



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2025 – 01:26 pm BST

PDB ID : 9H29 / pdb\_00009h29  
Title : Crystal structure of tyrosinase from *Priestia megaterium* F227Y mutant soaked in Cu(II)  
Authors : Englund, A.N.B.; Rohr, A.K.  
Deposited on : 2024-10-11  
Resolution : 2.17 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](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

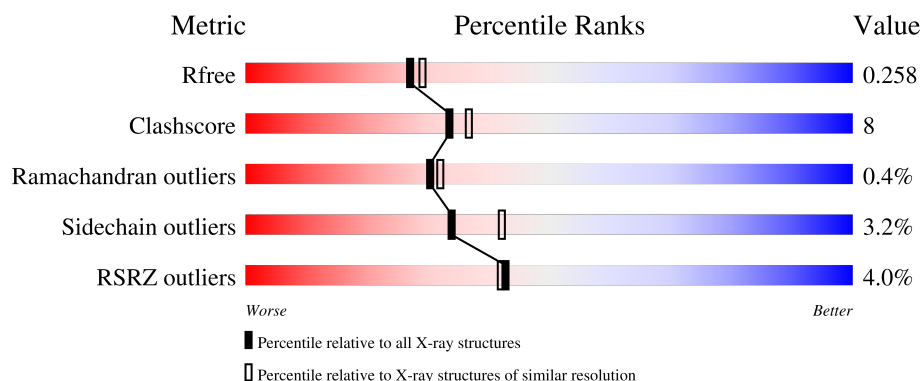
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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))
$R_{free}$	164625	8336 (2.20-2.16)
Clashscore	180529	9404 (2.20-2.16)
Ramachandran outliers	177936	9297 (2.20-2.16)
Sidechain outliers	177891	9297 (2.20-2.16)
RSRZ outliers	164620	8337 (2.20-2.16)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	303	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• 6%</div> </div> </div>
1	B	303	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4984 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 Tyrosinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	1	0
			2358	1498	427	425	8			
1	B	288	Total	C	N	O	S	0	0	0
			2364	1502	428	426	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	TYR	PHE	engineered mutation	UNP B2ZB02
A	298	HIS	-	expression tag	UNP B2ZB02
A	299	HIS	-	expression tag	UNP B2ZB02
A	300	HIS	-	expression tag	UNP B2ZB02
A	301	HIS	-	expression tag	UNP B2ZB02
A	302	HIS	-	expression tag	UNP B2ZB02
A	303	HIS	-	expression tag	UNP B2ZB02
B	227	TYR	PHE	engineered mutation	UNP B2ZB02
B	298	HIS	-	expression tag	UNP B2ZB02
B	299	HIS	-	expression tag	UNP B2ZB02
B	300	HIS	-	expression tag	UNP B2ZB02
B	301	HIS	-	expression tag	UNP B2ZB02
B	302	HIS	-	expression tag	UNP B2ZB02
B	303	HIS	-	expression tag	UNP B2ZB02

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cu	0	0
			3	3		
2	B	3	Total	Cu	0	0
			3	3		

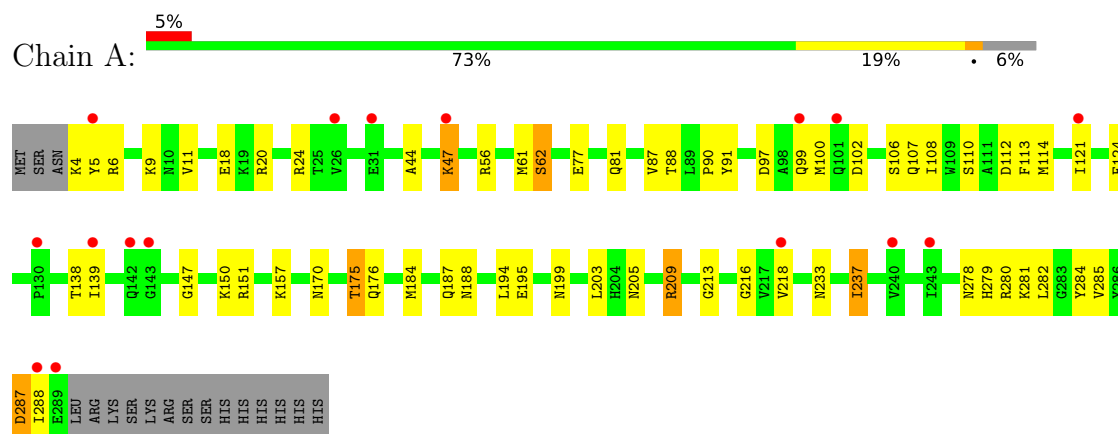
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total 109	O 109	0	0
3	B	147	Total 147	O 147	0	0

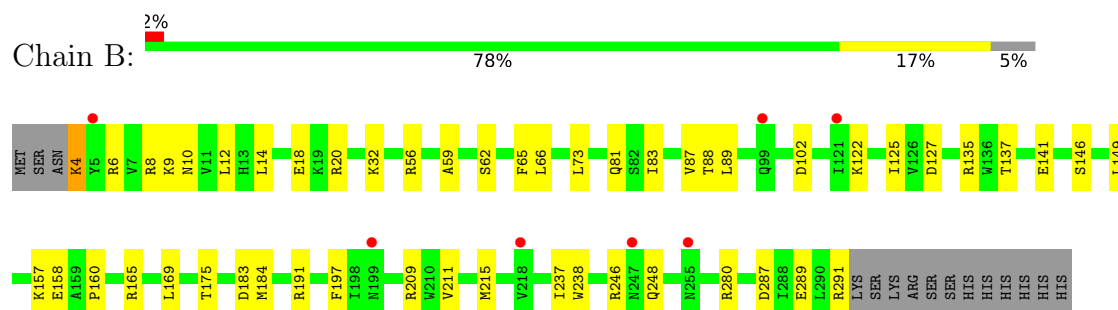
### 3 Residue-property plots [i](#)

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: Tyrosinase



#### • Molecule 1: Tyrosinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.42Å 78.90Å 83.05Å 90.00° 106.05° 90.00°	Depositor
Resolution (Å)	39.91 – 2.17 39.91 – 2.17	Depositor EDS
% Data completeness (in resolution range)	95.7 (39.91-2.17) 95.7 (39.91-2.17)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.202 , 0.258 0.204 , 0.258	Depositor DCC
$R_{free}$ test set	1661 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4984	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.33	0/2436	0.54	1/3319 (0.0%)
1	B	0.40	0/2442	0.60	0/3327
All	All	0.37	0/4878	0.57	1/6646 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ILE	N-CA-C	-8.00	105.52	113.20

There are no chirality outliers.

There are no planarity outliers.

### 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	2358	0	2238	38	0
1	B	2364	0	2243	32	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	109	0	0	5	0
3	B	147	0	0	7	0
All	All	4984	0	4481	70	1

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 8.

All (70) 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:A:44:ALA:HA	1:A:47:LYS:HE3	1.59	0.85
1:A:187:GLN:NE2	3:A:502:HOH:O	2.21	0.73
1:A:233:ASN:O	1:A:237:ILE:HG12	1.91	0.71
1:B:127:ASP:OD1	3:B:501:HOH:O	2.08	0.69
1:B:9:LYS:NZ	1:B:18:GLU:OE2	2.23	0.69
1:A:4:LYS:HA	1:A:285:VAL:HG13	1.78	0.66
1:B:175:THR:O	1:B:248:GLN:HG2	1.95	0.66
1:B:141:GLU:N	1:B:141:GLU:OE1	2.31	0.63
1:A:6:ARG:NH1	1:A:77:GLU:OE1	2.32	0.63
1:A:6:ARG:NH2	1:A:282:LEU:O	2.32	0.63
1:A:175:THR:HG22	1:A:176:GLN:HG2	1.82	0.62
1:B:135:ARG:NH1	3:B:512:HOH:O	2.34	0.60
1:B:184:MET:HG2	1:B:197:PHE:CD1	2.38	0.58
1:A:205:ASN:O	1:A:209[A]:ARG:HG2	2.04	0.58
1:A:278:ASN:ND2	1:A:281:LYS:HD2	2.18	0.57
1:B:157:LYS:NZ	3:B:511:HOH:O	2.33	0.57
1:A:81:GLN:NE2	1:A:87:VAL:O	2.34	0.57
1:A:170:ASN:ND2	3:A:506:HOH:O	2.37	0.57
1:A:61:MET:HE3	1:A:184:MET:SD	2.45	0.57
1:B:165:ARG:HH21	1:B:169:LEU:HD11	1.68	0.57
1:B:122:LYS:NZ	3:B:515:HOH:O	2.37	0.56
1:A:100:MET:HE1	1:A:106:SER:N	2.20	0.56
1:A:209[B]:ARG:NH1	1:A:216:GLY:O	2.40	0.54
1:B:280:ARG:NH2	1:B:289:GLU:OE1	2.40	0.54
1:A:188:ASN:ND2	3:A:507:HOH:O	2.40	0.54
1:A:88:THR:O	1:A:90:PRO:HD3	2.08	0.54
1:B:183:ASP:HB2	3:B:583:HOH:O	2.08	0.53
1:B:14:LEU:HD22	1:B:18:GLU:HB3	1.90	0.53
1:B:81:GLN:NE2	1:B:87:VAL:O	2.42	0.52
1:A:11:VAL:HG11	1:A:108:ILE:HG13	1.92	0.52
1:A:56:ARG:HD3	1:A:62:SER:OG	2.10	0.51
1:A:107:GLN:NE2	3:A:511:HOH:O	2.43	0.51
1:B:287:ASP:N	1:B:287:ASP:OD1	2.42	0.51
1:A:110:SER:OG	1:A:112:ASP:OD1	2.27	0.50
1:A:279:HIS:HB2	1:A:284:TYR:CZ	2.47	0.50
1:B:56:ARG:HB3	1:B:62:SER:HB2	1.94	0.50
1:A:124:PHE:HB3	1:A:151:ARG:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LYS:HB3	1:B:280:ARG:HB3	1.93	0.49
1:A:97:ASP:O	1:A:100:MET:HB2	2.11	0.49
1:B:6:ARG:HG2	1:B:88:THR:HG22	1.94	0.49
1:A:4:LYS:HD3	1:A:280:ARG:CZ	2.42	0.49
1:B:165:ARG:HD2	1:B:165:ARG:HA	1.67	0.48
1:A:91:TYR:OH	1:A:287:ASP:OD1	2.25	0.47
1:B:158:GLU:OE1	1:B:209:ARG:NE	2.47	0.47
1:B:211:VAL:HG11	1:B:215:MET:HG3	1.97	0.47
1:B:184:MET:HG2	1:B:197:PHE:CG	2.50	0.47
1:A:20:ARG:CZ	1:A:24:ARG:HH22	2.28	0.47
1:B:20:ARG:NH2	3:B:528:HOH:O	2.49	0.46
1:A:9:LYS:NZ	1:A:18:GLU:OE2	2.39	0.46
1:A:4:LYS:HA	1:A:285:VAL:CG1	2.46	0.46
1:A:20:ARG:NE	1:A:24:ARG:HH22	2.14	0.45
1:B:157:LYS:O	1:B:160:PRO:HD3	2.16	0.45
1:A:150:LYS:O	1:A:213:GLY:HA3	2.18	0.44
1:B:62:SER:O	1:B:191:ARG:HD3	2.18	0.44
1:B:66:LEU:HD13	1:B:238:TRP:CG	2.53	0.44
1:B:59:ALA:O	1:B:65:PHE:HA	2.18	0.43
1:A:138:THR:O	1:A:139:ILE:HD13	2.18	0.43
1:B:10:ASN:HD21	1:B:12:LEU:HD12	1.83	0.43
1:A:195:GLU:OE2	3:A:501:HOH:O	2.21	0.43
1:A:209[A]:ARG:HG2	1:A:209[A]:ARG:H	1.65	0.42
1:A:100:MET:HE2	1:A:102:ASP:O	2.19	0.42
1:B:158:GLU:H	1:B:158:GLU:CD	2.28	0.42
1:A:184:MET:HE2	1:A:184:MET:HB2	1.79	0.41
1:A:157:LYS:HB3	1:A:157:LYS:HE2	1.81	0.41
1:B:8:ARG:NH2	3:B:525:HOH:O	2.46	0.41
1:B:73:LEU:HG	1:B:89:LEU:HD21	2.03	0.41
1:A:113:PHE:HB3	1:A:114:MET:H	1.74	0.40
1:A:194:LEU:HA	1:A:203:LEU:HD13	2.03	0.40
1:B:32:LYS:HE3	1:B:83:ILE:HD11	2.04	0.40
1:B:149:LEU:HA	1:B:149:LEU:HD12	1.91	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ASP:OD1	1:B:246:ARG:NH1[2_646]	2.15	0.05

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/303 (94%)	271 (95%)	12 (4%)	2 (1%)	19	18
1	B	286/303 (94%)	277 (97%)	9 (3%)	0	100	100
All	All	571/606 (94%)	548 (96%)	21 (4%)	2 (0%)	30	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	GLY
1	A	287	ASP

### 5.3.2 Protein sidechains

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	250/266 (94%)	239 (96%)	11 (4%)	24	28
1	B	250/266 (94%)	244 (98%)	6 (2%)	44	54
All	All	500/532 (94%)	483 (97%)	17 (3%)	34	39

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	47	LYS
1	A	62	SER
1	A	99	GLN

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Mol	Chain	Res	Type
1	A	121	ILE
1	A	175	THR
1	A	199	ASN
1	A	209[A]	ARG
1	A	209[B]	ARG
1	A	218	VAL
1	A	237	ILE
1	B	4	LYS
1	B	125	ILE
1	B	137	THR
1	B	146	SER
1	B	237	ILE
1	B	291	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	A	176	GLN
1	A	187	GLN
1	B	193	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	286/303 (94%)	0.71	16 (5%) 31 31	17, 34, 48, 73	1 (0%)
1	B	288/303 (95%)	0.51	7 (2%) 59 58	20, 28, 42, 60	0
All	All	574/606 (94%)	0.61	23 (4%) 43 42	17, 31, 47, 73	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	218	VAL	4.4
1	B	5	TYR	3.4
1	A	5	TYR	3.1
1	B	199	ASN	3.1
1	A	142	GLN	3.0
1	A	47	LYS	2.7
1	A	139	ILE	2.6
1	A	101	GLN	2.6
1	A	99	GLN	2.5
1	A	218	VAL	2.4
1	A	243	ILE	2.4
1	A	288	ILE	2.3
1	A	289	GLU	2.2
1	A	26	VAL	2.2
1	A	143	GLY	2.2
1	B	255	ASN	2.2
1	B	99	GLN	2.2
1	B	247	ASN	2.1
1	B	121	ILE	2.1
1	A	130	PRO	2.1
1	A	121	ILE	2.1
1	A	31	GLU	2.0
1	A	240	VAL	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

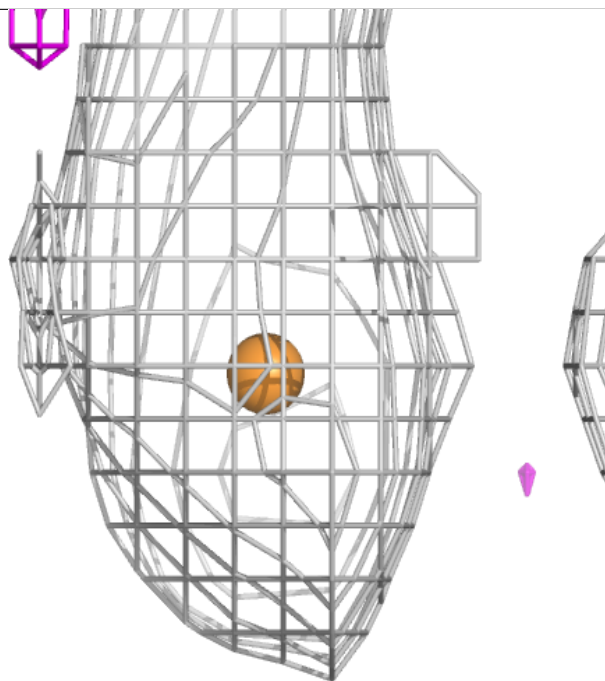
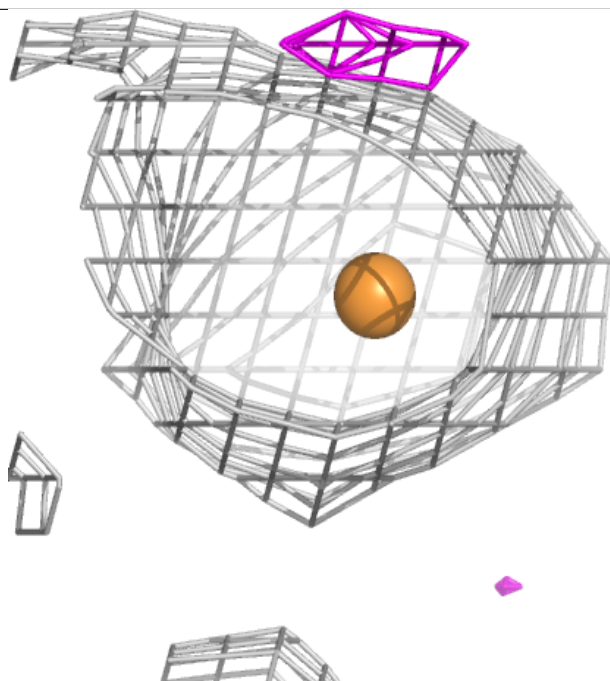
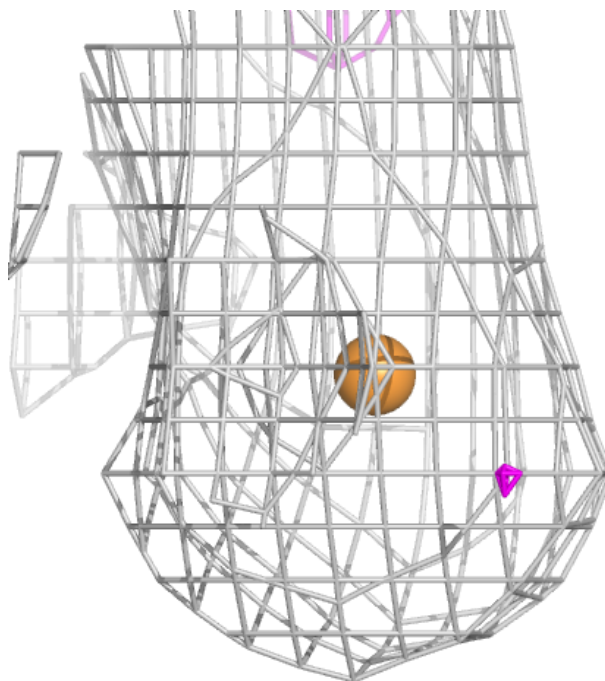
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CU	B	403	1/1	0.93	0.11	80,80,80,80	0
2	CU	A	403	1/1	0.96	0.08	73,73,73,73	0
2	CU	A	401	1/1	0.99	0.03	41,41,41,41	0
2	CU	B	401	1/1	0.99	0.01	32,32,32,32	0
2	CU	B	402	1/1	0.99	0.03	34,34,34,34	0
2	CU	A	402	1/1	0.99	0.03	38,38,38,38	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.

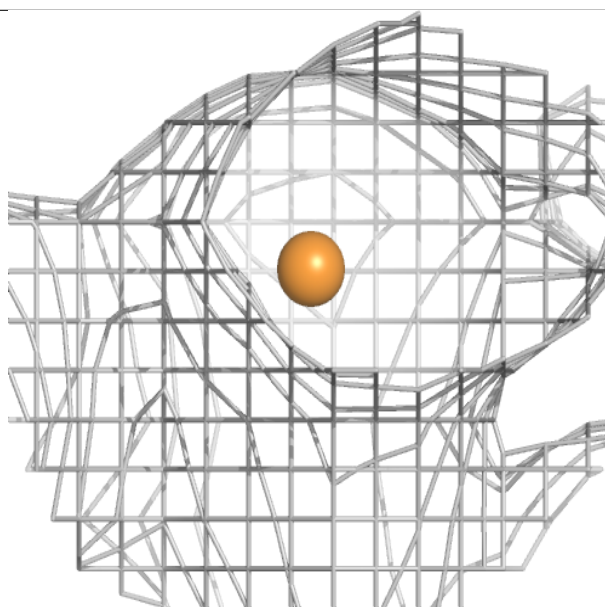
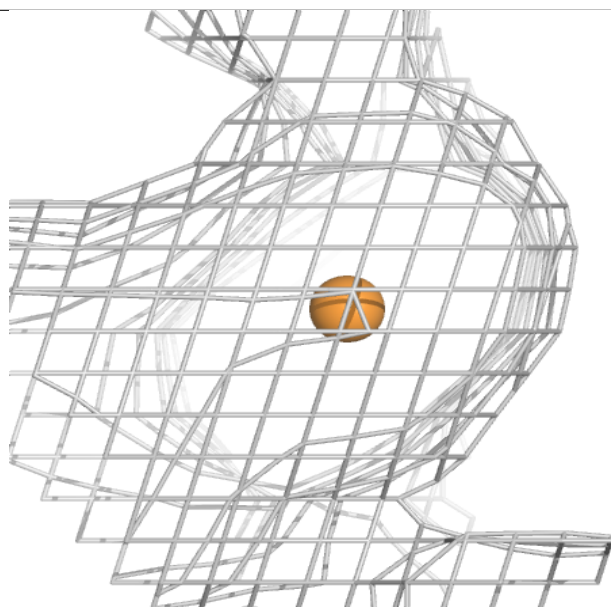
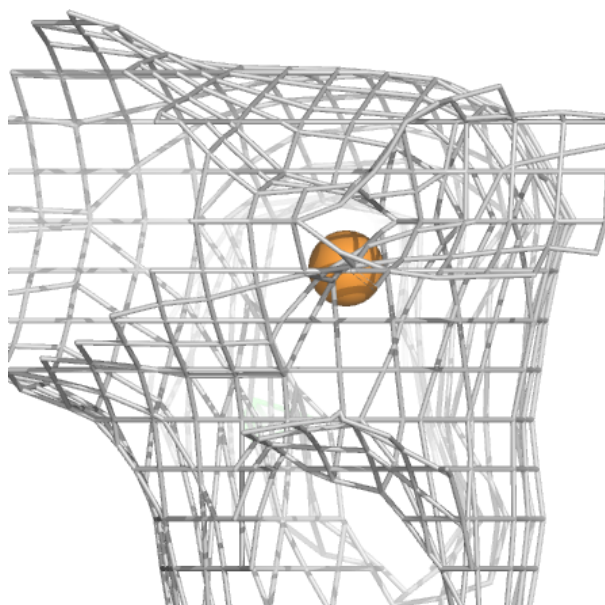
**Electron density around CU B 403:**

$2mF_o-DF_c$  (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:**

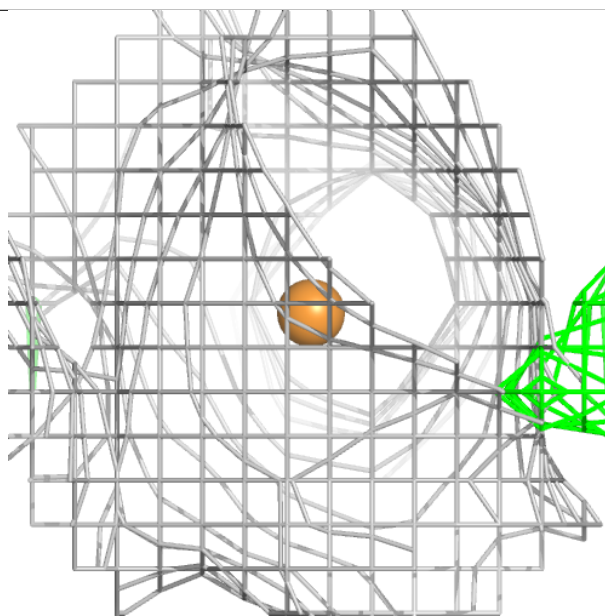
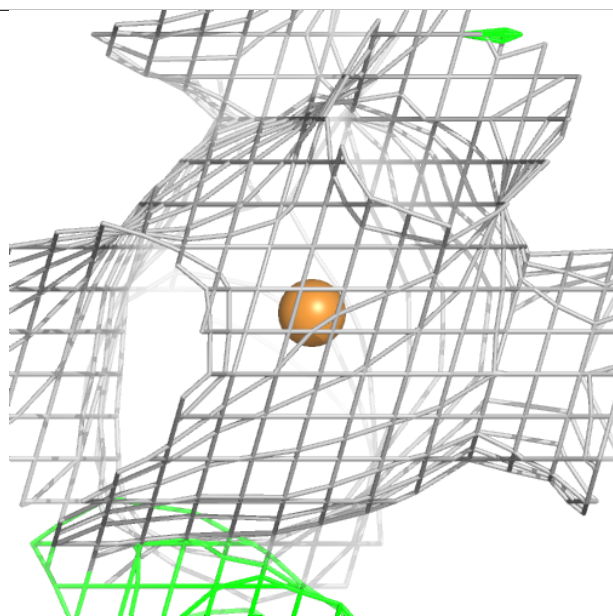
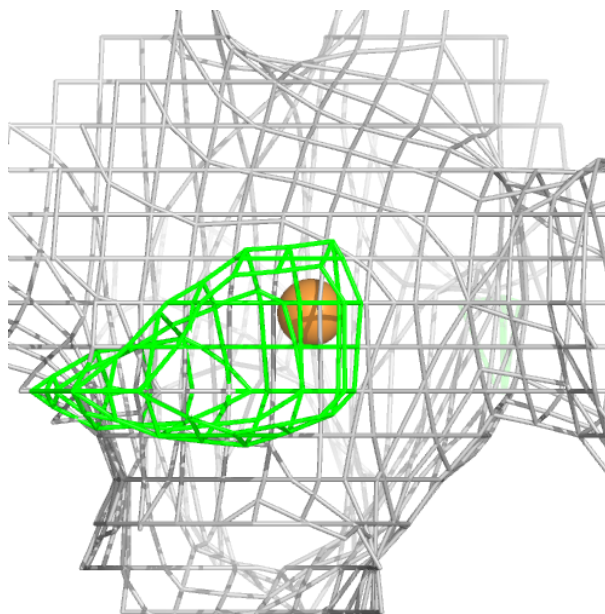
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





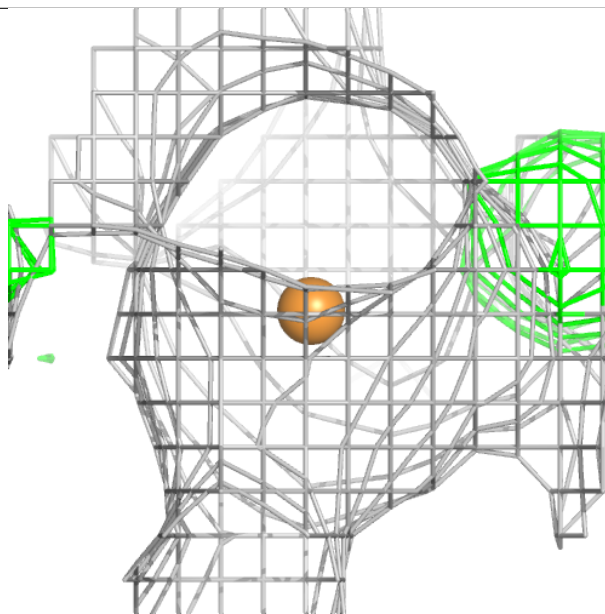
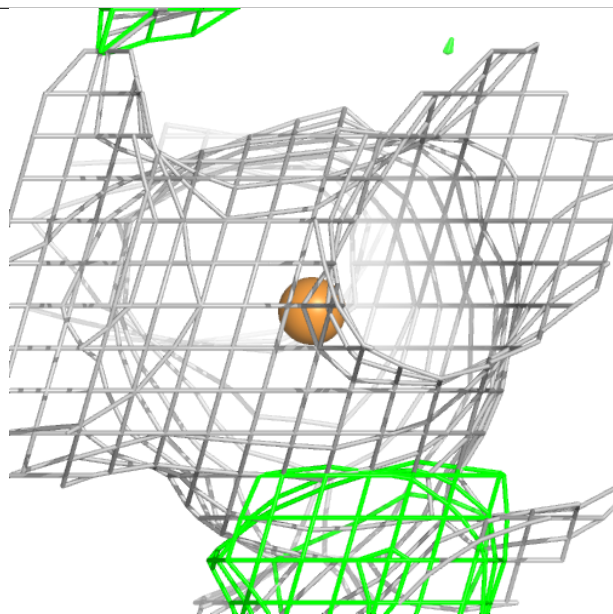
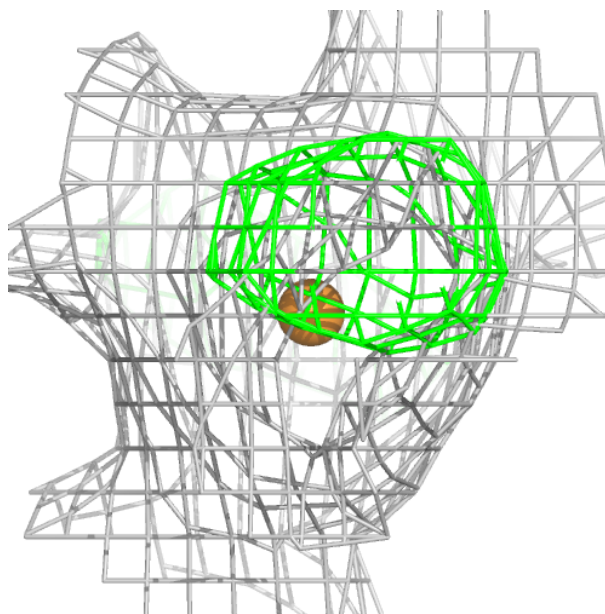
**Electron density around CU A 401:**

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



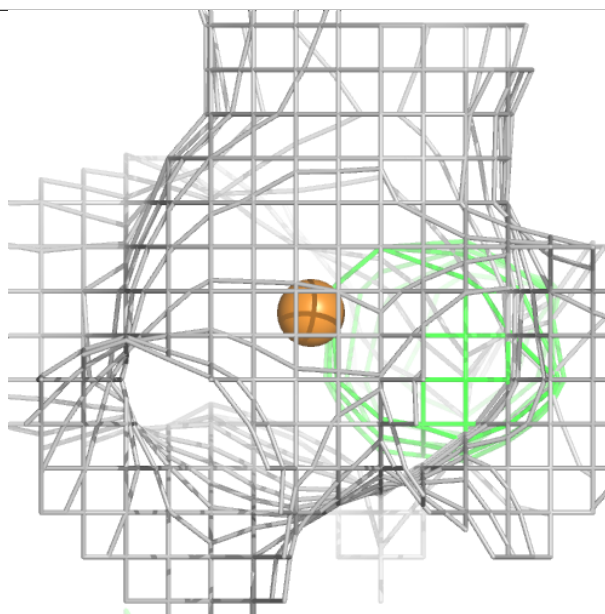
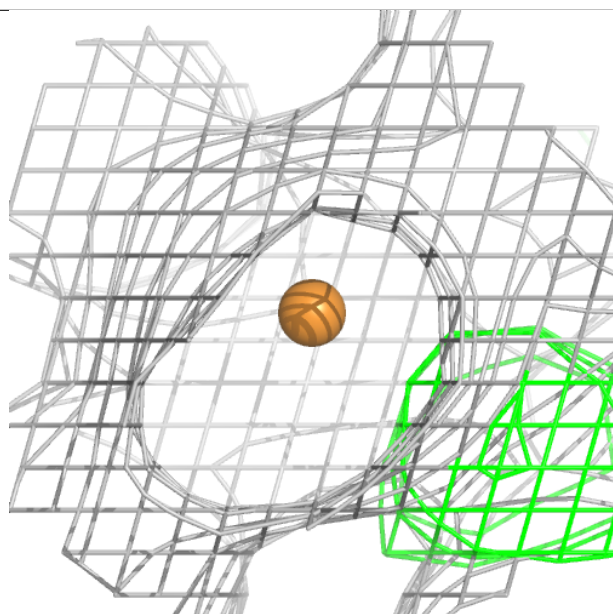
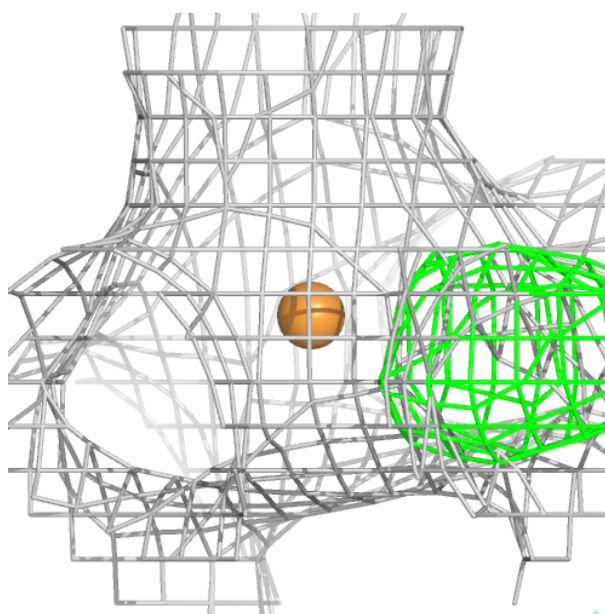
**Electron density around CU B 401:**

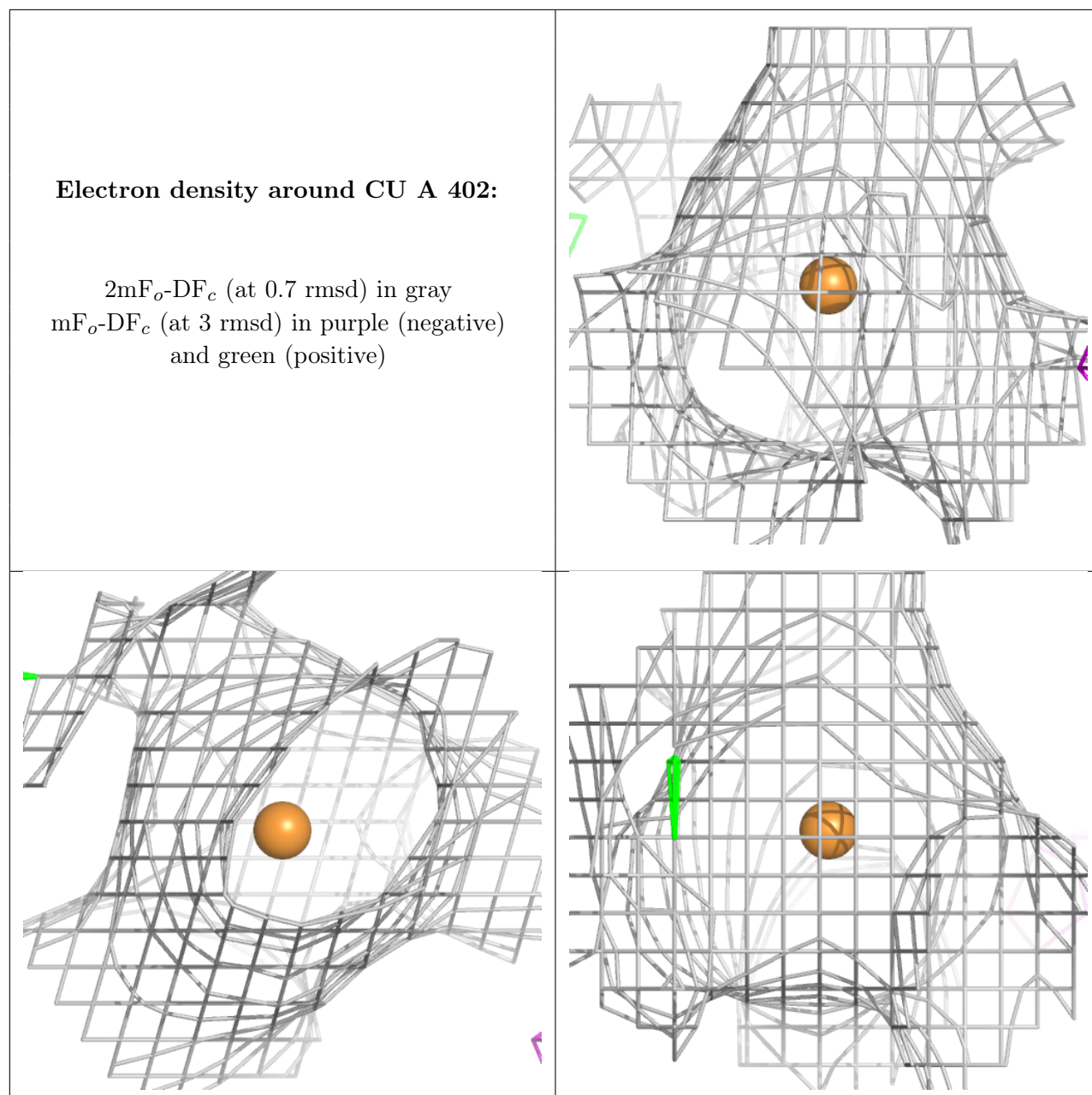
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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.