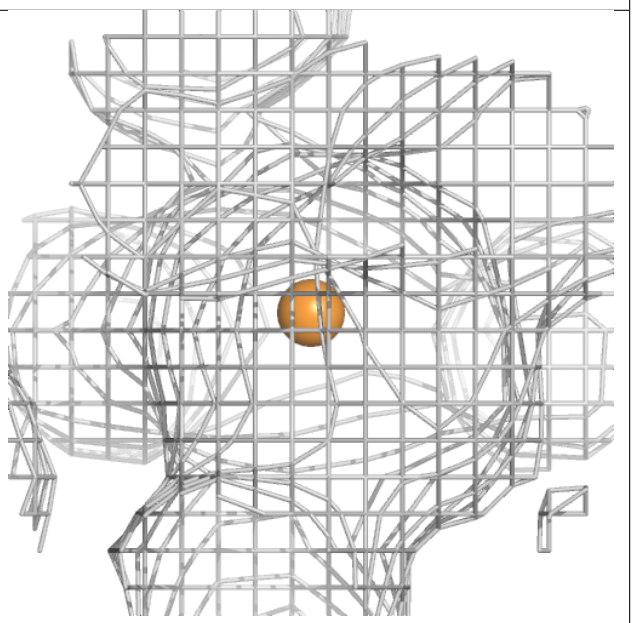


Electron density around CU B 604 (B):

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

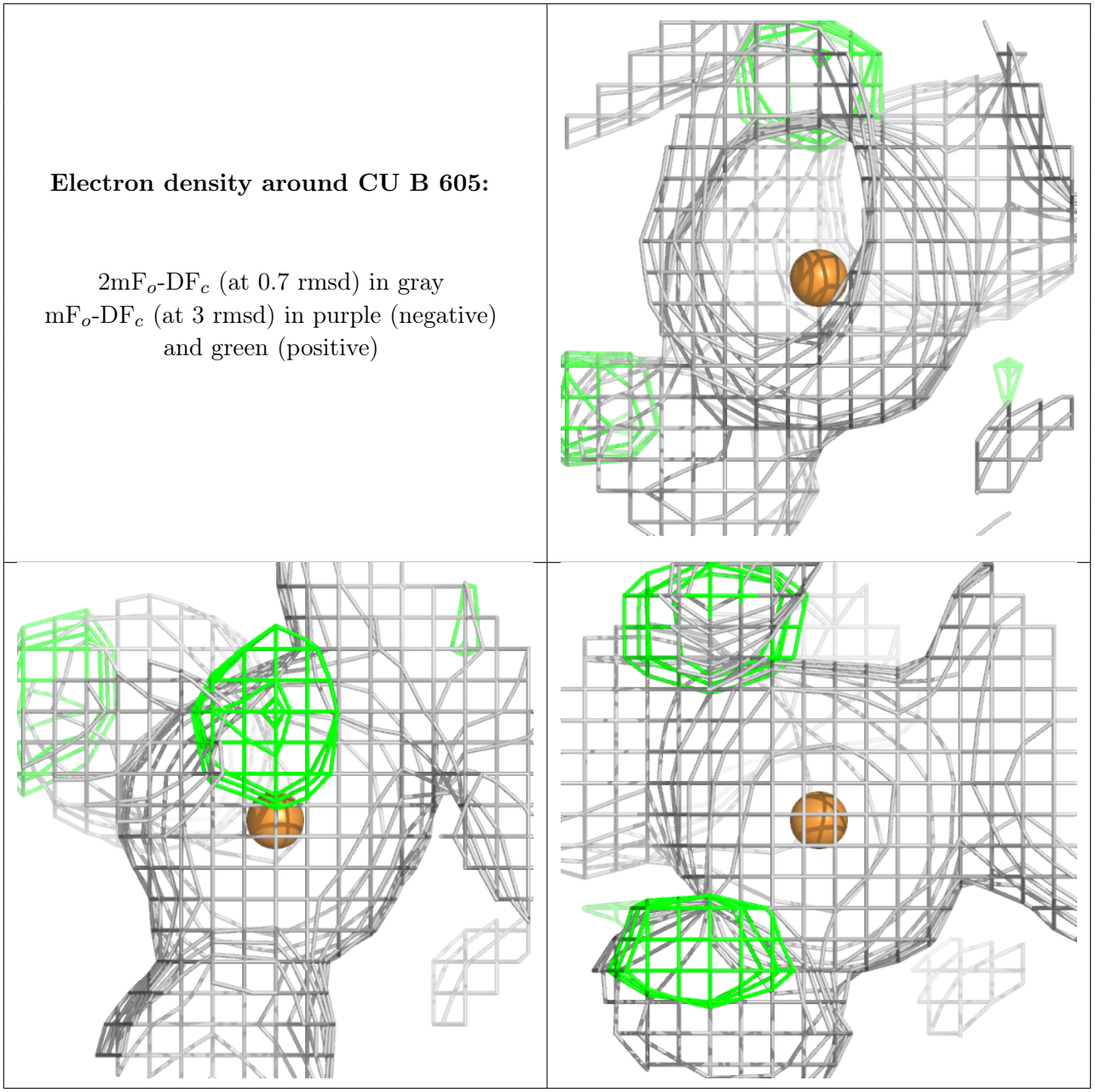






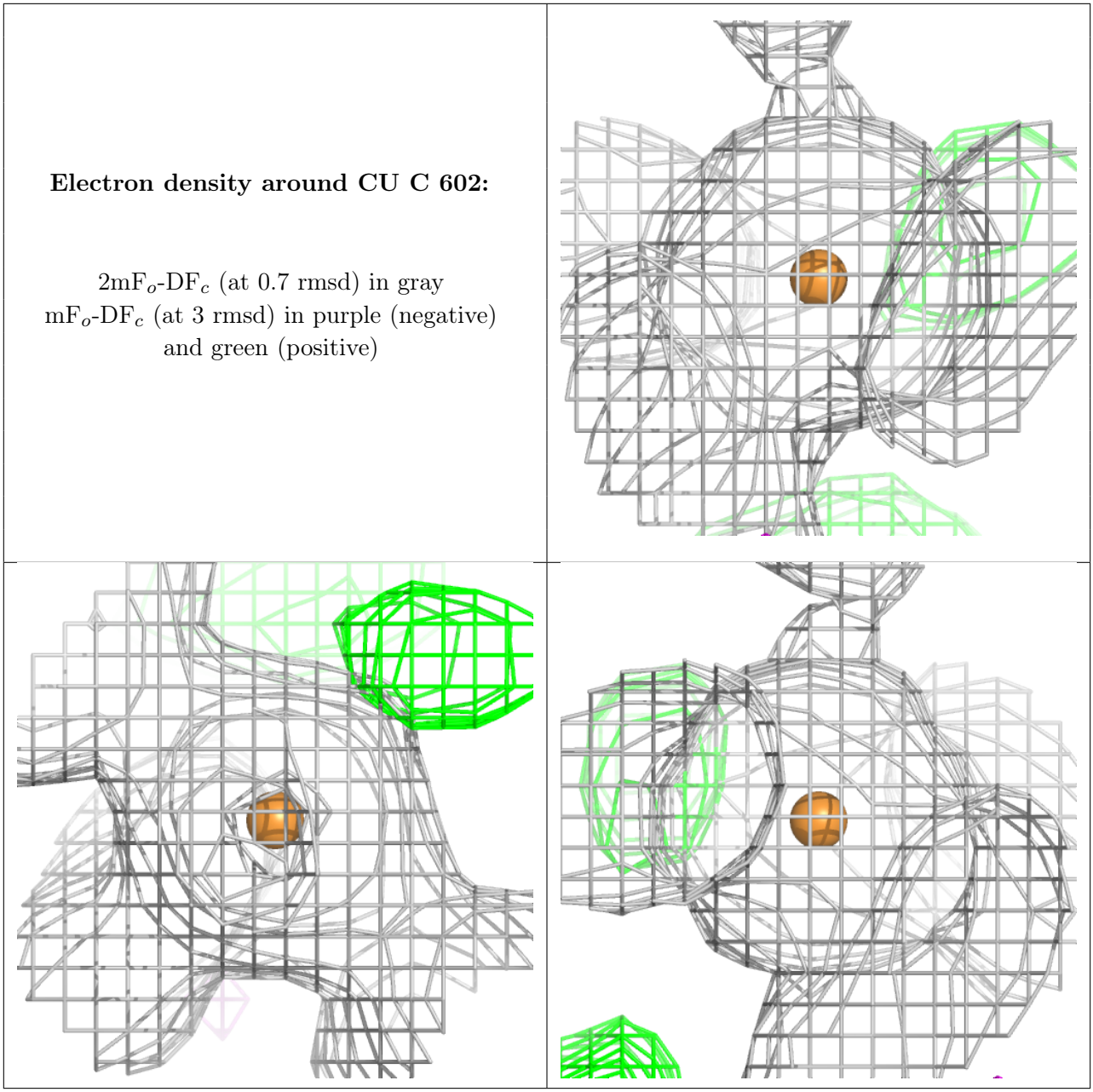
Electron density around CU B 605:

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



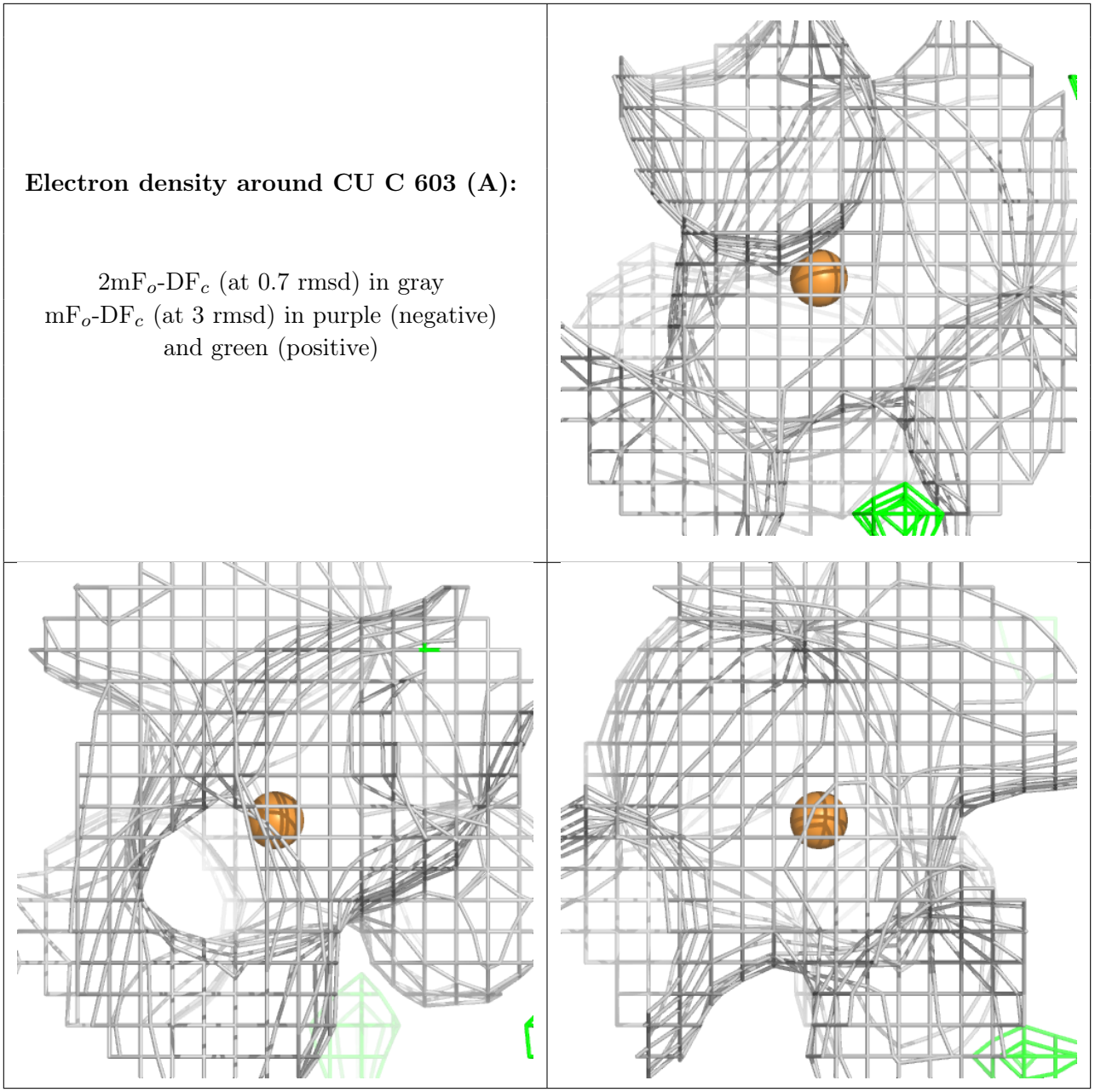
Electron density around CU C 602:

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



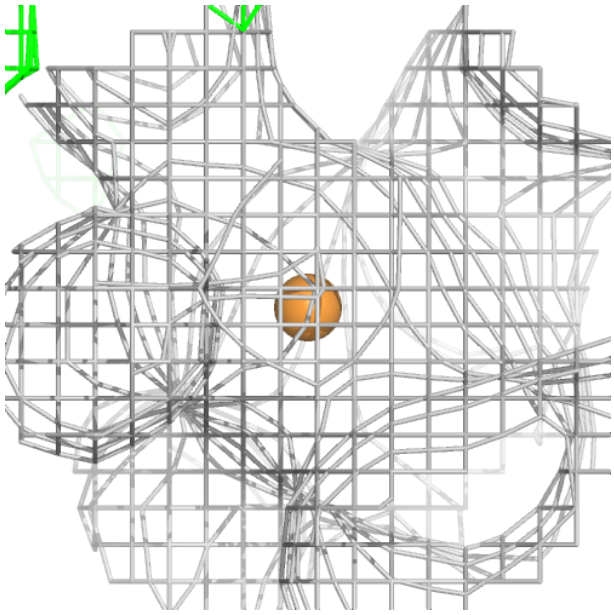
Electron density around CU C 603 (A):

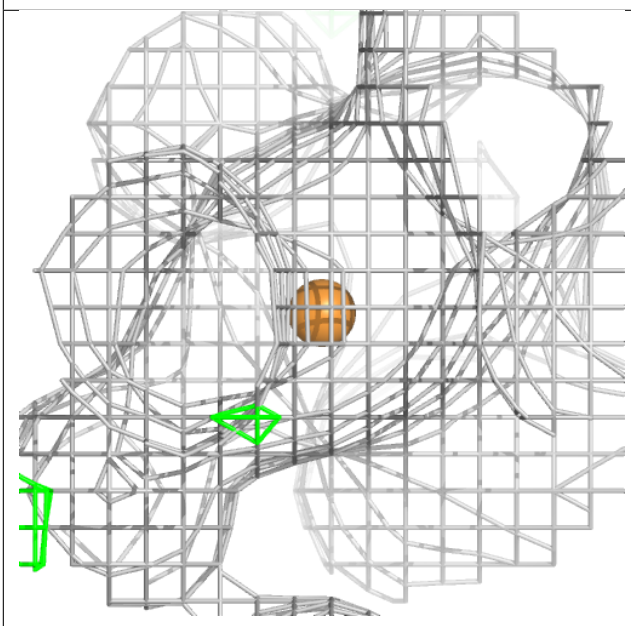
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

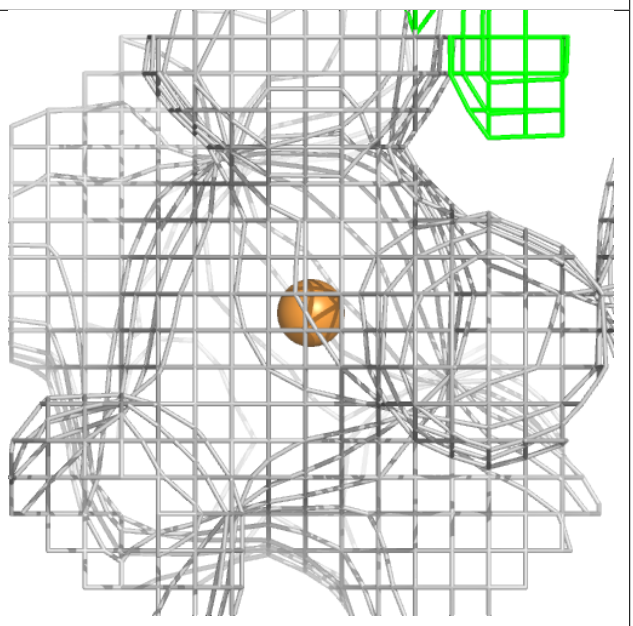


Electron density around CU C 603 (B):

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

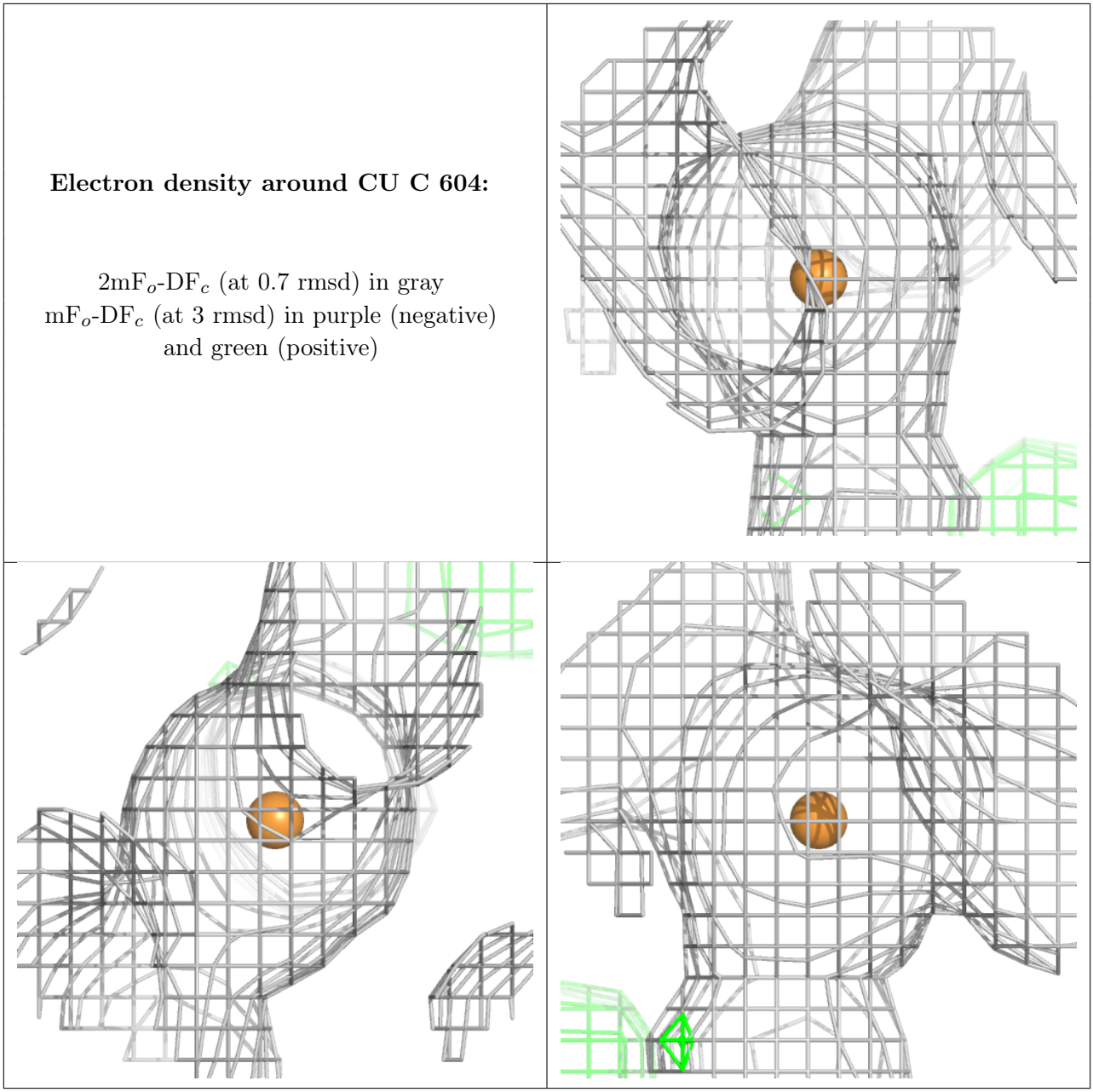






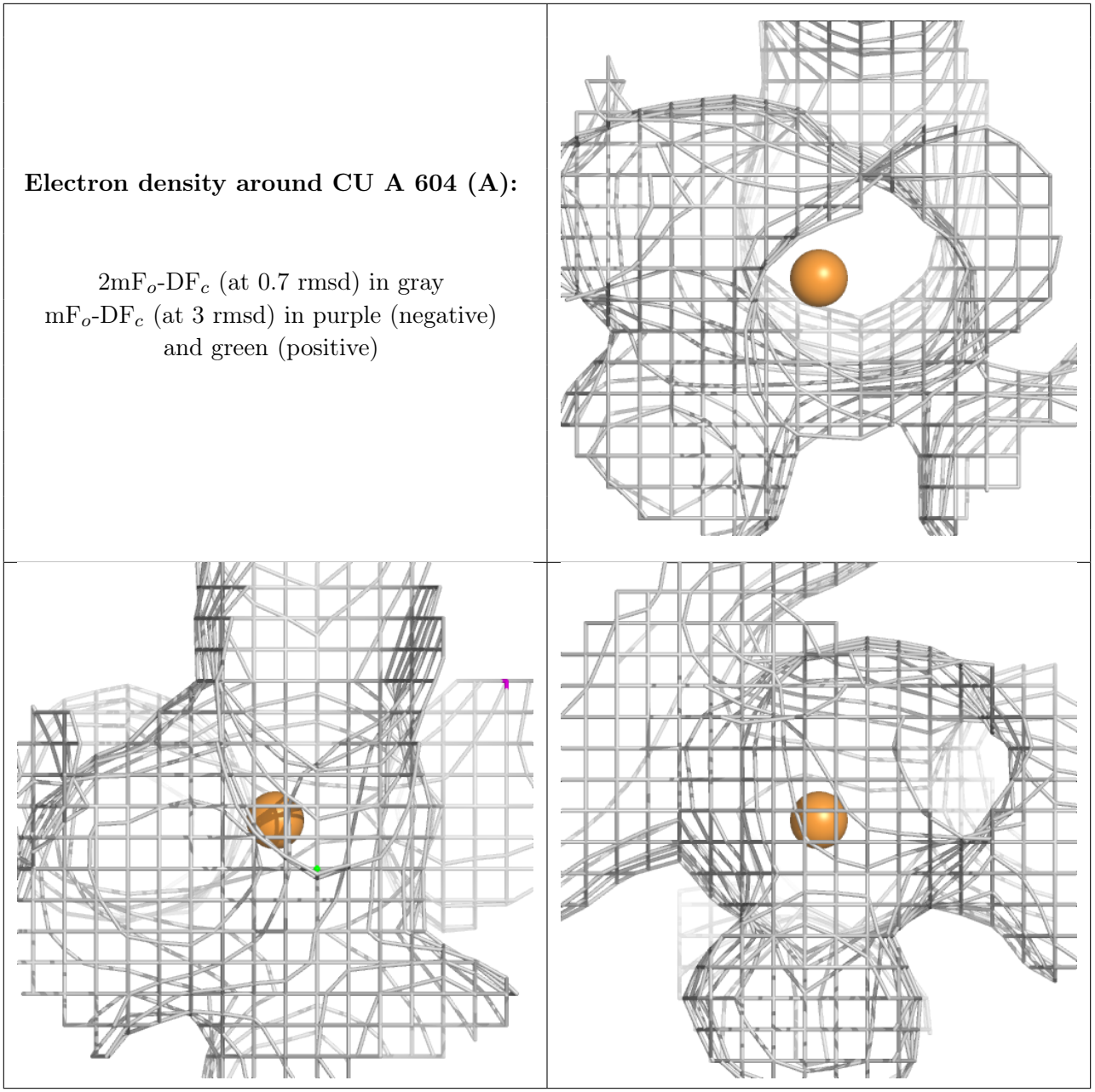
Electron density around CU C 604:

$2mF_o$-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 604 (A):

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



6.5 Other polymers (i)

There are no such residues in this entry.