wwPDB X-ray Structure Validation Summary Report (i)

Oct 19, 2026 – 11:27 PM JST

PDB ID	:	9X9P / pdb_00009x9p
Title	:	crystal structure of Cd(II)Ca(II)Mg(II)-bound human calprotectin
Authors	:	Tao, X.
Deposited on	:	2025-10-21
Resolution	:	1.85 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:

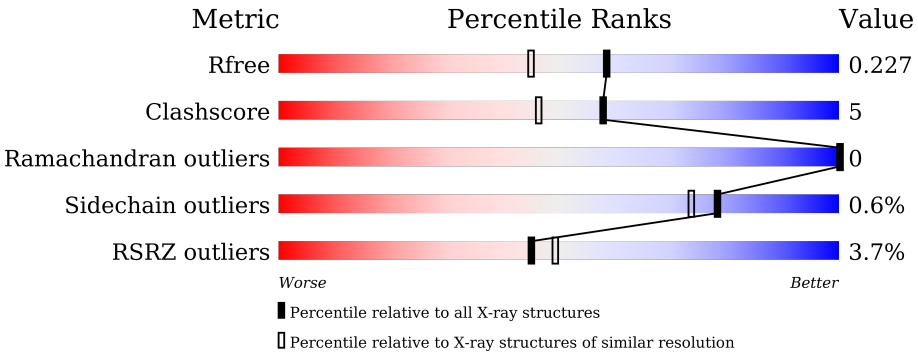
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	114	4% 84% 11% ·
1	C	114	4% 85% 10% · ·
1	E	114	3% 89% · 6%
1	G	114	4% 83% 11% 5%
2	B	94	3% 89% 5% · ·
2	D	94	2% 87% 9% ·

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Mol	Chain	Length	Quality of chain
2	F	94	
2	H	94	

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
7	CL	C	207	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 7537 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 Protein S100-A9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	2	0
			904	567	159	172	6			
1	C	109	Total	C	N	O	S	0	3	0
			911	572	159	174	6			
1	E	107	Total	C	N	O	S	0	2	0
			889	557	155	171	6			
1	G	108	Total	C	N	O	S	0	2	0
			901	566	160	170	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	CYS	conflict	UNP P06702
C	3	SER	CYS	conflict	UNP P06702
E	3	SER	CYS	conflict	UNP P06702
G	3	SER	CYS	conflict	UNP P06702

- Molecule 2 is a protein called Protein S100-A8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	90	Total	C	N	O	S	0	4	0
			756	489	125	140	2			
2	D	90	Total	C	N	O	S	0	3	0
			749	484	125	138	2			
2	F	90	Total	C	N	O	S	0	2	0
			743	481	124	136	2			
2	H	89	Total	C	N	O	S	0	2	0
			733	475	121	135	2			

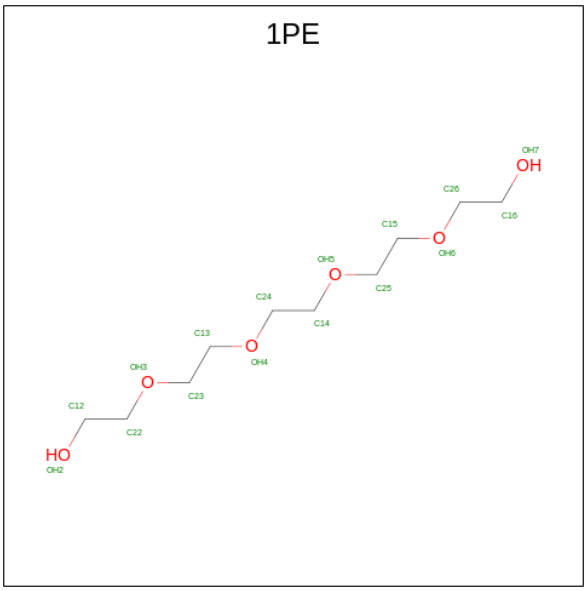
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P05109
B	42	SER	CYS	conflict	UNP P05109
D	0	GLY	-	expression tag	UNP P05109
D	42	SER	CYS	conflict	UNP P05109
F	0	GLY	-	expression tag	UNP P05109
F	42	SER	CYS	conflict	UNP P05109
H	0	GLY	-	expression tag	UNP P05109
H	42	SER	CYS	conflict	UNP P05109

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

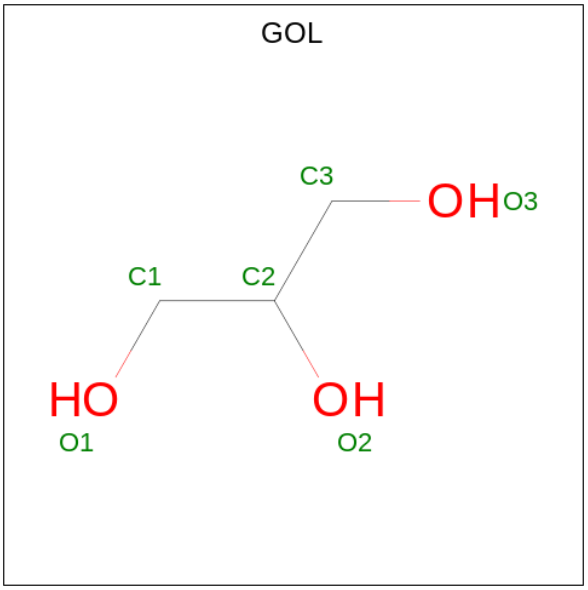
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0
3	B	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0
3	D	2	Total Ca 2 2	0	0
3	E	2	Total Ca 2 2	0	0
3	F	2	Total Ca 2 2	0	0
3	G	2	Total Ca 2 2	0	0
3	H	2	Total Ca 2 2	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 16 10 6	0	0
4	G	1	Total C O 16 10 6	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0

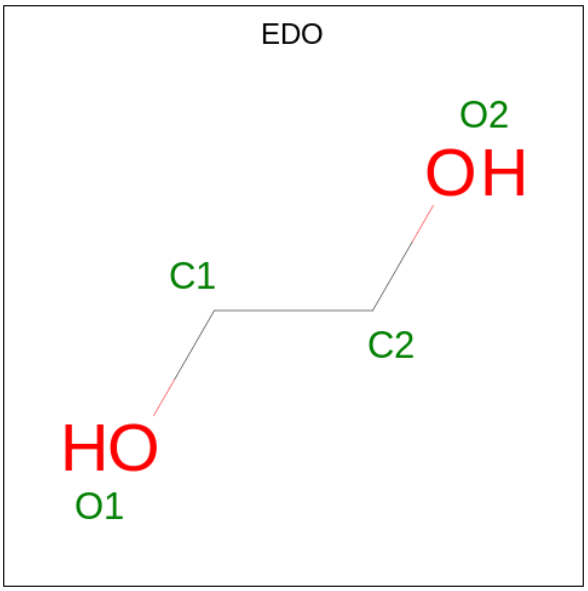
- Molecule 6 is CADMIUM ION (CCD ID: CD) (formula: Cd) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Cd 2 2	0	0
6	C	2	Total Cd 2 2	0	0
6	E	1	Total Cd 1 1	0	0
6	G	1	Total Cd 1 1	0	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0
7	C	1	Total Cl 1 1	0	0
7	D	1	Total Cl 1 1	0	0
7	E	1	Total Cl 1 1	0	0

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	G	1	Total C O 4 2 2	0	0
8	H	1	Total C O 4 2 2	0	0

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total Mg 1 1	0	0
9	G	1	Total Mg 1 1	0	0

- Molecule 10 is water.

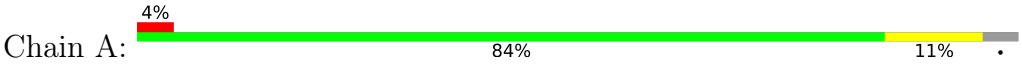
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	125	Total O 125 125	0	0
10	B	100	Total O 100 100	0	0
10	C	136	Total O 136 136	0	0
10	D	86	Total O 86 86	0	0
10	E	135	Total O 135 135	0	0
10	F	67	Total O 67 67	0	0
10	G	99	Total O 99 99	0	0
10	H	77	Total O 77 77	0	0

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.

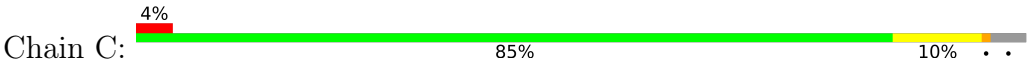
• Molecule 1: Protein S100-A9

Chain A:



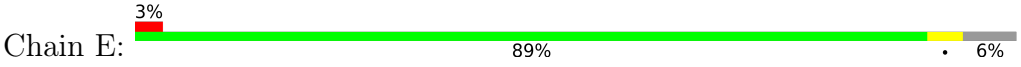
• Molecule 1: Protein S100-A9

Chain C:



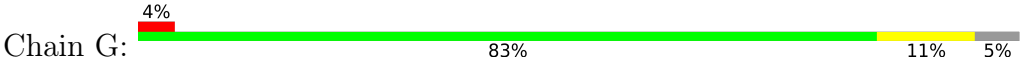
• Molecule 1: Protein S100-A9

Chain E:



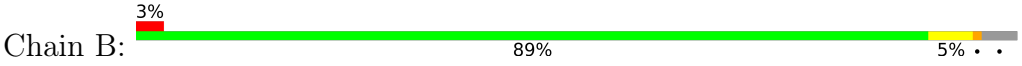
• Molecule 1: Protein S100-A9

Chain G:



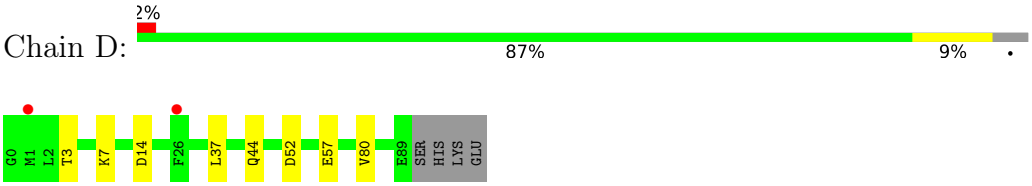
• Molecule 2: Protein S100-A8

Chain B:



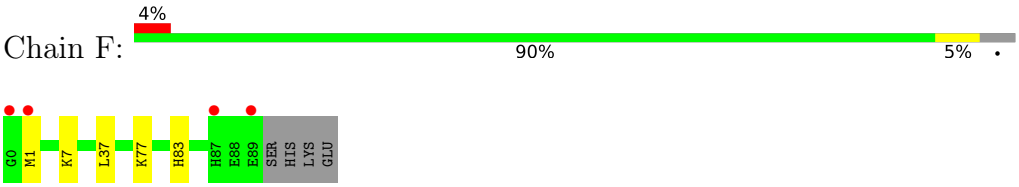
• Molecule 2: Protein S100-A8

Chain D:



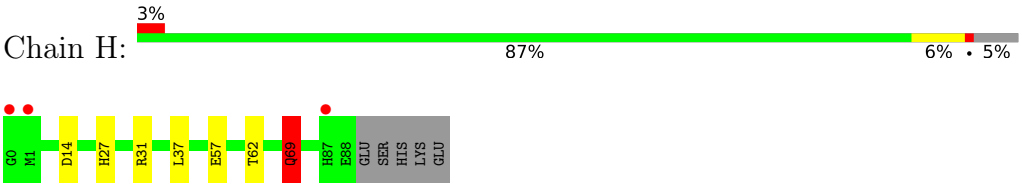
• Molecule 2: Protein S100-A8

Chain F:



• Molecule 2: Protein S100-A8

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.45Å 78.23Å 223.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.94 – 1.85 73.94 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.7 (73.94-1.85) 98.7 (73.94-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.167 , 0.219 0.177 , 0.227	Depositor DCC
R_{free} test set	4355 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7537	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% 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: 1PE, CL, EDO, MG, CD, GOL, CA

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	0.62	0/925	1.07	2/1238 (0.2%)
1	C	0.62	0/935	1.04	2/1251 (0.2%)
1	E	0.62	0/913	1.04	0/1223
1	G	0.61	0/925	1.03	3/1238 (0.2%)
2	B	0.63	0/782	0.99	0/1050
2	D	0.63	0/772	1.05	0/1037
2	F	0.59	0/764	1.05	0/1026
2	H	0.66	0/753	1.02	1/1012 (0.1%)
All	All	0.62	0/6769	1.04	8/9075 (0.1%)

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	1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	98	ASP	CA-CB-CG	6.94	119.54	112.60
2	H	69	GLN	N-CA-CB	6.48	119.75	110.16
1	C	76	PHE	CA-CB-CG	-5.79	108.01	113.80
1	C	98	ASP	CA-CB-CG	5.66	118.25	112.60
1	G	14	THR	CA-CB-OG1	-5.53	101.31	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	ARG	Sidechain

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	904	0	882	13	0
1	C	911	0	891	8	0
1	E	889	0	862	4	0
1	G	901	0	886	7	0
2	B	756	0	775	6	0
2	D	749	0	767	7	0
2	F	743	0	757	5	0
2	H	733	0	750	13	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	16	0	22	1	0
4	G	16	0	22	0	0
5	A	6	0	8	0	0
5	B	6	0	8	2	0
5	C	6	0	8	0	0
5	E	6	0	8	0	0
5	G	6	0	8	2	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	4	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	C	4	0	6	0	0
8	D	12	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	12	0	18	1	0
8	G	4	0	6	0	0
8	H	4	0	6	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
10	A	125	0	0	6	0
10	B	100	0	0	6	0
10	C	136	0	0	2	0
10	D	86	0	0	5	0
10	E	135	0	0	2	1
10	F	67	0	0	0	0
10	G	99	0	0	2	1
10	H	77	0	0	4	0
All	All	7537	0	6708	61	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 5.

The worst 5 of 61 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)
8:D:105:EDO:H11	10:D:214:HOH:O	1.60	1.01
7:C:207:CL:CL	2:H:69:GLN:CG	2.65	0.81
2:B:88:GLU:OE1	10:B:202:HOH:O	2.04	0.76
5:B:103:GOL:H2	10:B:221:HOH:O	1.86	0.76
2:B:39:GLU:OE2	10:B:203:HOH:O	2.05	0.75

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)
10:E:339:HOH:O	10:G:375:HOH:O[2_554]	1.88	0.32

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	109/114 (96%)	109 (100%)	0	0	100	100
1	C	110/114 (96%)	108 (98%)	2 (2%)	0	100	100
1	E	107/114 (94%)	105 (98%)	2 (2%)	0	100	100
1	G	108/114 (95%)	107 (99%)	1 (1%)	0	100	100
2	B	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
2	D	91/94 (97%)	91 (100%)	0	0	100	100
2	F	90/94 (96%)	89 (99%)	1 (1%)	0	100	100
2	H	89/94 (95%)	89 (100%)	0	0	100	100
All	All	796/832 (96%)	789 (99%)	7 (1%)	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	100/103 (97%)	100 (100%)	0	100	100
1	C	101/103 (98%)	99 (98%)	2 (2%)	48	36
1	E	99/103 (96%)	97 (98%)	2 (2%)	48	36
1	G	100/103 (97%)	100 (100%)	0	100	100
2	B	83/83 (100%)	82 (99%)	1 (1%)	63	55
2	D	82/83 (99%)	82 (100%)	0	100	100
2	F	81/83 (98%)	81 (100%)	0	100	100
2	H	80/83 (96%)	79 (99%)	1 (1%)	61	51
All	All	726/744 (98%)	720 (99%)	6 (1%)	78	67

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	81[A]	MET
1	E	81[B]	MET
2	H	69	GLN
1	C	81[A]	MET
2	B	69	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	10	ASN
1	G	73	GLN
2	H	69	GLN
2	H	10	ASN
2	D	10	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 28 are monoatomic - leaving 16 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	$\#\|Z\|>2$
5	GOL	G	204	-	5,5,5	0.18	0	5,5,5	0.45	0
8	EDO	E	204	-	3,3,3	0.06	0	2,2,2	0.26	0
4	1PE	A	203	-	15,15,15	0.24	0	14,14,14	0.16	0
5	GOL	E	201	-	5,5,5	0.12	0	5,5,5	0.33	0
8	EDO	D	104	-	3,3,3	0.10	0	2,2,2	0.29	0
8	EDO	G	203	-	3,3,3	0.18	0	2,2,2	0.30	0
8	EDO	D	103	-	3,3,3	0.15	0	2,2,2	0.07	0
8	EDO	H	103	-	3,3,3	0.21	0	2,2,2	0.22	0
5	GOL	B	103	-	5,5,5	0.09	0	5,5,5	0.45	0
8	EDO	D	105	-	3,3,3	0.35	0	2,2,2	0.38	0
8	EDO	E	205	-	3,3,3	0.05	0	2,2,2	0.13	0
5	GOL	A	204	-	5,5,5	0.10	0	5,5,5	0.37	0
8	EDO	E	206	-	3,3,3	0.12	0	2,2,2	0.09	0
8	EDO	C	203	-	3,3,3	0.14	0	2,2,2	0.11	0
4	1PE	G	205	-	15,15,15	0.27	0	14,14,14	0.21	0
5	GOL	C	204	-	5,5,5	0.14	0	5,5,5	0.42	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
5	GOL	G	204	-	-	3/4/4/4	-
8	EDO	E	204	-	-	0/1/1/1	-
4	1PE	A	203	-	-	5/13/13/13	-
5	GOL	E	201	-	-	2/4/4/4	-
8	EDO	D	104	-	-	0/1/1/1	-
8	EDO	G	203	-	-	1/1/1/1	-
8	EDO	D	103	-	-	0/1/1/1	-
8	EDO	H	103	-	-	1/1/1/1	-
5	GOL	B	103	-	-	4/4/4/4	-
8	EDO	D	105	-	-	1/1/1/1	-
8	EDO	E	205	-	-	0/1/1/1	-
5	GOL	A	204	-	-	0/4/4/4	-
8	EDO	E	206	-	-	0/1/1/1	-
8	EDO	C	203	-	-	0/1/1/1	-
4	1PE	G	205	-	-	6/13/13/13	-
5	GOL	C	204	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	103	GOL	O1-C1-C2-C3
5	C	204	GOL	C1-C2-C3-O3
5	E	201	GOL	C1-C2-C3-O3
5	G	204	GOL	O1-C1-C2-C3
8	D	105	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	204	GOL	2	0
4	A	203	1PE	1	0
5	B	103	GOL	2	0
8	D	105	EDO	1	0
8	E	206	EDO	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	109/114 (95%)	0.16	4 (3%)	45	49	12, 30, 52, 69	2 (1%)
1	C	109/114 (95%)	-0.10	5 (4%)	37	40	9, 28, 48, 75	3 (2%)
1	E	107/114 (93%)	0.02	3 (2%)	55	58	14, 30, 44, 61	2 (1%)
1	G	108/114 (94%)	0.44	5 (4%)	37	40	15, 37, 53, 76	3 (2%)
2	B	90/94 (95%)	-0.28	3 (3%)	49	53	13, 22, 43, 89	4 (4%)
2	D	90/94 (95%)	-0.09	2 (2%)	62	66	17, 26, 42, 71	3 (3%)
2	F	90/94 (95%)	0.29	4 (4%)	39	42	21, 30, 55, 99	2 (2%)
2	H	89/94 (94%)	-0.09	3 (3%)	48	52	14, 24, 55, 88	3 (3%)
All	All	792/832 (95%)	0.05	29 (3%)	45	49	9, 28, 52, 99	22 (2%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	LYS	4.0
2	H	0	GLY	3.3
1	C	102	GLY	3.1
2	F	1	MET	3.0
2	H	1	MET	3.0

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 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^{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
8	EDO	E	205	4/4	0.79	0.19	67,68,70,72	0
8	EDO	D	104	4/4	0.81	0.18	50,61,64,64	0
8	EDO	H	103	4/4	0.81	0.18	54,55,55,58	0
8	EDO	E	206	4/4	0.82	0.17	56,60,60,62	0
5	GOL	E	201	6/6	0.82	0.17	44,57,59,66	0
8	EDO	C	203	4/4	0.83	0.15	40,50,53,54	0
5	GOL	G	204	6/6	0.84	0.15	32,51,53,53	0
8	EDO	G	203	4/4	0.84	0.13	58,61,64,64	0
5	GOL	A	204	6/6	0.84	0.17	65,69,70,72	0
5	GOL	B	103	6/6	0.85	0.17	49,52,53,57	0
8	EDO	D	105	4/4	0.85	0.20	42,43,48,49	0
5	GOL	C	204	6/6	0.86	0.15	44,57,61,63	0
8	EDO	E	204	4/4	0.88	0.15	55,56,62,69	0
4	1PE	G	205	16/16	0.89	0.17	62,66,74,74	0
8	EDO	D	103	4/4	0.89	0.12	60,61,61,64	0
4	1PE	A	203	16/16	0.89	0.18	56,67,72,74	0
3	CA	D	102	1/1	0.92	0.14	32,32,32,32	1
7	CL	E	208	1/1	0.93	0.12	46,46,46,46	0
3	CA	G	202	1/1	0.93	0.09	34,34,34,34	0
9	MG	F	103	1/1	0.93	0.10	36,36,36,36	0
3	CA	G	201	1/1	0.94	0.08	41,41,41,41	0
3	CA	F	102	1/1	0.94	0.15	33,33,33,33	1
7	CL	C	207	1/1	0.95	0.13	51,51,51,51	0
9	MG	G	207	1/1	0.95	0.07	32,32,32,32	0
3	CA	A	201	1/1	0.96	0.06	34,34,34,34	0
3	CA	E	203	1/1	0.97	0.09	34,34,34,34	0
7	CL	D	106	1/1	0.97	0.08	41,41,41,41	0
3	CA	A	202	1/1	0.98	0.09	32,32,32,32	0
3	CA	E	202	1/1	0.98	0.04	28,28,28,28	0
3	CA	H	102	1/1	0.98	0.08	27,27,27,27	1
3	CA	C	202	1/1	0.98	0.05	32,32,32,32	0
3	CA	F	101	1/1	0.98	0.03	25,25,25,25	0
3	CA	D	101	1/1	0.98	0.04	27,27,27,27	0
6	CD	A	206	1/1	0.99	0.03	26,26,26,26	0
6	CD	C	205	1/1	0.99	0.03	25,25,25,25	0
6	CD	E	207	1/1	0.99	0.03	25,25,25,25	0
7	CL	A	207	1/1	0.99	0.08	37,37,37,37	0

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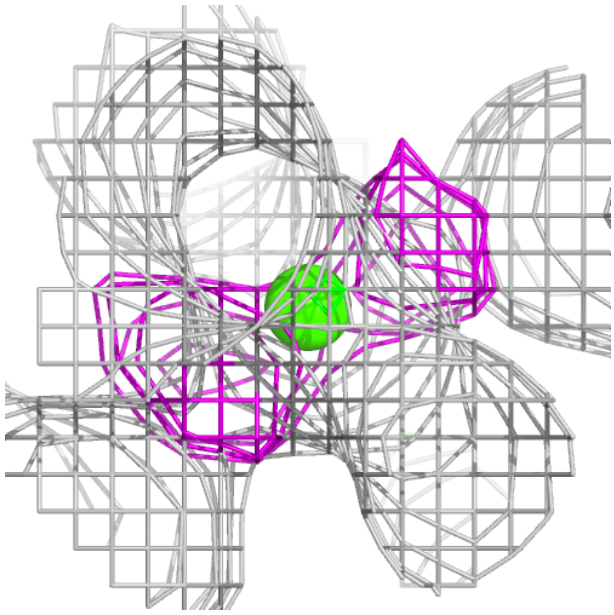
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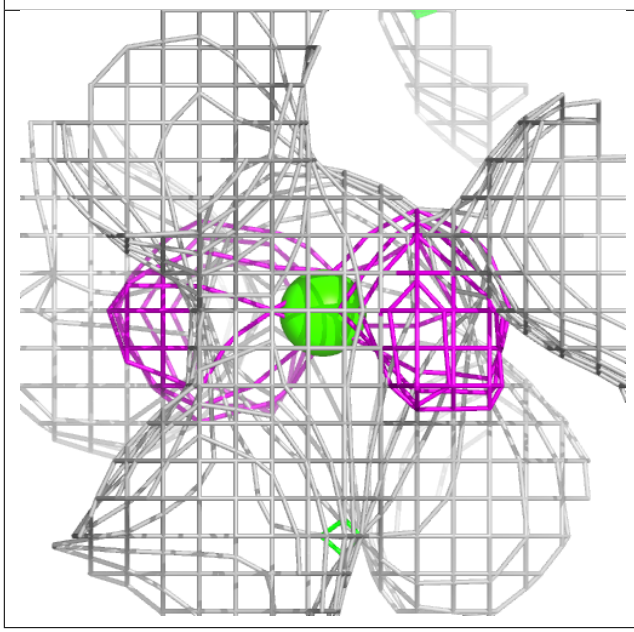
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	C	201	1/1	0.99	0.12	29,29,29,29	1
3	CA	B	102	1/1	0.99	0.13	27,27,27,27	1
3	CA	B	101	1/1	1.00	0.02	21,21,21,21	0
3	CA	H	101	1/1	1.00	0.01	19,19,19,19	0
6	CD	C	206	1/1	1.00	0.01	21,21,21,21	0
6	CD	A	205	1/1	1.00	0.01	19,19,19,19	0
6	CD	G	206	1/1	1.00	0.01	23,23,23,23	0

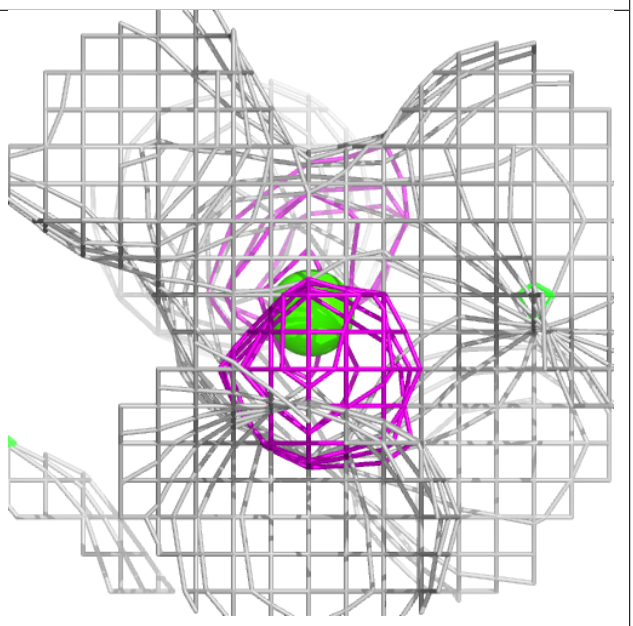
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CA D 102:

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

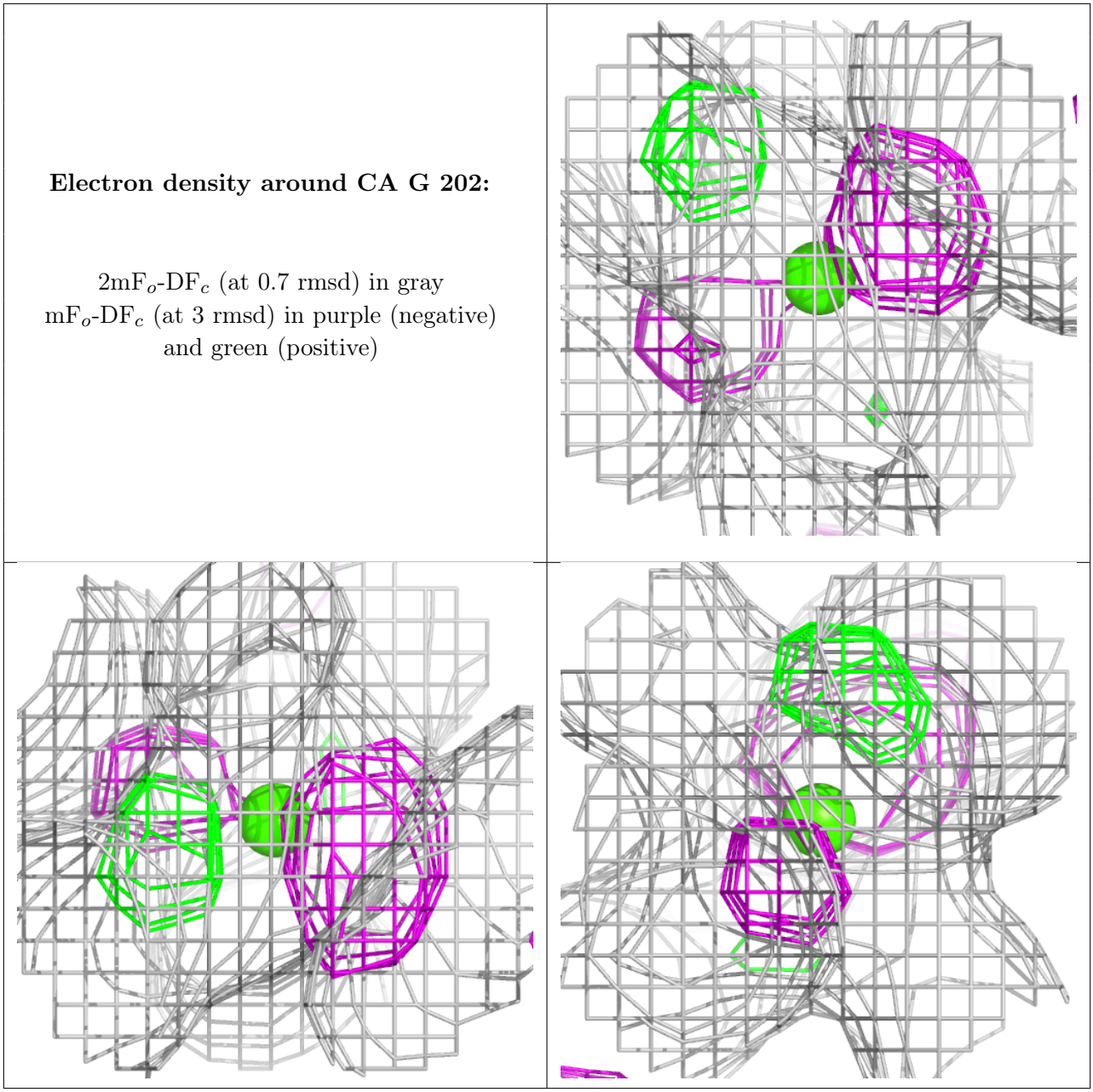






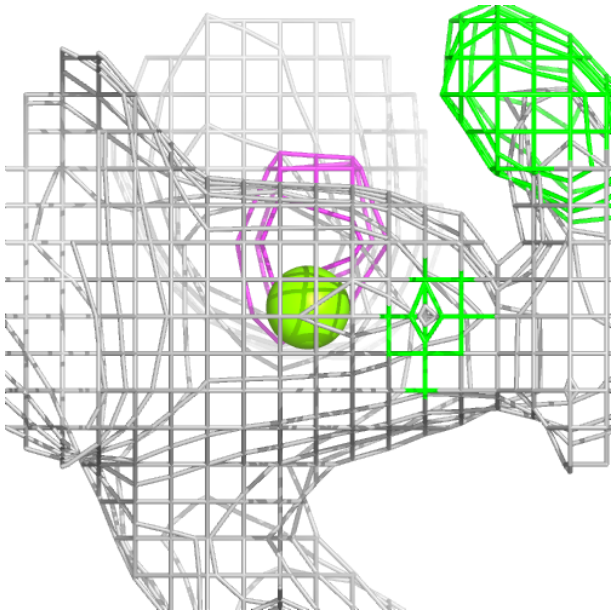
Electron density around CA G 202:

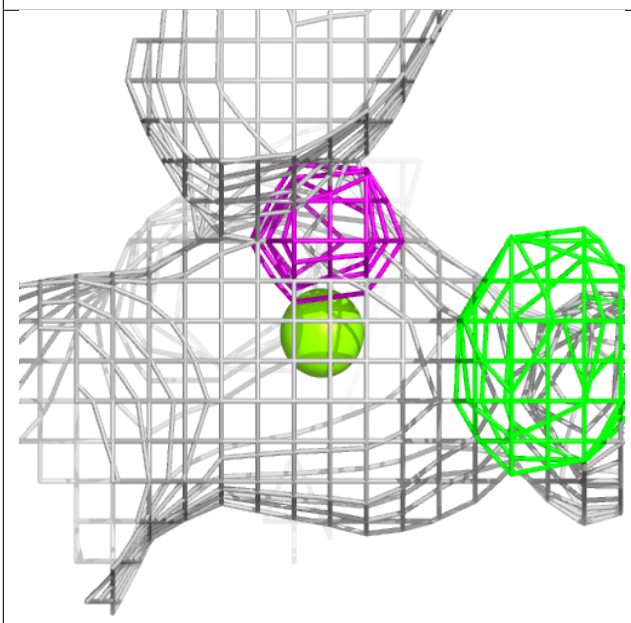
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

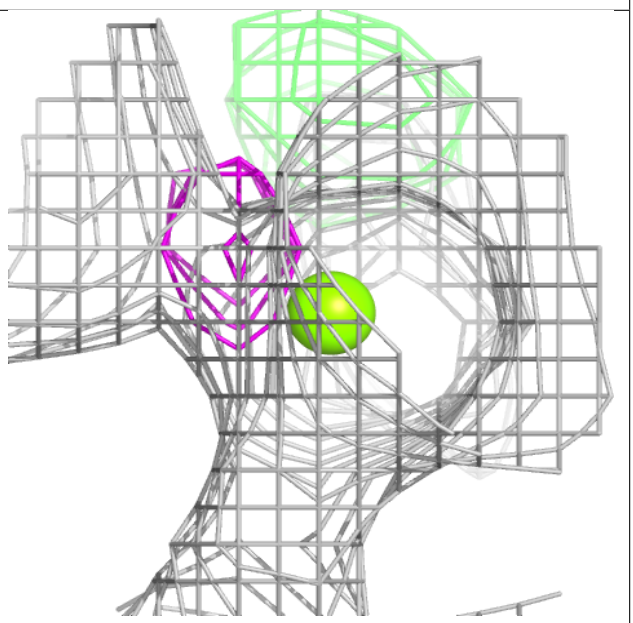


Electron density around MG F 103:

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

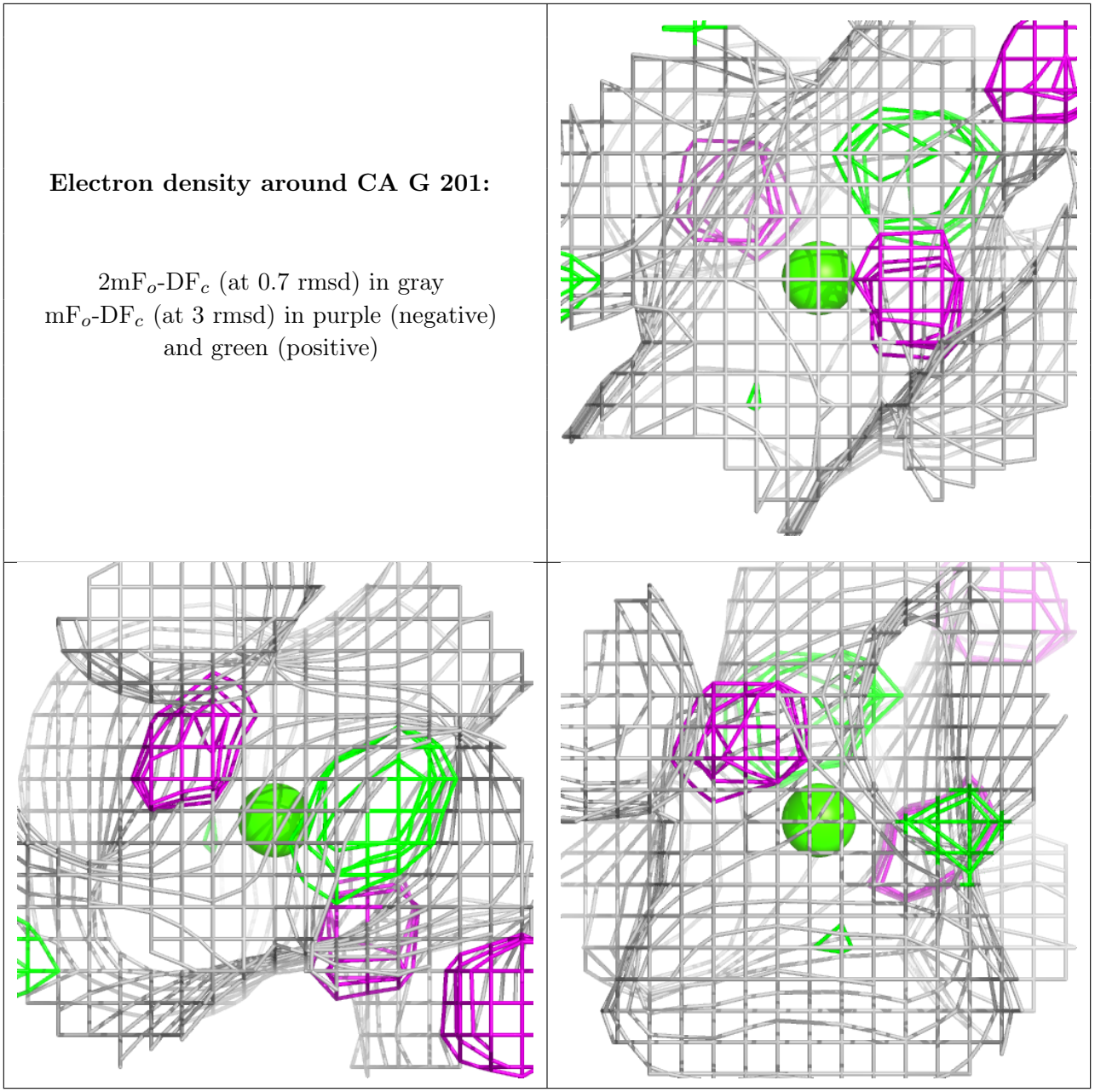






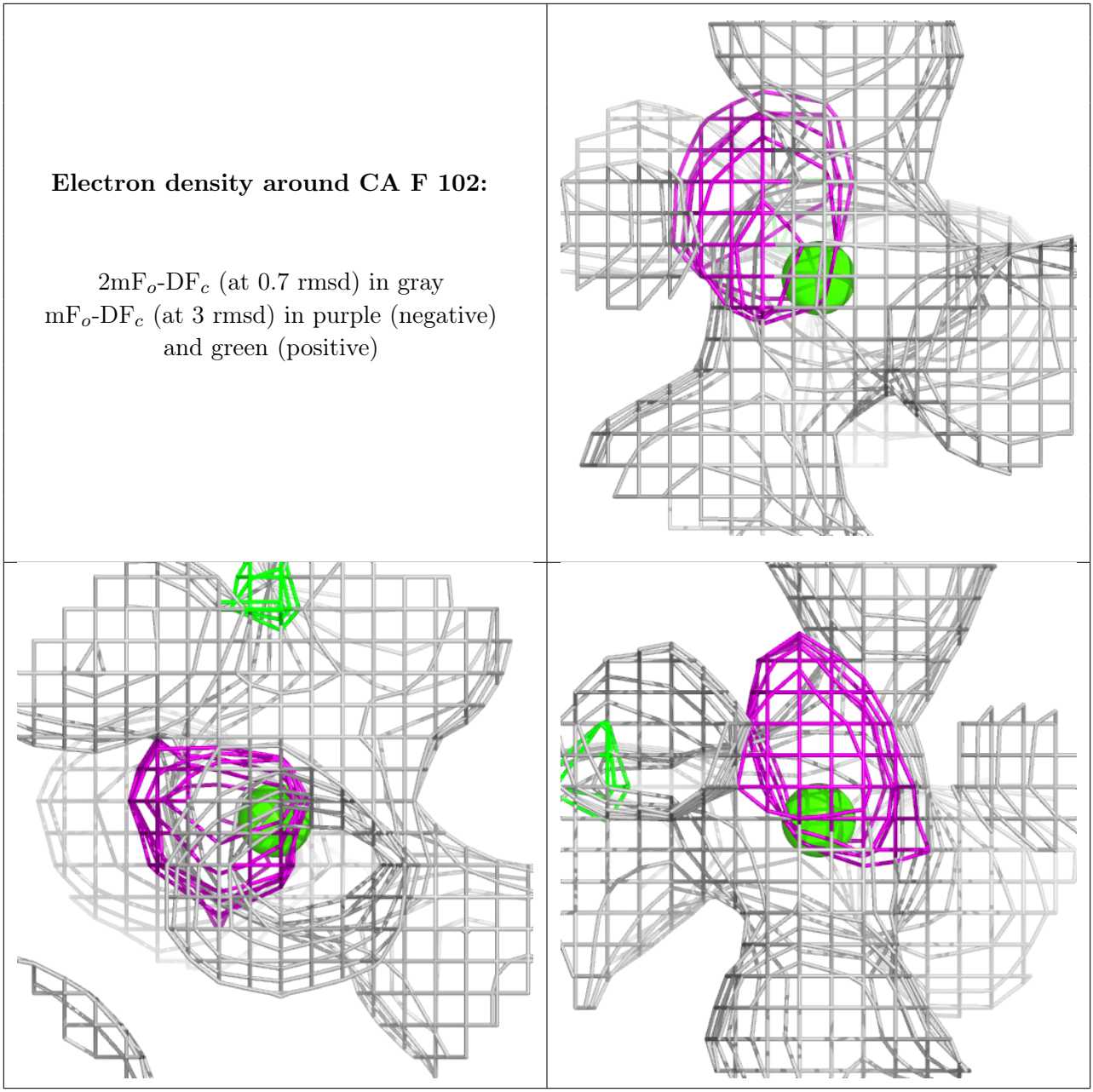
Electron density around CA G 201:

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



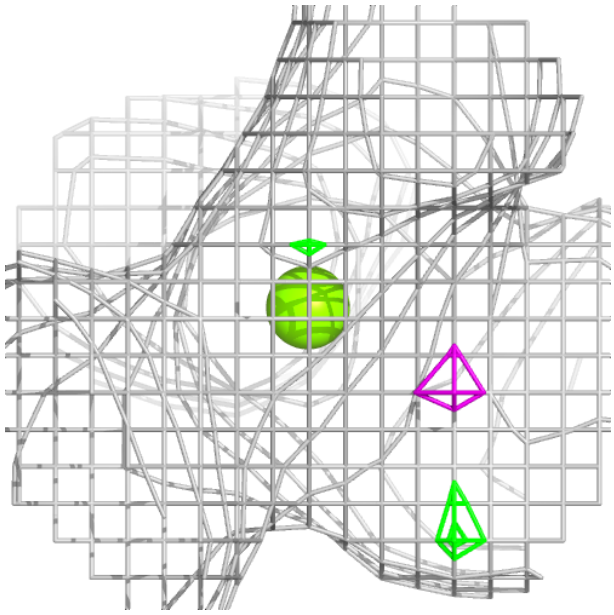
Electron density around CA F 102:

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



Electron density around MG G 207:

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

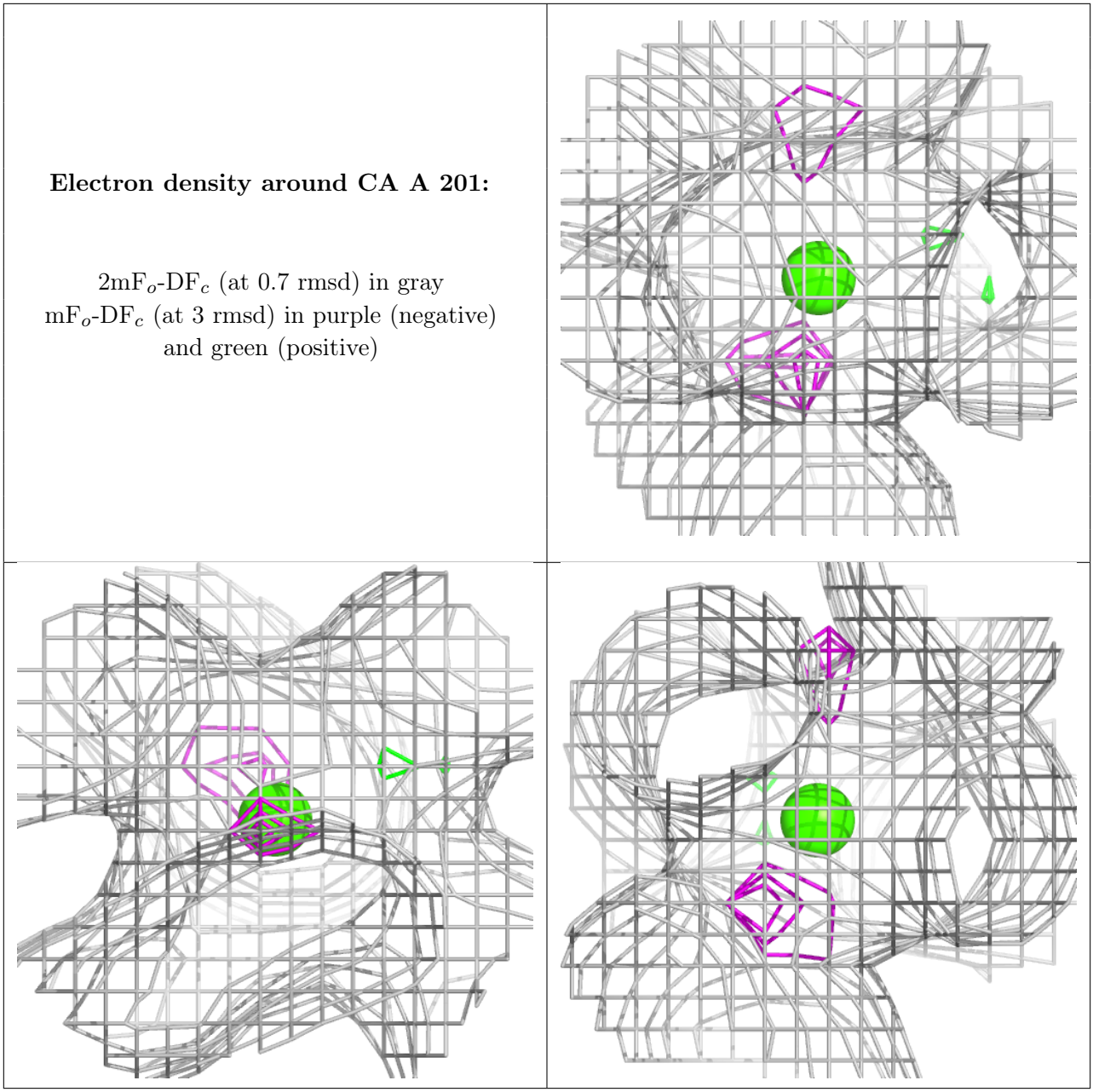






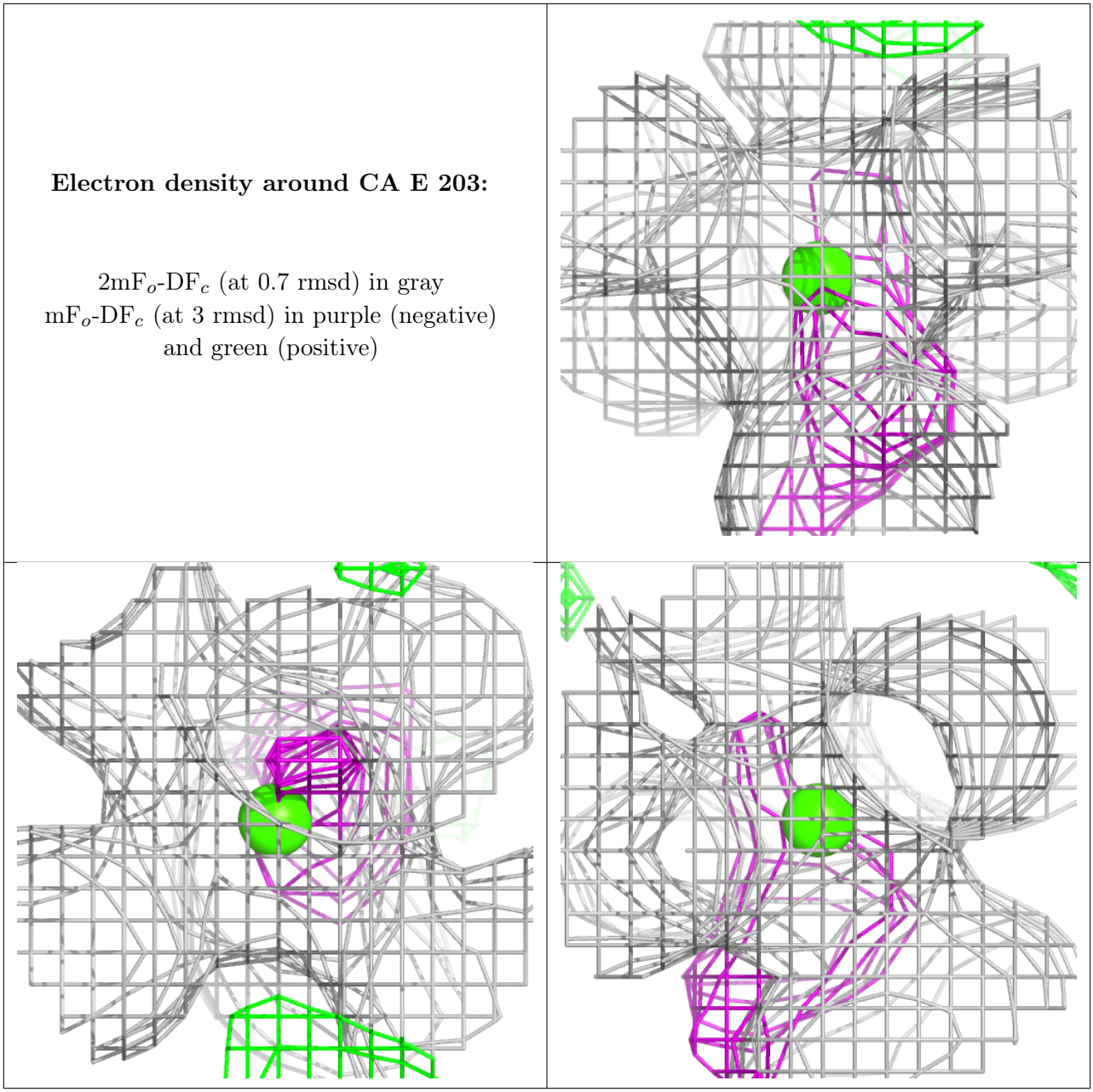
Electron density around CA A 201:

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



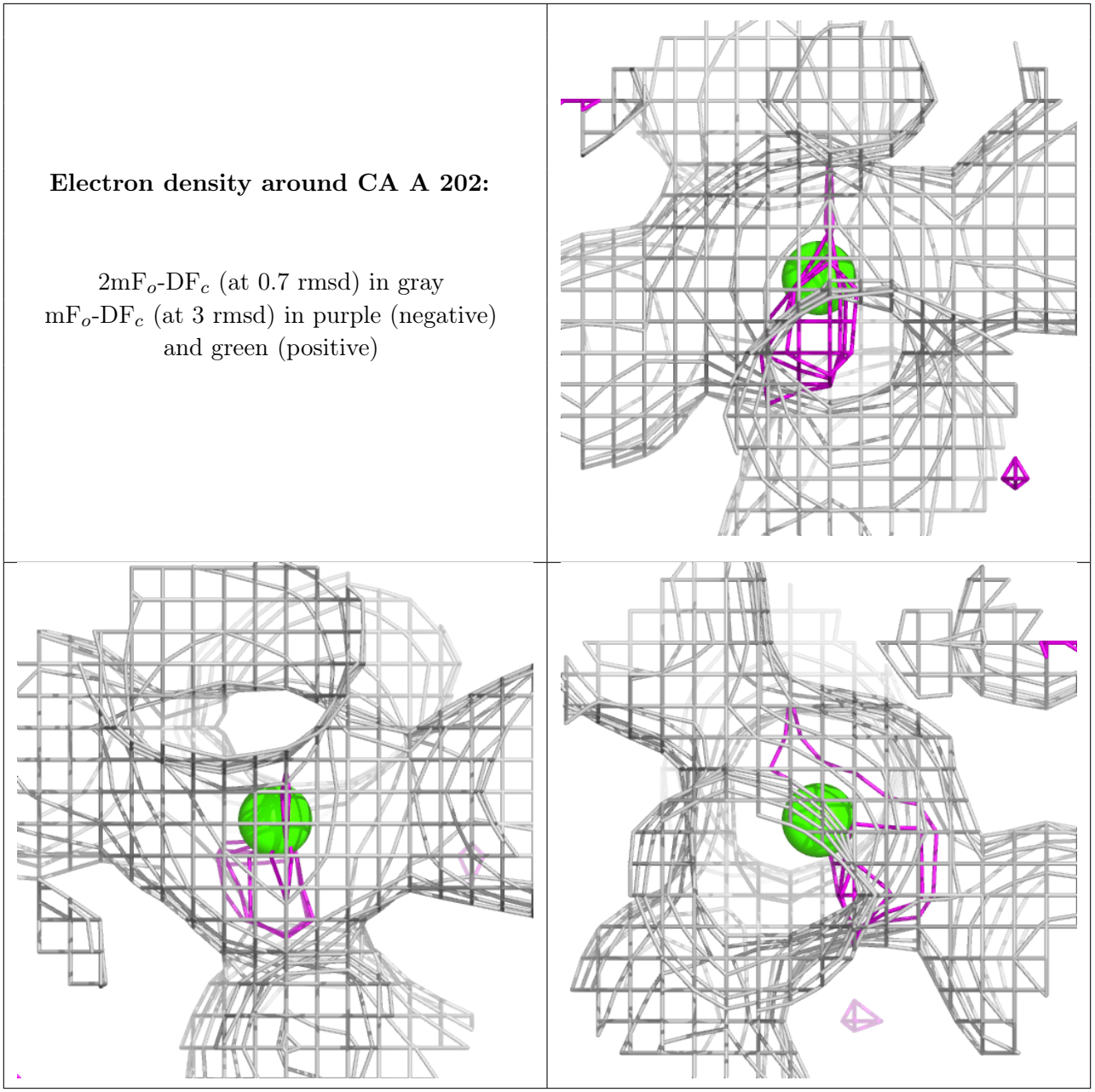
Electron density around CA E 203:

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



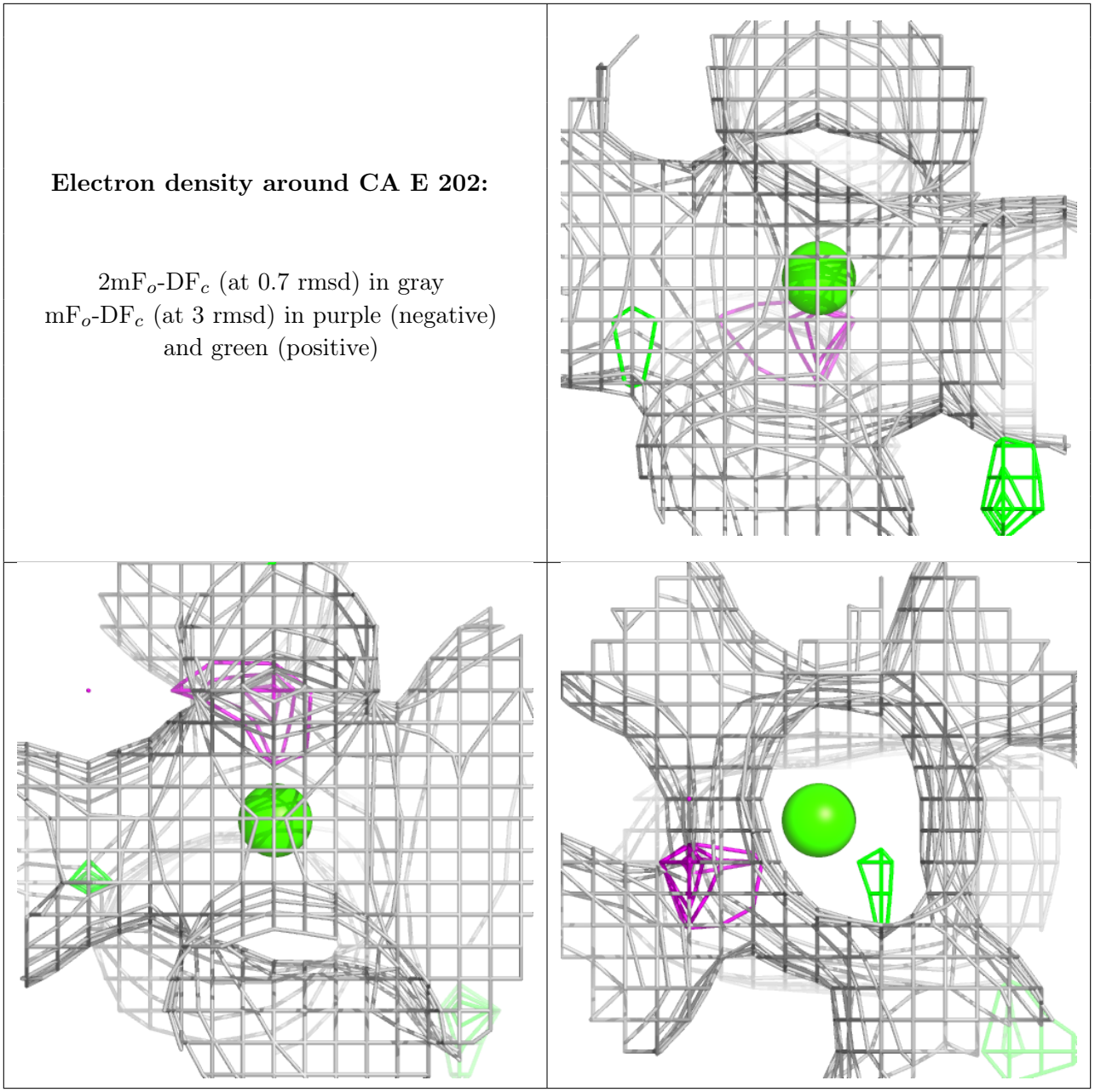
Electron density around CA A 202:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



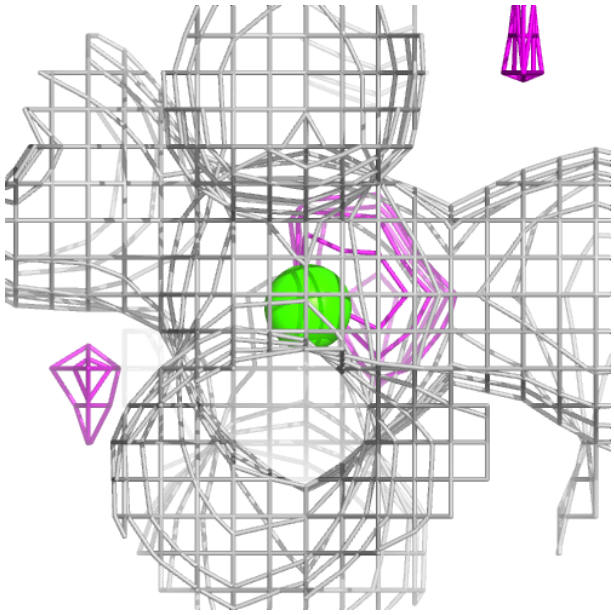
Electron density around CA E 202:

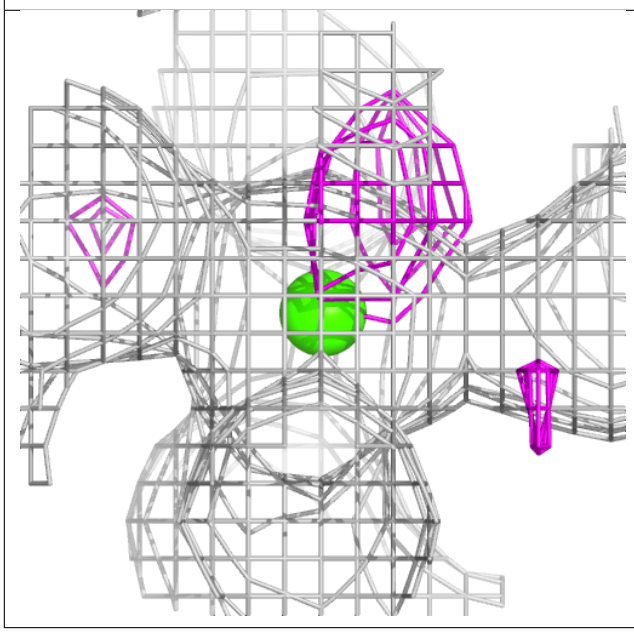
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

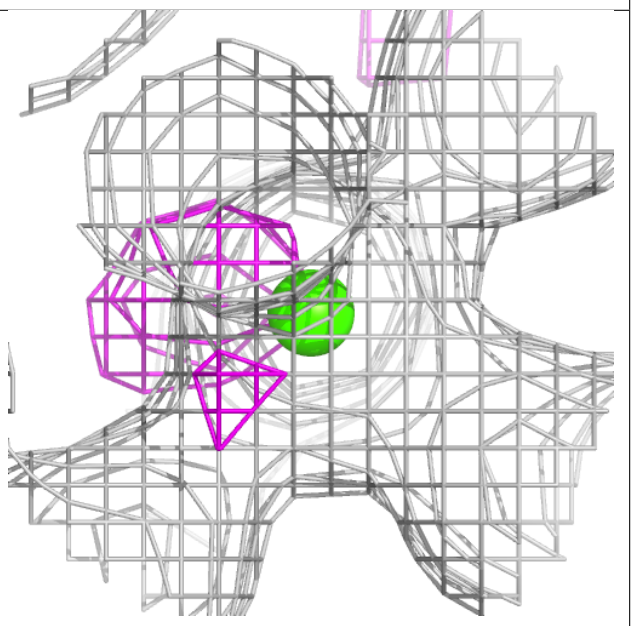


Electron density around CA H 102:

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

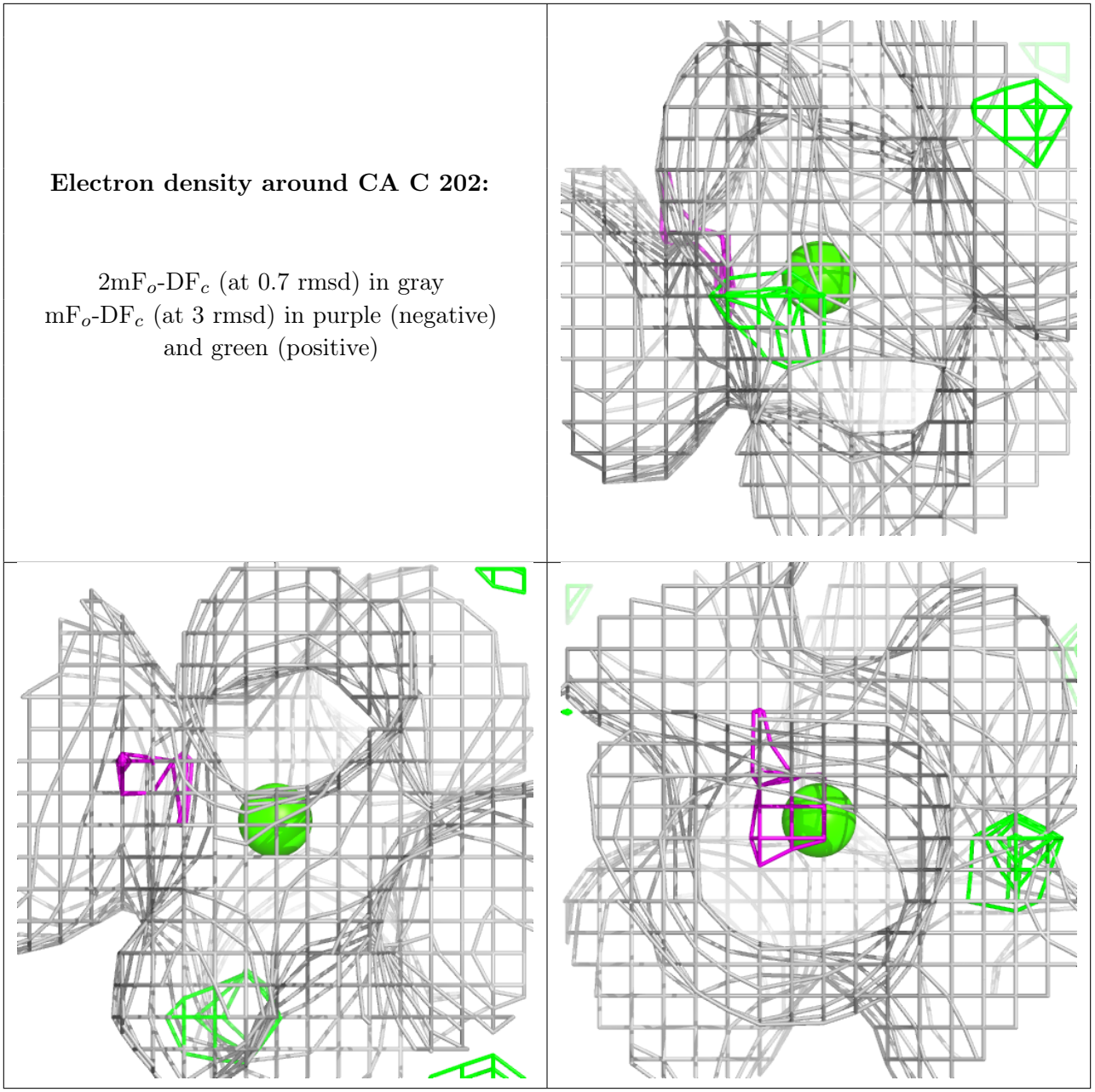






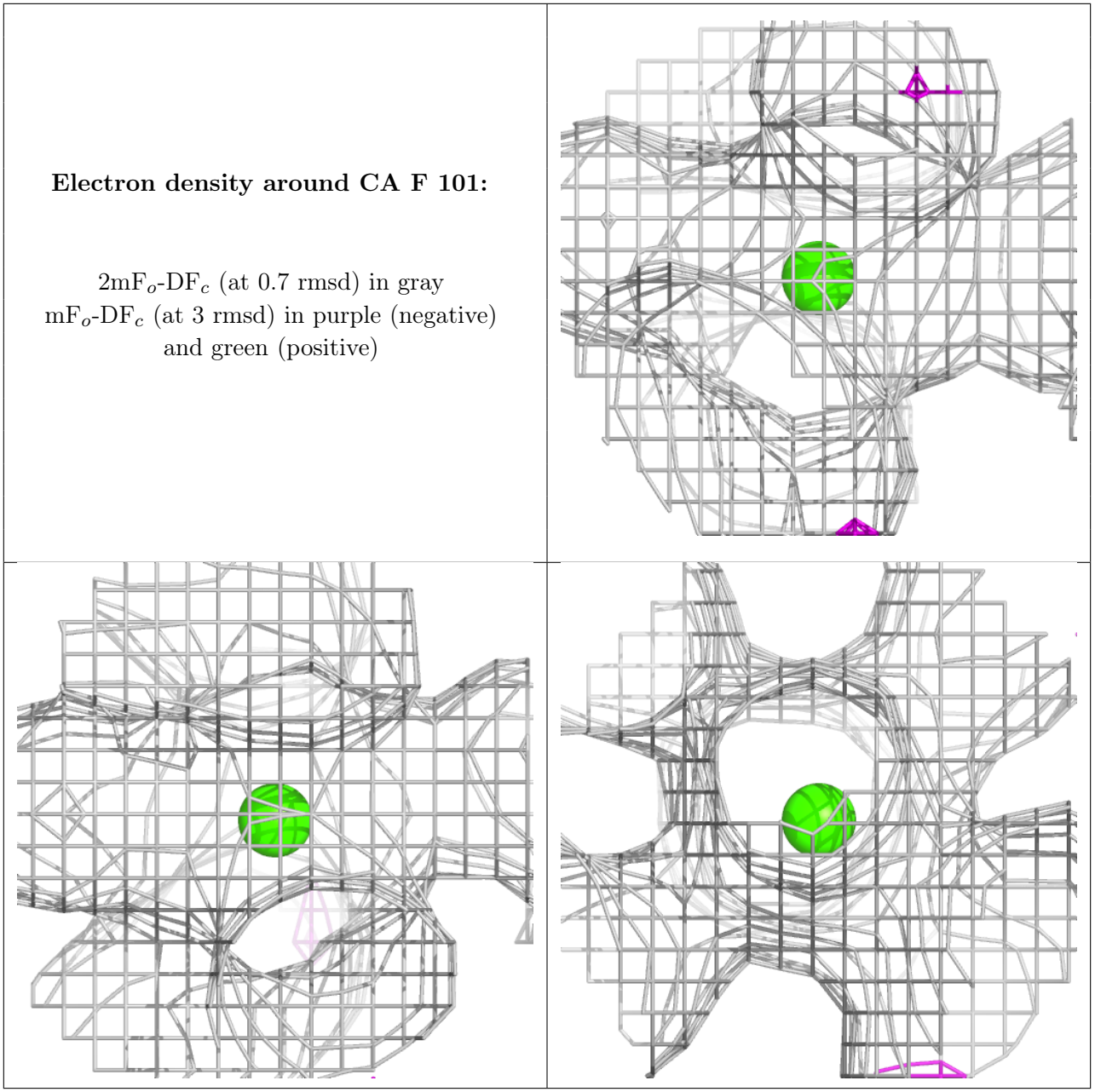
Electron density around CA C 202:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



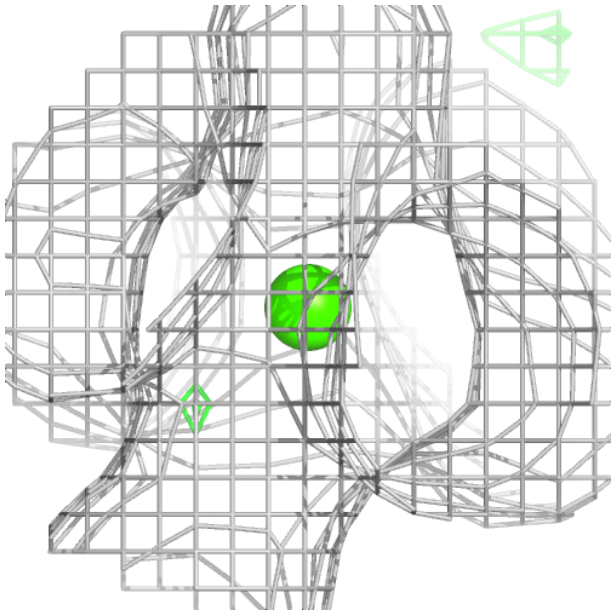
Electron density around CA F 101:

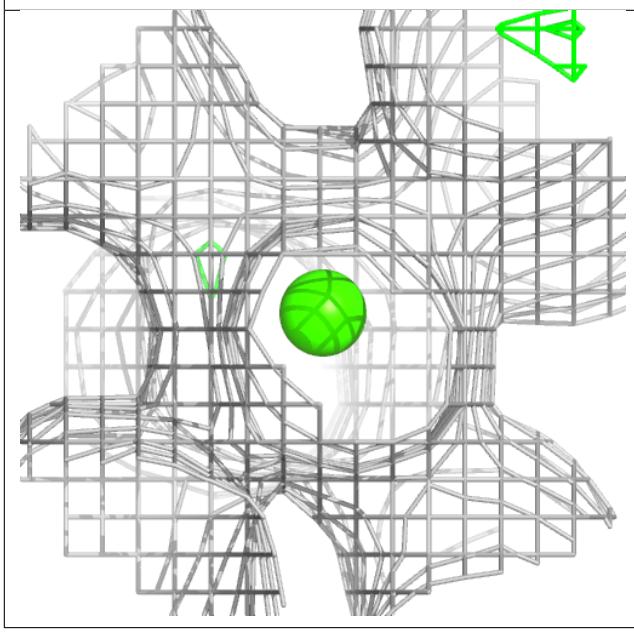
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

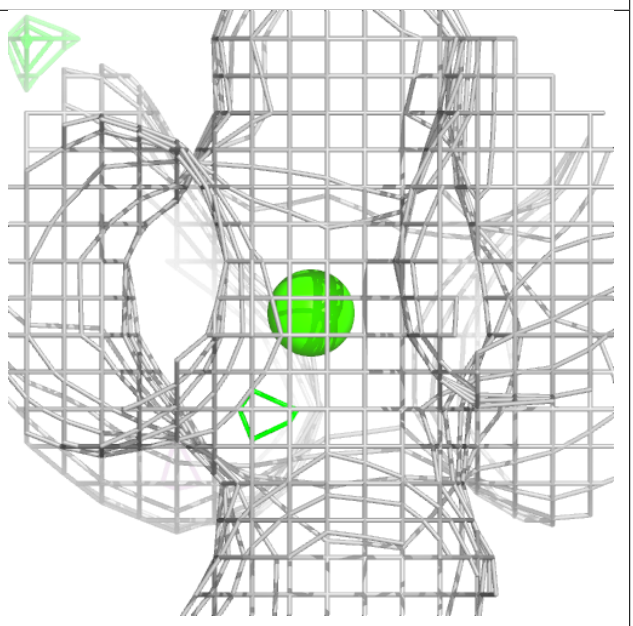


Electron density around CA D 101:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

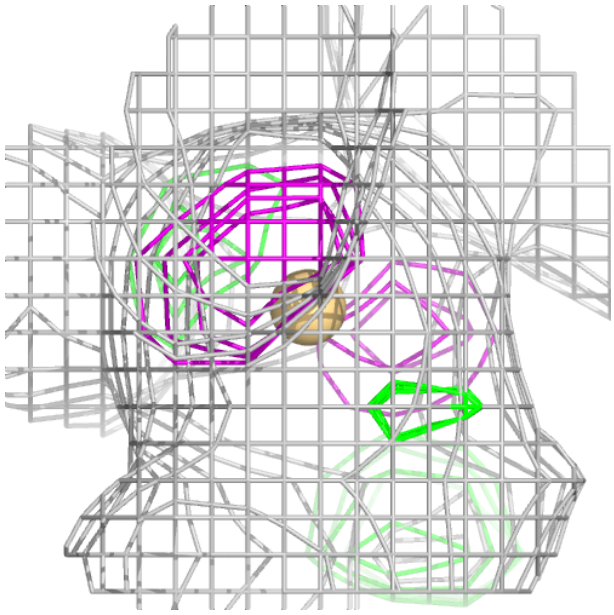


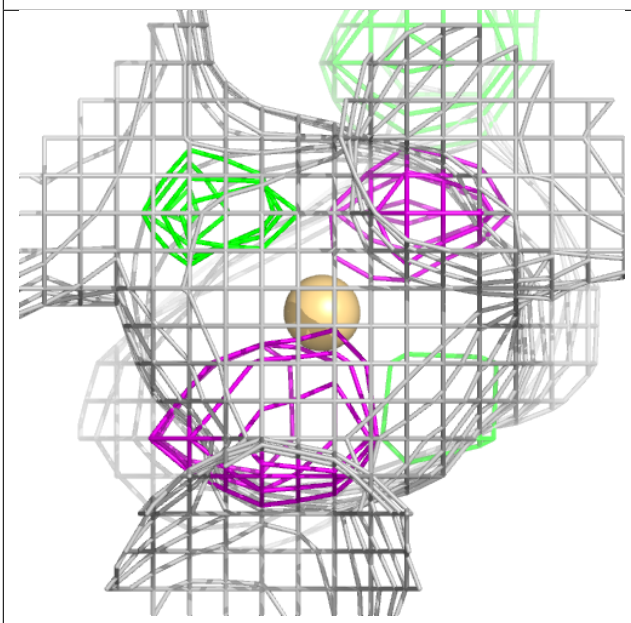


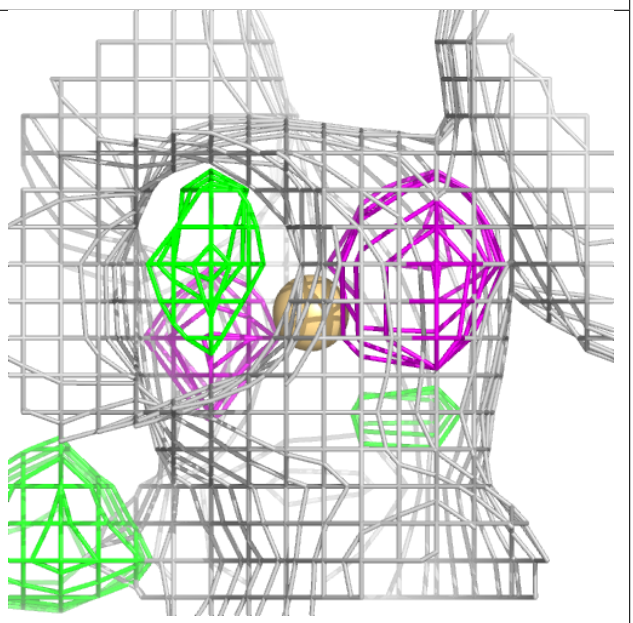


Electron density around CD A 206:

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

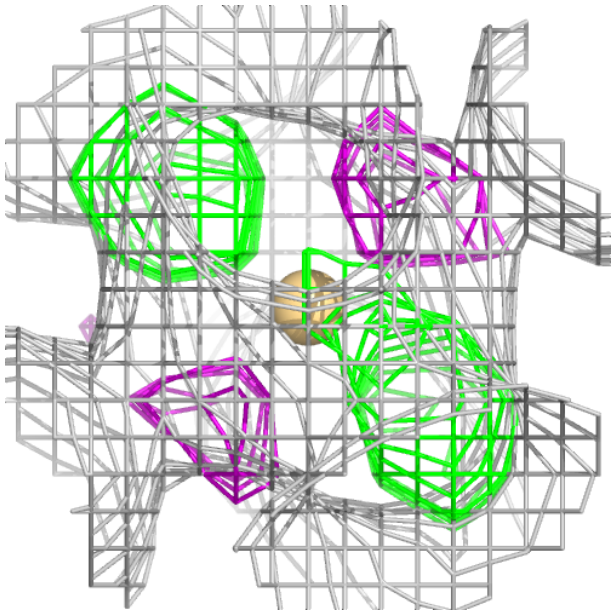


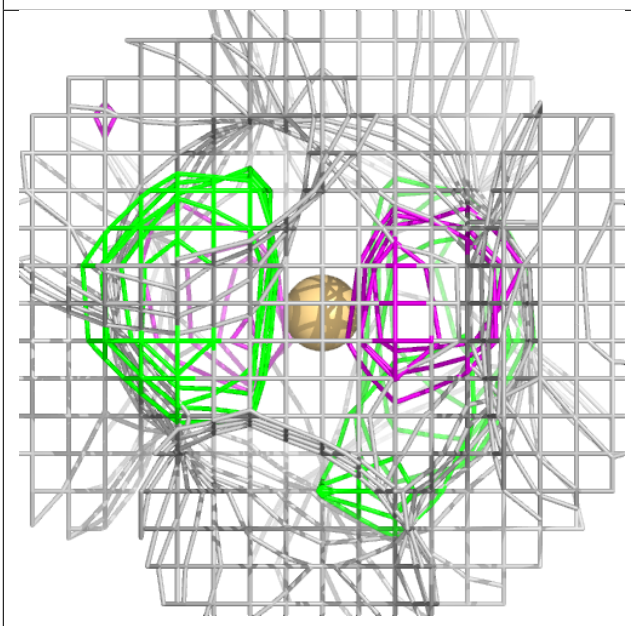


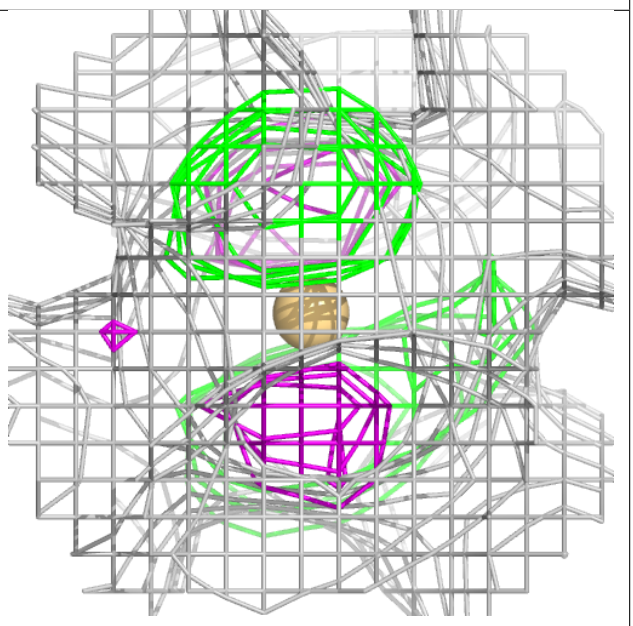


Electron density around CD C 205:

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

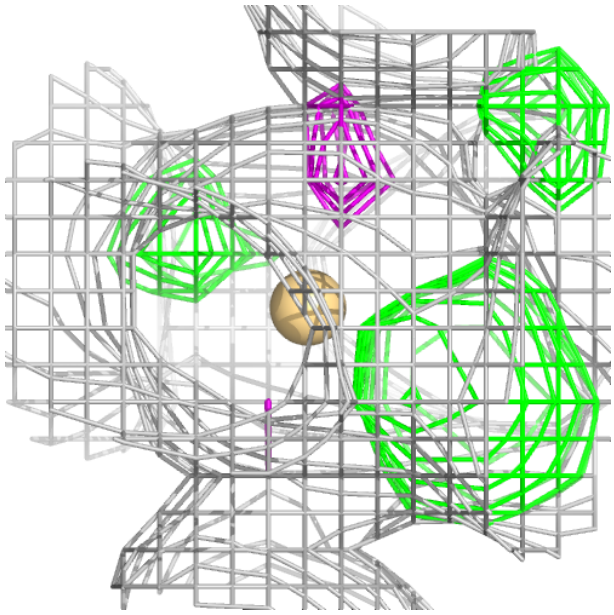


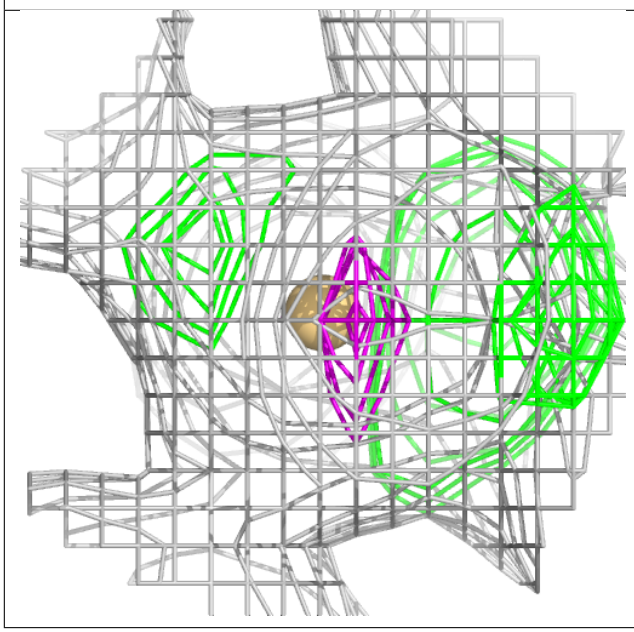


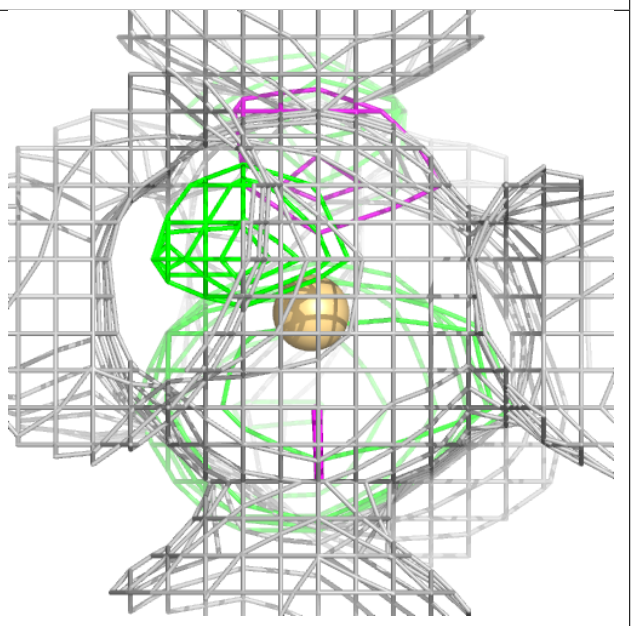


Electron density around CD E 207:

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

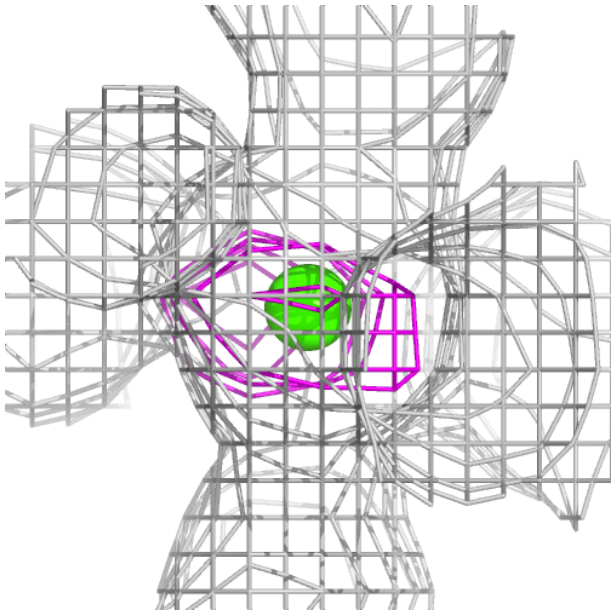


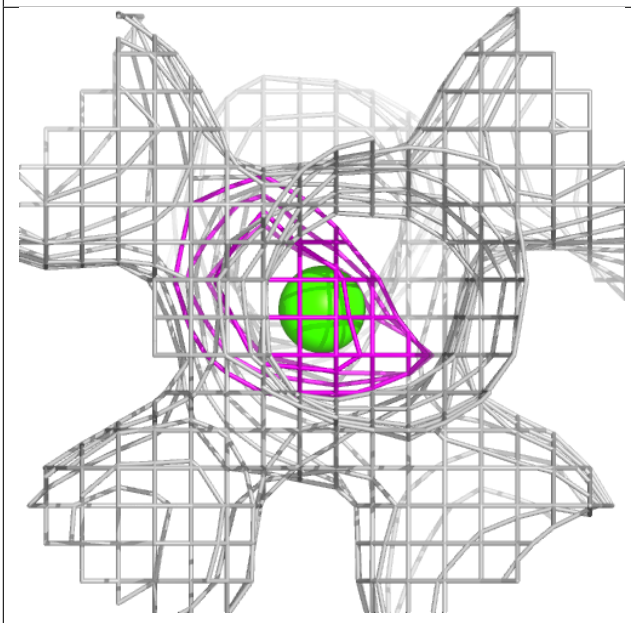


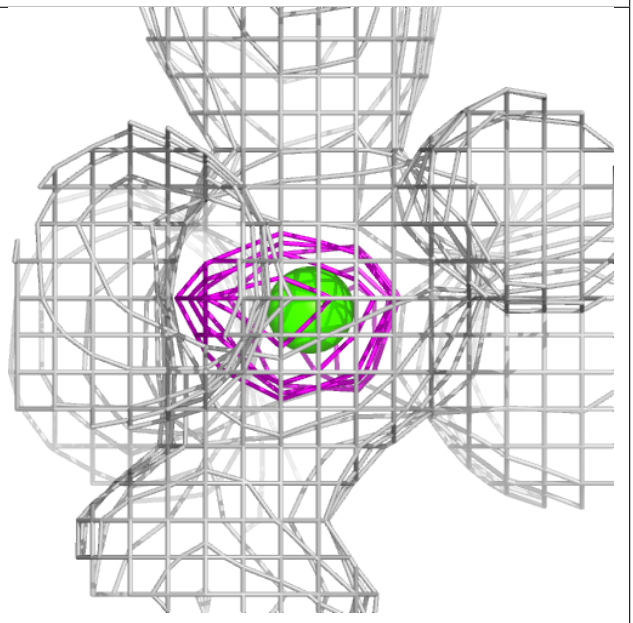


Electron density around CA C 201:

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

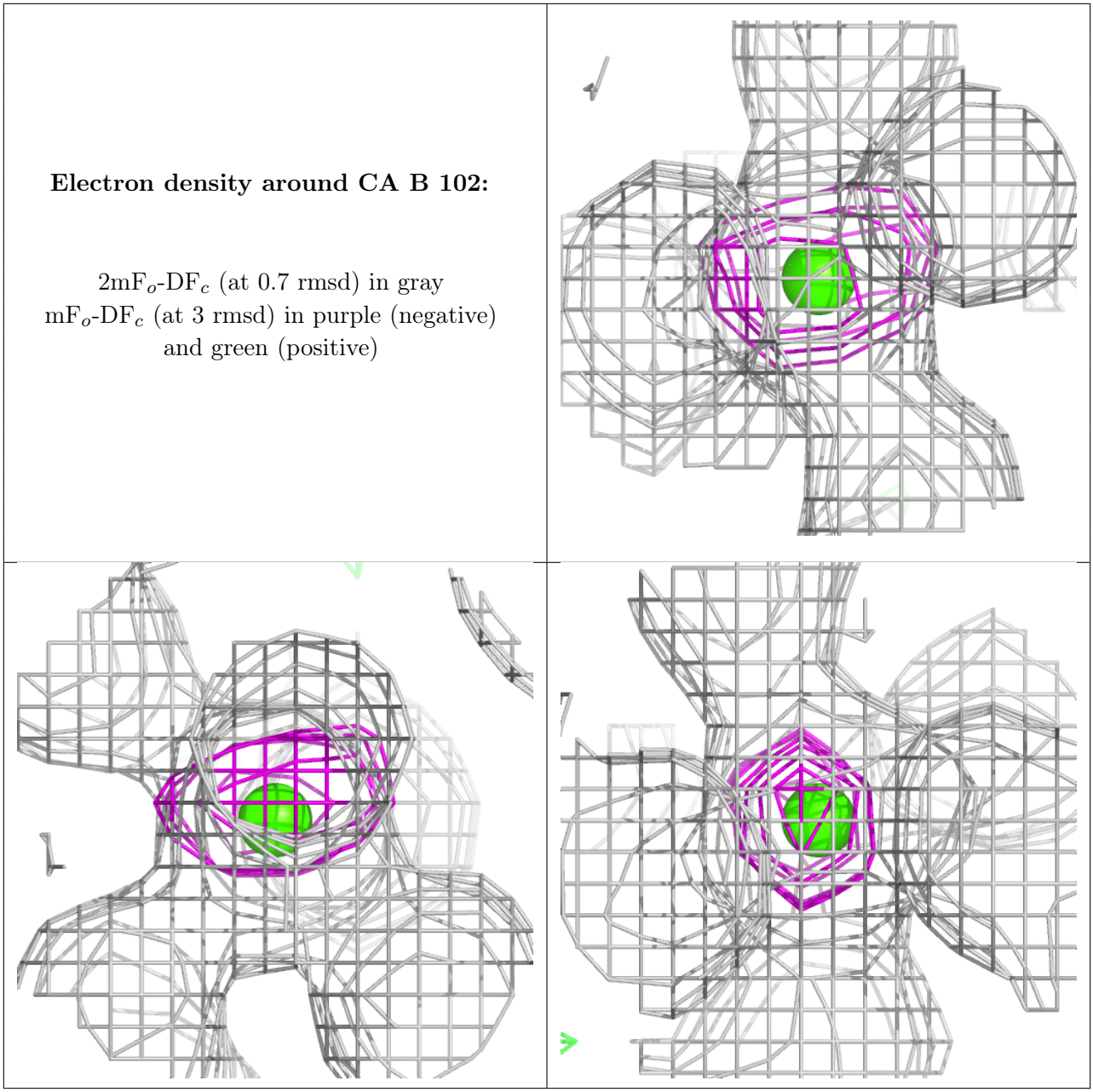






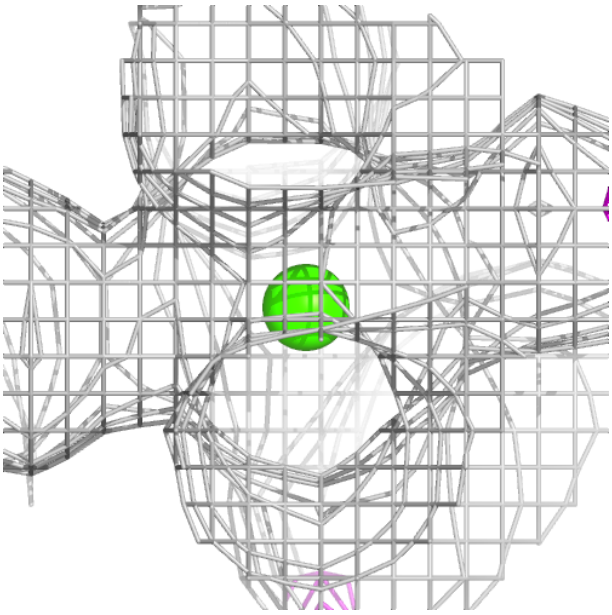
Electron density around CA B 102:

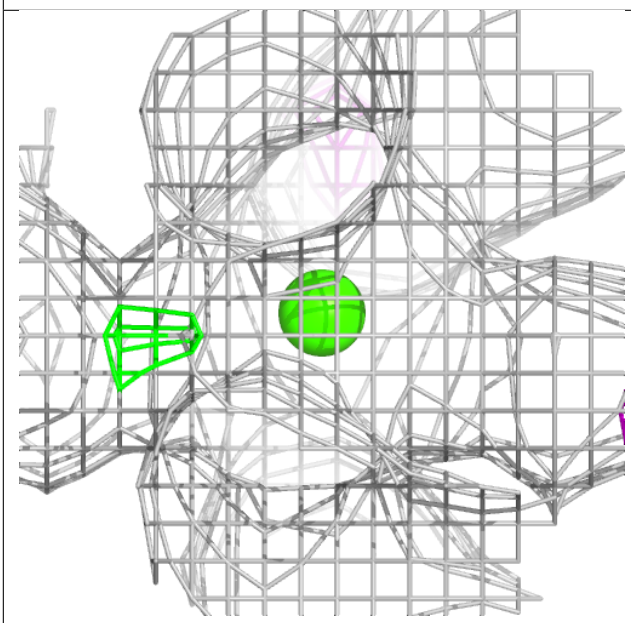
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

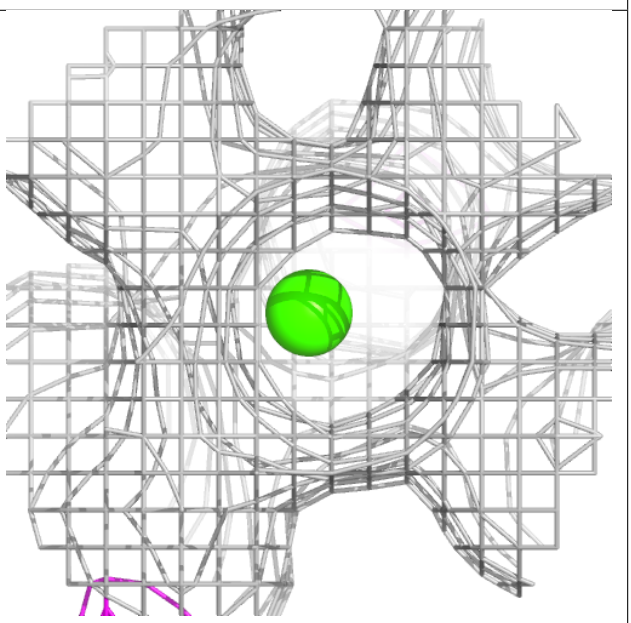


Electron density around CA B 101:

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

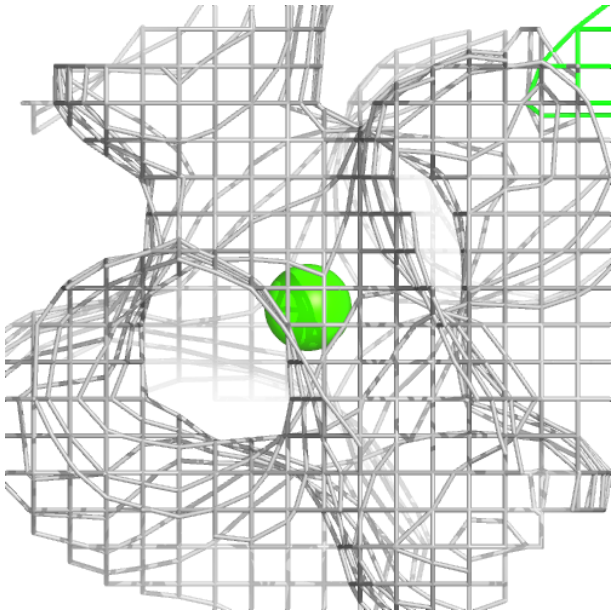


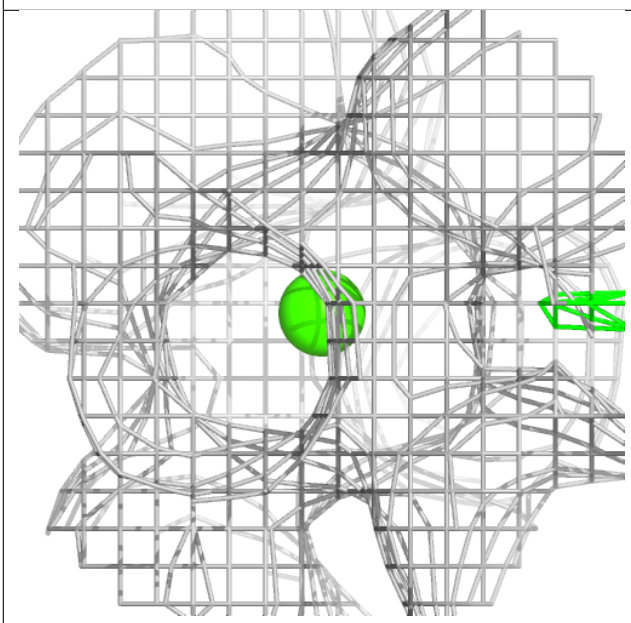


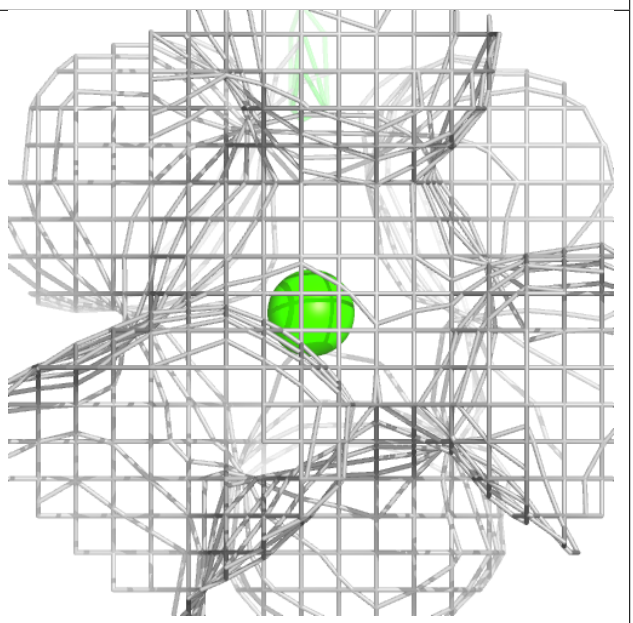


Electron density around CA H 101:

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

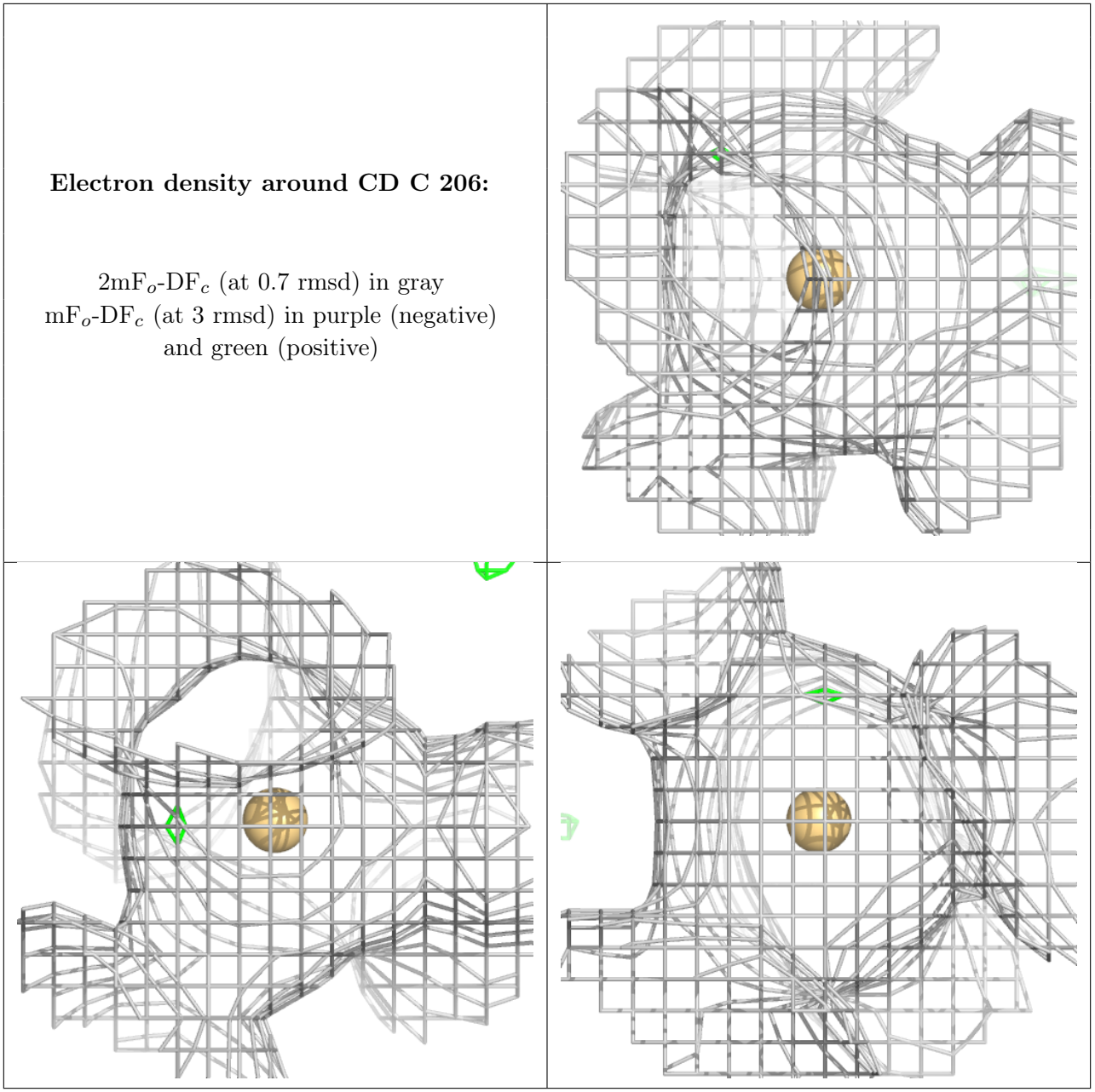






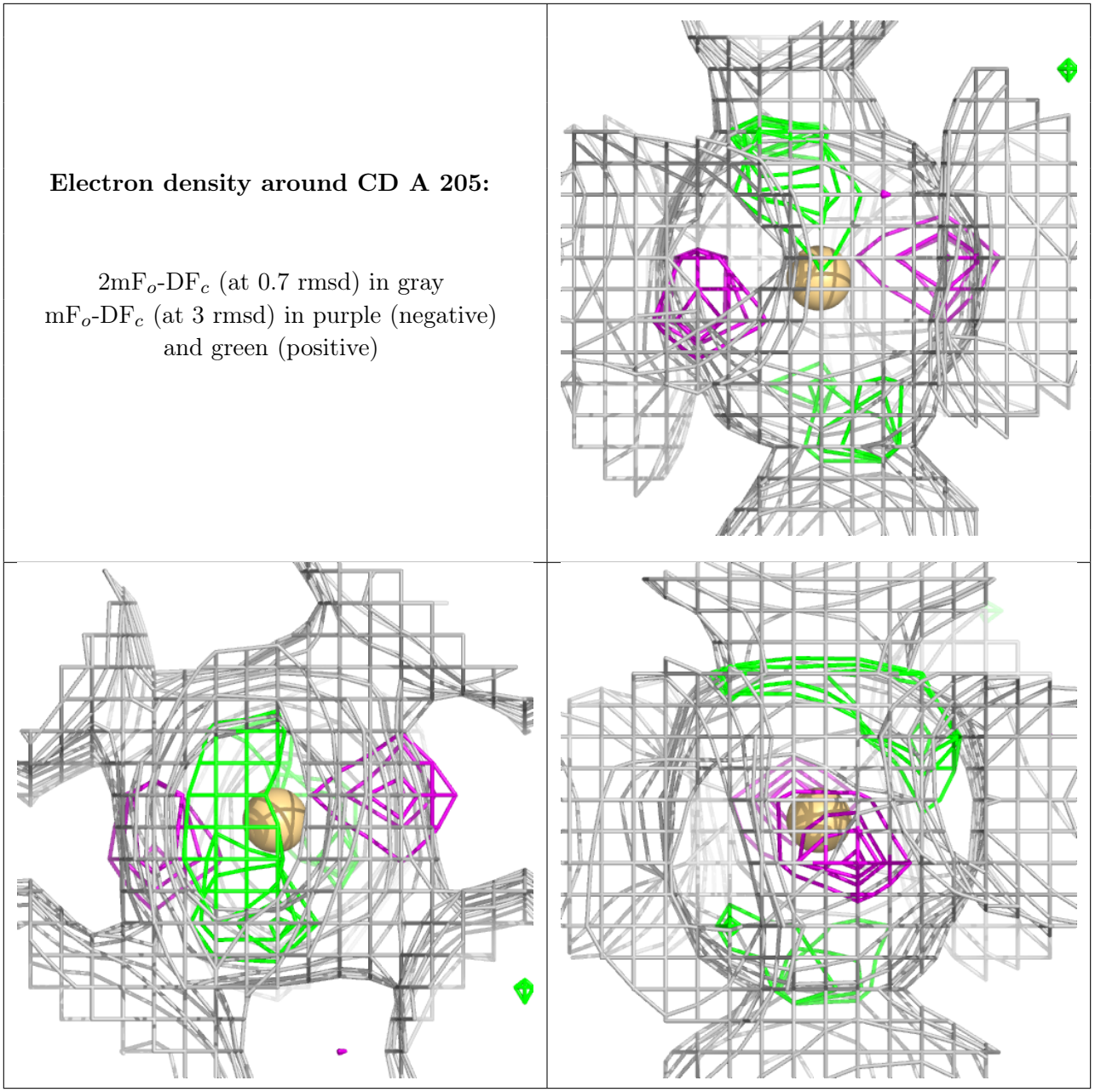
Electron density around CD C 206:

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



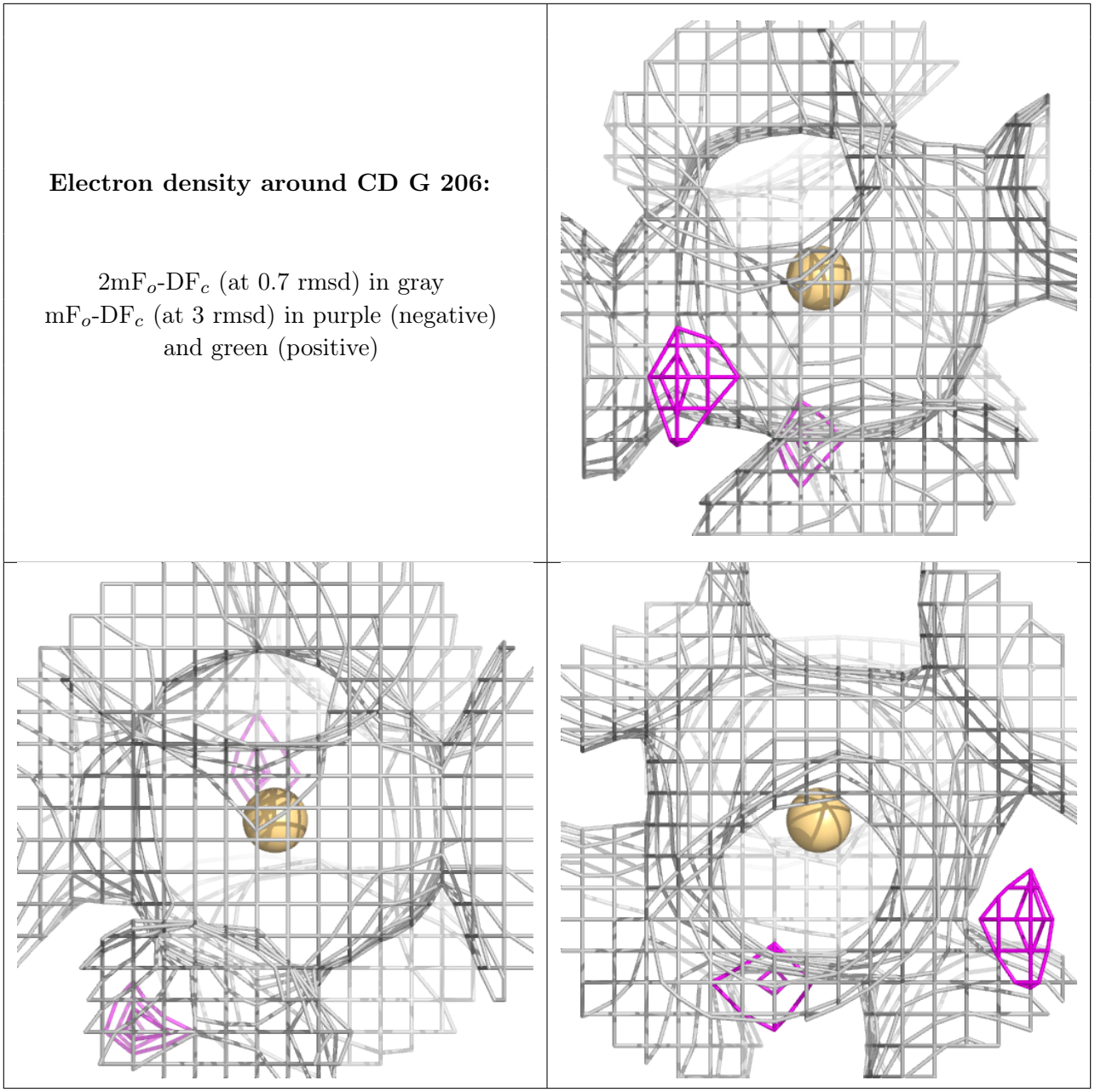
Electron density around CD A 205:

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



Electron density around CD G 206:

$2mF_o$-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.