Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 04:36 AM JST

PDB ID	:	6KR6
Title	:	Crystal structure of Drosophila Piwi
Authors	:	Yamaguchi, S.; Oe, A.; Yamashita, K.; Hirano, S.; Mastumoto, N.; Ishitani, R.; Nishimasu, H.; Nureki, O.
Deposited on	:	2019-08-21
Resolution	:	2.90 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:

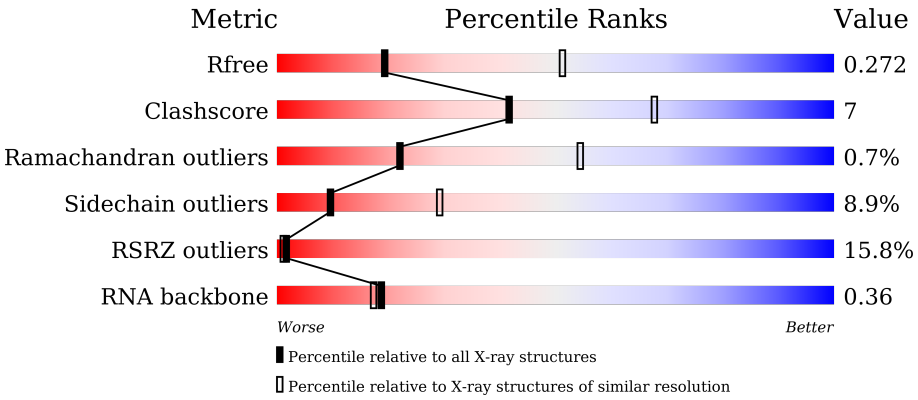
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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	810	14%, 69%, 17%, ·, 12%
2	B	5	80%, 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5504 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein piwi.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	713	5402	3463	907	1002	30	0	1	0

- Molecule 2 is a RNA chain called piRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	5	87	37	11	34	5	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	8	8	8	0	0

- Molecule 4 is MERCURY (II) ION (three-letter code: HG) (formula: Hg) (labeled as "Ligand of Interest" by depositor).

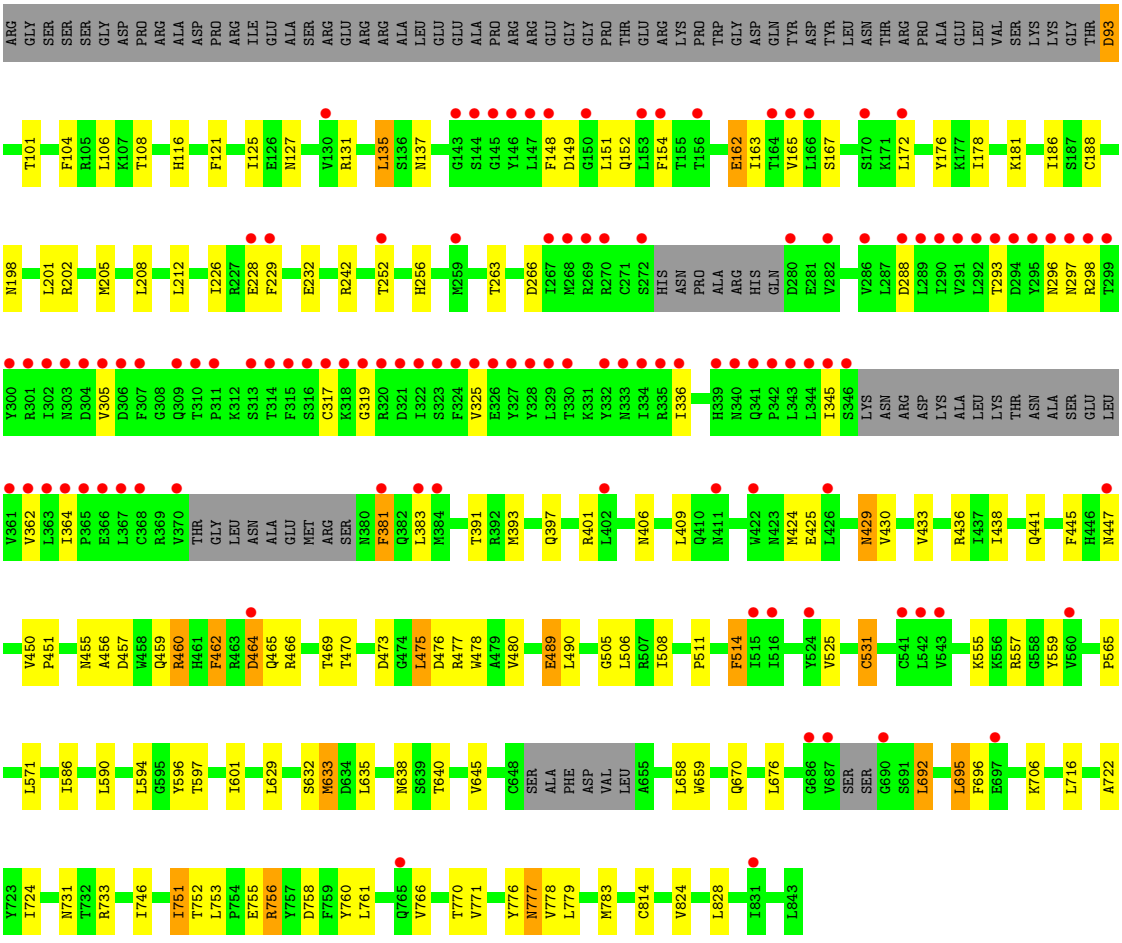
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
4	A	6	7	7	0	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Protein piwi

Chain A:



- Molecule 2: piRNA

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	62.09Å 115.64Å 119.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 2.90 39.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.90-2.90) 100.0 (39.90-2.90)	Depositor EDS
R_{merge}	0.55	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.239 , 0.259 0.247 , 0.272	Depositor DCC
R_{free} test set	947 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	94.7	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 85.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.039 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5504	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: ZN, HG

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	0.25	0/5516	0.44	1/7525 (0.0%)
2	B	1.14	1/91 (1.1%)	0.70	0/137
All	All	0.29	1/5607 (0.0%)	0.45	1/7662 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.76	1.48	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	695	LEU	CA-CB-CG	6.29	129.77	115.30

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	5402	0	5097	74	0
2	B	87	0	41	0	0
3	A	8	0	0	0	0
4	A	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5504	0	5138	74	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 (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HE	1:A:212:LEU:HD21	1.50	0.76
1:A:469:THR:HB	1:A:597:THR:H	1.55	0.70
1:A:393:MET:HE1	1:A:401:ARG:HD2	1.75	0.68
1:A:692:LEU:HD11	1:A:756:ARG:HH21	1.59	0.67
1:A:559:TYR:HE1	1:A:565:PRO:HA	1.59	0.67
1:A:462:PHE:HA	1:A:465:GLN:HB3	1.78	0.65
1:A:149:ASP:OD1	1:A:152:GLN:N	2.30	0.65
1:A:441:GLN:HB3	1:A:601:ILE:HD11	1.79	0.64
1:A:208:LEU:HD11	1:A:409:LEU:HD12	1.79	0.63
1:A:761:LEU:HB3	1:A:776:TYR:HE2	1.64	0.62
1:A:226:ILE:HG22	1:A:229:PHE:H	1.64	0.61
1:A:475:LEU:HD23	1:A:506:LEU:HD11	1.85	0.59
1:A:208:LEU:HD21	1:A:409:LEU:HA	1.83	0.59
1:A:469:THR:HG22	1:A:596:TYR:HD2	1.71	0.56
1:A:632:SER:HB2	1:A:635:LEU:HD21	1.87	0.55
1:A:162:GLU:HG2	1:A:181:LYS:HA	1.89	0.54
1:A:201:LEU:O	1:A:205:MET:HG2	2.07	0.54
1:A:525:VAL:HG13	1:A:557:ARG:HG3	1.89	0.54
1:A:475:LEU:HB2	1:A:508:ILE:HA	1.89	0.53
1:A:758:ASP:HB3	1:A:777:ASN:HA	1.91	0.53
1:A:429:ASN:OD1	1:A:429:ASN:N	2.42	0.52
1:A:101:THR:HG21	1:A:433:VAL:HG23	1.91	0.52
1:A:756:ARG:NH2	1:A:777:ASN:OD1	2.43	0.52
1:A:761:LEU:HB3	1:A:776:TYR:CE2	2.43	0.52
1:A:753:LEU:HD23	1:A:756:ARG:HH11	1.75	0.51
1:A:459:GLN:HA	1:A:462:PHE:CZ	2.46	0.51
1:A:824:VAL:HA	1:A:828:LEU:HB2	1.92	0.51
1:A:480:VAL:HG11	1:A:490:LEU:HD11	1.92	0.51
1:A:381:PHE:H	1:A:381:PHE:HD2	1.60	0.50
1:A:670:GLN:HB3	1:A:676:LEU:HD23	1.93	0.49
1:A:163:ILE:HD12	1:A:163:ILE:HA	1.82	0.47
1:A:766:VAL:HG22	1:A:771:VAL:HG22	1.96	0.47
1:A:296:ASN:O	1:A:298:ARG:N	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:ILE:HG12	1:A:778:VAL:HG22	1.97	0.47
1:A:125:ILE:HG22	1:A:127:ASN:H	1.80	0.46
1:A:263:THR:HG23	1:A:266:ASP:H	1.81	0.46
1:A:108:THR:HG22	1:A:424:MET:HB3	1.96	0.46
1:A:165:VAL:HG23	1:A:178:ILE:HB	1.97	0.46
1:A:514:PHE:CE2	1:A:531:CYS:HB2	2.51	0.45
1:A:455:ASN:O	1:A:457:ASP:N	2.43	0.45
1:A:475:LEU:HG	1:A:508:ILE:HG12	1.97	0.45
1:A:633:MET:O	1:A:638:ASN:HB3	2.16	0.45
1:A:121:PHE:CD1	1:A:178:ILE:HG12	2.52	0.45
1:A:489:GLU:HG3	1:A:571:LEU:HD11	1.99	0.45
1:A:659:TRP:CZ2	1:A:706:LYS:HB3	2.52	0.44
1:A:256:HIS:CE1	1:A:391:THR:HG21	2.52	0.44
1:A:460:ARG:H	1:A:460:ARG:HG3	1.43	0.44
1:A:722:ALA:HB2	1:A:783:MET:HG3	1.99	0.44
1:A:121:PHE:CE2	1:A:131:ARG:HB3	2.53	0.43
1:A:692:LEU:HD11	1:A:777:ASN:OD1	2.18	0.43
1:A:293:THR:OG1	1:A:296:ASN:O	2.32	0.43
1:A:758:ASP:N	1:A:758:ASP:OD1	2.52	0.43
1:A:696:PHE:HD2	1:A:779:LEU:HB3	1.85	0.42
1:A:154:PHE:CE1	1:A:186:ILE:HD11	2.55	0.42
1:A:464:ASP:N	1:A:464:ASP:OD1	2.51	0.42
1:A:135:LEU:HD12	1:A:148:PHE:CZ	2.55	0.42
1:A:475:LEU:HD22	1:A:594:LEU:HD11	2.01	0.42
1:A:397:GLN:HB3	1:A:401:ARG:NH2	2.35	0.42
1:A:445:PHE:HB3	1:A:466:ARG:O	2.20	0.42
1:A:478:TRP:CE2	1:A:511:PRO:HB3	2.55	0.42
1:A:104:PHE:CE1	1:A:430:VAL:HG22	2.55	0.41
1:A:383:LEU:HD23	1:A:383:LEU:HA	1.78	0.41
1:A:393:MET:HE2	1:A:393:MET:HB3	1.99	0.41
1:A:450:VAL:HG22	1:A:451:PRO:HD2	2.02	0.41
1:A:470:THR:HG21	1:A:505:GLY:O	2.21	0.41
1:A:93:ASP:OD1	1:A:93:ASP:N	2.53	0.41
1:A:116:HIS:CE1	1:A:152:GLN:OE1	2.73	0.41
1:A:167:SER:HB3	1:A:176:TYR:CZ	2.55	0.41
1:A:555:LYS:HD3	1:A:555:LYS:HA	1.94	0.41
1:A:586:ILE:O	1:A:590:LEU:HG	2.21	0.40
1:A:242:ARG:NH1	1:A:760:TYR:OH	2.55	0.40
1:A:433:VAL:HG21	1:A:751:ILE:HG12	2.03	0.40
1:A:336:ILE:HD13	1:A:364:ILE:HG12	2.02	0.40
1:A:438:ILE:HD11	1:A:746:ILE:HD12	2.02	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	701/810 (86%)	666 (95%)	30 (4%)	5 (1%)	22 54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	CYS
1	A	288	ASP
1	A	456	ALA
1	A	297	ASN
1	A	319	GLY

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	553/730 (76%)	504 (91%)	49 (9%)	9 29

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	ASP
1	A	106	LEU
1	A	135	LEU

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	151	LEU
1	A	162	GLU
1	A	172	LEU
1	A	188	CYS
1	A	198	ASN
1	A	228	GLU
1	A	232	GLU
1	A	252	THR
1	A	305	VAL
1	A	325	VAL
1	A	345	ILE
1	A	362	VAL
1	A	381	PHE
1	A	406	ASN
1	A	425	GLU
1	A	429	ASN
1	A	436	ARG
1	A	447	ASN
1	A	460	ARG
1	A	462	PHE
1	A	464	ASP
1	A	473	ASP
1	A	475	LEU
1	A	476	ASP
1	A	477	ARG
1	A	489	GLU
1	A	514	PHE
1	A	531	CYS
1	A	629	LEU
1	A	633	MET
1	A	640	THR
1	A	645	VAL
1	A	658	LEU
1	A	692	LEU
1	A	695	LEU
1	A	716	LEU
1	A	731	ASN
1	A	733	ARG
1	A	751	ILE
1	A	752	THR
1	A	755	GLU

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Mol	Chain	Res	Type
1	A	756	ARG
1	A	770	THR
1	A	777	ASN
1	A	814	CYS

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

Mol	Chain	Res	Type
1	A	406	ASN
1	A	407	HIS
1	A	440	GLN
1	A	636	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	3/5 (60%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	713/810 (88%)	0.96	113 (15%) 2 1	64, 103, 193, 206	0
2	B	4/5 (80%)	0.82	0 100 100	86, 88, 98, 115	0
All	All	717/815 (87%)	0.96	113 (15%) 2 1	64, 103, 193, 206	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	302	ILE	10.0
1	A	329	LEU	10.0
1	A	367	LEU	8.8
1	A	335	ARG	8.4
1	A	344	LEU	8.3
1	A	687	VAL	8.3
1	A	327	TYR	8.2
1	A	364	ILE	8.1
1	A	334	ILE	8.0
1	A	328	TYR	7.9
1	A	332	TYR	7.9
1	A	324	PHE	7.8
1	A	309	GLN	7.2
1	A	343	LEU	7.2
1	A	362	VAL	7.0
1	A	297	ASN	6.9
1	A	296	ASN	6.7
1	A	303	ASN	6.5
1	A	316	SER	6.5
1	A	686	GLY	6.2
1	A	315	PHE	6.1
1	A	311	PRO	6.0
1	A	268	MET	5.8
1	A	294	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	295	TYR	5.8
1	A	361	VAL	5.7
1	A	299	THR	5.7
1	A	322	ILE	5.5
1	A	300	TYR	5.4
1	A	321	ASP	5.2
1	A	336	ILE	5.2
1	A	326	GLU	5.0
1	A	363	LEU	5.0
1	A	144	SER	5.0
1	A	291	VAL	5.0
1	A	345	ILE	5.0
1	A	292	LEU	5.0
1	A	314	THR	5.0
1	A	333	ASN	5.0
1	A	346	SER	5.0
1	A	325	VAL	4.9
1	A	298	ARG	4.9
1	A	293	THR	4.8
1	A	342	PRO	4.8
1	A	143	GLY	4.7
1	A	172	LEU	4.7
1	A	272	SER	4.7
1	A	320	ARG	4.7
1	A	164	THR	4.7
1	A	370	VAL	4.7
1	A	147	LEU	4.6
1	A	259	MET	4.5
1	A	317	CYS	4.5
1	A	339	HIS	4.4
1	A	269	ARG	4.4
1	A	383	LEU	4.3
1	A	156	THR	4.2
1	A	340	ASN	4.1
1	A	464	ASP	4.1
1	A	341	GLN	3.9
1	A	290	ILE	3.7
1	A	313	SER	3.7
1	A	228	GLU	3.6
1	A	166	LEU	3.6
1	A	366	GLU	3.6
1	A	368	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	280	ASP	3.4
1	A	384	MET	3.4
1	A	323	SER	3.4
1	A	542	LEU	3.3
1	A	304	ASP	3.3
1	A	426	LEU	3.3
1	A	267	ILE	3.3
1	A	270	ARG	3.2
1	A	365	PRO	3.1
1	A	318	LYS	3.1
1	A	282	VAL	3.0
1	A	330	THR	3.0
1	A	145	GLY	3.0
1	A	148	PHE	3.0
1	A	697	GLU	2.9
1	A	289	LEU	2.9
1	A	319	GLY	2.9
1	A	288	ASP	2.8
1	A	301	ARG	2.8
1	A	541	CYS	2.8
1	A	146	TYR	2.7
1	A	411	ASN	2.7
1	A	165	VAL	2.7
1	A	402	LEU	2.6
1	A	524	TYR	2.6
1	A	229	PHE	2.6
1	A	252	THR	2.5
1	A	516	ILE	2.4
1	A	153	LEU	2.4
1	A	310	THR	2.4
1	A	130	VAL	2.4
1	A	831	ILE	2.4
1	A	381	PHE	2.3
1	A	306	ASP	2.3
1	A	150	GLY	2.2
1	A	690	GLY	2.2
1	A	170	SER	2.2
1	A	560	VAL	2.1
1	A	765	GLN	2.1
1	A	154	PHE	2.1
1	A	307	PHE	2.1
1	A	515	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	305	VAL	2.1
1	A	543	VAL	2.1
1	A	286	VAL	2.0
1	A	422	TRP	2.0
1	A	447	ASN	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.

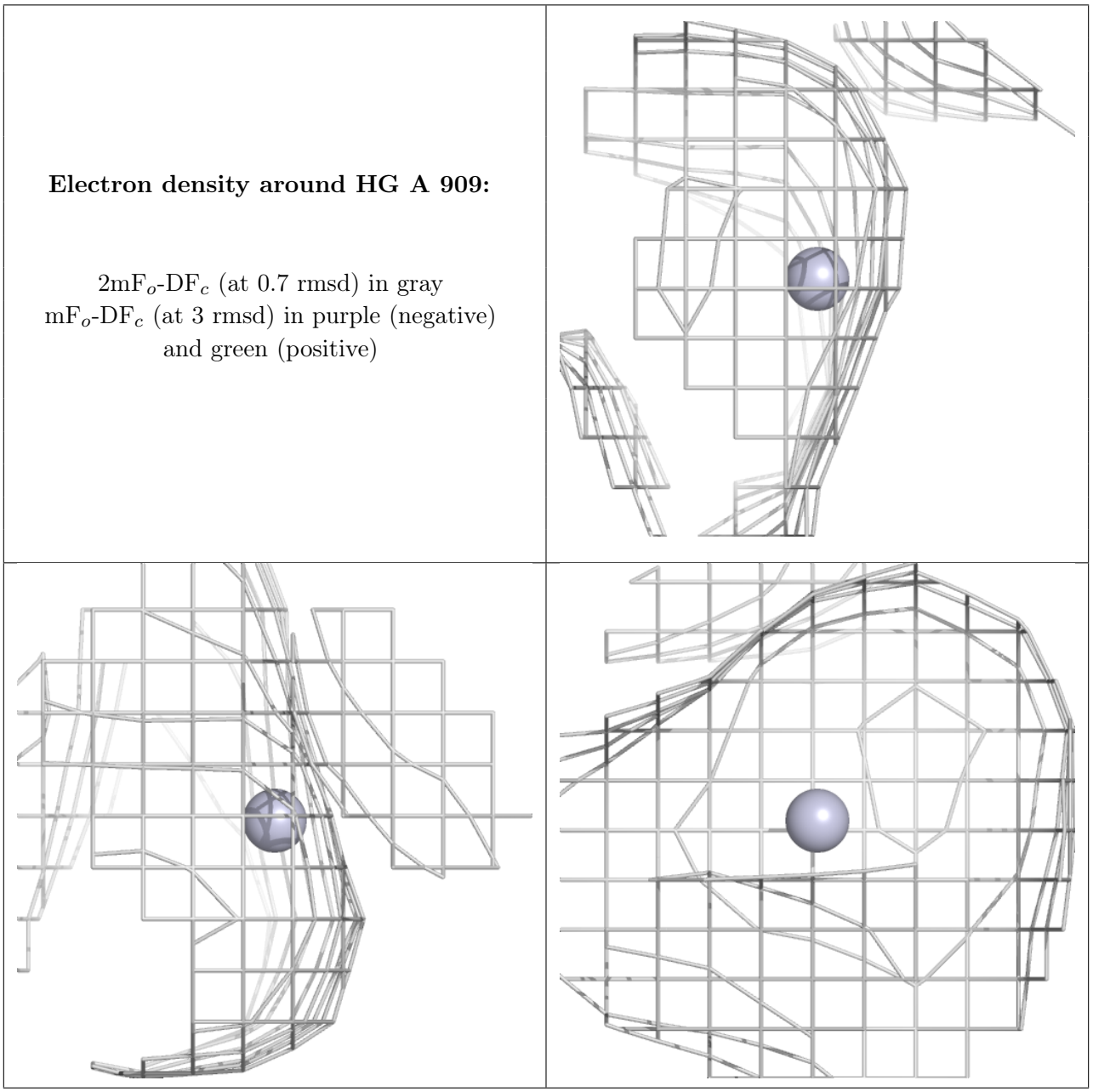
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	HG	A	909	1/1	0.31	0.19	232,232,232,232	1
4	HG	A	904	1/1	0.36	0.16	204,204,204,204	1
3	ZN	A	914	1/1	0.68	0.14	151,151,151,151	0
3	ZN	A	913	1/1	0.75	0.16	113,113,113,113	1
3	ZN	A	911	1/1	0.75	0.24	121,121,121,121	0
3	ZN	A	903	1/1	0.85	0.16	112,112,112,112	0
4	HG	A	908	1/1	0.86	0.08	169,169,169,169	1
3	ZN	A	902	1/1	0.94	0.37	128,128,128,128	0
3	ZN	A	912	1/1	0.95	0.25	112,112,112,112	1
3	ZN	A	910	1/1	0.96	0.17	99,99,99,99	0
4	HG	A	905	1/1	0.96	0.12	71,71,71,71	1
4	HG	A	907[A]	1/1	0.97	0.07	127,127,127,127	1
4	HG	A	907[B]	1/1	0.97	0.07	151,151,151,151	1
3	ZN	A	901	1/1	0.98	0.25	71,71,71,71	0
4	HG	A	906	1/1	0.99	0.11	117,117,117,117	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.

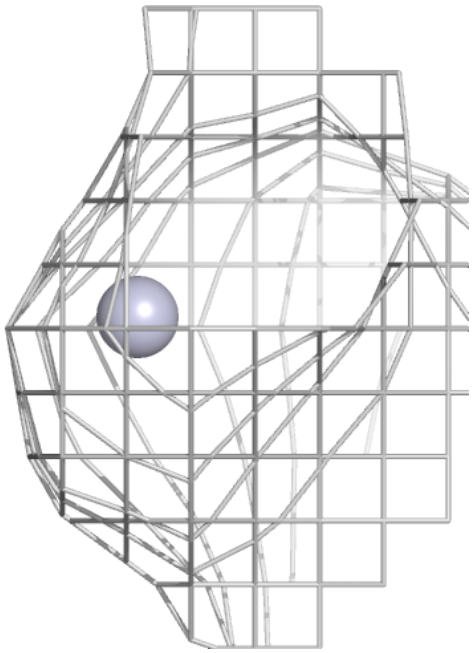
Electron density around HG A 909:

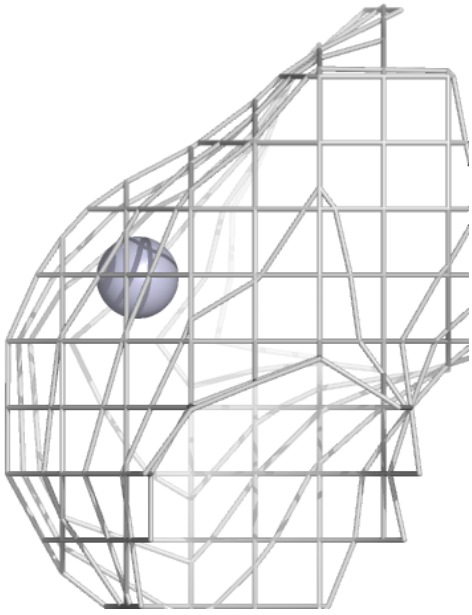
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

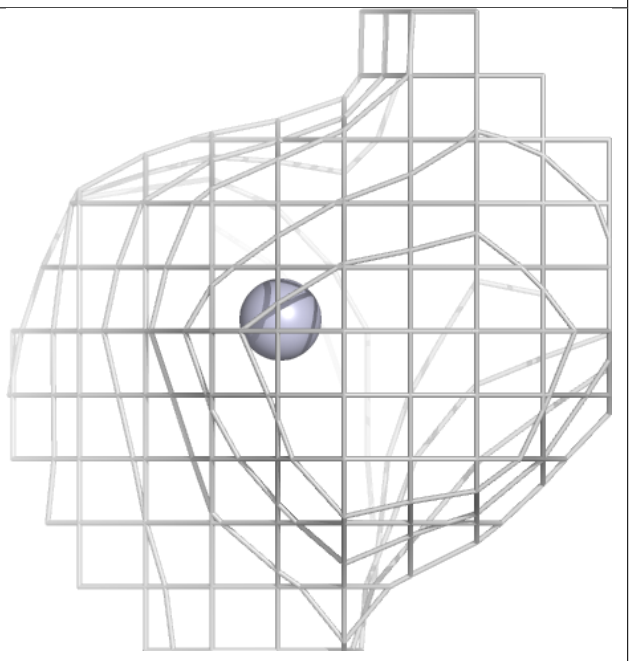


Electron density around HG A 904:

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

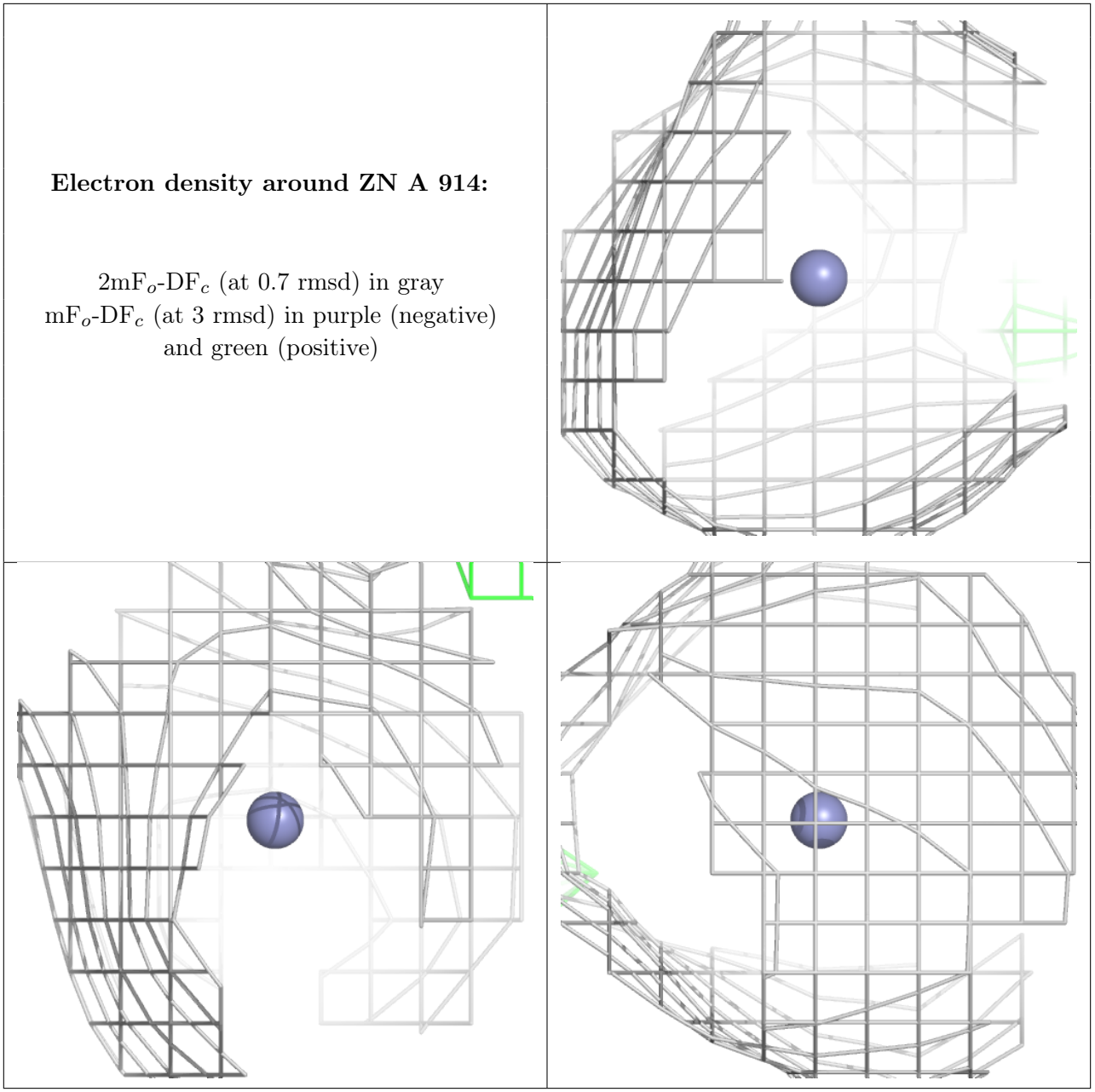






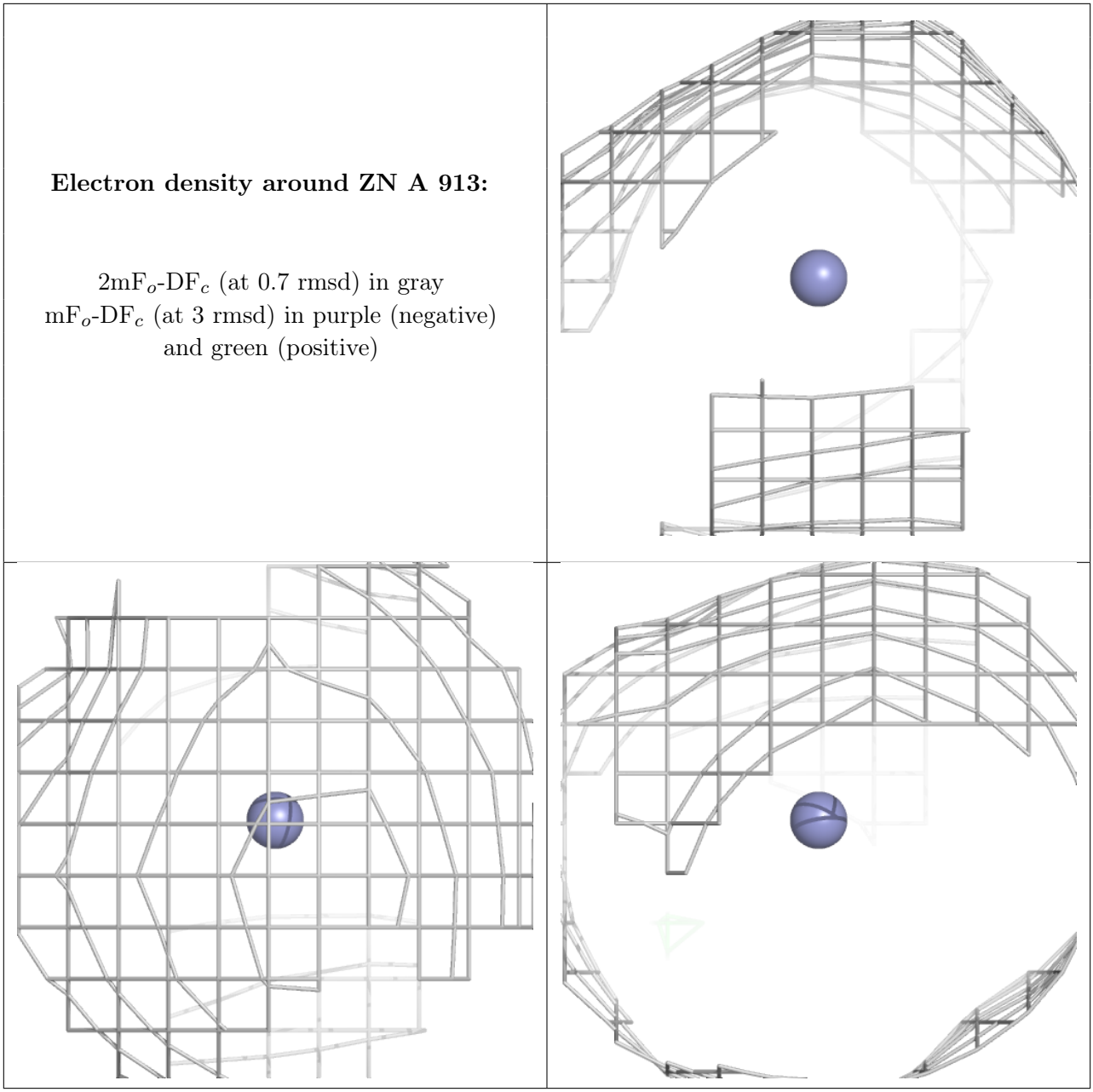
Electron density around ZN A 914:

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



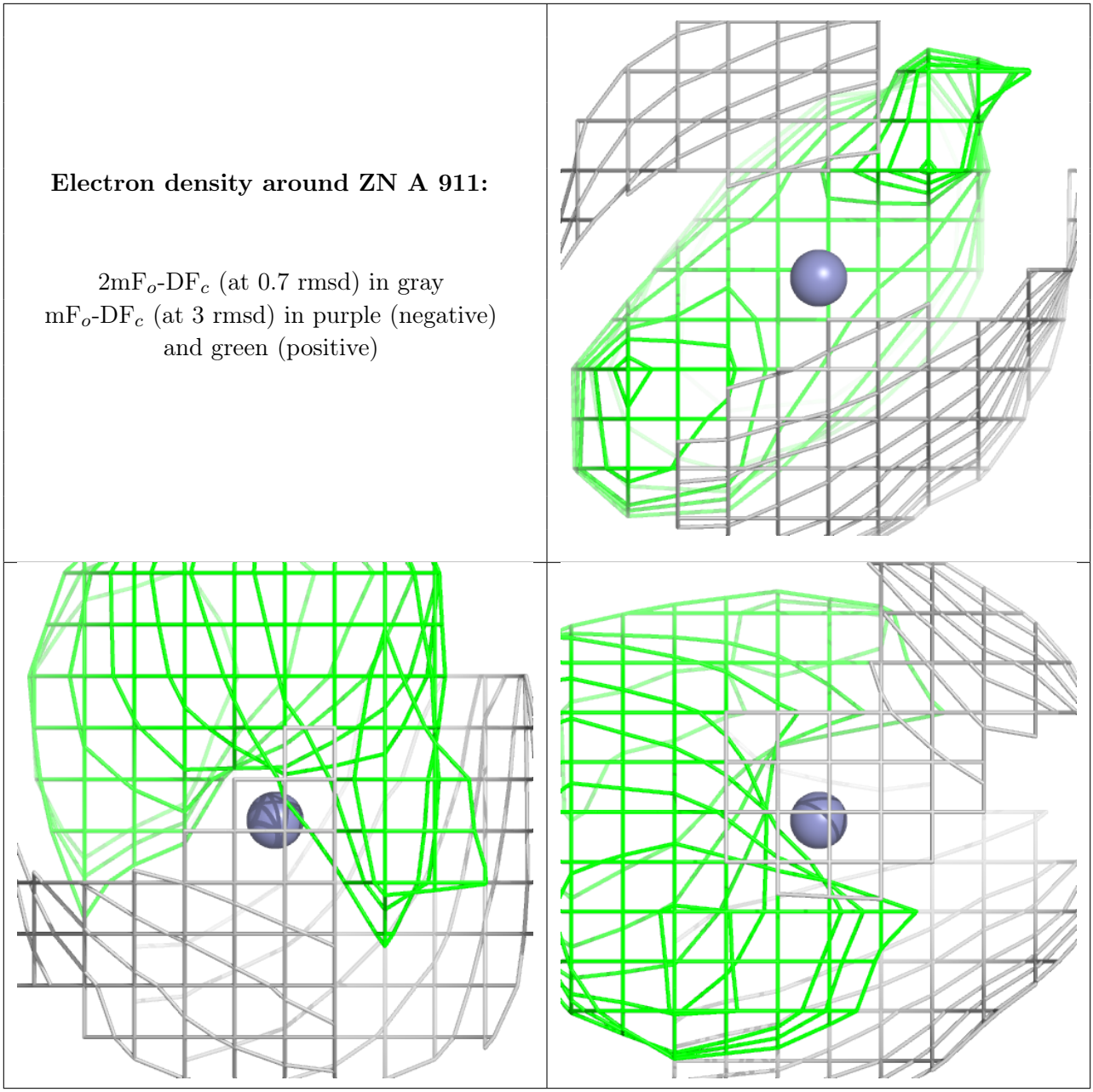
Electron density around ZN A 913:

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



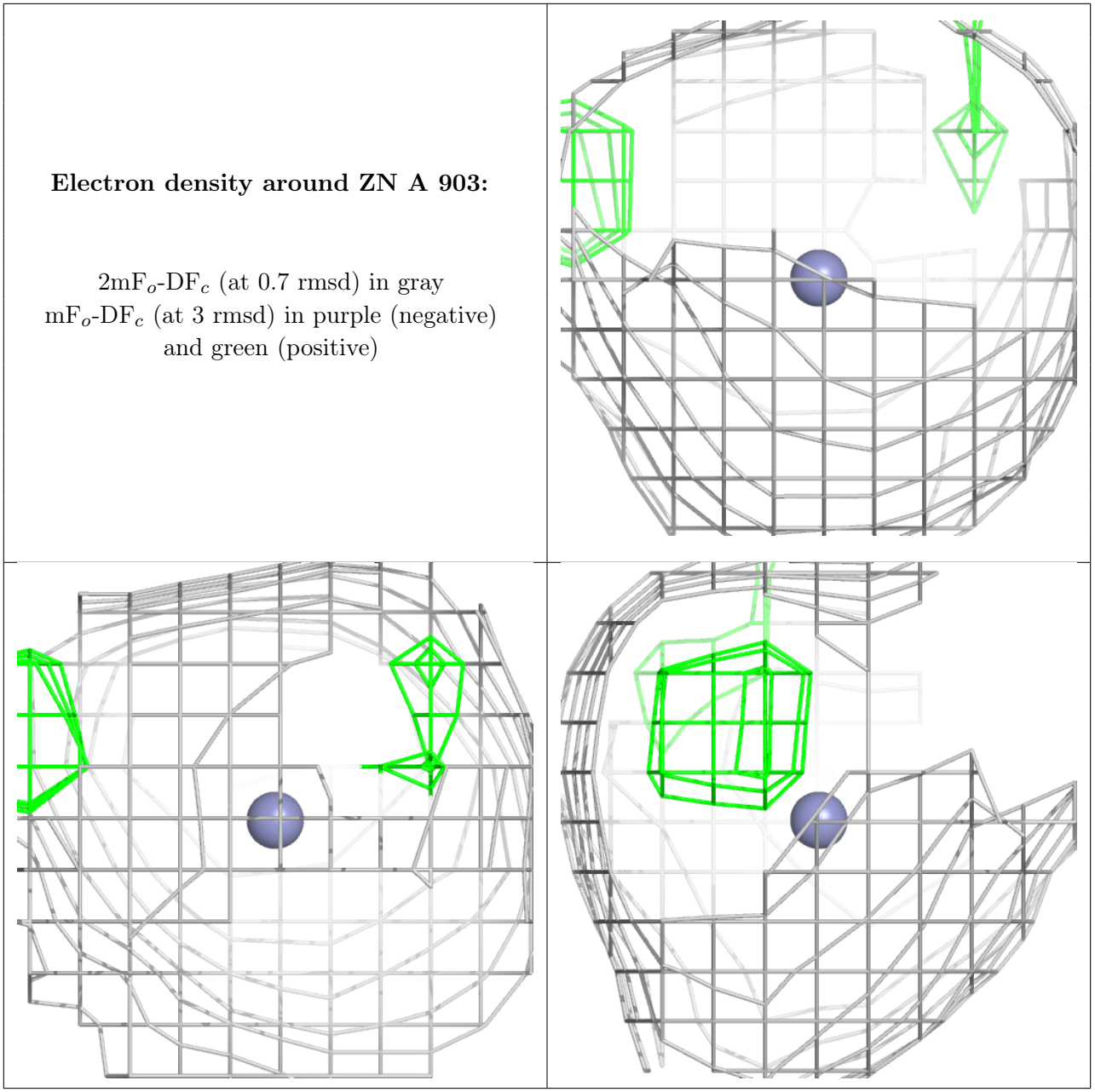
Electron density around ZN A 911:

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



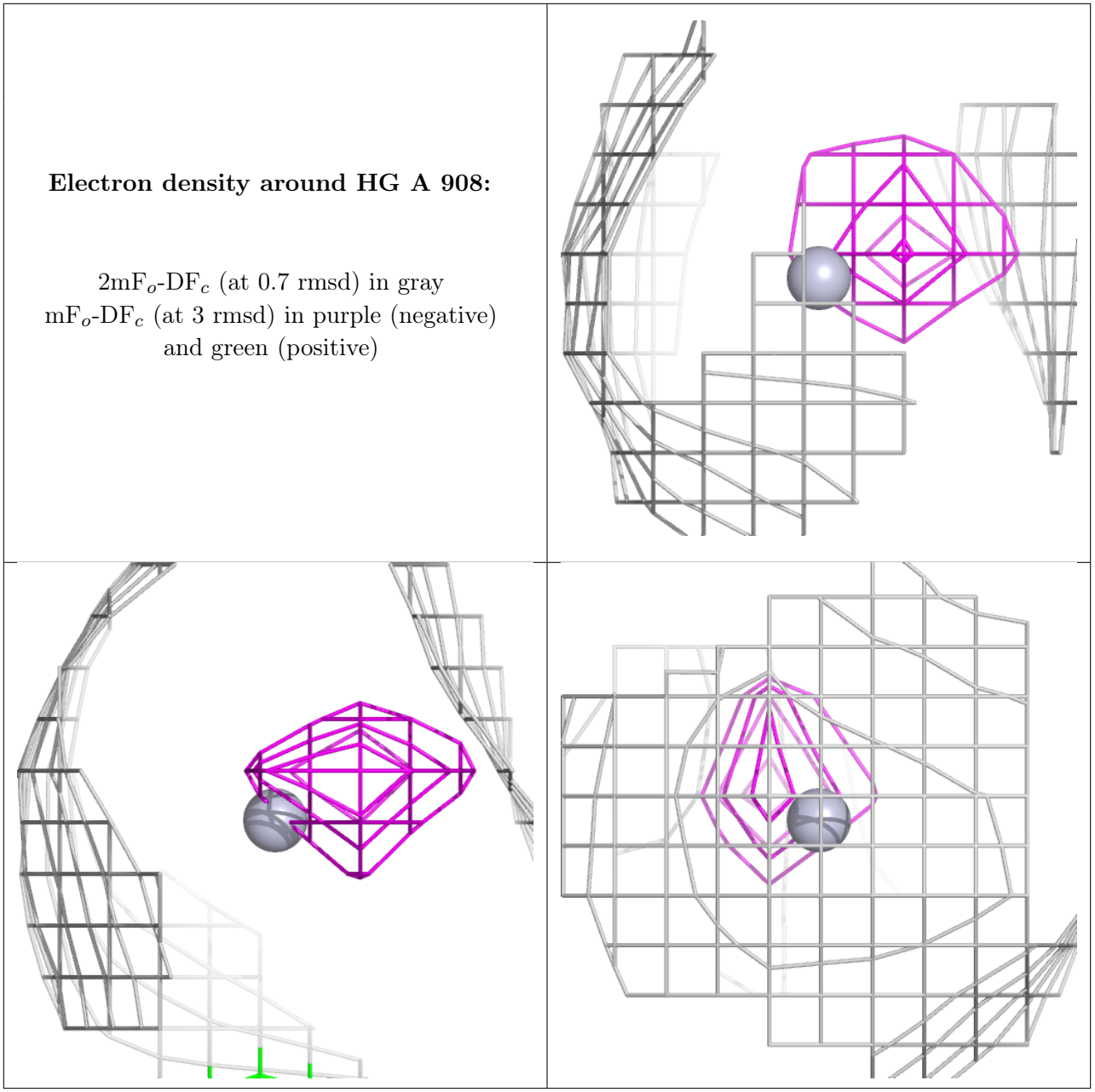
Electron density around ZN A 903:

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



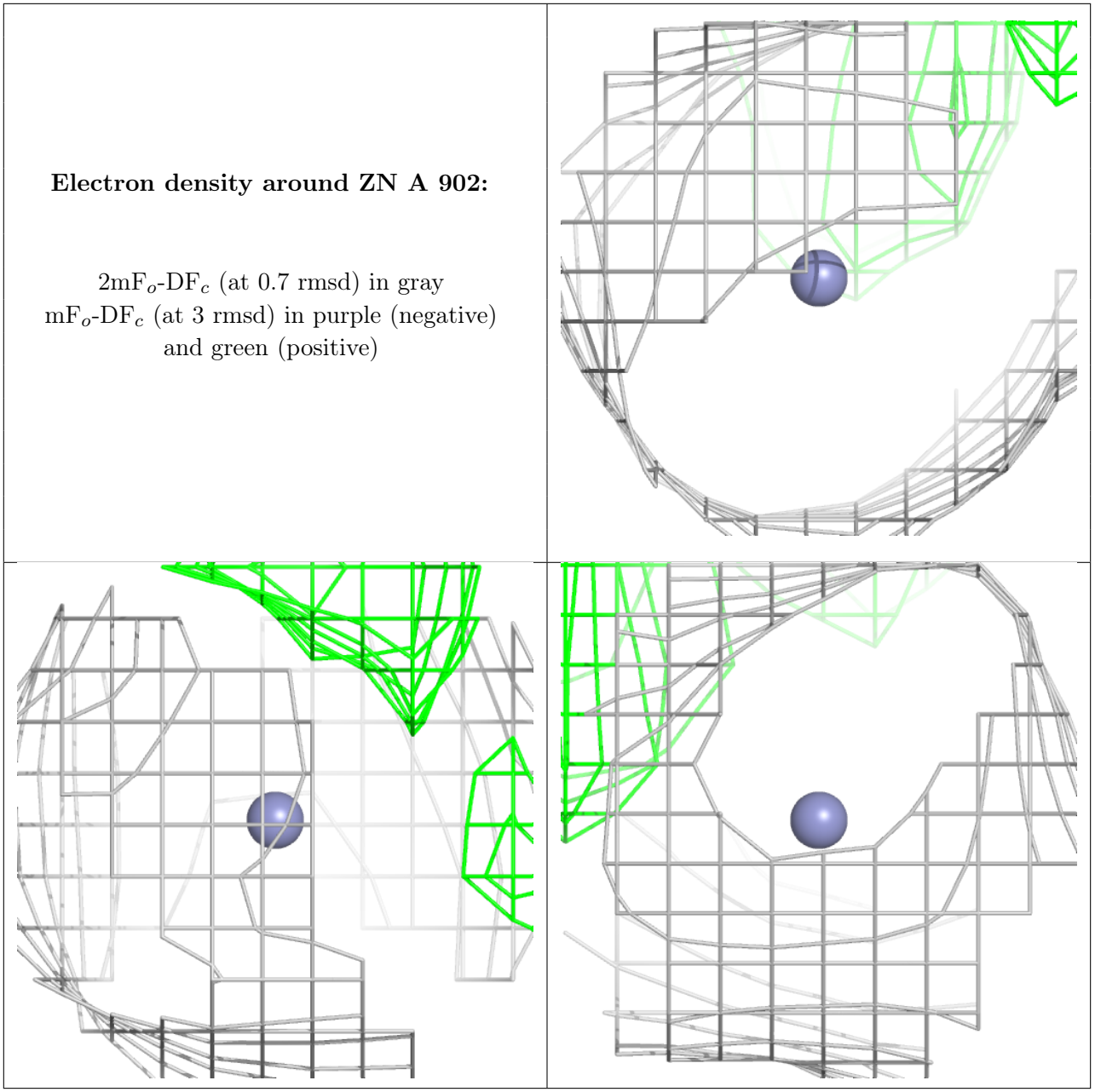
Electron density around HG A 908:

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



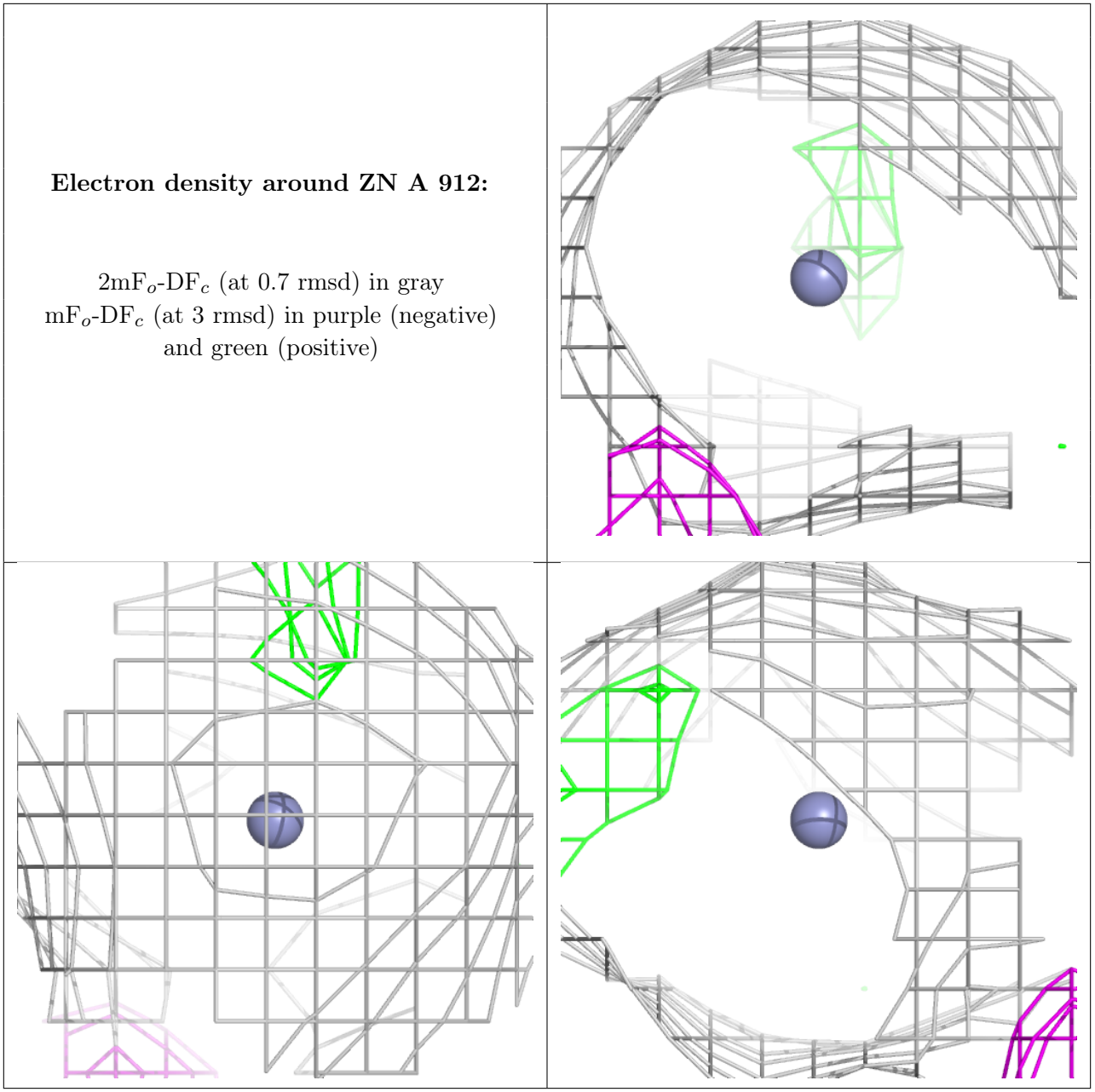
Electron density around ZN A 902:

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



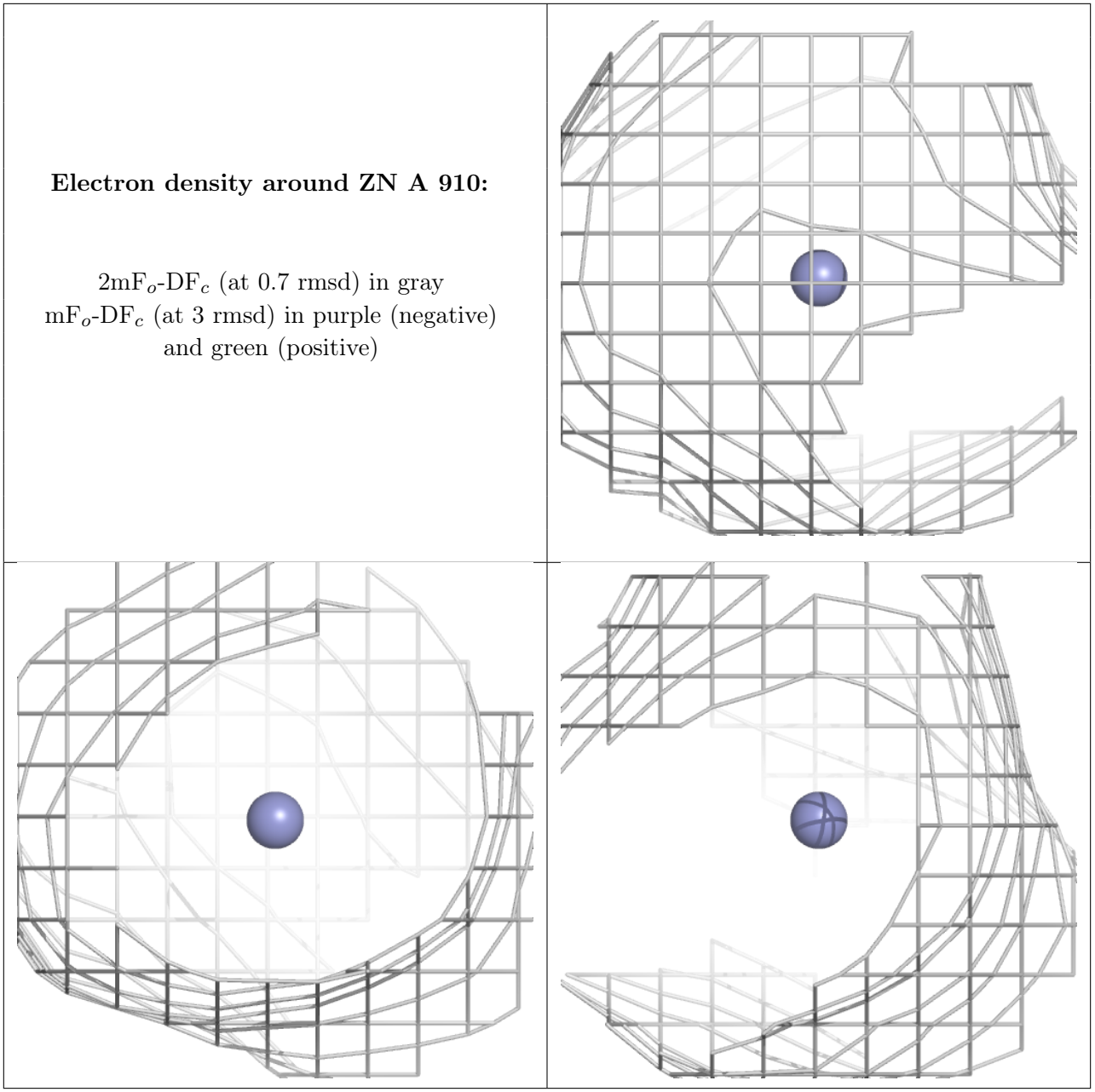
Electron density around ZN A 912:

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



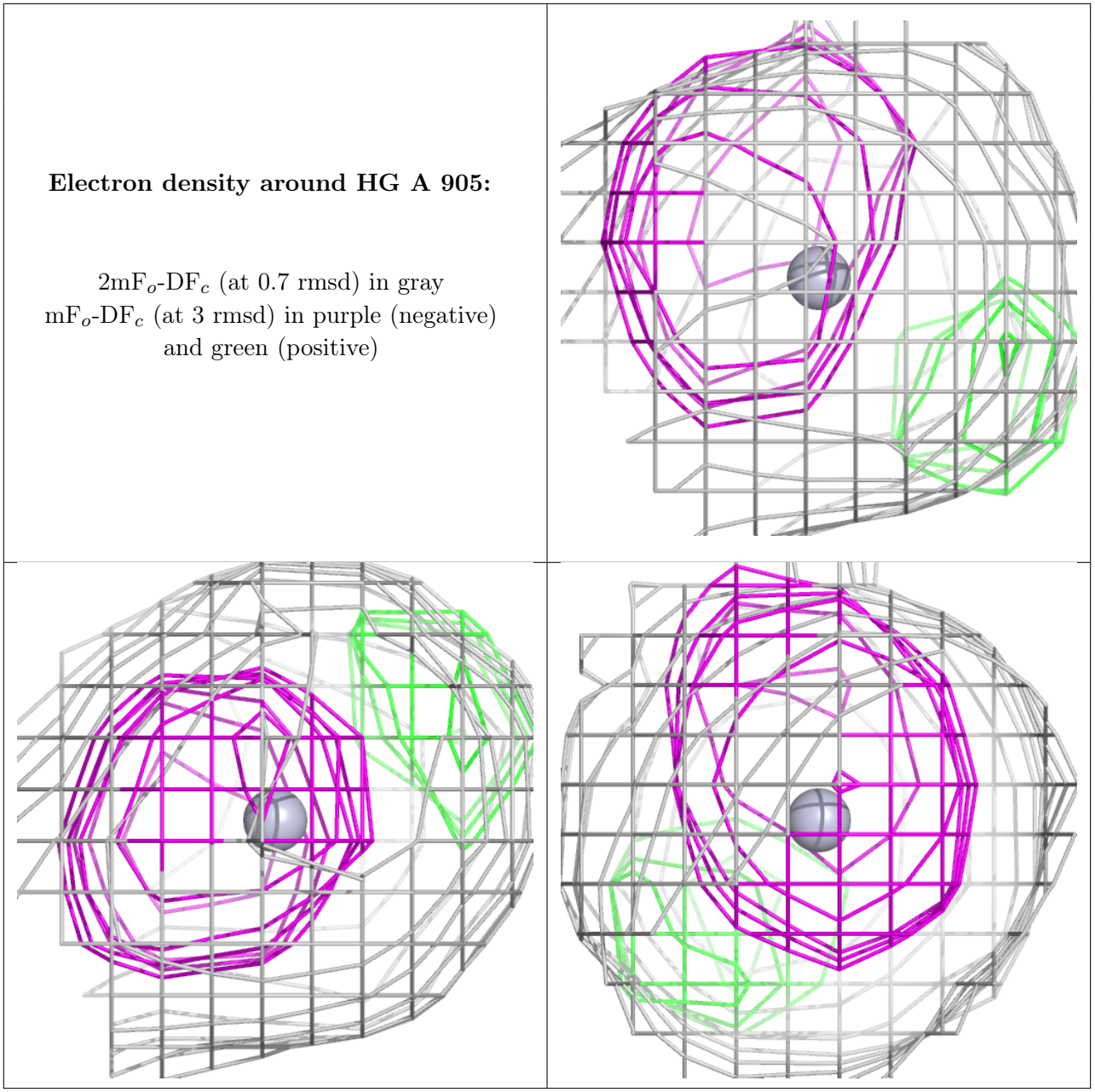
Electron density around ZN A 910:

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



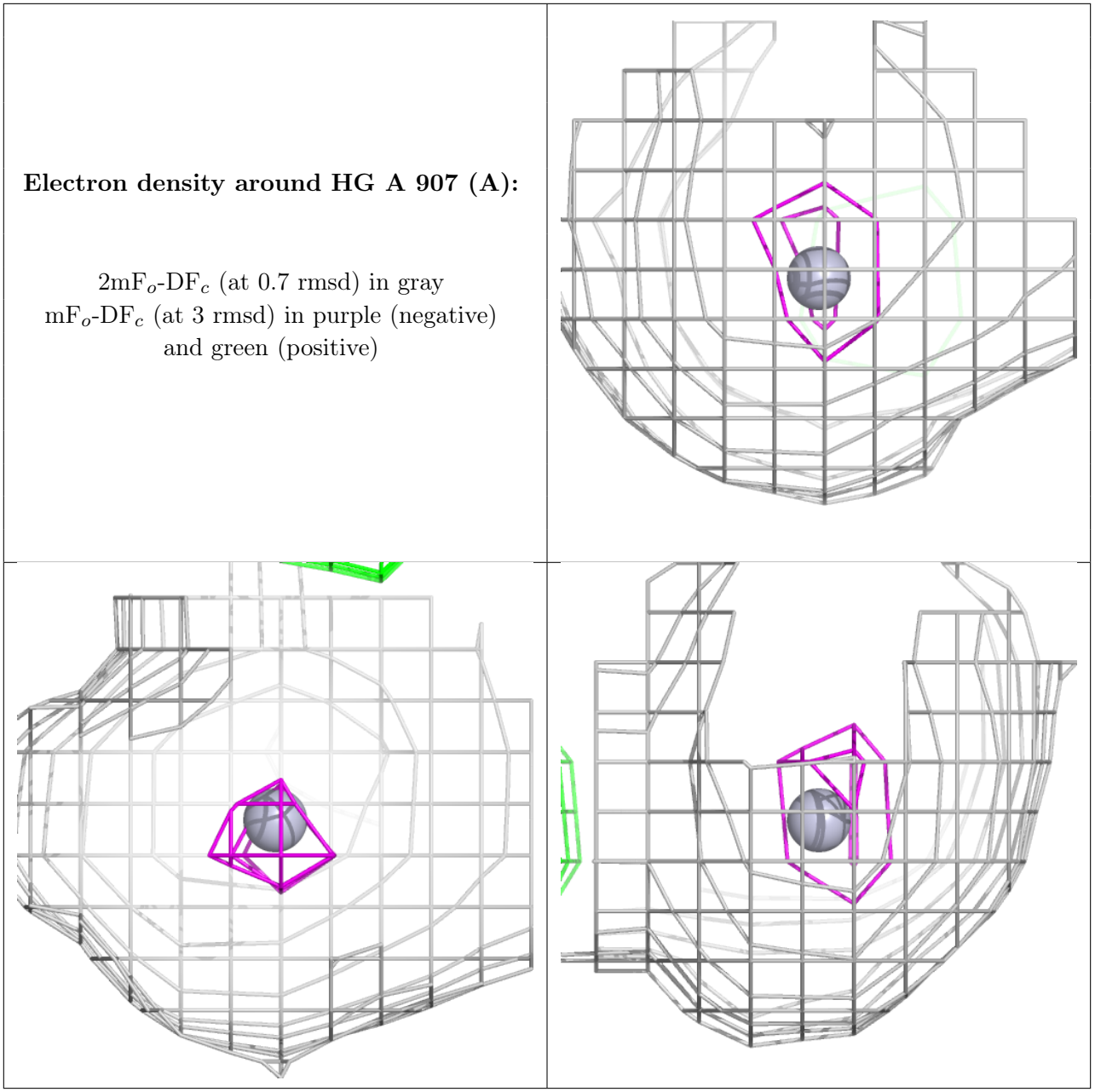
Electron density around HG A 905:

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



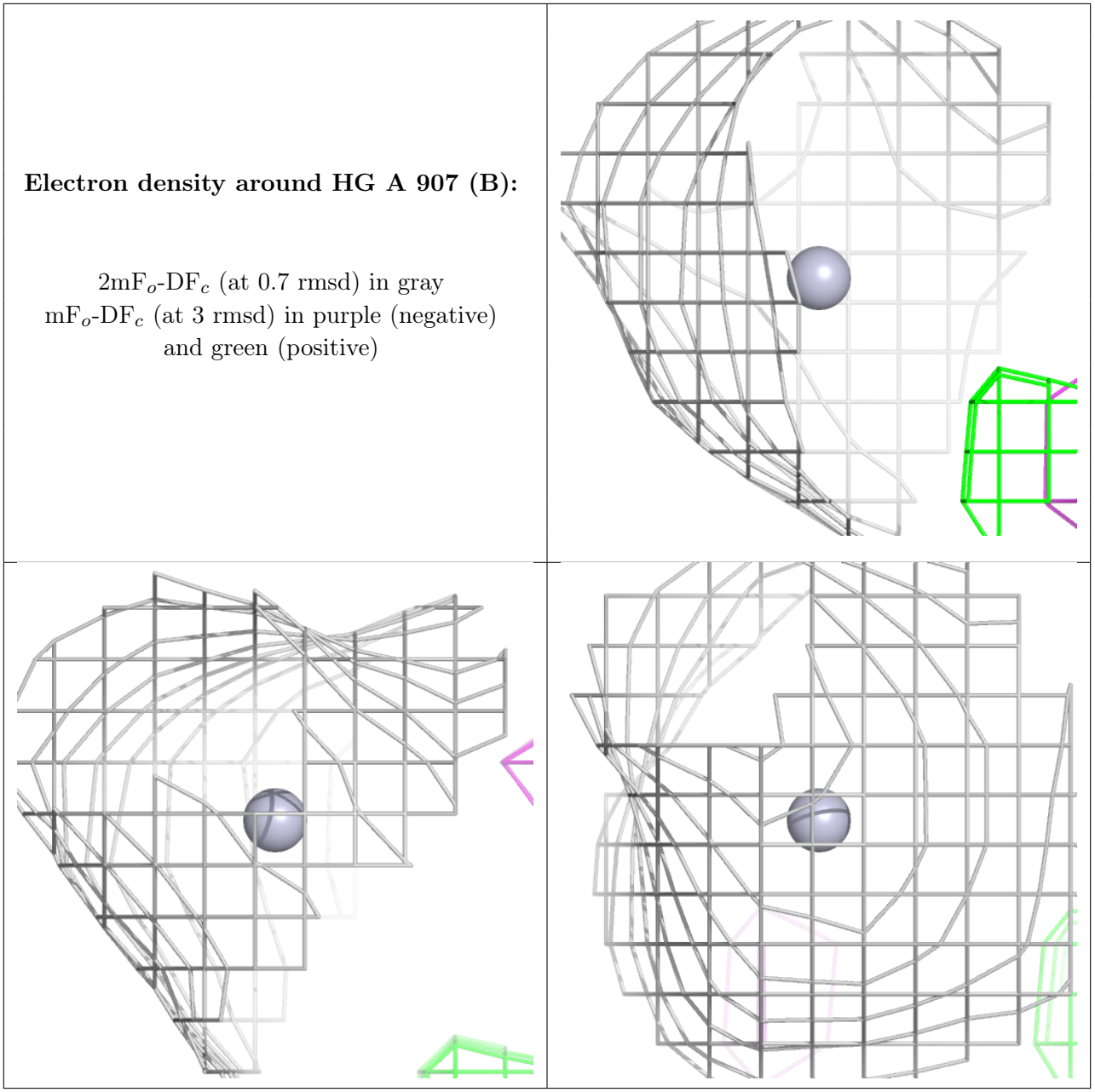
Electron density around HG A 907 (A):

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



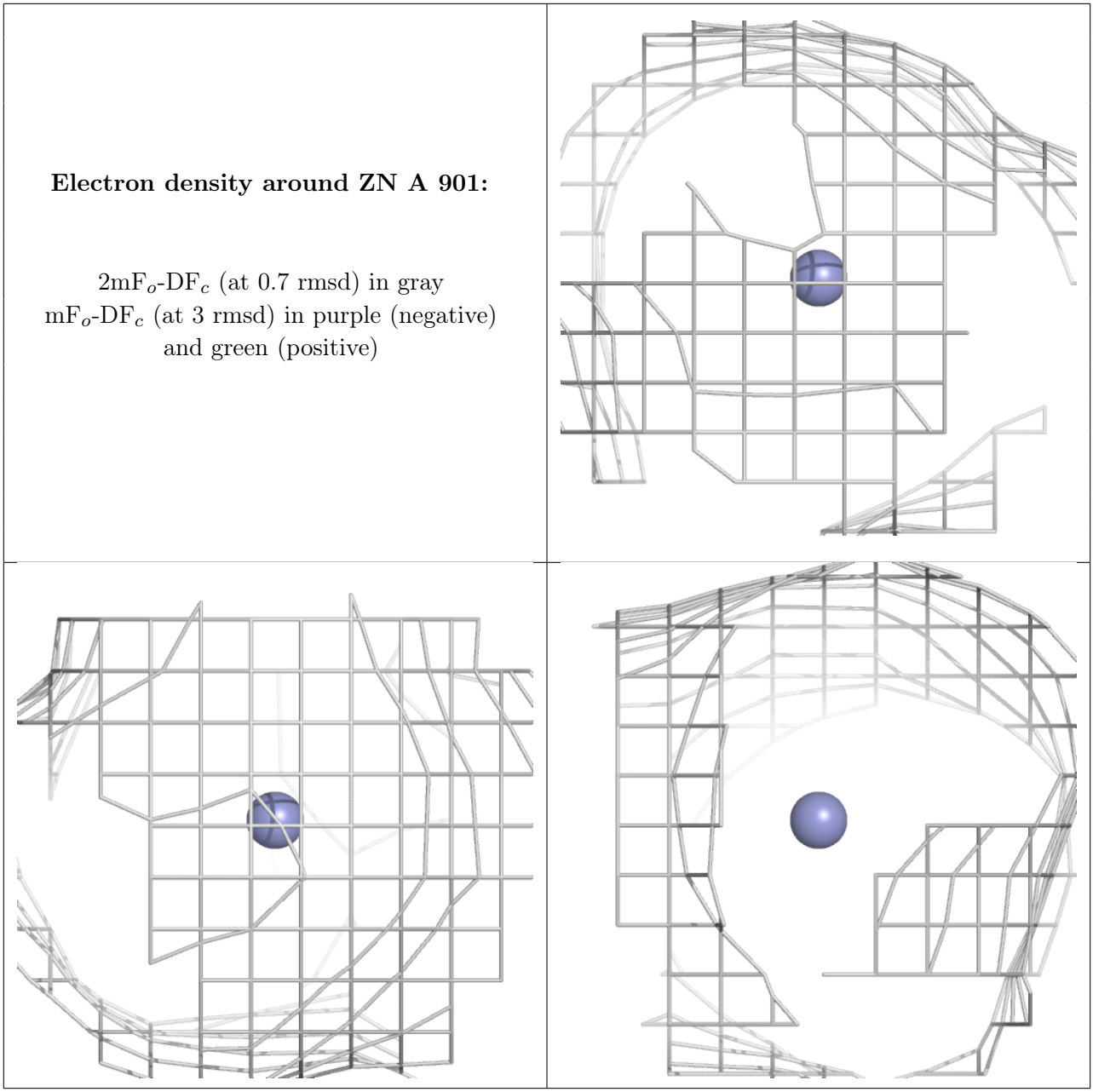
Electron density around HG A 907 (B):

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



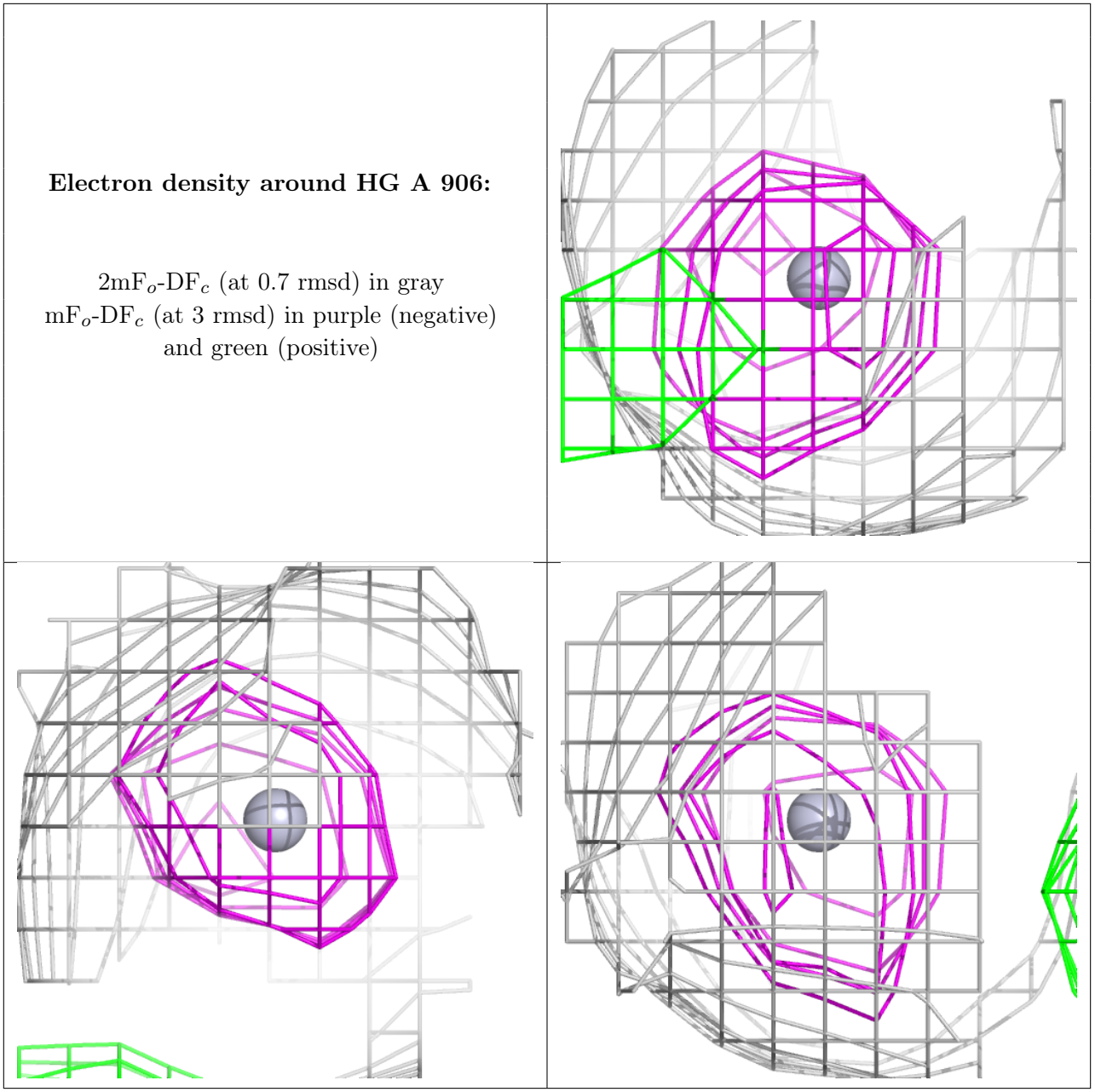
Electron density around ZN A 901:

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



Electron density around HG A 906:

$2mF_o$-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.