wwPDB X-ray Structure Validation Summary Report (i)

Oct 9, 2023 – 09:57 AM EDT

PDB ID	:	6WEF
Title	:	Copper-bound D92H variant of Campylobacter jejuni P19
Authors	:	Chan, A.C.; Murphy, M.E.
Deposited on	:	2020-04-02
Resolution	:	2.50 Å(reported)

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

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

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

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

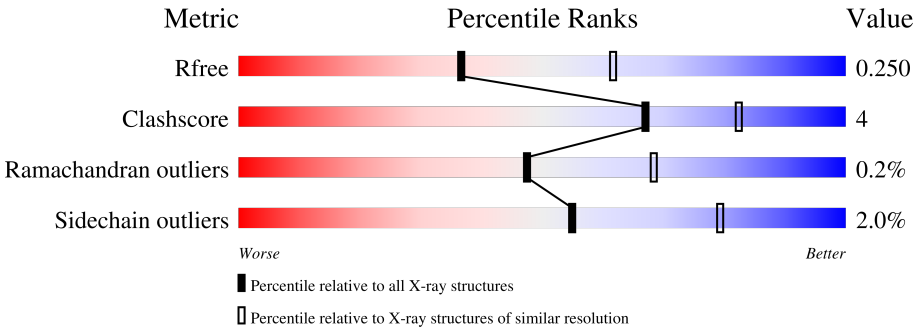
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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%

Mol	Chain	Length	Quality of chain
1	A	159	87% 13%
1	B	159	86% 14%
1	C	159	86% 13%
1	D	159	94% 6%
1	E	159	94% 6%
1	F	159	93% 6%
1	G	159	92% 8%

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Mol	Chain	Length	Quality of chain
1	H	159	87% 13%
1	I	159	90% 9%
1	J	159	91% 9%
1	K	159	89% 10%
1	L	159	84% 16%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 29768 atoms, of which 14307 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	158	Total	C	H	N	O	S	0	0	0
			2431	797	1194	202	232	6			
1	D	159	Total	C	H	N	O	S	0	0	0
			2422	795	1187	202	232	6			
1	A	158	Total	C	H	N	O	S	0	0	0
			2412	792	1183	201	230	6			
1	B	159	Total	C	H	N	O	S	0	0	0
			2441	799	1200	203	233	6			
1	E	158	Total	C	H	N	O	S	0	0	0
			2431	797	1194	202	232	6			
1	F	158	Total	C	H	N	O	S	0	0	0
			2425	796	1190	202	231	6			
1	G	158	Total	C	H	N	O	S	0	0	0
			2431	797	1194	202	232	6			
1	H	159	Total	C	H	N	O	S	0	0	0
			2442	799	1201	203	233	6			
1	I	158	Total	C	H	N	O	S	0	0	0
			2418	794	1185	201	232	6			
1	J	159	Total	C	H	N	O	S	0	0	0
			2415	793	1182	201	233	6			
1	K	158	Total	C	H	N	O	S	0	0	0
			2428	796	1194	202	230	6			
1	L	159	Total	C	H	N	O	S	0	0	0
			2428	796	1191	202	233	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	GLY	-	expression tag	UNP A0A0H3PA01
C	92	HIS	ASP	engineered mutation	UNP A0A0H3PA01
D	1	GLY	-	expression tag	UNP A0A0H3PA01
D	92	HIS	ASP	engineered mutation	UNP A0A0H3PA01
A	1	GLY	-	expression tag	UNP A0A0H3PA01

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Chain	Residue	Modelled	Actual	Comment	Reference
A	92	HIS	ASP	engineered mutation	UNP A0A0H3PA01
B	1	GLY	-	expression tag	UNP A0A0H3PA01
B	92	HIS	ASP	engineered mutation	UNP A0A0H3PA01
E	1	GLY	-	expression tag	UNP A0A0H3PA01
E	92	HIS	ASP	engineered mutation	UNP A0A0H3PA01
F	1	GLY	-	expression tag	UNP A0A0H3PA01
F	92	HIS	ASP	engineered mutation	UNP A0A0H3PA01
G	1	GLY	-	expression tag	UNP A0A0H3PA01
G	92	HIS	ASP	engineered mutation	UNP A0A0H3PA01
H	1	GLY	-	expression tag	UNP A0A0H3PA01
H	92	HIS	ASP	engineered mutation	UNP A0A0H3PA01
I	1	GLY	-	expression tag	UNP A0A0H3PA01
I	92	HIS	ASP	engineered mutation	UNP A0A0H3PA01
J	1	GLY	-	expression tag	UNP A0A0H3PA01
J	92	HIS	ASP	engineered mutation	UNP A0A0H3PA01
K	1	GLY	-	expression tag	UNP A0A0H3PA01
K	92	HIS	ASP	engineered mutation	UNP A0A0H3PA01
L	1	GLY	-	expression tag	UNP A0A0H3PA01
L	92	HIS	ASP	engineered mutation	UNP A0A0H3PA01

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

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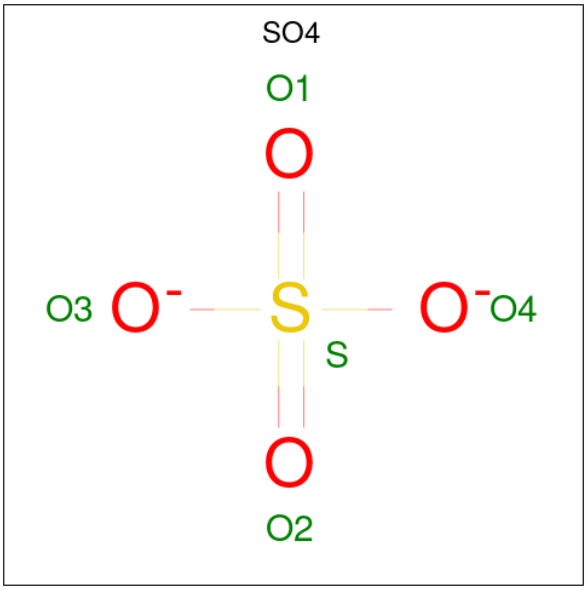
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total Cu 1 1	0	0
2	K	1	Total Cu 1 1	0	0
2	L	1	Total Cu 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

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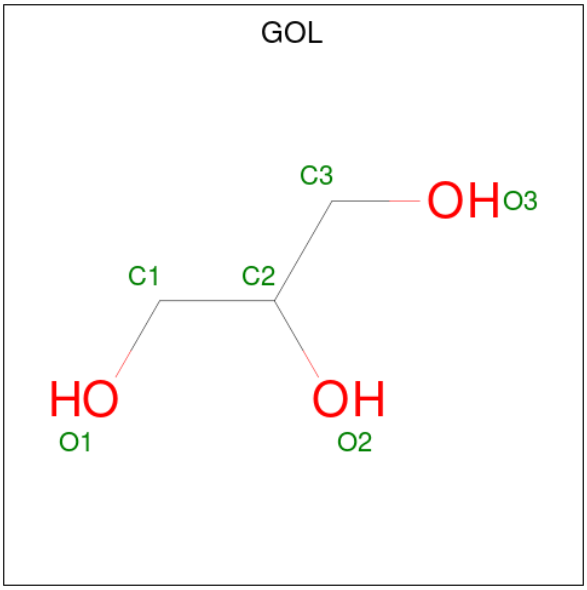
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C H O 9 3 3 3	0	0
4	H	1	Total C H O 9 3 3 3	0	0
4	H	1	Total C H O 9 3 3 3	0	0
4	K	1	Total C H O 9 3 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	32	Total O 32 32	0	0
5	D	53	Total O 53 53	0	0

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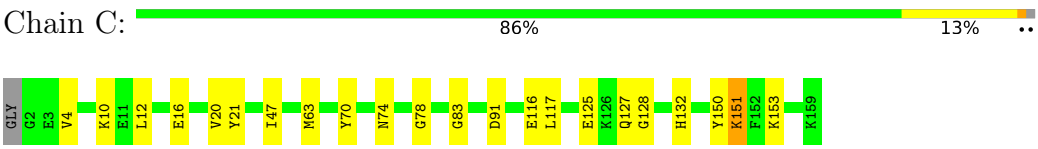
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	65	Total O 65 65	0	0
5	B	38	Total O 38 38	0	0
5	E	42	Total O 42 42	0	0
5	F	45	Total O 45 45	0	0
5	G	38	Total O 38 38	0	0
5	H	49	Total O 49 49	0	0
5	I	52	Total O 52 52	0	0
5	J	48	Total O 48 48	0	0
5	K	45	Total O 45 45	0	0
5	L	34	Total O 34 34	0	0

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. 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. 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.

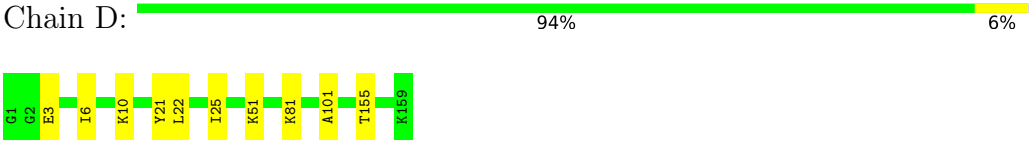
• Molecule 1: Uncharacterized protein

Chain C:



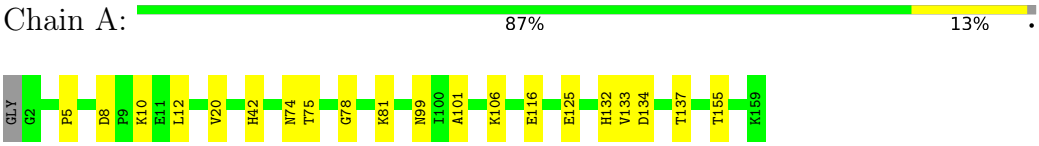
• Molecule 1: Uncharacterized protein

Chain D:



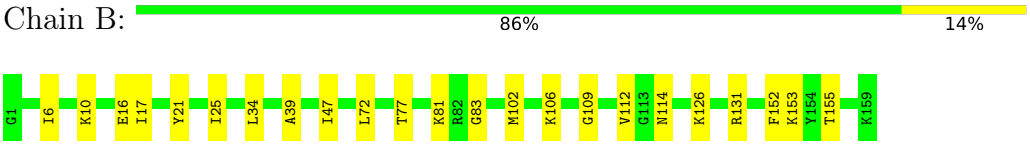
• Molecule 1: Uncharacterized protein

Chain A:



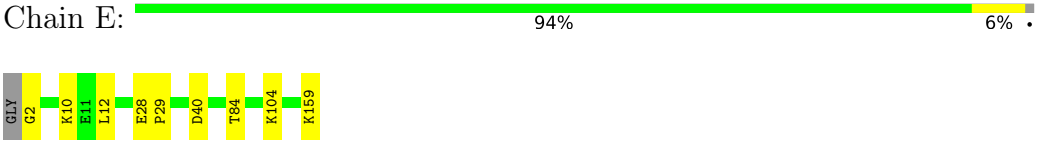
• Molecule 1: Uncharacterized protein

Chain B:



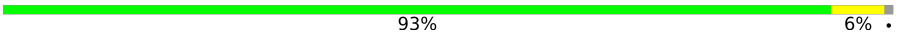
• Molecule 1: Uncharacterized protein

Chain E:



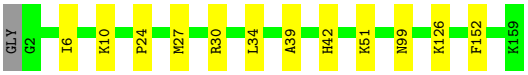
• Molecule 1: Uncharacterized protein

Chain F:



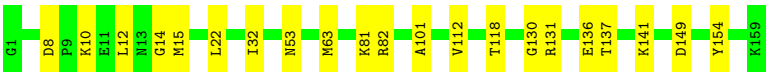
• Molecule 1: Uncharacterized protein

Chain G:



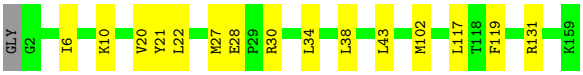
• Molecule 1: Uncharacterized protein

Chain H:



• Molecule 1: Uncharacterized protein

Chain I:

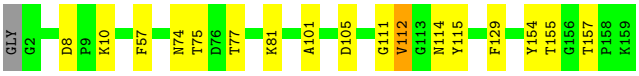


• Molecule 1: Uncharacterized protein

Chain J:

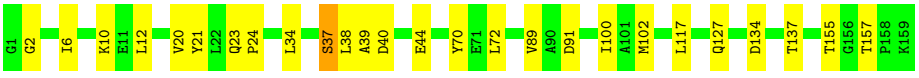
• Molecule 1: Uncharacterized protein

Chain K:



• Molecule 1: Uncharacterized protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	132.46Å 132.46Å 104.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.68 – 2.50 28.68 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (28.68-2.50) 78.1 (28.68-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.270 , 0.299 0.220 , 0.250	Depositor DCC
R_{free} test set	2028 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 23.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.479 for -h,-k,l 0.479 for h,-h-k,-l 0.479 for -k,-h,-l	Xtriage
Reported twinning fraction	0.490 for -h,-k,l	Depositor
Outliers	0 of 69955 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	29768	wwPDB-VP
Average B, all atoms (Å^2)	51.0	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 74.29 % 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 1.5703e-06. 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: GOL, SO4, CU

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	0.27	0/1265	0.46	0/1714
1	B	0.28	0/1277	0.44	0/1728
1	C	0.27	0/1273	0.46	0/1723
1	D	0.27	0/1271	0.46	0/1721
1	E	0.26	0/1273	0.45	0/1723
1	F	0.27	0/1271	0.44	0/1720
1	G	0.26	0/1273	0.44	0/1723
1	H	0.27	0/1277	0.44	0/1728
1	I	0.26	0/1269	0.45	0/1719
1	J	0.27	0/1269	0.44	0/1720
1	K	0.27	0/1270	0.47	0/1719
1	L	0.27	0/1273	0.44	0/1724
All	All	0.27	0/15261	0.45	0/20662

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	1229	1183	1179	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1241	1200	1200	14	0
1	C	1237	1194	1194	12	0
1	D	1235	1187	1184	7	0
1	E	1237	1194	1194	4	0
1	F	1235	1190	1189	6	0
1	G	1237	1194	1194	8	0
1	H	1241	1201	1200	13	0
1	I	1233	1185	1183	9	0
1	J	1233	1182	1178	9	0
1	K	1234	1194	1192	15	0
1	L	1237	1191	1189	20	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	10	0	0	1	0
3	B	5	0	0	1	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
3	F	10	0	0	0	0
3	G	5	0	0	0	0
3	I	5	0	0	1	0
3	J	5	0	0	0	0
4	G	6	3	8	3	0
4	H	12	6	16	2	0
4	K	6	3	8	0	0
5	A	65	0	0	1	0
5	B	38	0	0	0	0
5	C	32	0	0	0	0
5	D	53	0	0	0	0
5	E	42	0	0	0	0
5	F	45	0	0	1	0
5	G	38	0	0	0	0
5	H	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	52	0	0	1	0
5	J	48	0	0	2	0
5	K	45	0	0	1	0
5	L	34	0	0	1	0
All	All	15461	14307	14308	115	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 115 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:G:34:LEU:HD23	1:G:39:ALA:HB2	1.68	0.73
1:L:34:LEU:HD23	1:L:39:ALA:HB2	1.70	0.73
1:H:81:LYS:NZ	1:H:101:ALA:O	2.24	0.69
1:G:27:MET:HE2	1:H:130:GLY:HA3	1.78	0.65
1:A:81:LYS:NZ	1:A:101:ALA:O	2.30	0.64

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	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	B	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
1	C	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	D	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
1	E	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	F	156/159 (98%)	146 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	H	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
1	I	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	J	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
1	K	156/159 (98%)	147 (94%)	7 (4%)	2 (1%)	12	21
1	L	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	43
All	All	1877/1908 (98%)	1790 (95%)	84 (4%)	3 (0%)	47	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	112	VAL
1	L	2	GLY
1	K	105	ASP

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	125/127 (98%)	122 (98%)	3 (2%)	49	74
1	B	127/127 (100%)	124 (98%)	3 (2%)	49	74
1	C	127/127 (100%)	122 (96%)	5 (4%)	32	57
1	D	125/127 (98%)	124 (99%)	1 (1%)	81	93
1	E	127/127 (100%)	125 (98%)	2 (2%)	62	84
1	F	126/127 (99%)	125 (99%)	1 (1%)	81	93
1	G	127/127 (100%)	125 (98%)	2 (2%)	62	84
1	H	127/127 (100%)	124 (98%)	3 (2%)	49	74
1	I	126/127 (99%)	124 (98%)	2 (2%)	62	84
1	J	125/127 (98%)	121 (97%)	4 (3%)	39	65
1	K	126/127 (99%)	124 (98%)	2 (2%)	62	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	126/127 (99%)	123 (98%)	3 (2%)	49 74
All	All	1514/1524 (99%)	1483 (98%)	31 (2%)	55 79

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	10	LYS
1	K	10	LYS
1	H	8	ASP
1	L	12	LEU
1	J	86	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	127	GLN
1	G	23	GLN
1	L	52	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 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 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	SO4	E	202	-	4,4,4	0.13	0	6,6,6	0.06	0
3	SO4	I	202	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	A	202	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	F	203	-	4,4,4	0.16	0	6,6,6	0.06	0
4	GOL	H	202	-	5,5,5	0.91	0	5,5,5	0.99	0
3	SO4	B	202	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	D	203	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	D	202	-	4,4,4	0.13	0	6,6,6	0.08	0
4	GOL	G	202	-	5,5,5	0.92	0	5,5,5	0.94	0
4	GOL	H	203	-	5,5,5	0.85	0	5,5,5	1.03	0
3	SO4	A	203	-	4,4,4	0.13	0	6,6,6	0.09	0
4	GOL	K	202	-	5,5,5	0.92	0	5,5,5	1.02	0
3	SO4	F	202	-	4,4,4	0.15	0	6,6,6	0.05	0
3	SO4	J	202	-	4,4,4	0.13	0	6,6,6	0.06	0
3	SO4	G	203	-	4,4,4	0.15	0	6,6,6	0.08	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
4	GOL	H	203	-	-	0/4/4/4	-
4	GOL	K	202	-	-	0/4/4/4	-
4	GOL	G	202	-	-	0/4/4/4	-
4	GOL	H	202	-	-	0/4/4/4	-

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.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	202	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	202	SO4	1	0
4	G	202	GOL	3	0
4	H	203	GOL	2	0
3	A	203	SO4	1	0

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

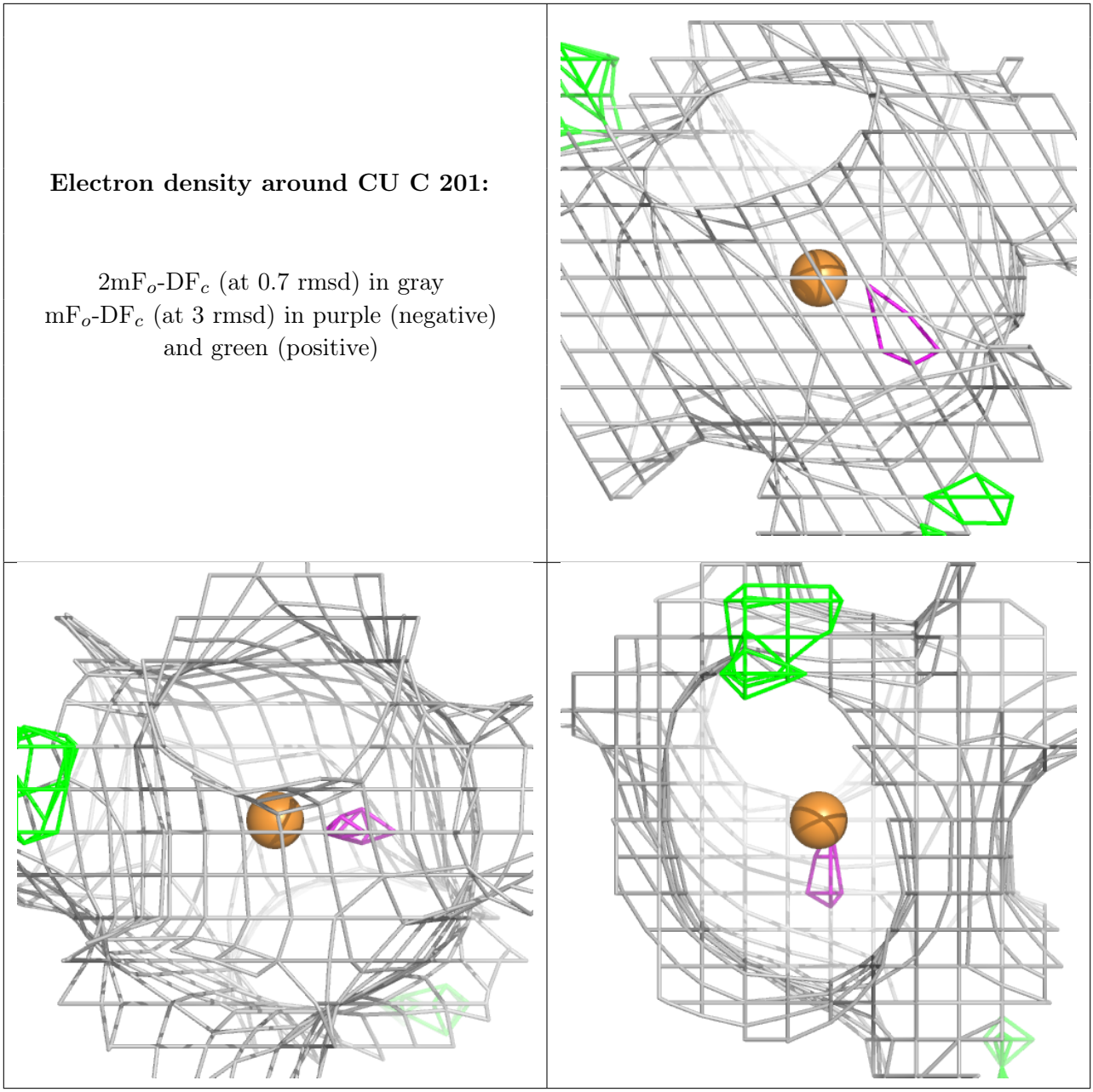
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

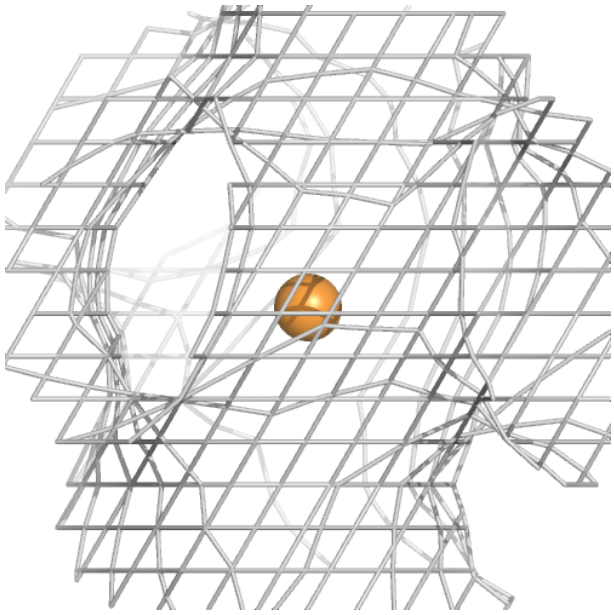
Electron density around CU C 201:

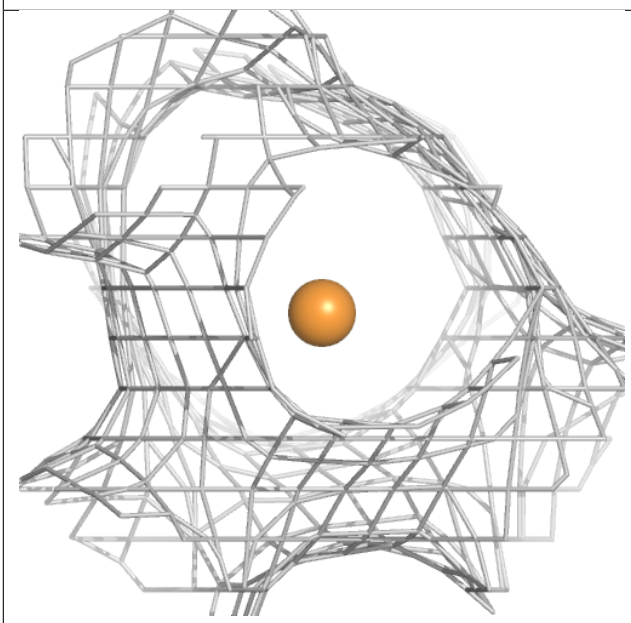
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

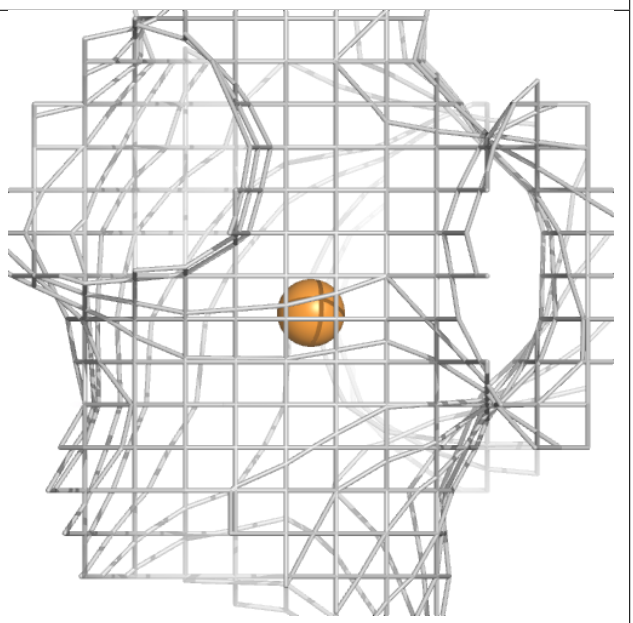


Electron density around CU D 201:

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

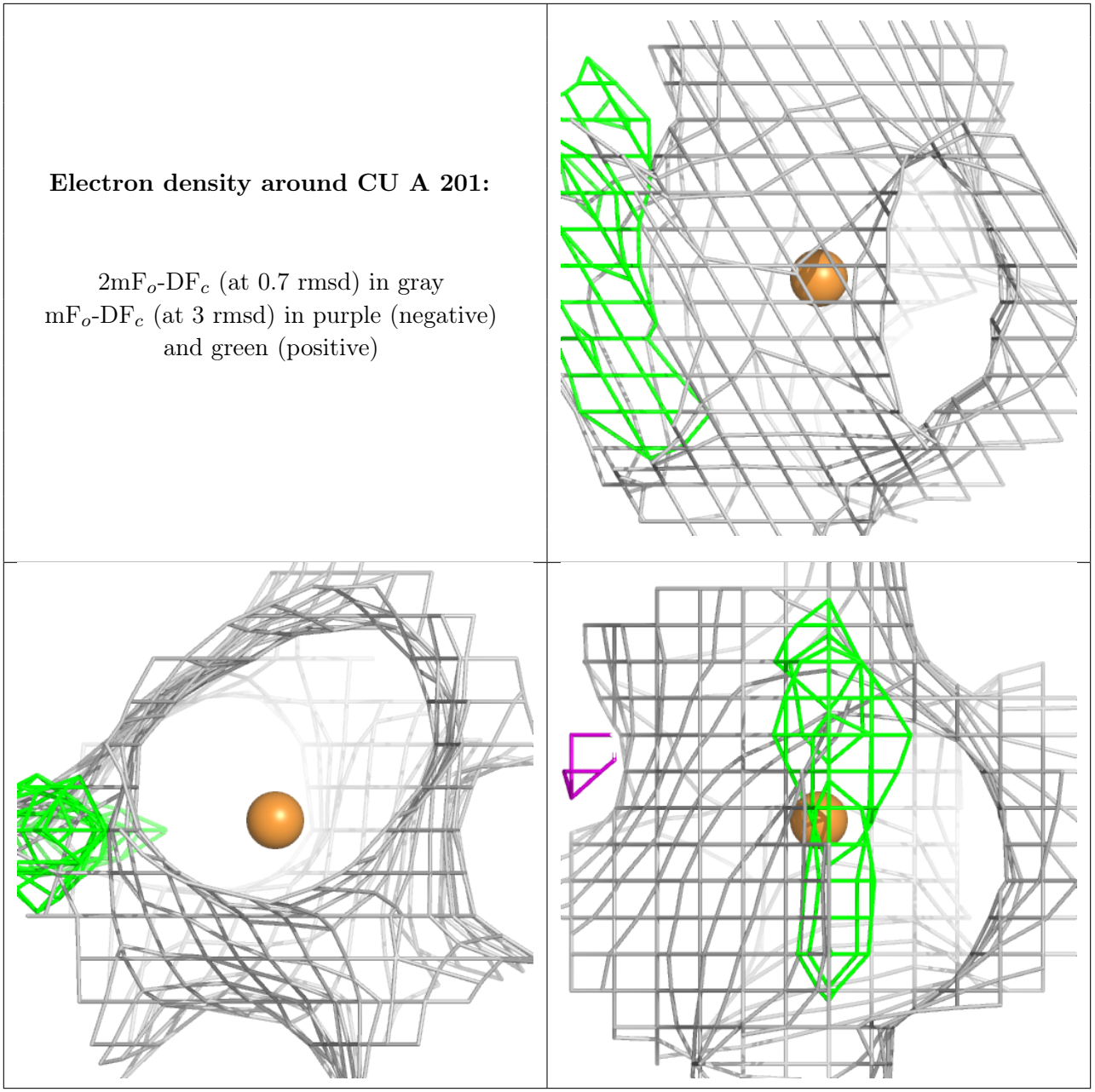






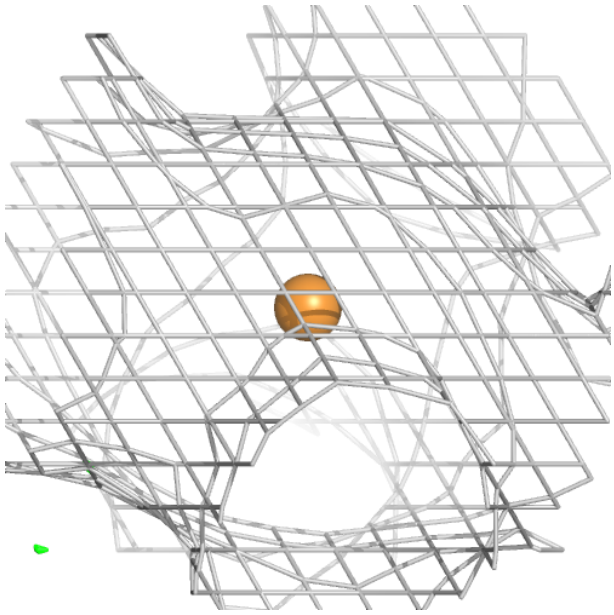
Electron density around CU A 201:

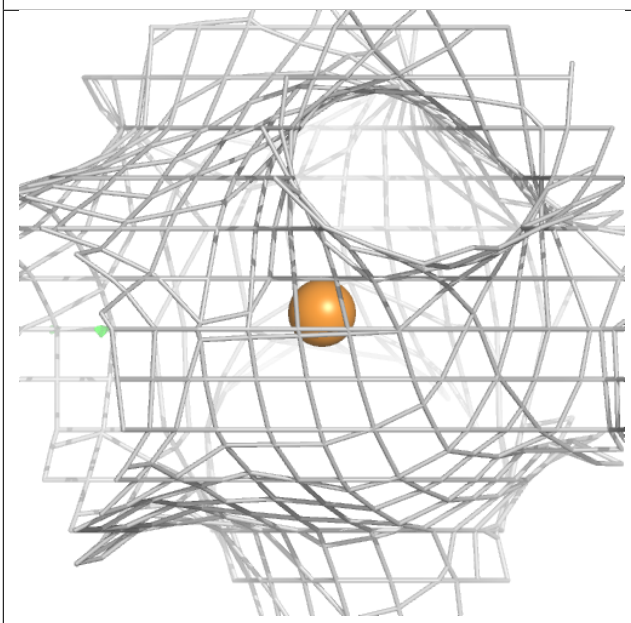
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

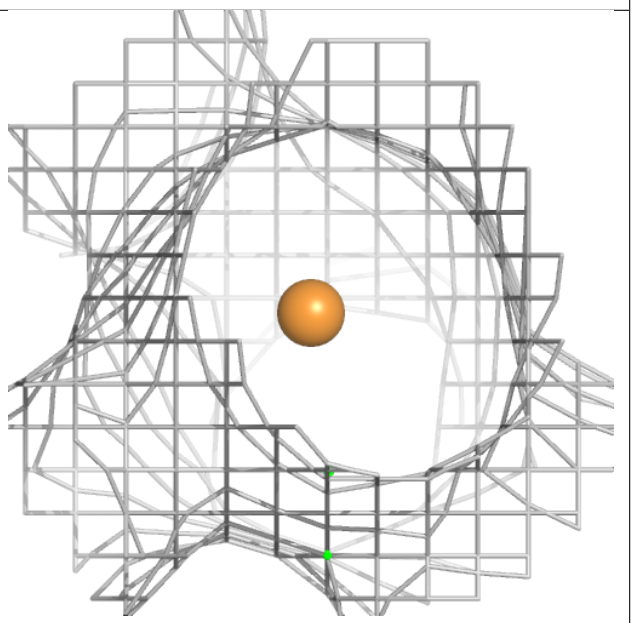


Electron density around CU B 201:

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

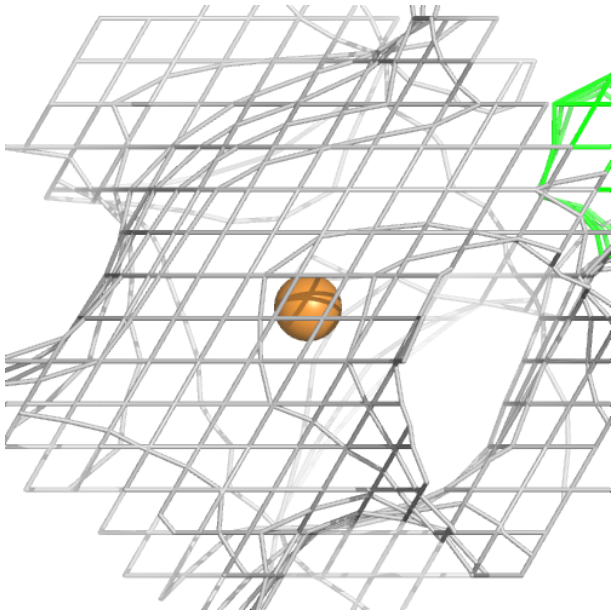


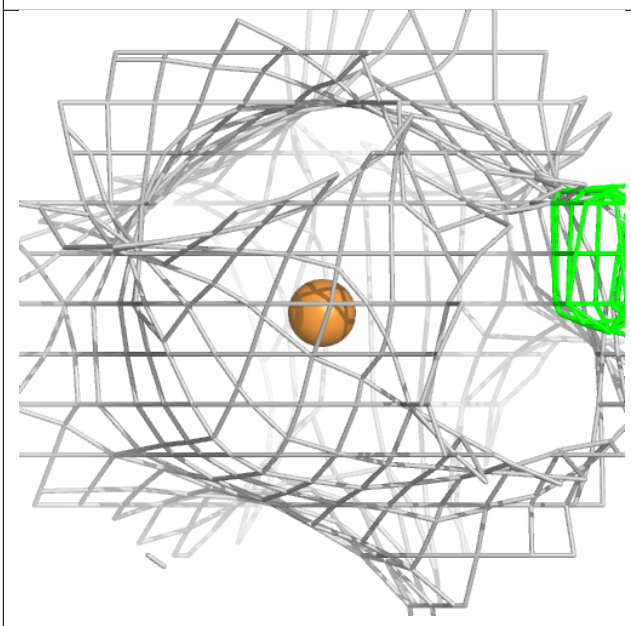


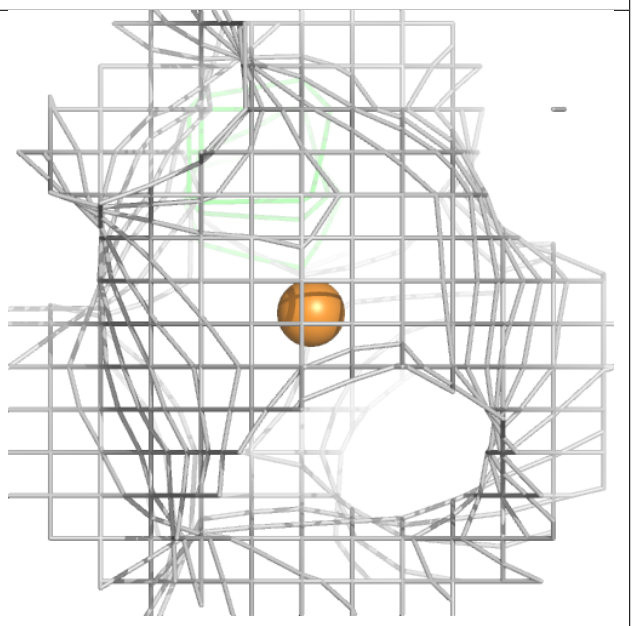


Electron density around CU E 201:

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

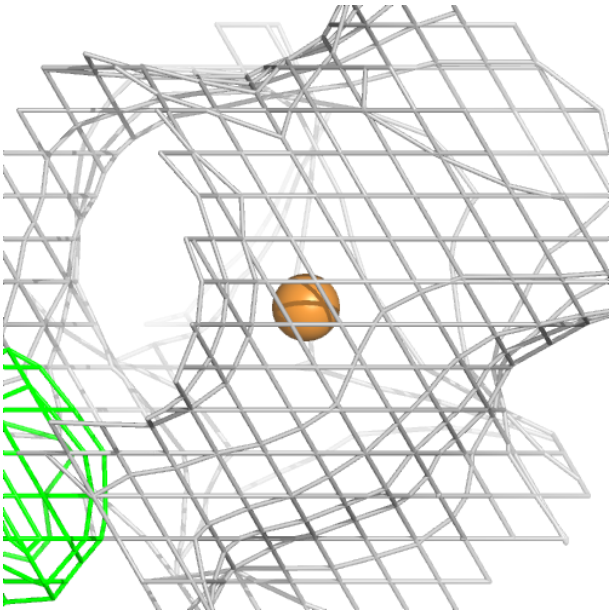


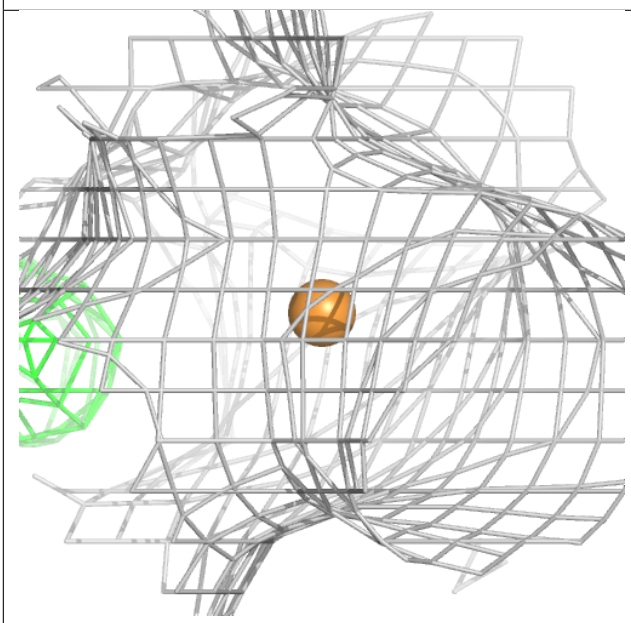


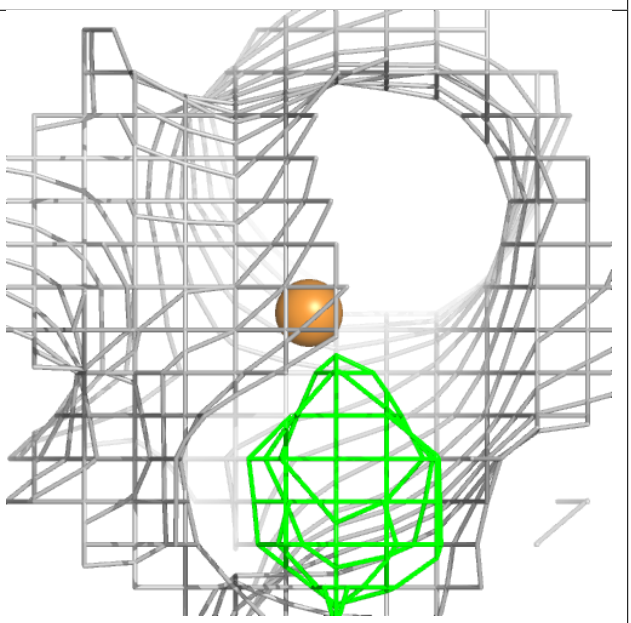


Electron density around CU F 201:

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

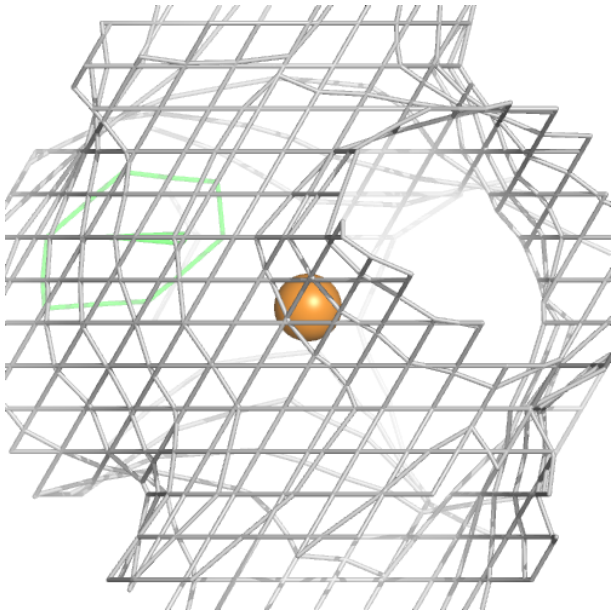


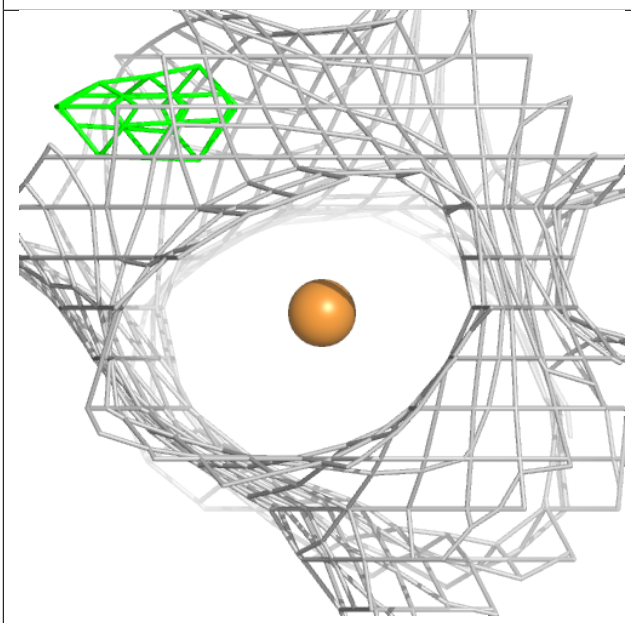


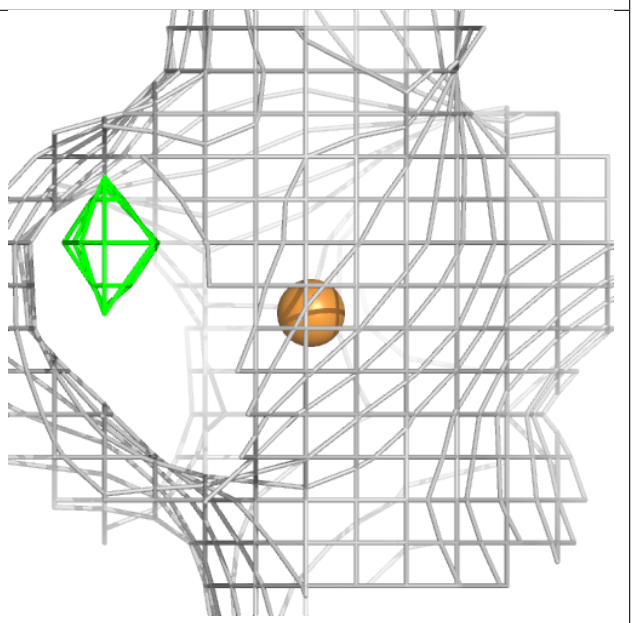


Electron density around CU G 201:

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

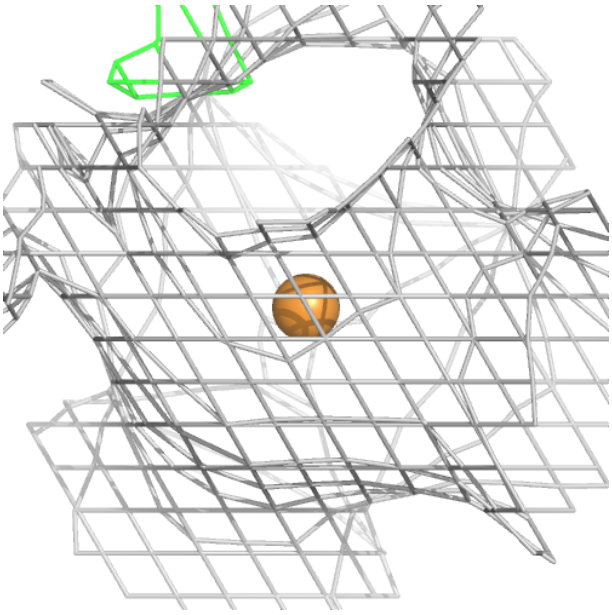


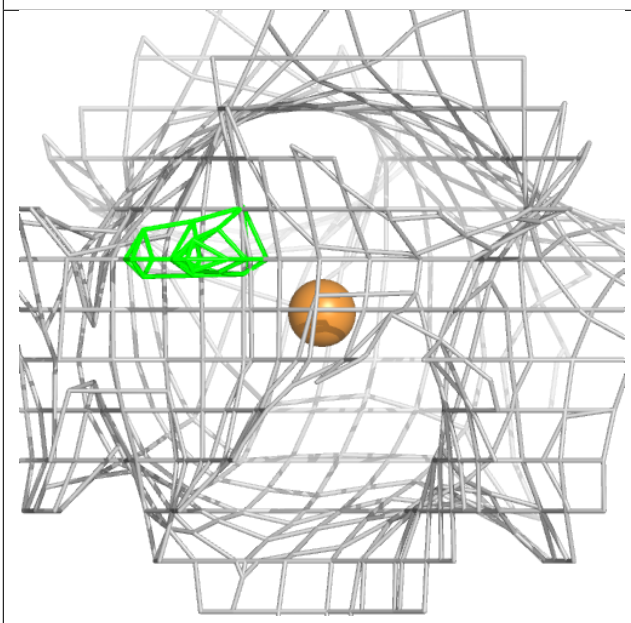


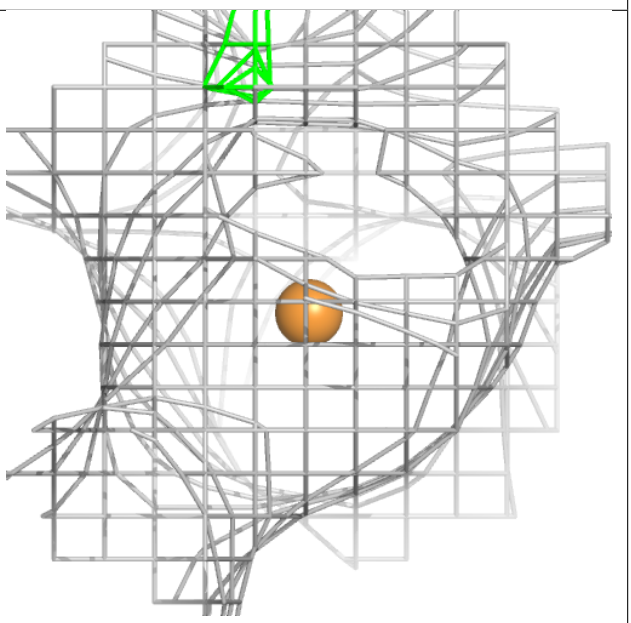


Electron density around CU H 201:

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

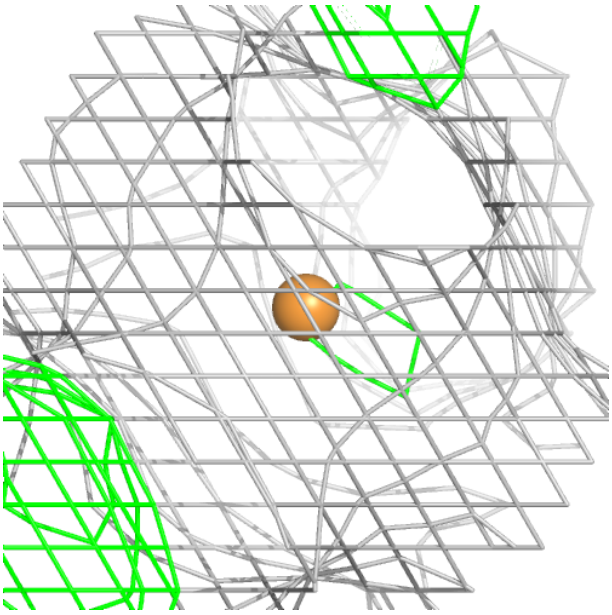


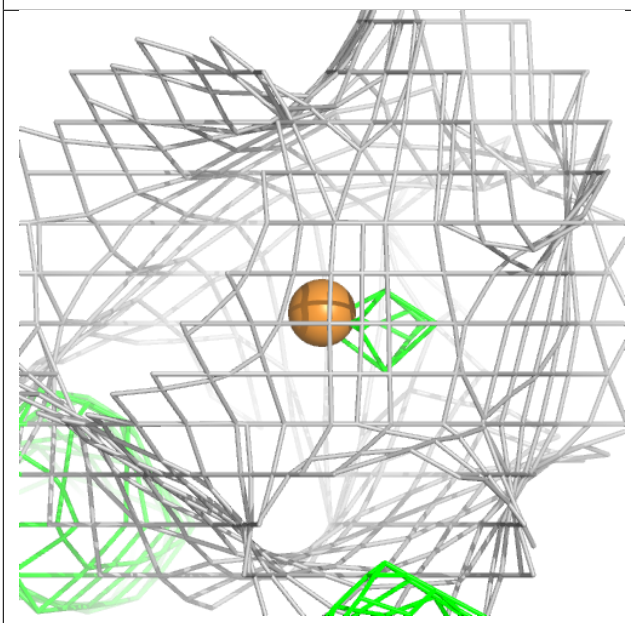


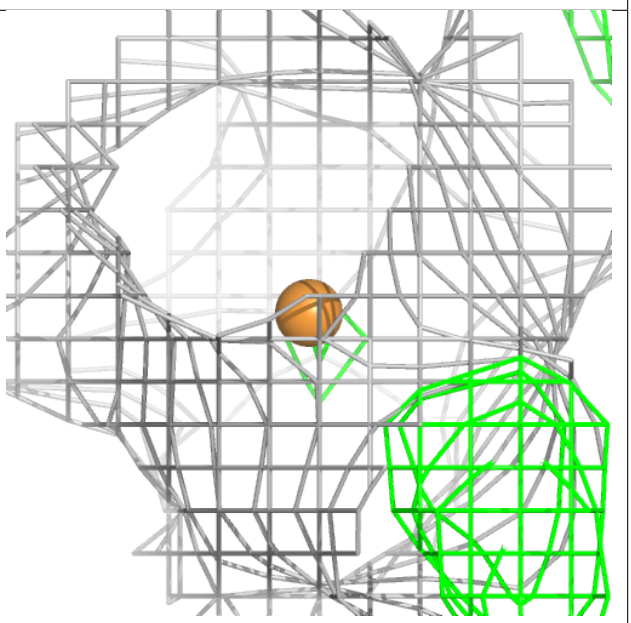


Electron density around CU I 201:

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

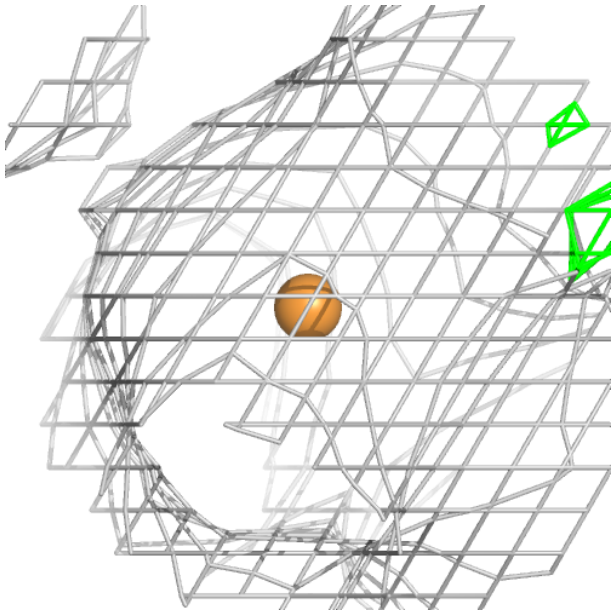


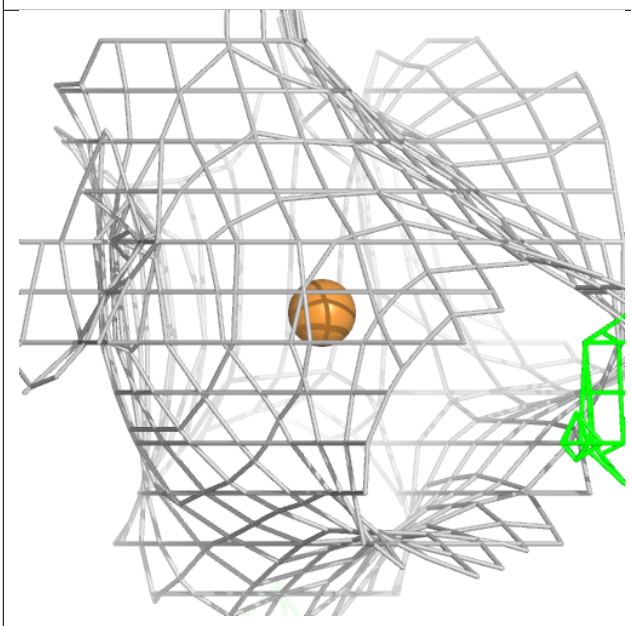


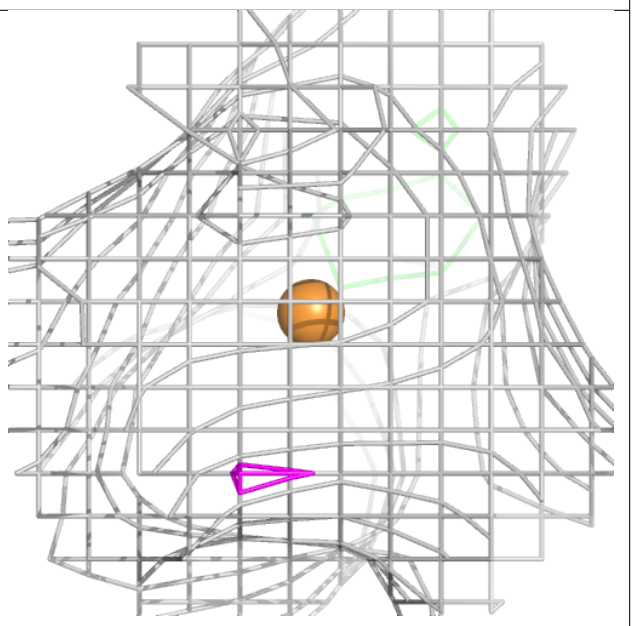


Electron density around CU J 201:

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

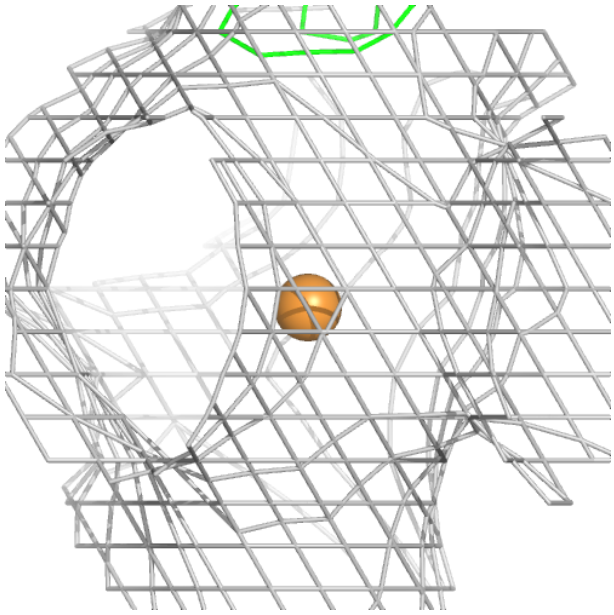


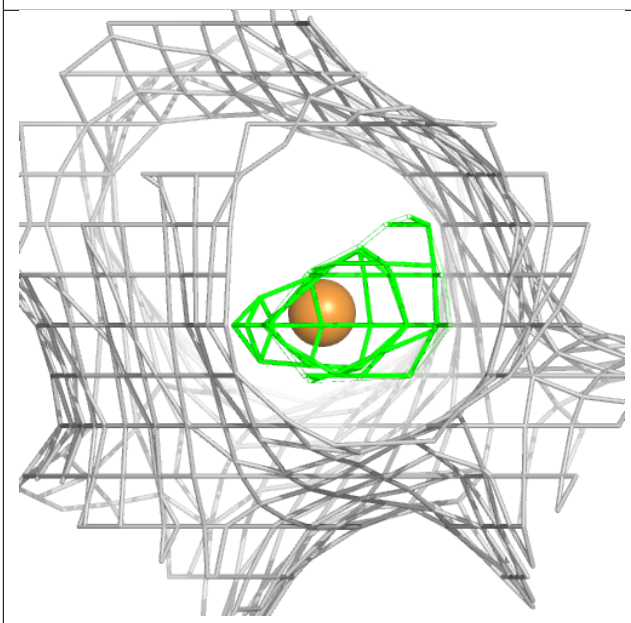


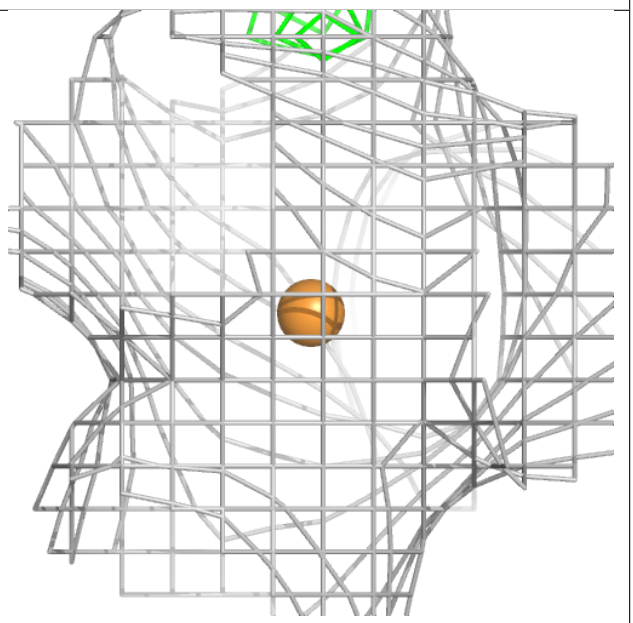


Electron density around CU K 201:

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

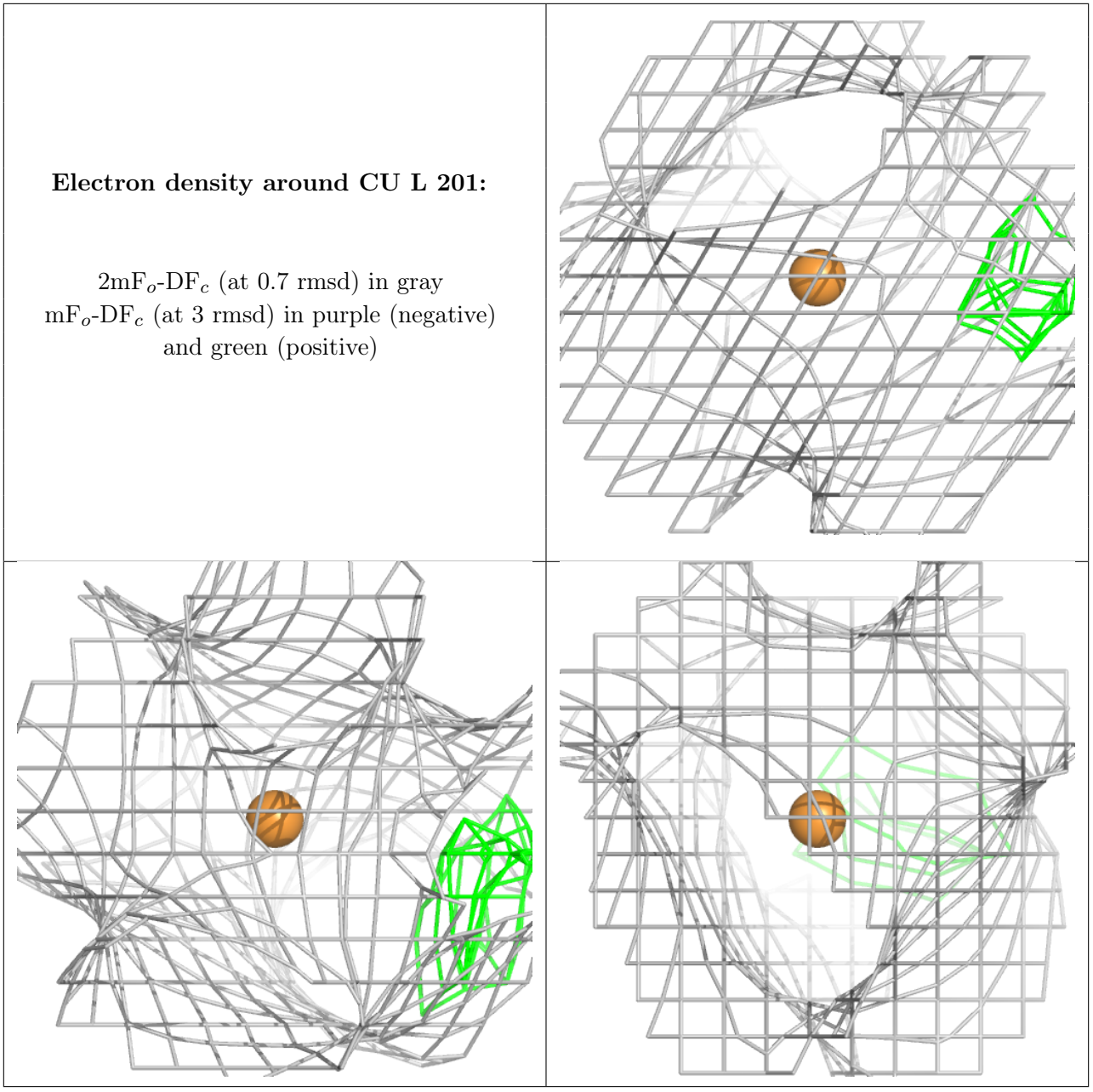






Electron density around CU L 201:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.