Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2025 – 01:49 am GMT

PDB ID	:	9H4V
Title	:	Crystal structure of the adduct formed upon reaction of aurothiomalate with human serum transferrin (apo-form)
Authors	:	Troisi, R.; Galardo, F.; Messori, L.; Sica, F.; Merlino, A.
Deposited on	:	2024-10-21
Resolution	:	3.02 Å(reported)

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

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

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

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

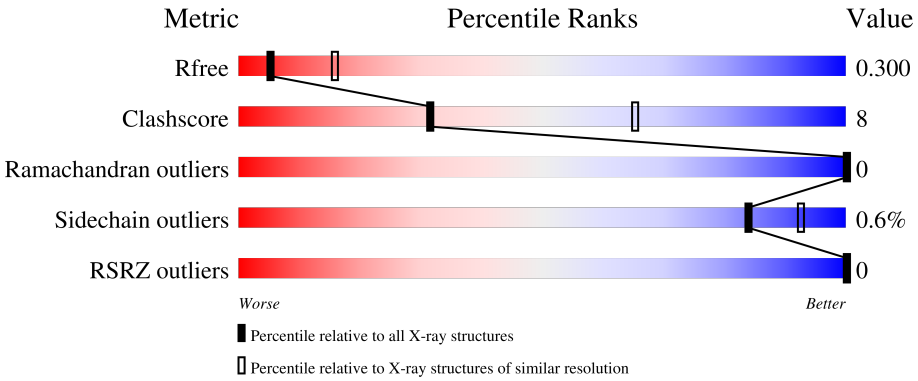
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.02 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2927 (3.04-3.00)
Clashscore	180529	3300 (3.04-3.00)
Ramachandran outliers	177936	3188 (3.04-3.00)
Sidechain outliers	177891	3191 (3.04-3.00)
RSRZ outliers	164620	2939 (3.04-3.00)

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	679	83% 17%
1	B	679	79% 20%

2 Entry composition

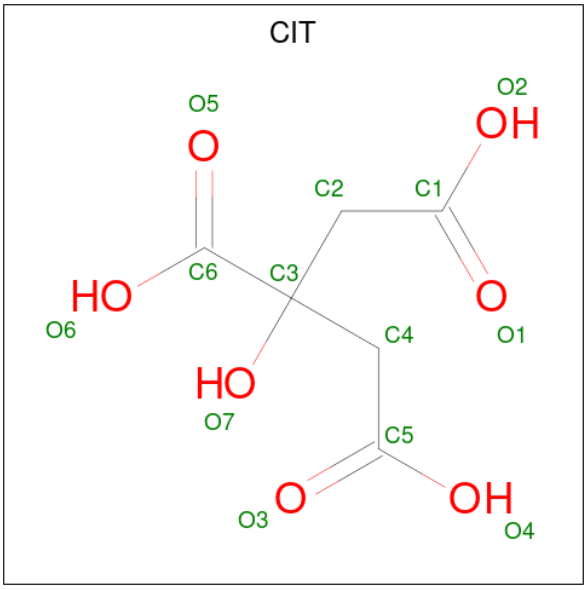
There are 5 unique types of molecules in this entry. The entry contains 10649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	676	Total	C	N	O	S	0	1	0
			5250	3295	911	997	47			
1	B	676	Total	C	N	O	S	0	2	0
			5252	3297	911	997	47			

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			13	6	7			
2	A	1	Total	C	O		0	0
			13	6	7			
2	A	1	Total	C	O		0	0
			13	6	7			
2	A	1	Total	C	O		0	0
			13	6	7			

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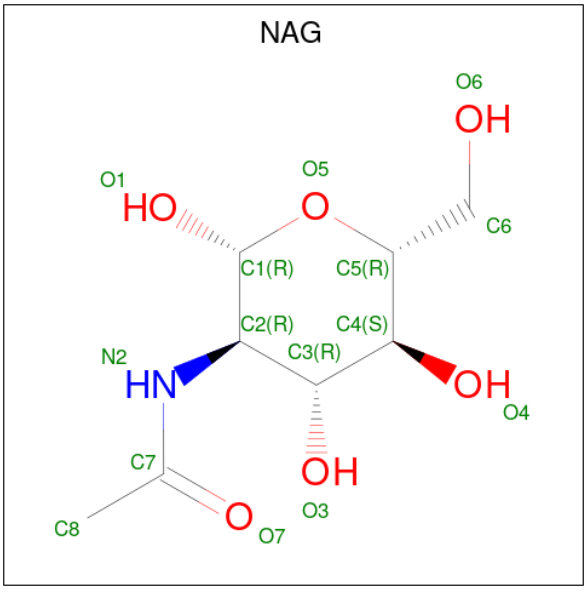
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0

- Molecule 3 is GOLD ION (three-letter code: AU) (formula: Au) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total Au 11 11	0	1
3	B	10	Total Au 10 10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is water.

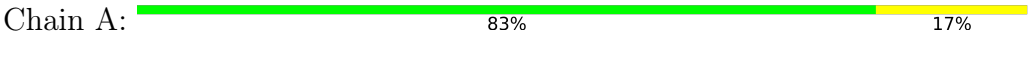
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total O 6 6	0	0
5	B	2	Total O 2 2	0	0

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.

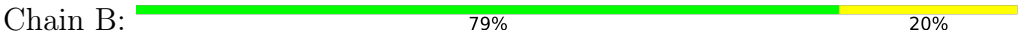
• Molecule 1: Serotransferrin

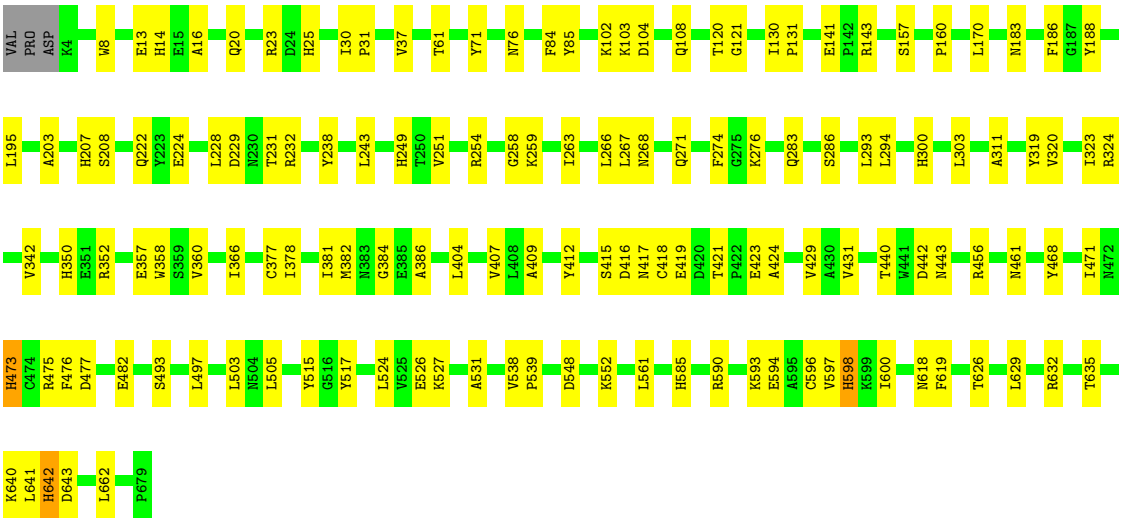
Chain A:



• Molecule 1: Serotransferrin

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.47Å 99.71Å 198.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.25 – 3.02 89.25 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.8 (89.25-3.02) 99.8 (89.25-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.243 , 0.296 0.247 , 0.300	Depositor DCC
R_{free} test set	1598 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	69.9	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10649	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: NAG, AU, CIT

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	0.29	0/5374	0.62	0/7262
1	B	0.29	0/5382	0.63	0/7273
All	All	0.29	0/10756	0.63	0/14535

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5250	0	5071	71	0
1	B	5252	0	5073	96	0
2	A	52	0	20	1	0
2	B	52	0	20	1	0
3	A	11	0	0	0	0
3	B	10	0	0	0	0
4	B	14	0	13	1	0
5	A	6	0	0	1	0
5	B	2	0	0	0	0
All	All	10649	0	10197	166	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 8.

All (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:GLU:HG2	1:B:424:ALA:H	1.24	1.00
1:B:598[B]:HIS:CE1	1:B:640:LYS:HD3	2.08	0.88
1:A:570:PRO:HG2	1:A:573:GLU:HG3	1.56	0.88
1:A:61:THR:HG21	1:A:294:LEU:O	1.75	0.85
1:B:61:THR:HG21	1:B:294:LEU:O	1.77	0.84
1:B:103:LYS:HD2	1:B:224:GLU:HG3	1.61	0.80
1:B:283:GLN:HB2	1:B:286:SER:HB3	1.65	0.78
1:B:320:VAL:O	1:B:324:ARG:HB2	1.84	0.77
1:B:342:VAL:HG13	1:B:366:ILE:HD13	1.66	0.77
1:A:61:THR:CG2	1:A:294:LEU:O	2.33	0.75
1:A:320:VAL:O	1:A:324:ARG:HB2	1.86	0.75
1:A:382:MET:HG2	1:A:404:LEU:HD21	1.68	0.74
1:A:468:TYR:HA	1:A:471:ILE:HB	1.69	0.73
1:A:350:HIS:HB3	1:A:629:LEU:HD21	1.70	0.71
1:B:30:ILE:HG13	1:B:31:PRO:HD2	1.73	0.70
1:A:229:ASP:OD1	1:A:231:THR:HG22	1.92	0.69
1:B:259:LYS:O	1:B:263:ILE:HD12	1.93	0.69
1:B:526:GLU:HB3	1:B:527:LYS:HE2	1.75	0.68
1:B:229:ASP:OD1	1:B:231:THR:HG22	1.93	0.68
1:B:61:THR:CG2	1:B:294:LEU:O	2.41	0.67
1:B:440:THR:HG22	1:B:443:ASN:OD1	1.94	0.67
1:B:423:GLU:HG2	1:B:424:ALA:N	2.05	0.67
1:A:349:HIS:HB2	2:A:701:CIT:O7	1.95	0.66
1:B:382:MET:HG2	1:B:404:LEU:HD21	1.76	0.66
1:B:283:GLN:CB	1:B:286:SER:HB3	2.25	0.66
1:A:16:ALA:O	1:A:20:GLN:HG3	1.96	0.66
1:A:382:MET:SD	1:A:402:CYS:HB3	2.36	0.65
1:B:378:ILE:O	1:B:382:MET:HG3	1.97	0.65
1:A:378:ILE:O	1:A:382:MET:HG3	1.95	0.65
1:A:96:TYR:H	1:A:207:HIS:HD2	1.45	0.65
1:B:461:ASN:HA	1:B:662:LEU:HD11	1.80	0.64
1:B:160:PRO:HB3	1:B:186:PHE:HD1	1.63	0.64
1:A:404:LEU:HB3	1:A:588:VAL:HG13	1.80	0.64
1:A:538:VAL:HG11	1:A:571:VAL:HG11	1.80	0.63
1:A:409:ALA:HB2	1:A:641:LEU:HD11	1.81	0.63
1:A:461:ASN:HA	1:A:662:LEU:HD11	1.81	0.62
1:A:410:GLU:HB3	1:A:635:THR:HG22	1.82	0.61
1:A:276:LYS:HD2	1:A:300:HIS:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ALA:HB3	1:A:456:ARG:HG3	1.82	0.61
1:B:8:TRP:HZ3	1:B:267:LEU:HD11	1.65	0.60
1:A:377:CYS:O	1:A:381:ILE:HG12	2.02	0.60
1:A:271:GLN:O	1:A:275:GLY:HA3	2.02	0.60
1:A:103:LYS:HG2	1:A:224:GLU:HG3	1.84	0.59
1:B:183:ASN:HB3	1:B:186:PHE:HB2	1.83	0.59
1:A:342:VAL:HG13	1:A:366:ILE:HD13	1.83	0.59
1:A:130:ILE:HB	1:A:131:PRO:HD3	1.84	0.58
1:A:37:VAL:HG22	1:A:266:LEU:HD11	1.84	0.58
1:A:96:TYR:H	1:A:207:HIS:CD2	2.22	0.58
1:B:130:ILE:HB	1:B:131:PRO:HD3	1.84	0.58
1:B:642:HIS:O	1:B:643:ASP:HB3	2.04	0.58
1:B:8:TRP:CZ3	1:B:267:LEU:HD11	2.39	0.57
1:A:259:LYS:O	1:A:263:ILE:HD12	2.04	0.57
1:A:500:GLY:O	1:A:505:LEU:HA	2.05	0.57
1:B:319:TYR:HE1	1:B:323:ILE:HD13	1.70	0.57
1:A:283:GLN:HB2	1:A:286:SER:HB3	1.87	0.56
1:B:141:GLU:HG2	1:B:143:ARG:NH2	2.20	0.56
1:A:415:SER:HB3	1:A:418:CYS:HB3	1.89	0.55
1:B:268:ASN:HA	1:B:271:GLN:HE21	1.70	0.55
1:B:418:CYS:HA	1:B:421:THR:HB	1.86	0.55
1:B:84:PHE:C	1:B:85:TYR:HD1	2.11	0.55
1:B:108:GLN:HE22	1:B:232:ARG:HG3	1.72	0.54
1:A:143:ARG:HH21	1:A:331:CYS:CB	2.20	0.54
1:B:71:TYR:O	1:B:76:ASN:HA	2.08	0.54
1:A:538:VAL:HB	1:A:539:PRO:HD3	1.89	0.53
1:B:228:LEU:HD21	1:B:243:LEU:HA	1.91	0.53
1:A:124:ARG:HD3	1:B:13:GLU:OE2	2.08	0.53
1:B:381:ILE:O	1:B:590:ARG:NH1	2.41	0.53
1:B:37:VAL:HG22	1:B:266:LEU:HD11	1.92	0.52
1:A:143:ARG:HH21	1:A:331:CYS:HB2	1.74	0.52
1:B:350:HIS:HB3	1:B:629:LEU:HD21	1.92	0.52
1:B:431:VAL:HG21	1:B:538:VAL:HG21	1.91	0.52
1:A:287:SER:HB3	1:A:293:LEU:HD22	1.91	0.51
1:B:598[B]:HIS:HE1	1:B:640:LYS:HD3	1.67	0.51
1:A:440:THR:HG22	1:A:443:ASN:OD1	2.11	0.51
1:B:456:ARG:NH2	1:B:515:TYR:OH	2.41	0.51
1:B:319:TYR:CE1	1:B:323:ILE:HD13	2.45	0.51
1:B:386:ALA:O	1:B:590:ARG:NH1	2.39	0.51
1:B:468:TYR:HA	1:B:471:ILE:HB	1.93	0.50
1:A:549:PRO:HA	1:A:552:LYS:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LEU:HB2	1:B:203:ALA:HB2	1.94	0.50
1:B:377:CYS:O	1:B:381:ILE:HG12	2.11	0.50
1:A:432:VAL:HG21	1:A:439:LEU:HD13	1.94	0.49
1:B:473:HIS:C	1:B:475:ARG:H	2.14	0.49
1:B:120:THR:HG21	1:B:188:TYR:CD1	2.47	0.49
1:B:416:ASP:C	1:B:418:CYS:H	2.14	0.49
1:B:342:VAL:CG1	1:B:366:ILE:HD13	2.39	0.49
1:B:440:THR:HG23	1:B:442:ASP:H	1.76	0.49
1:B:471:ILE:HD13	1:B:476:PHE:HD1	1.77	0.49
1:B:412:TYR:HE1	1:B:635:THR:HG22	1.77	0.49
1:B:14:HIS:HB3	1:B:293:LEU:HD21	1.95	0.49
1:B:409:ALA:HB2	1:B:641:LEU:HD11	1.93	0.49
1:B:538:VAL:HB	1:B:539:PRO:HD3	1.94	0.49
1:A:569:LYS:HG3	1:A:570:PRO:HD2	1.94	0.49
1:B:503:LEU:C	1:B:505:LEU:H	2.15	0.49
1:A:377:CYS:HB3	1:A:389:MET:SD	2.53	0.48
1:A:63:ASP:O	1:A:67:VAL:HG23	2.12	0.48
1:B:102:LYS:HB3	1:B:104:ASP:OD1	2.13	0.48
1:B:23:ARG:HA	1:B:37:VAL:HB	1.96	0.48
1:A:308:ARG:HB2	1:A:669:SER:HB2	1.94	0.48
1:B:16:ALA:O	1:B:20:GLN:HG3	2.14	0.48
1:A:8:TRP:CZ3	1:A:267:LEU:HD11	2.49	0.47
1:B:626:THR:OG1	1:B:629:LEU:HD11	2.15	0.47
1:A:559:TYR:O	1:A:571:VAL:HG13	2.14	0.47
1:A:422:PRO:HG2	5:A:801:HOH:O	2.13	0.47
1:B:524:LEU:HB2	1:B:531:ALA:HB2	1.95	0.47
1:A:605:GLN:O	1:A:609:GLY:HA3	2.15	0.47
1:A:254:ARG:HB2	1:A:258:GLY:HA2	1.96	0.47
1:A:284:LEU:HD21	1:A:302:PHE:HE2	1.81	0.46
1:B:596:CYS:O	1:B:600:ILE:HG12	2.16	0.46
1:A:376:ASP:O	1:A:380:LYS:HG2	2.15	0.46
1:B:431:VAL:HG21	1:B:538:VAL:CG2	2.46	0.46
1:A:342:VAL:CG1	1:A:366:ILE:HD13	2.46	0.45
1:B:461:ASN:HA	1:B:662:LEU:CD1	2.44	0.45
1:B:632:ARG:O	1:B:635:THR:HG23	2.15	0.45
1:B:415:SER:HB3	4:B:715:NAG:O5	2.17	0.45
1:B:418:CYS:HA	1:B:421:THR:CB	2.46	0.45
1:A:45:TYR:O	1:A:49:ILE:HG13	2.16	0.45
1:A:482:GLU:HB3	1:A:497:LEU:HD13	1.98	0.45
1:B:157:SER:HB2	1:B:170:LEU:HA	1.99	0.45
1:A:84:PHE:C	1:A:85:TYR:HD1	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:HA	1:A:38:ALA:HB3	1.98	0.44
1:B:417:ASN:C	1:B:419:GLU:H	2.20	0.44
1:B:121:GLY:HA2	1:B:160:PRO:HB2	2.00	0.44
1:A:409:ALA:CB	1:A:641:LEU:HD11	2.47	0.44
1:A:437:SER:HA	1:A:568:ARG:HH12	1.83	0.44
1:B:276:LYS:HD2	1:B:300:HIS:O	2.18	0.43
1:A:84:PHE:C	1:A:85:TYR:CD1	2.92	0.43
1:B:471:ILE:HD13	1:B:476:PHE:CD1	2.54	0.43
1:B:84:PHE:CD2	1:B:303:LEU:HG	2.54	0.43
1:A:61:THR:HB	1:A:251:VAL:HG22	2.00	0.43
1:A:62:LEU:HD13	1:A:66:LEU:HB3	2.01	0.43
1:A:23:ARG:HA	1:A:37:VAL:HB	2.00	0.42
1:B:207:HIS:CD2	1:B:208:SER:N	2.87	0.42
1:A:525:VAL:HG23	1:A:526:GLU:HG3	2.02	0.42
1:B:61:THR:HB	1:B:251:VAL:HG22	2.01	0.42
1:B:103:LYS:HB2	1:B:222:GLN:C	2.39	0.42
1:B:25:HIS:HB3	1:B:274:PHE:CZ	2.54	0.42
1:A:71:TYR:O	1:A:76:ASN:HA	2.20	0.42
1:A:103:LYS:CG	1:A:224:GLU:HG3	2.47	0.42
1:B:358:TRP:CE2	1:B:366:ILE:HG13	2.55	0.42
1:B:384:GLY:HA2	1:B:590:ARG:CZ	2.49	0.42
1:A:452:THR:OG1	1:A:459:GLY:HA3	2.20	0.42
1:A:160:PRO:C	1:A:161:CYS:SG	2.98	0.41
1:A:169:GLN:C	1:A:171:CYS:H	2.24	0.41
1:A:125:SER:HA	1:A:129:ASN:HB2	2.01	0.41
1:A:669:SER:HA	1:A:672:GLU:HG2	2.02	0.41
1:B:71:TYR:HB2	1:B:311:ALA:CB	2.51	0.41
1:B:207:HIS:HB2	1:B:238:TYR:CG	2.55	0.41
1:B:482:GLU:HB3	1:B:497:LEU:HD13	2.03	0.41
1:B:412:TYR:CE1	1:B:635:THR:HG22	2.54	0.41
1:B:471:ILE:HG22	1:B:473:HIS:O	2.20	0.41
1:B:84:PHE:C	1:B:85:TYR:CD1	2.93	0.41
1:B:641:LEU:O	1:B:642:HIS:C	2.59	0.41
1:B:254:ARG:HB2	1:B:258:GLY:HA2	2.02	0.40
1:B:357:GLU:O	1:B:360:VAL:HG12	2.21	0.40
1:A:429:VAL:HB	1:A:561:LEU:HD22	2.03	0.40
1:B:143:ARG:HH21	1:B:143:ARG:HG2	1.86	0.40
1:B:429:VAL:HB	1:B:561:LEU:HD12	2.02	0.40
1:B:593:LYS:O	1:B:597:VAL:HG23	2.21	0.40
1:B:618:ASN:CG	1:B:619:PHE:H	2.23	0.40
1:B:407:VAL:CG1	1:B:594:GLU:HG3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:TYR:CD2	2:B:704:CIT:H22	2.56	0.40
1:B:548:ASP:O	1:B:552:LYS:HG3	2.22	0.40
1:A:139:LEU:O	1:A:143:ARG:NH1	2.55	0.40
1:B:352:ARG:HA	1:B:352:ARG:HD2	1.89	0.40
1:B:477:ASP:HB2	1:B:493:SER:OG	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	675/679 (99%)	625 (93%)	50 (7%)	0	100	100
1	B	676/679 (100%)	625 (92%)	51 (8%)	0	100	100
All	All	1351/1358 (100%)	1250 (92%)	101 (8%)	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	570/572 (100%)	568 (100%)	2 (0%)	89	95
1	B	571/572 (100%)	565 (99%)	6 (1%)	70	87
All	All	1141/1144 (100%)	1133 (99%)	8 (1%)	84	91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	TYR
1	A	249	HIS
1	B	249	HIS
1	B	473	HIS
1	B	585	HIS
1	B	598[A]	HIS
1	B	598[B]	HIS
1	B	642	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	585	HIS

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 30 ligands modelled in this entry, 21 are monoatomic - leaving 9 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	$\#\|Z\|>2$
2	CIT	B	704	-	12,12,12	1.16	1 (8%)	17,17,17	1.33	2 (11%)
2	CIT	A	701	-	12,12,12	1.18	1 (8%)	17,17,17	1.30	2 (11%)
2	CIT	B	702	-	12,12,12	1.16	1 (8%)	17,17,17	1.31	2 (11%)
2	CIT	B	703	-	12,12,12	1.14	1 (8%)	17,17,17	1.34	2 (11%)
2	CIT	B	701	-	12,12,12	1.12	1 (8%)	17,17,17	1.26	2 (11%)
2	CIT	A	703	-	12,12,12	1.15	1 (8%)	17,17,17	1.28	2 (11%)
4	NAG	B	715	1	14,14,15	0.28	0	17,19,21	1.26	2 (11%)
2	CIT	A	704	-	12,12,12	1.15	1 (8%)	17,17,17	1.27	2 (11%)
2	CIT	A	702	-	12,12,12	1.17	1 (8%)	17,17,17	1.26	2 (11%)

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
2	CIT	B	704	-	-	0/16/16/16	-
2	CIT	A	701	-	-	7/16/16/16	-
2	CIT	B	702	-	-	11/16/16/16	-
2	CIT	B	703	-	-	0/16/16/16	-
2	CIT	B	701	-	-	7/16/16/16	-
2	CIT	A	703	-	-	4/16/16/16	-
4	NAG	B	715	1	-	3/6/23/26	0/1/1/1
2	CIT	A	704	-	-	9/16/16/16	-
2	CIT	A	702	-	-	12/16/16/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	CIT	C3-C6	2.34	1.55	1.53
2	A	702	CIT	C3-C6	2.31	1.55	1.53
2	B	704	CIT	C3-C6	2.30	1.55	1.53
2	B	702	CIT	C3-C6	2.25	1.55	1.53
2	A	703	CIT	C3-C6	2.23	1.55	1.53
2	B	703	CIT	C3-C6	2.21	1.55	1.53
2	A	704	CIT	C3-C6	2.14	1.55	1.53
2	B	701	CIT	C3-C6	2.11	1.55	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	715	NAG	C2-N2-C7	3.76	128.25	122.90
2	B	703	CIT	O5-C6-C3	-3.50	117.29	122.25
2	B	704	CIT	O5-C6-C3	-3.46	117.36	122.25
2	B	702	CIT	O5-C6-C3	-3.29	117.59	122.25
2	A	701	CIT	O5-C6-C3	-3.29	117.59	122.25
2	A	703	CIT	O5-C6-C3	-3.29	117.59	122.25
2	B	701	CIT	O5-C6-C3	-3.26	117.64	122.25
2	A	704	CIT	O5-C6-C3	-3.17	117.77	122.25
2	A	702	CIT	O5-C6-C3	-3.06	117.91	122.25
4	B	715	NAG	C1-C2-N2	2.92	115.47	110.49
2	B	703	CIT	O6-C6-C3	2.65	117.65	113.05
2	B	704	CIT	O6-C6-C3	2.58	117.54	113.05
2	A	701	CIT	O6-C6-C3	2.56	117.49	113.05
2	A	703	CIT	O6-C6-C3	2.54	117.46	113.05
2	B	702	CIT	O6-C6-C3	2.53	117.44	113.05
2	B	701	CIT	O6-C6-C3	2.37	117.17	113.05
2	A	704	CIT	O6-C6-C3	2.36	117.15	113.05
2	A	702	CIT	O6-C6-C3	2.33	117.10	113.05

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	CIT	C1-C2-C3-O7
2	A	701	CIT	C1-C2-C3-C4
2	A	701	CIT	C1-C2-C3-C6
2	A	701	CIT	O7-C3-C6-O5
2	A	701	CIT	O7-C3-C6-O6
2	A	701	CIT	C4-C3-C6-O5
2	A	701	CIT	C4-C3-C6-O6
2	A	702	CIT	C1-C2-C3-O7
2	A	702	CIT	C1-C2-C3-C4
2	A	702	CIT	C1-C2-C3-C6
2	A	702	CIT	C2-C3-C4-C5
2	A	702	CIT	O7-C3-C4-C5
2	A	703	CIT	O7-C3-C6-O5
2	A	703	CIT	O7-C3-C6-O6
2	A	703	CIT	C4-C3-C6-O5
2	A	703	CIT	C4-C3-C6-O6
2	A	704	CIT	O7-C3-C6-O5
2	A	704	CIT	O7-C3-C6-O6
2	A	704	CIT	C4-C3-C6-O5
2	A	704	CIT	C4-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	701	CIT	C1-C2-C3-C4
2	B	701	CIT	C1-C2-C3-C6
2	B	701	CIT	O7-C3-C6-O5
2	B	701	CIT	O7-C3-C6-O6
2	B	701	CIT	C4-C3-C6-O5
2	B	701	CIT	C4-C3-C6-O6
2	B	702	CIT	C2-C3-C4-C5
2	B	702	CIT	O7-C3-C4-C5
2	B	702	CIT	C6-C3-C4-C5
4	B	715	NAG	C8-C7-N2-C2
4	B	715	NAG	O7-C7-N2-C2
2	A	704	CIT	C1-C2-C3-C4
2	A	704	CIT	C1-C2-C3-C6
2	B	702	CIT	C2-C3-C6-O6
2	A	702	CIT	C6-C3-C4-C5
2	B	701	CIT	C1-C2-C3-O7
4	B	715	NAG	C3-C2-N2-C7
2	B	702	CIT	O7-C3-C6-O5
2	A	702	CIT	C2-C3-C6-O5
2	A	702	CIT	C2-C3-C6-O6
2	A	702	CIT	C4-C3-C6-O5
2	A	702	CIT	C4-C3-C6-O6
2	B	702	CIT	C4-C3-C6-O5
2	B	702	CIT	C4-C3-C6-O6
2	B	702	CIT	C2-C3-C6-O5
2	A	704	CIT	C1-C2-C3-O7
2	A	702	CIT	O7-C3-C6-O5
2	A	702	CIT	O7-C3-C6-O6
2	B	702	CIT	O7-C3-C6-O6
2	B	702	CIT	O2-C1-C2-C3
2	B	702	CIT	O1-C1-C2-C3
2	A	704	CIT	O1-C1-C2-C3
2	A	704	CIT	O2-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	704	CIT	1	0
2	A	701	CIT	1	0
4	B	715	NAG	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	676/679 (99%)	-0.37	0	100	100	49, 76, 133, 155	1 (0%)
1	B	676/679 (99%)	-0.30	0	100	100	49, 77, 131, 158	2 (0%)
All	All	1352/1358 (99%)	-0.34	0	100	100	49, 77, 133, 158	3 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	B	715	14/15	0.58	0.12	110,113,115,117	0
2	CIT	B	704	13/13	0.64	0.10	144,147,149,149	0
2	CIT	B	701	13/13	0.69	0.11	115,118,119,119	0
2	CIT	A	703	13/13	0.73	0.10	113,116,118,119	0
2	CIT	A	702	13/13	0.77	0.09	113,118,119,119	0
3	AU	A	708	1/1	0.78	0.12	97,97,97,97	1
2	CIT	B	703	13/13	0.79	0.10	118,122,124,125	0

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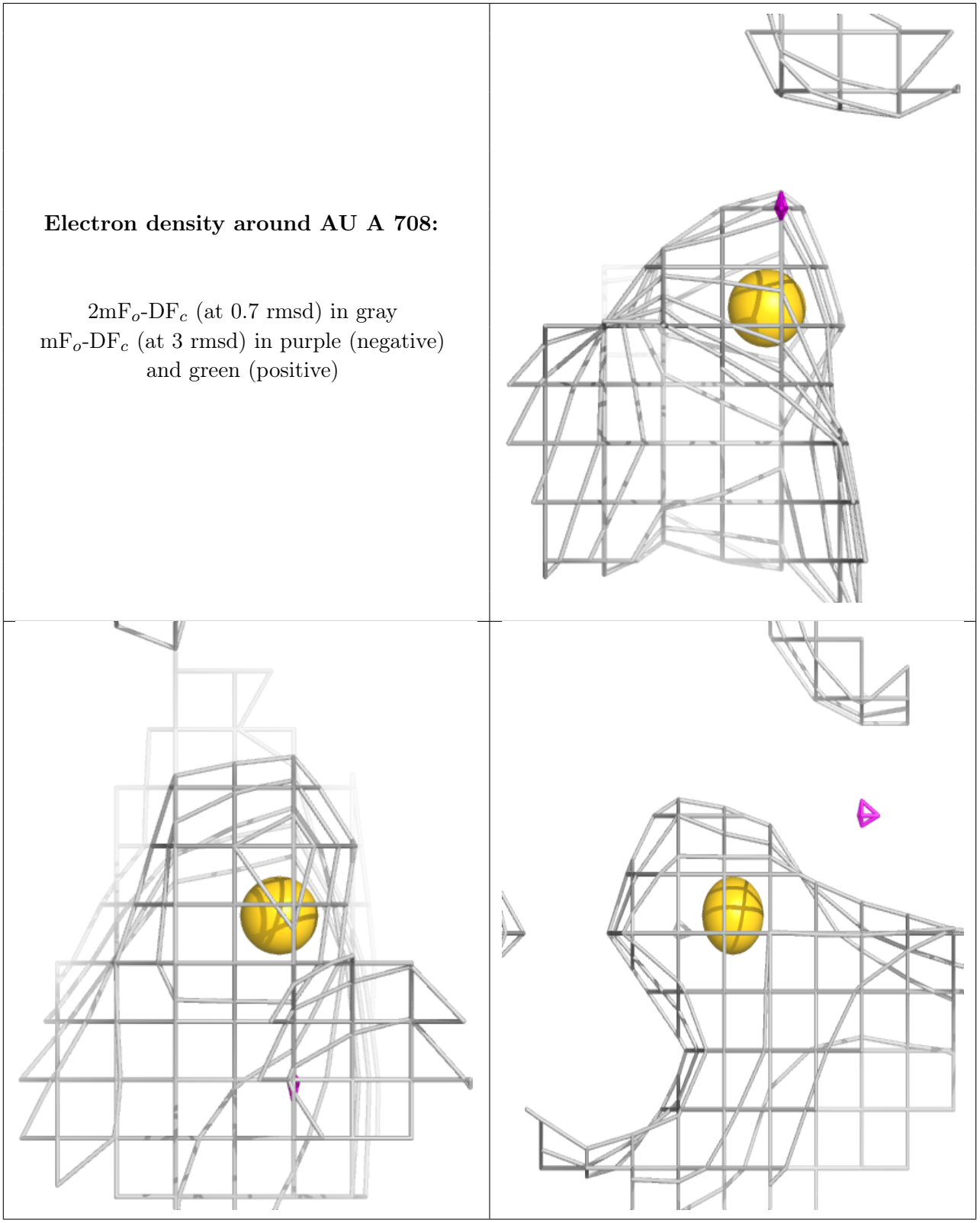
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CIT	A	701	13/13	0.79	0.10	114,116,118,118	0
2	CIT	B	702	13/13	0.83	0.08	116,118,119,120	0
3	AU	A	713	1/1	0.85	0.07	76,76,76,76	1
2	CIT	A	704	13/13	0.85	0.07	98,102,102,102	0
3	AU	A	707	1/1	0.87	0.09	99,99,99,99	1
3	AU	A	709[C]	1/1	0.88	0.10	77,77,77,77	1
3	AU	A	709[A]	1/1	0.88	0.10	95,95,95,95	1
3	AU	B	711	1/1	0.88	0.09	140,140,140,140	1
3	AU	A	709[B]	1/1	0.88	0.10	95,95,95,95	1
3	AU	A	710	1/1	0.89	0.07	76,76,76,76	1
3	AU	B	708	1/1	0.89	0.18	91,91,91,91	1
3	AU	A	711	1/1	0.90	0.07	80,80,80,80	1
3	AU	B	712	1/1	0.93	0.07	94,94,94,94	1
3	AU	B	710	1/1	0.93	0.07	80,80,80,80	1
3	AU	B	706	1/1	0.95	0.06	121,121,121,121	1
3	AU	B	707	1/1	0.96	0.11	80,80,80,80	1
3	AU	B	713	1/1	0.96	0.10	97,97,97,97	1
3	AU	B	714	1/1	0.96	0.10	79,79,79,79	1
3	AU	B	705	1/1	0.96	0.04	107,107,107,107	1
3	AU	A	705	1/1	0.98	0.04	71,71,71,71	1
3	AU	B	709	1/1	0.98	0.03	117,117,117,117	1
3	AU	A	712	1/1	0.98	0.03	90,90,90,90	1
3	AU	A	706	1/1	0.98	0.06	103,103,103,103	1

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

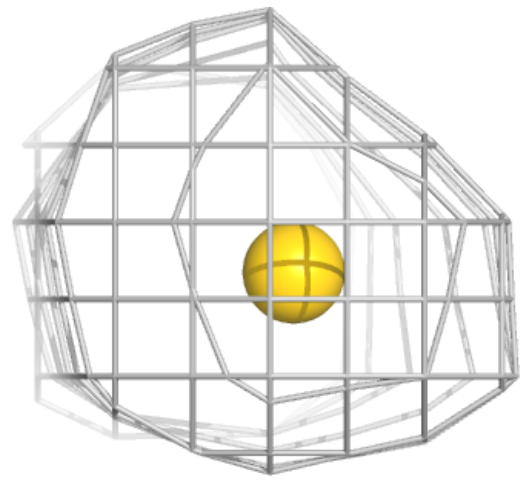
Electron density around AU A 708:

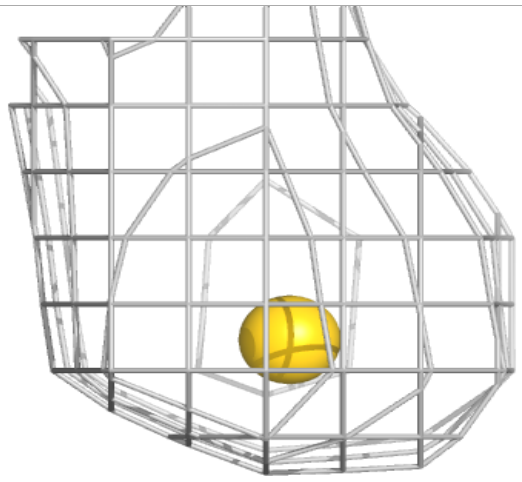
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

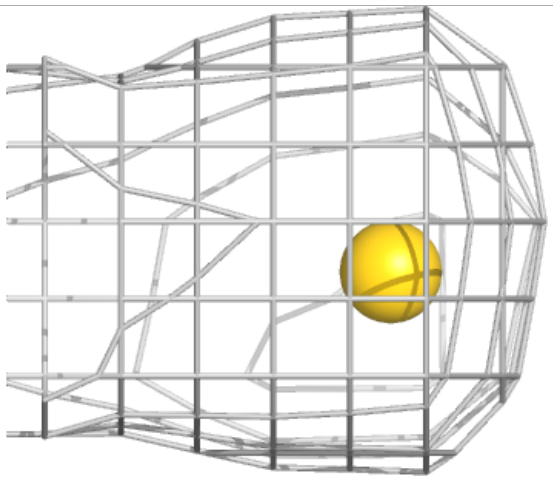


Electron density around AU A 713:

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

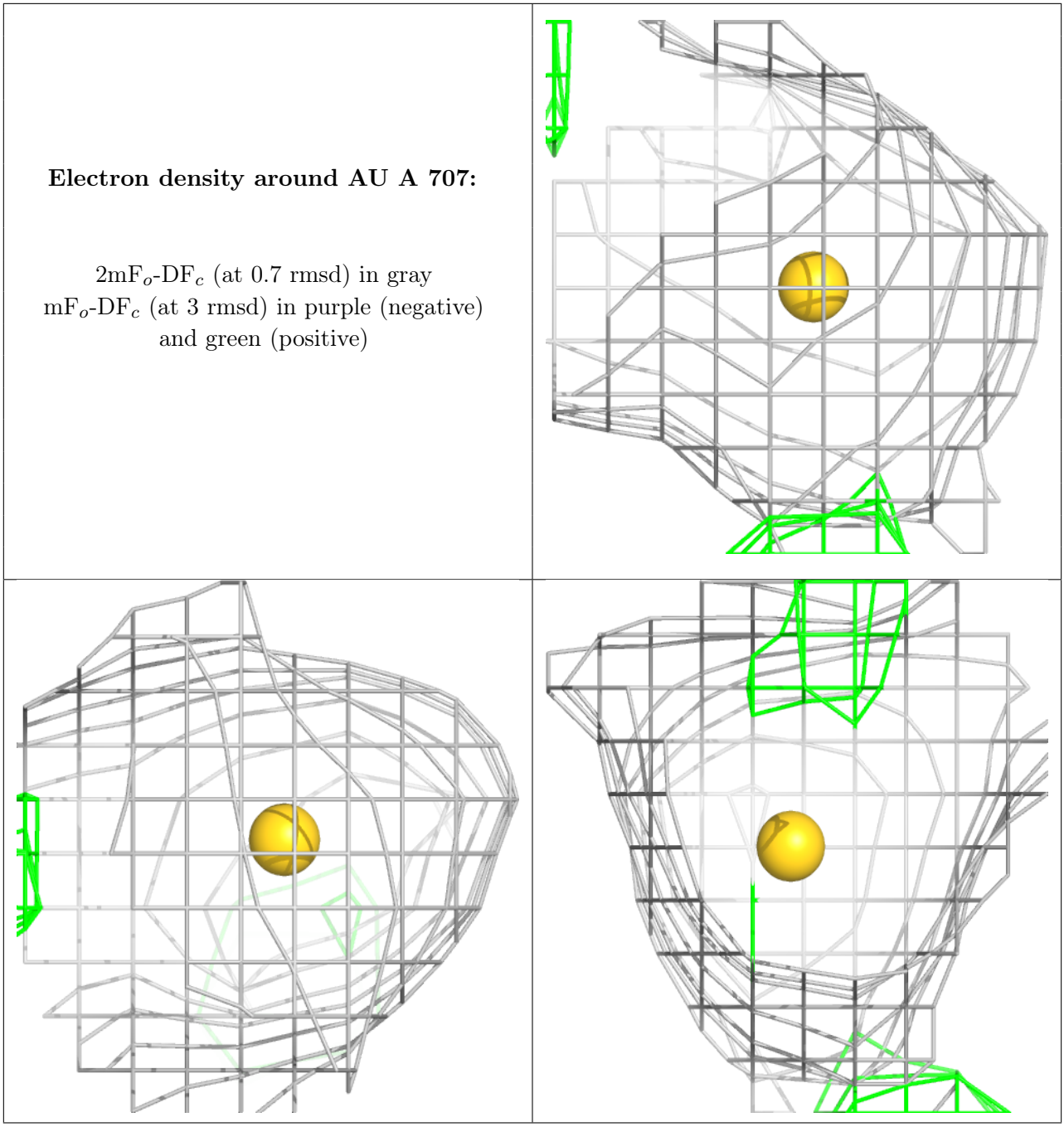






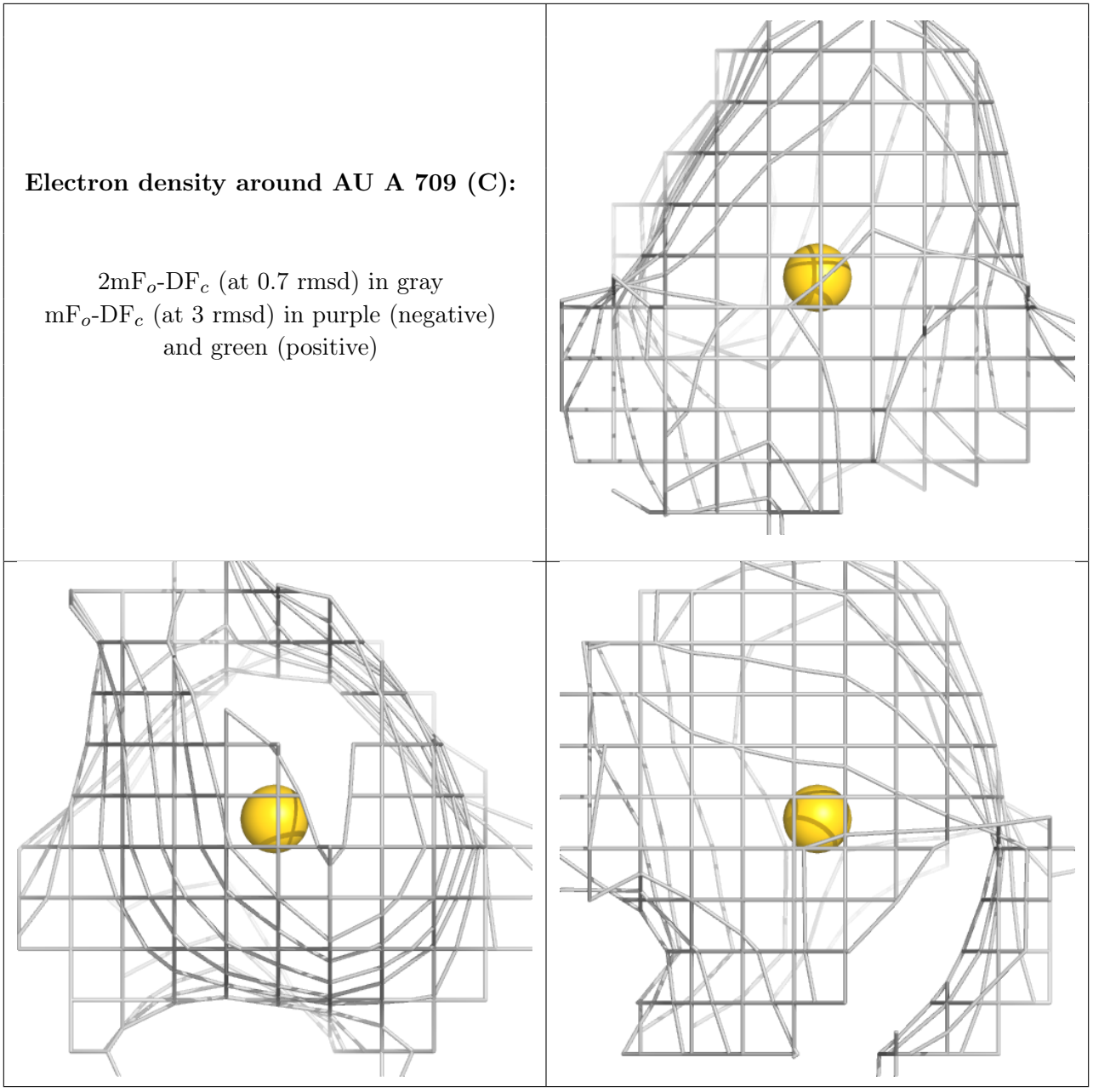
Electron density around AU A 707:

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



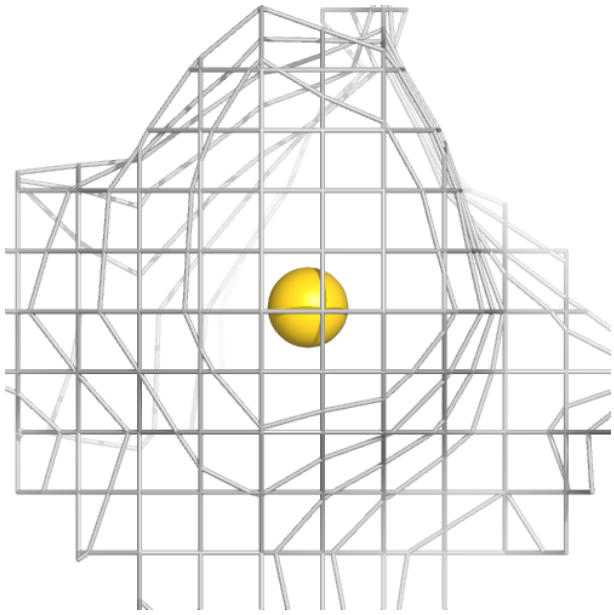
Electron density around AU A 709 (C):

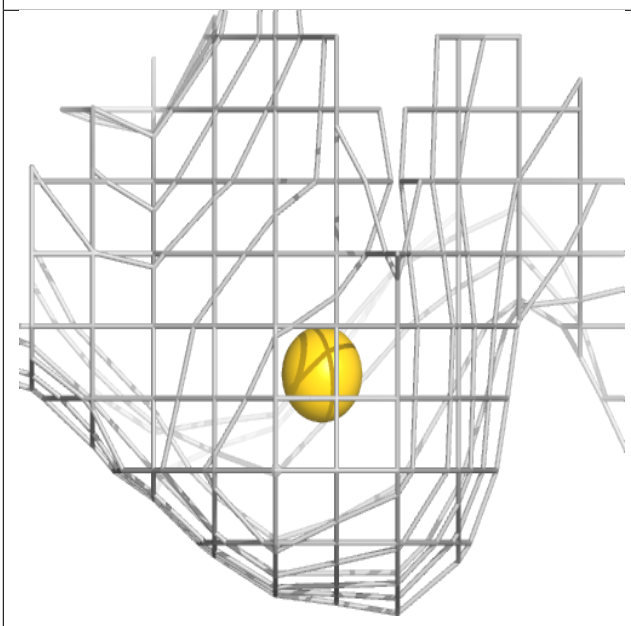
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

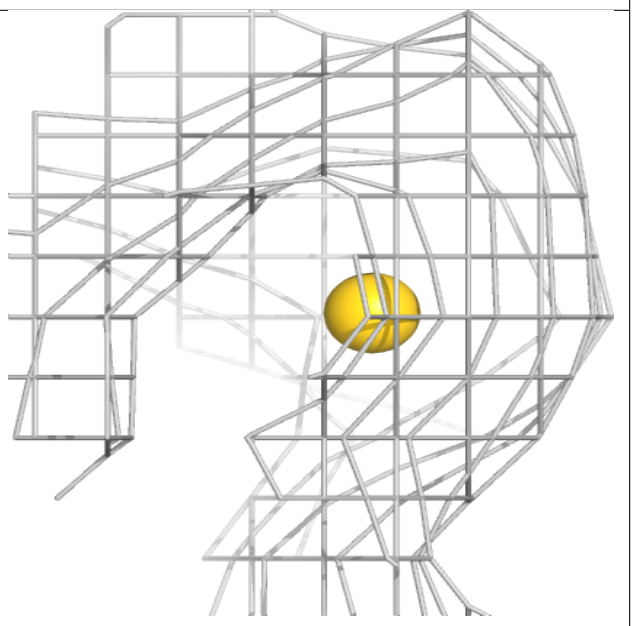


Electron density around AU A 709 (A):

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

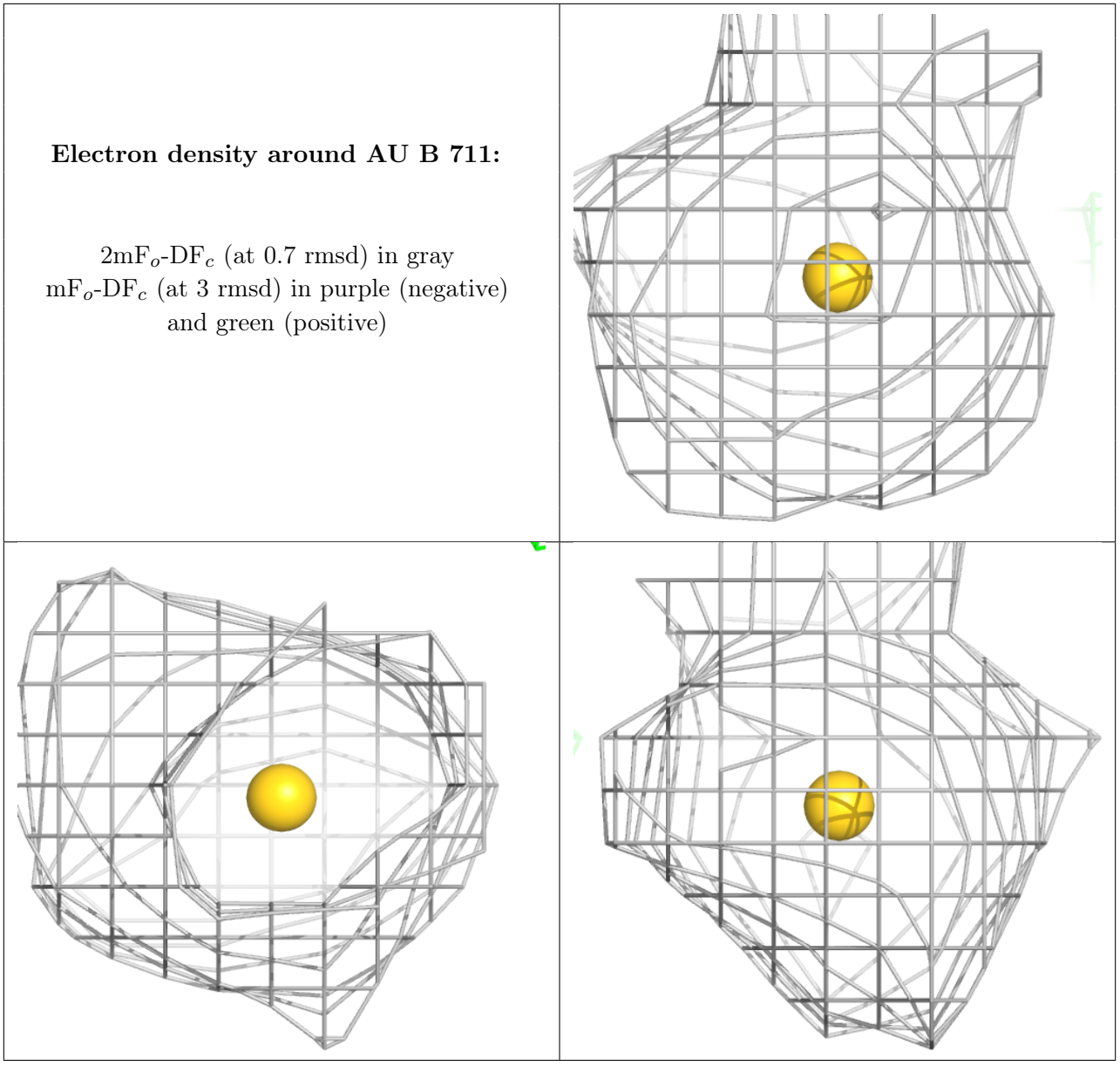






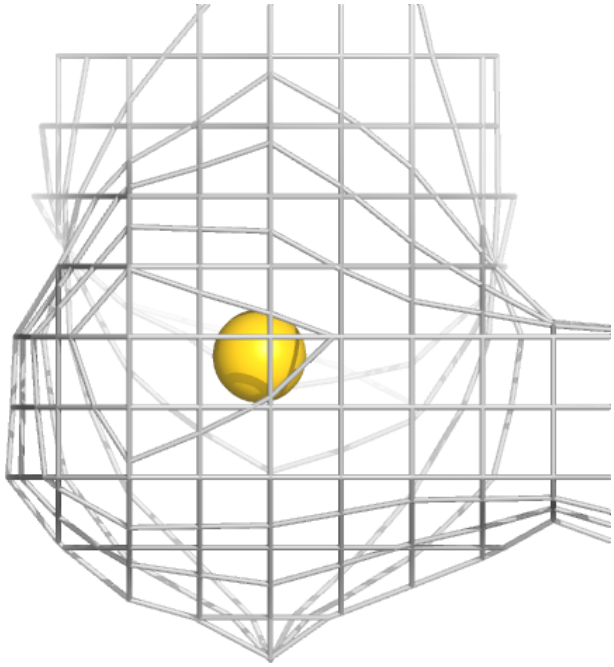
Electron density around AU B 711:

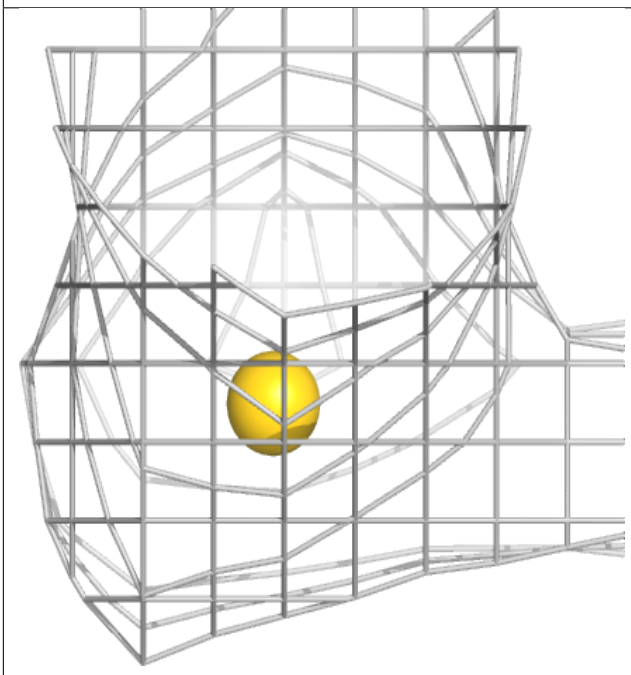
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

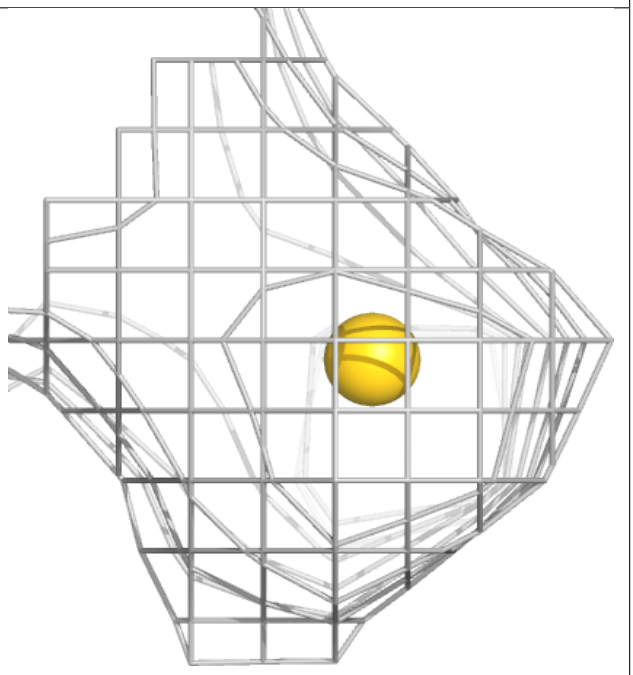


Electron density around AU A 709 (B):

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

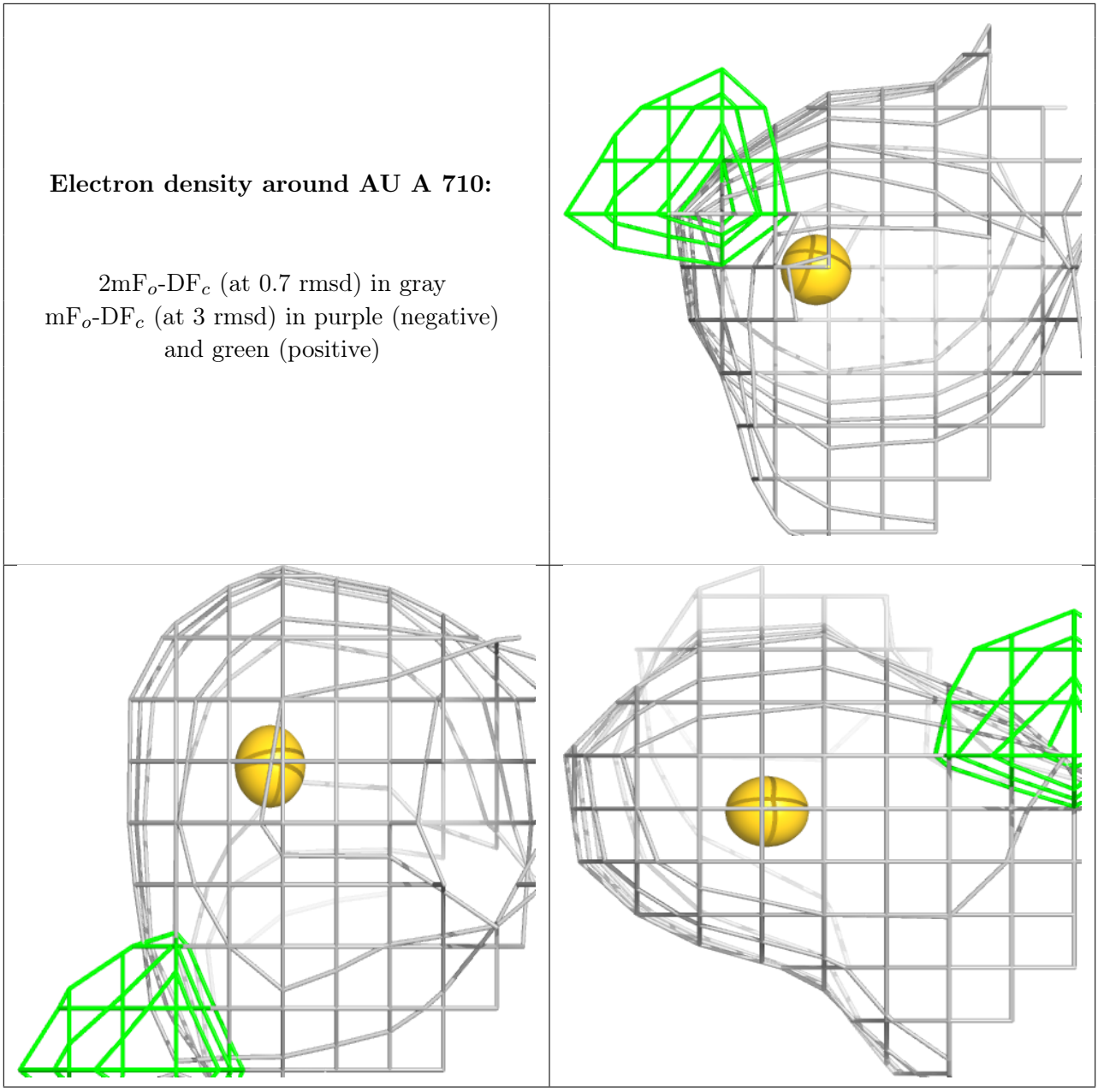






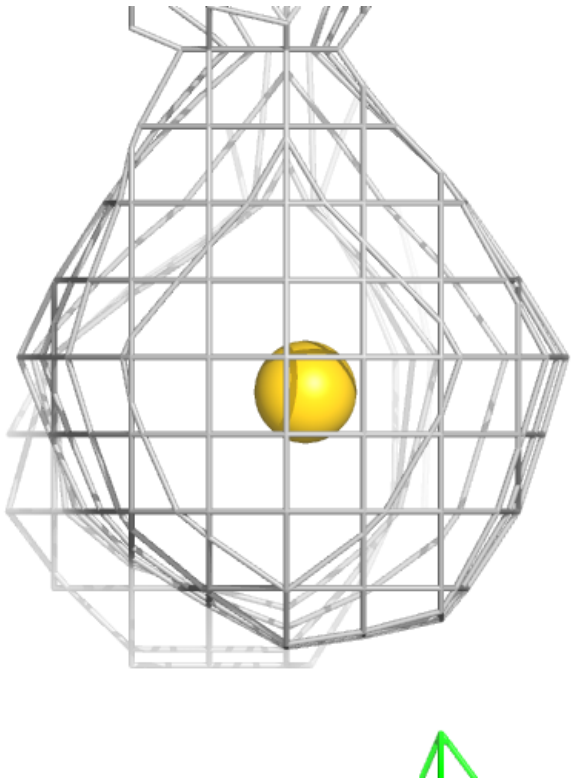
Electron density around AU A 710:

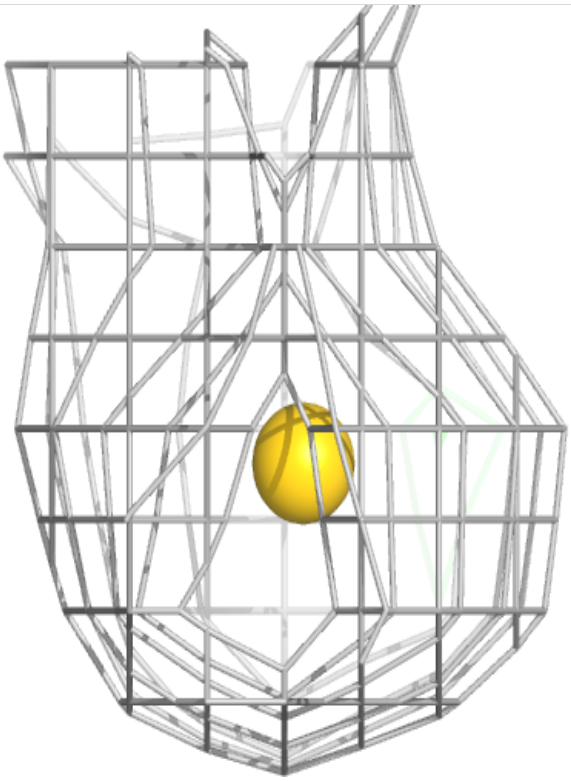
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

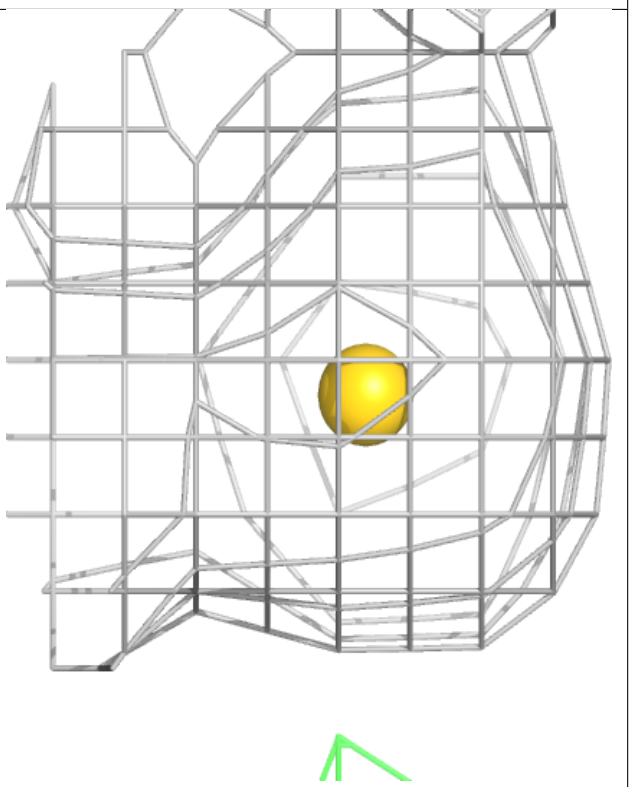


Electron density around AU B 708:

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

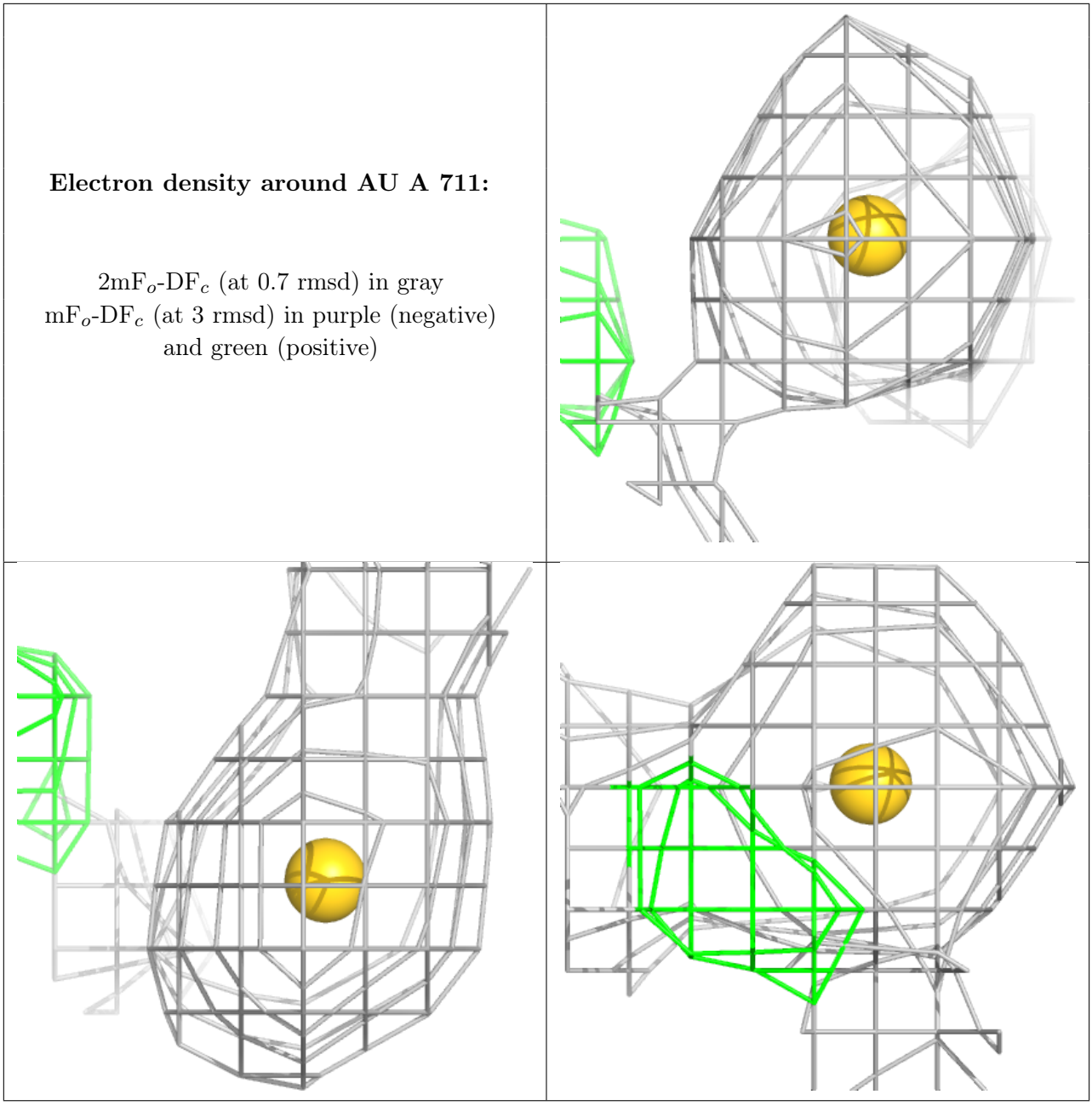






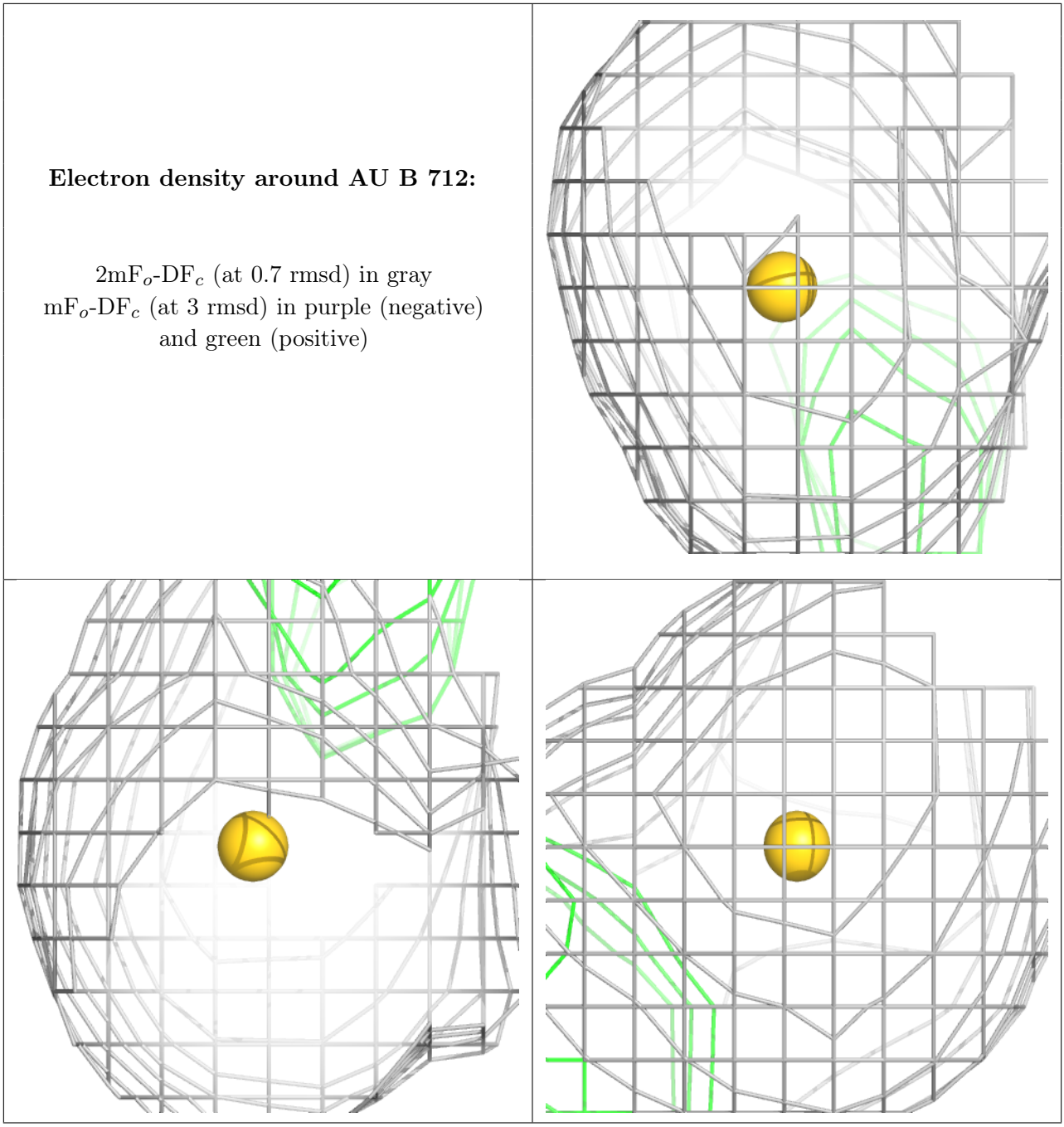
Electron density around AU A 711:

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



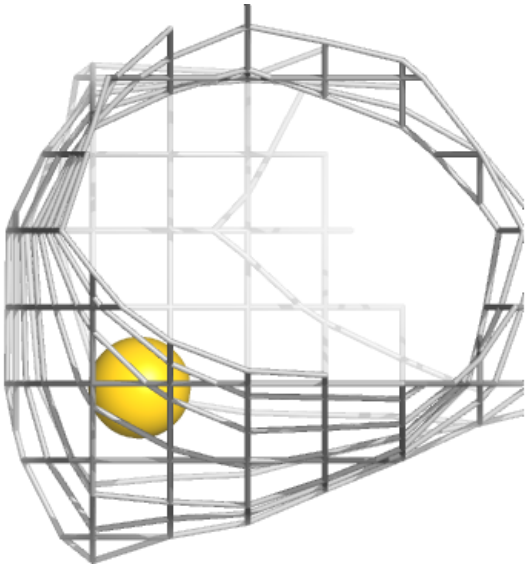
Electron density around AU B 712:

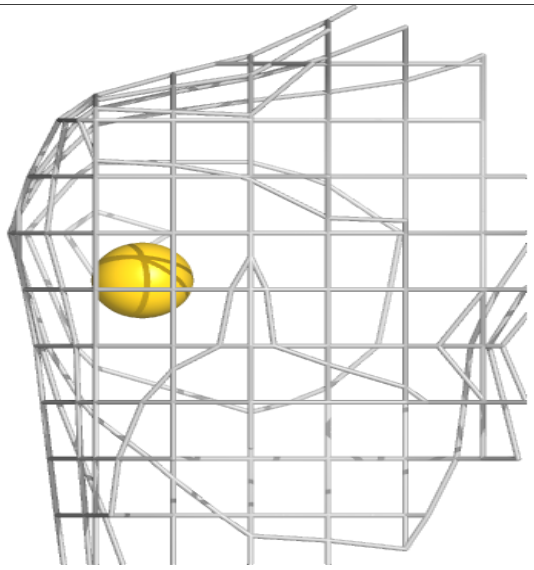
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

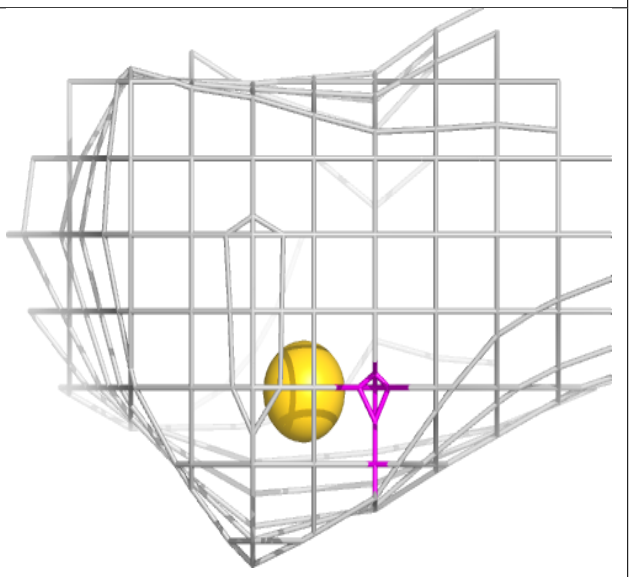


Electron density around AU B 710:

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

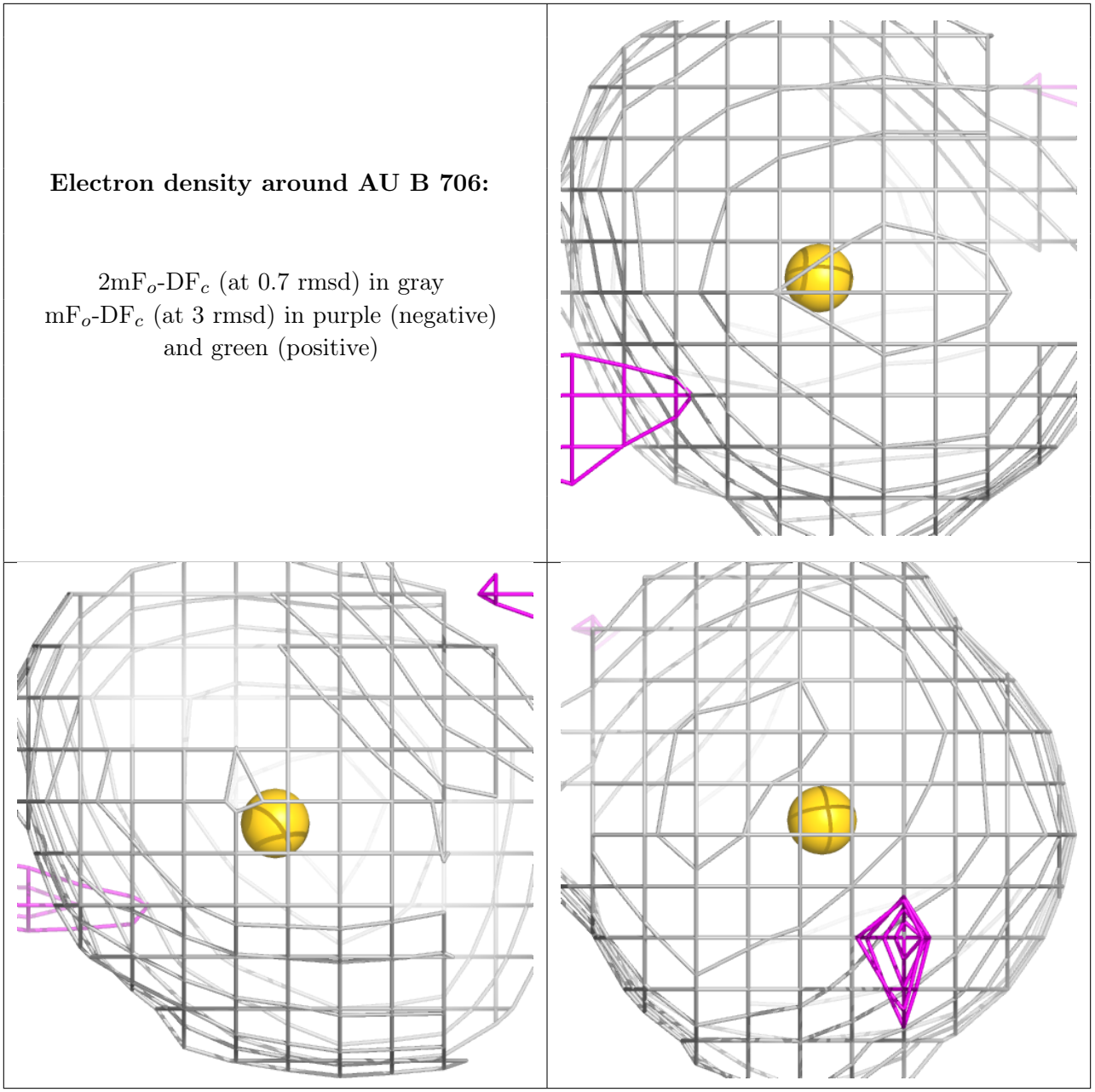






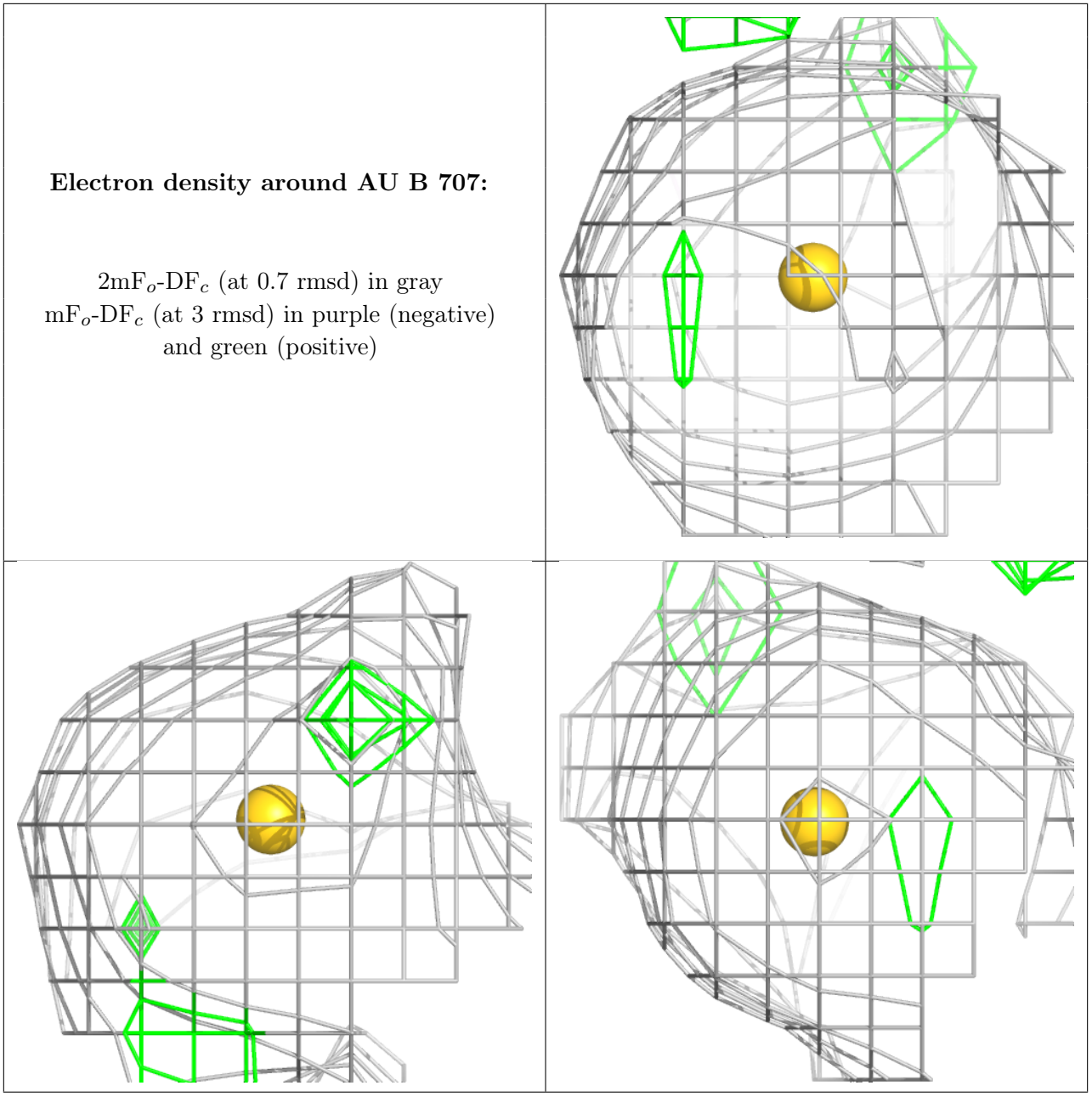
Electron density around AU B 706:

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



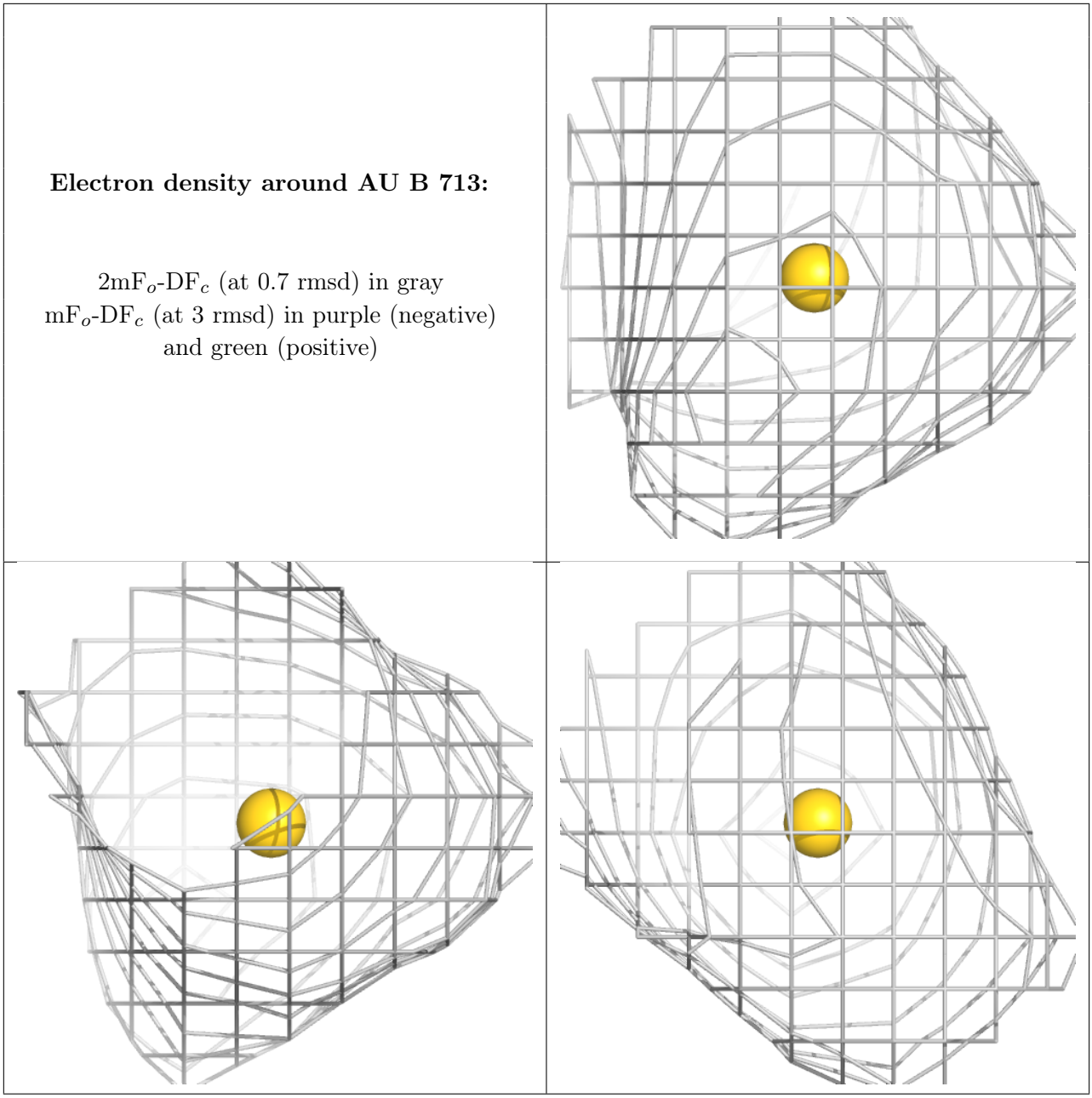
Electron density around AU B 707:

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



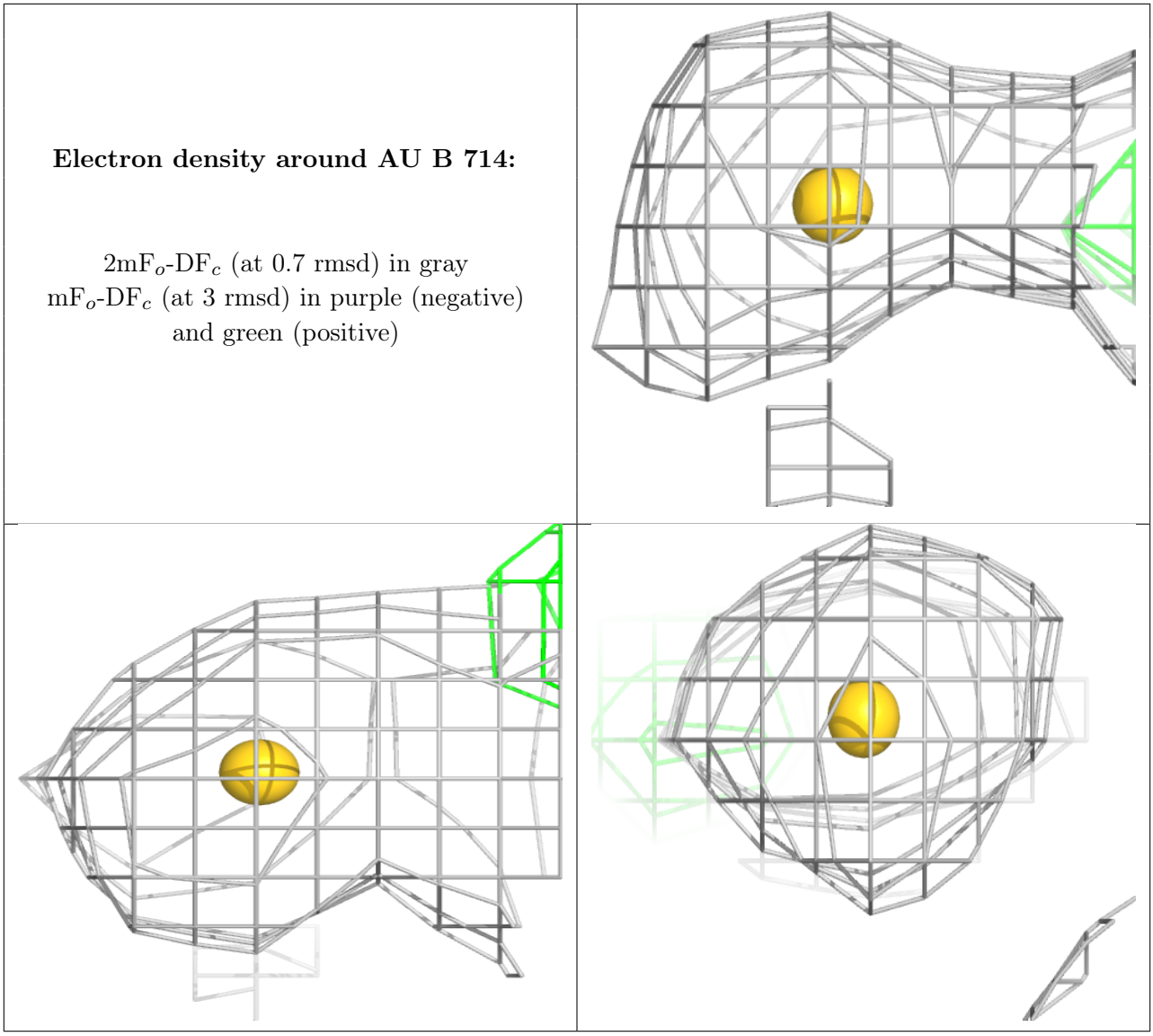
Electron density around AU B 713:

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



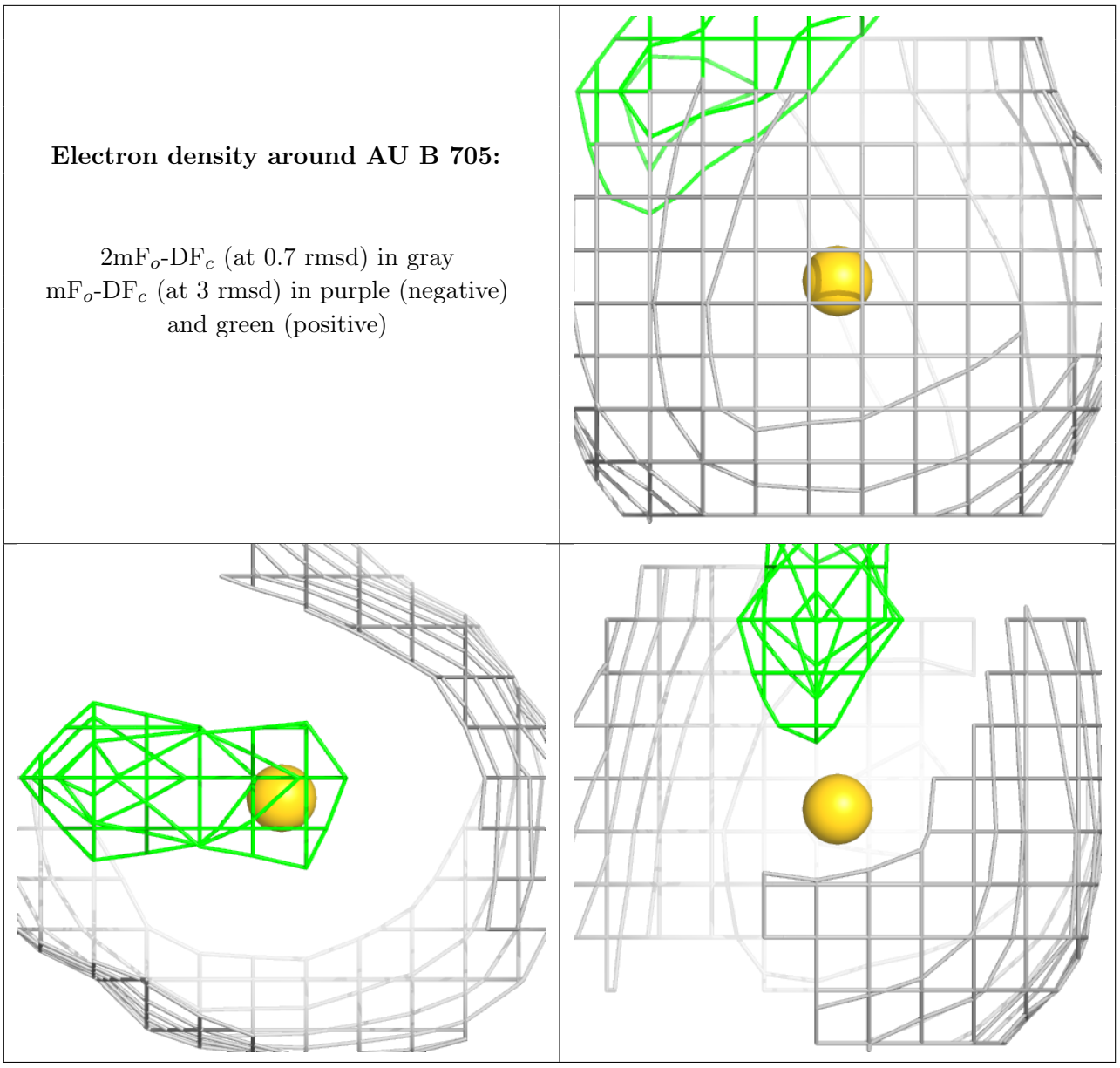
Electron density around AU B 714:

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



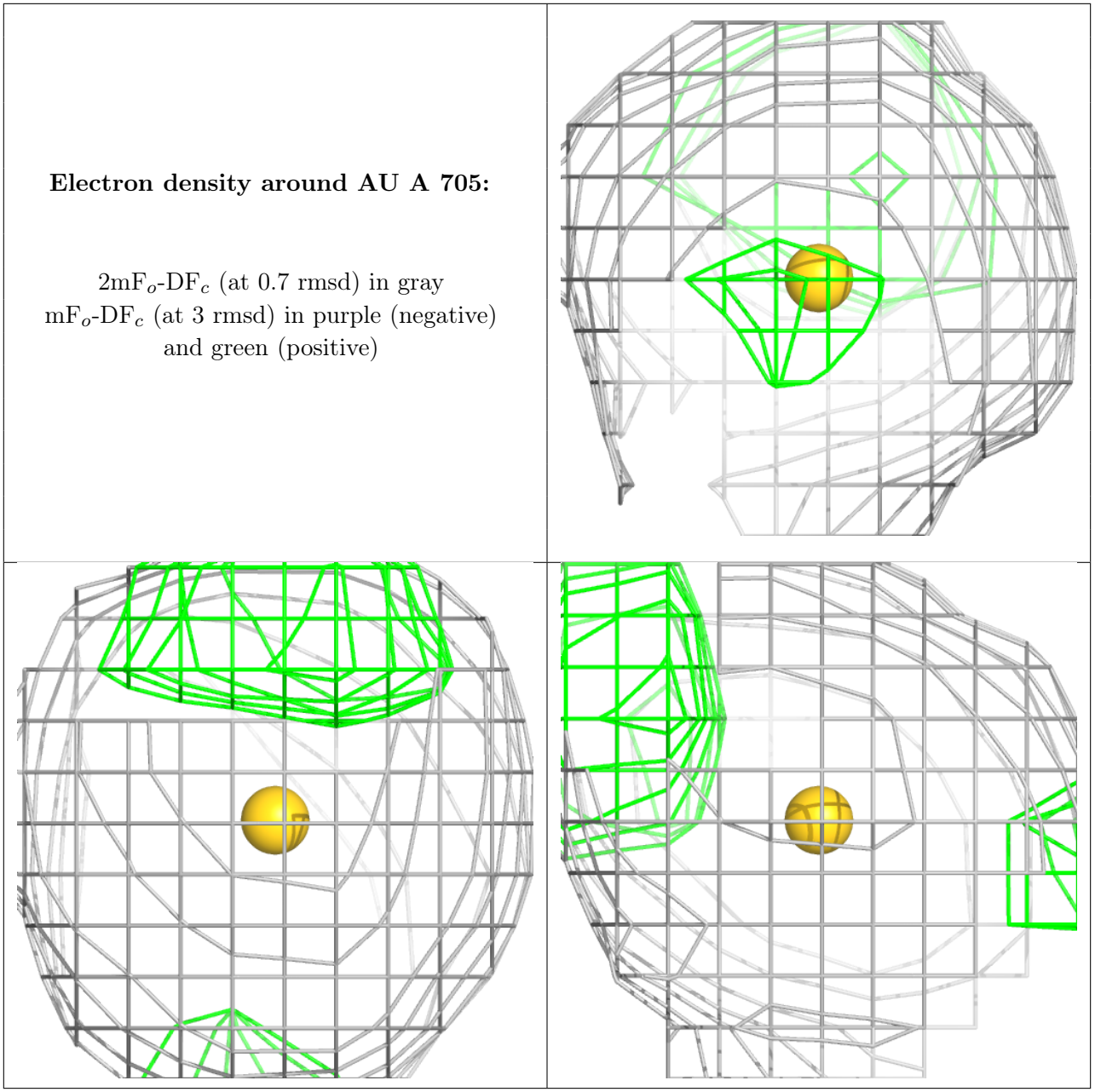
Electron density around AU B 705:

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



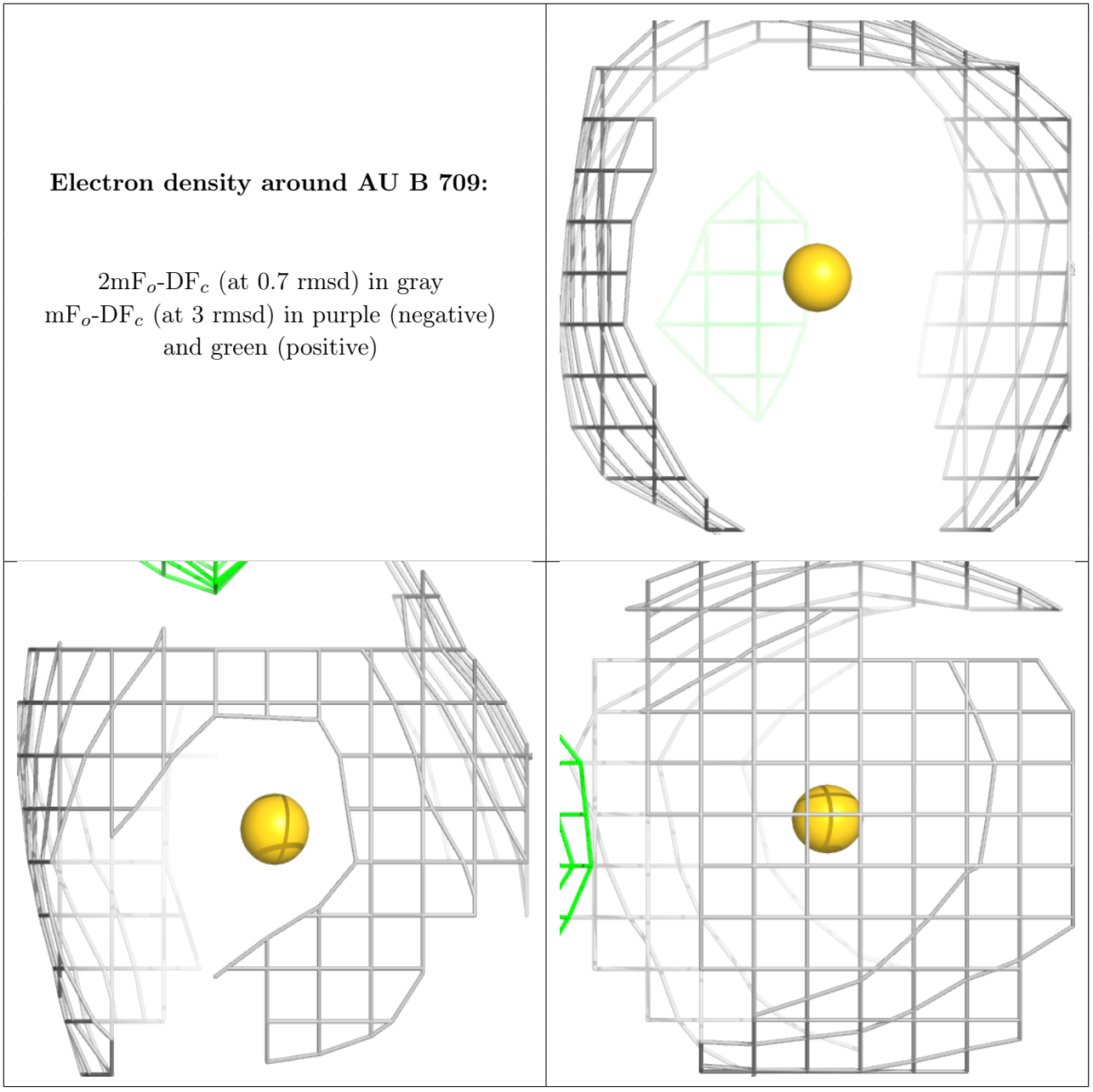
Electron density around AU A 705:

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



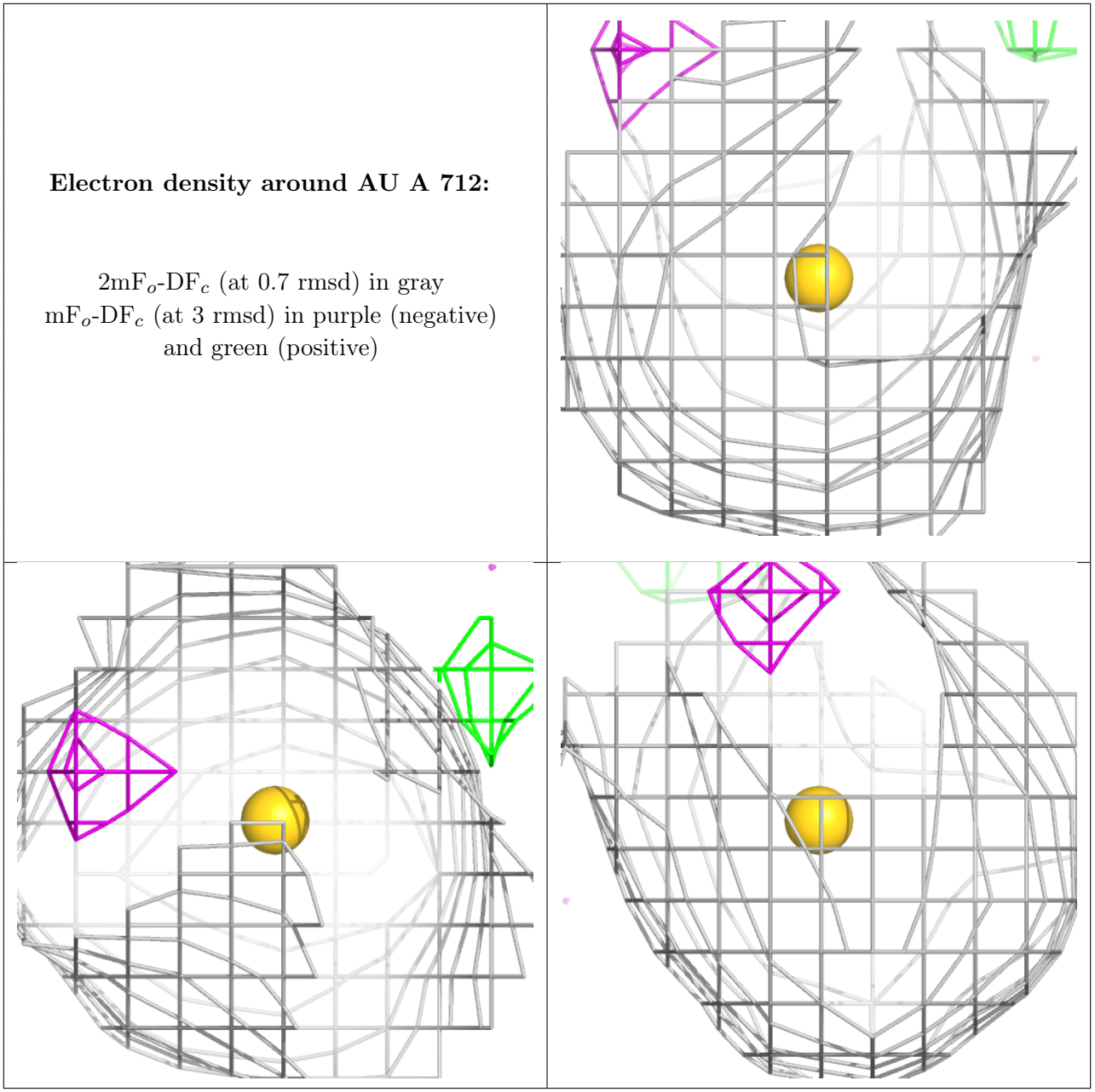
Electron density around AU B 709:

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



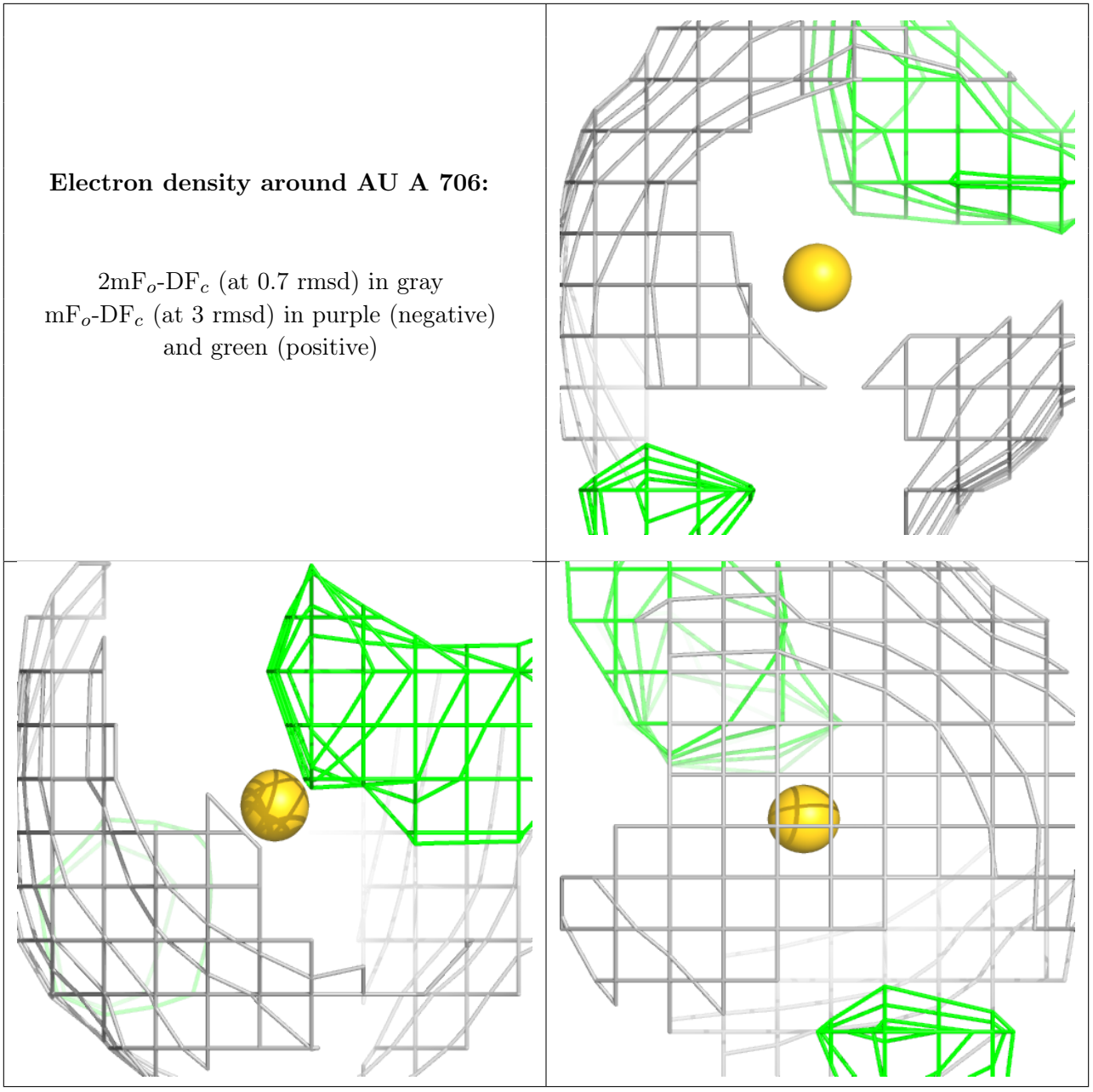
Electron density around AU A 712:

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



Electron density around AU A 706:

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



6.5 Other polymers (i)

There are no such residues in this entry.