Full wwPDB X-ray Structure Validation Report (i)

Mar 18, 2024 – 04:46 PM JST

PDB ID	:	6K83
Title	:	Structure of RGLG1 mutant-D207G
Authors	:	Wang, Q.; Wu, Y.
Deposited on	:	2019-06-11
Resolution	:	2.39 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 (i) symbol.

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

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

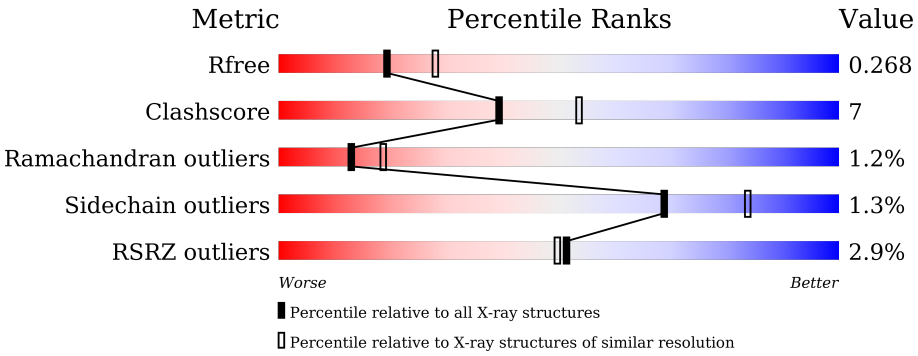
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	301	3% 78% 14% • 7%
1	B	301	3% 74% 18% • 7%
1	C	301	2% 80% 13% 7%
1	D	301	3% 79% 13% • 7%
1	E	301	2% 72% 20% • 7%
1	F	301	4% 75% 16% •• 7%

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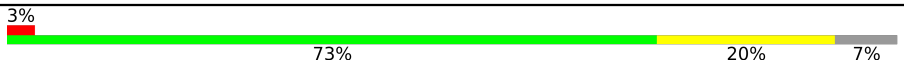
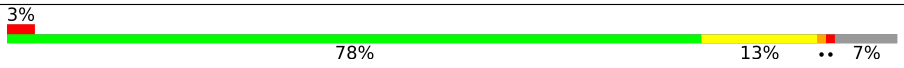
Mol	Chain	Length	Quality of chain
1	G	301	
1	H	301	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17985 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 E3 ubiquitin-protein ligase RGLG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	280	Total	C	N	O	S	0	0	0
			2181	1381	369	423	8			
1	A	280	Total	C	N	O	S	0	0	0
			2181	1381	369	423	8			
1	C	280	Total	C	N	O	S	0	0	0
			2181	1381	369	423	8			
1	D	280	Total	C	N	O	S	0	0	0
			2181	1381	369	423	8			
1	E	280	Total	C	N	O	S	0	0	0
			2181	1381	369	423	8			
1	F	280	Total	C	N	O	S	0	0	0
			2181	1381	369	423	8			
1	G	280	Total	C	N	O	S	0	0	0
			2181	1381	369	423	8			
1	H	280	Total	C	N	O	S	0	0	0
			2181	1381	369	423	8			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	119	GLY	-	expression tag	UNP Q9SS90
B	120	THR	-	expression tag	UNP Q9SS90
B	121	SER	-	expression tag	UNP Q9SS90
B	122	SER	-	expression tag	UNP Q9SS90
B	123	MET	-	expression tag	UNP Q9SS90
B	124	ALA	-	expression tag	UNP Q9SS90
B	125	ASP	-	expression tag	UNP Q9SS90
B	126	ILE	-	expression tag	UNP Q9SS90
B	127	GLY	-	expression tag	UNP Q9SS90
B	128	SER	-	expression tag	UNP Q9SS90
B	207	GLY	ASP	engineered mutation	UNP Q9SS90
A	119	GLY	-	expression tag	UNP Q9SS90
A	120	THR	-	expression tag	UNP Q9SS90

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Chain	Residue	Modelled	Actual	Comment	Reference
A	121	SER	-	expression tag	UNP Q9SS90
A	122	SER	-	expression tag	UNP Q9SS90
A	123	MET	-	expression tag	UNP Q9SS90
A	124	ALA	-	expression tag	UNP Q9SS90
A	125	ASP	-	expression tag	UNP Q9SS90
A	126	ILE	-	expression tag	UNP Q9SS90
A	127	GLY	-	expression tag	UNP Q9SS90
A	128	SER	-	expression tag	UNP Q9SS90
A	207	GLY	ASP	engineered mutation	UNP Q9SS90
C	119	GLY	-	expression tag	UNP Q9SS90
C	120	THR	-	expression tag	UNP Q9SS90
C	121	SER	-	expression tag	UNP Q9SS90
C	122	SER	-	expression tag	UNP Q9SS90
C	123	MET	-	expression tag	UNP Q9SS90
C	124	ALA	-	expression tag	UNP Q9SS90
C	125	ASP	-	expression tag	UNP Q9SS90
C	126	ILE	-	expression tag	UNP Q9SS90
C	127	GLY	-	expression tag	UNP Q9SS90
C	128	SER	-	expression tag	UNP Q9SS90
C	207	GLY	ASP	engineered mutation	UNP Q9SS90
D	119	GLY	-	expression tag	UNP Q9SS90
D	120	THR	-	expression tag	UNP Q9SS90
D	121	SER	-	expression tag	UNP Q9SS90
D	122	SER	-	expression tag	UNP Q9SS90
D	123	MET	-	expression tag	UNP Q9SS90
D	124	ALA	-	expression tag	UNP Q9SS90
D	125	ASP	-	expression tag	UNP Q9SS90
D	126	ILE	-	expression tag	UNP Q9SS90
D	127	GLY	-	expression tag	UNP Q9SS90
D	128	SER	-	expression tag	UNP Q9SS90
D	207	GLY	ASP	engineered mutation	UNP Q9SS90
E	119	GLY	-	expression tag	UNP Q9SS90
E	120	THR	-	expression tag	UNP Q9SS90
E	121	SER	-	expression tag	UNP Q9SS90
E	122	SER	-	expression tag	UNP Q9SS90
E	123	MET	-	expression tag	UNP Q9SS90
E	124	ALA	-	expression tag	UNP Q9SS90
E	125	ASP	-	expression tag	UNP Q9SS90
E	126	ILE	-	expression tag	UNP Q9SS90
E	127	GLY	-	expression tag	UNP Q9SS90
E	128	SER	-	expression tag	UNP Q9SS90
E	207	GLY	ASP	engineered mutation	UNP Q9SS90

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Chain	Residue	Modelled	Actual	Comment	Reference
F	119	GLY	-	expression tag	UNP Q9SS90
F	120	THR	-	expression tag	UNP Q9SS90
F	121	SER	-	expression tag	UNP Q9SS90
F	122	SER	-	expression tag	UNP Q9SS90
F	123	MET	-	expression tag	UNP Q9SS90
F	124	ALA	-	expression tag	UNP Q9SS90
F	125	ASP	-	expression tag	UNP Q9SS90
F	126	ILE	-	expression tag	UNP Q9SS90
F	127	GLY	-	expression tag	UNP Q9SS90
F	128	SER	-	expression tag	UNP Q9SS90
F	207	GLY	ASP	engineered mutation	UNP Q9SS90
G	119	GLY	-	expression tag	UNP Q9SS90
G	120	THR	-	expression tag	UNP Q9SS90
G	121	SER	-	expression tag	UNP Q9SS90
G	122	SER	-	expression tag	UNP Q9SS90
G	123	MET	-	expression tag	UNP Q9SS90
G	124	ALA	-	expression tag	UNP Q9SS90
G	125	ASP	-	expression tag	UNP Q9SS90
G	126	ILE	-	expression tag	UNP Q9SS90
G	127	GLY	-	expression tag	UNP Q9SS90
G	128	SER	-	expression tag	UNP Q9SS90
G	207	GLY	ASP	engineered mutation	UNP Q9SS90
H	119	GLY	-	expression tag	UNP Q9SS90
H	120	THR	-	expression tag	UNP Q9SS90
H	121	SER	-	expression tag	UNP Q9SS90
H	122	SER	-	expression tag	UNP Q9SS90
H	123	MET	-	expression tag	UNP Q9SS90
H	124	ALA	-	expression tag	UNP Q9SS90
H	125	ASP	-	expression tag	UNP Q9SS90
H	126	ILE	-	expression tag	UNP Q9SS90
H	127	GLY	-	expression tag	UNP Q9SS90
H	128	SER	-	expression tag	UNP Q9SS90
H	207	GLY	ASP	engineered mutation	UNP Q9SS90

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	65	Total O 65 65	0	0
4	A	58	Total O 58 58	0	0
4	C	80	Total O 80 80	0	0

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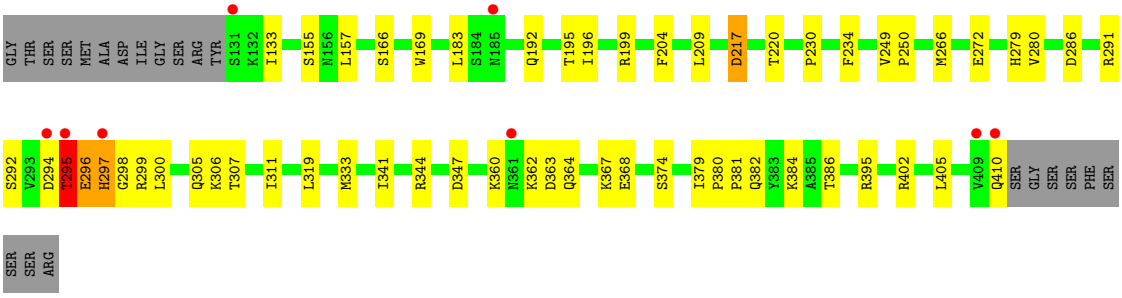
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	55	Total O 55 55	0	0
4	E	58	Total O 58 58	0	0
4	F	71	Total O 71 71	0	0
4	G	56	Total O 56 56	0	0
4	H	62	Total O 62 62	0	0

3 Residue-property plots

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.

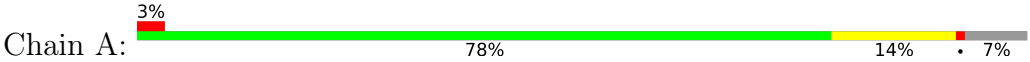
• Molecule 1: E3 ubiquitin-protein ligase RGLG1

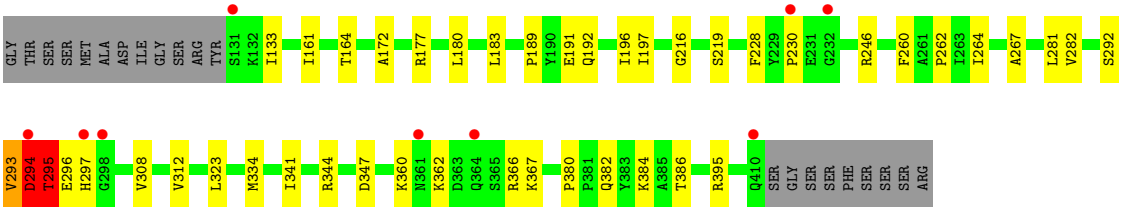
Chain B:



• Molecule 1: E3 ubiquitin-protein ligase RGLG1

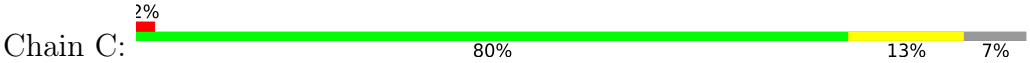
Chain A:

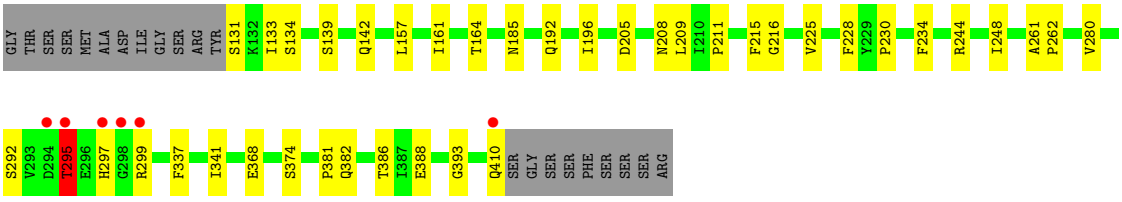




• Molecule 1: E3 ubiquitin-protein ligase RGLG1

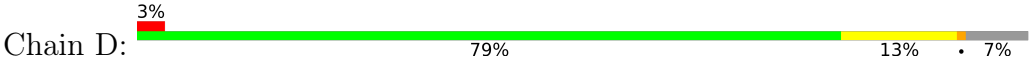
Chain C:

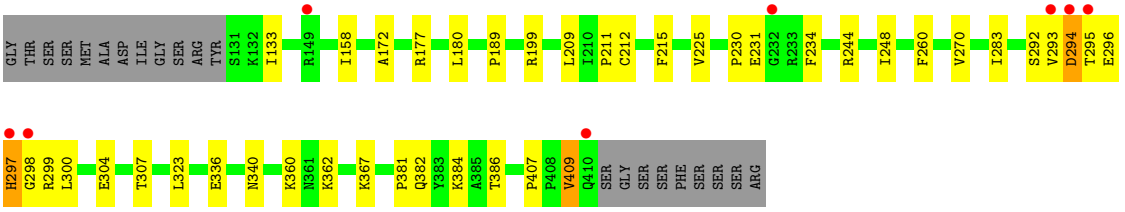




• Molecule 1: E3 ubiquitin-protein ligase RGLG1

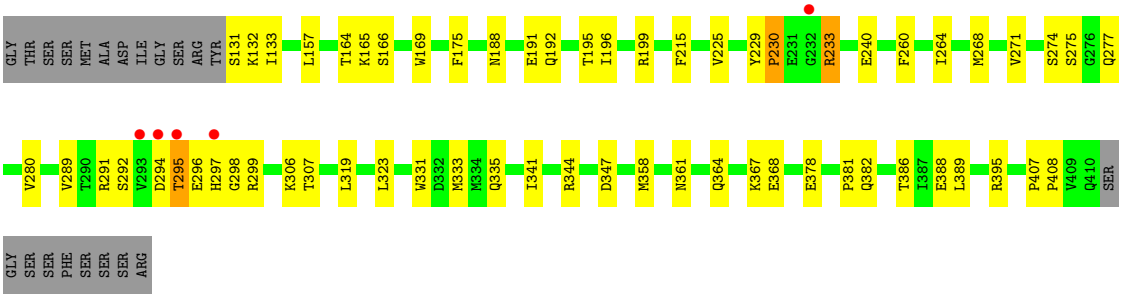
Chain D:





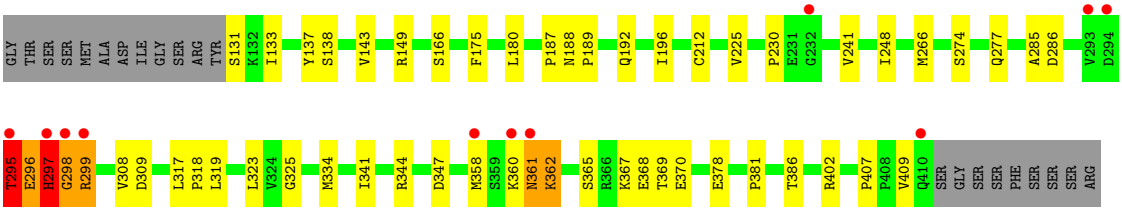
• Molecule 1: E3 ubiquitin-protein ligase RGLG1

Chain E:



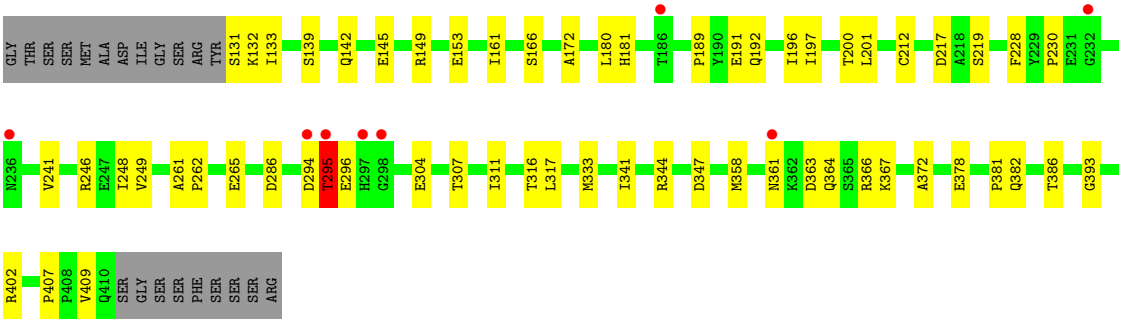
• Molecule 1: E3 ubiquitin-protein ligase RGLG1

Chain F:



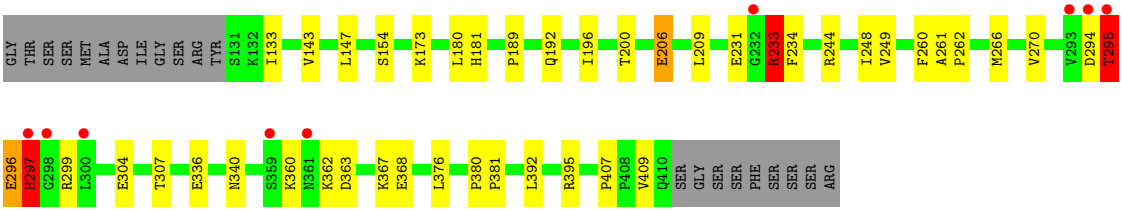
• Molecule 1: E3 ubiquitin-protein ligase RGLG1

Chain G:



• Molecule 1: E3 ubiquitin-protein ligase RGLG1

Chain H:


GLY THR SER SER MET ALA ASP ILE GLY SER ARG TYR S131 K132 I133 V143 L147 S154 K173 L180 H181 P189 Q192 I196 T200 E206 L209 E231 Q232 R233 F234 R244 I248 V249 F260 A261 P262 M266 V270 V293 D294 T295
E296 H297 G298 R299 L300 E304 T307 E336 N340 S359 K360 N361 K362 D363 K367 E368 L376 P380 P381 L392 R395 P407 P408 V409 Q410 SER GLY SER SER PHE SER SER SER ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	141.12Å 42.18Å 243.44Å 90.00° 91.08° 90.00°	Depositor
Resolution (Å)	46.51 – 2.39 46.51 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.51-2.39) 98.5 (46.51-2.39)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.205 , 0.268 0.208 , 0.268	Depositor DCC
R_{free} test set	5656 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17985	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.10% 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: CA, MG

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	0.46	0/2229	0.63	2/3028 (0.1%)
1	B	0.47	0/2229	0.60	1/3028 (0.0%)
1	C	0.46	0/2229	0.64	1/3028 (0.0%)
1	D	0.45	0/2229	0.63	0/3028
1	E	0.44	0/2229	0.59	0/3028
1	F	0.48	0/2229	0.64	1/3028 (0.0%)
1	G	0.42	0/2229	0.60	1/3028 (0.0%)
1	H	0.43	0/2229	0.64	2/3028 (0.1%)
All	All	0.45	0/17832	0.62	8/24224 (0.0%)

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
1	C	0	1
1	E	0	1
1	F	0	3
1	H	0	1
All	All	0	7

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	295	THR	N-CA-C	7.50	131.24	111.00
1	C	295	THR	N-CA-C	6.78	129.30	111.00
1	F	295	THR	N-CA-C	6.38	128.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	295	THR	N-CA-C	5.83	126.73	111.00
1	A	294	ASP	C-N-CA	5.76	136.10	121.70
1	H	295	THR	N-CA-C	5.60	126.13	111.00
1	H	296	GLU	C-N-CA	5.36	135.11	121.70
1	G	295	THR	N-CA-C	5.30	125.32	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	THR	Peptide
1	C	295	THR	Peptide
1	E	295	THR	Peptide
1	F	295	THR	Peptide
1	F	296	GLU	Peptide
1	F	297	HIS	Peptide
1	H	297	HIS	Peptide

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	2181	0	2138	27	0
1	B	2181	0	2139	44	0
1	C	2181	0	2139	24	0
1	D	2181	0	2138	26	0
1	E	2181	0	2139	36	0
1	F	2181	0	2139	38	0
1	G	2181	0	2138	34	0
1	H	2181	0	2138	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
4	A	58	0	0	2	0
4	B	65	0	0	6	0
4	C	80	0	0	3	0
4	D	55	0	0	7	0
4	E	58	0	0	1	0
4	F	71	0	0	3	0
4	G	56	0	0	0	0
4	H	62	0	0	8	0
All	All	17985	0	17108	256	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (256) 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:H:295:THR:HB	1:H:297:HIS:CD2	1.76	1.20
1:H:295:THR:HB	1:H:297:HIS:HD2	1.08	1.09
1:B:292:SER:HB3	1:B:295:THR:HG22	1.59	0.83
1:D:199:ARG:NH2	4:D:601:HOH:O	2.09	0.82
1:F:297:HIS:CG	1:F:298:GLY:H	1.99	0.81
1:H:304:GLU:OE2	4:H:601:HOH:O	2.01	0.77
1:G:304:GLU:HG2	1:G:333:MET:HE1	1.67	0.77
1:B:384:LYS:HZ2	1:A:293:VAL:H	1.33	0.76
1:B:374:SER:OG	4:B:601:HOH:O	2.05	0.75
1:F:297:HIS:CG	1:F:298:GLY:N	2.55	0.75
1:C:131:SER:OG	4:C:601:HOH:O	2.06	0.73
1:F:149:ARG:HH12	1:G:364:GLN:H	1.37	0.72
1:B:272:GLU:OE1	4:B:603:HOH:O	2.08	0.72
1:H:180:LEU:HD22	1:H:189:PRO:HG2	1.74	0.70
1:B:220:THR:OG1	4:B:602:HOH:O	2.06	0.69
1:C:161:ILE:HD12	1:C:228:PHE:HZ	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:309:ASP:OD2	4:F:601:HOH:O	2.11	0.68
1:D:260:PHE:HB2	1:D:307:THR:HG23	1.76	0.67
1:F:308:VAL:HG13	1:F:341:ILE:HD12	1.77	0.66
1:G:197:ILE:HG23	1:G:201:LEU:HD12	1.78	0.66
1:H:173:LYS:NZ	4:H:609:HOH:O	2.28	0.66
1:C:215:PHE:HB3	1:C:225:VAL:HG12	1.78	0.65
1:B:286:ASP:OD1	4:B:604:HOH:O	2.14	0.64
1:A:292:SER:OG	1:A:294:ASP:O	2.16	0.64
1:H:395:ARG:NH1	4:H:612:HOH:O	2.32	0.63
1:F:360:LYS:HB3	1:F:362:LYS:HZ2	1.64	0.63
1:D:384:LYS:NZ	4:D:603:HOH:O	2.31	0.62
1:D:407:PRO:HB2	1:D:409:VAL:HG22	1.82	0.62
1:H:192:GLN:NE2	4:H:602:HOH:O	2.13	0.62
1:C:131:SER:N	4:C:604:HOH:O	2.32	0.61
1:C:133:ILE:HD13	1:C:381:PRO:HB2	1.81	0.61
1:E:192:GLN:O	1:E:196:ILE:HG12	1.99	0.61
1:F:149:ARG:NH1	1:G:364:GLN:H	1.97	0.61
1:H:336:GLU:OE2	1:H:340:ASN:ND2	2.34	0.61
1:F:297:HIS:CD2	1:F:298:GLY:N	2.69	0.61
1:E:331:TRP:O	1:E:335:GLN:HG3	2.00	0.60
1:F:296:GLU:O	1:F:297:HIS:HB3	1.99	0.60
1:A:180:LEU:HD22	1:A:189:PRO:HG2	1.84	0.59
1:A:360:LYS:O	1:A:367:LYS:NZ	2.31	0.59
1:F:180:LEU:HD22	1:F:189:PRO:HG2	1.85	0.59
1:H:297:HIS:CD2	1:H:297:HIS:H	2.20	0.59
1:B:294:ASP:HA	1:B:295:THR:C	2.22	0.59
1:G:217:ASP:OD2	1:G:219:SER:OG	2.19	0.58
1:D:298:GLY:N	4:D:607:HOH:O	2.35	0.58
1:A:395:ARG:NH1	4:A:605:HOH:O	2.28	0.58
1:E:233:ARG:NH2	1:E:240:GLU:OE2	2.36	0.58
1:D:172:ALA:HA	1:D:177:ARG:HA	1.86	0.58
1:E:165:LYS:HB3	1:G:153:GLU:HG2	1.86	0.58
1:D:209:LEU:HD22	1:D:234:PHE:HB2	1.86	0.57
1:F:360:LYS:HE3	1:F:362:LYS:HE3	1.85	0.57
1:C:131:SER:N	4:C:608:HOH:O	2.36	0.57
1:C:209:LEU:HD22	1:C:234:PHE:HB2	1.86	0.57
1:G:166:SER:OG	1:G:286:ASP:OD2	2.23	0.57
1:C:157:LEU:HD23	1:C:280:VAL:HB	1.86	0.57
1:G:200:THR:HB	1:G:372:ALA:HB2	1.87	0.56
1:D:360:LYS:HD3	1:D:362:LYS:HE2	1.88	0.56
1:E:271:VAL:HG21	1:E:319:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:PRO:HA	1:F:407:PRO:HD2	1.88	0.56
1:A:161:ILE:HD12	1:A:228:PHE:HZ	1.70	0.56
1:B:294:ASP:HA	1:B:295:THR:O	2.06	0.55
1:D:295:THR:HG22	4:D:607:HOH:O	2.06	0.55
1:F:138:SER:O	4:F:602:HOH:O	2.17	0.55
1:F:360:LYS:HB3	1:F:362:LYS:NZ	2.21	0.55
1:E:157:LEU:HD23	1:E:280:VAL:HB	1.88	0.55
1:B:364:GLN:O	1:B:368:GLU:HG3	2.07	0.54
1:C:337:PHE:HA	1:C:341:ILE:HD11	1.89	0.54
1:D:362:LYS:HZ2	1:D:367:LYS:HA	1.73	0.54
1:D:336:GLU:HG3	1:D:340:ASN:HB3	1.89	0.53
1:B:300:LEU:HD12	1:B:305:GLN:OE1	2.08	0.53
1:A:362:LYS:NZ	1:A:366:ARG:HD2	2.23	0.53
1:F:360:LYS:HE3	1:F:362:LYS:CE	2.39	0.53
1:B:217:ASP:HB3	4:B:602:HOH:O	2.08	0.53
1:H:231:GLU:N	4:H:604:HOH:O	2.21	0.53
1:H:154:SER:OG	1:H:206:GLU:OE1	2.16	0.53
1:D:299:ARG:NH2	4:D:612:HOH:O	2.41	0.53
1:G:145:GLU:O	1:G:149:ARG:HG3	2.10	0.52
1:B:291:ARG:NH2	1:B:333:MET:SD	2.83	0.52
1:D:293:VAL:O	1:D:294:ASP:HB2	2.09	0.52
1:F:360:LYS:HG2	1:F:361:ASN:H	1.75	0.52
1:B:217:ASP:OD1	4:B:605:HOH:O	2.19	0.51
1:B:382:GLN:O	1:B:386:THR:HG23	2.11	0.51
1:B:384:LYS:NZ	1:A:293:VAL:HG22	2.26	0.51
1:H:297:HIS:CD2	1:H:297:HIS:N	2.79	0.51
1:D:244:ARG:CZ	1:D:248:ILE:HD11	2.41	0.51
1:H:196:ILE:HD12	1:H:368:GLU:HG2	1.91	0.51
1:A:133:ILE:HD12	1:A:347:ASP:HB3	1.92	0.51
1:B:209:LEU:HD22	1:B:234:PHE:HB2	1.93	0.51
1:D:212:CYS:N	4:D:611:HOH:O	2.38	0.51
1:F:248:ILE:HG12	1:F:409:VAL:HG11	1.92	0.50
1:G:139:SER:OG	1:G:142:GLN:HG3	2.11	0.50
1:G:358:MET:HA	1:G:367:LYS:HD3	1.93	0.50
1:H:133:ILE:HD13	1:H:381:PRO:HB2	1.92	0.50
1:G:382:GLN:O	1:G:386:THR:HG23	2.12	0.50
1:F:358:MET:O	1:F:367:LYS:HE3	2.12	0.50
1:H:363:ASP:O	1:H:367:LYS:HG3	2.11	0.50
1:B:379:ILE:HB	1:B:380:PRO:HD3	1.94	0.50
1:E:378:GLU:O	1:E:381:PRO:HD2	2.11	0.50
1:F:137:TYR:CD2	1:F:143:VAL:HG12	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:231:GLU:O	4:H:603:HOH:O	2.20	0.50
1:B:133:ILE:HD13	1:B:381:PRO:HB2	1.94	0.50
1:D:180:LEU:HD22	1:D:189:PRO:HG2	1.94	0.49
1:G:191:GLU:OE2	1:G:246:ARG:HD2	2.12	0.49
1:C:164:THR:HG22	1:C:216:GLY:HA3	1.93	0.49
1:G:378:GLU:O	1:G:381:PRO:HD2	2.12	0.49
1:B:266:MET:HE2	1:B:402:ARG:HG2	1.93	0.49
1:G:265:GLU:OE1	1:G:402:ARG:NH2	2.36	0.49
1:H:260:PHE:HB2	1:H:307:THR:HG23	1.95	0.49
1:B:295:THR:HG1	1:B:297:HIS:HB2	1.77	0.49
1:B:362:LYS:O	1:B:367:LYS:NZ	2.37	0.49
1:A:192:GLN:O	1:A:196:ILE:HG12	2.13	0.48
1:F:365:SER:O	1:F:369:THR:HG23	2.13	0.48
1:C:139:SER:OG	1:C:142:GLN:HG3	2.13	0.48
1:F:133:ILE:HD13	1:F:381:PRO:HB2	1.95	0.48
1:G:230:PRO:HA	1:G:407:PRO:HD2	1.96	0.48
1:C:292:SER:HB3	1:C:295:THR:HG22	1.95	0.48
1:E:260:PHE:HB2	1:E:307:THR:HG23	1.95	0.48
1:G:161:ILE:HD12	1:G:228:PHE:HZ	1.79	0.48
1:E:133:ILE:HG13	1:E:347:ASP:HB3	1.94	0.48
1:E:364:GLN:O	1:E:368:GLU:HG3	2.13	0.48
1:F:341:ILE:O	1:F:344:ARG:HG2	2.14	0.48
1:G:261:ALA:HB3	1:G:262:PRO:HD3	1.95	0.48
1:E:292:SER:HB3	1:E:295:THR:OG1	2.13	0.48
1:A:267:ALA:HB2	1:A:281:LEU:HD22	1.96	0.48
1:H:297:HIS:HB3	1:H:299:ARG:N	2.29	0.47
1:A:308:VAL:O	1:A:312:VAL:HG23	2.14	0.47
1:D:211:PRO:HB3	1:D:234:PHE:CE1	2.49	0.47
1:B:272:GLU:OE2	1:B:395:ARG:HG3	2.14	0.47
1:A:164:THR:HG22	1:A:216:GLY:HA3	1.95	0.47
1:H:200:THR:N	4:H:613:HOH:O	2.47	0.47
1:H:209:LEU:HD22	1:H:234:PHE:HB2	1.95	0.47
1:B:291:ARG:HH21	1:B:333:MET:HB2	1.79	0.47
1:C:196:ILE:HG23	1:C:368:GLU:HG2	1.97	0.47
1:E:131:SER:OG	1:E:132:LYS:N	2.37	0.47
1:H:233:ARG:N	4:H:603:HOH:O	2.47	0.47
1:H:360:LYS:HB2	1:H:362:LYS:HE3	1.96	0.47
1:B:306:LYS:NZ	1:C:393:GLY:O	2.48	0.46
1:B:341:ILE:O	1:B:344:ARG:HG2	2.16	0.46
1:H:294:ASP:HA	1:H:295:THR:C	2.35	0.46
1:A:295:THR:CG2	1:A:297:HIS:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:LEU:O	1:F:319:LEU:N	2.48	0.46
1:A:191:GLU:OE1	1:A:246:ARG:HD3	2.14	0.46
1:E:275:SER:HB2	1:E:395:ARG:HD2	1.96	0.46
1:F:175:PHE:CZ	1:F:188:ASN:HA	2.50	0.46
1:E:294:ASP:HA	1:E:295:THR:O	2.16	0.46
1:D:296:GLU:O	1:D:298:GLY:N	2.49	0.46
1:E:289:VAL:HB	1:E:333:MET:SD	2.56	0.46
1:E:175:PHE:CZ	1:E:188:ASN:HA	2.51	0.46
1:F:402:ARG:HB2	4:F:626:HOH:O	2.16	0.45
1:A:172:ALA:HA	1:A:177:ARG:HA	1.99	0.45
1:D:133:ILE:HD13	1:D:381:PRO:HB2	1.98	0.45
1:E:395:ARG:HE	1:E:395:ARG:HB3	1.60	0.45
1:F:212:CYS:SG	1:F:241:VAL:HG22	2.57	0.45
1:B:183:LEU:HD11	1:B:249:VAL:HG13	1.97	0.45
1:A:262:PRO:HG2	4:A:628:HOH:O	2.16	0.45
1:A:260:PHE:O	1:A:264:ILE:HG13	2.15	0.45
1:A:323:LEU:HG	1:A:334:MET:SD	2.57	0.45
1:E:195:THR:O	1:E:199:ARG:HG2	2.16	0.45
1:C:297:HIS:HB3	1:C:299:ARG:HB3	1.98	0.45
1:G:361:ASN:OD1	1:G:361:ASN:N	2.50	0.45
1:B:166:SER:HA	1:B:169:TRP:CZ2	2.51	0.45
1:B:296:GLU:O	1:B:298:GLY:N	2.50	0.45
1:G:212:CYS:SG	1:G:241:VAL:HG22	2.57	0.45
1:H:181:HIS:HB3	1:H:249:VAL:HG21	1.97	0.45
1:G:131:SER:C	1:G:132:LYS:HD3	2.37	0.45
1:F:323:LEU:HG	1:F:334:MET:SD	2.56	0.45
1:G:294:ASP:HA	1:G:295:THR:O	2.17	0.45
1:D:300:LEU:HD12	1:D:304:GLU:HB3	1.98	0.44
1:B:384:LYS:HZ2	1:A:293:VAL:HG22	1.82	0.44
1:D:299:ARG:N	4:D:607:HOH:O	2.49	0.44
1:H:143:VAL:HG11	1:H:376:LEU:HB3	1.99	0.44
1:H:261:ALA:HB3	1:H:262:PRO:HD3	2.00	0.44
1:A:183:LEU:HD23	1:A:183:LEU:HA	1.74	0.44
1:G:307:THR:O	1:G:311:ILE:HG13	2.17	0.44
1:G:407:PRO:HB2	1:G:409:VAL:HG22	1.99	0.44
1:B:384:LYS:HD3	1:B:384:LYS:HA	1.53	0.44
1:A:296:GLU:CD	1:A:296:GLU:O	2.56	0.44
1:H:266:MET:O	1:H:270:VAL:HG23	2.18	0.44
1:B:266:MET:CE	1:B:402:ARG:HG2	2.47	0.44
1:D:297:HIS:HB3	1:D:299:ARG:HB3	2.00	0.44
1:E:296:GLU:C	1:E:298:GLY:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:THR:O	1:B:311:ILE:HG13	2.16	0.44
1:C:261:ALA:HB3	1:C:262:PRO:HD3	1.99	0.44
1:H:294:ASP:HA	1:H:295:THR:O	2.17	0.43
1:C:211:PRO:HB3	1:C:234:PHE:CE1	2.53	0.43
1:F:318:PRO:HB3	1:F:386:THR:HB	2.01	0.43
1:B:195:THR:HG22	1:B:199:ARG:HD2	2.01	0.43
1:A:380:PRO:O	1:A:384:LYS:HD3	2.19	0.43
1:C:192:GLN:O	1:C:196:ILE:HG12	2.18	0.43
1:E:133:ILE:HD13	1:E:381:PRO:HB2	2.00	0.43
1:D:283:ILE:HB	1:D:323:LEU:HD22	2.01	0.43
1:H:147:LEU:HG	1:H:380:PRO:HG3	2.01	0.43
1:F:297:HIS:O	1:F:299:ARG:N	2.47	0.43
1:F:378:GLU:O	1:F:381:PRO:HD2	2.19	0.43
1:E:306:LYS:NZ	1:G:393:GLY:O	2.52	0.43
1:H:244:ARG:O	1:H:248:ILE:HG13	2.19	0.43
1:E:388:GLU:O	1:H:299:ARG:NH2	2.52	0.42
1:D:215:PHE:HB3	1:D:225:VAL:HG12	2.01	0.42
1:E:188:ASN:OD1	1:E:191:GLU:HG3	2.20	0.42
1:E:215:PHE:HB3	1:E:225:VAL:HG12	2.00	0.42
1:G:341:ILE:O	1:G:344:ARG:HG2	2.19	0.42
1:C:292:SER:O	1:C:295:THR:HG23	2.20	0.42
1:E:131:SER:N	4:E:612:HOH:O	2.52	0.42
1:E:341:ILE:O	1:E:344:ARG:HG2	2.20	0.42
1:F:187:PRO:O	1:F:192:GLN:NE2	2.36	0.42
1:B:155:SER:OG	1:B:204:PHE:O	2.36	0.42
1:B:410:GLN:HA	1:B:410:GLN:OE1	2.20	0.42
1:A:294:ASP:OD1	1:A:294:ASP:N	2.52	0.42
1:C:382:GLN:O	1:C:386:THR:HG23	2.19	0.42
1:B:192:GLN:O	1:B:196:ILE:HG12	2.19	0.42
1:F:196:ILE:HD12	1:F:368:GLU:HG2	2.02	0.42
1:F:285:ALA:O	1:F:325:GLY:HA2	2.19	0.42
1:C:157:LEU:HD12	1:C:205:ASP:HB2	2.02	0.42
1:G:248:ILE:HG12	1:G:409:VAL:HG11	2.01	0.42
1:H:295:THR:CB	1:H:297:HIS:HD2	2.01	0.42
1:H:297:HIS:HB3	1:H:299:ARG:H	1.85	0.42
1:H:380:PRO:HB2	1:H:381:PRO:HD3	2.02	0.42
1:E:264:ILE:O	1:E:268:MET:HG3	2.20	0.41
1:G:133:ILE:HG13	1:G:347:ASP:HB3	2.02	0.41
1:G:180:LEU:HD22	1:G:189:PRO:HG2	2.02	0.41
1:G:181:HIS:HB3	1:G:249:VAL:HG21	2.02	0.41
1:E:294:ASP:HA	1:E:295:THR:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:363:ASP:HB3	1:G:366:ARG:HD3	2.01	0.41
1:E:382:GLN:O	1:E:386:THR:HG23	2.20	0.41
1:H:407:PRO:HB2	1:H:409:VAL:HG22	2.03	0.41
1:B:299:ARG:NH2	1:C:388:GLU:O	2.54	0.41
1:F:225:VAL:HG21	1:F:266:MET:HG2	2.03	0.41
1:H:336:GLU:CD	1:H:340:ASN:HD22	2.23	0.41
1:C:292:SER:HB3	1:C:295:THR:CG2	2.50	0.41
1:E:166:SER:HA	1:E:169:TRP:CE2	2.55	0.41
1:F:192:GLN:O	1:F:196:ILE:HG12	2.20	0.41
1:G:316:THR:O	1:G:317:LEU:HD23	2.20	0.41
1:E:274:SER:O	1:E:277:GLN:HG2	2.20	0.41
1:B:249:VAL:HG13	1:B:250:PRO:HD3	2.03	0.41
1:B:362:LYS:H	1:B:367:LYS:HZ1	1.69	0.41
1:A:197:ILE:HD13	1:A:282:VAL:HG11	2.03	0.41
1:A:341:ILE:O	1:A:344:ARG:HG2	2.21	0.41
1:E:164:THR:HB	1:G:153:GLU:OE2	2.21	0.41
1:E:229:TYR:HA	1:E:230:PRO:HD3	1.96	0.41
1:E:407:PRO:HA	1:E:408:PRO:HD3	1.93	0.41
1:G:192:GLN:O	1:G:196:ILE:HG12	2.21	0.41
1:B:220:THR:HG22	1:B:405:LEU:HD12	2.03	0.41
1:H:297:HIS:HB3	1:H:299:ARG:O	2.21	0.41
1:B:347:ASP:O	1:B:382:GLN:HG2	2.21	0.40
1:A:382:GLN:O	1:A:386:THR:HG23	2.21	0.40
1:F:131:SER:O	1:F:347:ASP:HB2	2.20	0.40
1:F:166:SER:OG	1:F:286:ASP:OD2	2.38	0.40
1:B:292:SER:HB3	1:B:295:THR:CG2	2.42	0.40
1:D:158:ILE:HD11	1:D:270:VAL:HG11	2.03	0.40
1:E:358:MET:HA	1:E:367:LYS:HD3	2.03	0.40
1:B:157:LEU:HD23	1:B:280:VAL:HB	2.03	0.40
1:H:392:LEU:HD12	1:H:392:LEU:HA	1.89	0.40
1:B:279:HIS:O	1:B:319:LEU:HD12	2.22	0.40
1:D:382:GLN:O	1:D:386:THR:HG23	2.22	0.40
1:C:244:ARG:NE	1:C:248:ILE:HD11	2.36	0.40
1:E:389:LEU:HA	1:E:389:LEU:HD23	1.90	0.40
1:F:274:SER:O	1:F:277:GLN:HG2	2.22	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	278/301 (92%)	266 (96%)	10 (4%)	2 (1%)	22	32
1	B	278/301 (92%)	260 (94%)	14 (5%)	4 (1%)	11	15
1	C	278/301 (92%)	265 (95%)	10 (4%)	3 (1%)	14	20
1	D	278/301 (92%)	266 (96%)	8 (3%)	4 (1%)	11	15
1	E	278/301 (92%)	261 (94%)	15 (5%)	2 (1%)	22	32
1	F	278/301 (92%)	261 (94%)	13 (5%)	4 (1%)	11	15
1	G	278/301 (92%)	259 (93%)	16 (6%)	3 (1%)	14	20
1	H	278/301 (92%)	260 (94%)	14 (5%)	4 (1%)	11	15
All	All	2224/2408 (92%)	2098 (94%)	100 (4%)	26 (1%)	13	19

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	295	THR
1	A	295	THR
1	C	230	PRO
1	C	295	THR
1	D	297	HIS
1	F	295	THR
1	F	297	HIS
1	F	298	GLY
1	G	295	THR
1	H	295	THR
1	H	297	HIS
1	B	297	HIS
1	C	185	ASN
1	E	297	HIS
1	F	361	ASN
1	B	230	PRO
1	D	294	ASP

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Mol	Chain	Res	Type
1	H	233	ARG
1	D	230	PRO
1	E	230	PRO
1	G	296	GLU
1	H	206	GLU
1	B	360	LYS
1	G	172	ALA
1	D	409	VAL
1	A	230	PRO

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	242/259 (93%)	239 (99%)	3 (1%)	71	85
1	B	242/259 (93%)	239 (99%)	3 (1%)	71	85
1	C	242/259 (93%)	237 (98%)	5 (2%)	53	72
1	D	242/259 (93%)	240 (99%)	2 (1%)	81	91
1	E	242/259 (93%)	237 (98%)	5 (2%)	53	72
1	F	242/259 (93%)	238 (98%)	4 (2%)	60	78
1	G	242/259 (93%)	242 (100%)	0	100	100
1	H	242/259 (93%)	239 (99%)	3 (1%)	71	85
All	All	1936/2072 (93%)	1911 (99%)	25 (1%)	69	84

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	217	ASP
1	B	296	GLU
1	B	363	ASP
1	A	219	SER
1	A	293	VAL
1	A	294	ASP

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Mol	Chain	Res	Type
1	C	134	SER
1	C	208	ASN
1	C	295	THR
1	C	374	SER
1	C	410	GLN
1	D	231	GLU
1	D	292	SER
1	E	233	ARG
1	E	291	ARG
1	E	299	ARG
1	E	323	LEU
1	E	361	ASN
1	F	295	THR
1	F	299	ARG
1	F	362	LYS
1	F	370	GLU
1	H	233	ARG
1	H	296	GLU
1	H	297	HIS

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

Mol	Chain	Res	Type
1	B	273	GLN
1	D	236	ASN
1	F	297	HIS
1	H	297	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 32 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	280/301 (93%)	0.07	9 (3%)	47	46	28, 38, 63, 91	0
1	B	280/301 (93%)	0.15	8 (2%)	51	50	30, 40, 66, 93	0
1	C	280/301 (93%)	0.03	6 (2%)	63	61	30, 39, 57, 93	0
1	D	280/301 (93%)	0.10	8 (2%)	51	50	29, 39, 63, 92	0
1	E	280/301 (93%)	0.04	5 (1%)	68	66	30, 40, 59, 100	0
1	F	280/301 (93%)	0.13	11 (3%)	39	38	29, 41, 64, 87	0
1	G	280/301 (93%)	0.11	8 (2%)	51	50	32, 43, 66, 92	0
1	H	280/301 (93%)	0.09	9 (3%)	47	46	30, 41, 67, 95	0
All	All	2240/2408 (93%)	0.09	64 (2%)	51	50	28, 40, 65, 100	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	297	HIS	9.0
1	B	297	HIS	8.3
1	B	361	ASN	7.3
1	E	297	HIS	6.5
1	F	361	ASN	6.4
1	C	294	ASP	5.8
1	C	298	GLY	5.7
1	D	232	GLY	5.5
1	G	297	HIS	5.5
1	E	294	ASP	5.2
1	A	232	GLY	5.1
1	D	297	HIS	4.9
1	E	293	VAL	4.8
1	G	232	GLY	4.6
1	A	361	ASN	4.6
1	F	410	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	H	294	ASP	4.2
1	H	361	ASN	4.2
1	B	295	THR	4.2
1	B	410	GLN	3.8
1	D	294	ASP	3.7
1	G	295	THR	3.7
1	F	294	ASP	3.6
1	H	297	HIS	3.5
1	C	295	THR	3.5
1	F	298	GLY	3.3
1	F	293	VAL	3.3
1	F	360	LYS	3.2
1	F	299	ARG	3.2
1	H	232	GLY	3.2
1	H	298	GLY	3.2
1	B	294	ASP	3.1
1	G	294	ASP	3.1
1	F	232	GLY	3.1
1	E	295	THR	3.1
1	H	295	THR	3.0
1	C	299	ARG	2.9
1	E	232	GLY	2.8
1	F	295	THR	2.8
1	B	409	VAL	2.7
1	A	297	HIS	2.7
1	C	410	GLN	2.7
1	D	298	GLY	2.5
1	G	186	THR	2.4
1	F	297	HIS	2.4
1	H	293	VAL	2.4
1	D	293	VAL	2.3
1	B	131	SER	2.3
1	H	359	SER	2.3
1	A	298	GLY	2.2
1	G	361	ASN	2.2
1	D	410	GLN	2.2
1	A	230	PRO	2.2
1	A	294	ASP	2.2
1	D	295	THR	2.2
1	A	410	GLN	2.2
1	D	149	ARG	2.2
1	B	185	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	358	MET	2.1
1	A	364	GLN	2.1
1	G	298	GLY	2.1
1	H	300	LEU	2.0
1	G	236	ASN	2.0
1	A	131	SER	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 monosaccharides 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
3	CA	D	502	1/1	0.90	0.05	57,57,57,57	0
3	CA	F	504	1/1	0.91	0.06	59,59,59,59	0
2	MG	F	501	1/1	0.92	0.19	28,28,28,28	0
3	CA	C	502	1/1	0.94	0.09	45,45,45,45	0
2	MG	C	501	1/1	0.95	0.12	31,31,31,31	0
3	CA	A	502	1/1	0.95	0.10	41,41,41,41	0
3	CA	E	503	1/1	0.95	0.08	53,53,53,53	0
3	CA	A	504	1/1	0.95	0.05	56,56,56,56	0
2	MG	E	501	1/1	0.96	0.10	34,34,34,34	0
3	CA	F	502	1/1	0.96	0.04	38,38,38,38	0
3	CA	F	503	1/1	0.96	0.08	42,42,42,42	0
3	CA	B	502	1/1	0.96	0.05	54,54,54,54	0
2	MG	A	501	1/1	0.97	0.14	34,34,34,34	0
2	MG	D	501	1/1	0.97	0.18	31,31,31,31	0
3	CA	E	504	1/1	0.97	0.12	40,40,40,40	0
3	CA	G	503	1/1	0.97	0.12	42,42,42,42	0
3	CA	H	502	1/1	0.97	0.07	52,52,52,52	0

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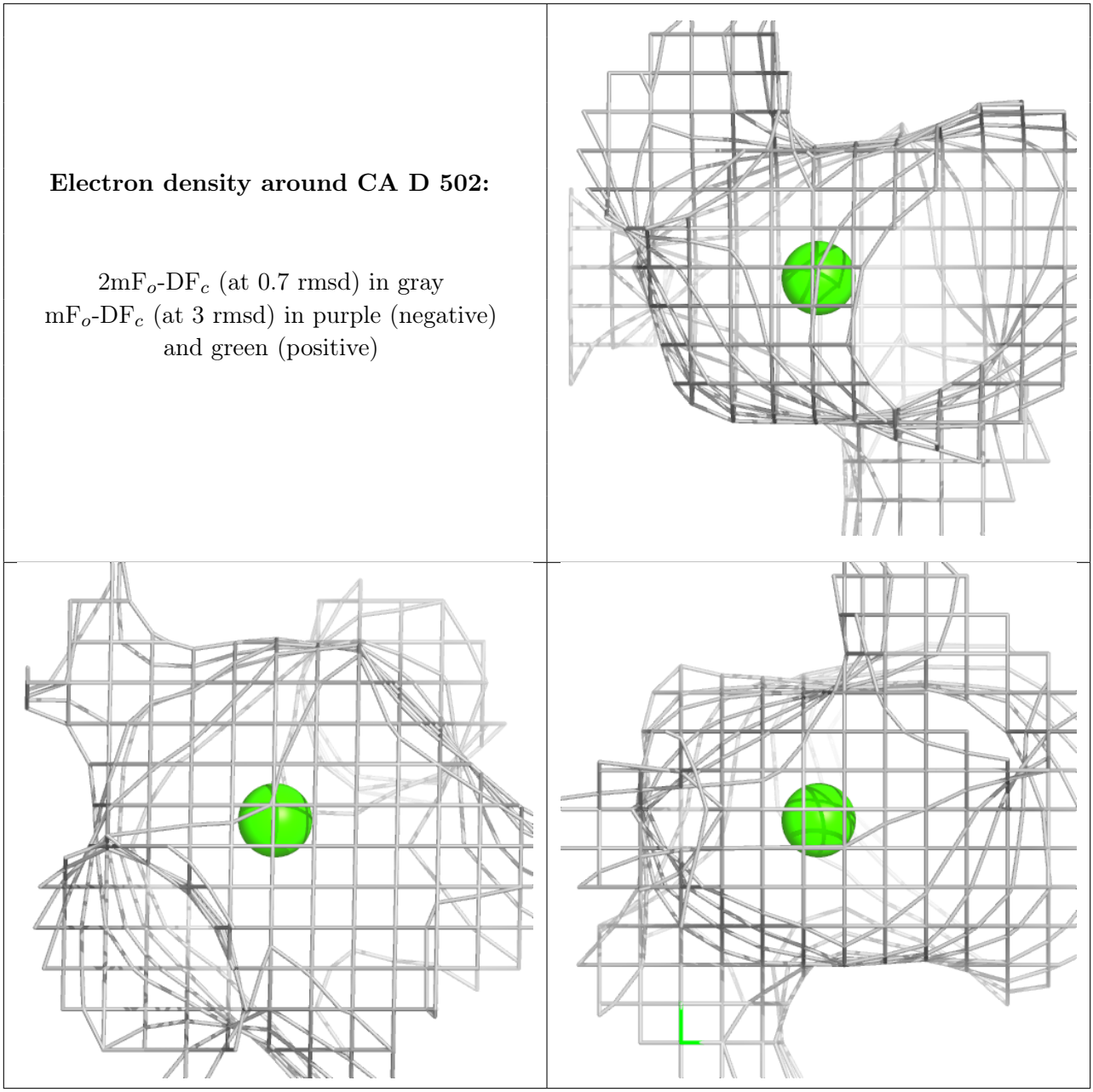
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	C	504	1/1	0.98	0.12	40,40,40,40	0
2	MG	H	501	1/1	0.98	0.15	28,28,28,28	0
3	CA	D	504	1/1	0.98	0.11	35,35,35,35	0
3	CA	G	502	1/1	0.98	0.11	37,37,37,37	0
2	MG	B	501	1/1	0.98	0.14	24,24,24,24	0
3	CA	G	504	1/1	0.98	0.09	51,51,51,51	0
3	CA	B	503	1/1	0.98	0.11	34,34,34,34	0
3	CA	H	503	1/1	0.98	0.11	37,37,37,37	0
2	MG	G	501	1/1	0.99	0.23	36,36,36,36	0
3	CA	E	502	1/1	0.99	0.10	28,28,28,28	0
3	CA	C	503	1/1	0.99	0.16	33,33,33,33	0
3	CA	A	503	1/1	0.99	0.12	31,31,31,31	0
3	CA	B	504	1/1	0.99	0.11	41,41,41,41	0
3	CA	D	503	1/1	0.99	0.14	36,36,36,36	0
3	CA	H	504	1/1	0.99	0.07	43,43,43,43	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.

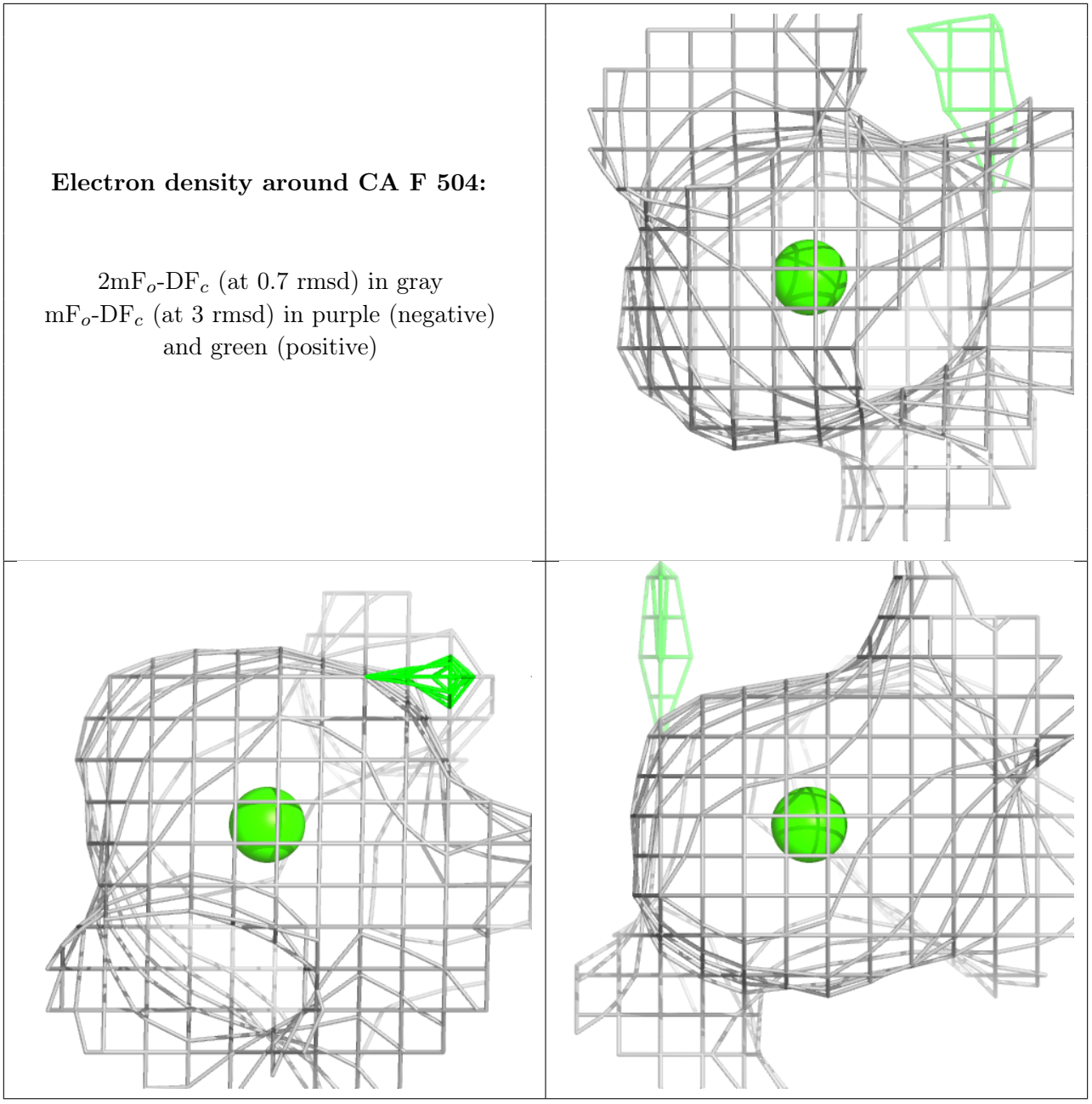
Electron density around CA D 502:

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



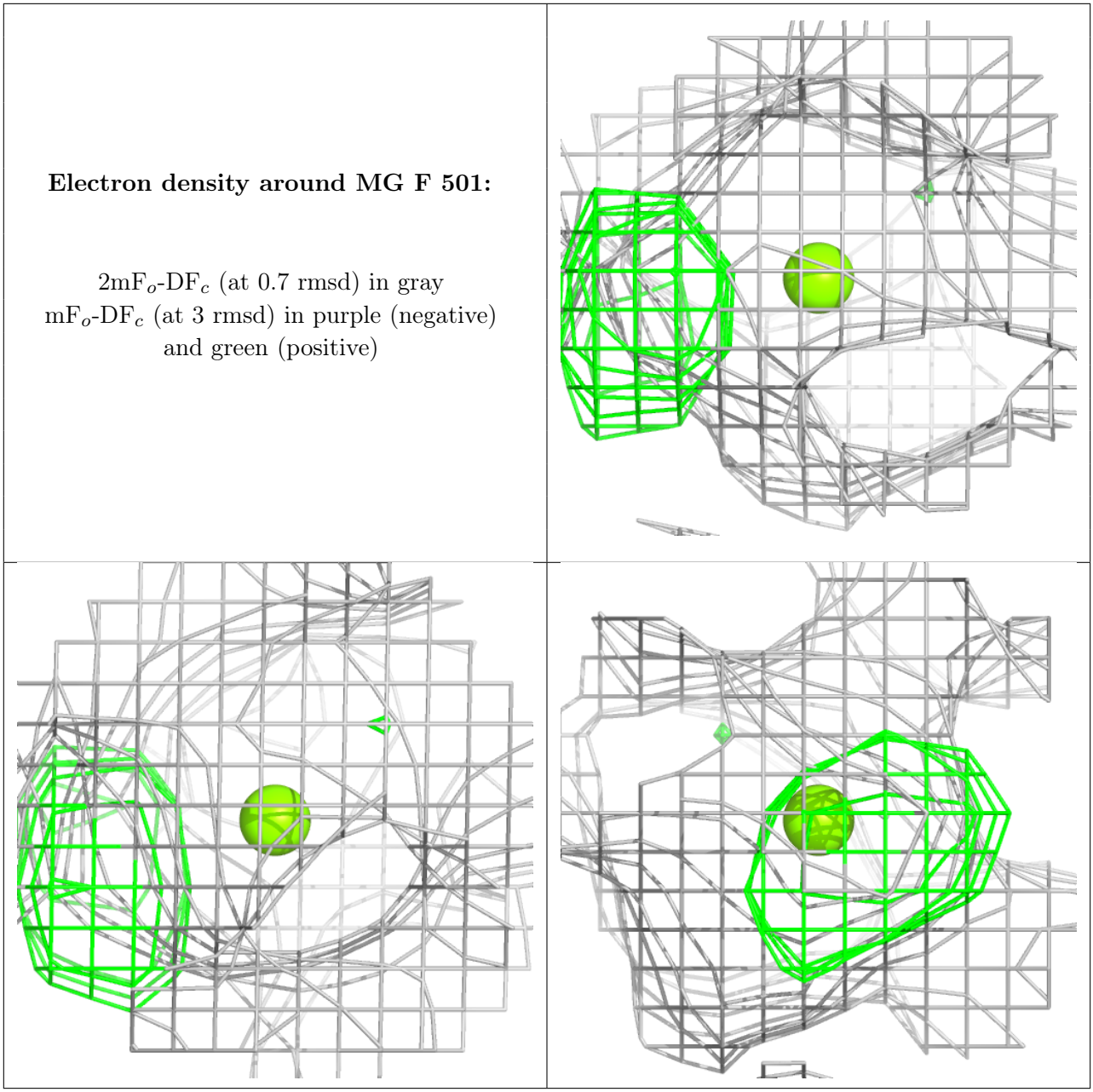
Electron density around CA F 504:

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



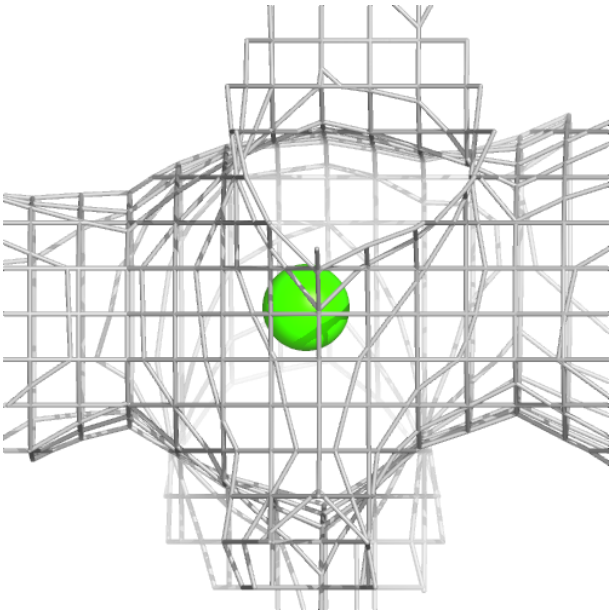
Electron density around MG F 501:

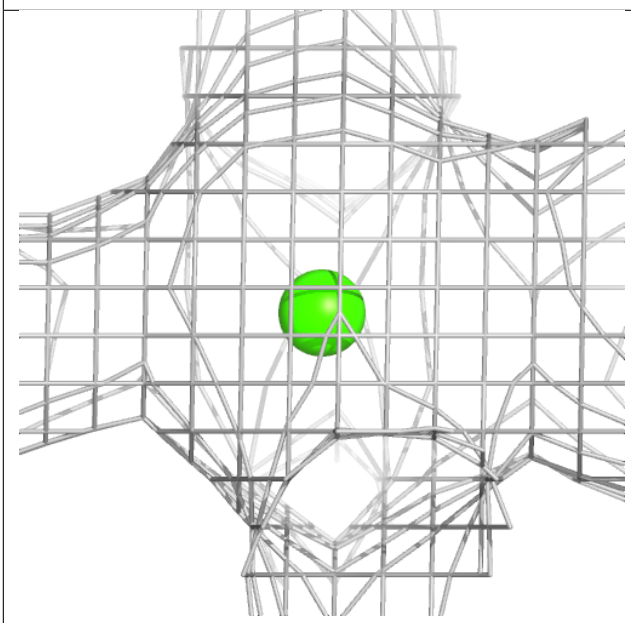
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

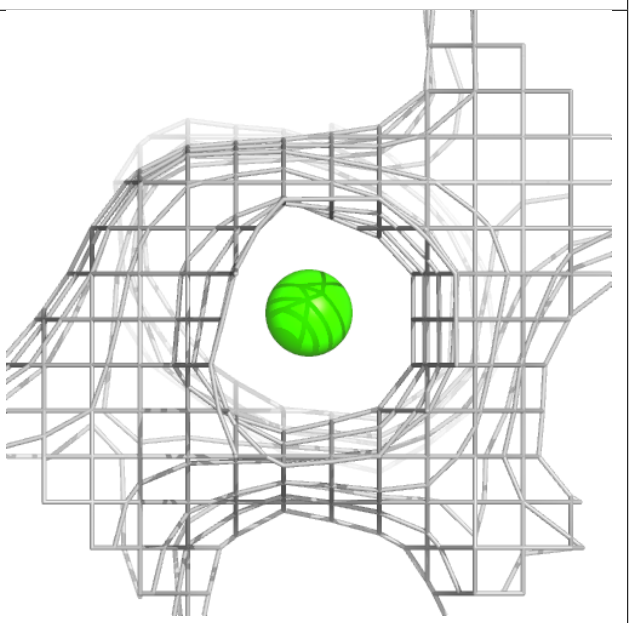


Electron density around CA C 502:

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

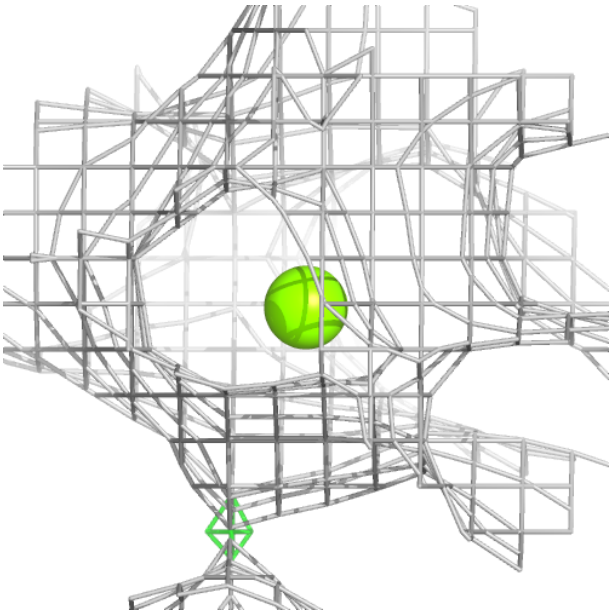


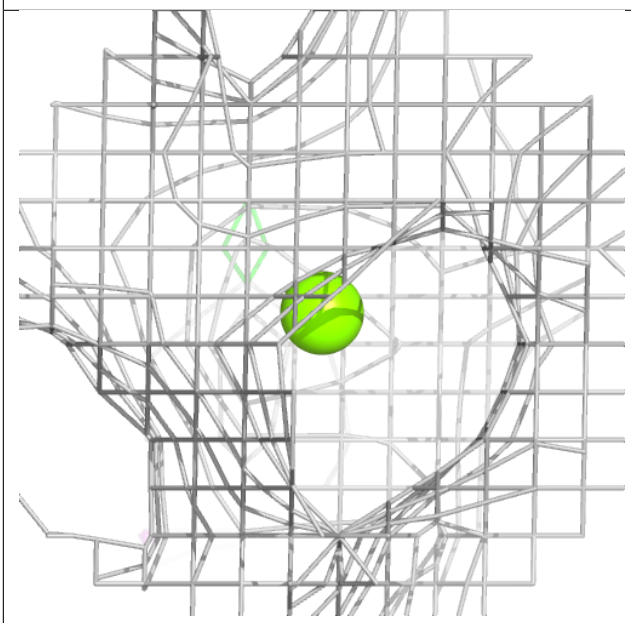


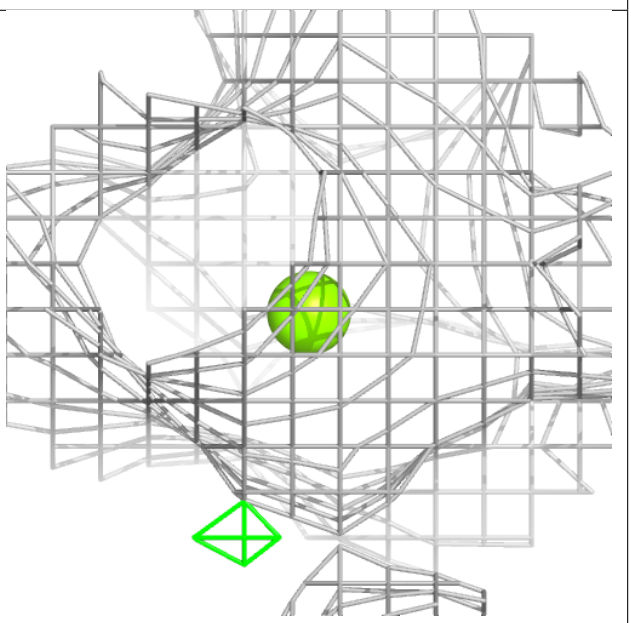


Electron density around MG C 501:

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

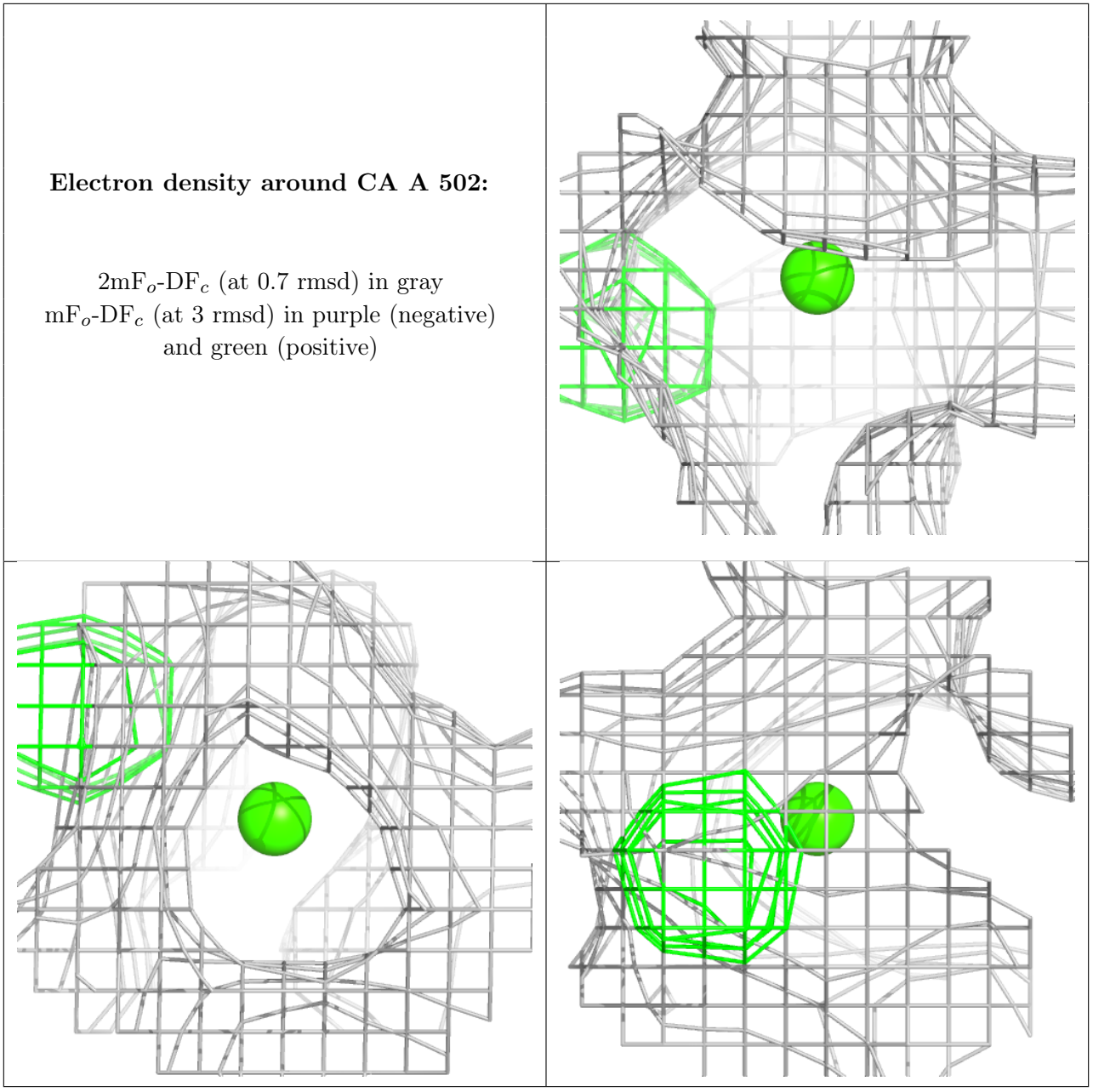






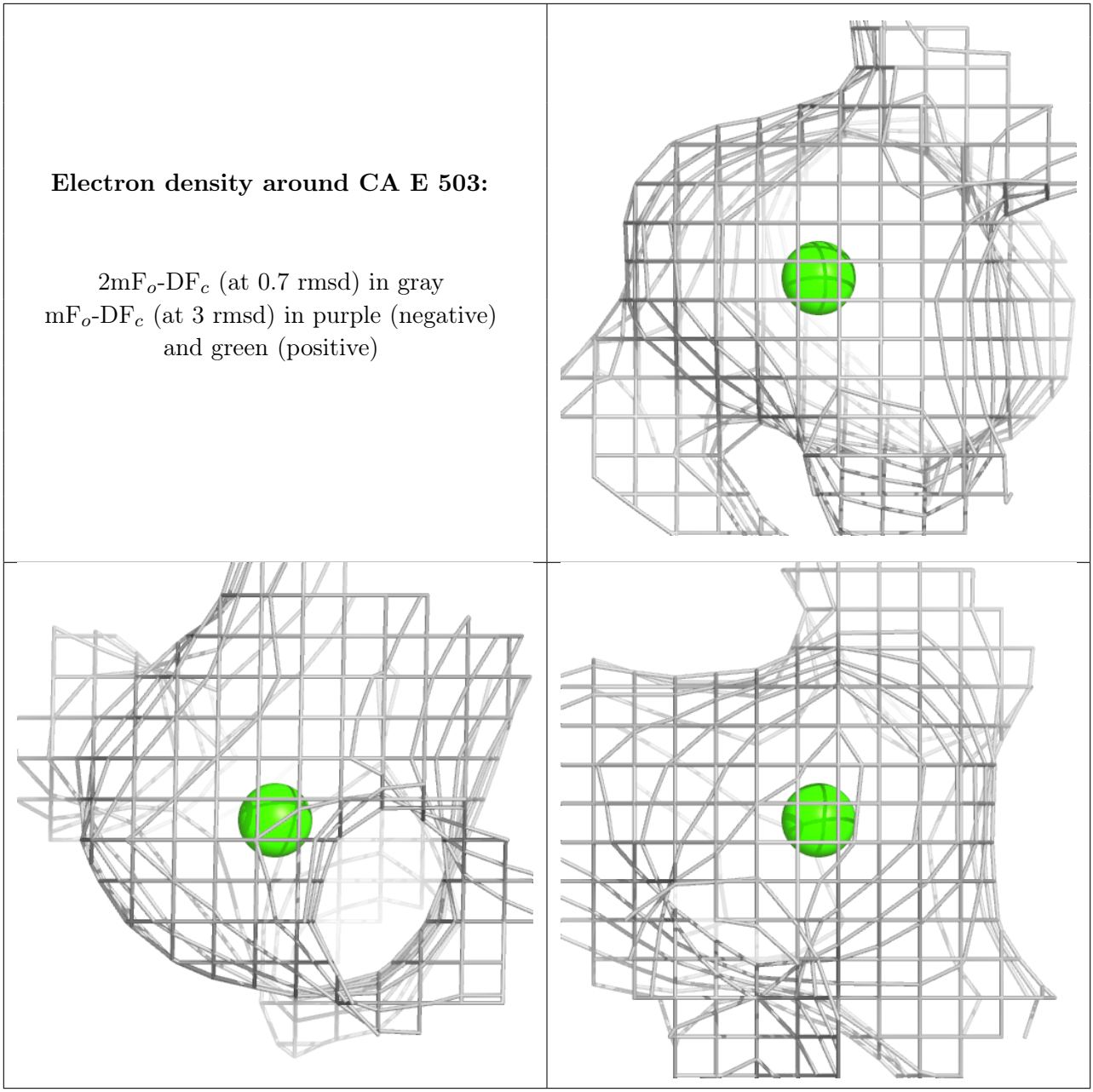
Electron density around CA A 502:

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



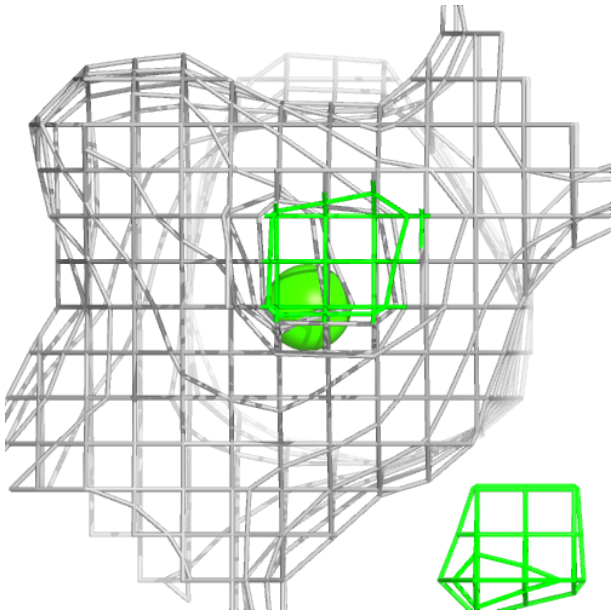
Electron density around CA E 503:

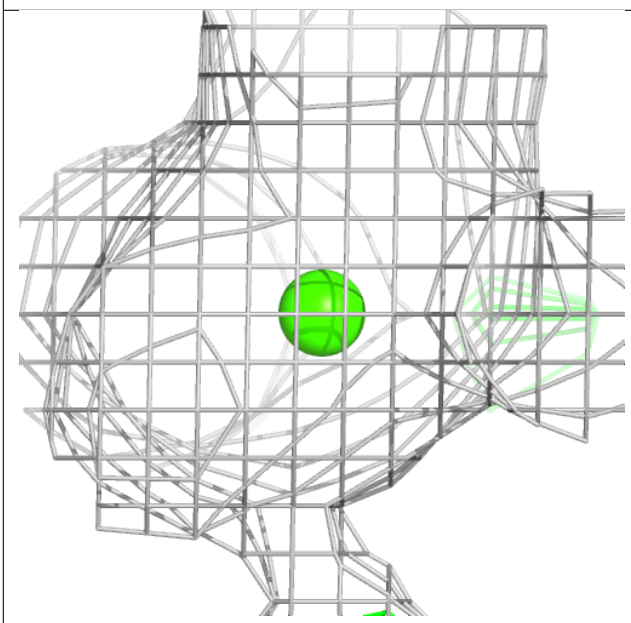
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

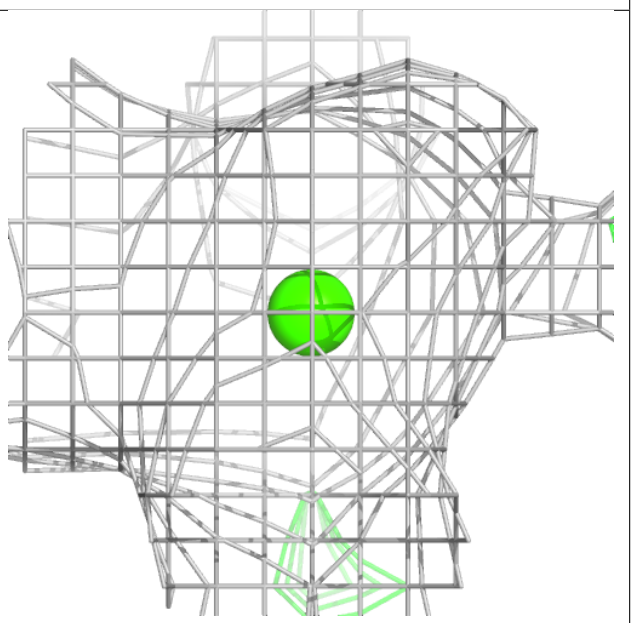


Electron density around CA A 504:

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

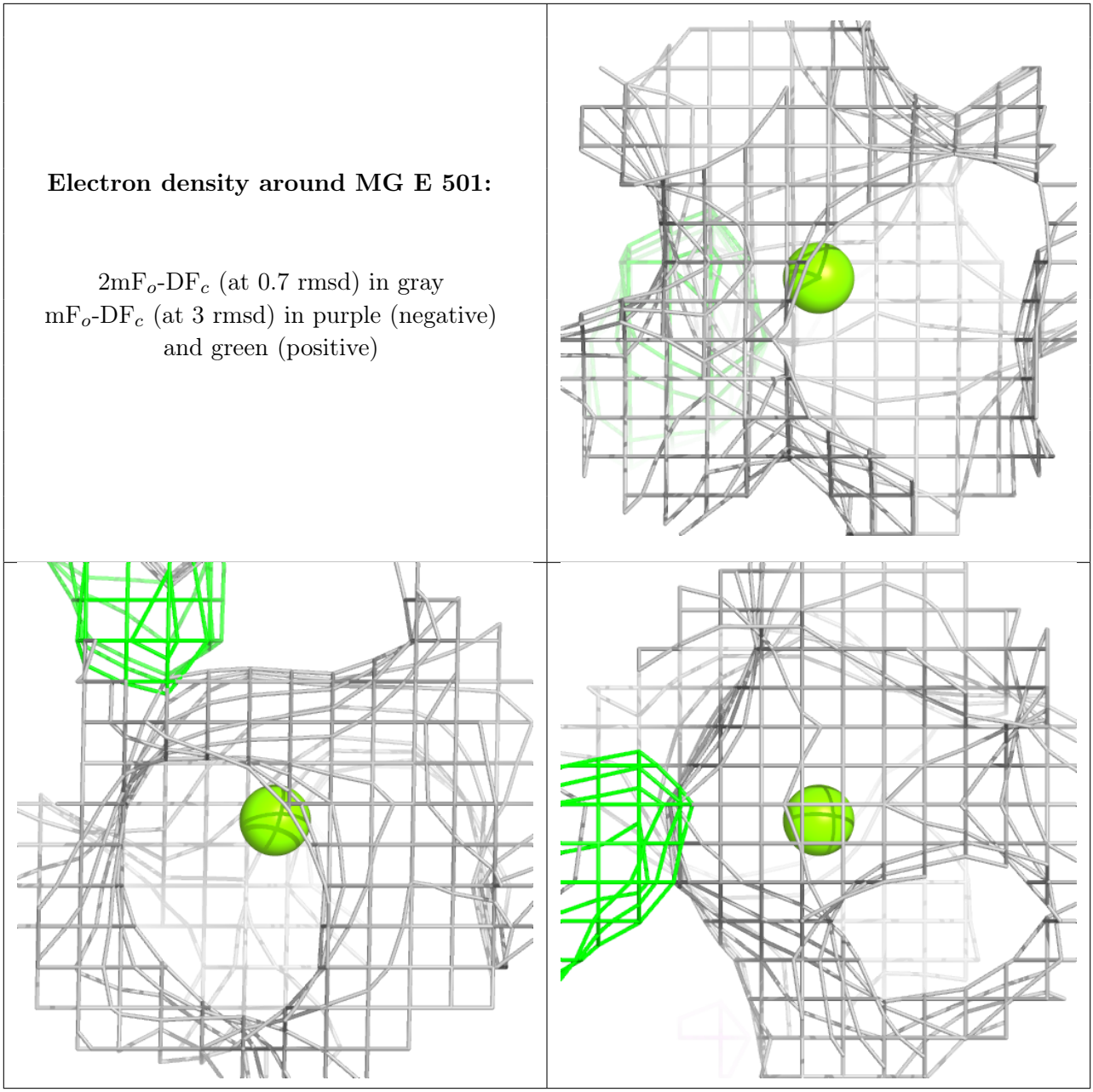






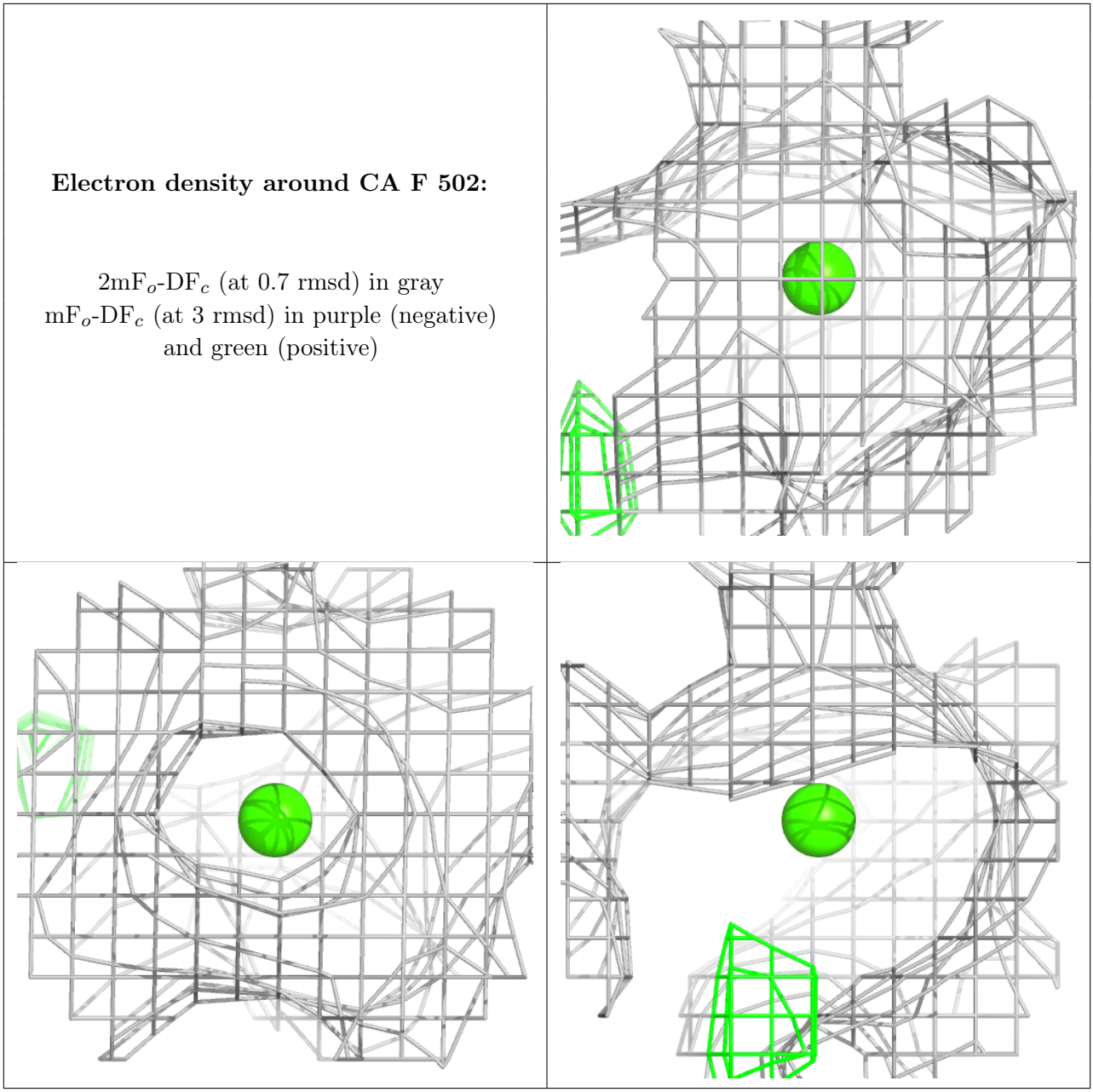
Electron density around MG E 501:

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



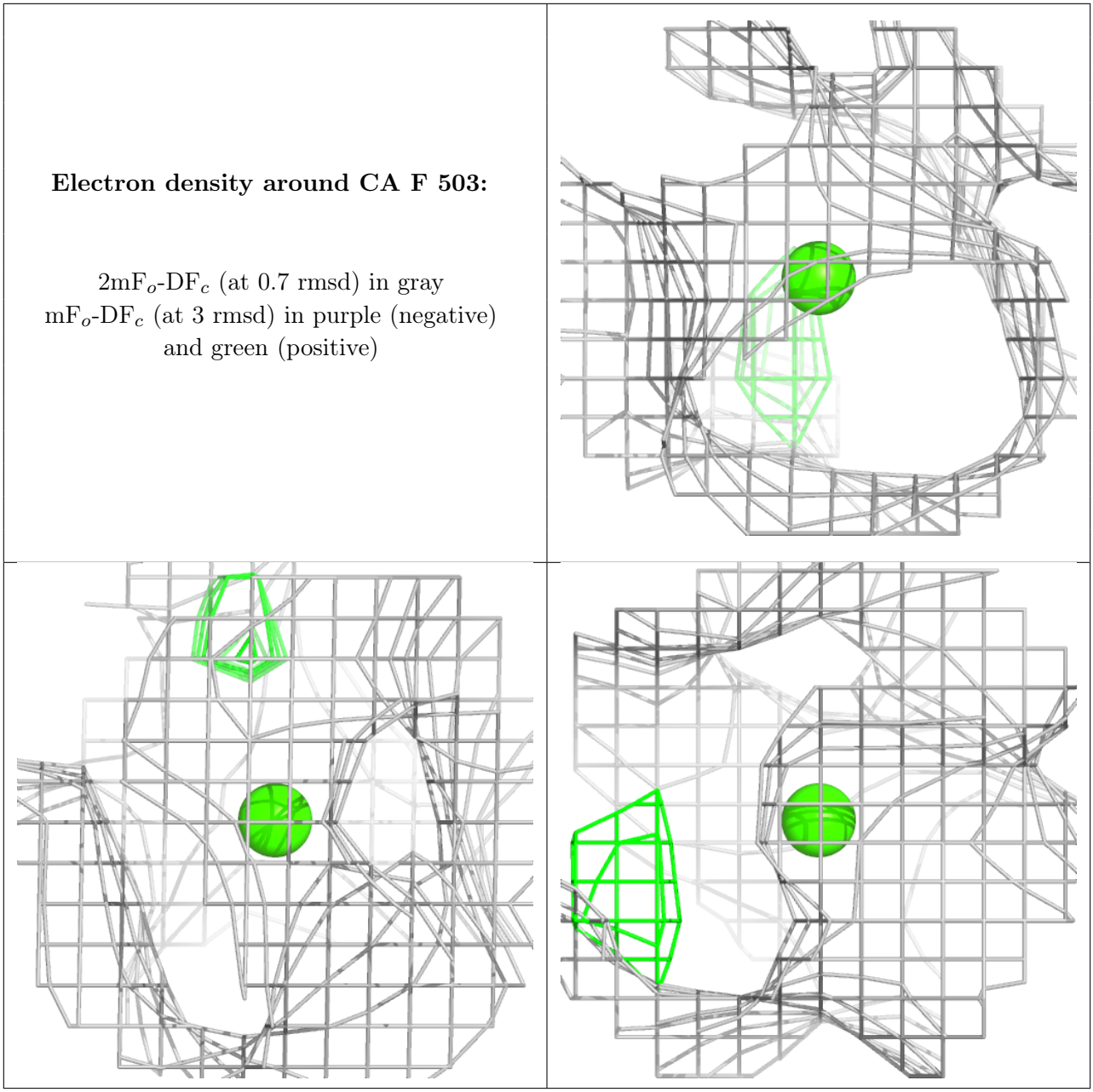
Electron density around CA F 502:

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



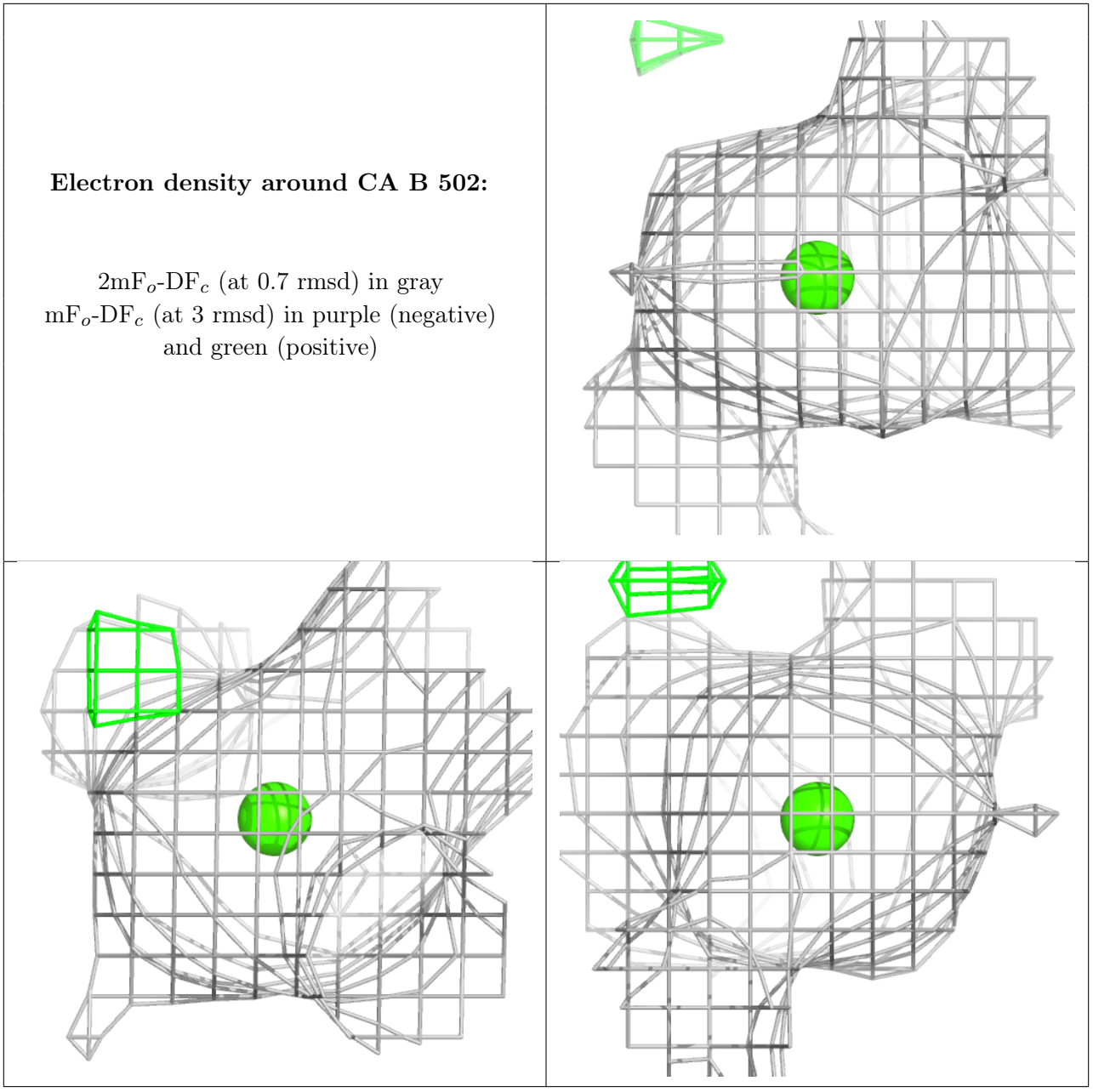
Electron density around CA F 503:

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



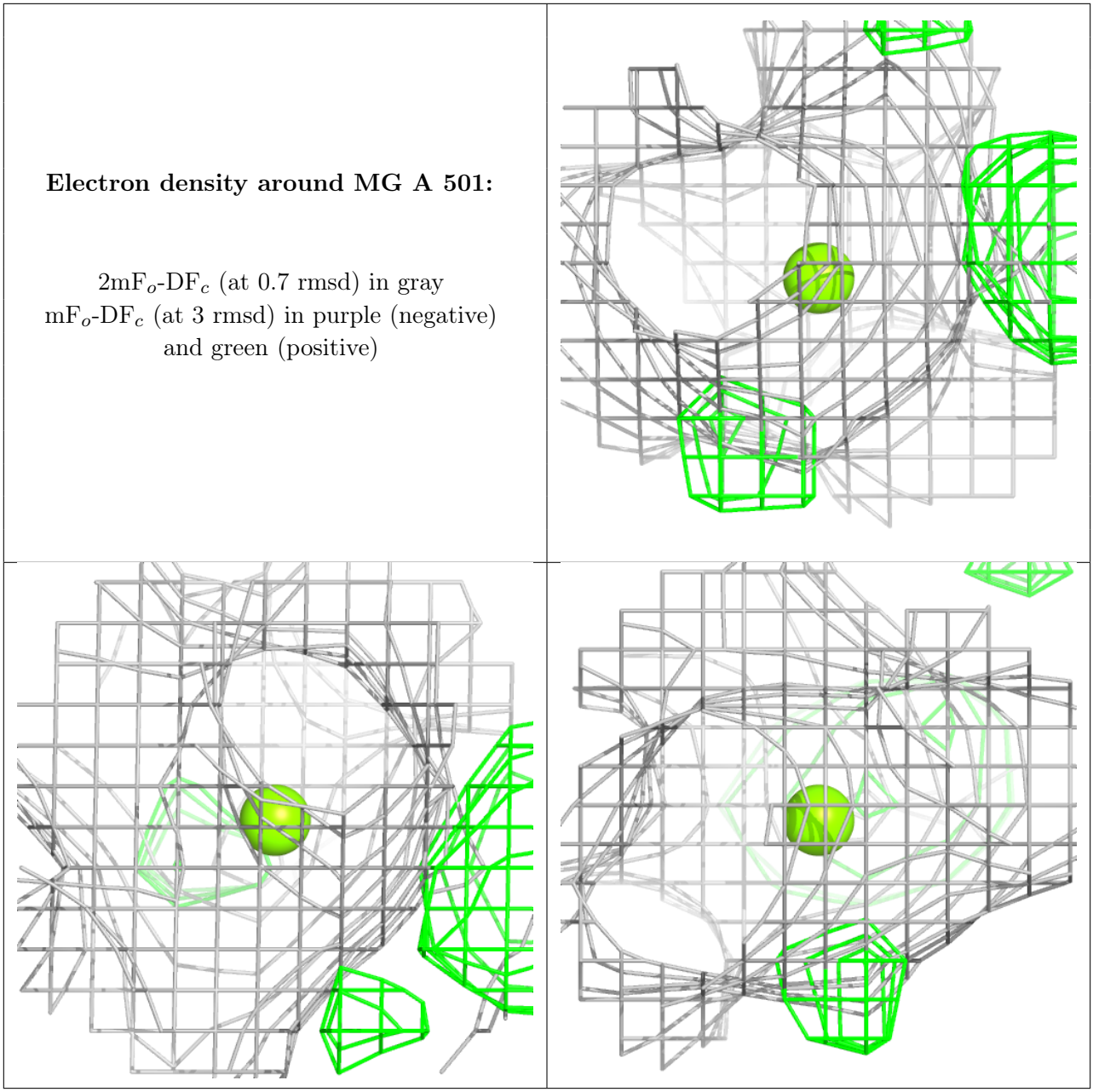
Electron density around CA B 502:

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



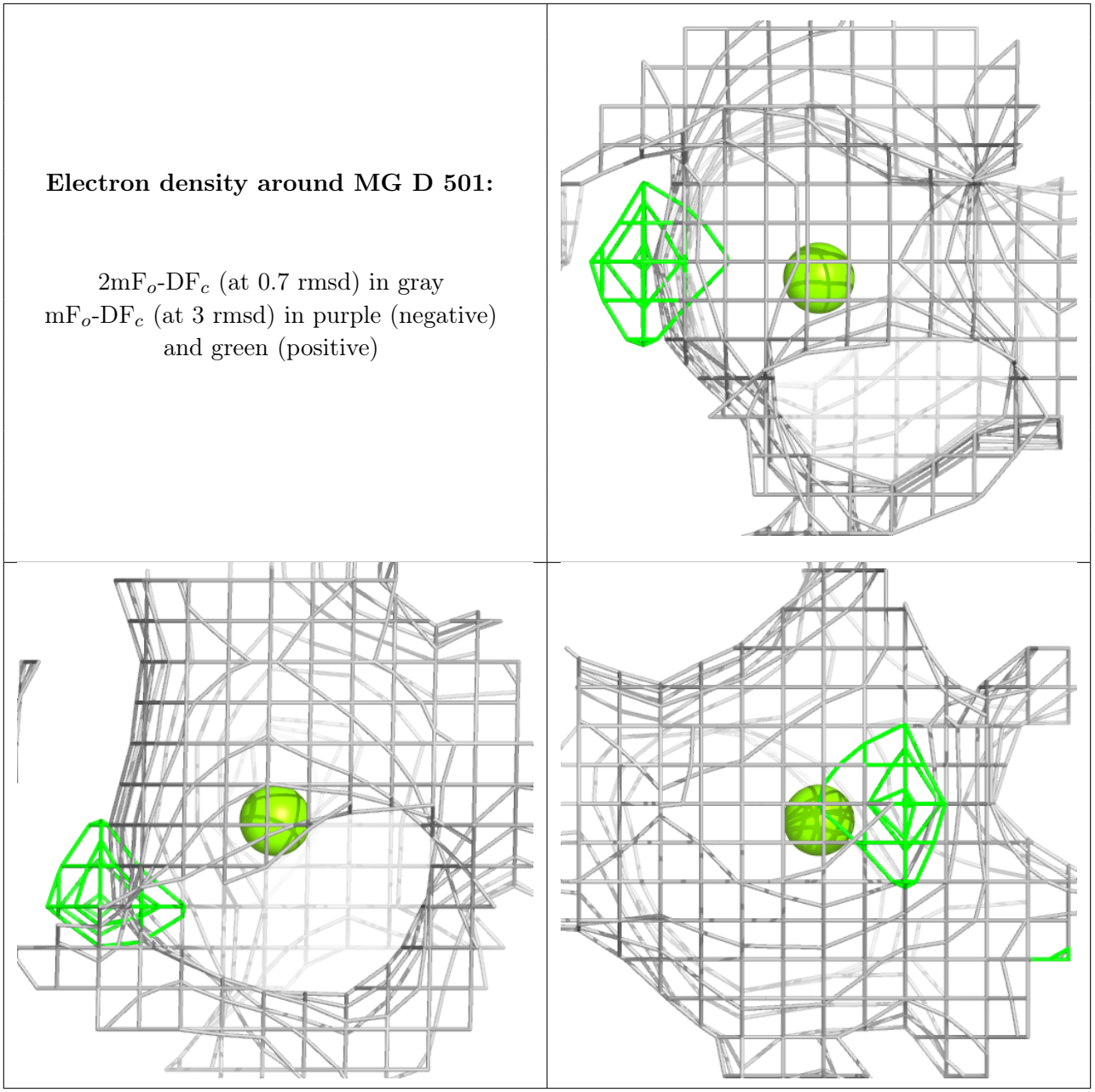
Electron density around MG A 501:

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



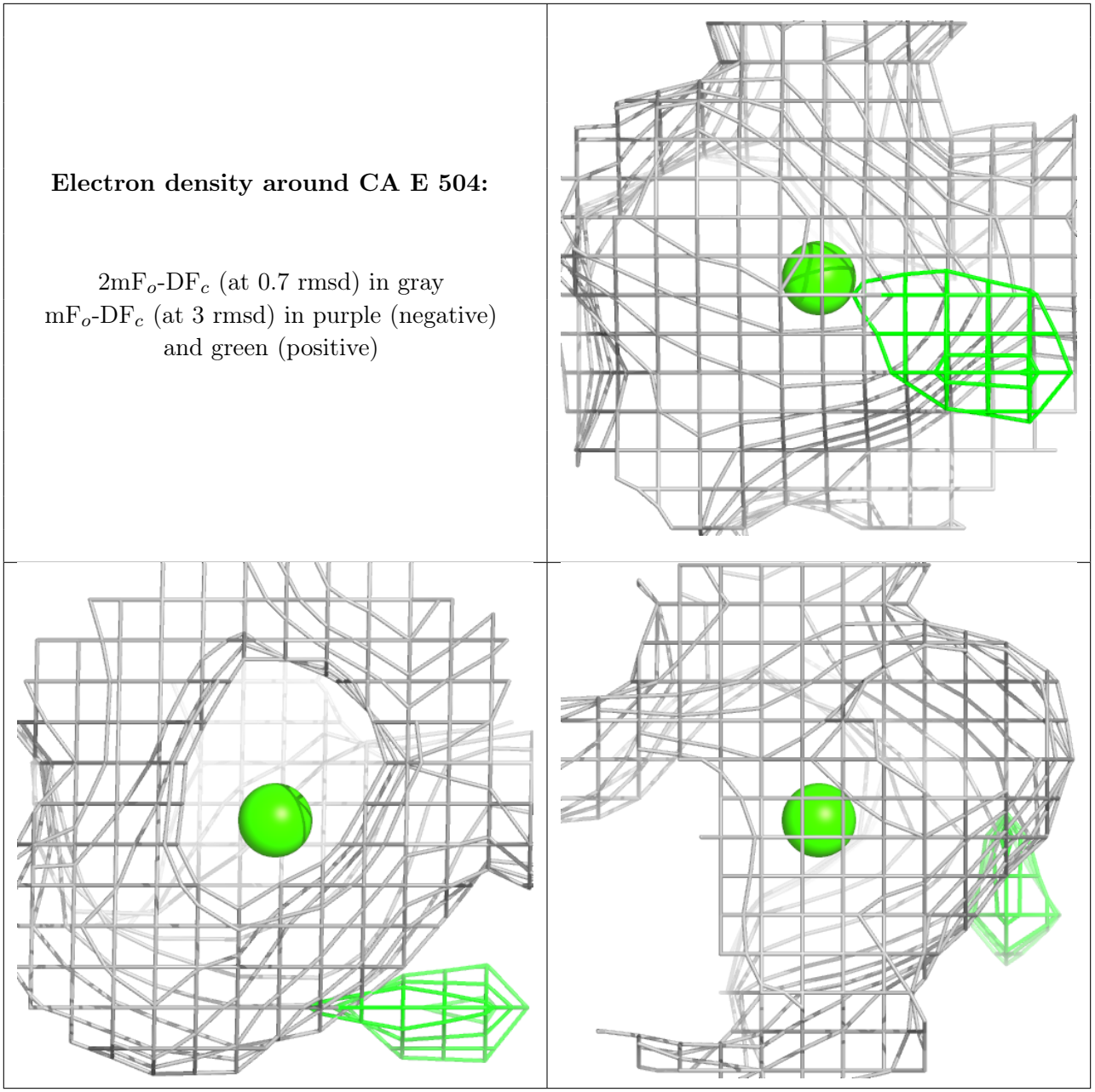
Electron density around MG D 501:

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



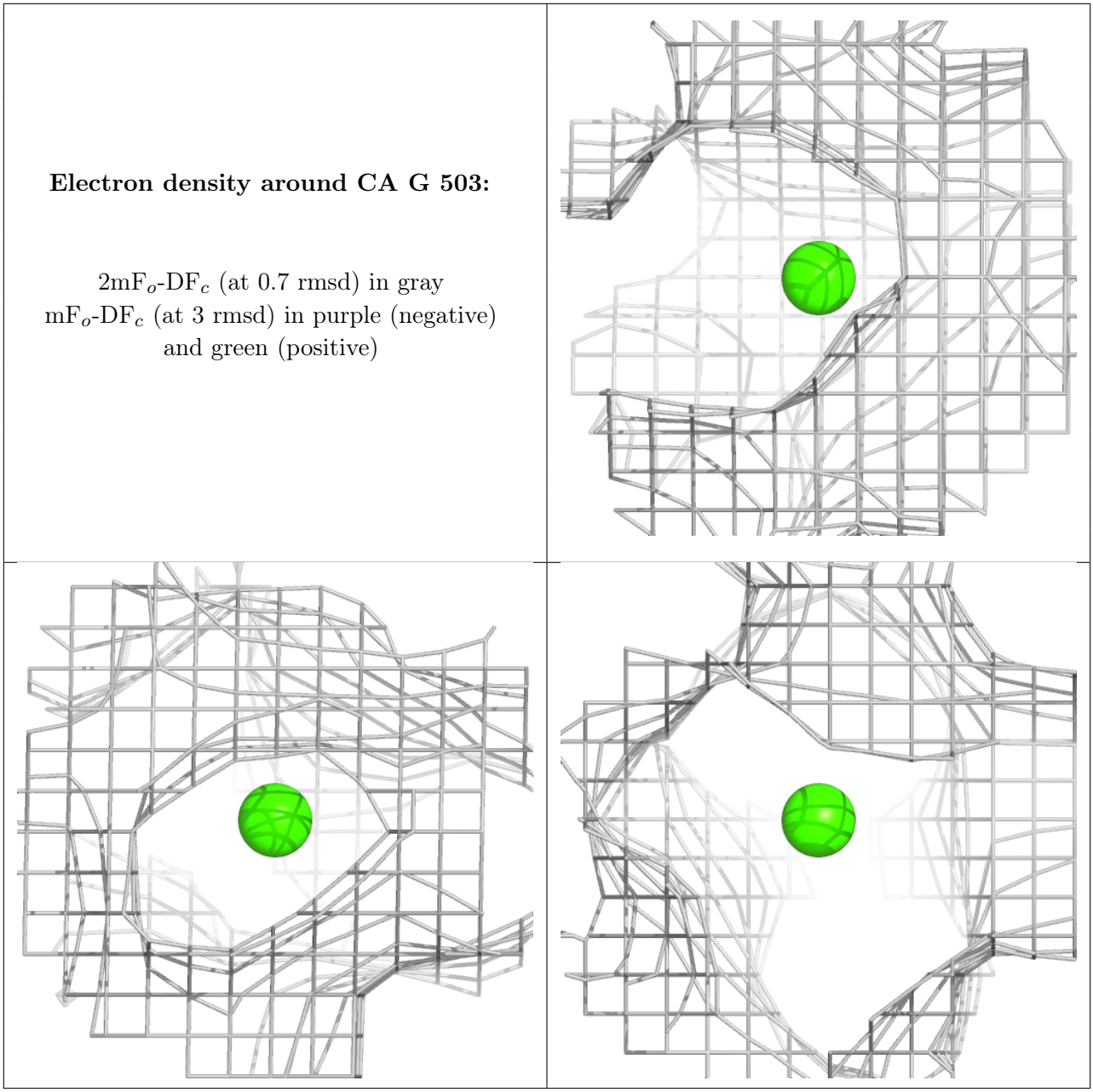
Electron density around CA E 504:

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



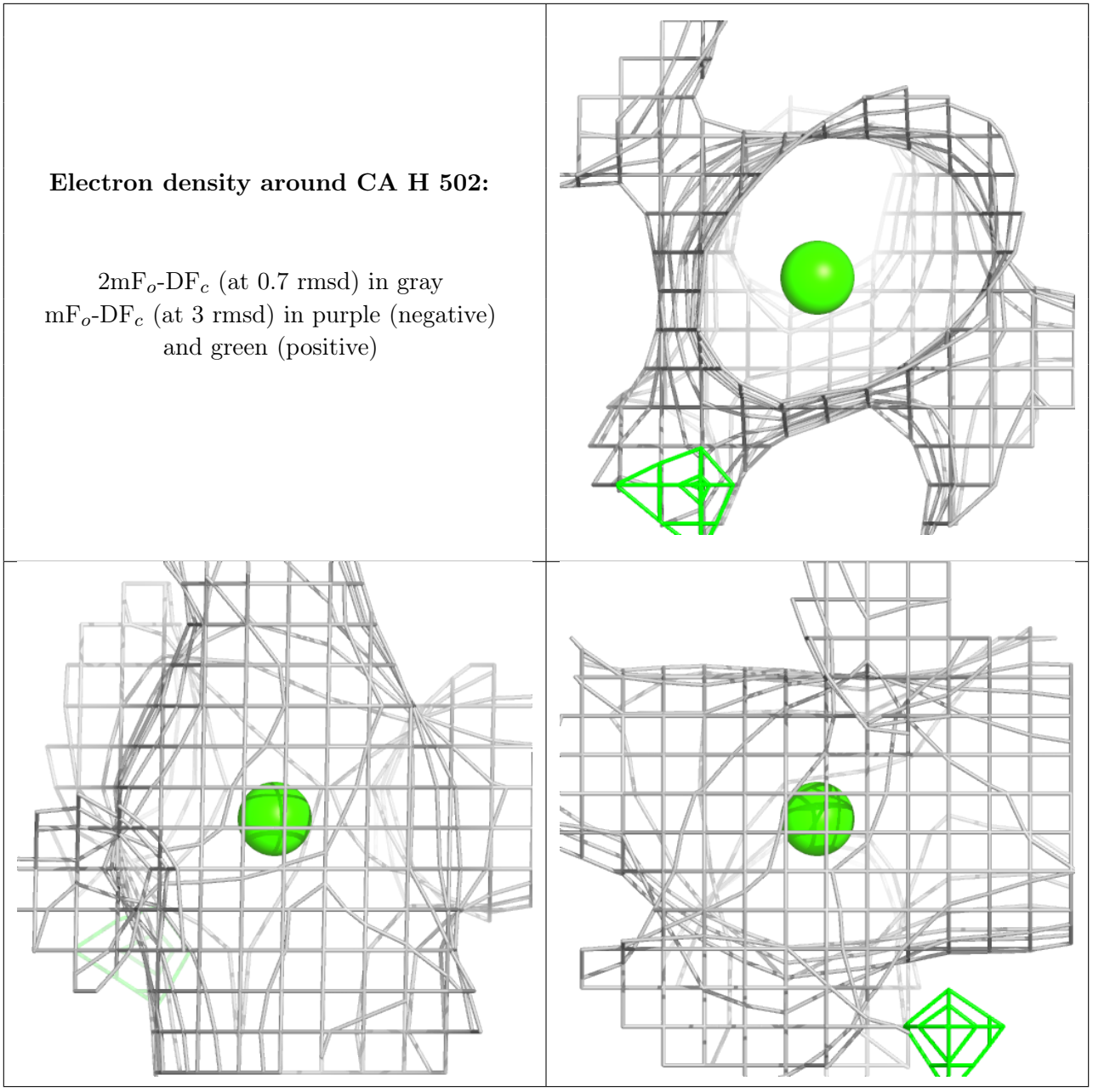
Electron density around CA G 503:

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



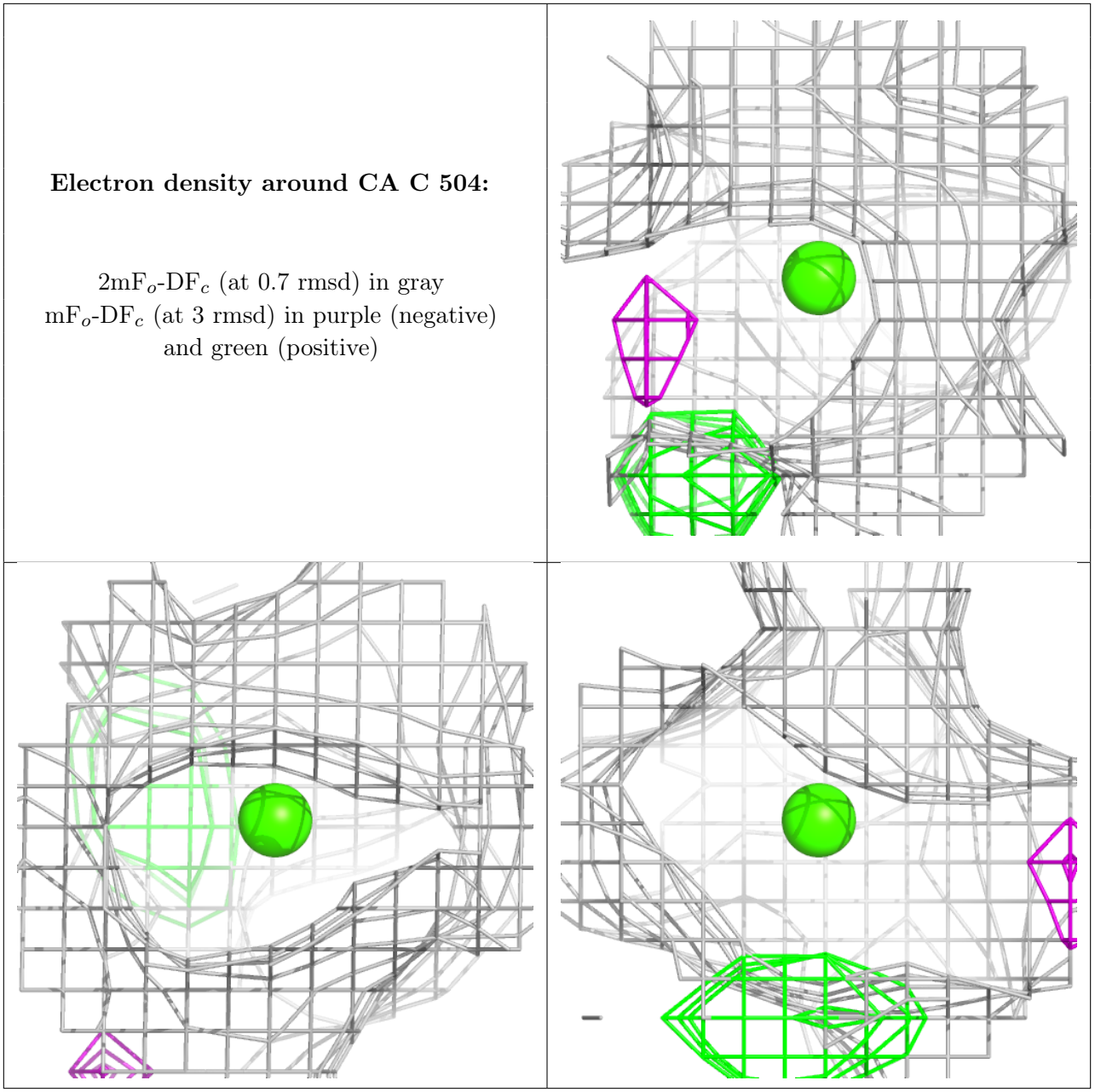
Electron density around CA H 502:

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



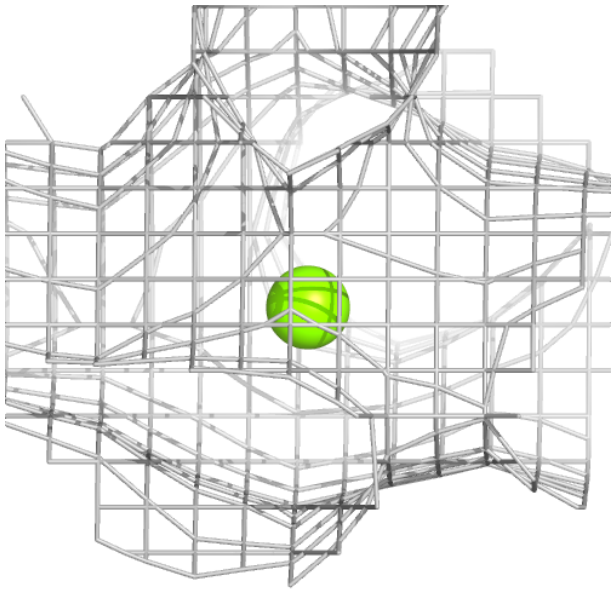
Electron density around CA C 504:

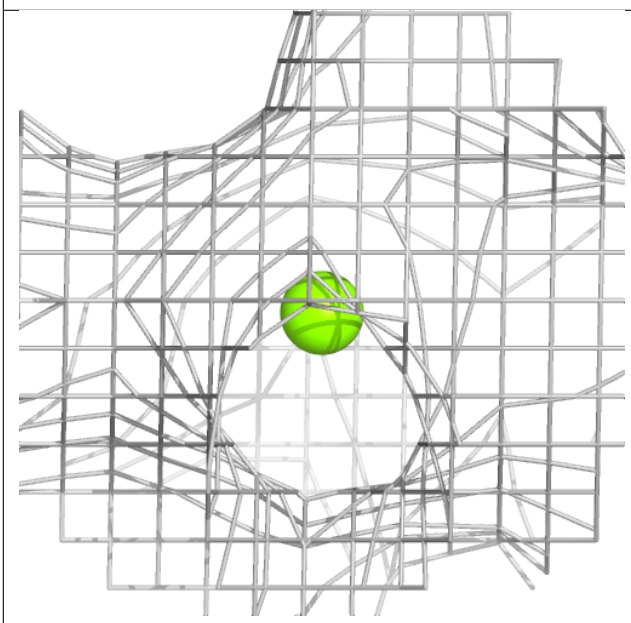
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

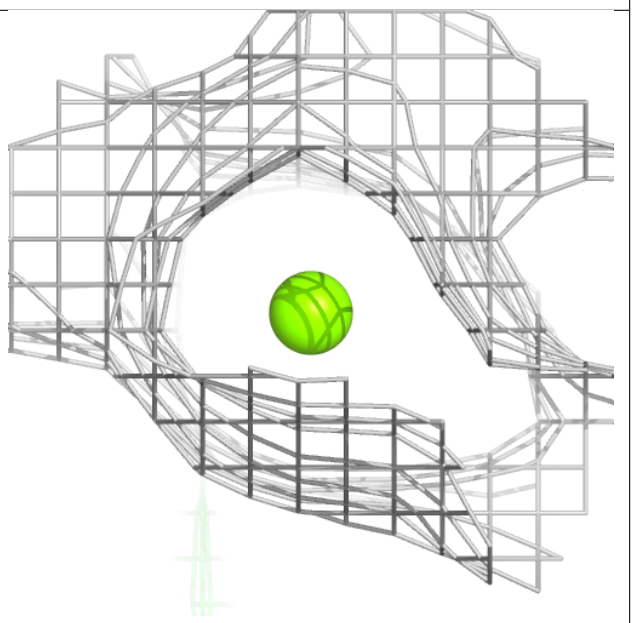


Electron density around MG H 501:

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

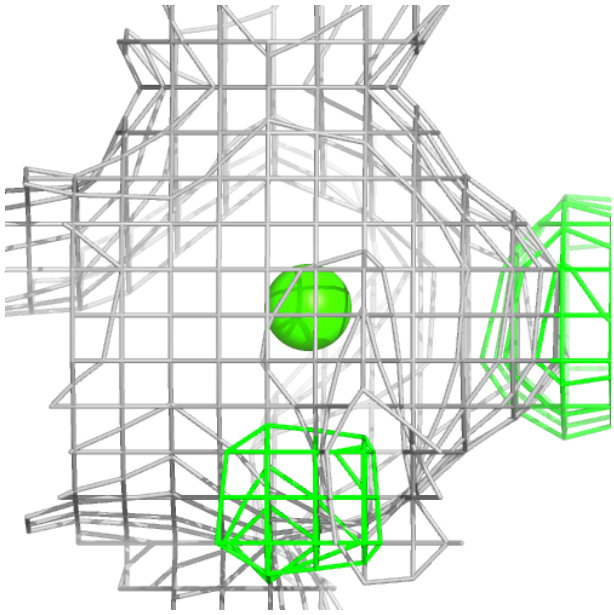


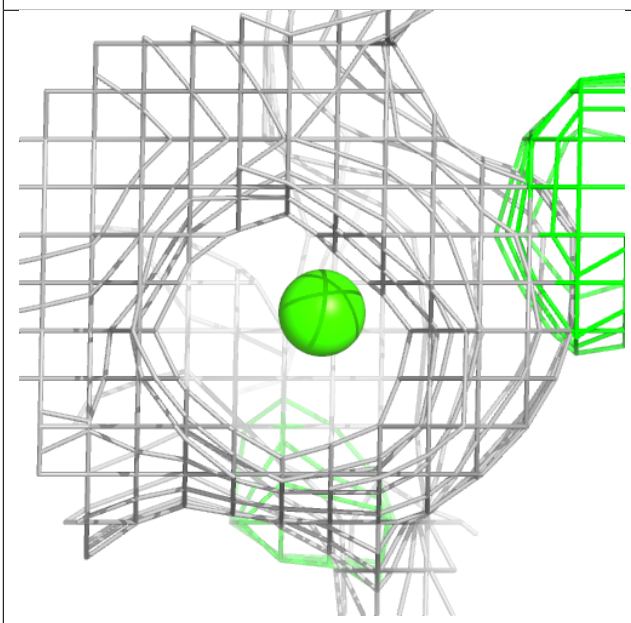


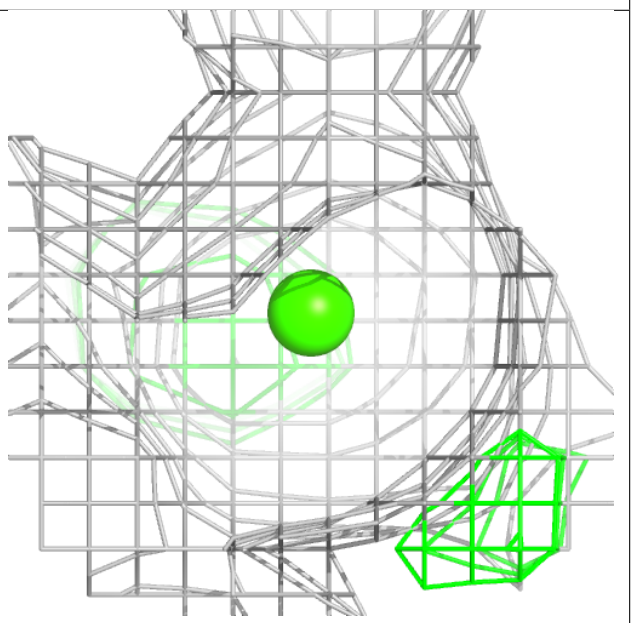


Electron density around CA D 504:

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

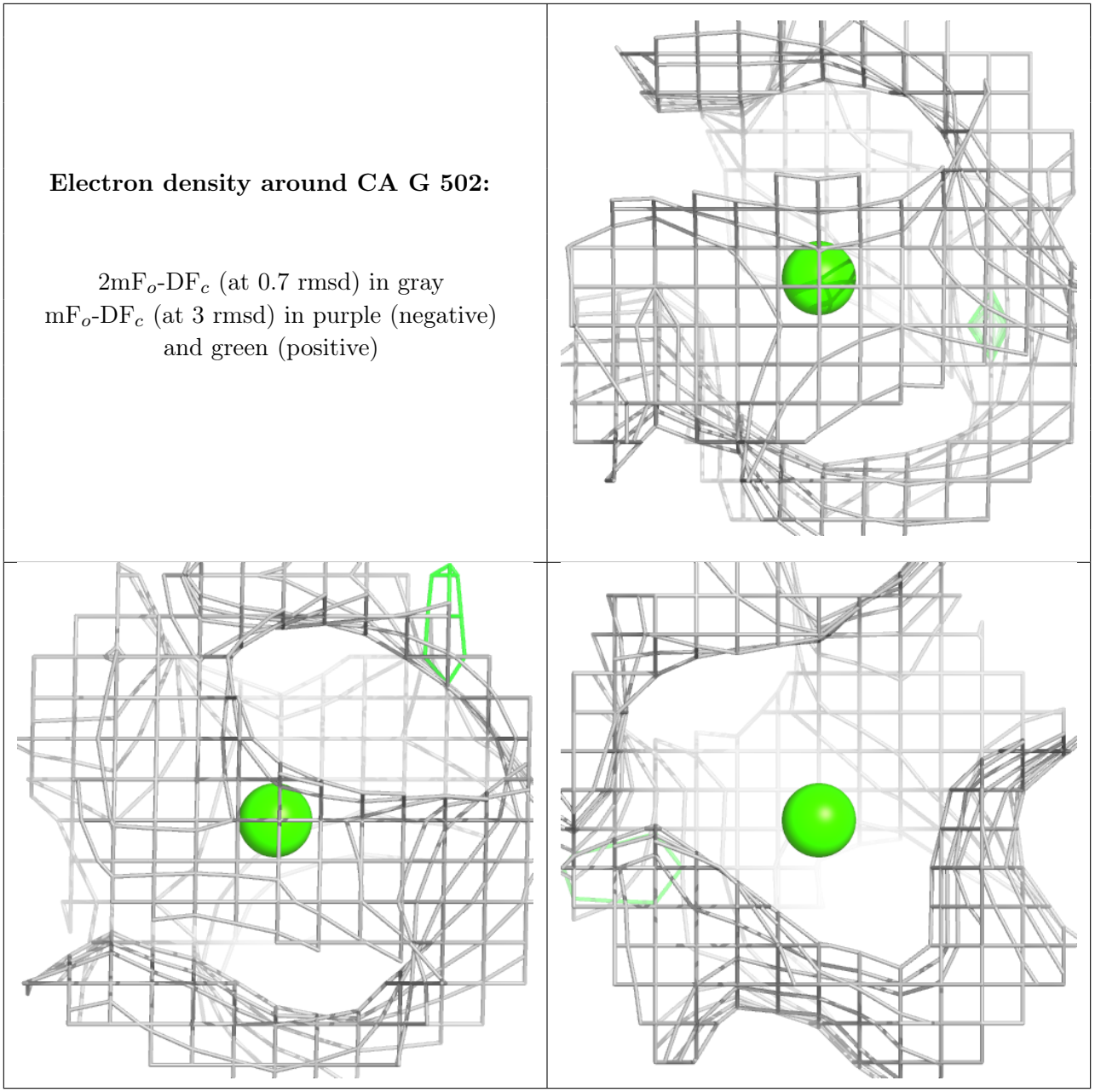






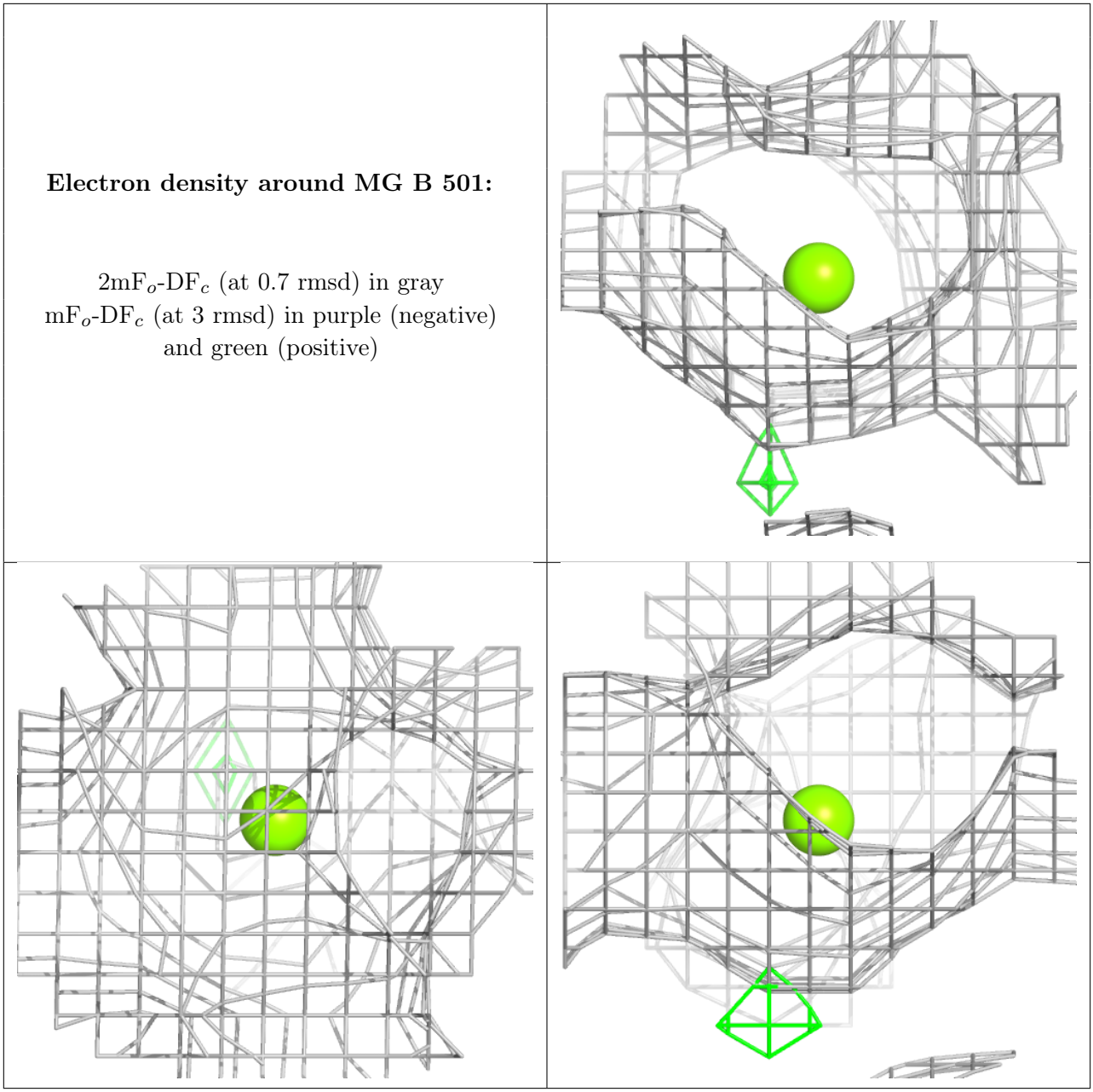
Electron density around CA G 502:

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



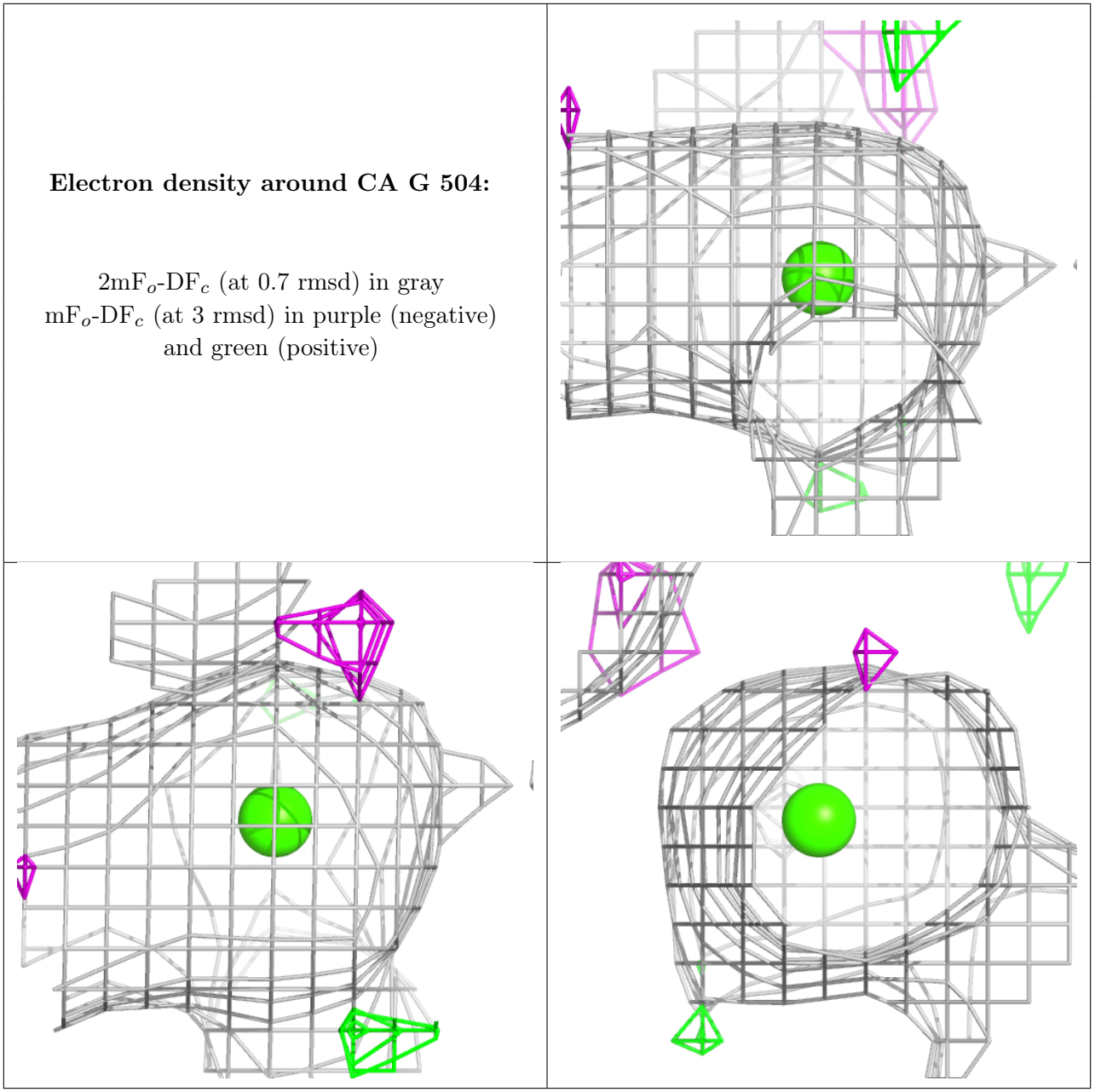
Electron density around MG B 501:

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



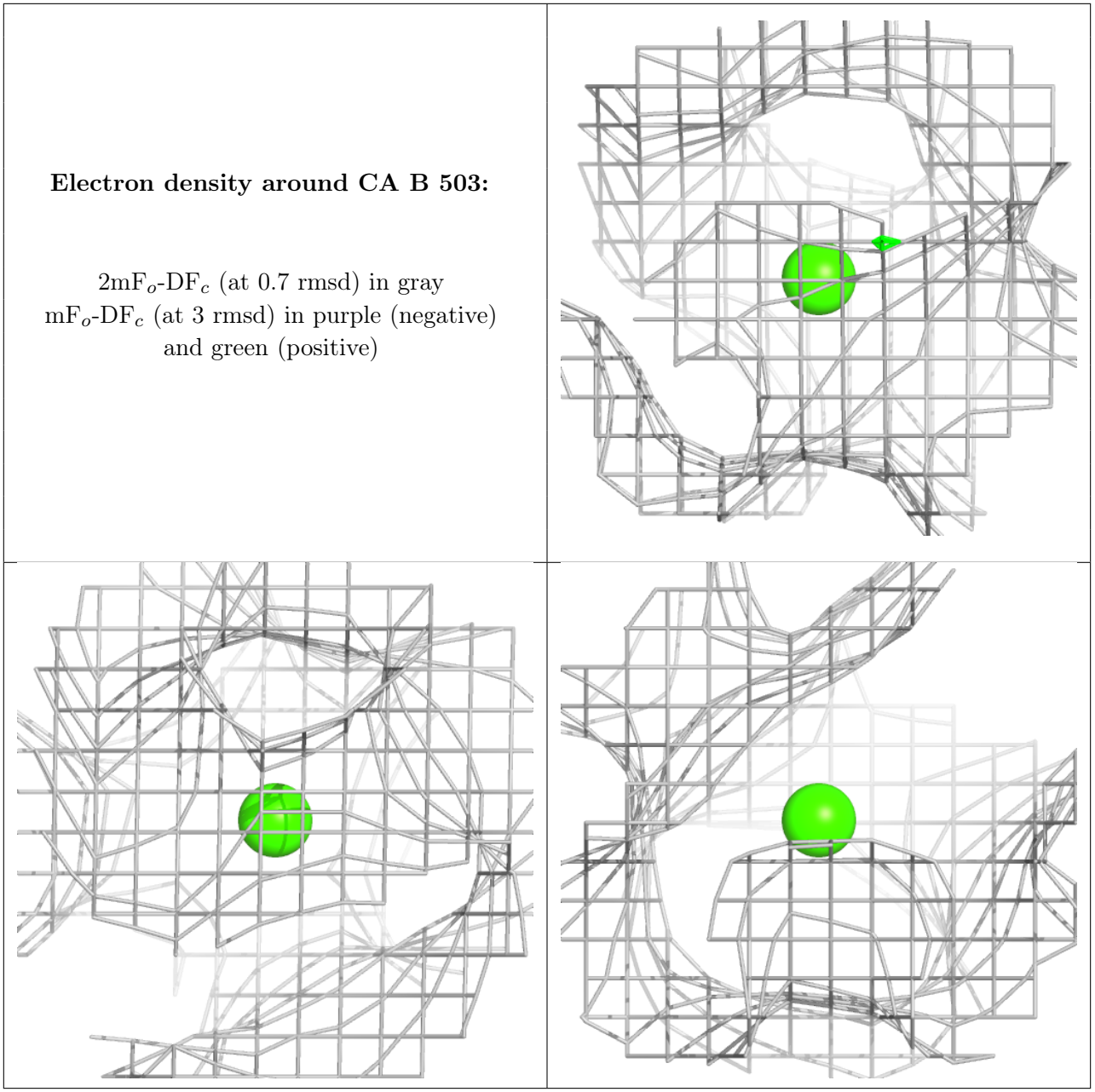
Electron density around CA G 504:

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



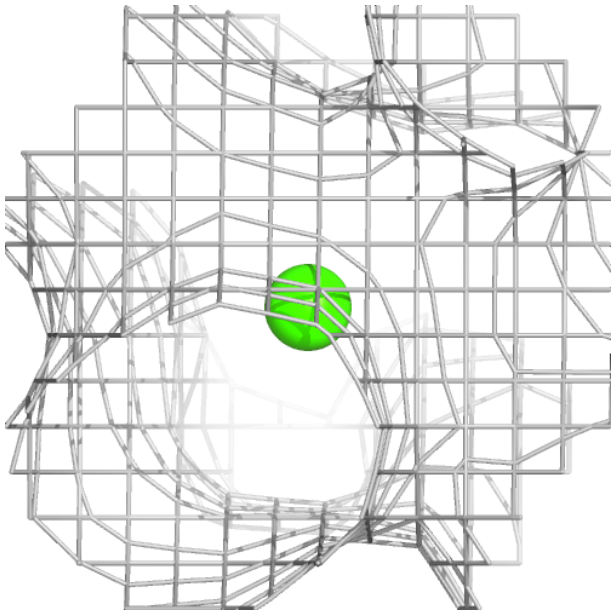
Electron density around CA B 503:

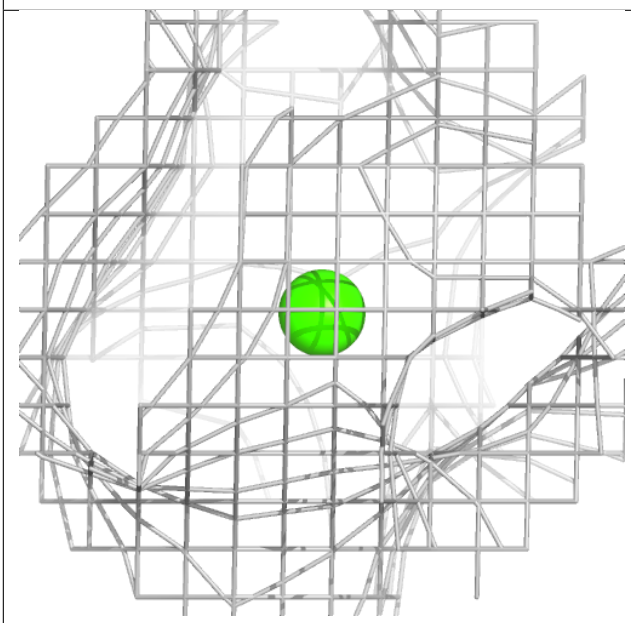
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

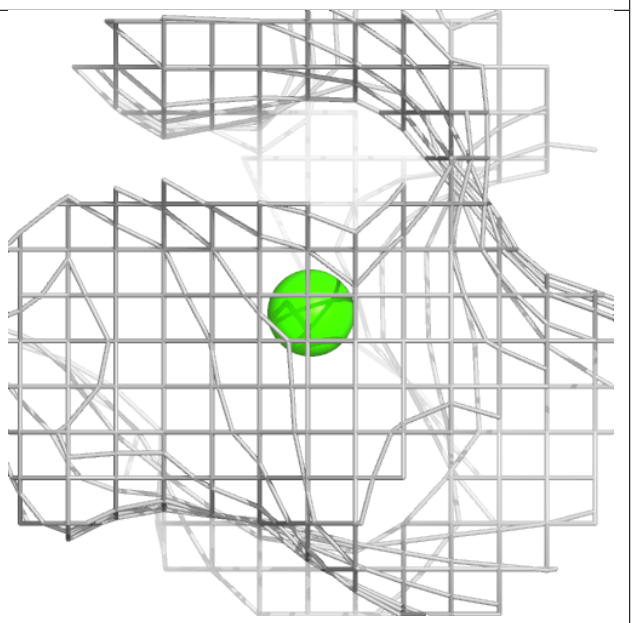


Electron density around CA H 503:

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

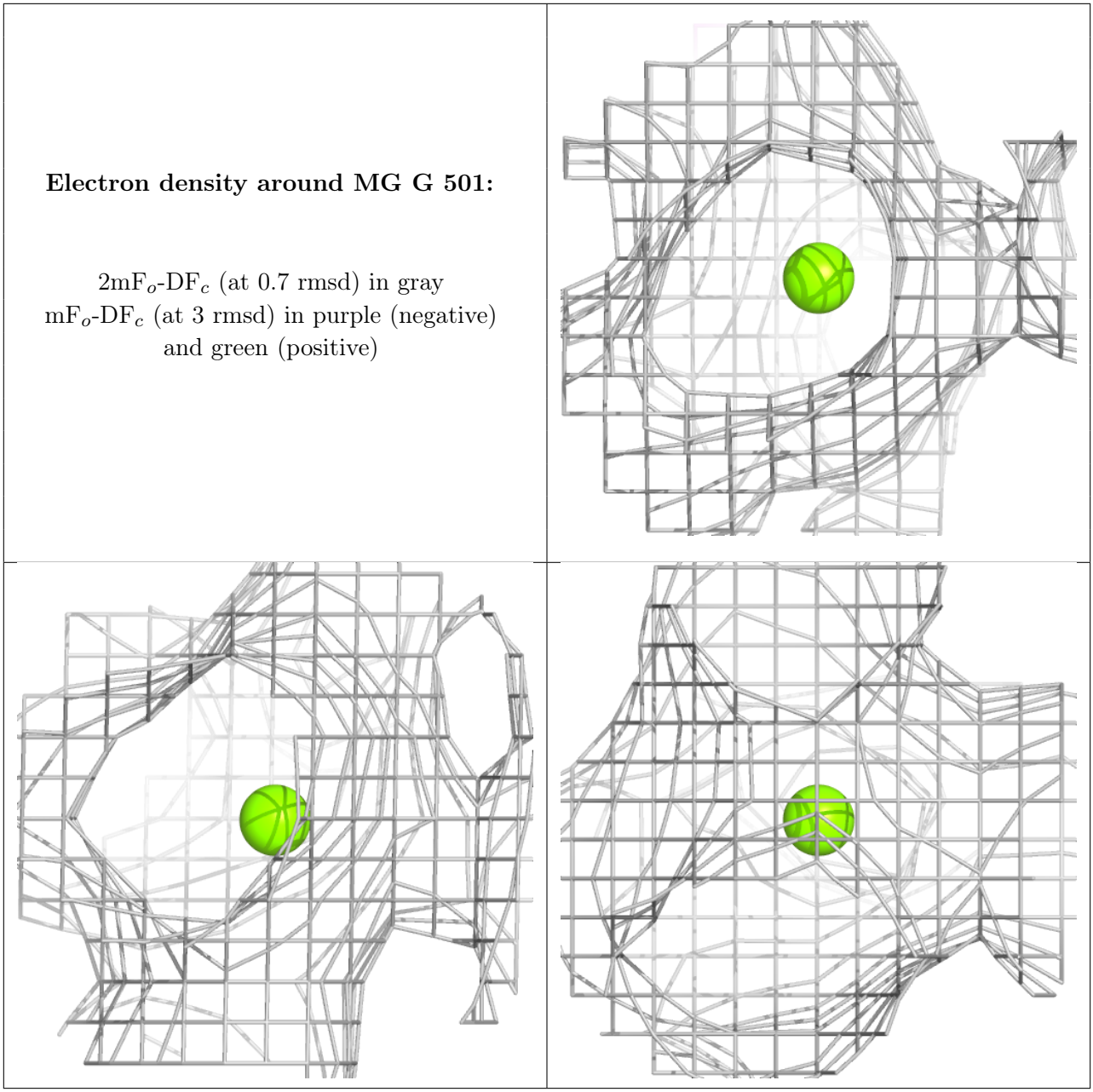






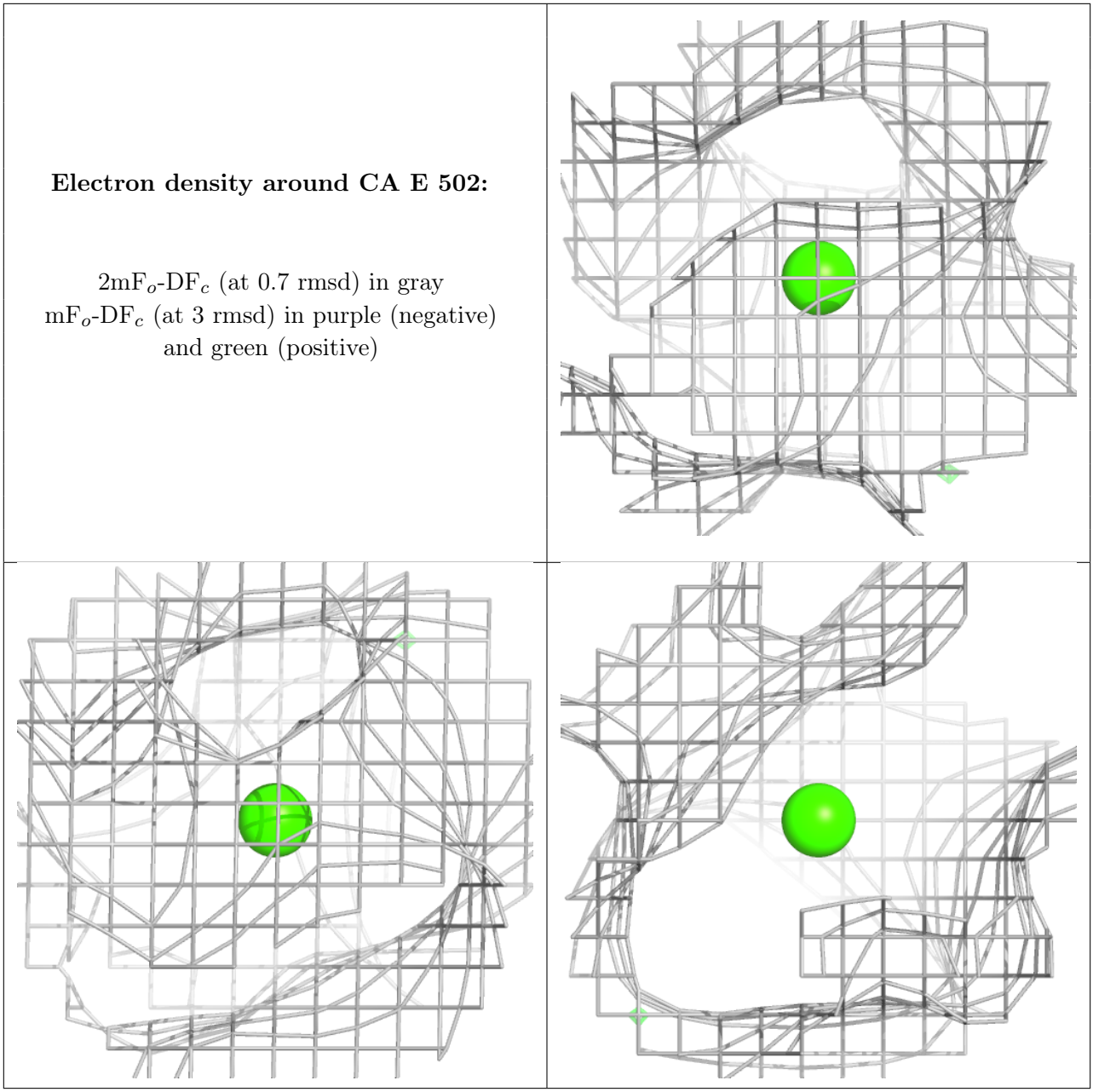
Electron density around MG G 501:

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



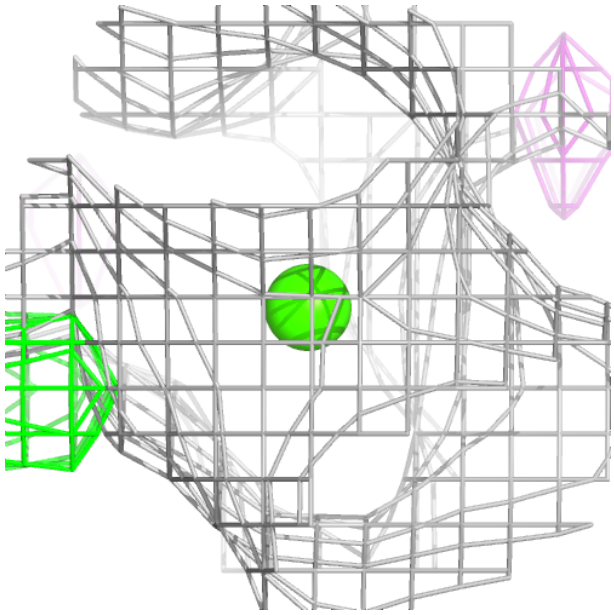
Electron density around CA E 502:

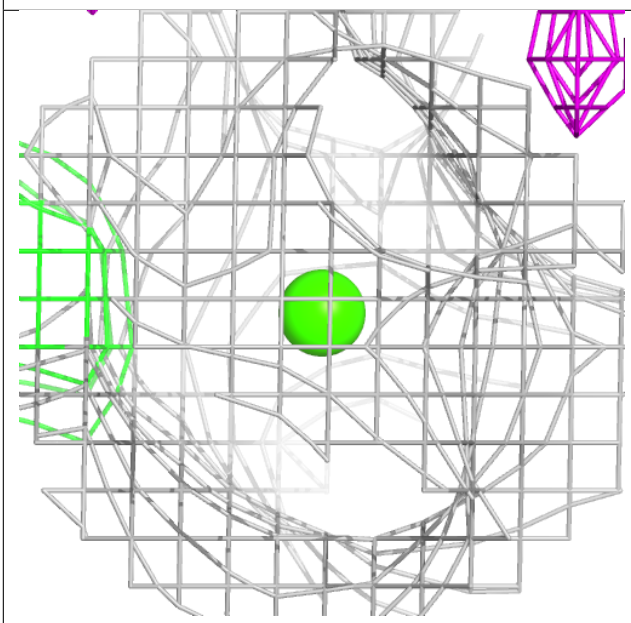
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

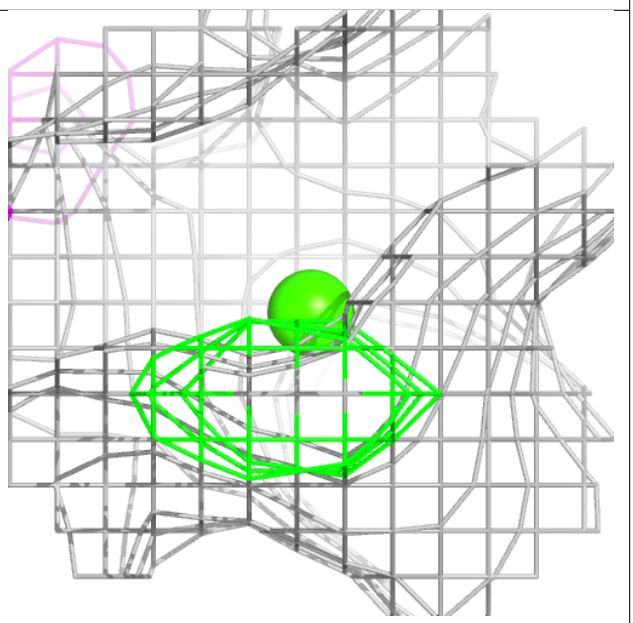


Electron density around CA C 503:

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

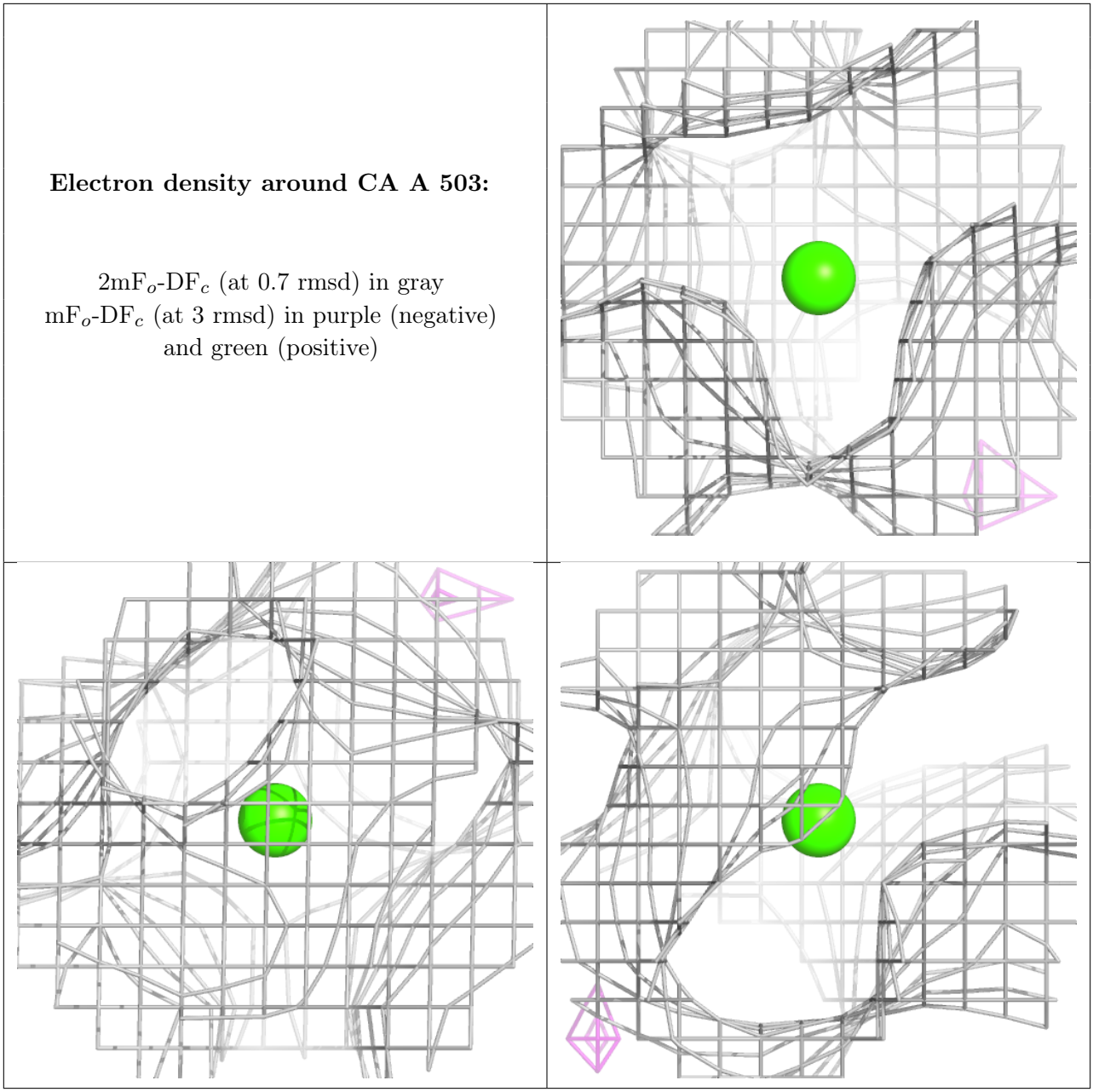






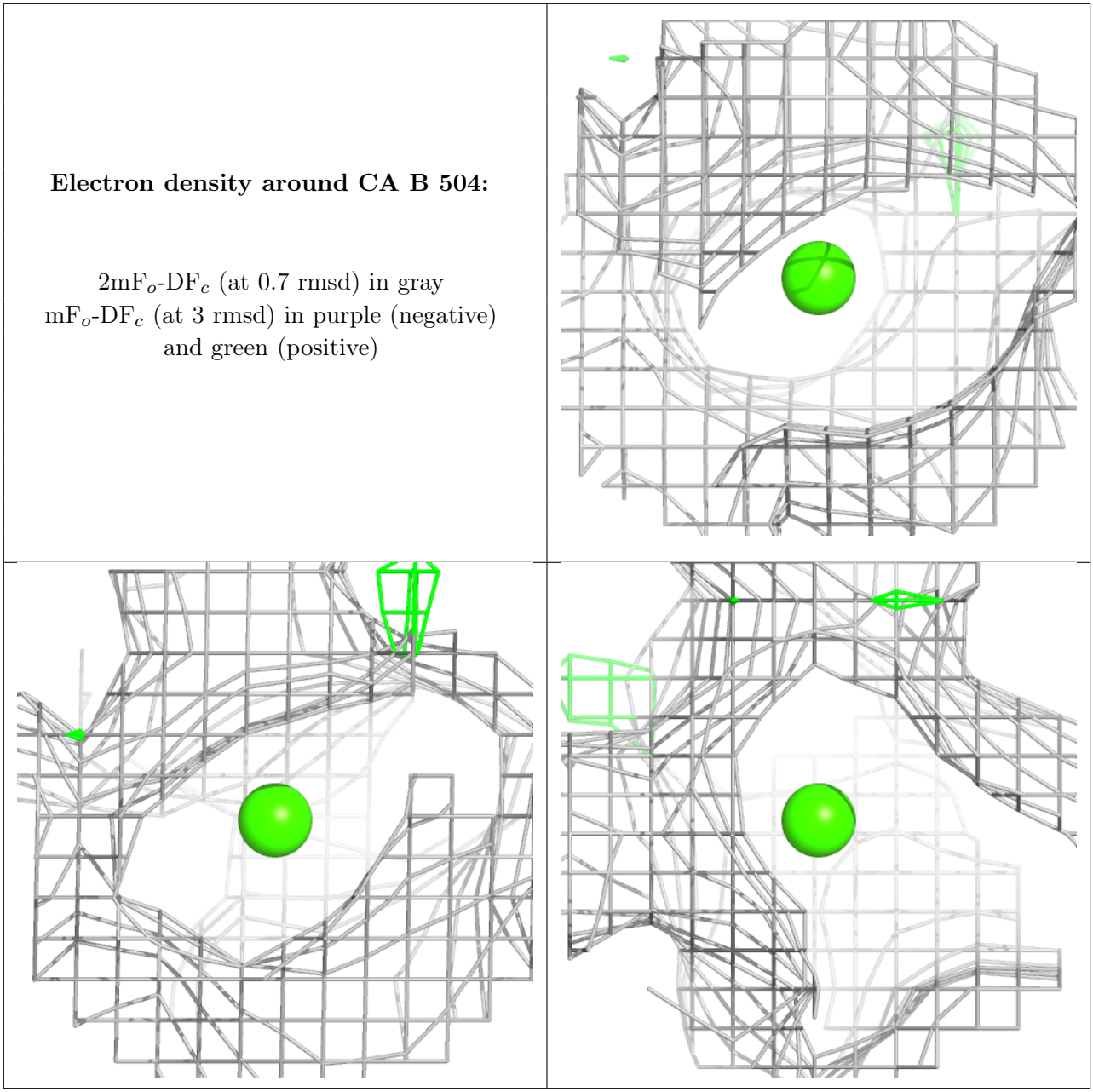
Electron density around CA A 503:

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



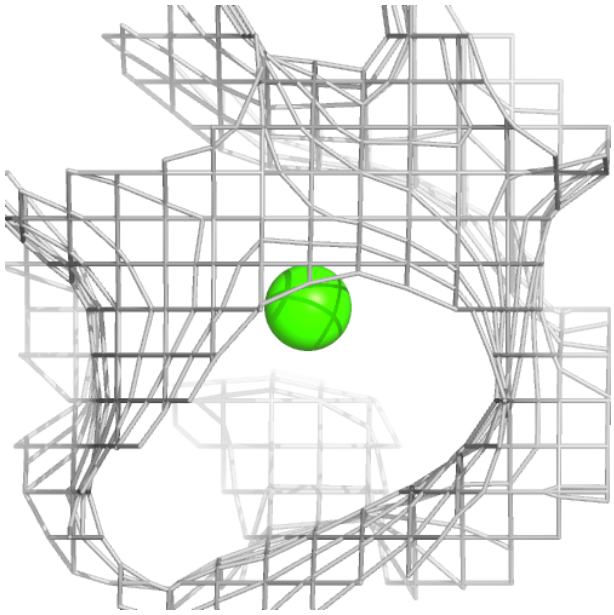
Electron density around CA B 504:

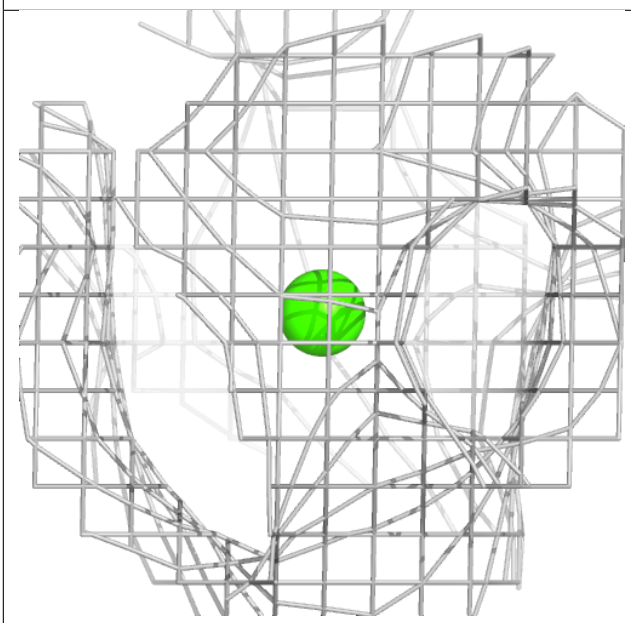
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

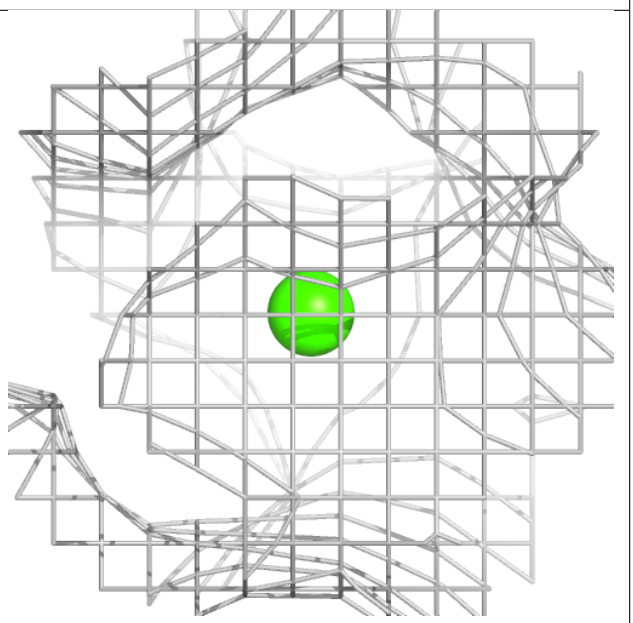


Electron density around CA D 503:

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

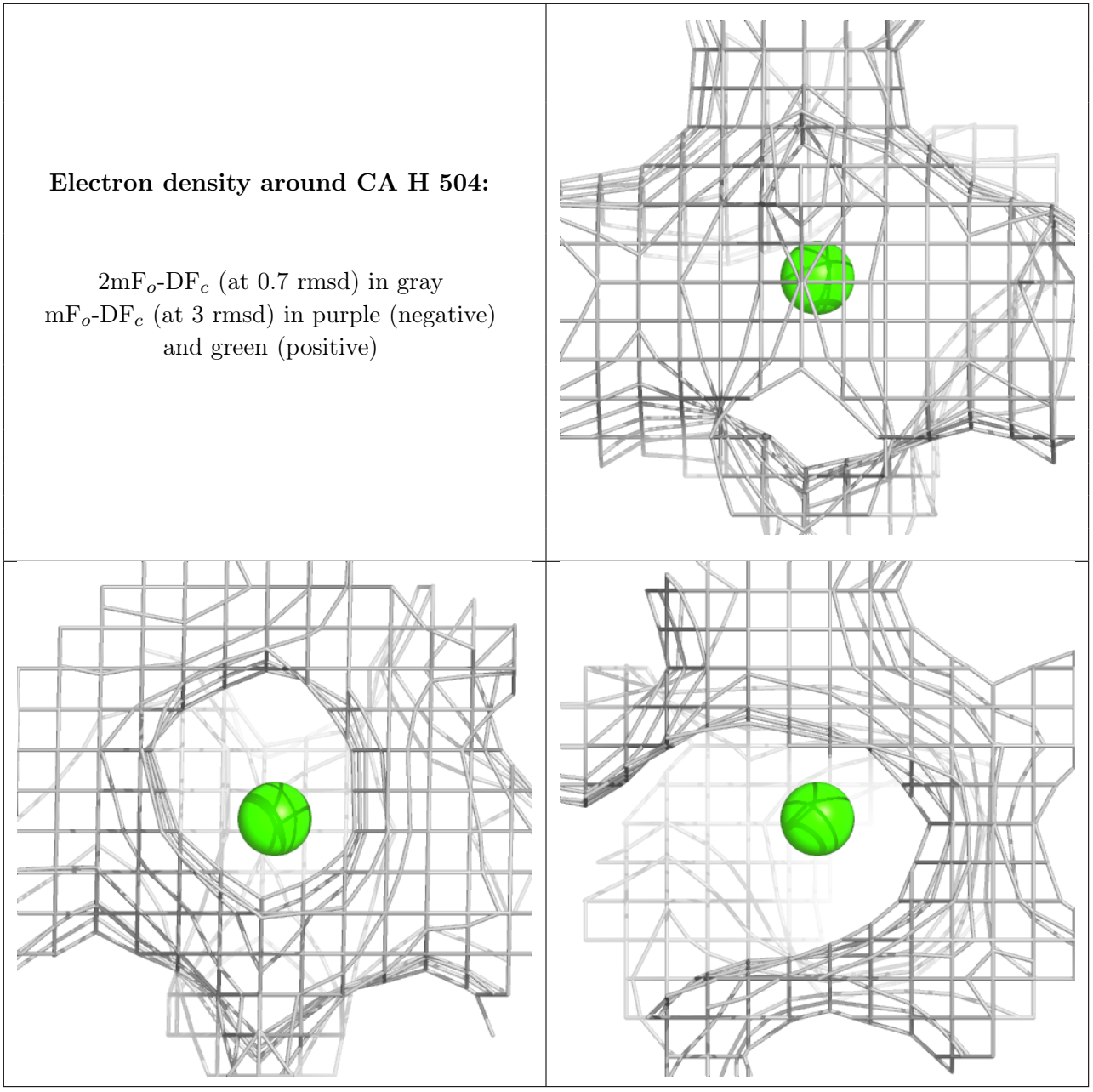






Electron density around CA H 504:

$2mF_o$-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.