Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2023 – 12:22 PM EST

PDB ID	:	8U8Q
Title	:	V290N/S292F Streptomyces coelicolor Laccase
Authors	:	Wang, J.-X.; Lu, Y.
Deposited on	:	2023-09-18
Resolution	:	2.70 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:

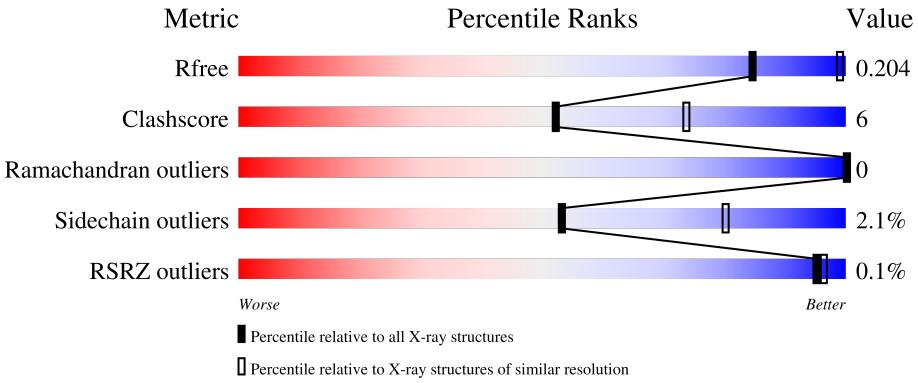
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	351	70% 10% 21%
1	B	351	69% 10% 21%
1	C	351	70% 9% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLY	A	408	-	X	-	-
3	GLY	B	409	-	X	-	-
3	GLY	C	407	-	X	-	-
3	GLY	C	409	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7128 atoms, of which 258 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 Copper oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2156	1349	393	403	11			
1	B	278	Total	C	N	O	S	0	0	0
			2156	1349	393	403	11			
1	C	278	Total	C	N	O	S	0	0	0
			2156	1349	393	403	11			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ASN	VAL	engineered mutation	UNP Q9XAL8
A	292	PHE	SER	engineered mutation	UNP Q9XAL8
A	344	LEU	-	expression tag	UNP Q9XAL8
A	345	GLU	-	expression tag	UNP Q9XAL8
A	346	HIS	-	expression tag	UNP Q9XAL8
A	347	HIS	-	expression tag	UNP Q9XAL8
A	348	HIS	-	expression tag	UNP Q9XAL8
A	349	HIS	-	expression tag	UNP Q9XAL8
A	350	HIS	-	expression tag	UNP Q9XAL8
A	351	HIS	-	expression tag	UNP Q9XAL8
B	290	ASN	VAL	engineered mutation	UNP Q9XAL8
B	292	PHE	SER	engineered mutation	UNP Q9XAL8
B	344	LEU	-	expression tag	UNP Q9XAL8
B	345	GLU	-	expression tag	UNP Q9XAL8
B	346	HIS	-	expression tag	UNP Q9XAL8
B	347	HIS	-	expression tag	UNP Q9XAL8
B	348	HIS	-	expression tag	UNP Q9XAL8
B	349	HIS	-	expression tag	UNP Q9XAL8
B	350	HIS	-	expression tag	UNP Q9XAL8
B	351	HIS	-	expression tag	UNP Q9XAL8
C	290	ASN	VAL	engineered mutation	UNP Q9XAL8
C	292	PHE	SER	engineered mutation	UNP Q9XAL8
C	344	LEU	-	expression tag	UNP Q9XAL8

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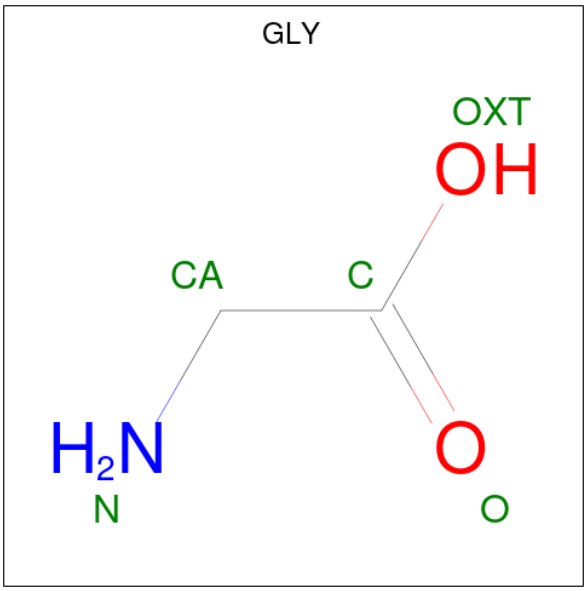
Chain	Residue	Modelled	Actual	Comment	Reference
C	345	GLU	-	expression tag	UNP Q9XAL8
C	346	HIS	-	expression tag	UNP Q9XAL8
C	347	HIS	-	expression tag	UNP Q9XAL8
C	348	HIS	-	expression tag	UNP Q9XAL8
C	349	HIS	-	expression tag	UNP Q9XAL8
C	350	HIS	-	expression tag	UNP Q9XAL8
C	351	HIS	-	expression tag	UNP Q9XAL8

- 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	A	4	Total Cu 4 4	0	0
2	B	4	Total Cu 4 4	0	0
2	C	4	Total Cu 4 4	0	0

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O 10 2 5 1 2	0	0
3	A	1	Total C H N O 10 2 5 1 2	0	0

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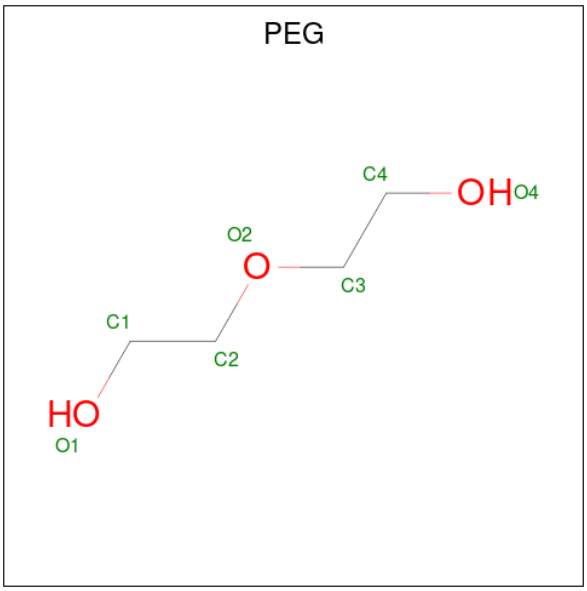
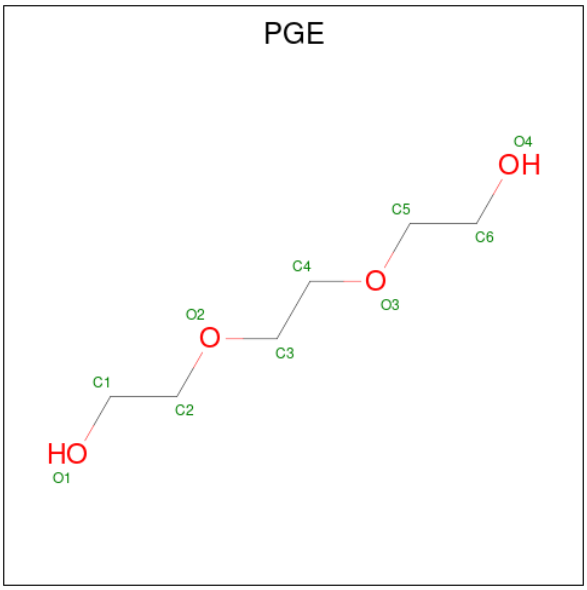
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	A	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	A	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	B	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	B	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	B	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	B	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	B	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			24	6	14	4		

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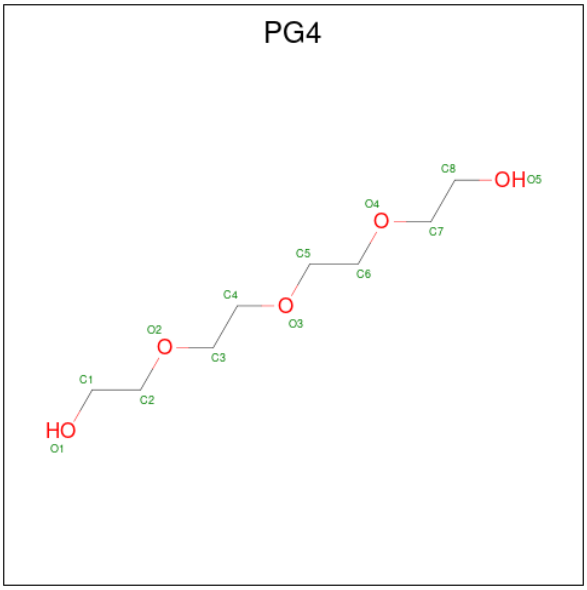
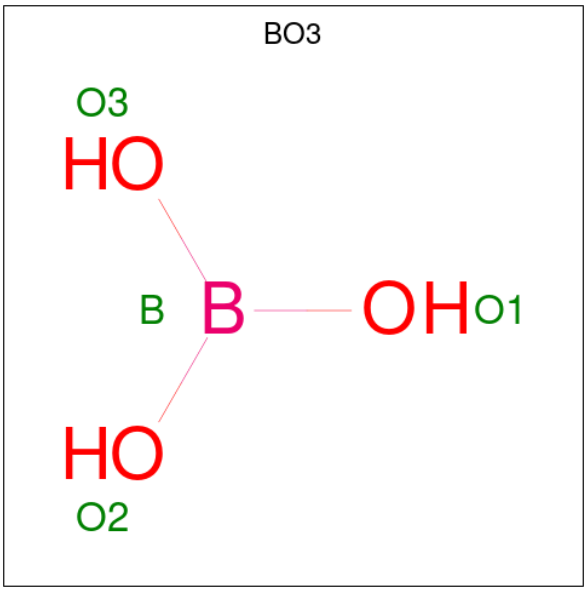
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C H O 24 6 14 4	0	0
5	C	1	Total C H O 24 6 14 4	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



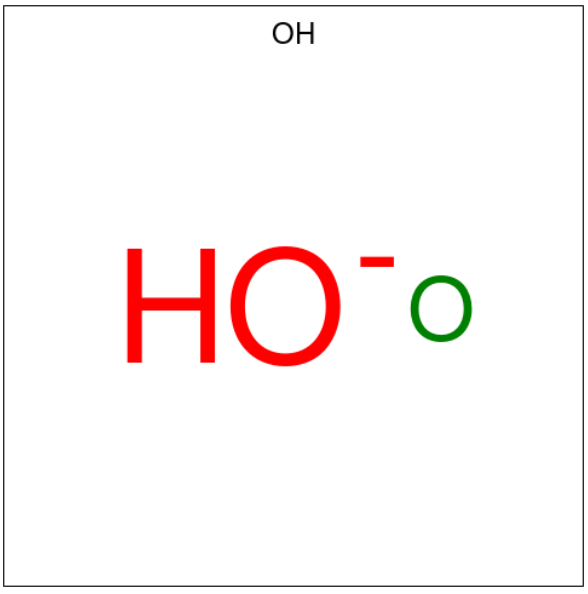
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 31 8 18 5	0	0
6	A	1	Total C H O 31 8 18 5	0	0
6	B	1	Total C H O 31 8 18 5	0	0
6	B	1	Total C H O 31 8 18 5	0	0
6	C	1	Total C H O 31 8 18 5	0	0
6	C	1	Total C H O 31 8 18 5	0	0

- Molecule 7 is BORIC ACID (three-letter code: BO3) (formula: BH_3O_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total B H O 7 1 3 3	0	0

- Molecule 8 is HYDROXIDE ION (three-letter code: OH) (formula: HO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 1 1	0	0
8	B	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O 1 1	0	0

- Molecule 9 is water.

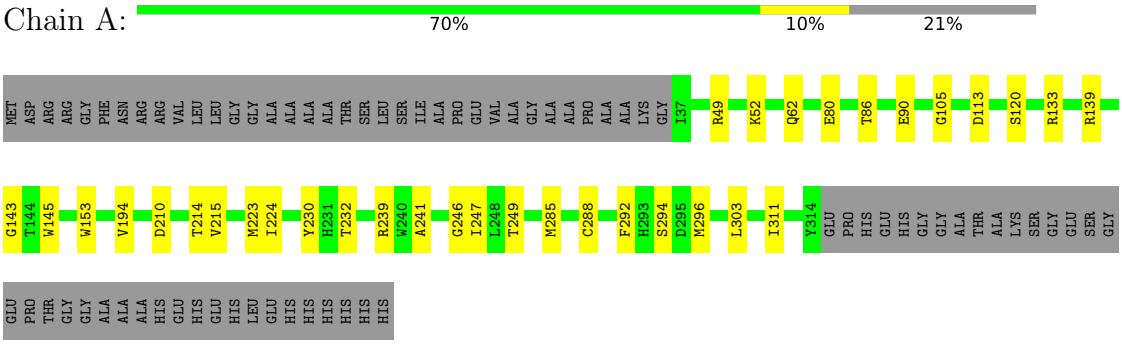
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	55	Total O 55 55	0	0
9	B	64	Total O 64 64	0	0
9	C	60	Total O 60 60	0	0

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.

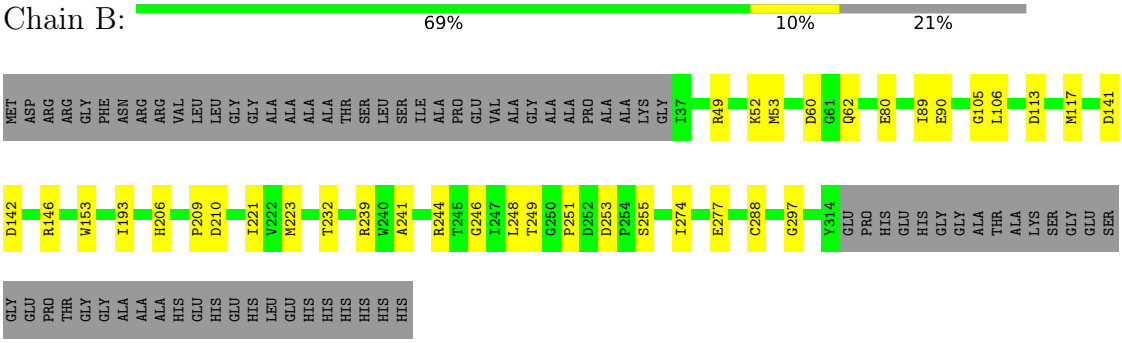
• Molecule 1: Copper oxidase

Chain A:



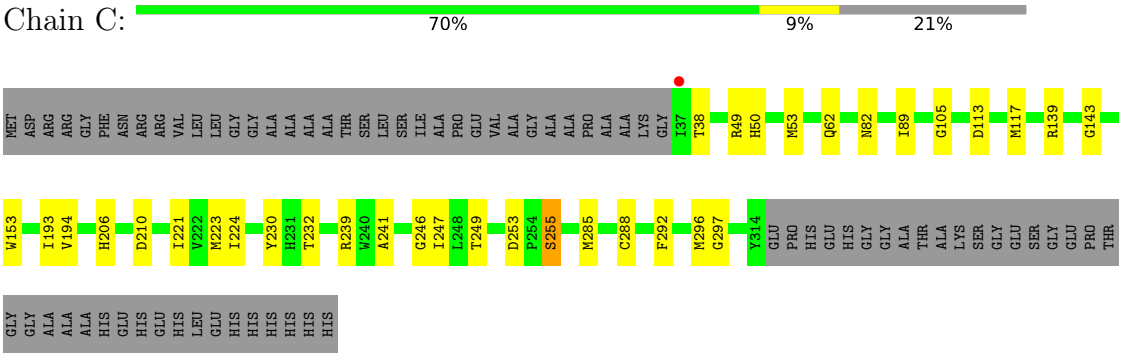
• Molecule 1: Copper oxidase

Chain B:



• Molecule 1: Copper oxidase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	178.34Å 178.34Å 179.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.42 – 2.70 59.57 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (56.42-2.70) 81.4 (59.57-2.40)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.31 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.173 , 0.205 0.173 , 0.204	Depositor DCC
R_{free} test set	5587 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.457 for -h,l,k 0.447 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7128	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: PGE, CU, OH, PG4, BO3, PEG

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	0.40	0/2219	0.65	0/3011
1	B	0.40	0/2219	0.65	0/3011
1	C	0.40	0/2219	0.65	0/3011
All	All	0.40	0/6657	0.65	0/9033

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	2156	0	2036	20	0
1	B	2156	0	2036	31	0
1	C	2156	0	2036	25	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	25	25	10	0	0
3	B	25	25	10	1	0
3	C	25	25	10	1	0
4	A	7	10	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	7	10	10	0	0
4	C	7	10	10	2	0
5	A	10	14	14	0	0
5	B	10	14	14	3	0
5	C	10	14	14	0	0
6	A	26	36	36	4	0
6	B	26	36	36	7	0
6	C	26	36	36	4	0
7	A	4	3	3	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	A	55	0	0	1	0
9	B	64	0	0	1	0
9	C	60	0	0	0	0
All	All	6870	258	6321	72	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 6.

All (72) 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:B:49:ARG:HD3	6:B:412:PG4:H51	1.58	0.84
1:B:249:THR:HG23	1:B:253:ASP:OD2	1.77	0.83
1:B:193:ILE:HD12	1:B:221:ILE:HG23	1.74	0.70
1:B:53:MET:HE3	1:B:89:ILE:HG21	1.72	0.69
1:B:146:ARG:HH11	5:B:411:PGE:H22	1.57	0.69
1:C:53:MET:HE3	1:C:89:ILE:HG21	1.79	0.65
1:B:52:LYS:HE2	1:B:90:GLU:OE2	1.97	0.65
1:C:253:ASP:OD1	1:C:255:SER:OG	2.14	0.64
1:B:146:ARG:HD3	5:B:411:PGE:H2	1.80	0.62
1:C:82:ASN:HD21	3:C:409:GLY:N	1.99	0.61
1:A:285:MET:HG2	1:C:117:MET:HE1	1.83	0.60
1:B:49:ARG:HH11	6:B:412:PG4:H51	1.68	0.59
1:C:206:HIS:CE1	1:C:297:GLY:HA2	2.39	0.58
1:A:145:TRP:CH2	1:B:251:PRO:HG3	2.39	0.57
1:B:193:ILE:HD12	1:B:221:ILE:CG2	2.32	0.57
1:B:253:ASP:OD1	1:B:255:SER:OG	2.17	0.56
1:C:210:ASP:H	6:C:414:PG4:H71	1.69	0.56
1:B:206:HIS:CE1	1:B:297:GLY:HA2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ARG:HE	6:C:413:PG4:H51	1.72	0.55
1:B:209:PRO:HA	6:B:413:PG4:H72	1.87	0.55
1:C:53:MET:HE3	1:C:89:ILE:CG2	2.37	0.55
1:A:49:ARG:HB3	6:A:412:PG4:H62	1.89	0.54
1:B:142:ASP:HA	1:C:38:THR:HG22	1.90	0.54
1:B:53:MET:HE3	1:B:89:ILE:CG2	2.38	0.53
1:A:232:THR:O	1:A:288:CYS:HA	2.09	0.52
1:B:80:GLU:H	6:B:412:PG4:H31	1.74	0.52
1:B:117:MET:HE1	1:C:285:MET:HG3	1.91	0.52
1:C:62:GLN:HE22	4:C:412:PEG:H42	1.74	0.52
1:C:50:HIS:H	6:C:413:PG4:H71	1.73	0.52
1:A:139:ARG:HD2	1:A:143:GLY:O	2.11	0.50
1:C:249:THR:HG23	1:C:253:ASP:OD2	2.11	0.50
1:C:193:ILE:HD12	1:C:221:ILE:HG23	1.93	0.50
1:A:62:GLN:HE22	4:A:410:PEG:H32	1.77	0.50
1:C:139:ARG:HD2	1:C:143:GLY:O	2.11	0.50
1:A:210:ASP:H	6:A:413:PG4:H71	1.77	0.50
1:B:53:MET:HE1	1:B:89:ILE:HD13	1.93	0.49
1:B:210:ASP:H	6:B:413:PG4:C7	2.25	0.49
1:B:60:ASP:OD1	1:B:62:GLN:HG3	2.12	0.49
1:B:210:ASP:OD2	6:B:413:PG4:H32	2.13	0.49
1:B:244:ARG:HH11	3:B:406:GLY:N	2.12	0.48
1:B:146:ARG:HD3	5:B:411:PGE:C2	2.44	0.48
1:A:105:GLY:HA3	1:A:153:TRP:CD2	2.49	0.47
1:A:62:GLN:HE22	4:A:410:PEG:C3	2.28	0.47
9:B:504:HOH:O	1:C:247:ILE:HG23	2.14	0.47
1:B:232:THR:O	1:B:288:CYS:HA	2.15	0.47
1:B:210:ASP:H	6:B:413:PG4:H71	1.80	0.46
1:A:292:PHE:O	1:A:296:MET:HG2	2.16	0.46
1:C:241:ALA:O	1:C:246:GLY:HA2	2.16	0.46
1:C:49:ARG:NE	6:C:413:PG4:H51	2.30	0.46
1:A:49:ARG:HB3	6:A:412:PG4:C6	2.46	0.45
1:B:106:LEU:HD12	1:B:106:LEU:N	2.31	0.45
1:C:232:THR:O	1:C:288:CYS:HA	2.16	0.45
1:C:194:VAL:HG22	1:C:224:ILE:HB	1.98	0.45
1:A:80:GLU:O	6:A:412:PG4:H42	2.17	0.44
1:B:248:LEU:HD22	1:B:253:ASP:HB3	1.98	0.44
1:C:38:THR:O	1:C:38:THR:HG23	2.16	0.44
1:A:247:ILE:HG21	9:A:543:HOH:O	2.18	0.44
1:B:105:GLY:HA3	1:B:153:TRP:CD2	2.52	0.44
1:A:303:LEU:HD22	1:A:311:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:TYR:CD1	1:C:230:TYR:N	2.87	0.42
1:A:86:THR:HG23	1:A:133:ARG:HG3	2.01	0.42
1:A:241:ALA:O	1:A:246:GLY:HA2	2.20	0.42
1:B:52:LYS:HD2	1:B:90:GLU:HB3	2.01	0.42
1:B:241:ALA:O	1:B:246:GLY:HA2	2.21	0.41
1:A:52:LYS:HE2	1:A:90:GLU:OE2	2.20	0.41
1:A:194:VAL:HA	1:A:224:ILE:O	2.20	0.41
1:C:62:GLN:HE22	4:C:412:PEG:C4	2.34	0.41
1:C:292:PHE:O	1:C:296:MET:HG2	2.20	0.41
1:A:214:THR:O	1:A:215:VAL:C	2.59	0.41
1:C:105:GLY:HA3	1:C:153:TRP:CD2	2.56	0.41
1:B:274:ILE:HB	1:B:277:GLU:HB2	2.03	0.40
1:A:230:TYR:CD1	1:A:230:TYR:N	2.90	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	276/351 (79%)	265 (96%)	11 (4%)	0	100	100
1	B	276/351 (79%)	266 (96%)	10 (4%)	0	100	100
1	C	276/351 (79%)	269 (98%)	7 (2%)	0	100	100
All	All	828/1053 (79%)	800 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	223/270 (83%)	217 (97%)	6 (3%)	44 74
1	B	223/270 (83%)	219 (98%)	4 (2%)	59 83
1	C	223/270 (83%)	219 (98%)	4 (2%)	59 83
All	All	669/810 (83%)	655 (98%)	14 (2%)	53 80

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ASP
1	A	120	SER
1	A	223	MET
1	A	239	ARG
1	A	249	THR
1	A	294	SER
1	B	113	ASP
1	B	141	ASP
1	B	223	MET
1	B	239	ARG
1	C	113	ASP
1	C	223	MET
1	C	239	ARG
1	C	255	SER

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

Mol	Chain	Res	Type
1	A	82	ASN
1	B	82	ASN
1	C	82	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 43 ligands modelled in this entry, 12 are monoatomic and 3 are modelled with single atom - leaving 28 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	GLY	C	406	-	4,4,4	1.17	1 (25%)	3,4,4	1.19	0
3	GLY	A	414	-	4,4,4	1.15	1 (25%)	3,4,4	1.43	0
6	PG4	C	413	-	12,12,12	0.26	0	11,11,11	0.50	0
6	PG4	A	412	-	12,12,12	0.22	0	11,11,11	0.66	0
6	PG4	B	412	-	12,12,12	0.24	0	11,11,11	0.43	0
3	GLY	C	409	-	4,4,4	1.12	1 (25%)	3,4,4	1.80	1 (33%)
3	GLY	B	409	-	4,4,4	1.10	1 (25%)	3,4,4	1.84	2 (66%)
5	PGE	B	411	-	9,9,9	0.37	0	8,8,8	0.43	0
3	GLY	A	407	-	4,4,4	1.26	1 (25%)	3,4,4	1.16	0
3	GLY	B	408	-	4,4,4	1.03	0	3,4,4	1.52	0
6	PG4	B	413	-	12,12,12	0.23	0	11,11,11	0.56	0
3	GLY	A	406	-	4,4,4	1.09	1 (25%)	3,4,4	1.73	1 (33%)
4	PEG	B	410	-	6,6,6	0.31	0	5,5,5	0.17	0
6	PG4	A	413	-	12,12,12	0.20	0	11,11,11	0.60	0
4	PEG	C	412	-	6,6,6	0.22	0	5,5,5	0.08	0
6	PG4	C	414	-	12,12,12	0.22	0	11,11,11	0.65	0
5	PGE	A	411	-	9,9,9	0.39	0	8,8,8	0.57	0
3	GLY	A	408	-	4,4,4	1.16	1 (25%)	3,4,4	1.66	1 (33%)
4	PEG	A	410	-	6,6,6	0.27	0	5,5,5	0.08	0
5	PGE	C	411	-	9,9,9	0.39	0	8,8,8	0.28	0
3	GLY	A	409	-	4,4,4	1.11	1 (25%)	3,4,4	1.73	2 (66%)
3	GLY	B	414	-	4,4,4	1.17	1 (25%)	3,4,4	1.30	0
3	GLY	B	407	-	4,4,4	1.25	1 (25%)	3,4,4	1.25	0
3	GLY	B	406	-	4,4,4	1.03	0	3,4,4	1.69	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GLY	C	410	-	4,4,4	0.99	0	3,4,4	1.74	1 (33%)
7	BO3	A	415	-	3,3,3	0.74	0	3,3,3	1.00	0
3	GLY	C	408	-	4,4,4	0.70	0	3,4,4	2.44	1 (33%)
3	GLY	C	407	-	4,4,4	1.09	1 (25%)	3,4,4	1.63	1 (33%)

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
3	GLY	C	406	-	-	0/2/2/2	-
3	GLY	A	414	-	-	0/2/2/2	-
6	PG4	C	413	-	-	9/10/10/10	-
6	PG4	A	412	-	-	6/10/10/10	-
6	PG4	B	412	-	-	4/10/10/10	-
3	GLY	C	409	-	-	2/2/2/2	-
3	GLY	B	409	-	-	2/2/2/2	-
5	PGE	B	411	-	-	4/7/7/7	-
3	GLY	A	407	-	-	0/2/2/2	-
3	GLY	B	408	-	-	2/2/2/2	-
6	PG4	B	413	-	-	4/10/10/10	-
3	GLY	A	406	-	-	0/2/2/2	-
4	PEG	B	410	-	-	3/4/4/4	-
6	PG4	A	413	-	-	4/10/10/10	-
4	PEG	C	412	-	-	2/4/4/4	-
6	PG4	C	414	-	-	5/10/10/10	-
5	PGE	A	411	-	-	5/7/7/7	-
3	GLY	A	408	-	-	2/2/2/2	-
4	PEG	A	410	-	-	2/4/4/4	-
5	PGE	C	411	-	-	5/7/7/7	-
3	GLY	A	409	-	-	0/2/2/2	-
3	GLY	B	414	-	-	0/2/2/2	-
3	GLY	B	407	-	-	0/2/2/2	-
3	GLY	B	406	-	-	2/2/2/2	-
3	GLY	C	410	-	-	0/2/2/2	-
3	GLY	C	408	-	-	1/2/2/2	-
3	GLY	C	407	-	-	2/2/2/2	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	407	GLY	OXT-C	-2.19	1.23	1.30
3	A	408	GLY	OXT-C	-2.18	1.23	1.30
3	B	407	GLY	OXT-C	-2.13	1.23	1.30
3	C	409	GLY	OXT-C	-2.13	1.23	1.30
3	A	414	GLY	OXT-C	-2.09	1.23	1.30
3	C	406	GLY	OXT-C	-2.09	1.23	1.30
3	B	414	GLY	OXT-C	-2.08	1.23	1.30
3	B	409	GLY	OXT-C	-2.07	1.23	1.30
3	A	409	GLY	OXT-C	-2.07	1.23	1.30
3	A	406	GLY	OXT-C	-2.06	1.23	1.30
3	C	407	GLY	OXT-C	-2.03	1.23	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	408	GLY	OXT-C-CA	3.29	126.53	113.45
3	A	406	GLY	OXT-C-O	-2.50	117.07	123.30
3	C	410	GLY	OXT-C-O	-2.40	117.33	123.30
3	C	409	GLY	OXT-C-O	-2.38	117.36	123.30
3	B	406	GLY	OXT-C-O	-2.28	117.60	123.30
3	B	409	GLY	OXT-C-O	-2.28	117.61	123.30
3	C	407	GLY	OXT-C-O	-2.22	117.76	123.30
3	A	409	GLY	OXT-C-O	-2.19	117.84	123.30
3	B	409	GLY	OXT-C-CA	2.16	122.06	113.45
3	A	408	GLY	OXT-C-O	-2.16	117.90	123.30
3	A	409	GLY	OXT-C-CA	2.01	121.44	113.45

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	408	GLY	O-C-CA-N
3	A	408	GLY	OXT-C-CA-N
3	B	406	GLY	O-C-CA-N
3	B	408	GLY	O-C-CA-N
3	B	409	GLY	O-C-CA-N
3	B	409	GLY	OXT-C-CA-N
3	C	407	GLY	O-C-CA-N
3	C	409	GLY	O-C-CA-N
3	C	409	GLY	OXT-C-CA-N
5	B	411	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
6	A	413	PG4	O3-C5-C6-O4
6	C	413	PG4	O3-C5-C6-O4
6	C	413	PG4	O2-C3-C4-O3
6	B	413	PG4	O2-C3-C4-O3
5	C	411	PGE	O2-C3-C4-O3
6	B	412	PG4	O3-C5-C6-O4
3	B	406	GLY	OXT-C-CA-N
3	B	408	GLY	OXT-C-CA-N
3	C	407	GLY	OXT-C-CA-N
5	C	411	PGE	O3-C5-C6-O4
6	B	412	PG4	O4-C7-C8-O5
6	C	414	PG4	O4-C7-C8-O5
5	A	411	PGE	O2-C3-C4-O3
6	C	414	PG4	O3-C5-C6-O4
4	A	410	PEG	O1-C1-C2-O2
5	A	411	PGE	O1-C1-C2-O2
5	A	411	PGE	O3-C5-C6-O4
6	A	413	PG4	O1-C1-C2-O2
6	A	412	PG4	O1-C1-C2-O2
4	A	410	PEG	O2-C3-C4-O4
6	C	413	PG4	O4-C7-C8-O5
6	A	412	PG4	O3-C5-C6-O4
4	B	410	PEG	O2-C3-C4-O4
4	C	412	PEG	O2-C3-C4-O4
6	C	413	PG4	O1-C1-C2-O2
6	C	414	PG4	O1-C1-C2-O2
6	B	413	PG4	O4-C7-C8-O5
6	A	413	PG4	C6-C5-O3-C4
4	C	412	PEG	C1-C2-O2-C3
6	C	413	PG4	C3-C4-O3-C5
6	C	414	PG4	C6-C5-O3-C4
6	B	413	PG4	C1-C2-O2-C3
6	B	412	PG4	C6-C5-O3-C4
5	C	411	PGE	C1-C2-O2-C3
6	A	413	PG4	C4-C3-O2-C2
4	B	410	PEG	C1-C2-O2-C3
5	A	411	PGE	C6-C5-O3-C4
5	C	411	PGE	O1-C1-C2-O2
5	B	411	PGE	C3-C4-O3-C5
6	C	413	PG4	C4-C3-O2-C2
5	B	411	PGE	C6-C5-O3-C4
6	C	413	PG4	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
6	A	412	PG4	C1-C2-O2-C3
5	A	411	PGE	C4-C3-O2-C2
6	A	412	PG4	C8-C7-O4-C6
6	A	412	PG4	O4-C7-C8-O5
6	C	413	PG4	C1-C2-O2-C3
6	B	413	PG4	O3-C5-C6-O4
6	C	413	PG4	C5-C6-O4-C7
5	B	411	PGE	O1-C1-C2-O2
4	B	410	PEG	C4-C3-O2-C2
6	B	412	PG4	C5-C6-O4-C7
5	C	411	PGE	C3-C4-O3-C5
6	C	414	PG4	O2-C3-C4-O3
3	C	408	GLY	O-C-CA-N
6	A	412	PG4	O2-C3-C4-O3

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	413	PG4	3	0
6	A	412	PG4	3	0
6	B	412	PG4	3	0
3	C	409	GLY	1	0
5	B	411	PGE	3	0
6	B	413	PG4	4	0
6	A	413	PG4	1	0
4	C	412	PEG	2	0
6	C	414	PG4	1	0
4	A	410	PEG	2	0
3	B	406	GLY	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

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	278/351 (79%)	-0.17	0	100	100	42, 52, 69, 91	0
1	B	278/351 (79%)	-0.17	0	100	100	41, 52, 69, 91	0
1	C	278/351 (79%)	-0.19	1 (0%)	92	93	42, 52, 69, 91	0
All	All	834/1053 (79%)	-0.18	1 (0%)	95	96	41, 52, 69, 91	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	ILE	2.3

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	PEG	B	410	7/7	0.69	0.27	70,98,125,125	0
4	PEG	A	410	7/7	0.77	0.26	75,95,114,114	0

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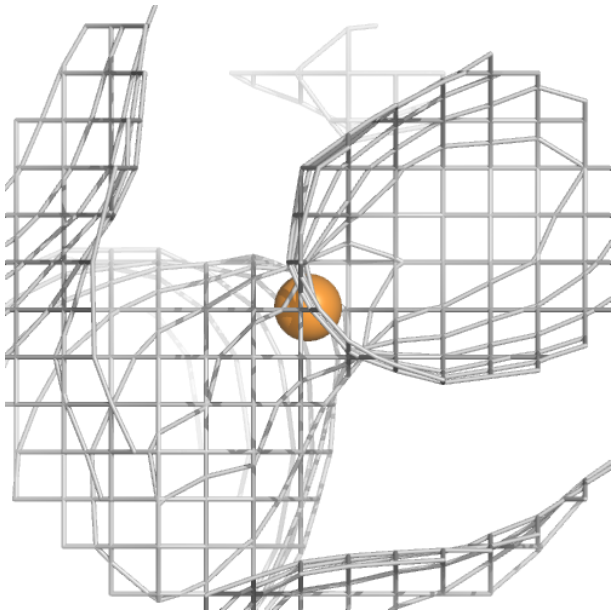
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	C	412	7/7	0.77	0.33	69,96,125,125	0
5	PGE	C	411	10/10	0.83	0.25	69,88,110,122	0
6	PG4	A	413	13/13	0.83	0.32	76,100,128,135	0
3	GLY	A	408	5/5	0.84	0.34	74,89,102,102	0
5	PGE	A	411	10/10	0.84	0.29	73,95,115,123	0
6	PG4	A	412	13/13	0.86	0.28	66,95,115,119	0
6	PG4	B	412	13/13	0.86	0.24	64,94,114,118	0
6	PG4	B	413	13/13	0.86	0.29	72,98,118,123	0
6	PG4	C	414	13/13	0.86	0.26	74,97,122,125	0
6	PG4	C	413	13/13	0.88	0.31	63,96,116,116	0
5	PGE	B	411	10/10	0.88	0.27	67,95,117,120	0
3	GLY	B	408	5/5	0.89	0.20	71,85,93,102	0
3	GLY	C	410	5/5	0.90	0.16	70,84,92,92	0
3	GLY	B	409	5/5	0.91	0.15	70,85,92,92	0
3	GLY	C	409	5/5	0.93	0.28	72,87,94,94	0
3	GLY	A	406	5/5	0.94	0.31	66,76,83,83	0
3	GLY	A	409	5/5	0.94	0.15	68,81,85,90	0
7	BO3	A	415	4/4	0.94	0.15	62,65,79,79	0
3	GLY	C	407	5/5	0.95	0.27	67,77,81,81	0
3	GLY	B	406	5/5	0.95	0.28	64,76,84,84	0
3	GLY	C	408	5/5	0.96	0.26	56,67,71,74	0
3	GLY	A	407	5/5	0.96	0.24	54,66,69,71	0
3	GLY	A	414	5/5	0.96	0.20	49,59,72,75	0
2	CU	A	403	1/1	0.96	0.34	54,54,54,54	1
3	GLY	B	407	5/5	0.97	0.23	53,64,68,73	0
3	GLY	B	414	5/5	0.97	0.14	54,65,79,82	0
3	GLY	C	406	5/5	0.97	0.16	55,67,76,76	0
2	CU	A	402	1/1	0.97	0.08	61,61,61,61	1
2	CU	B	403	1/1	0.98	0.18	55,55,55,55	1
2	CU	C	402	1/1	0.98	0.15	59,59,59,59	1
2	CU	B	402	1/1	0.98	0.10	57,57,57,57	1
2	CU	C	404	1/1	0.99	0.19	51,51,51,51	1
2	CU	C	401	1/1	0.99	0.22	55,55,55,55	0
2	CU	A	401	1/1	0.99	0.22	55,55,55,55	0
2	CU	C	403	1/1	0.99	0.33	56,56,56,56	1
8	OH	A	405	1/1	0.99	0.43	58,58,58,58	1
8	OH	B	405	1/1	0.99	0.22	57,57,57,57	1
8	OH	C	405	1/1	0.99	0.26	57,57,57,57	0
2	CU	B	404	1/1	1.00	0.21	55,55,55,55	1
2	CU	B	401	1/1	1.00	0.19	57,57,57,57	0
2	CU	A	404	1/1	1.00	0.21	52,52,52,52	1

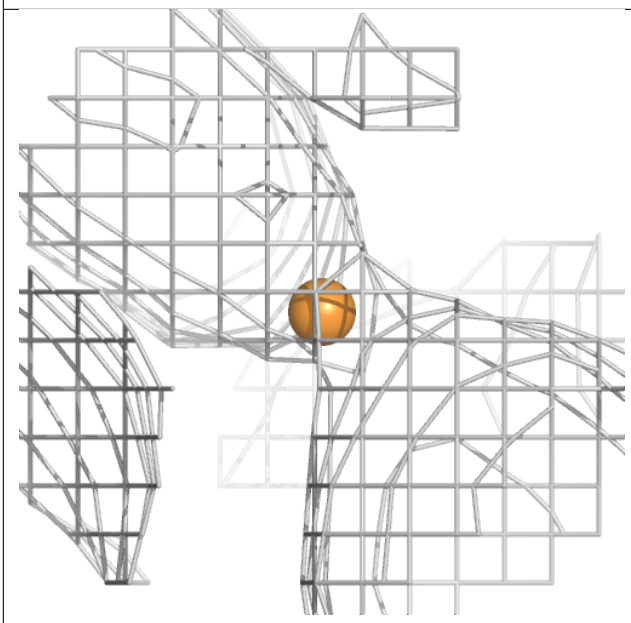
The following is a graphical depiction of the model fit to experimental electron density of all

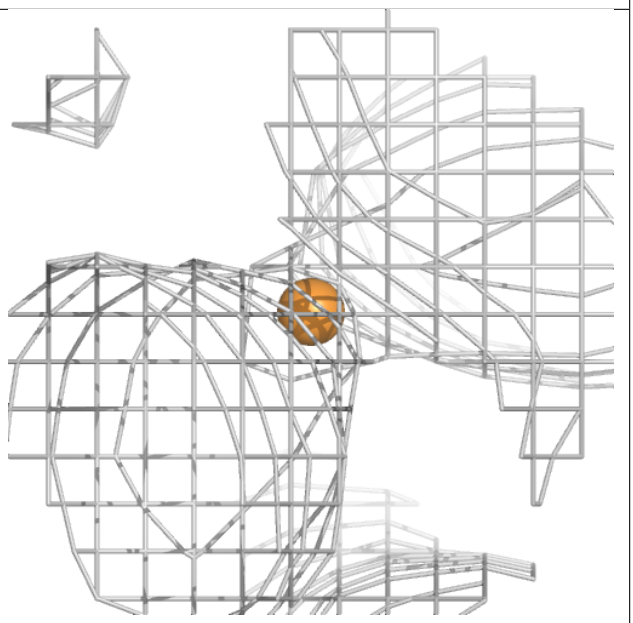
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CU A 403:

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

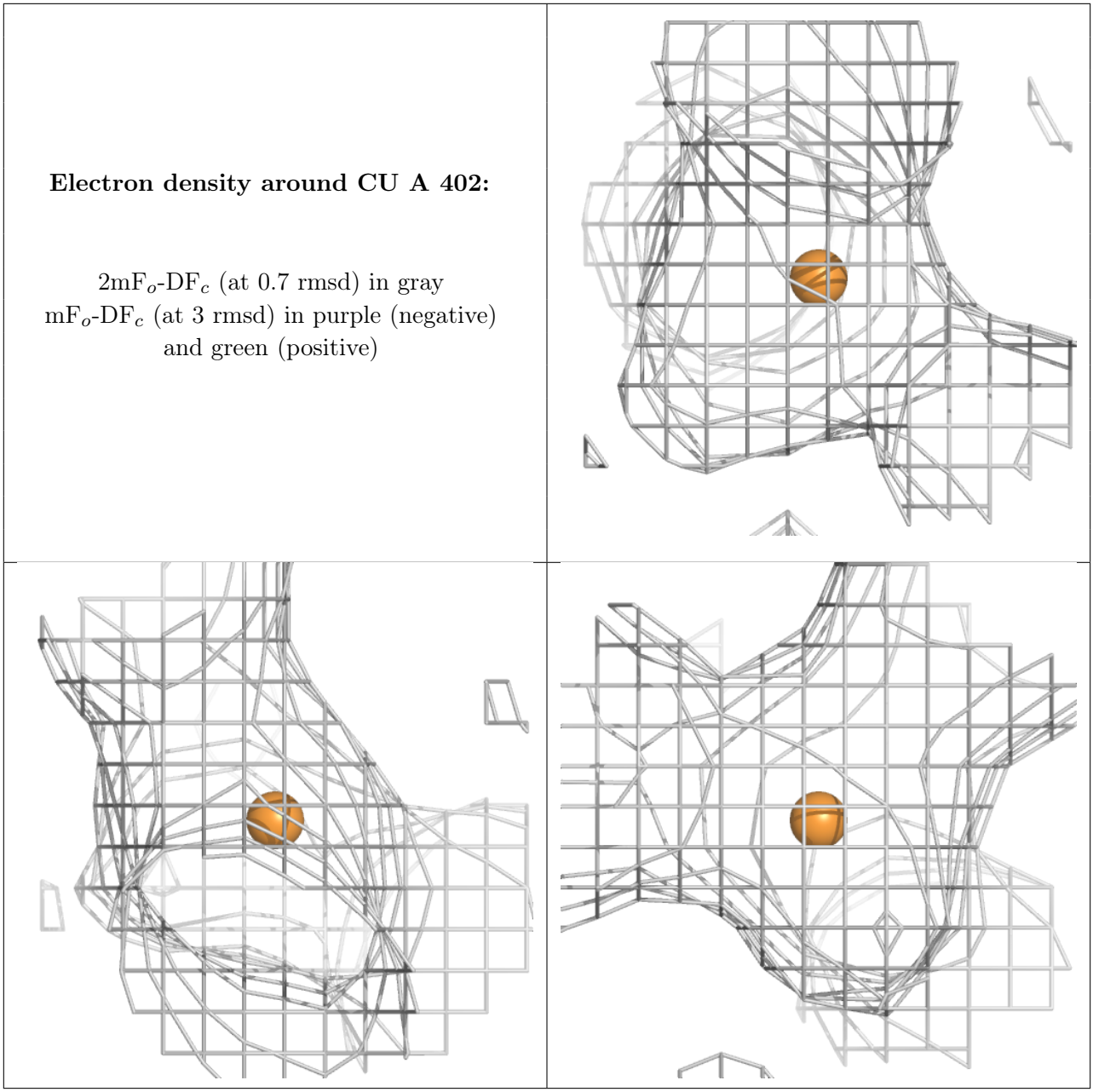






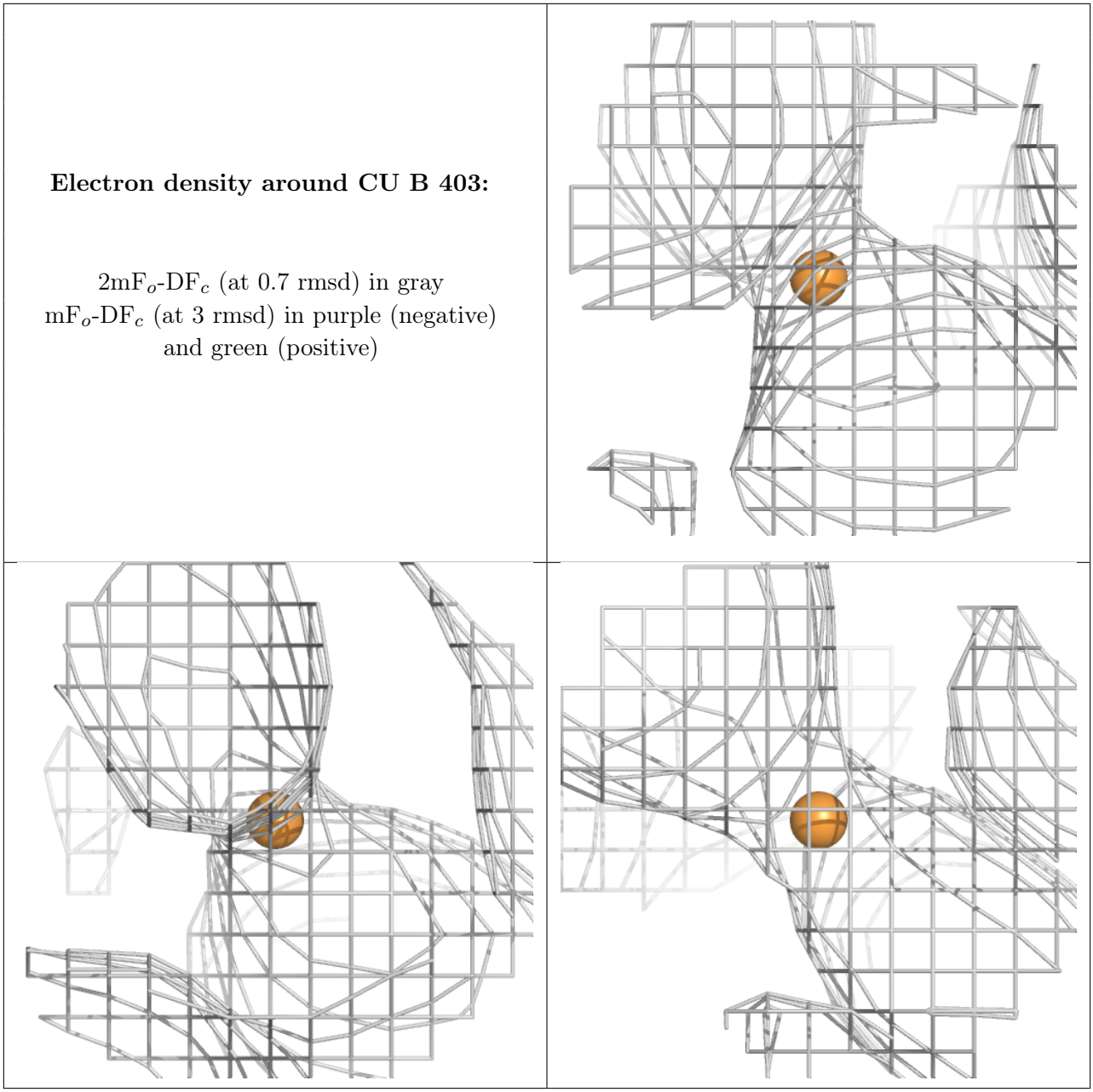
Electron density around CU A 402:

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



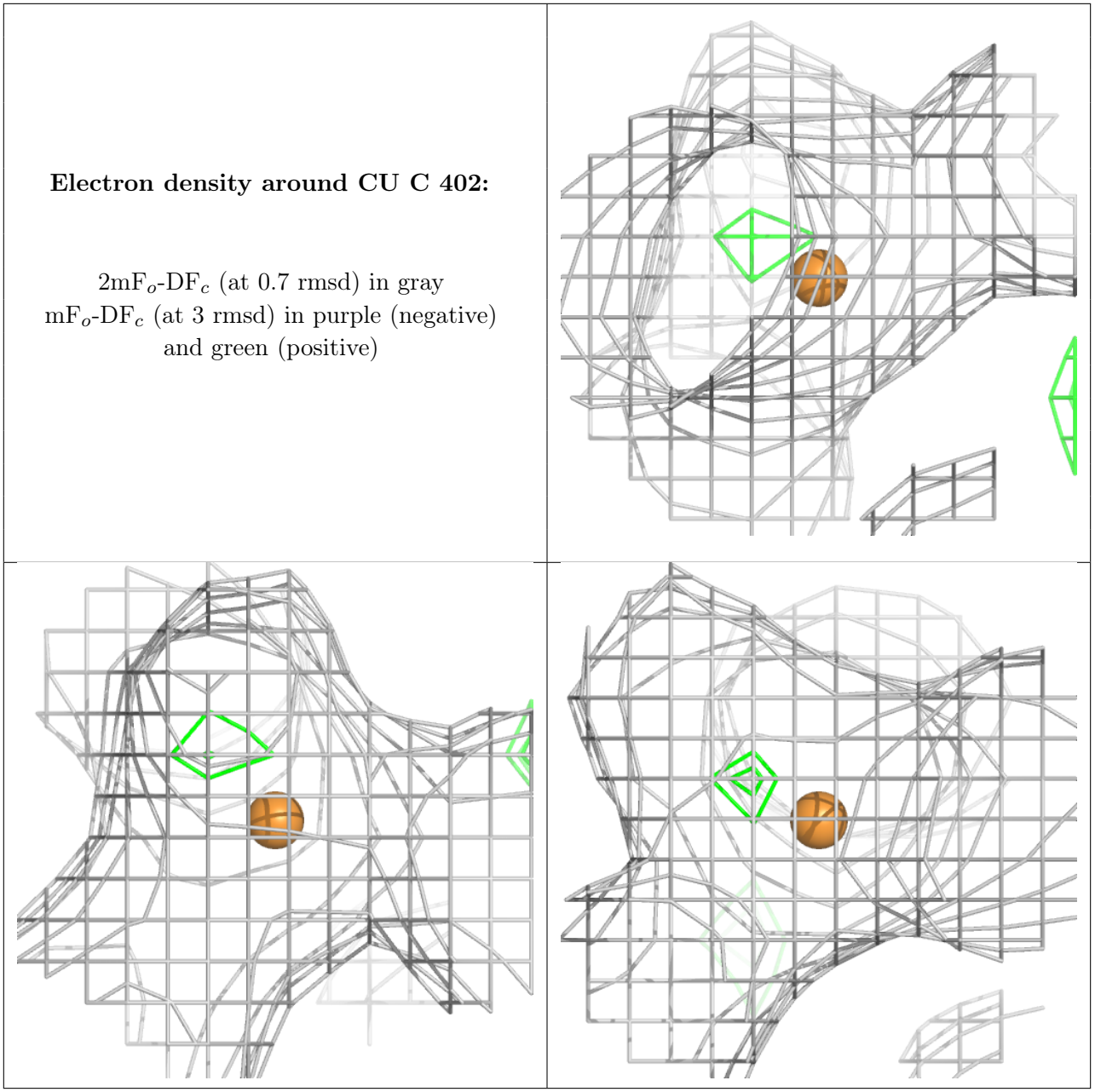
Electron density around CU B 403:

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



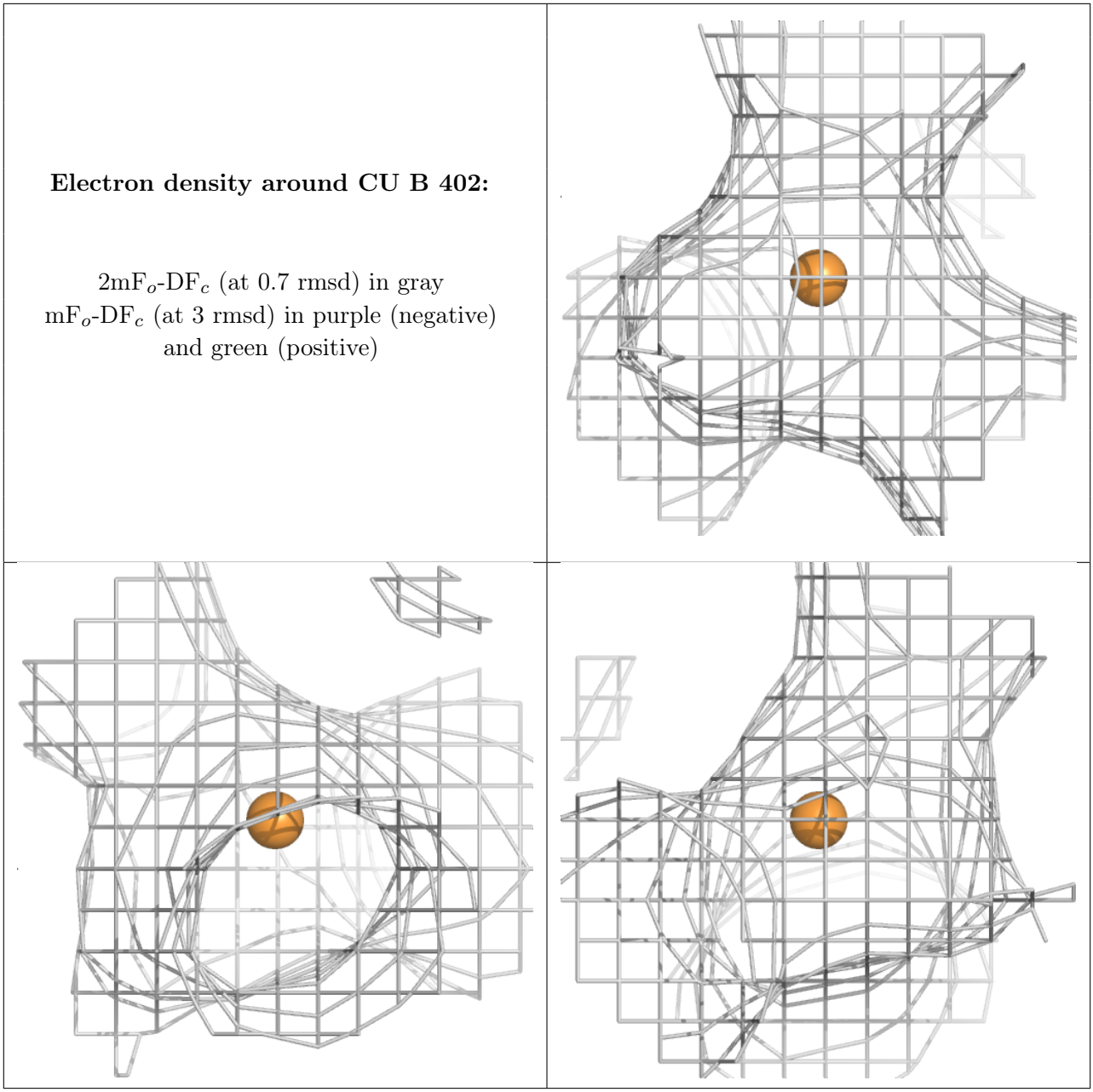
Electron density around CU C 402:

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



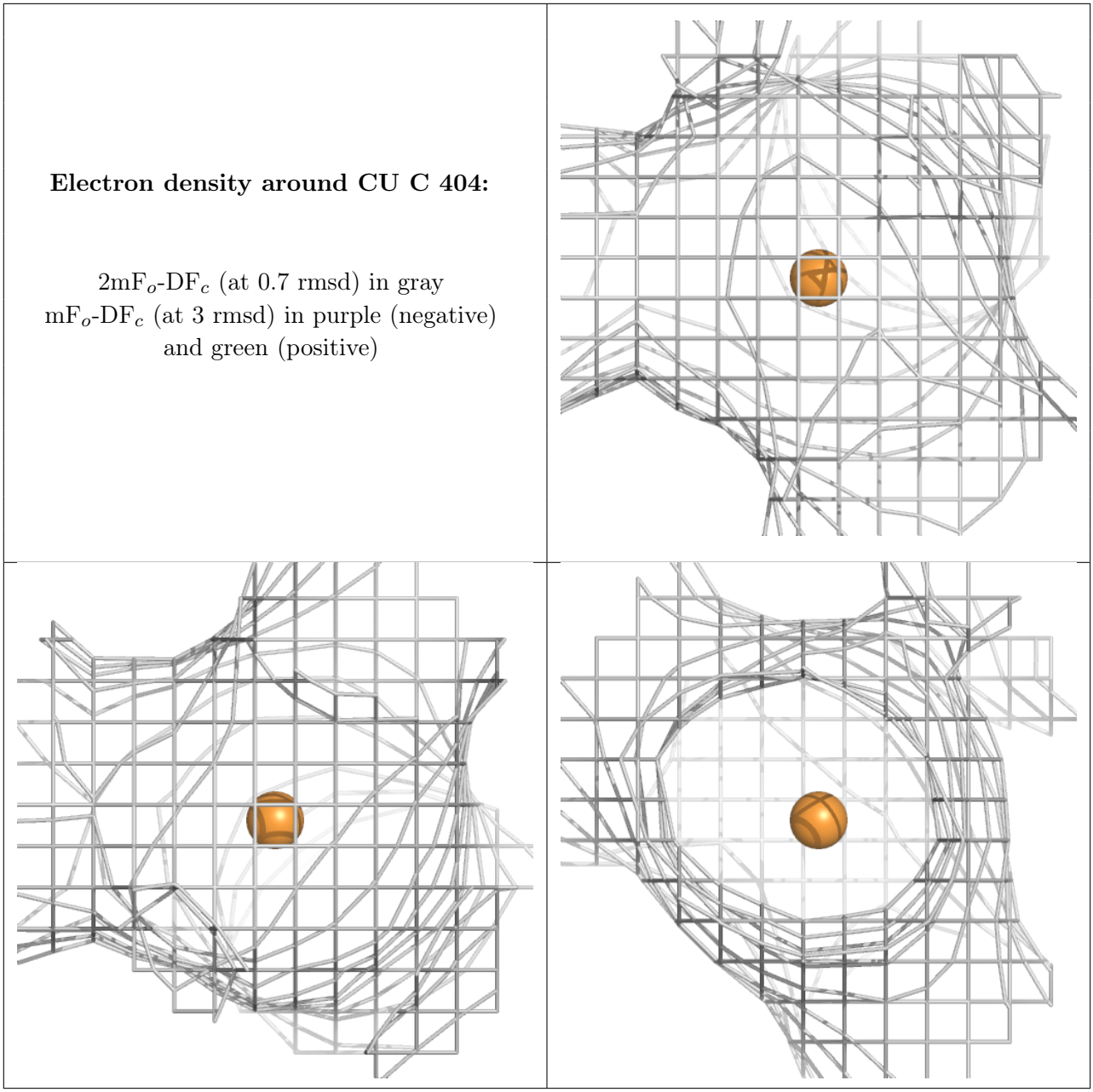
Electron density around CU B 402:

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



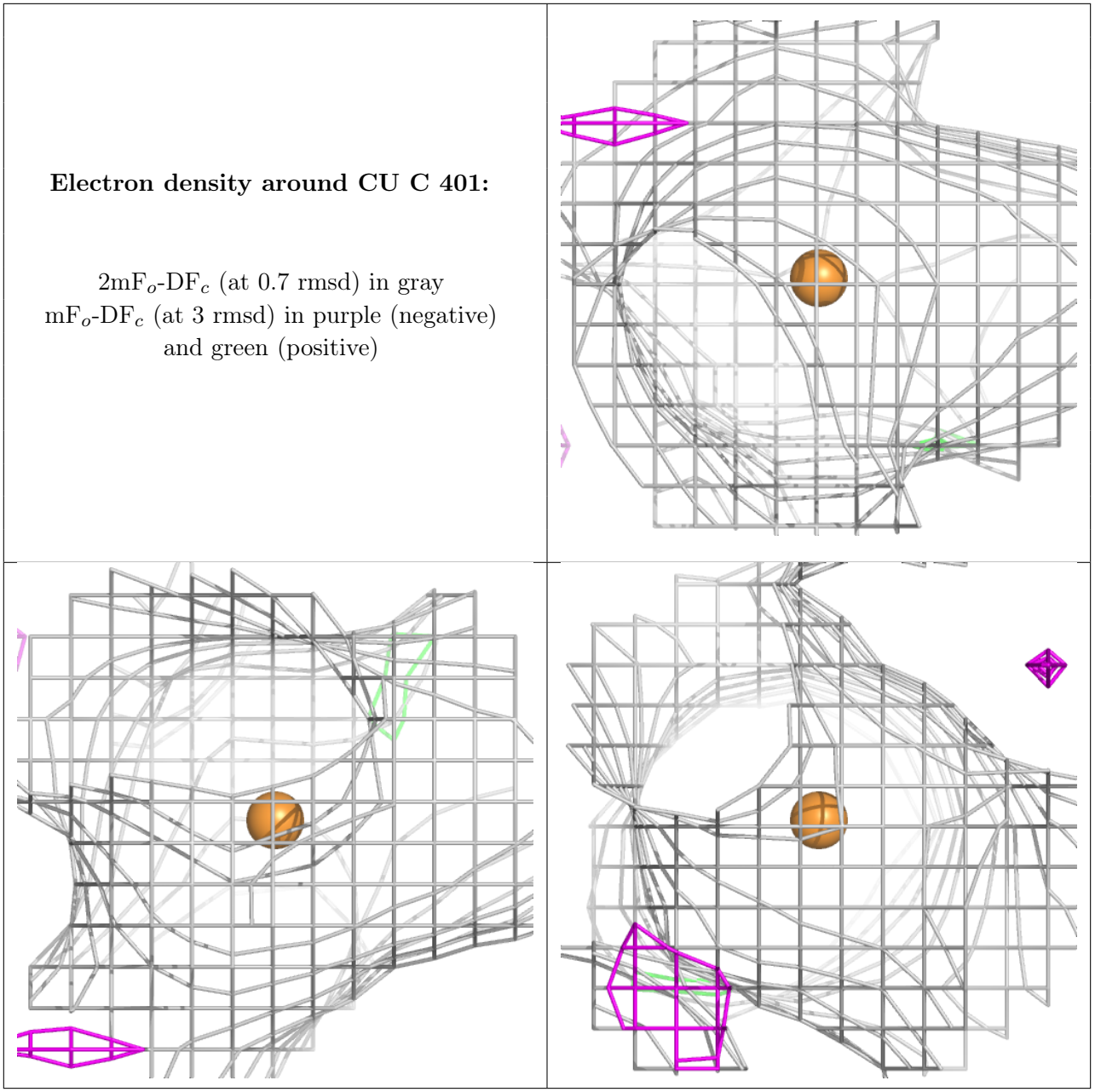
Electron density around CU C 404:

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



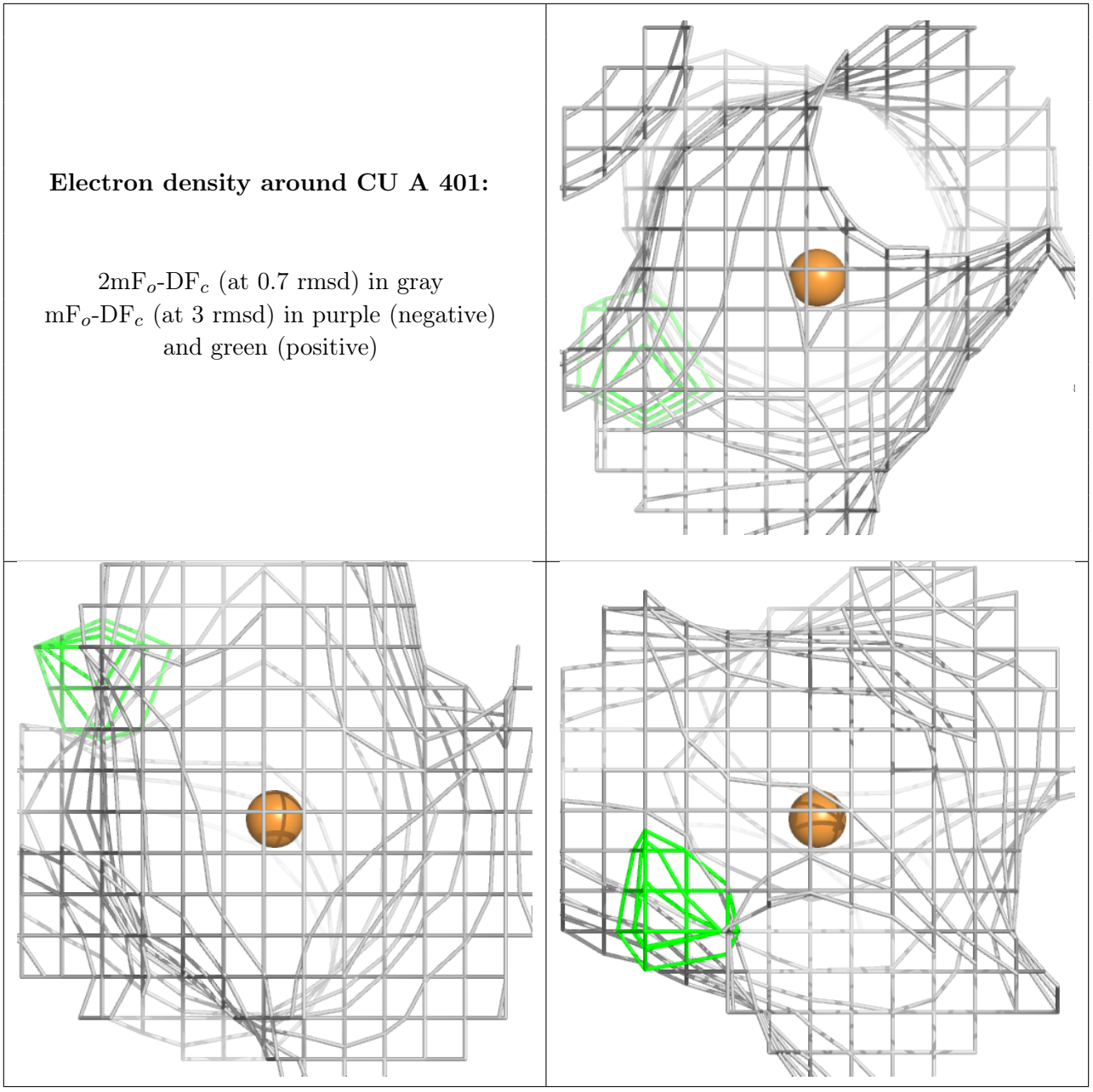
Electron density around CU C 401:

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



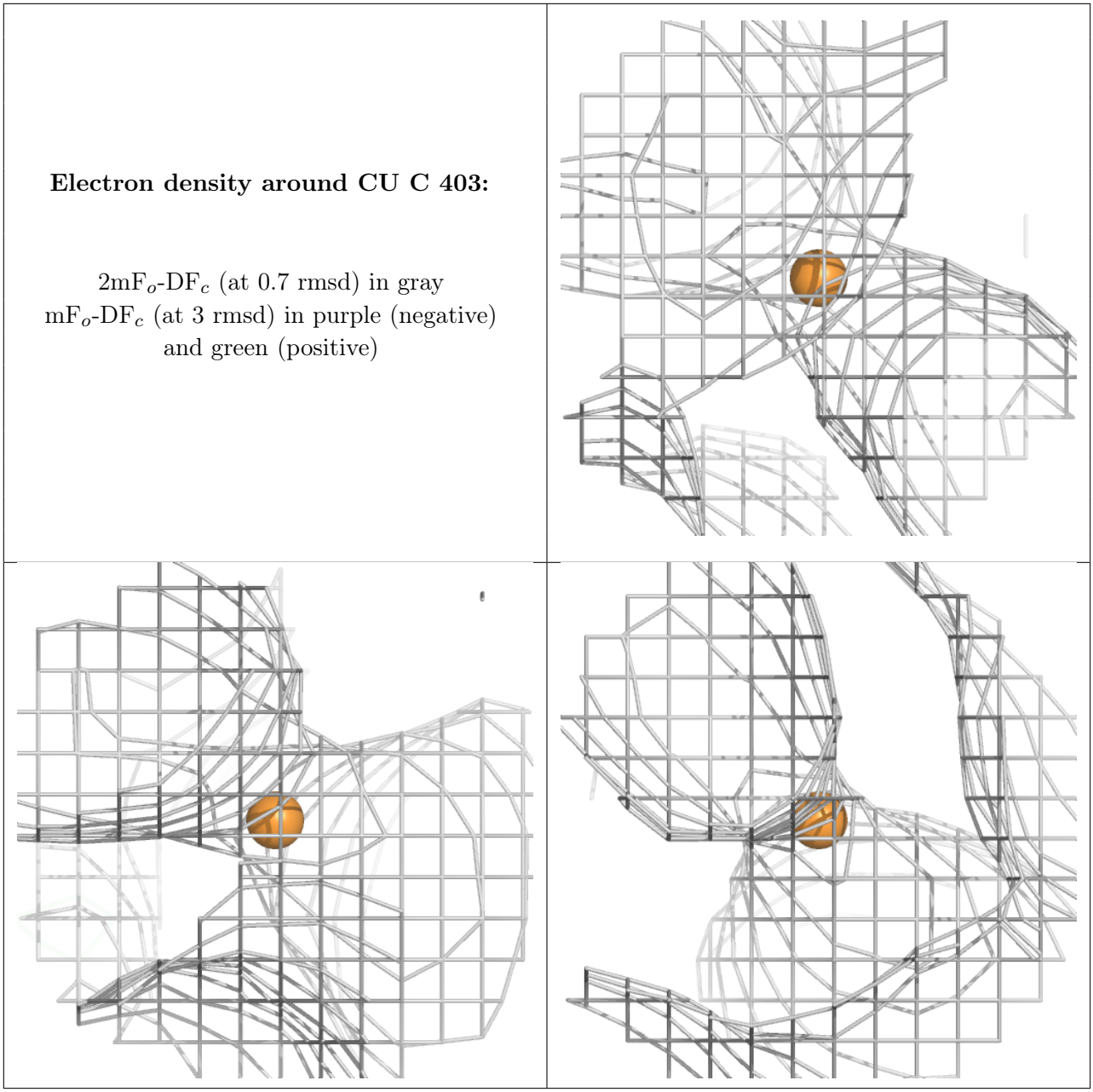
Electron density around CU A 401:

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



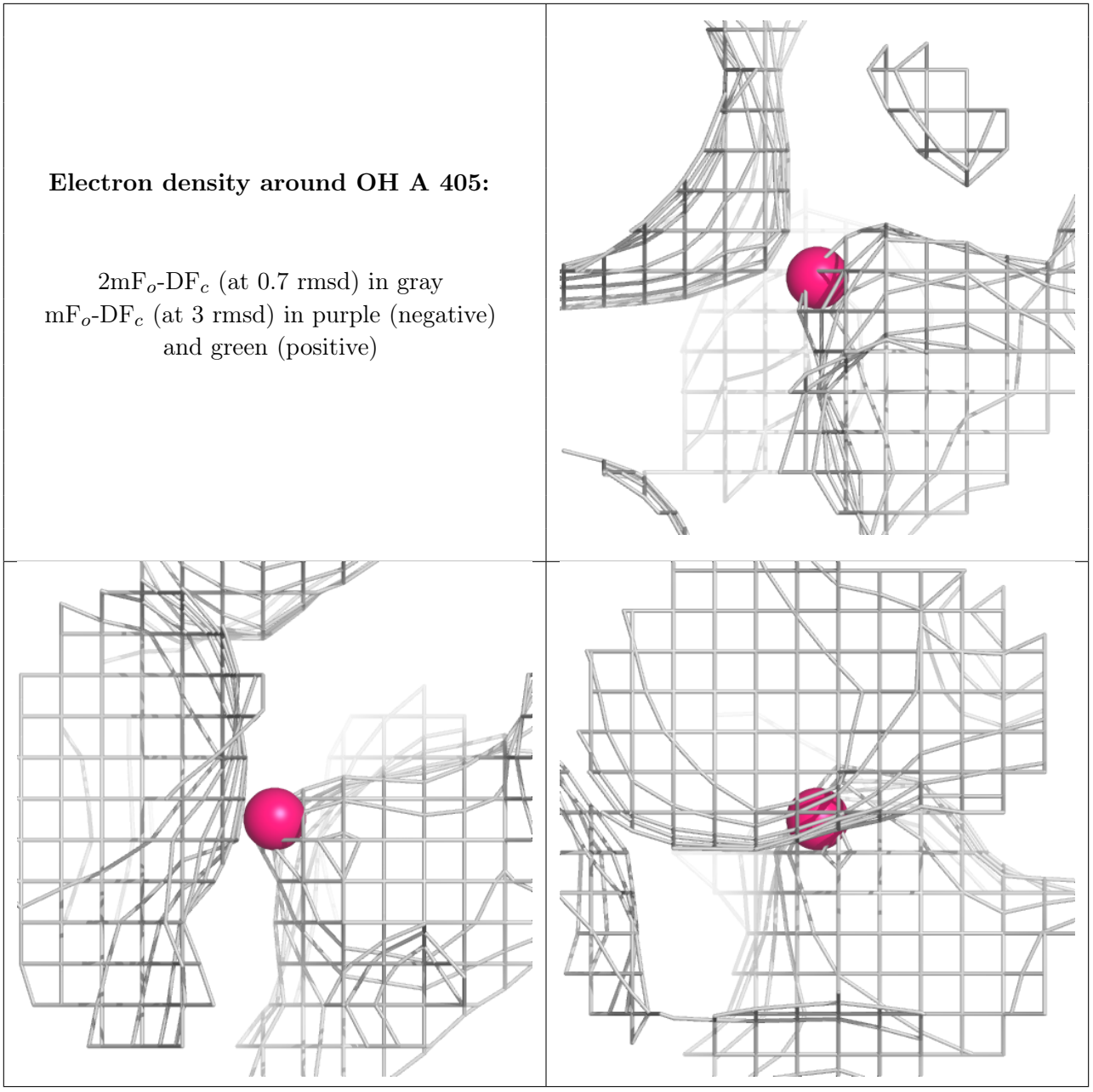
Electron density around CU C 403:

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



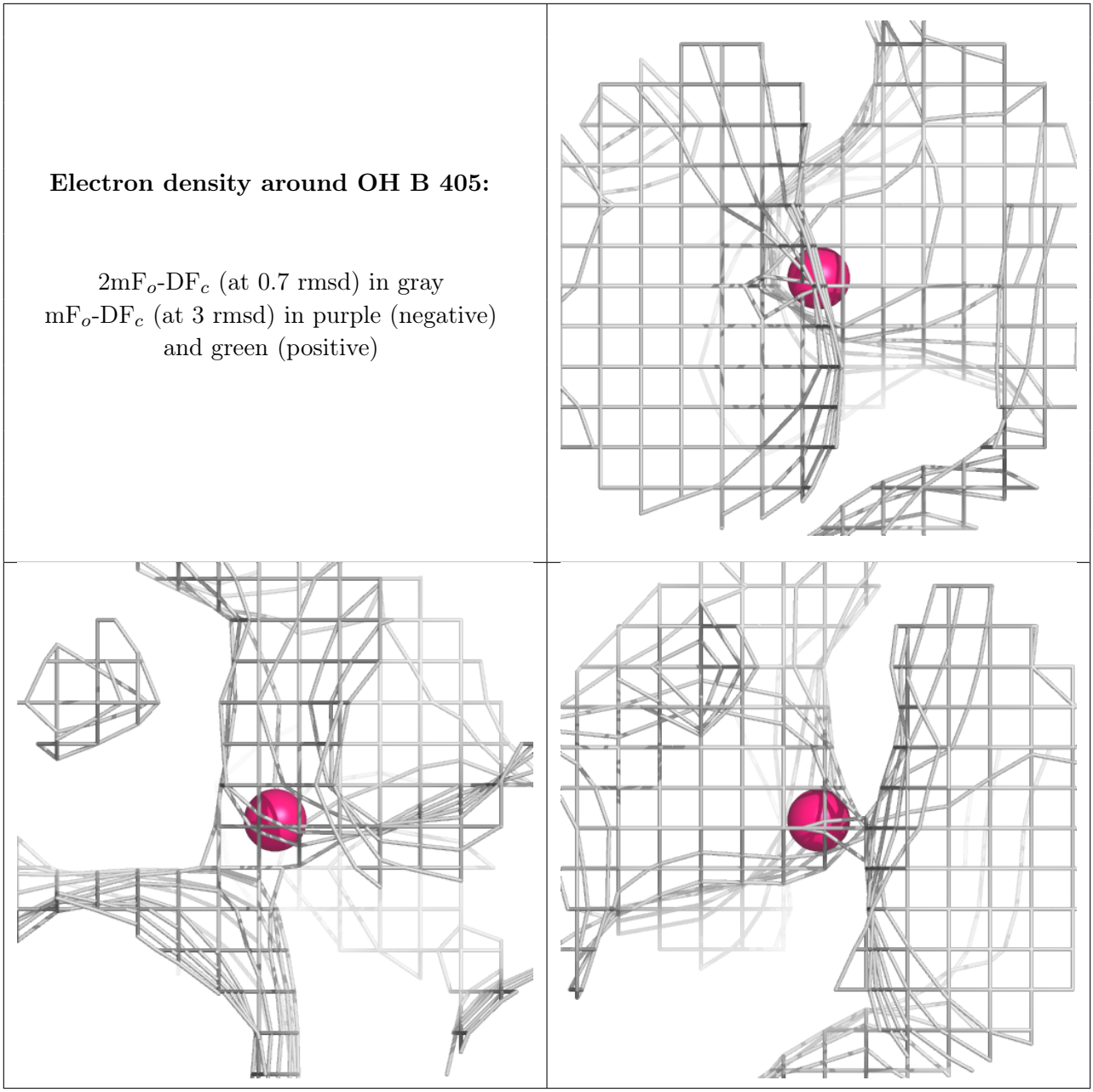
Electron density around OH A 405:

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



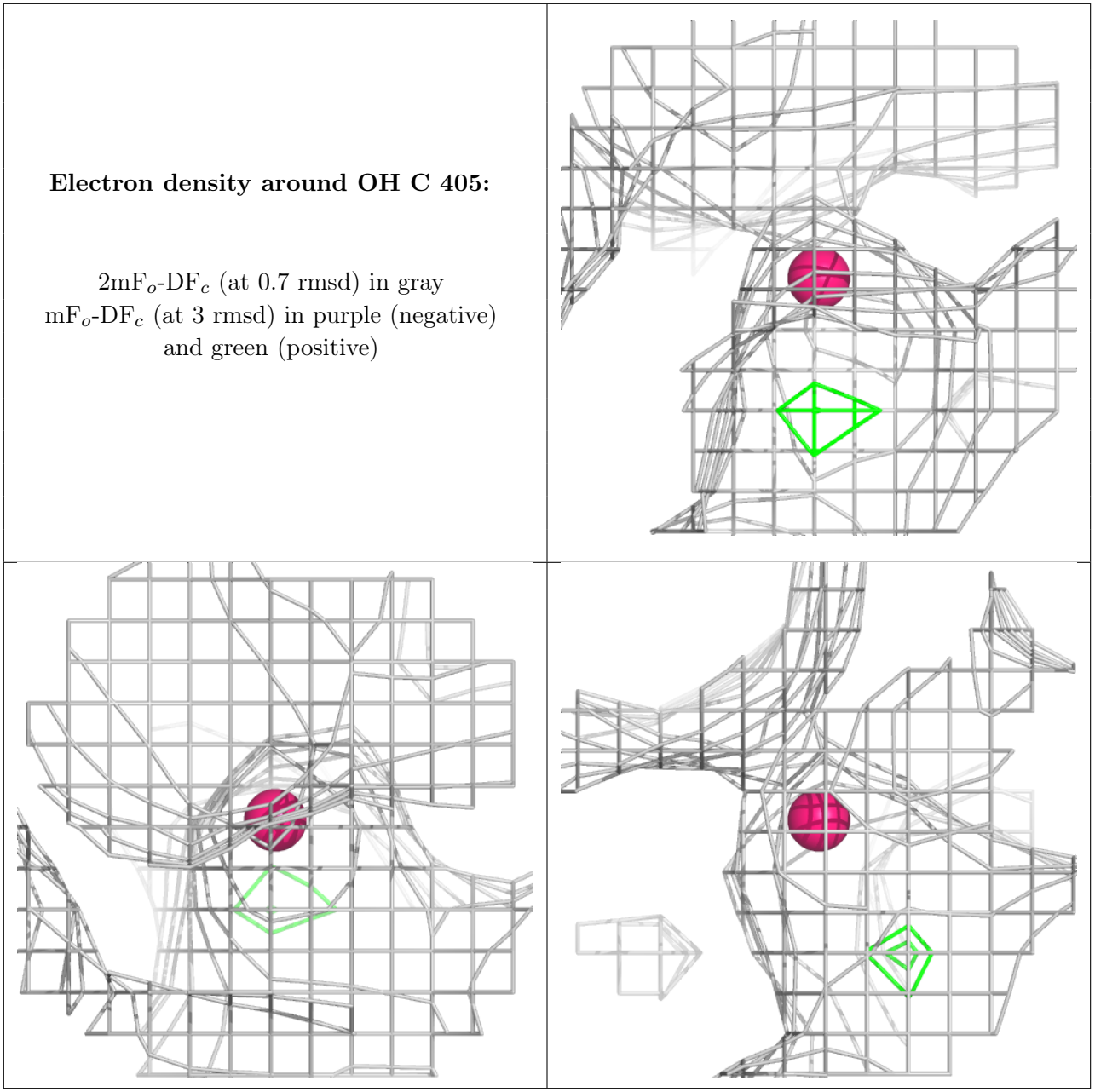
Electron density around OH B 405:

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



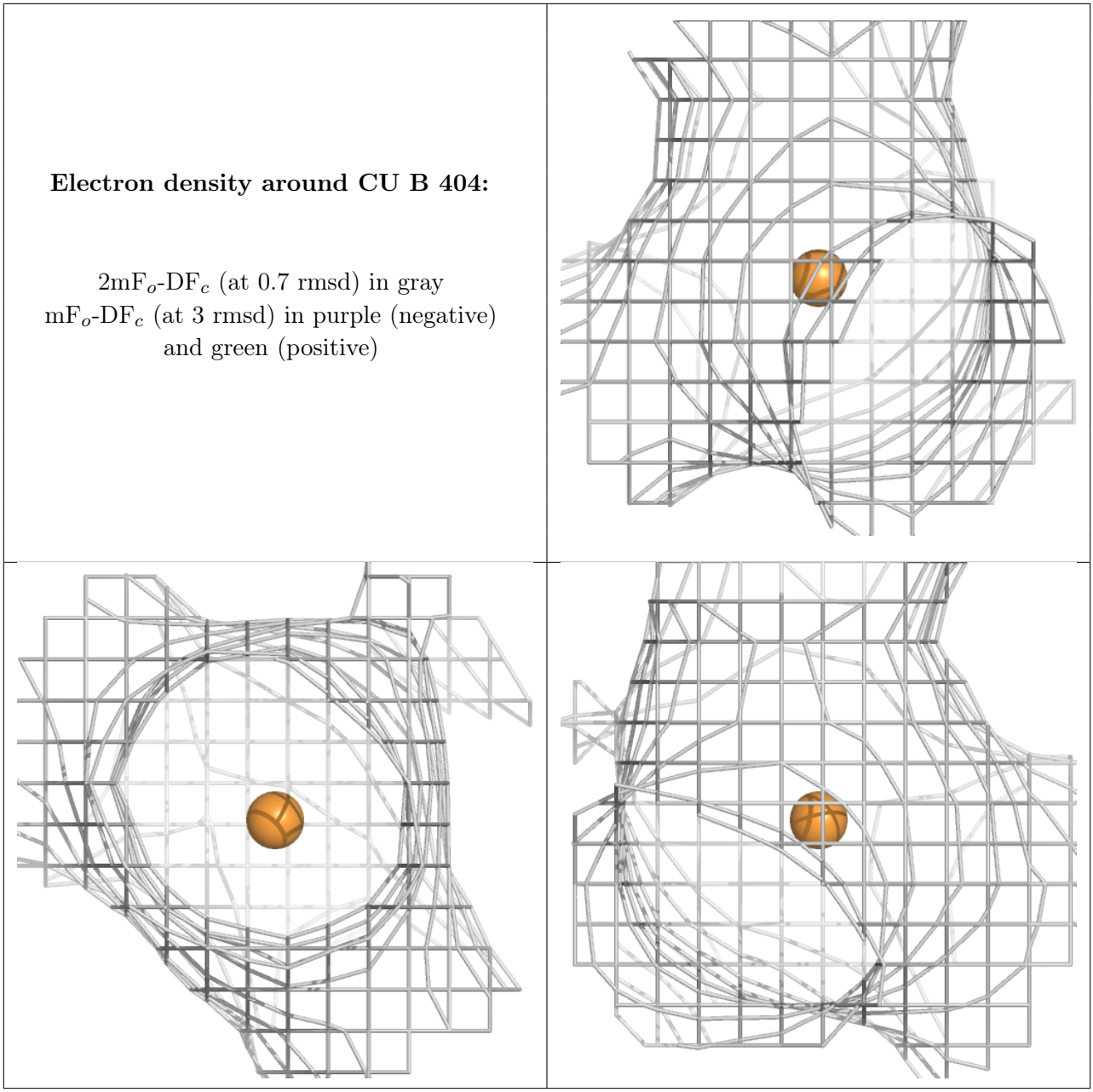
Electron density around OH C 405:

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



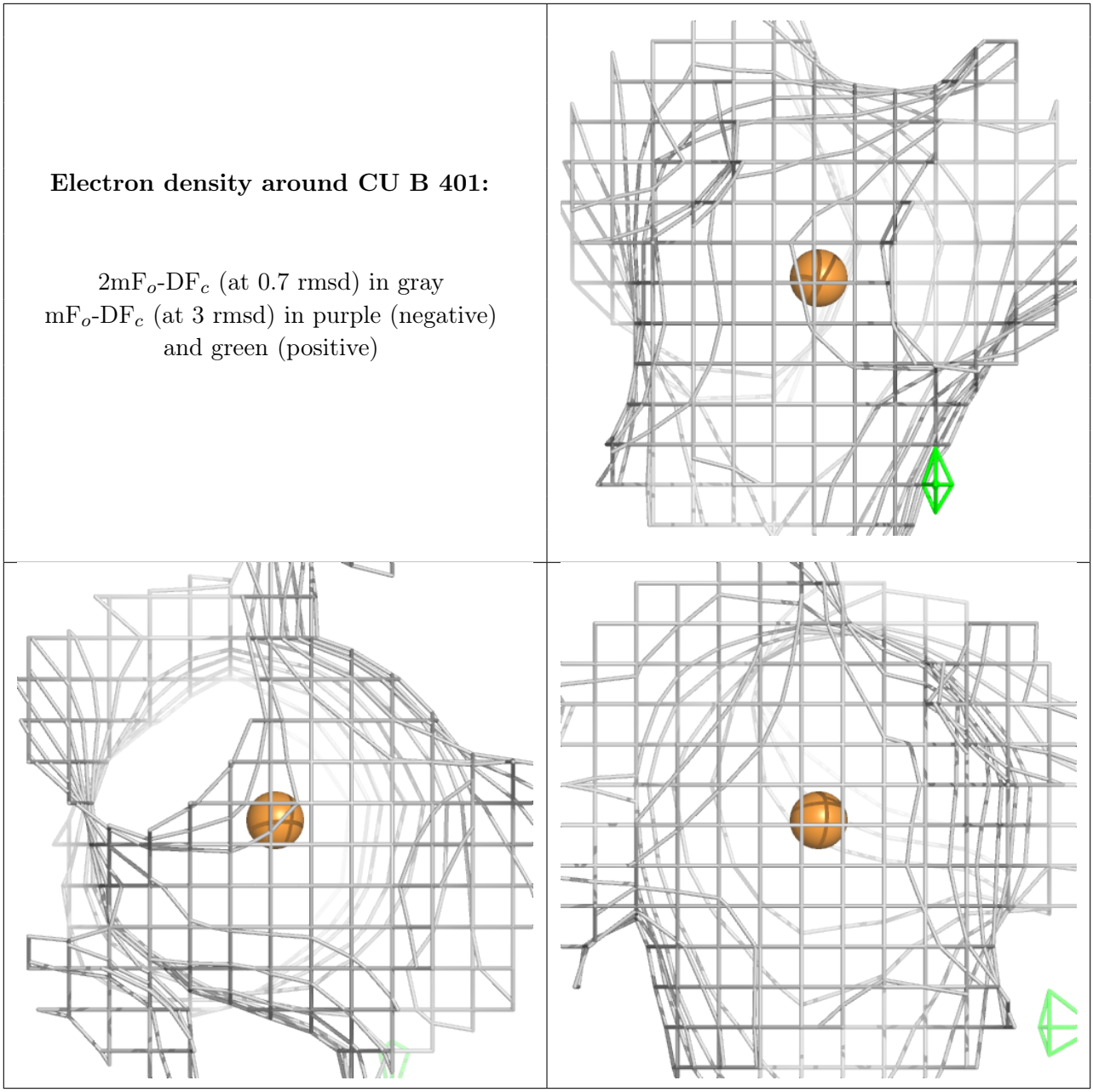
Electron density around CU B 404:

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



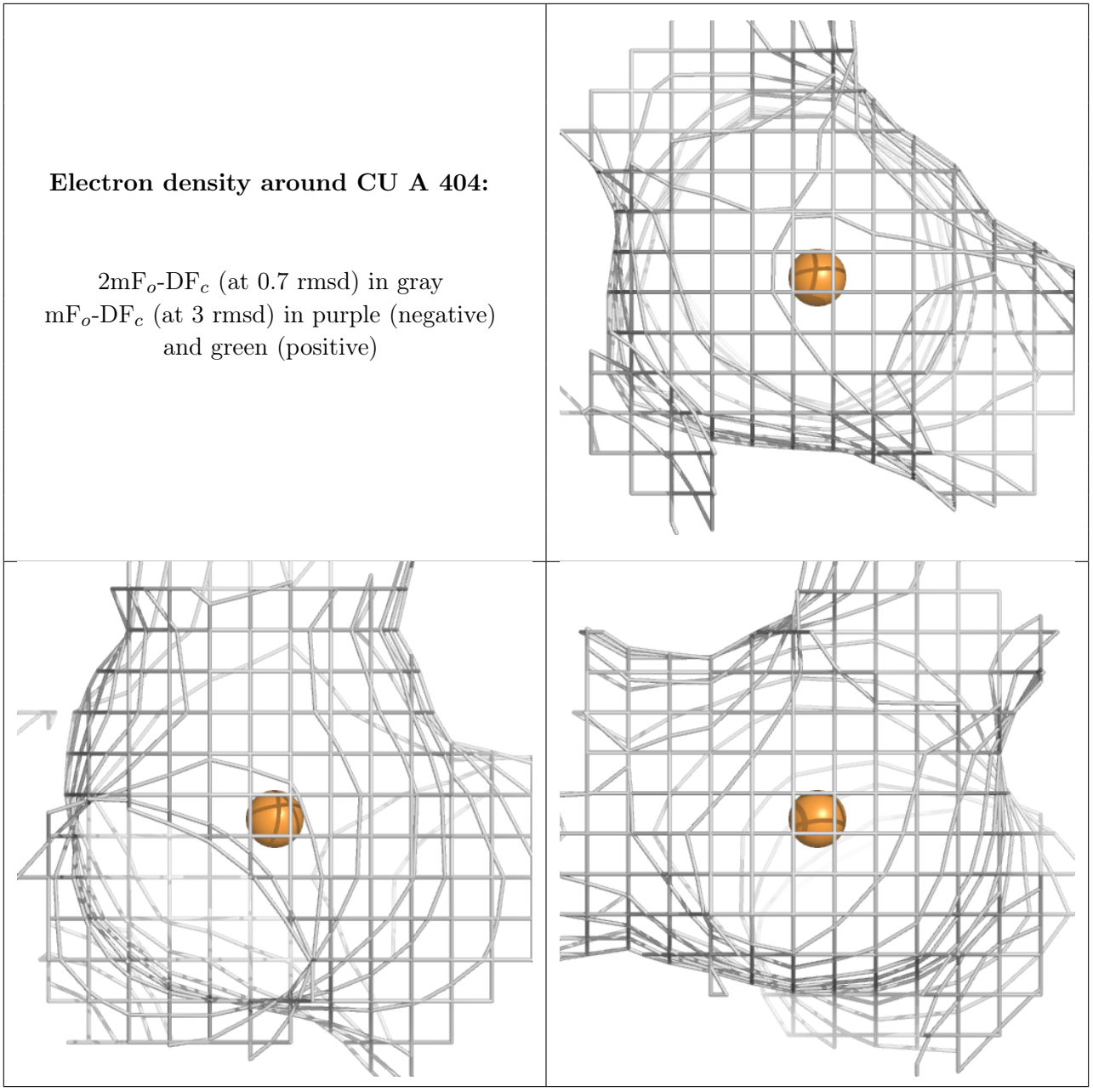
Electron density around CU B 401:

$2mF_o$-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 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)



6.5 Other polymers

There are no such residues in this entry.