Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 06:50 PM JST

PDB ID	:	7WYJ
Title	:	Structure of the complex of lactoperoxidase with nitric oxide catalytic product nitrite at 1.89 A resolution
Authors	:	Viswanathan, V.; Pandey, N.; Singh, A.K.; Sinha, M.; Singh, R.P.; Sharma, P.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2022-02-16
Resolution	:	1.89 Å(reported)

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

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

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

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

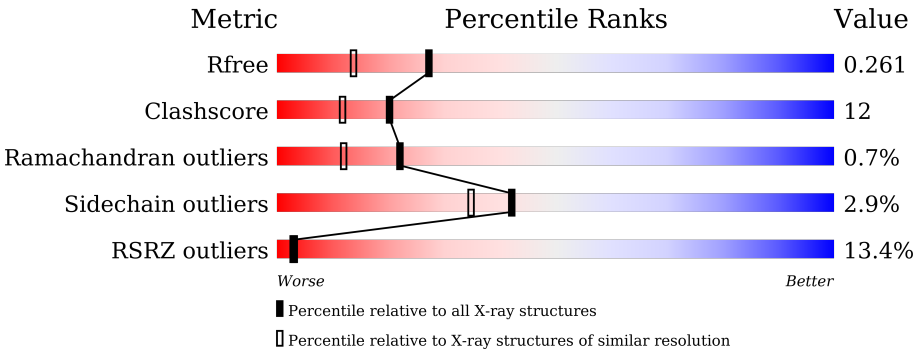
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	595	13%, 82%, 17%, ·
2	B	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IOD	A	608[B]	-	-	X	-
4	IOD	A	610	-	-	X	-
4	IOD	A	620[B]	-	-	X	-
4	IOD	A	621	-	-	X	-
4	IOD	A	622[B]	-	-	X	-
4	IOD	A	622[C]	-	-	X	-
4	IOD	A	626[A]	-	-	X	-
4	IOD	A	627[B]	-	-	X	-
4	IOD	A	627[C]	-	-	X	-
4	IOD	A	631[B]	-	-	X	-
7	NO2	A	614	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 5454 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 Lactoperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	2	0
			4783	3045	850	862	26			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

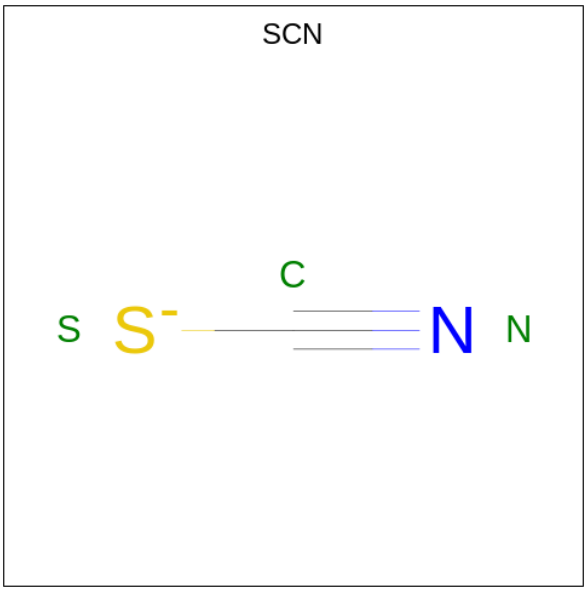
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I) (labeled as "Ligand of Interest" by depositor).

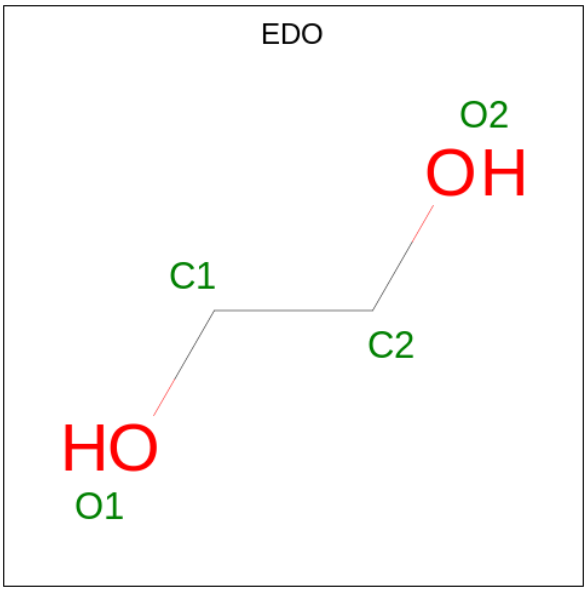
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	I	0	12
			38	38		

- Molecule 5 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS) (labeled as "Ligand of Interest" by depositor).



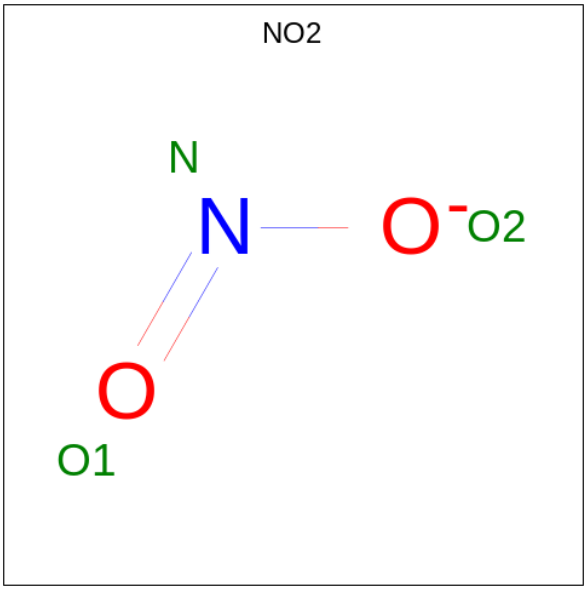
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N S 3 1 1 1	0	0
5	A	1	Total C N S 3 1 1 1	0	0
5	A	1	Total C N S 3 1 1 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



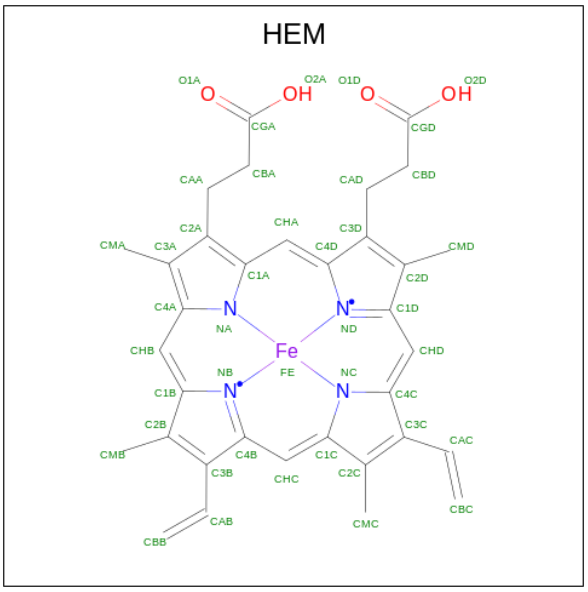
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0

- Molecule 7 is NITRITE ION (three-letter code: NO2) (formula: NO_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total N O 3 1 2	0	0

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

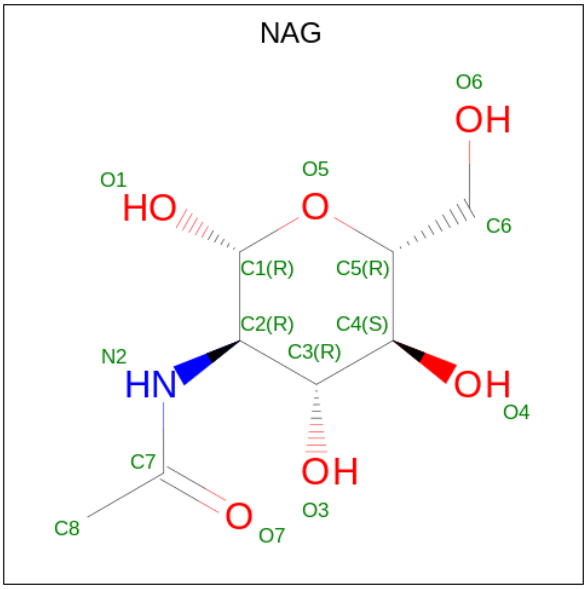


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	Fe	N	O	0	1
			48	37	1	4	6		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Zn	0	1
			2	2		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is water.

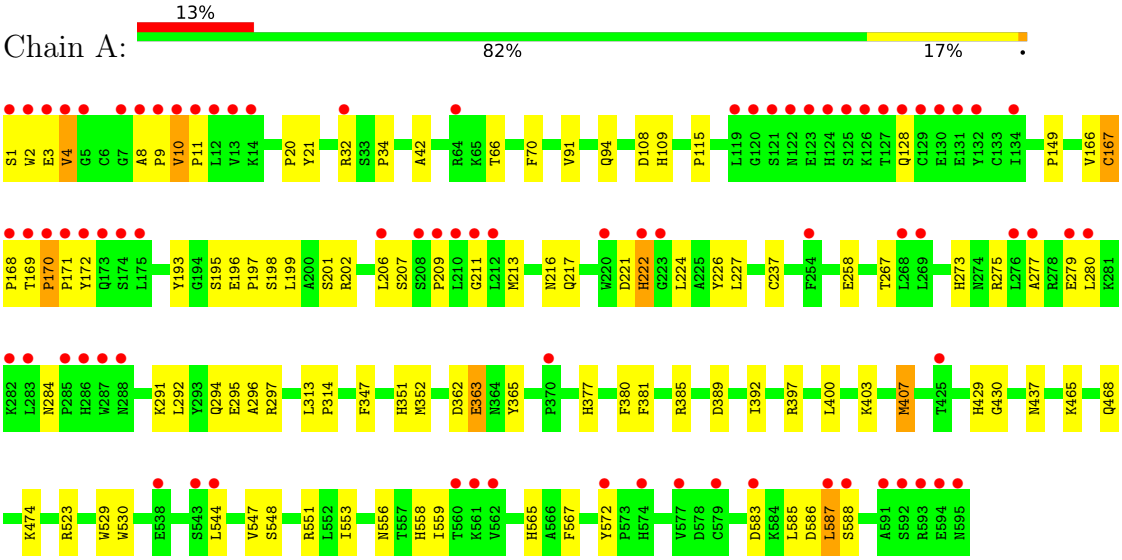
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	481	Total	O	0	7
			488	488		

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.

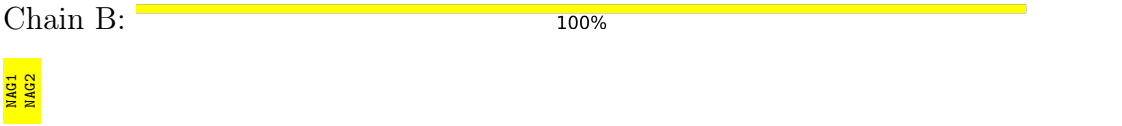
• Molecule 1: Lactoperoxidase

Chain A:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.99Å 79.93Å 76.31Å 90.00° 102.18° 90.00°	Depositor
Resolution (Å)	35.30 – 1.89 35.30 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.30-1.89) 100.0 (35.30-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.50 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.203 , 0.258 0.209 , 0.261	Depositor DCC
R_{free} test set	2580 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5454	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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, IOD, ZN, SCN, CA, EDO, HEM, NO2

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	0.73	0/4917	0.82	0/6670

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	4783	0	4705	111	0
2	B	28	0	25	0	0
3	A	1	0	0	0	0
4	A	38	0	0	41	0
5	A	9	0	0	2	0
6	A	12	0	18	2	0
7	A	3	0	0	5	0
8	A	48	0	8	2	0
9	A	2	0	0	0	0
10	A	42	0	39	0	0
11	A	488	0	0	16	0
All	All	5454	0	4795	120	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 12.

All (120) 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:559:ILE:HA	4:A:627[B]:IOD:I	1.97	1.35
1:A:222:HIS:HB3	4:A:626[A]:IOD:I	2.04	1.27
1:A:216:ASN:HA	4:A:608[B]:IOD:I	2.17	1.15
4:A:625:IOD:I	11:A:1039:HOH:O	2.36	1.14
1:A:429:HIS:O	4:A:621:IOD:I	2.43	1.06
7:A:614:NO2:O1	8:A:616[A]:HEM:O2D	1.74	1.03
7:A:614:NO2:N	4:A:619[A]:IOD:I	2.64	1.00
1:A:222:HIS:CB	4:A:626[A]:IOD:I	2.80	0.99
1:A:222:HIS:CG	4:A:626[A]:IOD:I	2.94	0.91
1:A:558:HIS:CE1	4:A:626[A]:IOD:I	2.94	0.91
1:A:207:SER:HA	11:A:908:HOH:O	1.72	0.88
4:A:610:IOD:I	11:A:1055:HOH:O	2.61	0.88
1:A:195:SER:O	11:A:701:HOH:O	1.92	0.85
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.57	0.85
1:A:558:HIS:ND1	4:A:626[A]:IOD:I	2.84	0.81
1:A:109:HIS:NE2	7:A:614:NO2:N	2.25	0.81
1:A:198:SER:OG	4:A:620[B]:IOD:I	2.69	0.80
1:A:199:LEU:HA	4:A:622[C]:IOD:I	2.55	0.77
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.30	0.77
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.16	0.75
1:A:363:GLU:HA	4:A:627[D]:IOD:I	2.57	0.75
1:A:109:HIS:NE2	7:A:614:NO2:O1	2.21	0.72
1:A:209:PRO:HB3	11:A:1089:HOH:O	1.91	0.69
1:A:202:ARG:HB2	4:A:622[B]:IOD:I	2.65	0.67
1:A:196:GLU:OE1	11:A:703:HOH:O	2.13	0.67
1:A:202:ARG:HD3	4:A:622[C]:IOD:I	2.65	0.66
1:A:558:HIS:ND1	4:A:626[B]:IOD:I	2.99	0.66
1:A:362:ASP:O	1:A:365:TYR:N	2.26	0.66
4:A:604[A]:IOD:I	11:A:857:HOH:O	2.82	0.66
1:A:222:HIS:ND1	4:A:626[A]:IOD:I	2.98	0.66
1:A:237:CYS:O	11:A:702:HOH:O	2.12	0.66
7:A:614:NO2:N	4:A:619[B]:IOD:I	2.98	0.65
1:A:559:ILE:CA	4:A:627[B]:IOD:I	2.93	0.65
1:A:216:ASN:CA	4:A:608[B]:IOD:I	3.08	0.64
4:A:603[B]:IOD:I	11:A:1137:HOH:O	2.85	0.64
1:A:397:ARG:NE	4:A:627[C]:IOD:I	2.99	0.62
6:A:615:EDO:H12	5:A:617:SCN:S	2.43	0.59
1:A:217:GLN:N	4:A:608[B]:IOD:I	3.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.33	0.57
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.86	0.57
1:A:352:MET:SD	1:A:407:MET:HE3	2.45	0.56
1:A:586:ASP:N	11:A:714:HOH:O	2.35	0.56
1:A:279:GLU:OE2	1:A:279:GLU:HA	2.06	0.56
1:A:565:HIS:HB3	4:A:631[B]:IOD:I	2.76	0.56
1:A:559:ILE:HA	4:A:627[C]:IOD:I	2.77	0.54
1:A:149:PRO:HB2	4:A:610:IOD:I	2.78	0.54
1:A:169:THR:OG1	1:A:170:PRO:HD3	2.08	0.53
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.43	0.53
1:A:170:PRO:HD2	1:A:171:PRO:HD2	1.91	0.53
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.91	0.52
1:A:385:ARG:O	1:A:389:ASP:HB3	2.10	0.52
1:A:558:HIS:HE1	4:A:626[A]:IOD:I	2.56	0.51
8:A:616[A]:HEM:O2D	11:A:704:HOH:O	2.19	0.51
1:A:207:SER:N	11:A:725:HOH:O	2.43	0.51
1:A:167:CYS:CB	1:A:168:PRO:CD	2.88	0.50
1:A:237:CYS:HA	1:A:381:PHE:O	2.11	0.50
1:A:530:TRP:NE1	4:A:603[A]:IOD:I	3.12	0.50
1:A:206:LEU:HD23	11:A:1035:HOH:O	2.12	0.50
1:A:42:ALA:HB2	1:A:166:VAL:HG21	1.94	0.50
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.93	0.49
1:A:567:PHE:HB2	4:A:631[B]:IOD:I	2.82	0.49
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.47	0.49
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.48	0.49
1:A:294:GLN:OE1	1:A:294:GLN:HA	2.14	0.47
1:A:352:MET:SD	1:A:407:MET:CE	3.01	0.47
1:A:363:GLU:OE1	4:A:627[C]:IOD:I	3.03	0.46
1:A:267:THR:CG2	1:A:392:ILE:HD13	2.45	0.46
1:A:363:GLU:HA	4:A:627[C]:IOD:I	2.85	0.46
1:A:227:LEU:CD1	1:A:267:THR:HA	2.46	0.46
1:A:556:ASN:HA	11:A:716:HOH:O	2.16	0.46
1:A:9:PRO:O	1:A:10:VAL:C	2.55	0.45
1:A:198:SER:CB	4:A:620[B]:IOD:I	3.34	0.45
1:A:66:THR:HB	1:A:70:PHE:N	2.32	0.45
1:A:198:SER:HB2	4:A:622[B]:IOD:I	2.87	0.45
1:A:211:GLY:HA2	11:A:787:HOH:O	2.17	0.45
1:A:34:PRO:HD2	4:A:624:IOD:I	2.87	0.44
1:A:430:GLY:HA2	4:A:621:IOD:I	2.88	0.44
1:A:199:LEU:CA	4:A:622[C]:IOD:I	3.33	0.44
1:A:585:LEU:HG	1:A:587:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:CB	4:A:622[B]:IOD:I	3.35	0.44
1:A:586:ASP:OD1	1:A:588:SER:HB3	2.17	0.44
1:A:551:ARG:HD3	1:A:583:ASP:O	2.18	0.44
1:A:1:SER:HB2	1:A:2:TRP:CE3	2.53	0.44
1:A:292:LEU:O	1:A:296:ALA:HB2	2.17	0.44
1:A:8:ALA:CB	1:A:167:CYS:O	2.66	0.44
1:A:548:SER:OG	1:A:551:ARG:HB2	2.17	0.43
1:A:291:LYS:O	1:A:295:GLU:HB2	2.18	0.43
1:A:20:PRO:HG3	11:A:1098:HOH:O	2.18	0.43
1:A:198:SER:C	4:A:622[B]:IOD:I	3.27	0.43
1:A:277:ALA:O	1:A:280:LEU:HB2	2.19	0.43
1:A:21:TYR:OH	1:A:295:GLU:HG2	2.18	0.43
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.53	0.43
1:A:313:LEU:N	1:A:314:PRO:CD	2.82	0.43
1:A:280:LEU:O	1:A:284:ASN:N	2.52	0.42
1:A:199:LEU:HD13	4:A:622[C]:IOD:I	2.89	0.42
1:A:377:HIS:NE2	5:A:618:SCN:S	2.91	0.42
1:A:544:LEU:O	1:A:547:VAL:HG22	2.20	0.41
1:A:8:ALA:HB3	1:A:167:CYS:O	2.20	0.41
1:A:9:PRO:O	1:A:11:PRO:N	2.54	0.41
1:A:94:GLN:OE1	1:A:403:LYS:HE2	2.21	0.41
1:A:224:LEU:HA	6:A:612:EDO:H22	2.02	0.41
1:A:193:TYR:CZ	1:A:297:ARG:HA	2.57	0.40
1:A:292:LEU:O	1:A:296:ALA:CB	2.69	0.40
1:A:365:TYR:CE2	1:A:397:ARG:HB3	2.55	0.40
1:A:365:TYR:CD1	1:A:572:TYR:CE2	3.10	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	595/595 (100%)	549 (92%)	42 (7%)	4 (1%)	22 12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	170	PRO
1	A	4	VAL
1	A	10	VAL

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	520/518 (100%)	505 (97%)	15 (3%)	42 35

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	VAL
1	A	32	ARG
1	A	91	VAL
1	A	115	PRO
1	A	128	GLN
1	A	172	TYR
1	A	197	PRO
1	A	201	SER
1	A	222	HIS
1	A	347	PHE
1	A	363	GLU
1	A	407	MET
1	A	465	LYS
1	A	587	LEU

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

Mol	Chain	Res	Type
1	A	124	HIS
1	A	138	ASN
1	A	570	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

2 monosaccharides are modelled in this entry.

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	NAG	B	1	1,2	14,14,15	0.63	0	17,19,21	1.55	4 (23%)
2	NAG	B	2	2	14,14,15	0.32	0	17,19,21	1.62	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	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	C1-O5-C5	5.37	119.47	112.19
2	B	2	NAG	C4-C3-C2	-3.07	106.52	111.02
2	B	1	NAG	O5-C1-C2	2.33	114.96	111.29
2	B	1	NAG	O7-C7-N2	2.29	126.16	121.95
2	B	1	NAG	C6-C5-C4	2.10	117.93	113.00
2	B	1	NAG	O4-C4-C3	-2.01	105.71	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

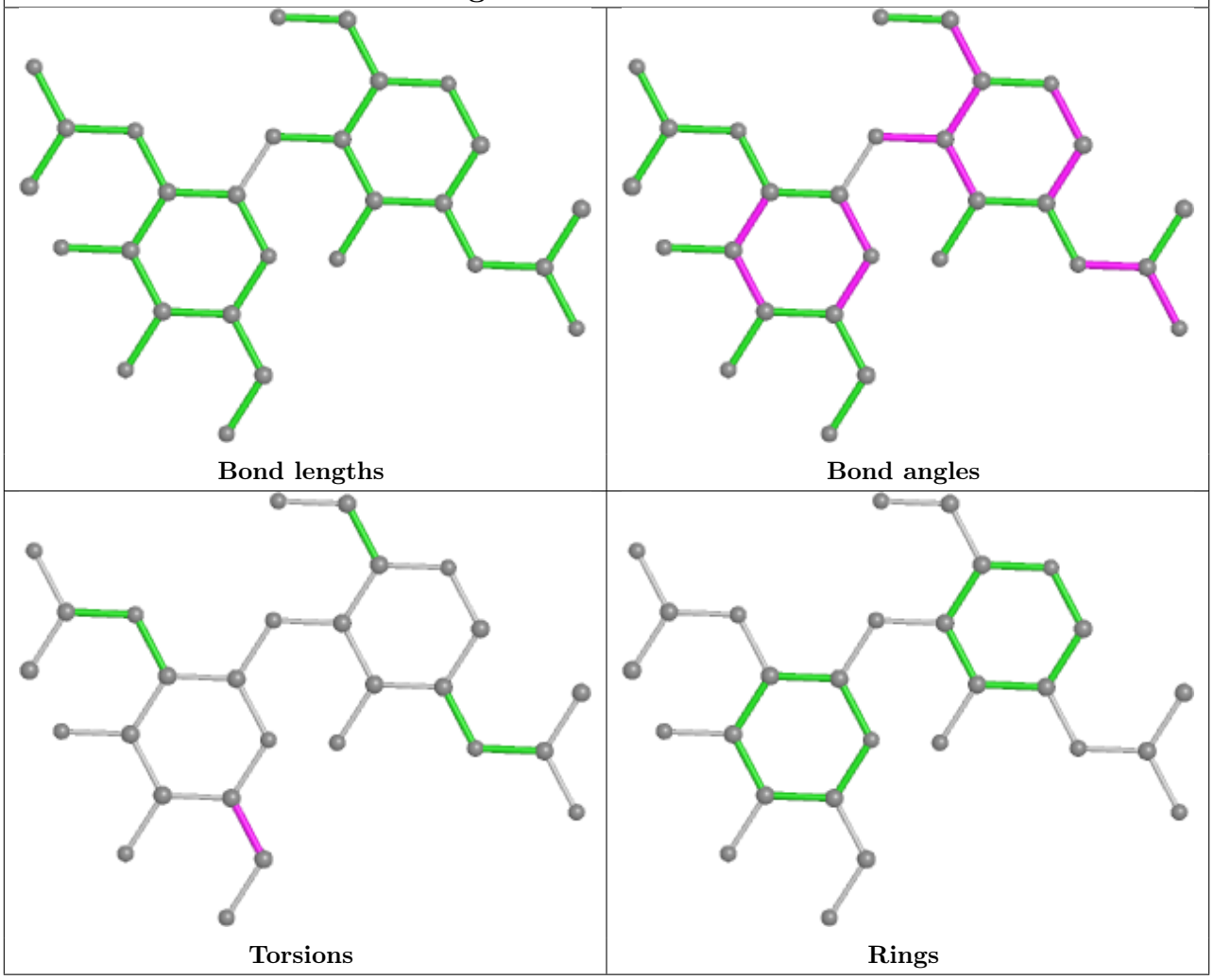
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain B



5.6 Ligand geometry (i)

Of 53 ligands modelled in this entry, 41 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
8	HEM	A	616[B]	-	41,50,50	1.37	8 (19%)	45,82,82	1.99	13 (28%)
5	SCN	A	611	-	1,2,2	0.92	0	0,1,1	-	-
6	EDO	A	615	-	3,3,3	0.13	0	2,2,2	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	A	633	1	14,14,15	0.57	0	17,19,21	0.98	1 (5%)
8	HEM	A	616[A]	-	41,50,50	1.23	6 (14%)	45,82,82	1.96	11 (24%)
7	NO2	A	614	8	1,2,2	0.15	0	0,1,1	-	-
10	NAG	A	635	1	14,14,15	0.29	0	17,19,21	1.60	4 (23%)
6	EDO	A	612	-	3,3,3	0.41	0	2,2,2	0.52	0
5	SCN	A	617	-	1,2,2	0.78	0	0,1,1	-	-
5	SCN	A	618	-	1,2,2	1.21	0	0,1,1	-	-
6	EDO	A	613	-	3,3,3	0.05	0	2,2,2	0.15	0
10	NAG	A	634	1	14,14,15	0.61	0	17,19,21	1.35	1 (5%)

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
8	HEM	A	616[B]	-	-	4/12/54/54	-
6	EDO	A	615	-	-	1/1/1/1	-
10	NAG	A	633	1	-	0/6/23/26	0/1/1/1
8	HEM	A	616[A]	-	-	5/12/54/54	-
10	NAG	A	635	1	-	0/6/23/26	0/1/1/1
6	EDO	A	612	-	-	0/1/1/1	-
6	EDO	A	613	-	-	0/1/1/1	-
10	NAG	A	634	1	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	616[B]	HEM	CBD-CGD	3.01	1.57	1.50
8	A	616[A]	HEM	C1B-NB	-2.88	1.35	1.40
8	A	616[B]	HEM	C1B-NB	-2.88	1.35	1.40
8	A	616[A]	HEM	C4B-NB	-2.56	1.33	1.38
8	A	616[B]	HEM	C4B-NB	-2.56	1.33	1.38
8	A	616[A]	HEM	CHB-C1B	2.49	1.41	1.35
8	A	616[B]	HEM	CHB-C1B	2.49	1.41	1.35
8	A	616[A]	HEM	C4D-ND	-2.44	1.36	1.40
8	A	616[B]	HEM	C4D-ND	-2.44	1.36	1.40
8	A	616[A]	HEM	C1A-CHA	-2.17	1.35	1.41
8	A	616[B]	HEM	C1A-CHA	-2.17	1.35	1.41
8	A	616[A]	HEM	FE-NB	2.17	2.07	1.96
8	A	616[B]	HEM	FE-NB	2.17	2.07	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	616[B]	HEM	O1D-CGD	2.01	1.28	1.22

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	616[A]	HEM	CHC-C4B-NB	5.03	129.90	124.43
8	A	616[B]	HEM	CHC-C4B-NB	5.03	129.90	124.43
8	A	616[A]	HEM	C1B-NB-C4B	4.42	109.63	105.07
8	A	616[B]	HEM	C1B-NB-C4B	4.42	109.63	105.07
10	A	635	NAG	C1-O5-C5	4.36	118.10	112.19
8	A	616[A]	HEM	CMD-C2D-C1D	4.34	131.65	125.04
8	A	616[B]	HEM	CMD-C2D-C1D	4.34	131.65	125.04
8	A	616[A]	HEM	CHD-C1D-ND	3.94	128.72	124.43
8	A	616[B]	HEM	CHD-C1D-ND	3.94	128.72	124.43
10	A	634	NAG	O5-C1-C2	-3.56	105.67	111.29
8	A	616[A]	HEM	CHA-C4D-ND	3.15	128.27	124.38
8	A	616[B]	HEM	CHA-C4D-ND	3.15	128.27	124.38
8	A	616[A]	HEM	CHA-C4D-C3D	-2.98	119.73	125.33
8	A	616[B]	HEM	CHA-C4D-C3D	-2.98	119.73	125.33
10	A	635	NAG	C3-C4-C5	-2.68	105.46	110.24
10	A	635	NAG	C4-C3-C2	-2.64	107.15	111.02
8	A	616[B]	HEM	O2D-CGD-O1D	-2.63	116.75	123.30
8	A	616[A]	HEM	CBD-CAD-C3D	-2.61	105.37	112.63
8	A	616[B]	HEM	O2D-CGD-CBD	2.55	122.23	114.03
8	A	616[B]	HEM	CAD-C3D-C4D	2.34	128.75	124.66
10	A	633	NAG	C1-O5-C5	2.33	115.35	112.19
8	A	616[A]	HEM	CHD-C1D-C2D	-2.26	121.44	124.98
8	A	616[B]	HEM	CHD-C1D-C2D	-2.26	121.44	124.98
8	A	616[A]	HEM	C4B-C3B-C2B	-2.24	105.34	107.11
8	A	616[B]	HEM	C4B-C3B-C2B	-2.24	105.34	107.11
8	A	616[A]	HEM	CMC-C2C-C3C	2.20	128.79	124.68
8	A	616[B]	HEM	CMC-C2C-C3C	2.20	128.79	124.68
8	A	616[A]	HEM	C2C-C3C-C4C	-2.18	105.38	106.90
8	A	616[B]	HEM	C2C-C3C-C4C	-2.18	105.38	106.90
10	A	635	NAG	C2-N2-C7	-2.02	120.03	122.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	616[A]	HEM	C3D-CAD-CBD-CGD
6	A	615	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
8	A	616[A]	HEM	CAA-CBA-CGA-O1A
8	A	616[B]	HEM	CAA-CBA-CGA-O1A
8	A	616[A]	HEM	CAA-CBA-CGA-O2A
8	A	616[B]	HEM	CAA-CBA-CGA-O2A
8	A	616[A]	HEM	CAD-CBD-CGD-O2D
8	A	616[A]	HEM	CAD-CBD-CGD-O1D
8	A	616[B]	HEM	CAD-CBD-CGD-O2D
8	A	616[B]	HEM	CAD-CBD-CGD-O1D

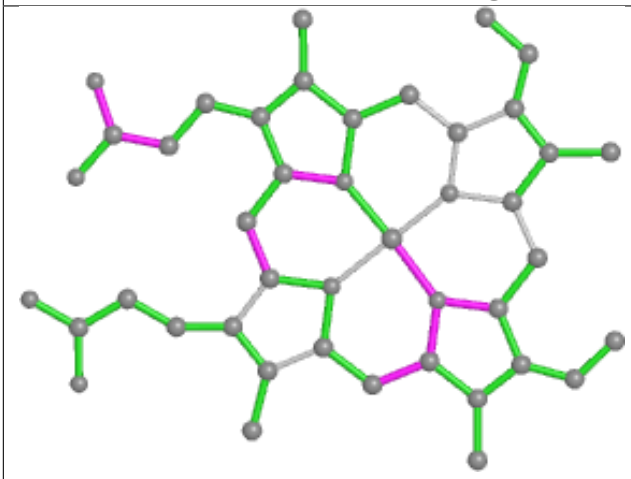
There are no ring outliers.

6 monomers are involved in 9 short contacts:

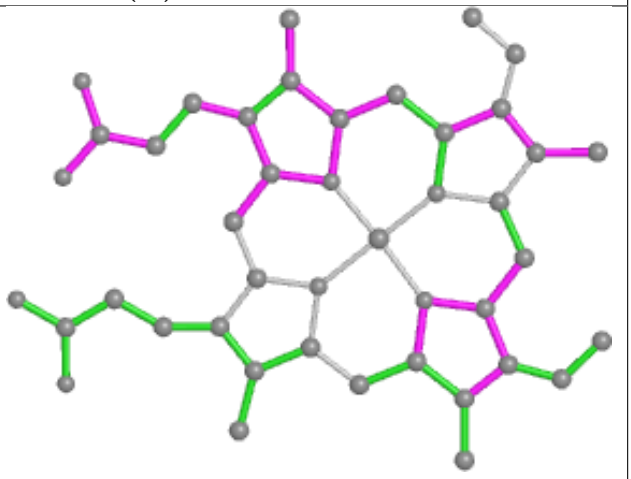
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	615	EDO	1	0
8	A	616[A]	HEM	2	0
7	A	614	NO2	5	0
6	A	612	EDO	1	0
5	A	617	SCN	1	0
5	A	618	SCN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

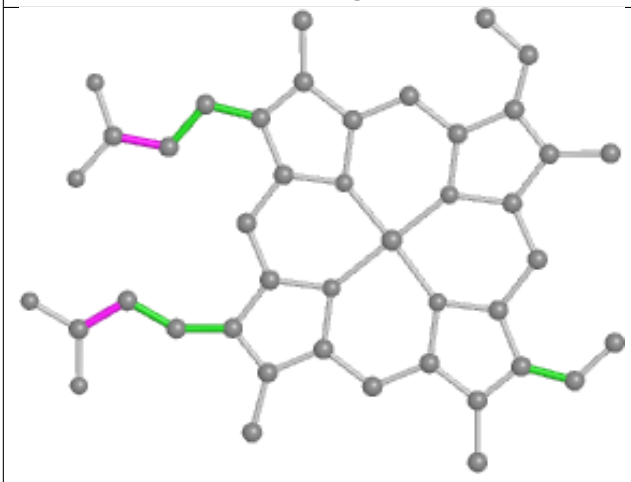
Ligand HEM A 616 (B)



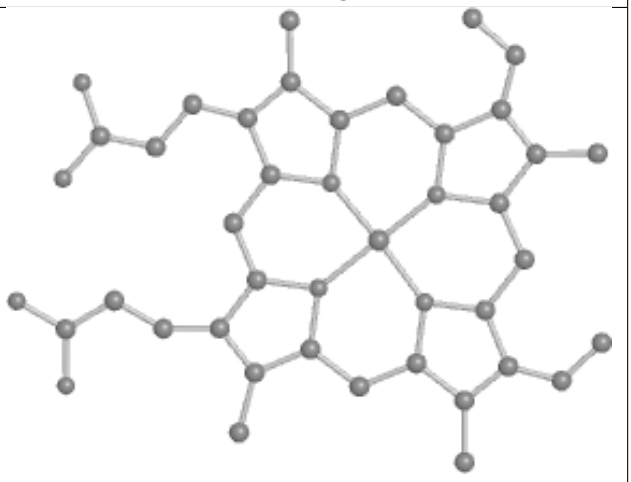
Bond lengths



Bond angles

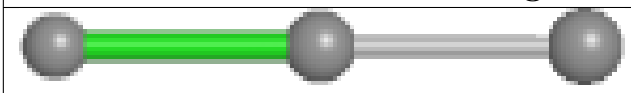


Torsions



Rings

Ligand SCN A 611



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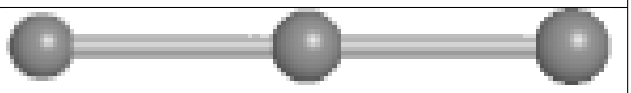

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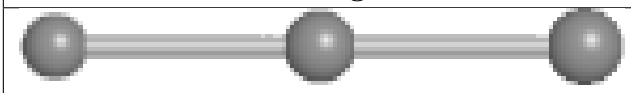
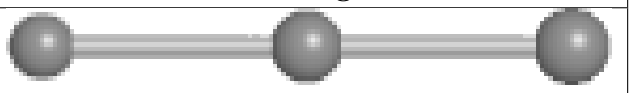
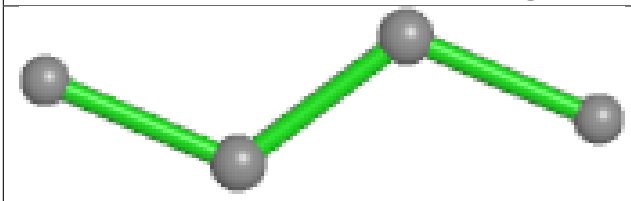


Torsions

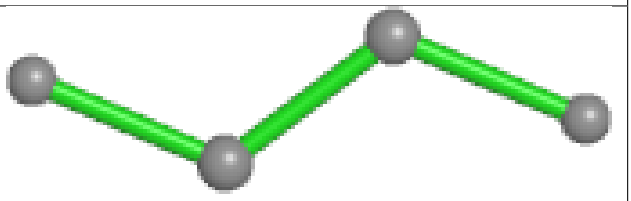


Rings

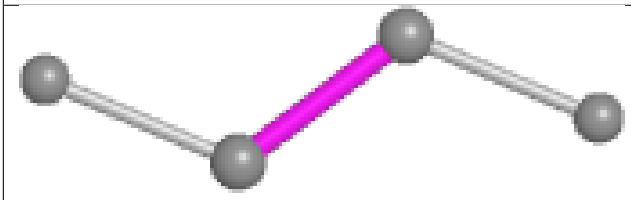
Ligand EDO A 615



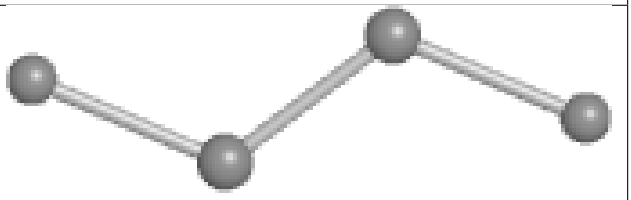
Bond lengths



Bond angles

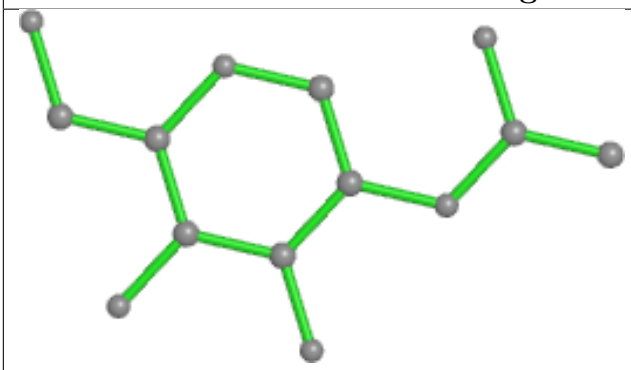


Torsions

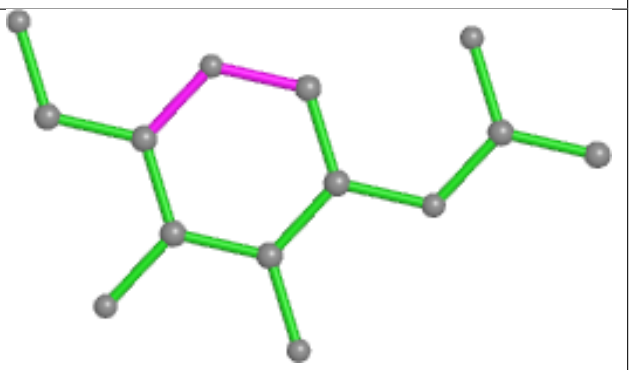


Rings

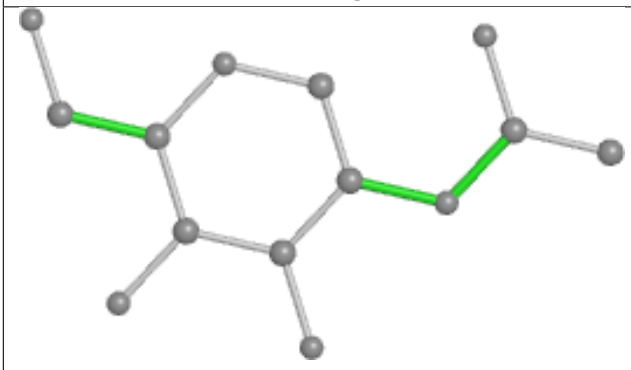
Ligand NAG A 633



Bond lengths



Bond angles



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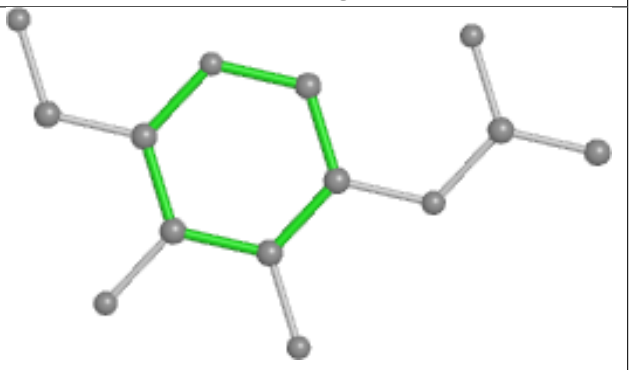
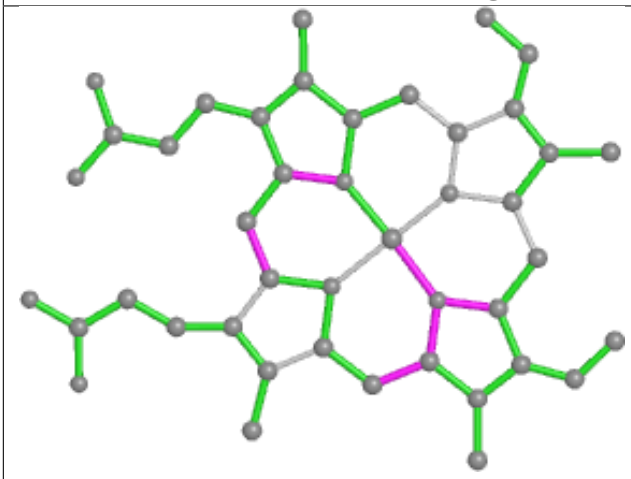
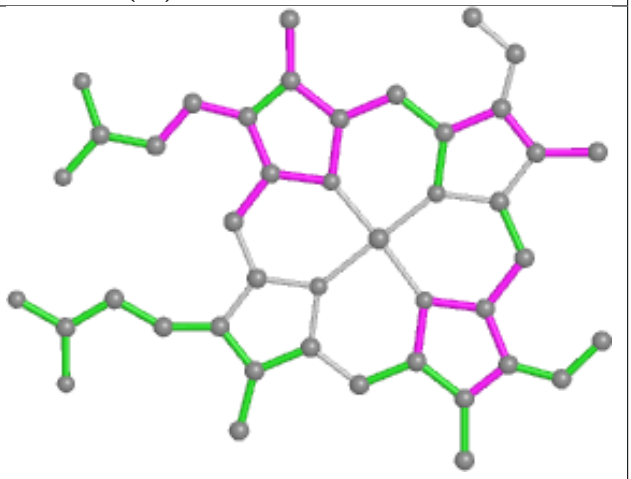


Rings

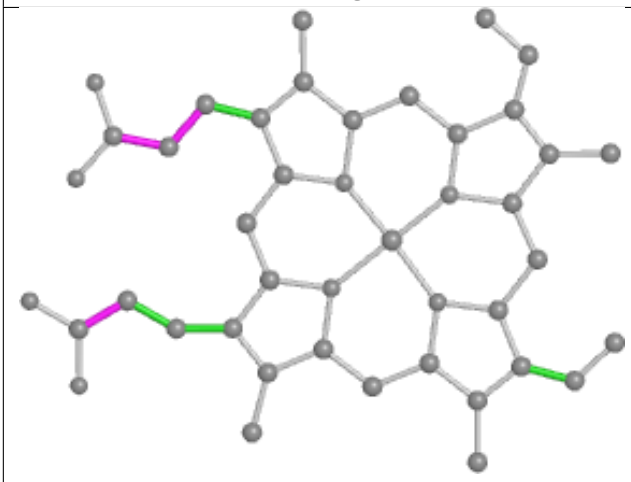
Ligand HEM A 616 (A)



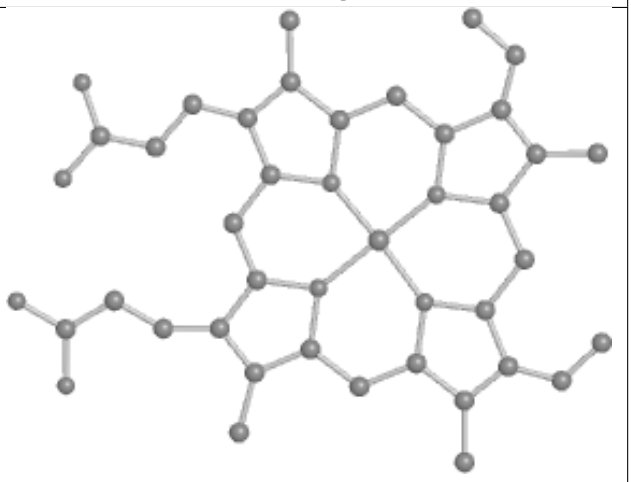
Bond lengths



Bond angles

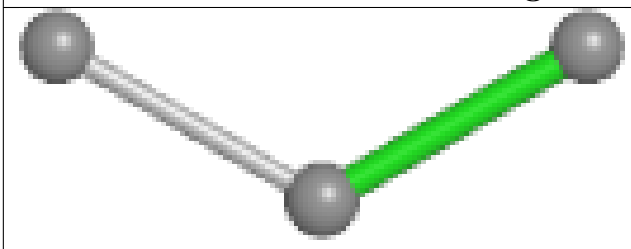


Torsions

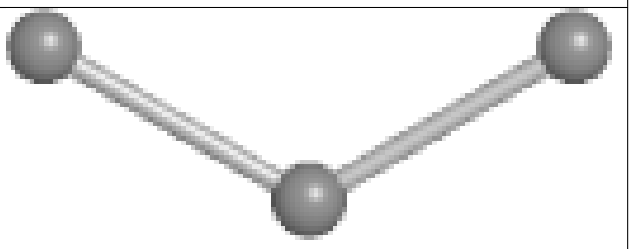


Rings

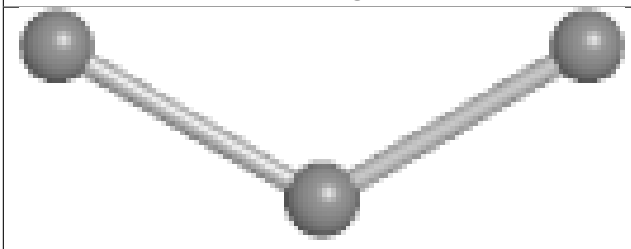
Ligand NO2 A 614



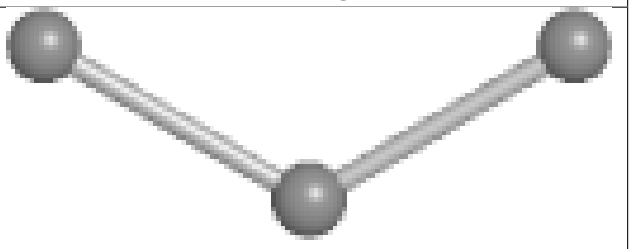
Bond lengths



Bond angles

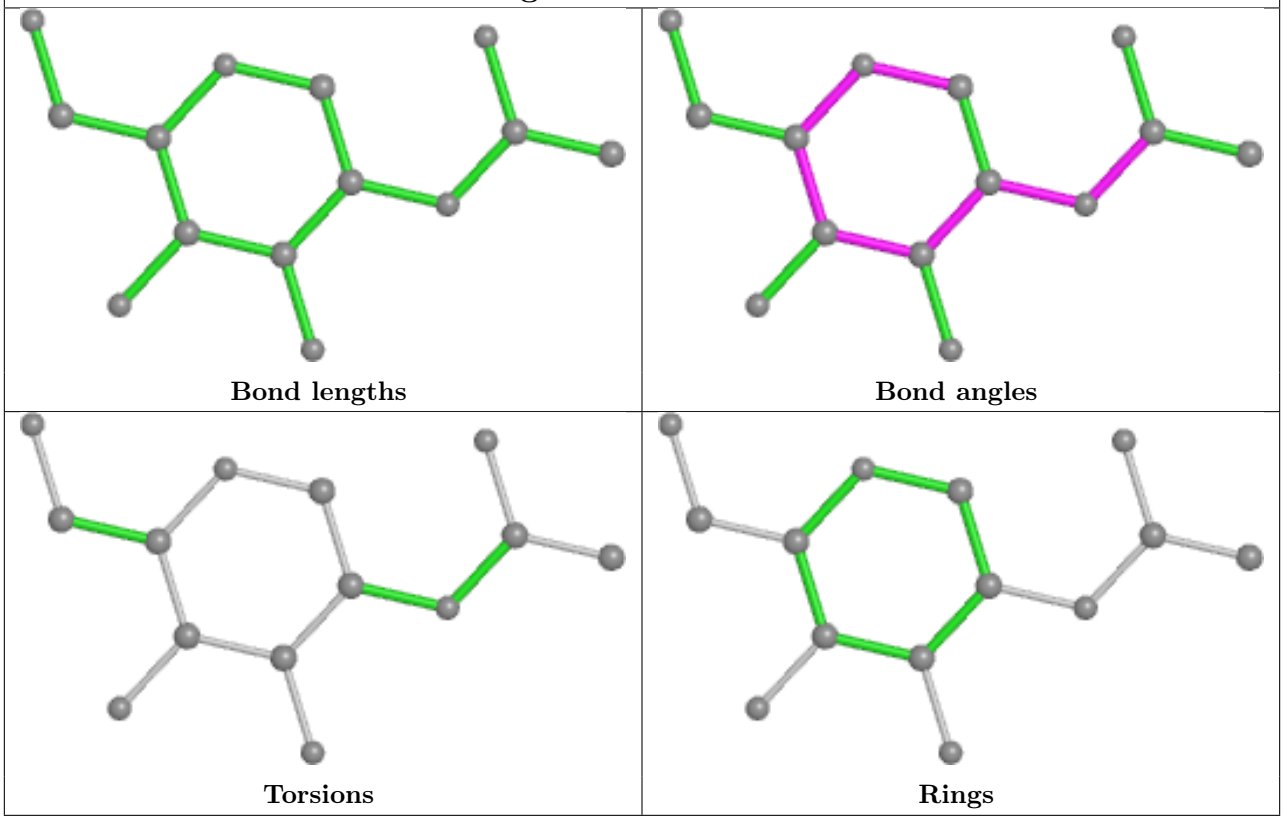


Torsions

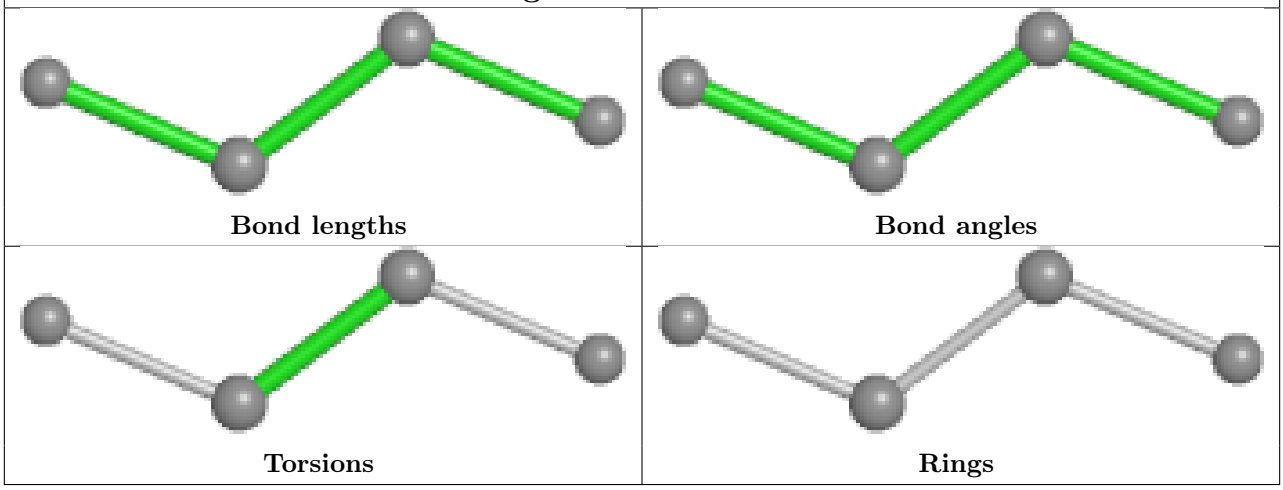


Rings

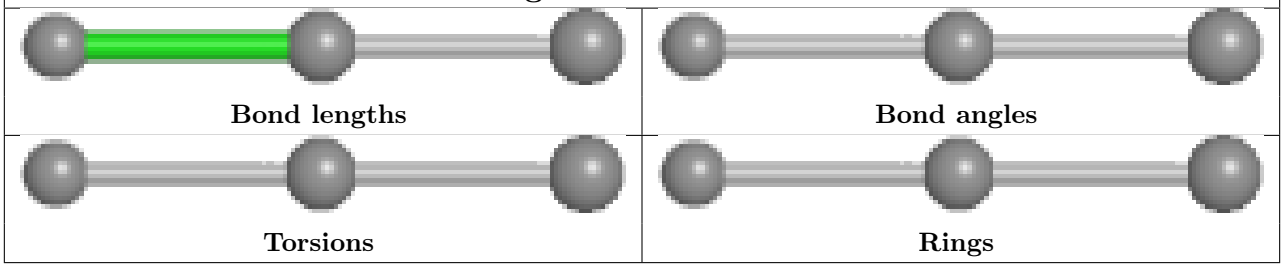
Ligand NAG A 635



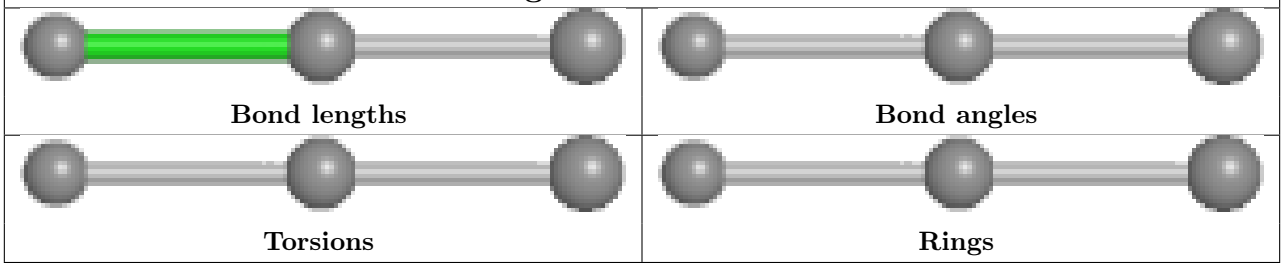
Ligand EDO A 612



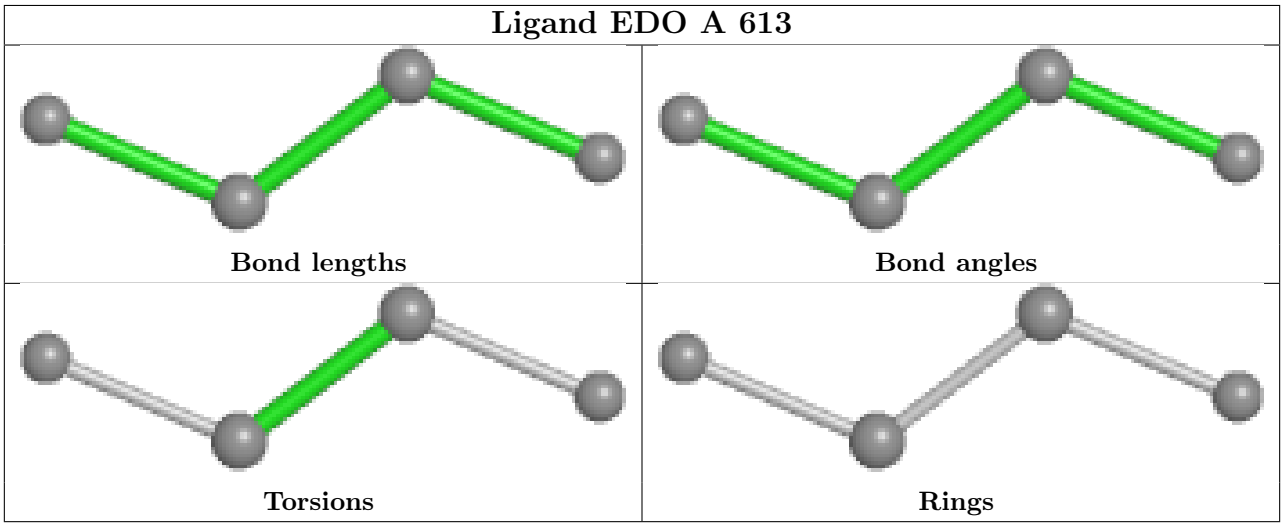
Ligand SCN A 617



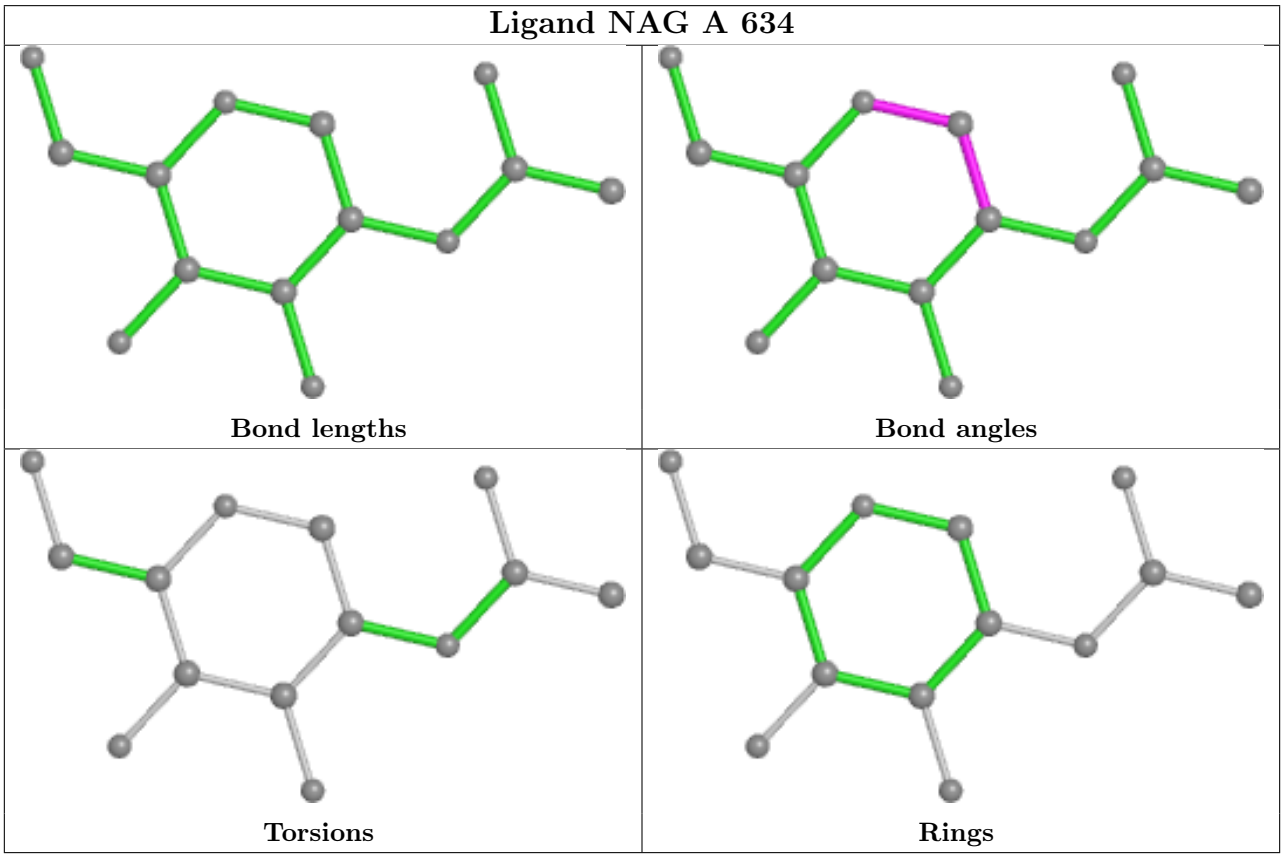
Ligand SCN A 618



Ligand EDO A 613



Ligand NAG A 634



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	595/595 (100%)	0.83	80 (13%)	3	3	12, 30, 81, 153	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	595	ASN	16.3
1	A	12	LEU	16.1
1	A	172	TYR	14.0
1	A	2	TRP	13.4
1	A	10	VAL	13.2
1	A	173	GLN	12.1
1	A	8	ALA	12.0
1	A	174	SER	11.8
1	A	1	SER	11.6
1	A	11	PRO	10.7
1	A	121	SER	10.6
1	A	119	LEU	10.2
1	A	9	PRO	9.7
1	A	171	PRO	9.3
1	A	122	ASN	8.9
1	A	593	ARG	8.7
1	A	4	VAL	8.6
1	A	594	GLU	7.8
1	A	280	LEU	7.7
1	A	283	LEU	7.6
1	A	13	VAL	7.1
1	A	124	HIS	6.6
1	A	170	PRO	5.7
1	A	425	THR	5.7
1	A	7	GLY	5.6
1	A	125	SER	5.0
1	A	287	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	220	TRP	4.6
1	A	123	GLU	4.4
1	A	574	HIS	4.4
1	A	169	THR	4.1
1	A	208	SER	4.1
1	A	592	SER	4.1
1	A	209	PRO	4.0
1	A	120	GLY	3.9
1	A	3	GLU	3.8
1	A	222	HIS	3.7
1	A	14	LYS	3.7
1	A	128	GLN	3.6
1	A	587	LEU	3.6
1	A	562	VAL	3.6
1	A	127	THR	3.6
1	A	561	LYS	3.5
1	A	282	LYS	3.5
1	A	254	PHE	3.4
1	A	212	LEU	3.4
1	A	285	PRO	3.3
1	A	175	LEU	3.3
1	A	5	GLY	3.0
1	A	279	GLU	3.0
1	A	132	TYR	3.0
1	A	286	HIS	3.0
1	A	130	GLU	2.8
1	A	591	ALA	2.7
1	A	288	ASN	2.7
1	A	588	SER	2.7
1	A	210	LEU	2.6
1	A	211	GLY	2.6
1	A	268	LEU	2.5
1	A	276	LEU	2.5
1	A	131	GLU	2.5
1	A	269	LEU	2.5
1	A	129	CYS	2.5
1	A	32	ARG	2.4
1	A	560	THR	2.3
1	A	223	GLY	2.3
1	A	126	LYS	2.3
1	A	206	LEU	2.3
1	A	168	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	538	GLU	2.3
1	A	64	ARG	2.3
1	A	277	ALA	2.3
1	A	579	CYS	2.2
1	A	577	VAL	2.2
1	A	134	ILE	2.2
1	A	583	ASP	2.1
1	A	572	TYR	2.1
1	A	544	LEU	2.1
1	A	543	SER	2.0
1	A	370	PRO	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)

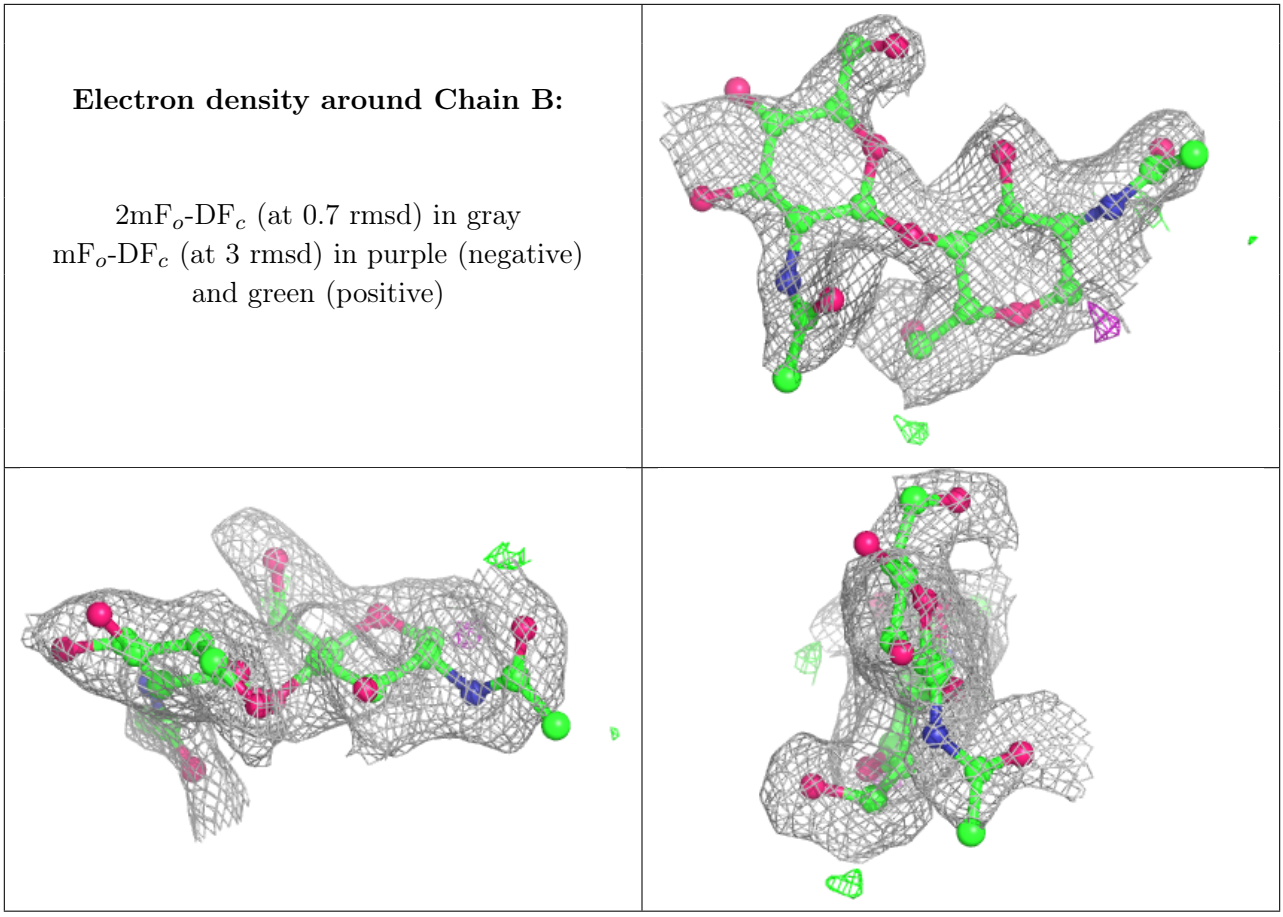
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	NAG	B	1	14/15	0.71	0.19	38,56,60,66	0
2	NAG	B	2	14/15	0.74	0.26	65,74,79,83	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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



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
10	NAG	A	633	14/15	0.66	0.30	51,61,70,72	0
10	NAG	A	635	14/15	0.81	0.16	48,58,64,64	0
6	EDO	A	612	4/4	0.83	0.18	24,24,27,30	0
10	NAG	A	634	14/15	0.89	0.10	34,38,40,42	0
6	EDO	A	613	4/4	0.90	0.22	40,48,50,50	0
5	SCN	A	611	3/3	0.90	0.10	47,47,54,54	0
6	EDO	A	615	4/4	0.92	0.13	31,31,33,35	0
4	IOD	A	609	1/1	0.95	0.04	50,50,50,50	1
9	ZN	A	632[B]	1/1	0.96	0.05	48,48,48,48	1
4	IOD	A	629	1/1	0.96	0.07	50,50,50,50	1
7	NO2	A	614	3/3	0.96	0.15	14,14,16,18	3
9	ZN	A	632[A]	1/1	0.96	0.05	40,40,40,40	1

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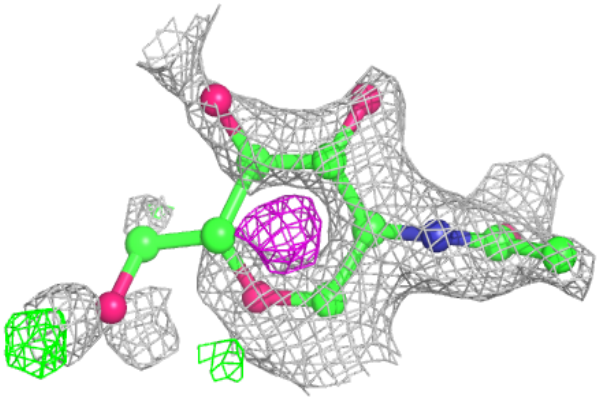
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	IOD	A	631[B]	1/1	0.97	0.08	41,41,41,41	1
4	IOD	A	605	1/1	0.97	0.03	50,50,50,50	1
5	SCN	A	617	3/3	0.97	0.08	40,40,41,49	0
4	IOD	A	604[A]	1/1	0.97	0.07	33,33,33,33	1
4	IOD	A	604[B]	1/1	0.97	0.07	46,46,46,46	1
4	IOD	A	631[A]	1/1	0.97	0.08	47,47,47,47	1
4	IOD	A	624	1/1	0.98	0.05	46,46,46,46	1
4	IOD	A	626[A]	1/1	0.98	0.07	46,46,46,46	1
4	IOD	A	626[B]	1/1	0.98	0.07	55,55,55,55	1
4	IOD	A	608[B]	1/1	0.98	0.04	26,26,26,26	1
8	HEM	A	616[A]	43/43	0.98	0.14	12,14,17,20	5
8	HEM	A	616[B]	43/43	0.98	0.14	12,14,19,20	5
4	IOD	A	608[A]	1/1	0.98	0.04	24,24,24,24	1
4	IOD	A	610	1/1	0.98	0.06	33,33,33,33	1
4	IOD	A	620[A]	1/1	0.98	0.03	28,28,28,28	1
4	IOD	A	620[B]	1/1	0.98	0.03	30,30,30,30	1
5	SCN	A	618	3/3	0.98	0.08	22,22,23,26	3
4	IOD	A	630	1/1	0.99	0.03	35,35,35,35	1
3	CA	A	601	1/1	0.99	0.05	17,17,17,17	0
4	IOD	A	622[A]	1/1	0.99	0.04	23,23,23,23	1
4	IOD	A	622[B]	1/1	0.99	0.04	39,39,39,39	1
4	IOD	A	622[C]	1/1	0.99	0.04	29,29,29,29	1
4	IOD	A	622[D]	1/1	0.99	0.04	30,30,30,30	1
4	IOD	A	603[A]	1/1	0.99	0.04	24,24,24,24	1
4	IOD	A	625	1/1	0.99	0.05	33,33,33,33	1
4	IOD	A	603[B]	1/1	0.99	0.04	25,25,25,25	1
4	IOD	A	606[A]	1/1	0.99	0.05	23,23,23,23	1
4	IOD	A	627[A]	1/1	0.99	0.04	21,21,21,21	1
4	IOD	A	627[B]	1/1	0.99	0.04	19,19,19,19	1
4	IOD	A	627[C]	1/1	0.99	0.04	25,25,25,25	1
4	IOD	A	627[D]	1/1	0.99	0.04	20,20,20,20	1
4	IOD	A	628[A]	1/1	0.99	0.03	26,26,26,26	1
4	IOD	A	628[B]	1/1	0.99	0.03	42,42,42,42	1
4	IOD	A	606[B]	1/1	0.99	0.05	22,22,22,22	1
4	IOD	A	607	1/1	1.00	0.03	27,27,27,27	1
4	IOD	A	621	1/1	1.00	0.02	30,30,30,30	1
4	IOD	A	602[B]	1/1	1.00	0.04	32,32,32,32	1
4	IOD	A	619[A]	1/1	1.00	0.05	20,20,20,20	1
4	IOD	A	619[B]	1/1	1.00	0.05	17,17,17,17	1
4	IOD	A	602[A]	1/1	1.00	0.04	21,21,21,21	1
4	IOD	A	623	1/1	1.00	0.04	18,18,18,18	0

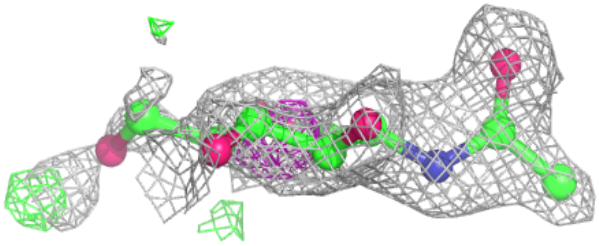
The following is a graphical depiction of the model fit to experimental electron density of all

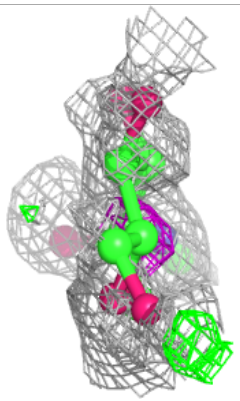
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG A 633:

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

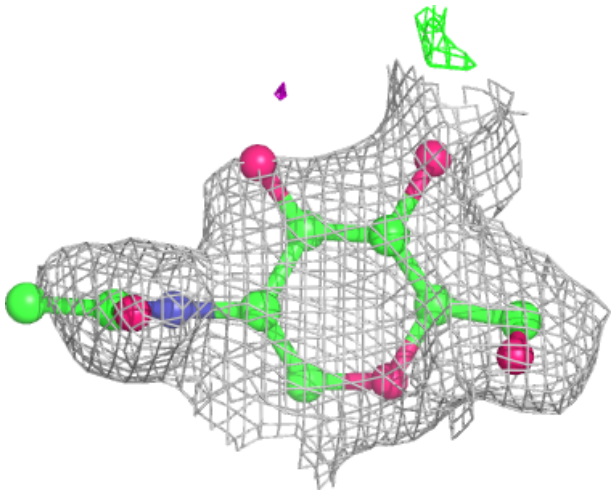


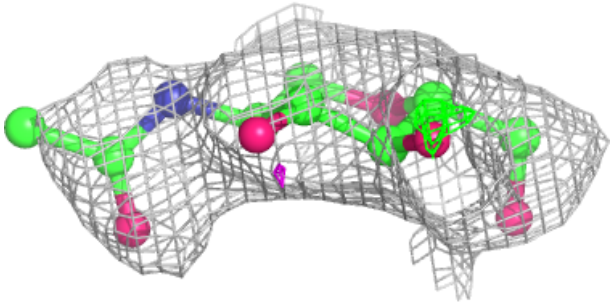


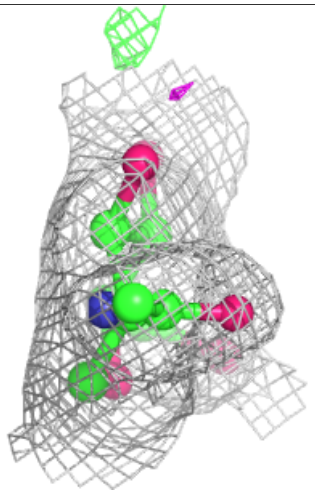


Electron density around NAG A 635:

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

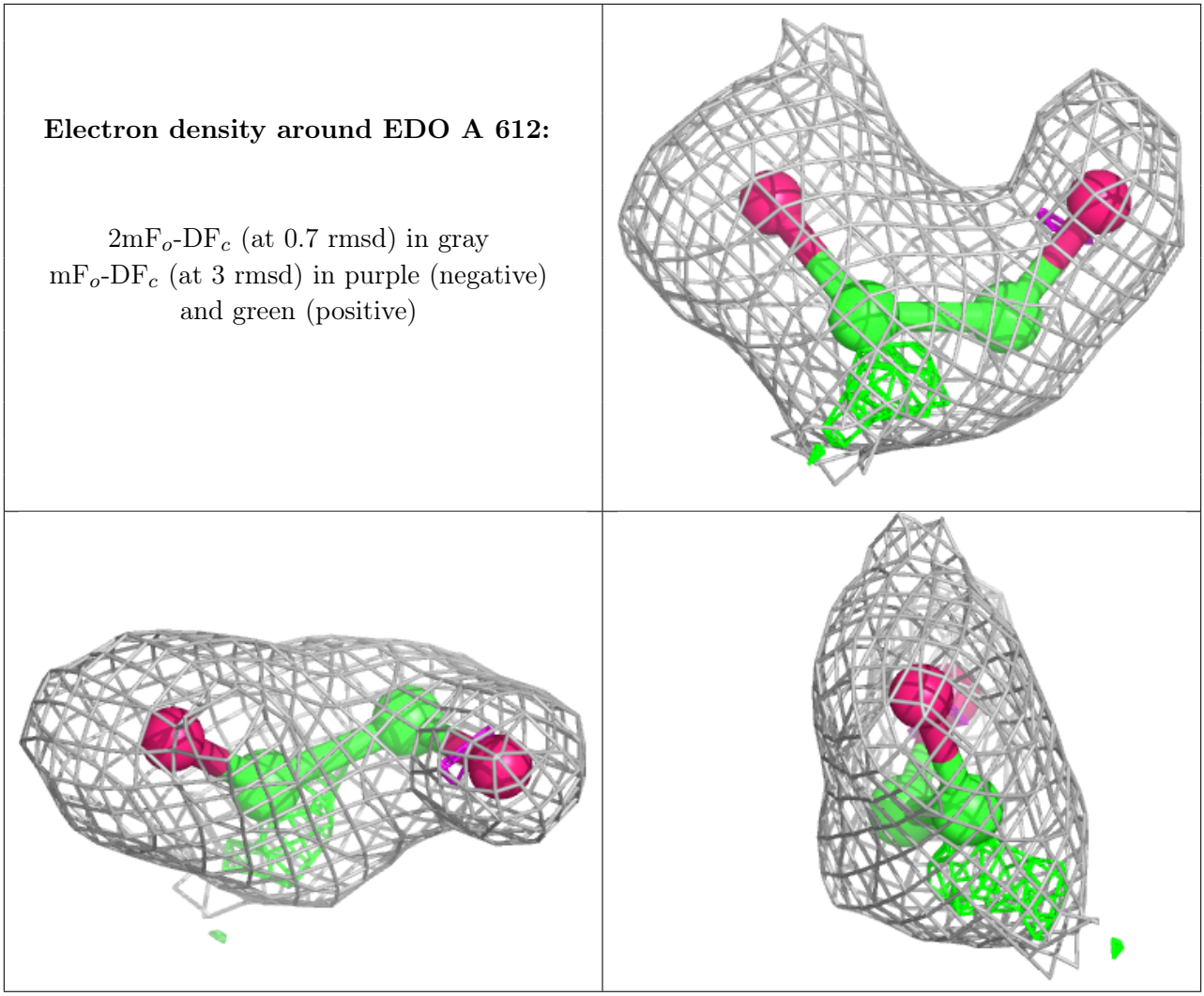






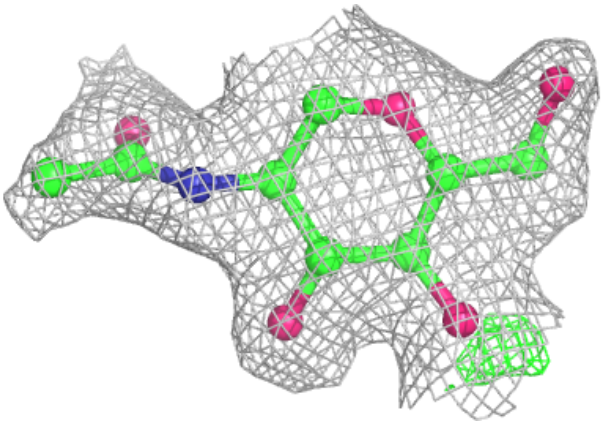
Electron density around EDO A 612:

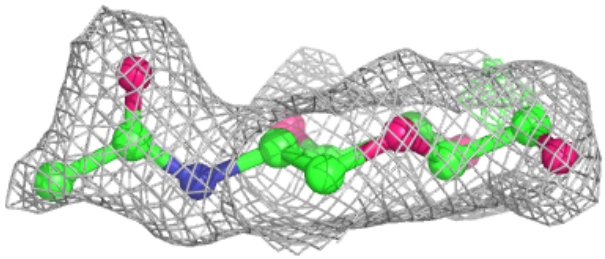
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

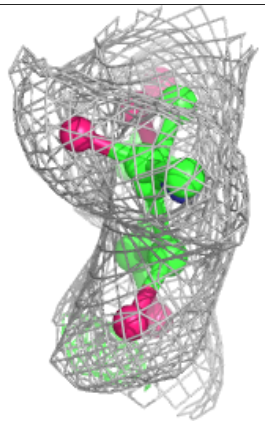


Electron density around NAG A 634:

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

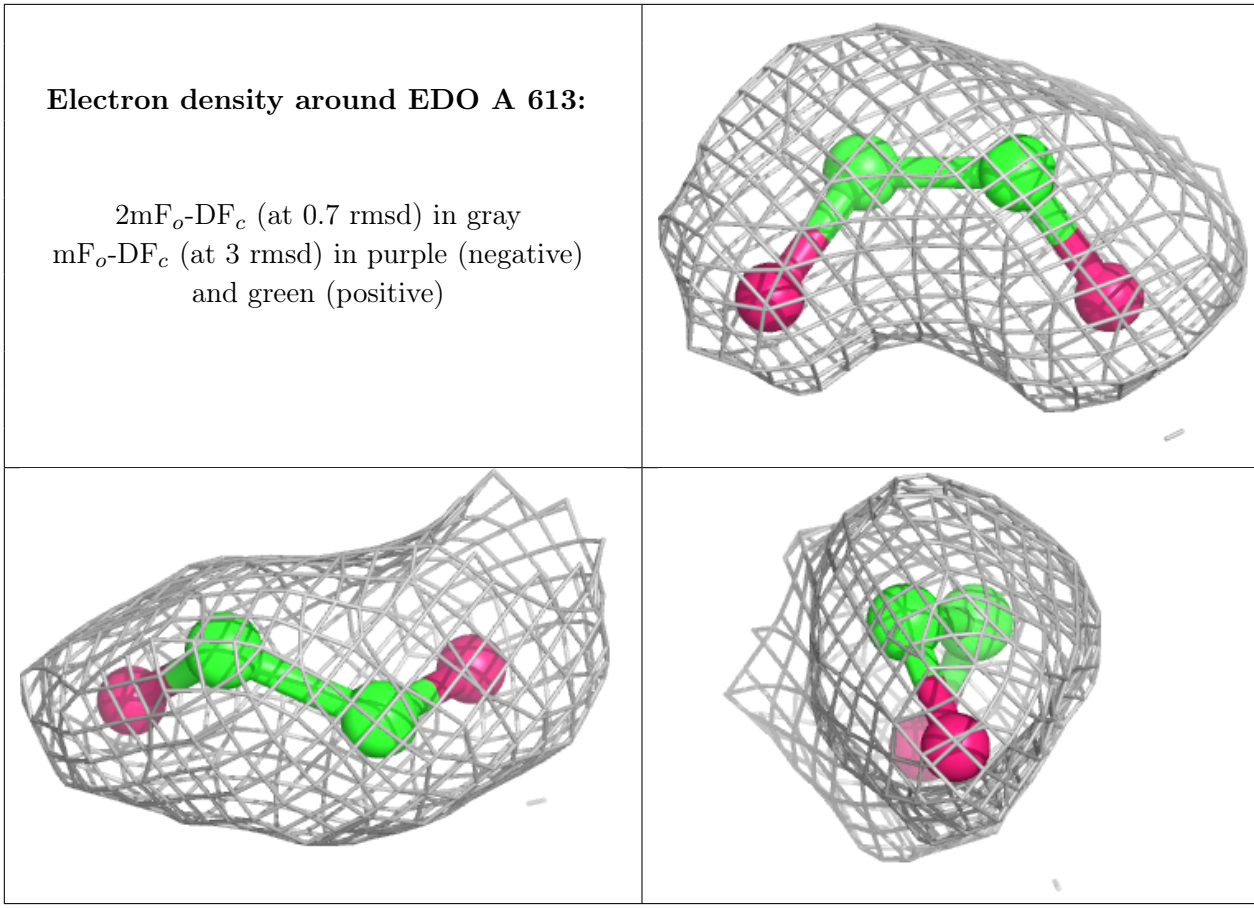






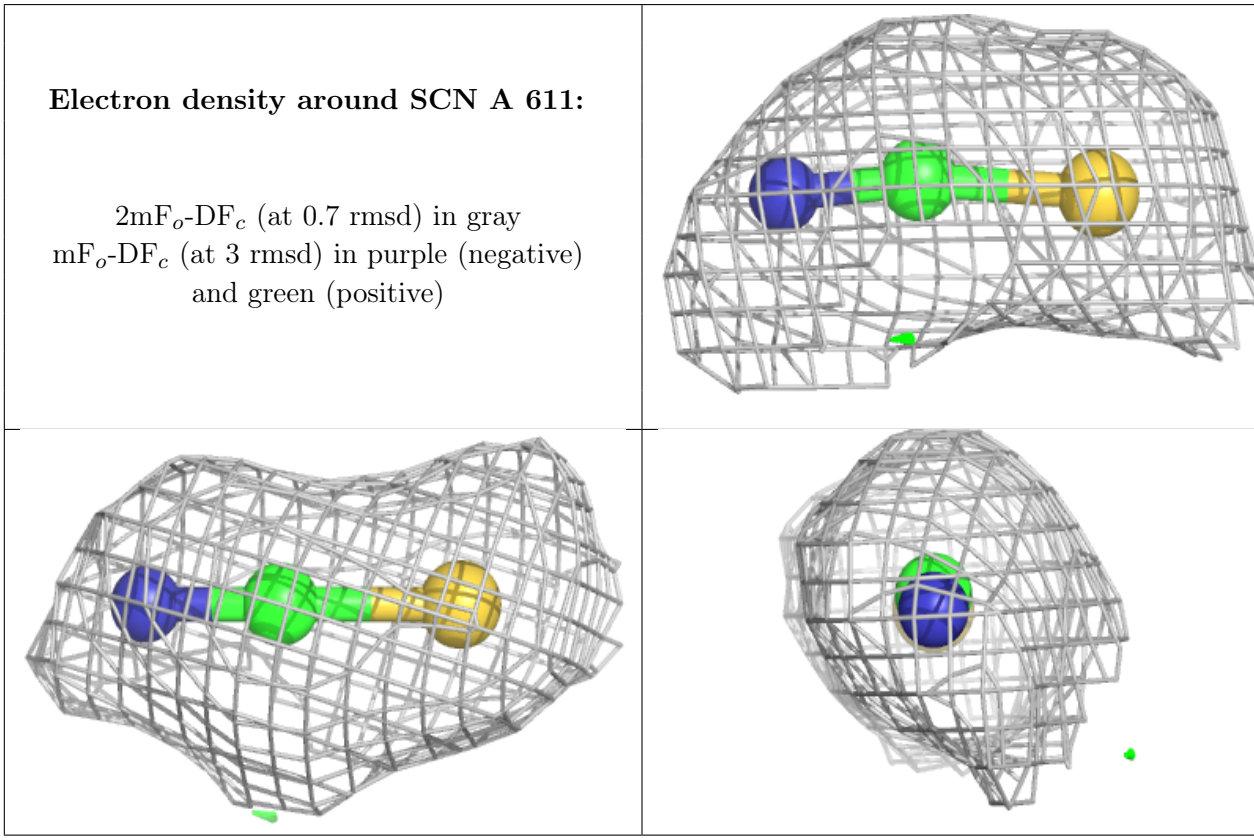
Electron density around EDO A 613:

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



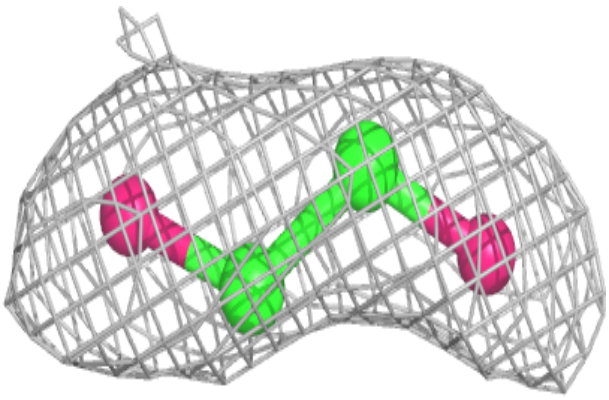
Electron density around SCN A 611:

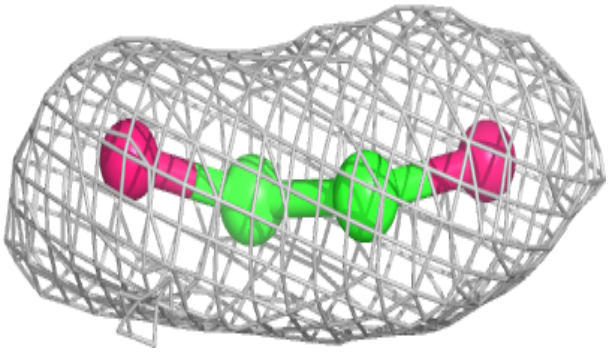
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

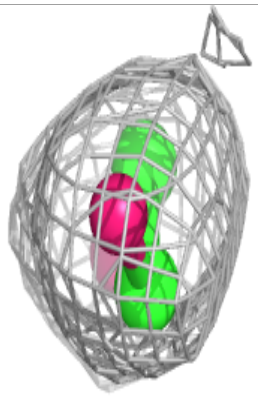


Electron density around EDO A 615:

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

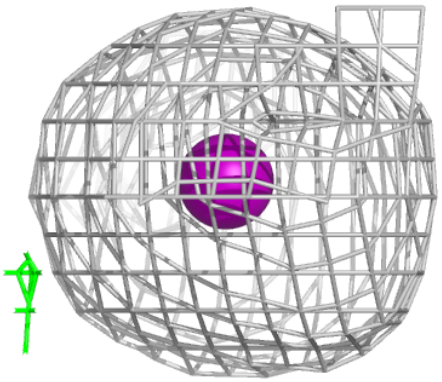


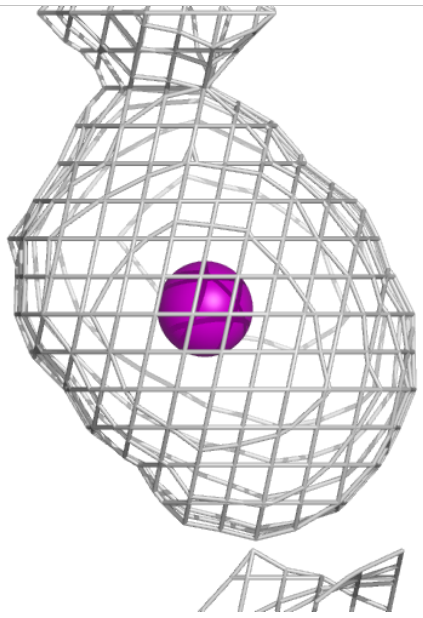


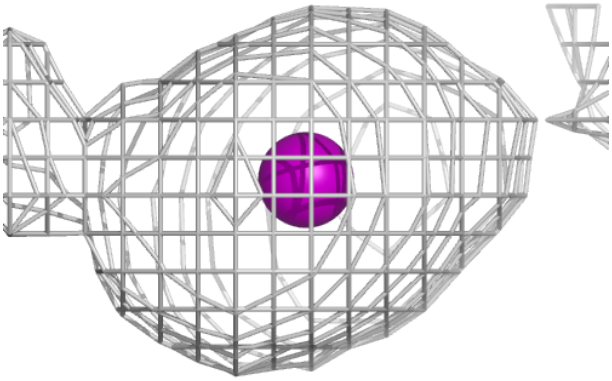


Electron density around IOD A 609:

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

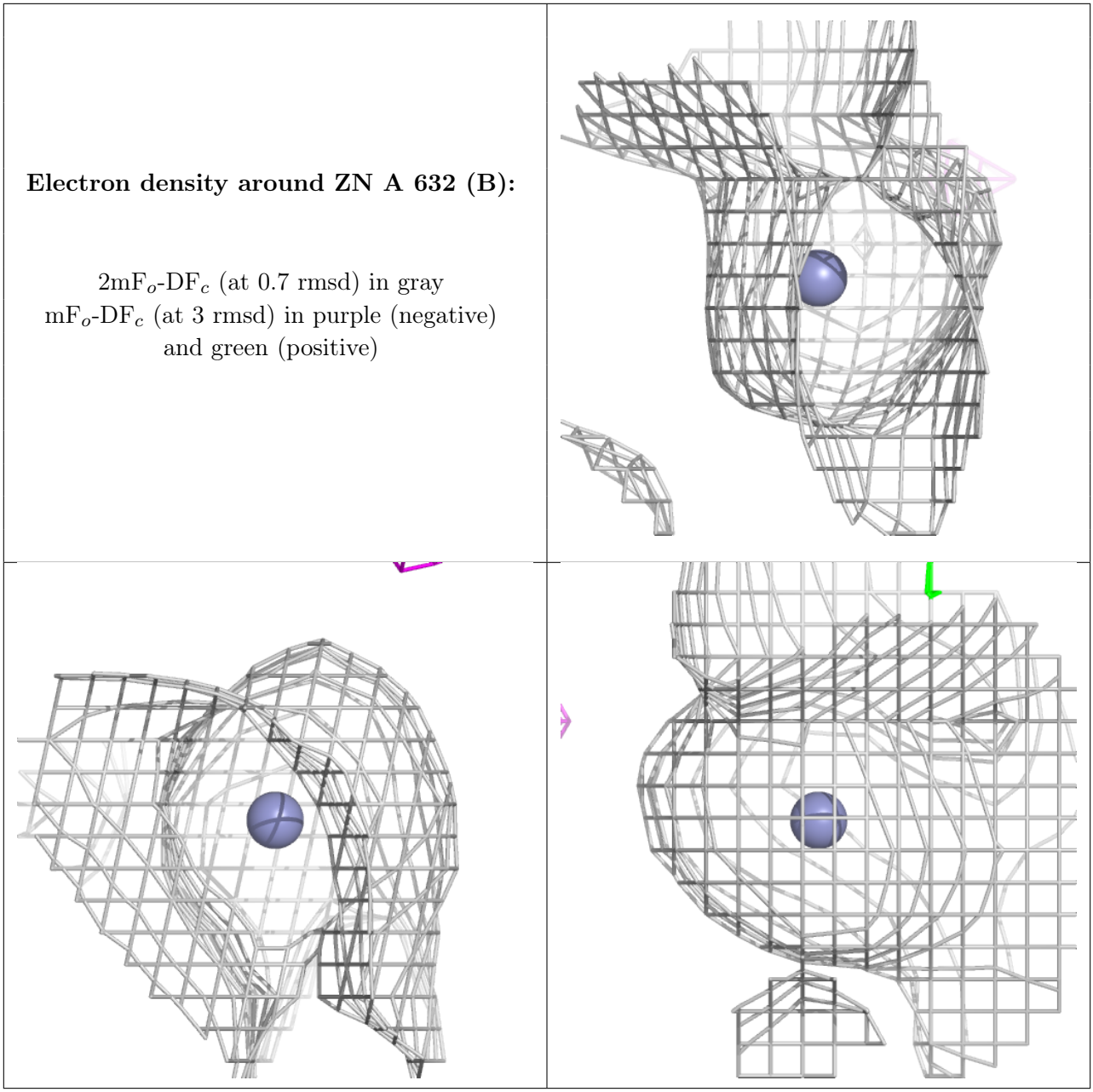






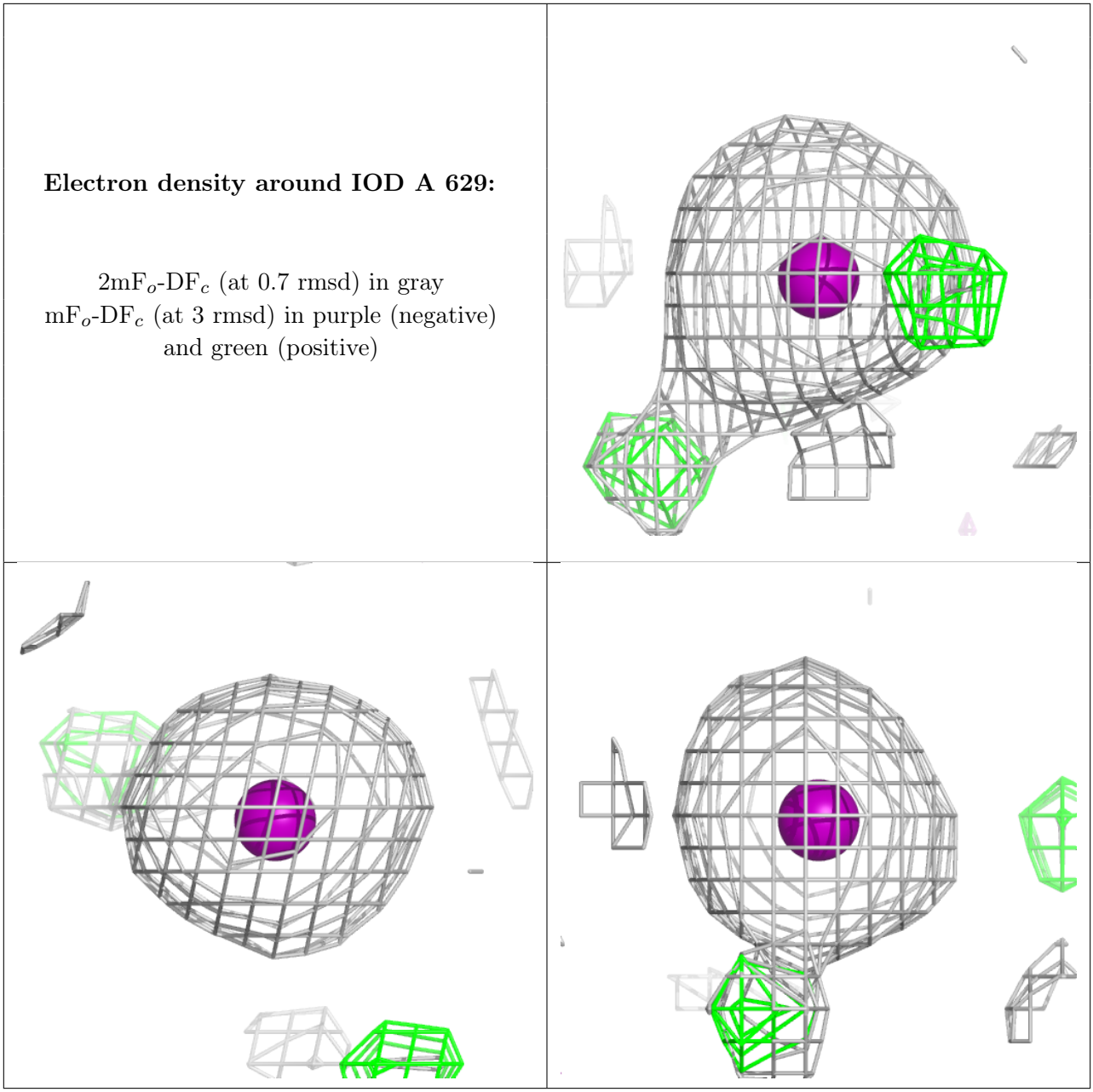
Electron density around ZN A 632 (B):

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



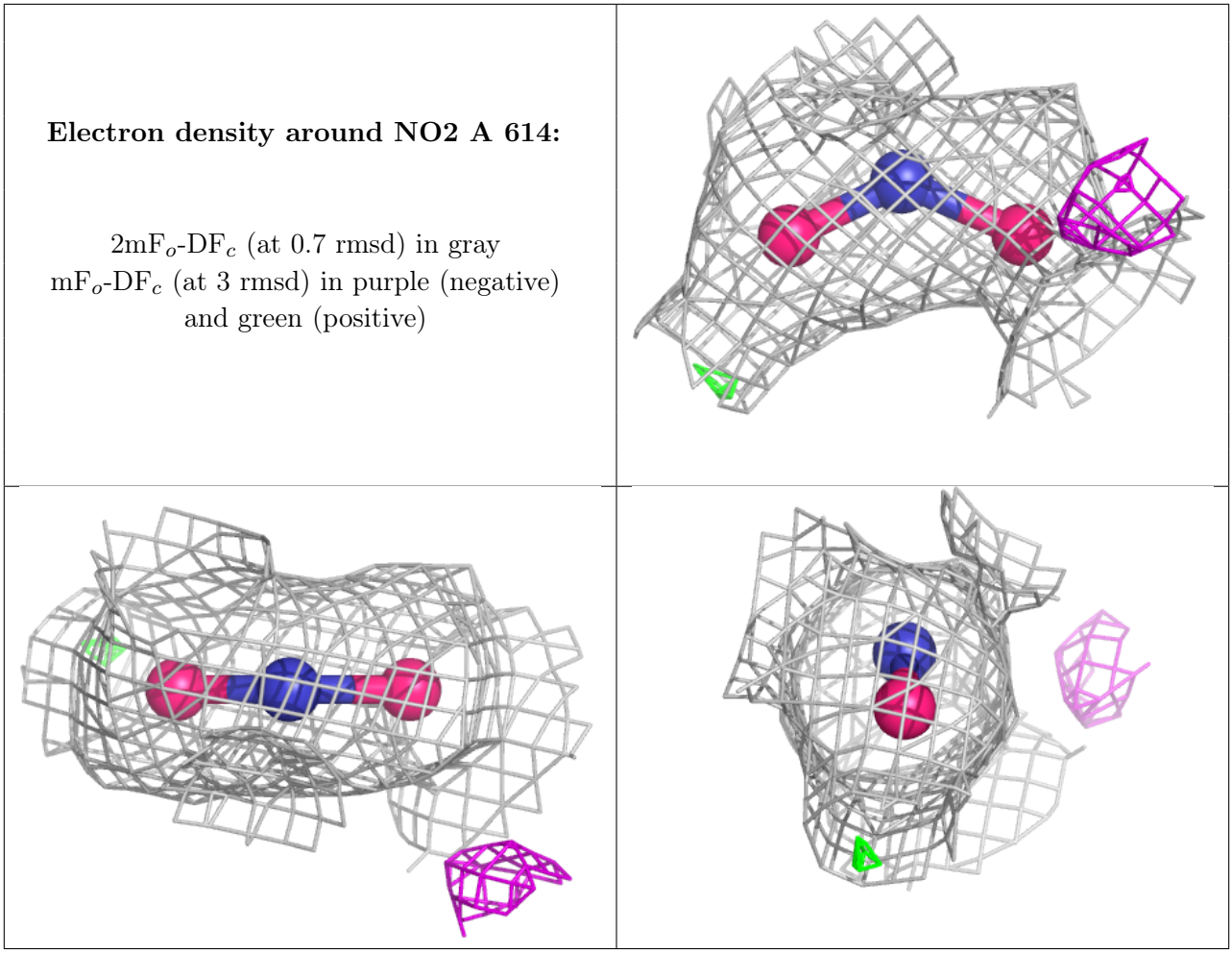
Electron density around IOD A 629:

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



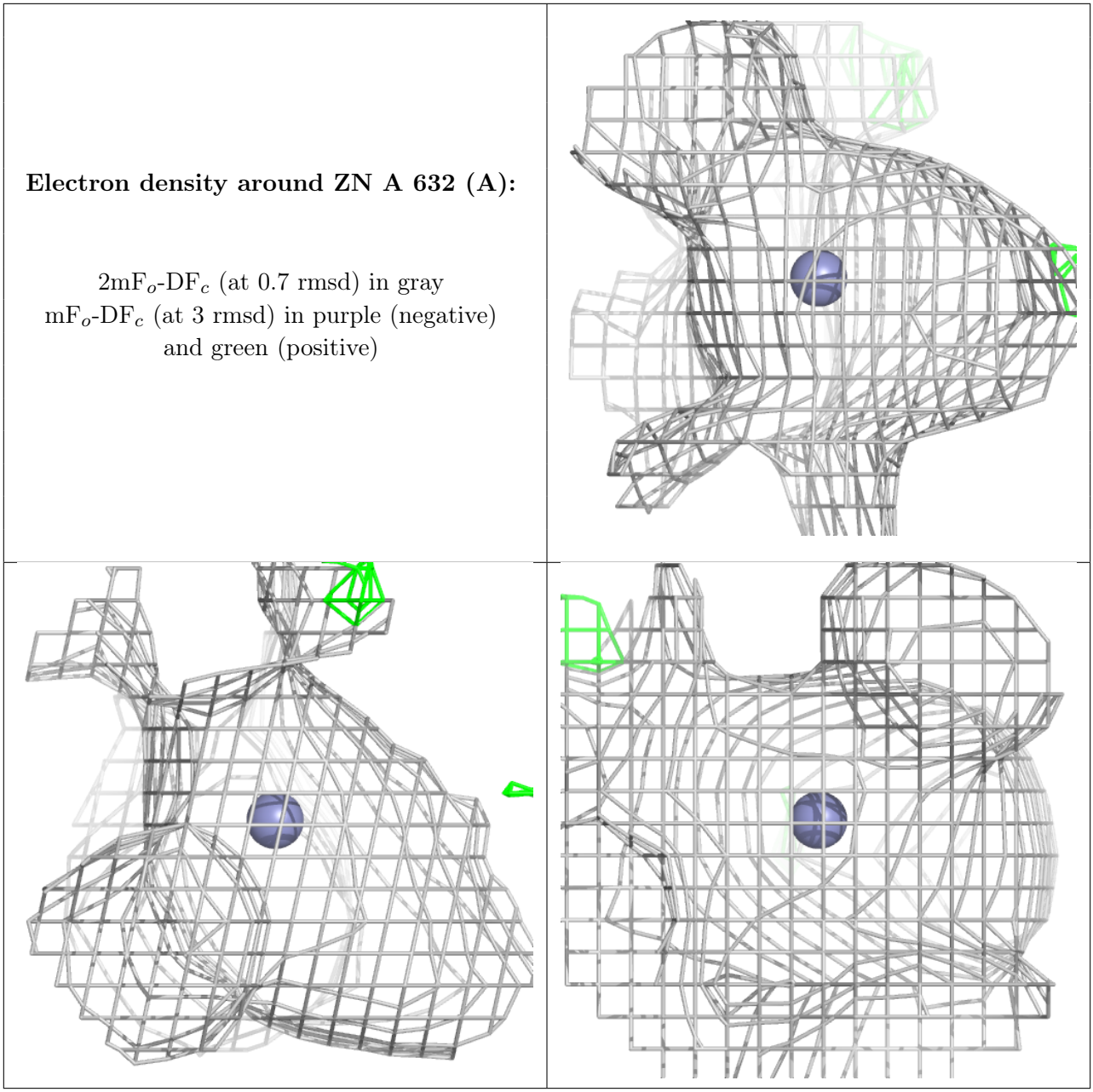
Electron density around NO2 A 614:

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



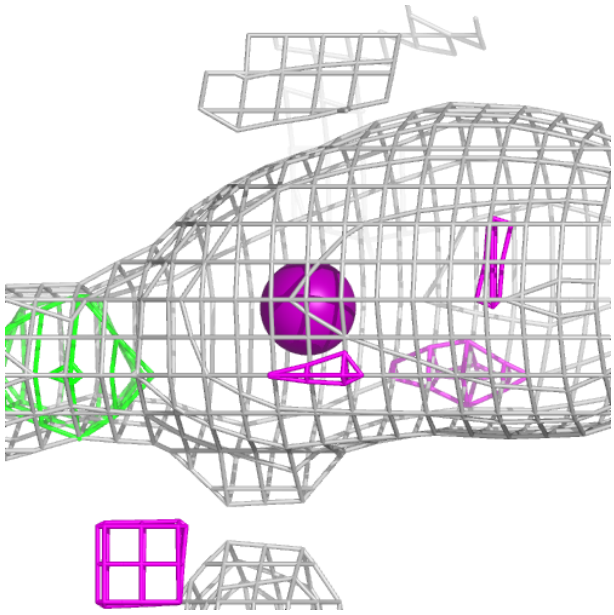
Electron density around ZN A 632 (A):

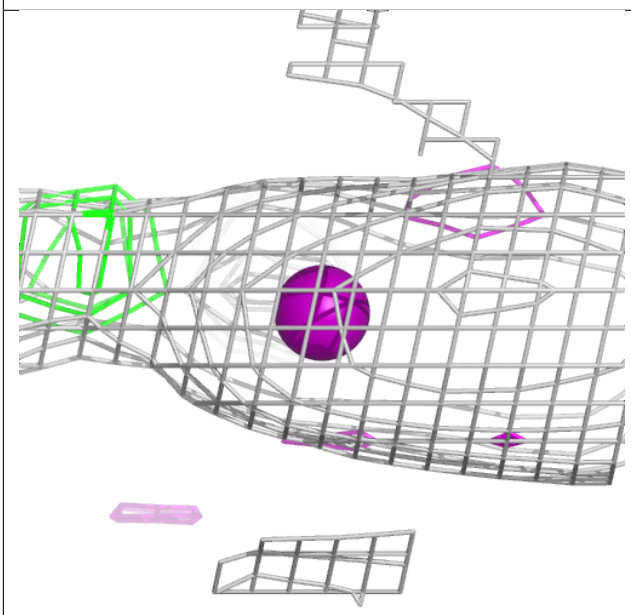
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

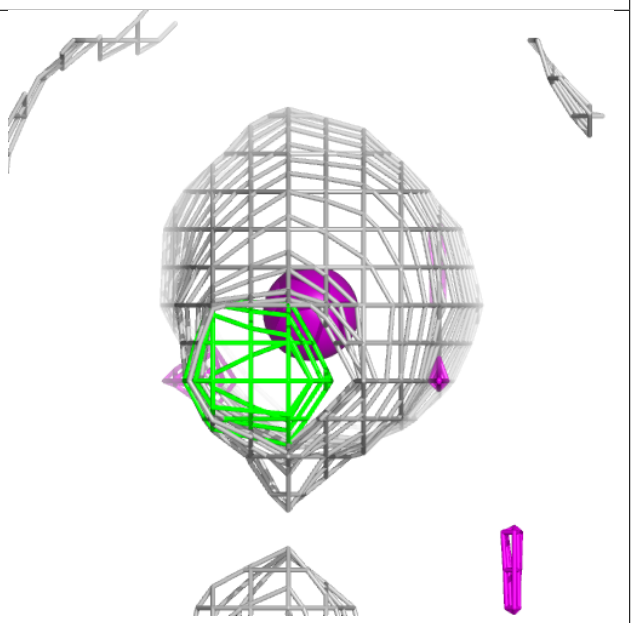


Electron density around IOD A 631 (B):

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

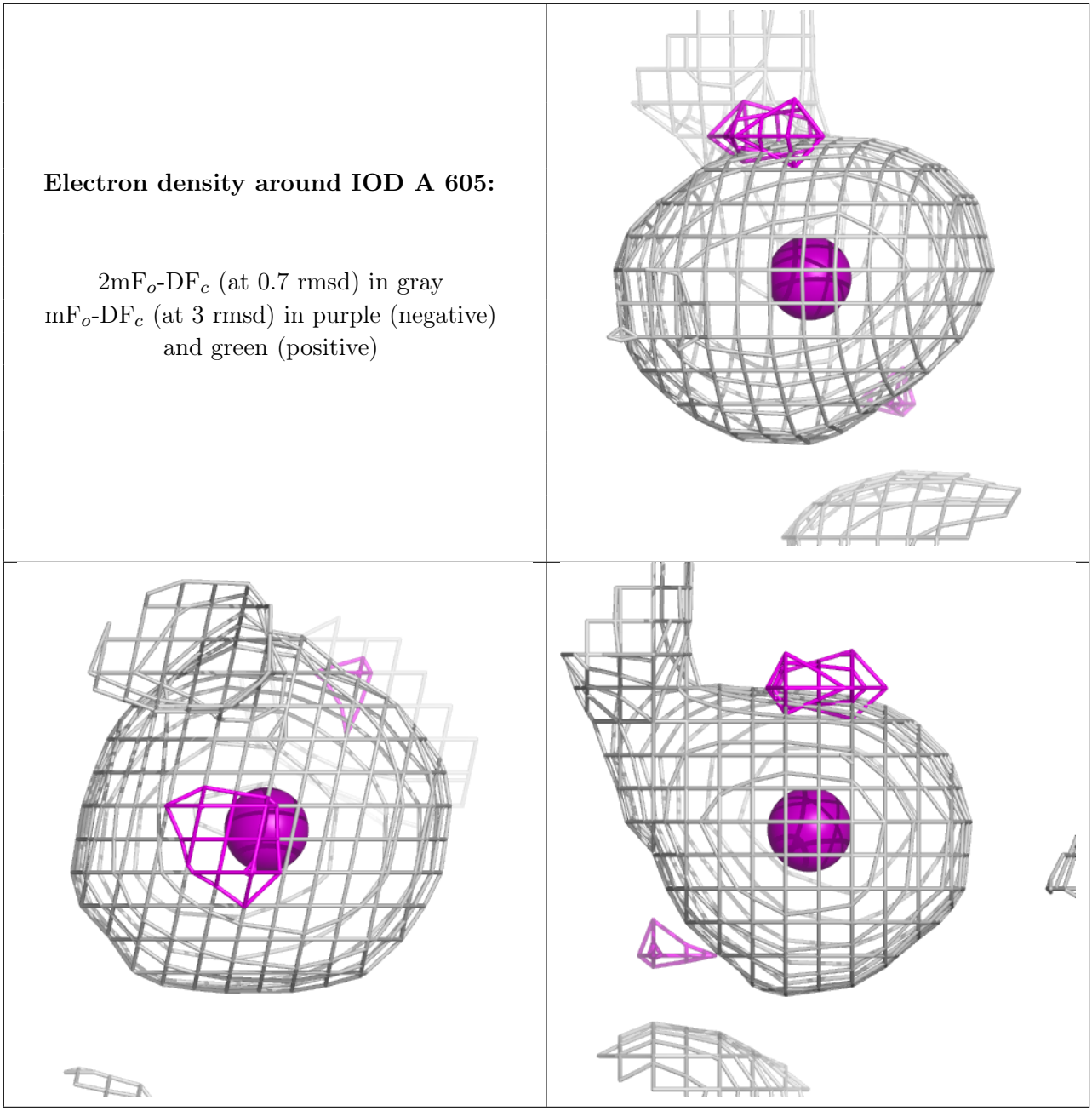






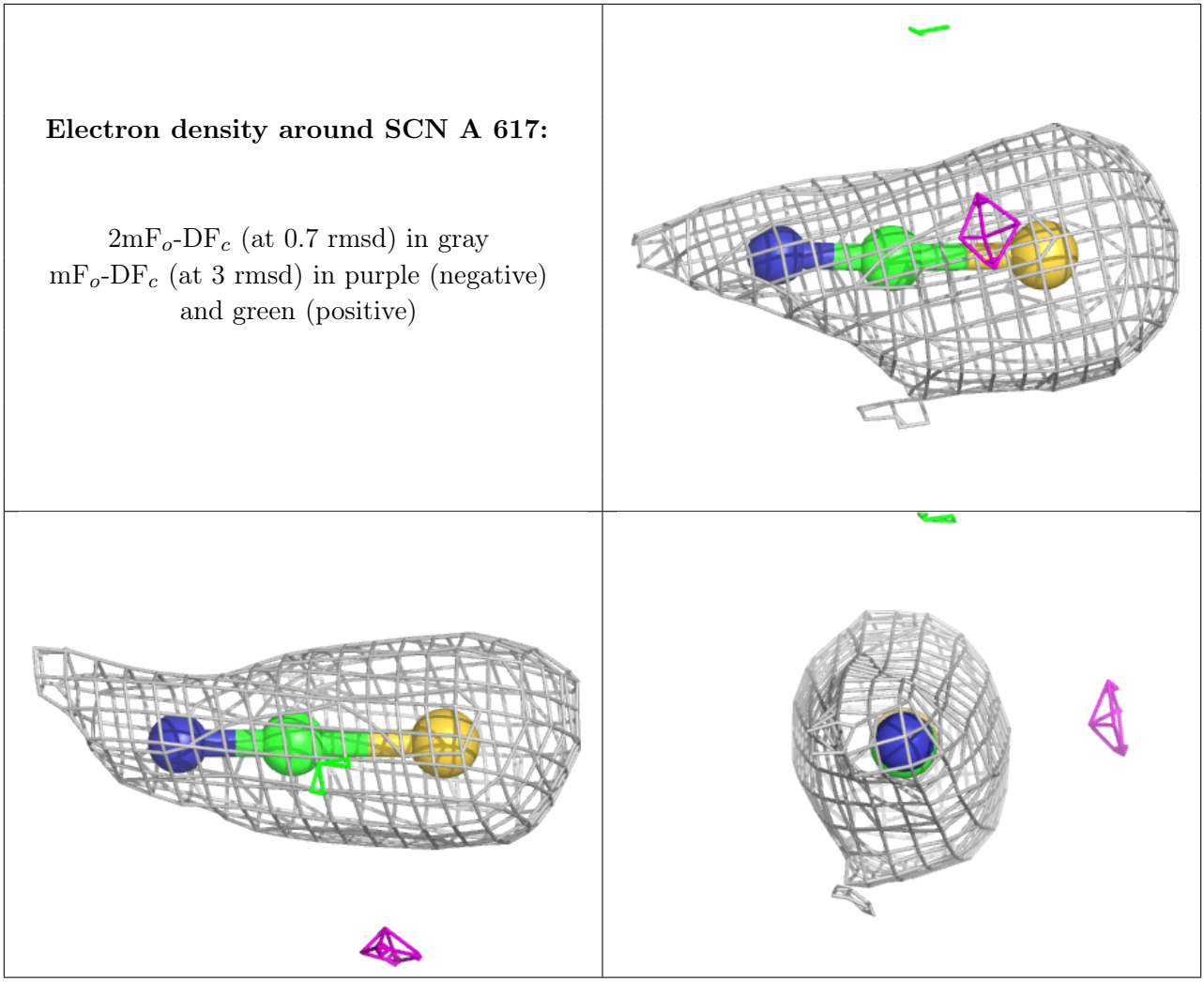
Electron density around IOD A 605:

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



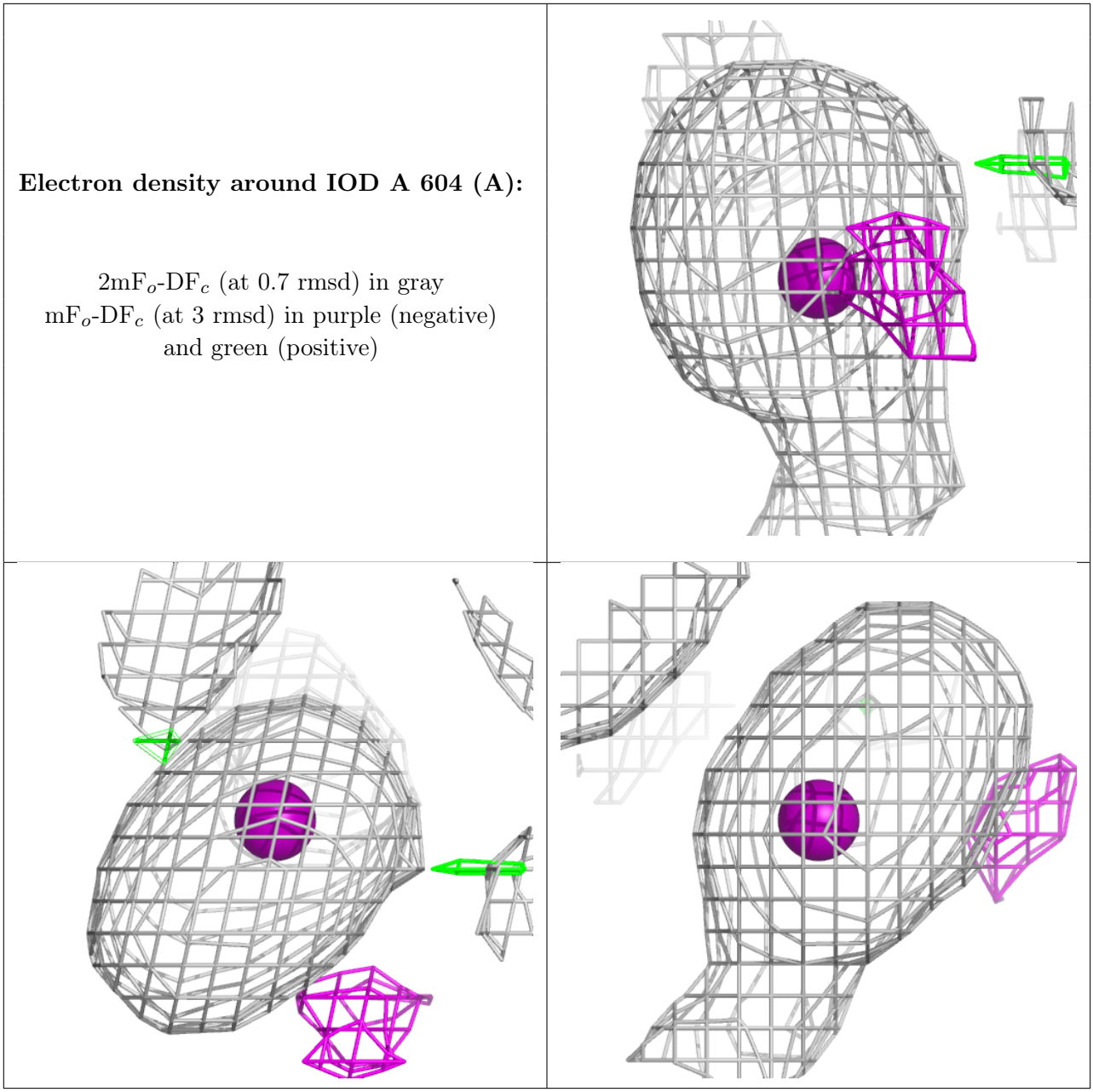
Electron density around SCN A 617:

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



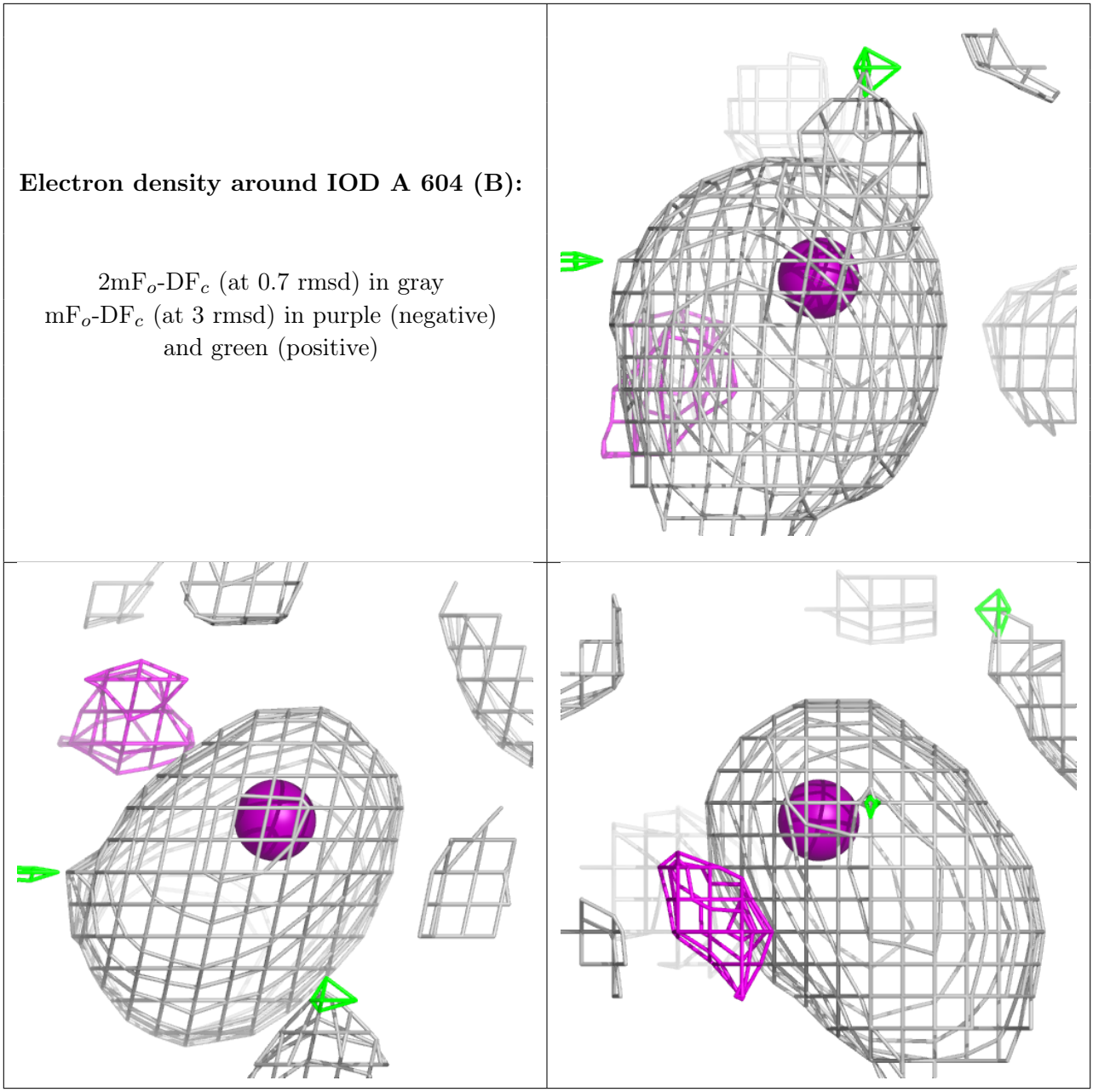
Electron density around IOD A 604 (A):

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



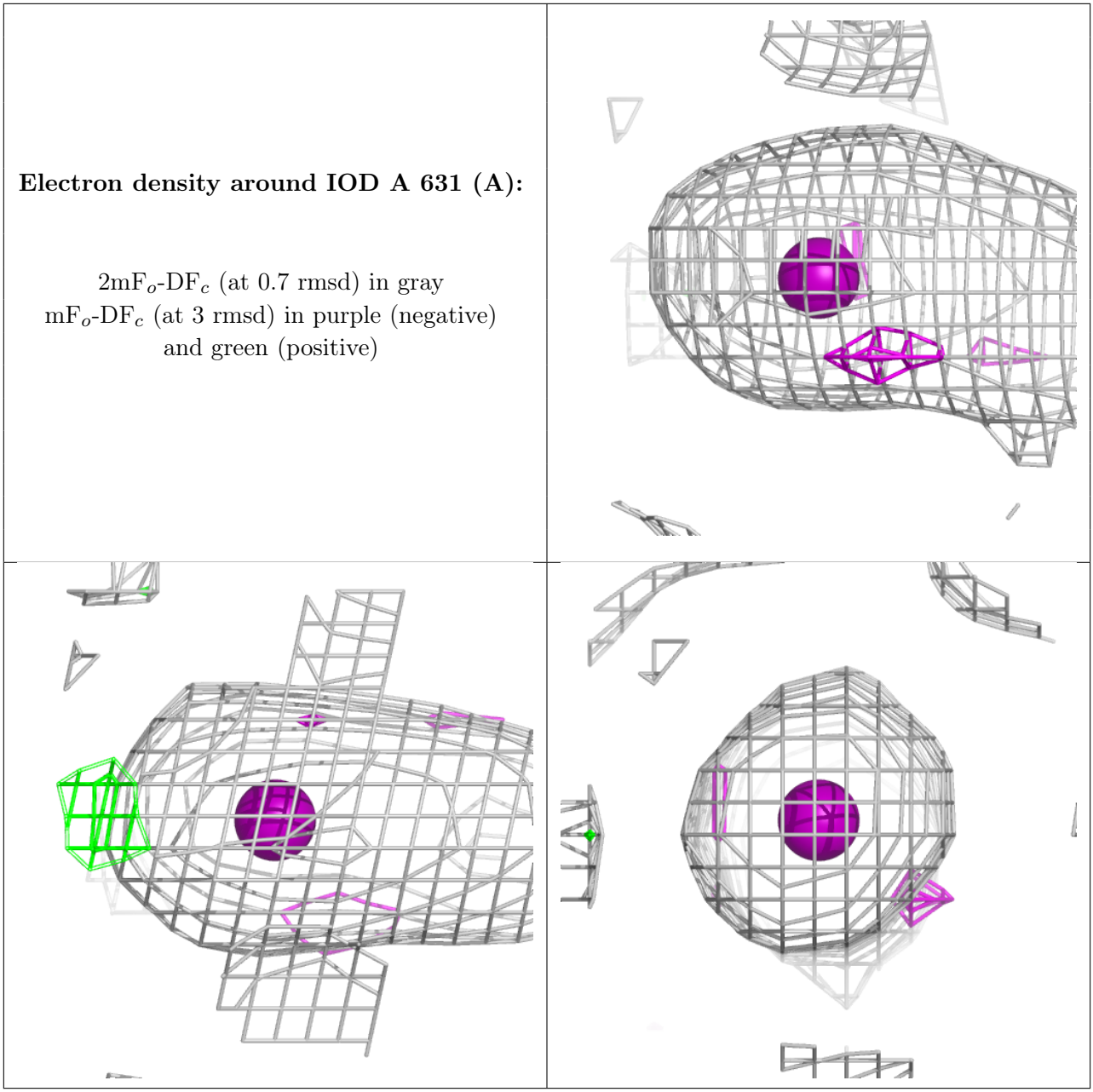
Electron density around IOD A 604 (B):

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



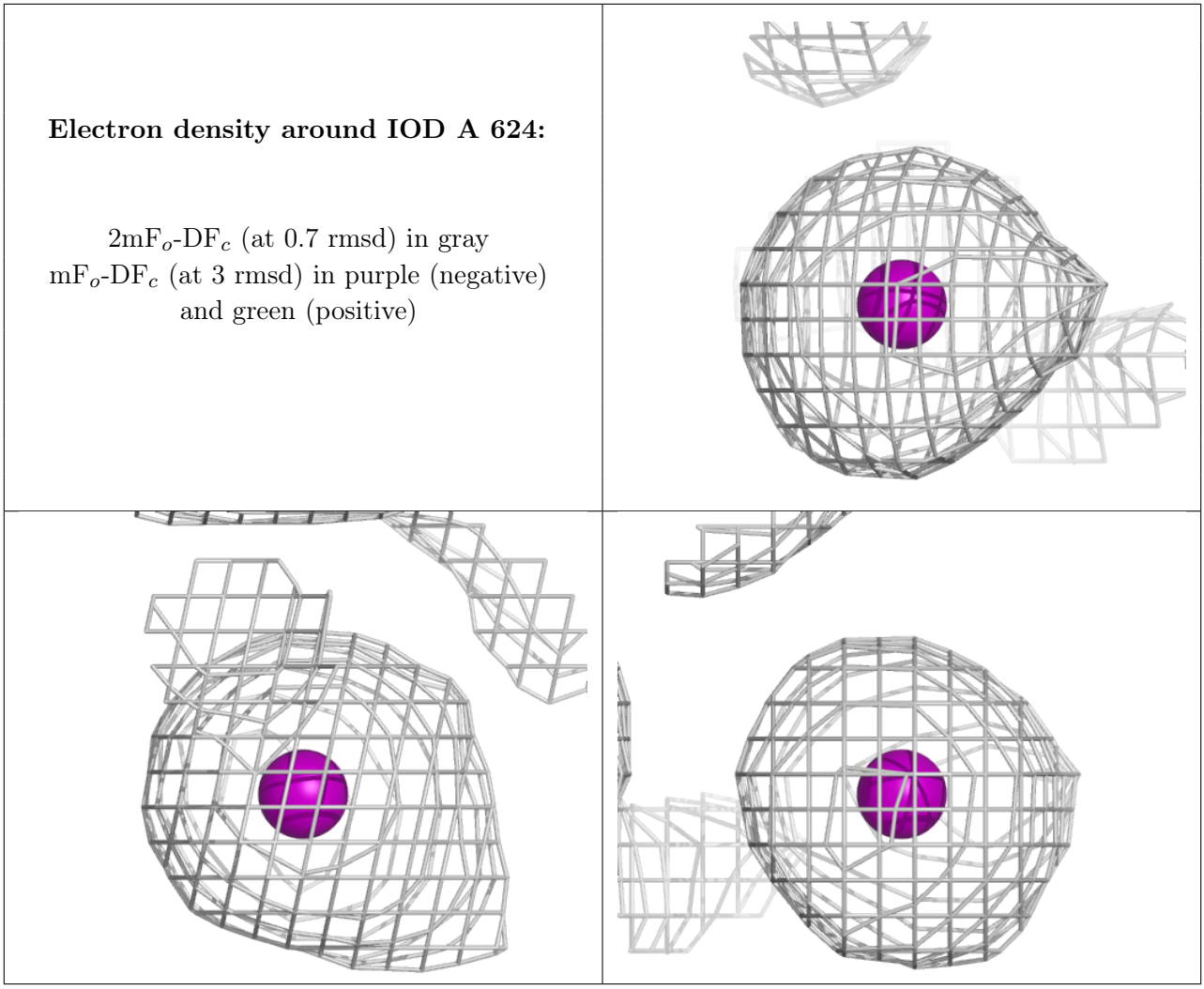
Electron density around IOD A 631 (A):

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



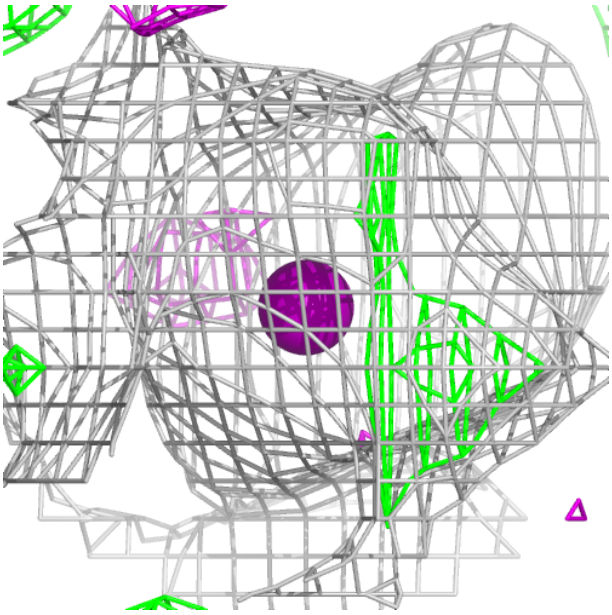
Electron density around IOD A 624:

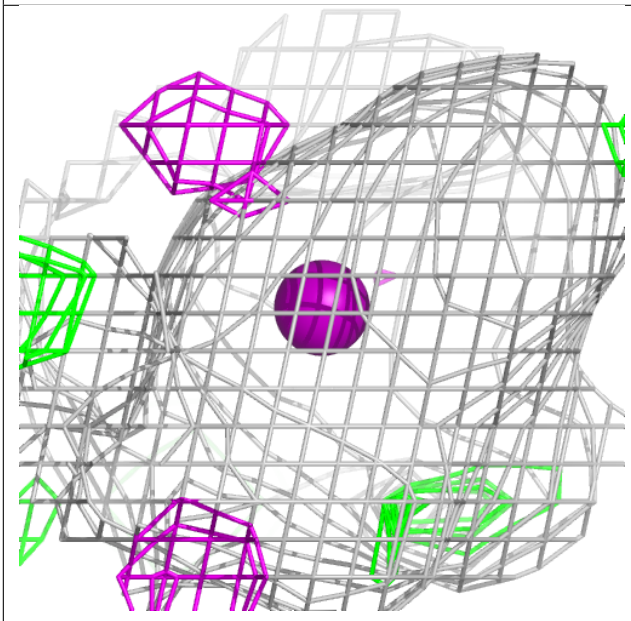
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

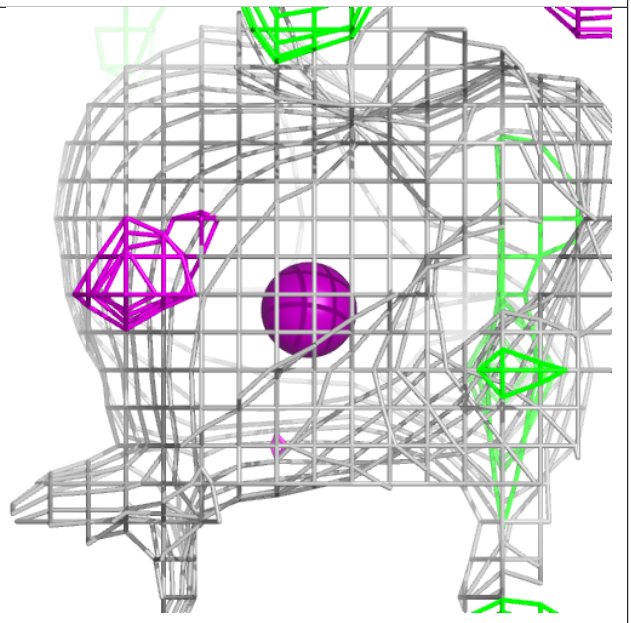


Electron density around IOD A 626 (A):

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

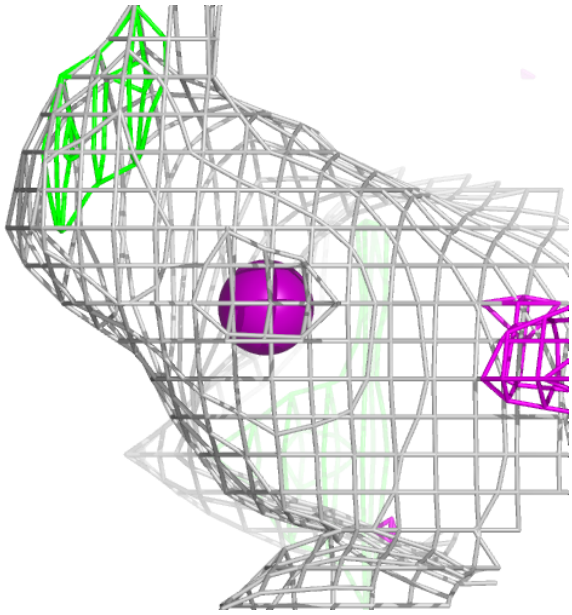


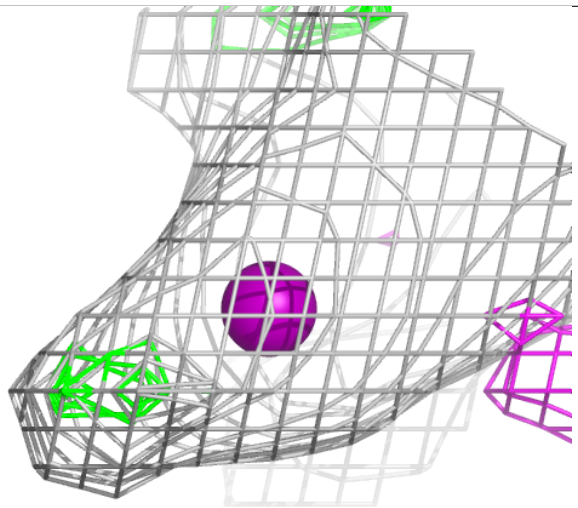


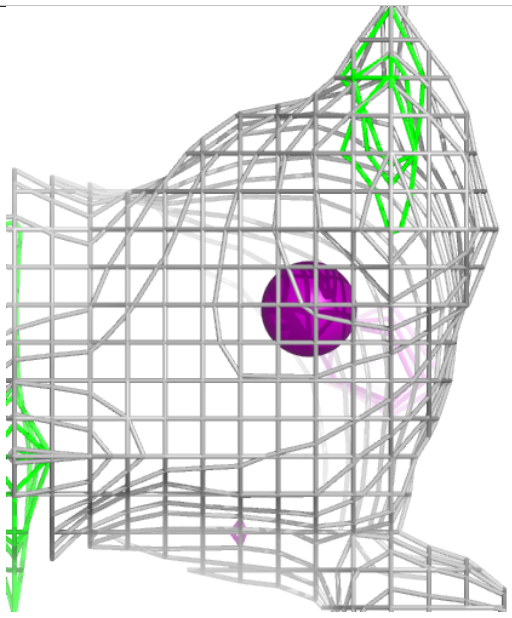


Electron density around IOD A 626 (B):

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

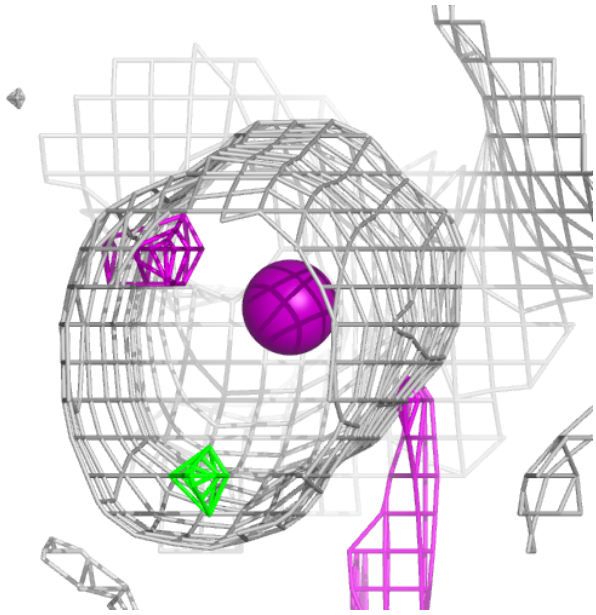


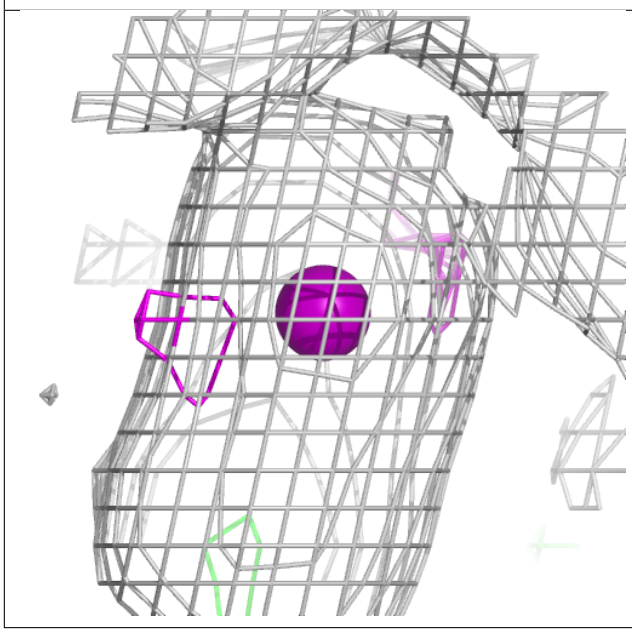


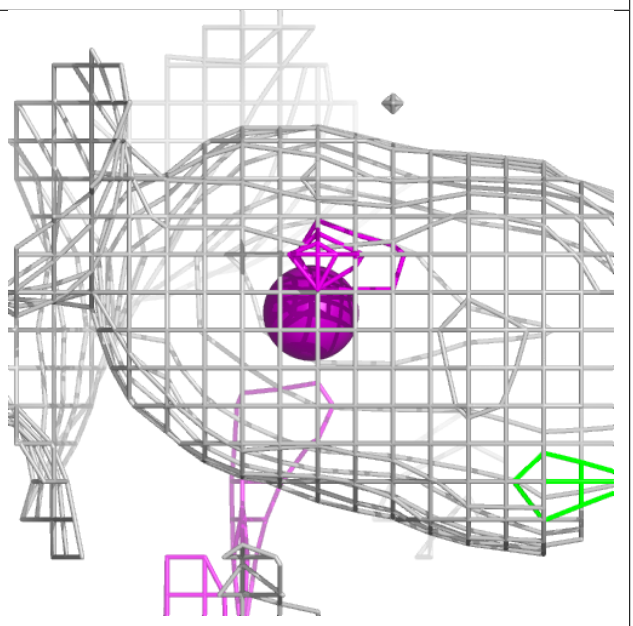


Electron density around IOD A 608 (B):

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

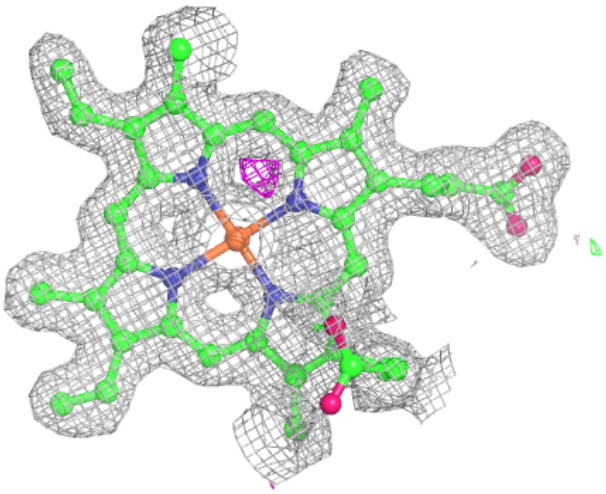


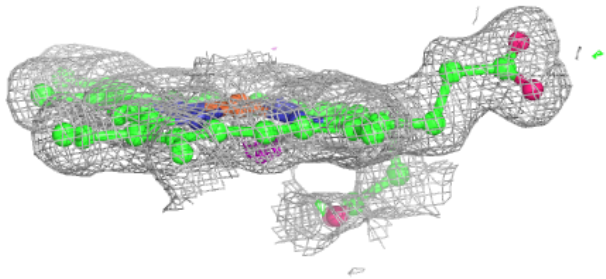


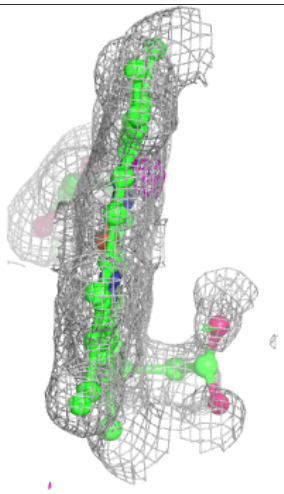


Electron density around HEM A 616 (A):

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

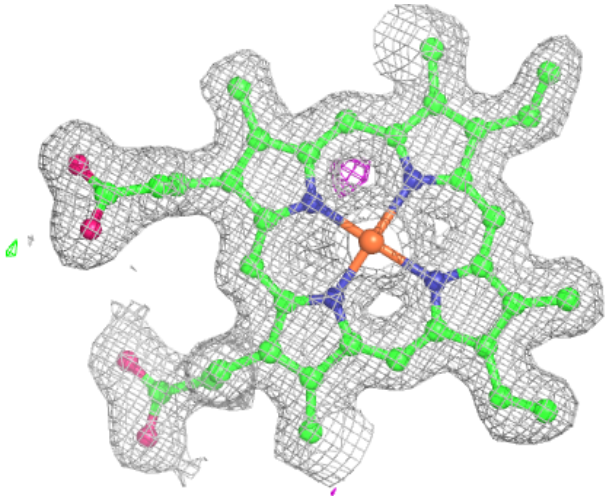


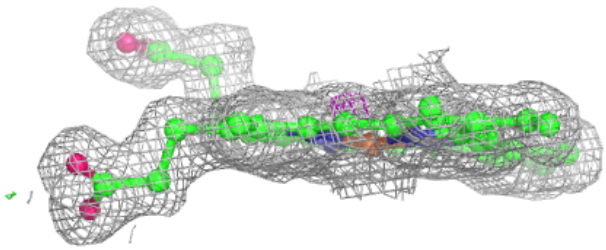


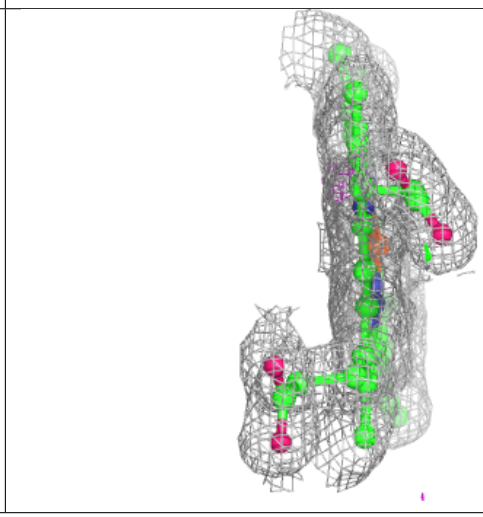


Electron density around HEM A 616 (B):

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

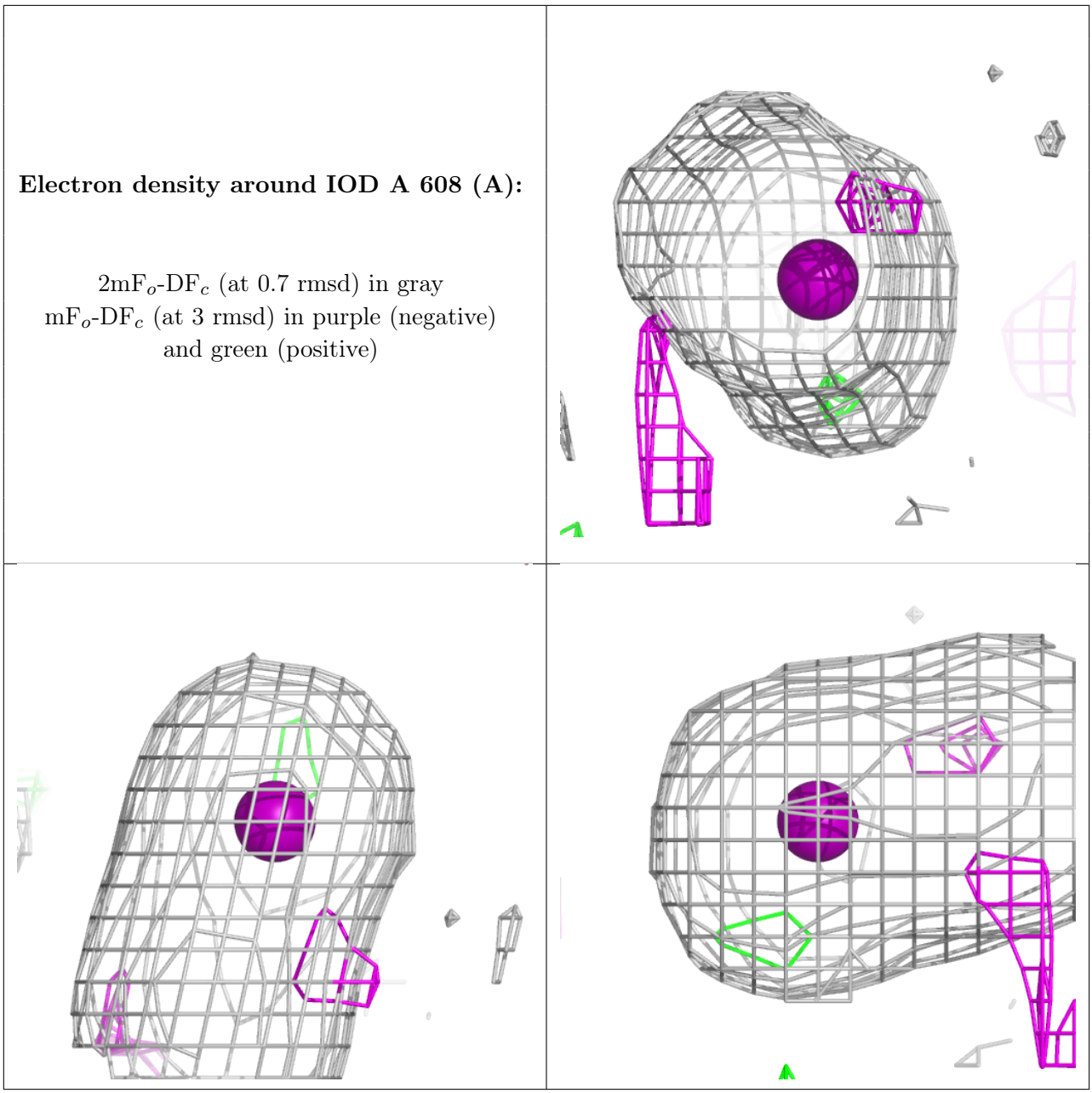






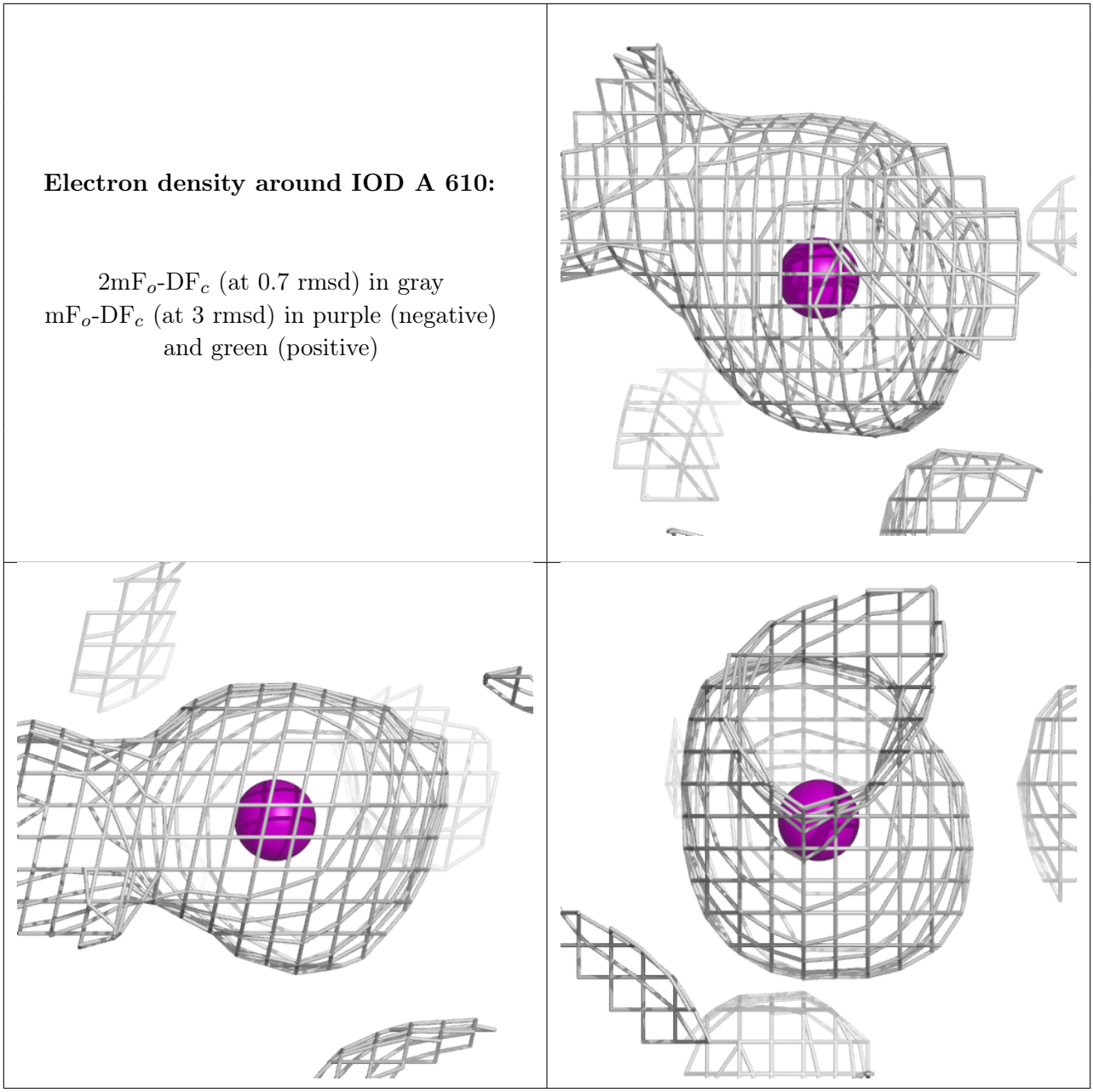
Electron density around IOD A 608 (A):

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



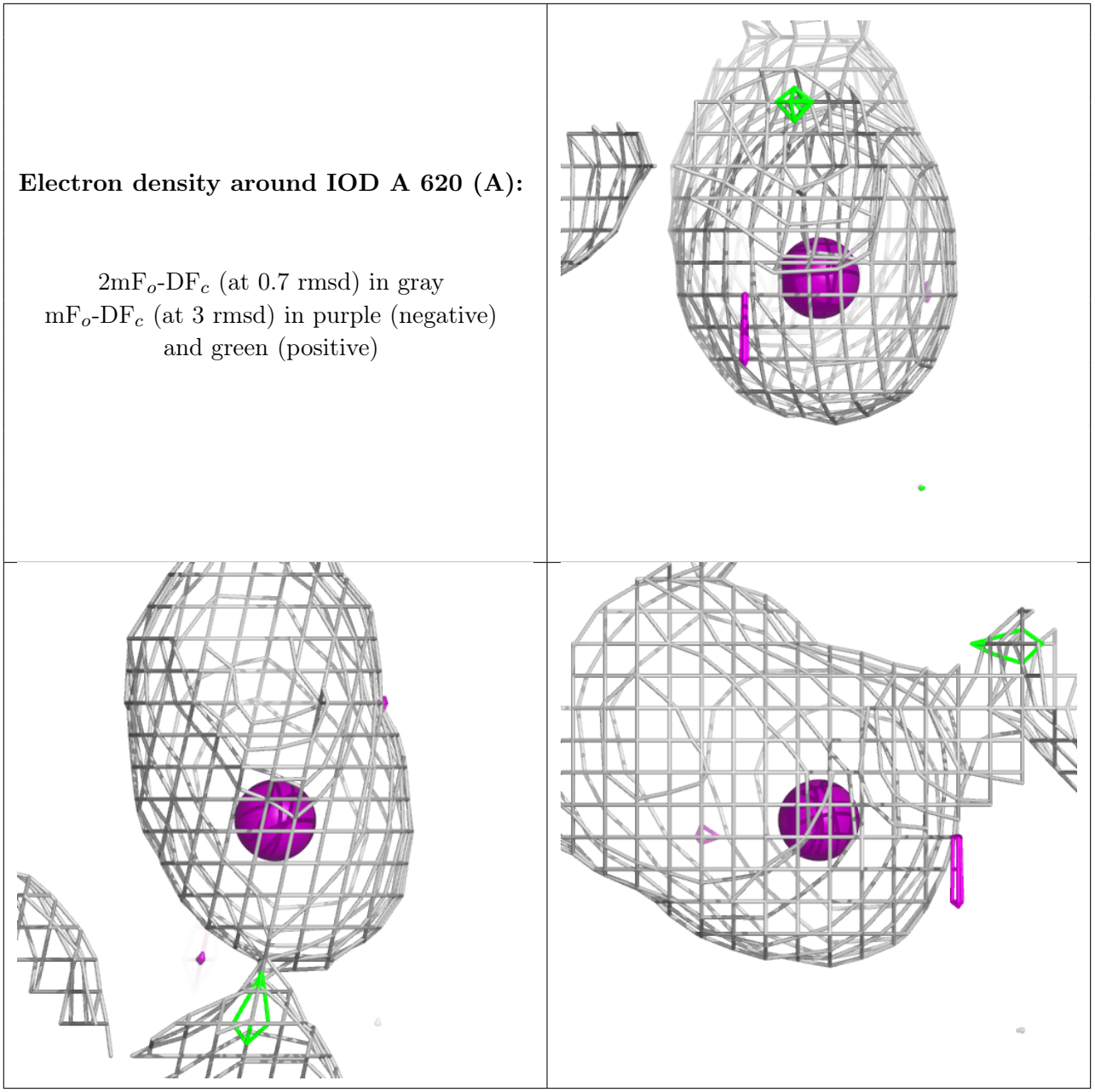
Electron density around IOD A 610:

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



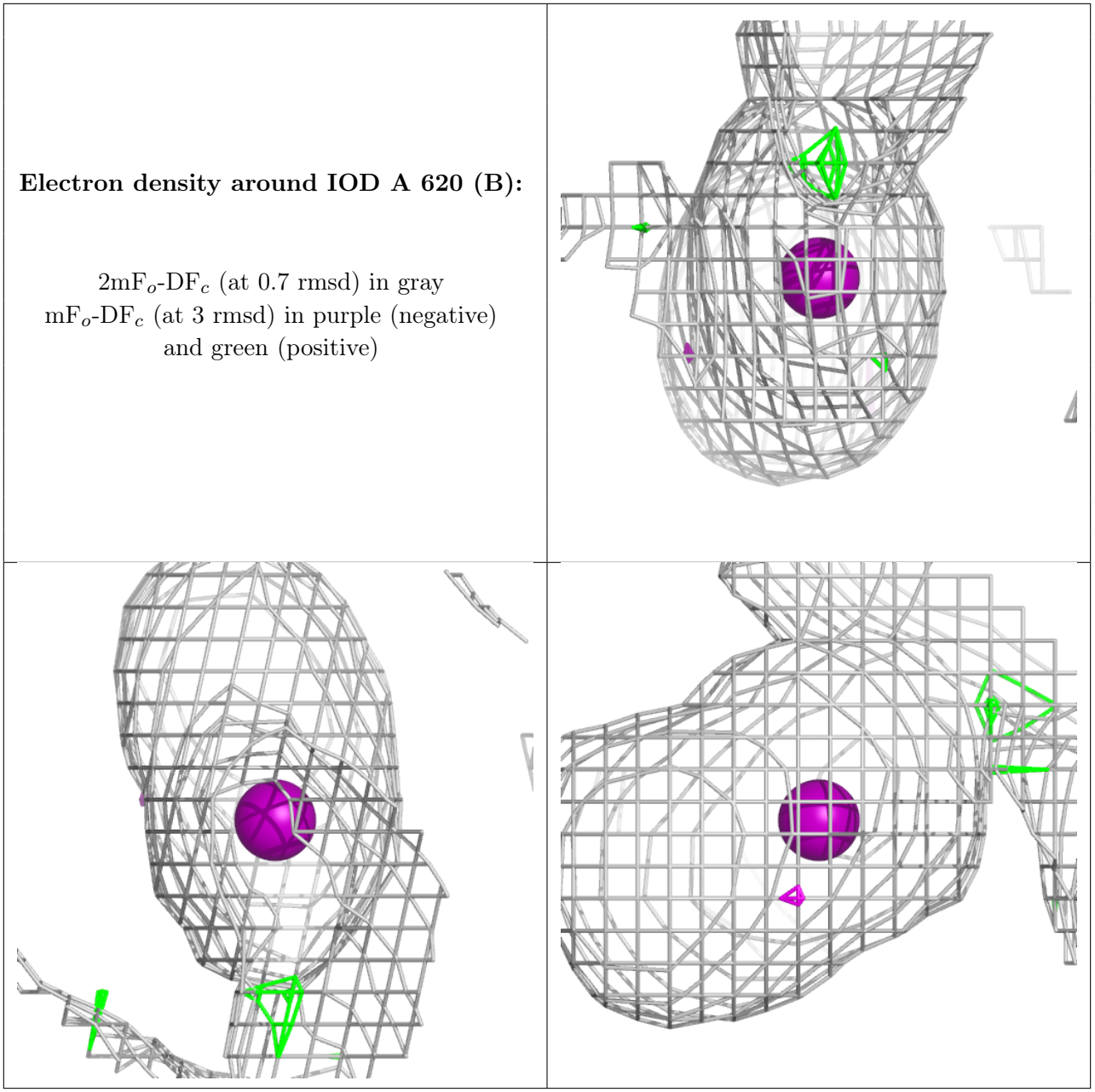
Electron density around IOD A 620 (A):

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



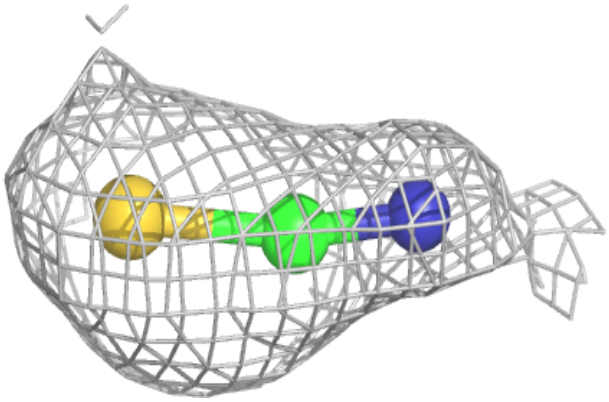
Electron density around IOD A 620 (B):

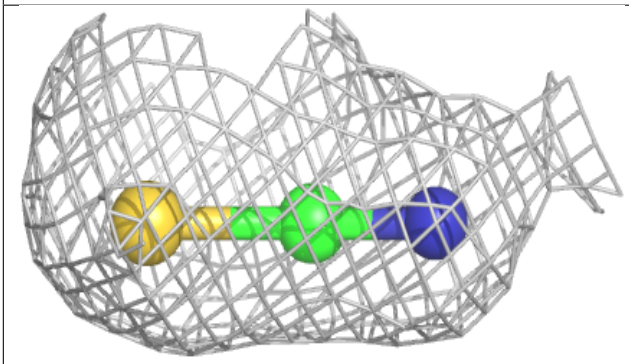
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

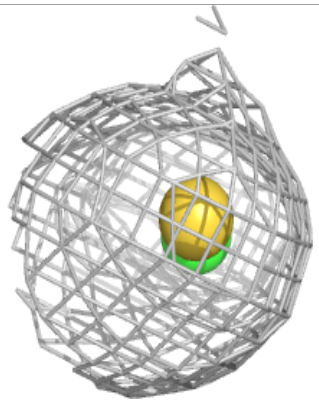


Electron density around SCN A 618:

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

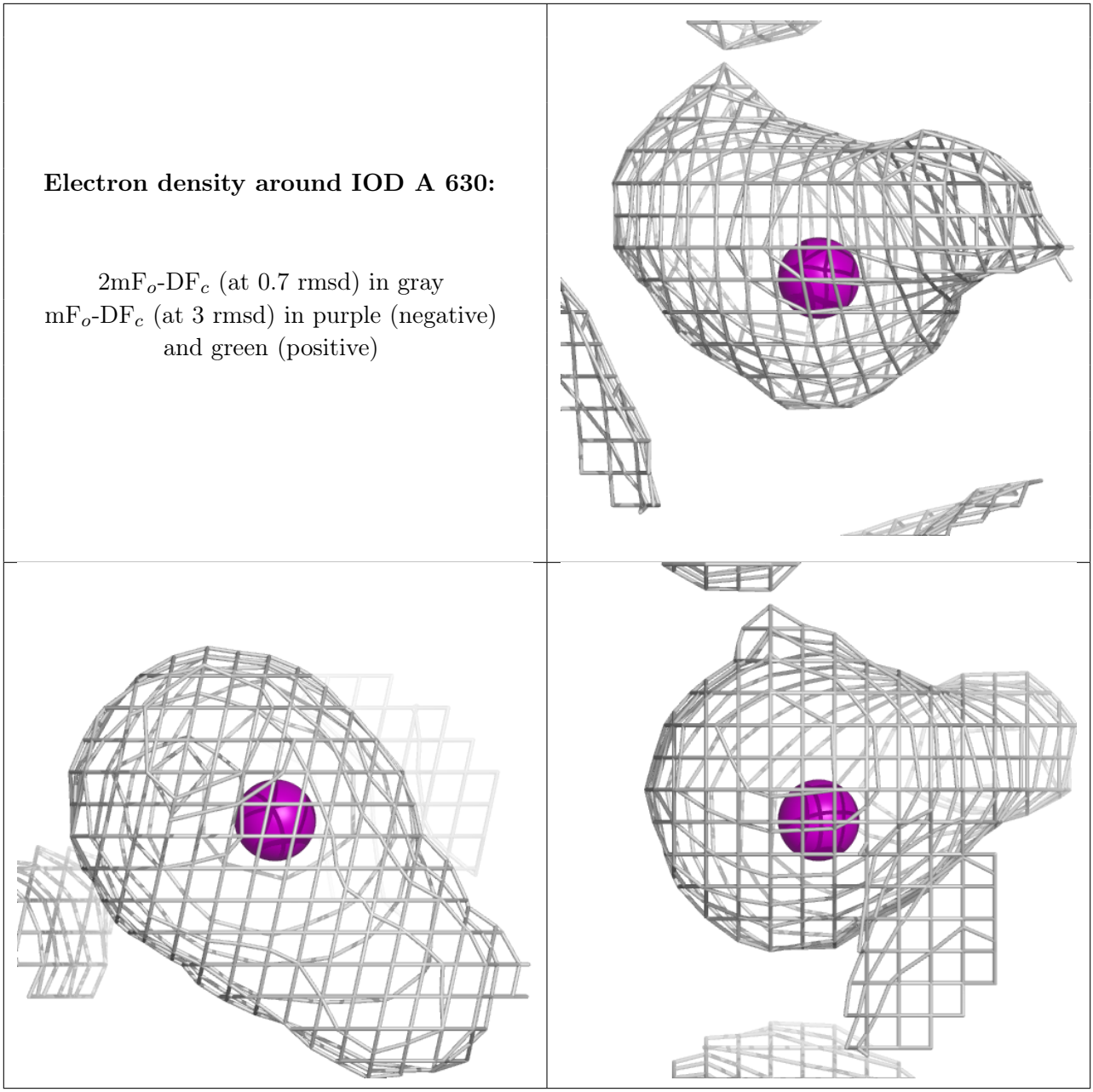






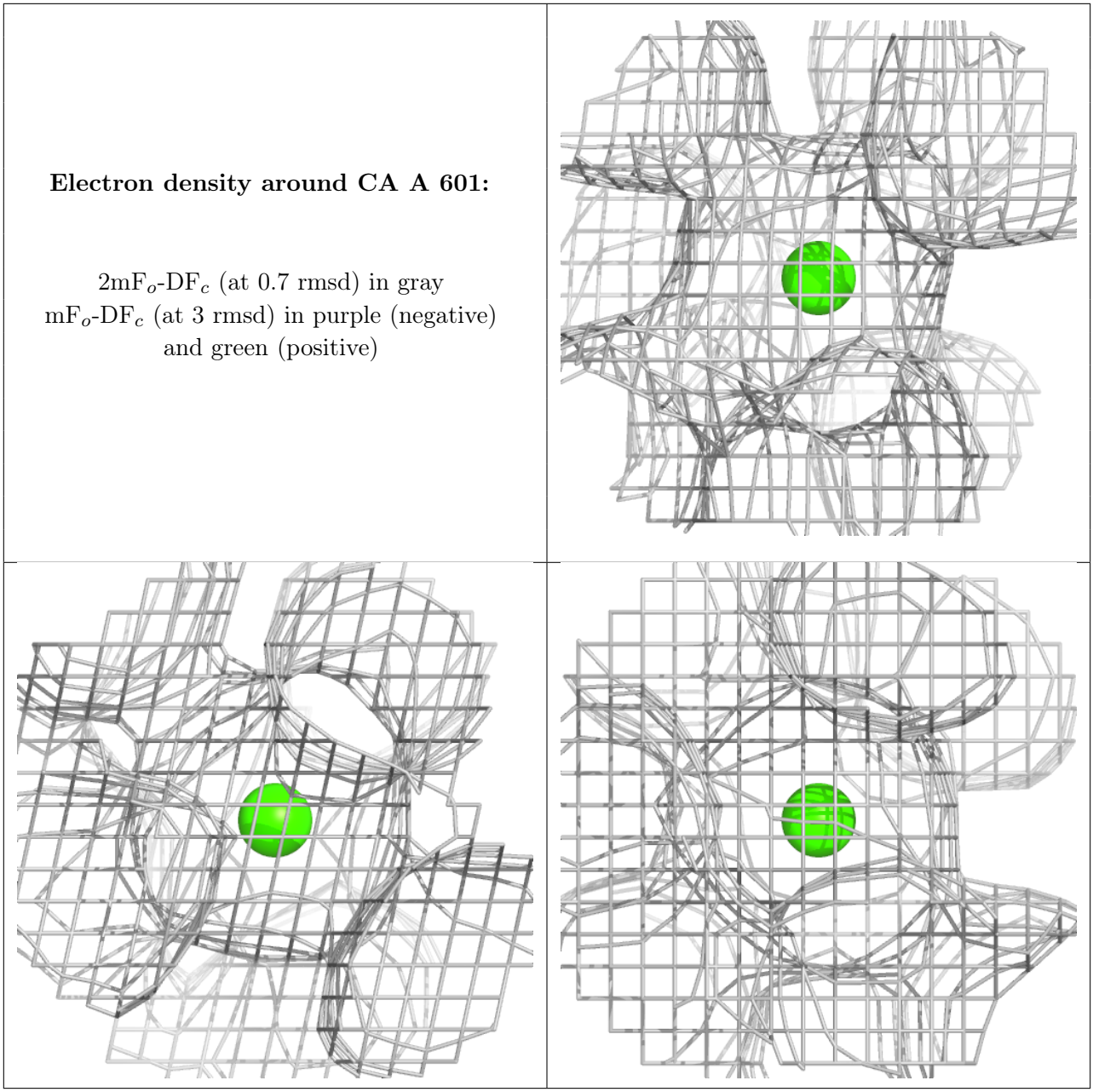
Electron density around IOD A 630:

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



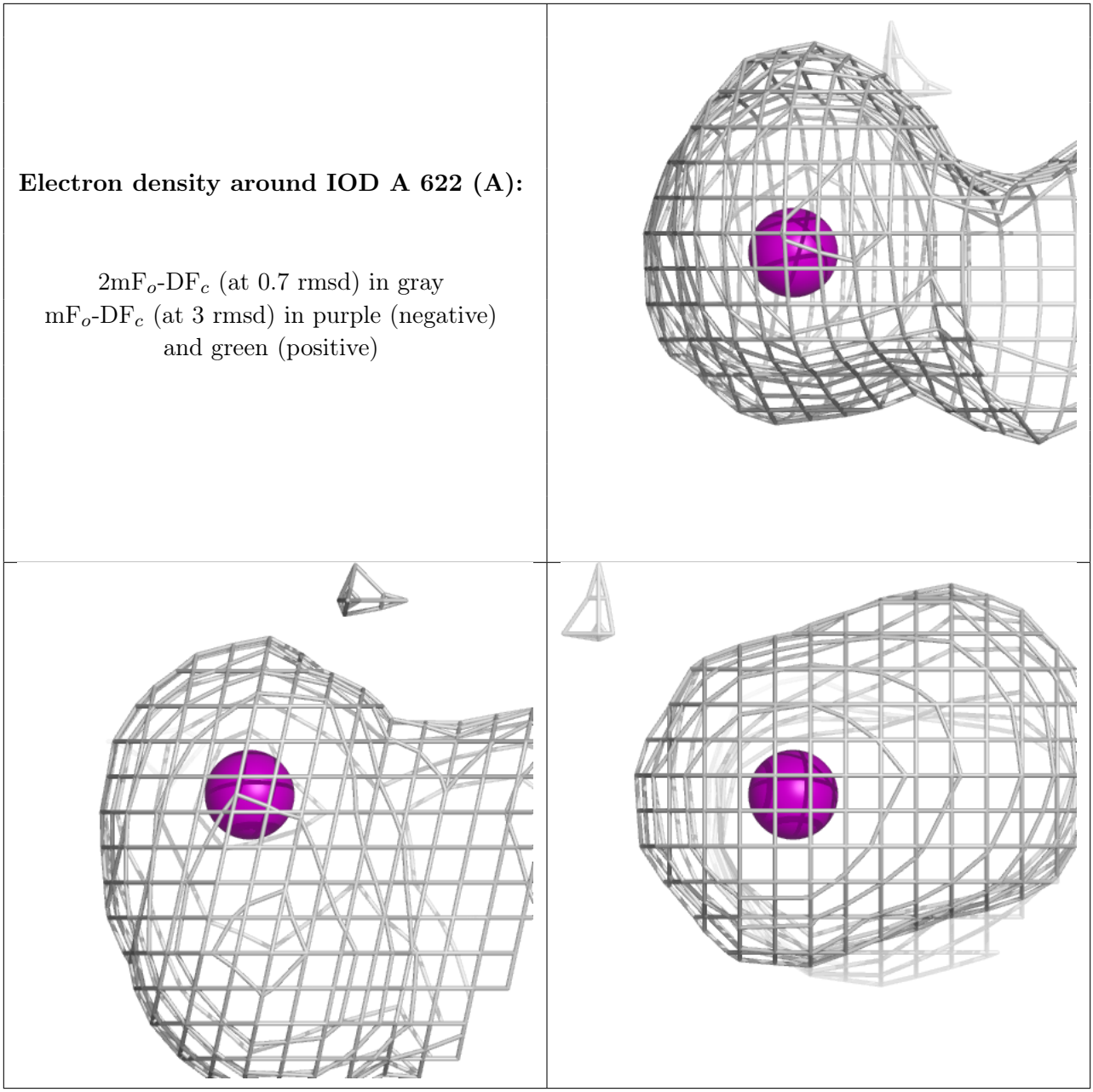
Electron density around CA A 601:

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



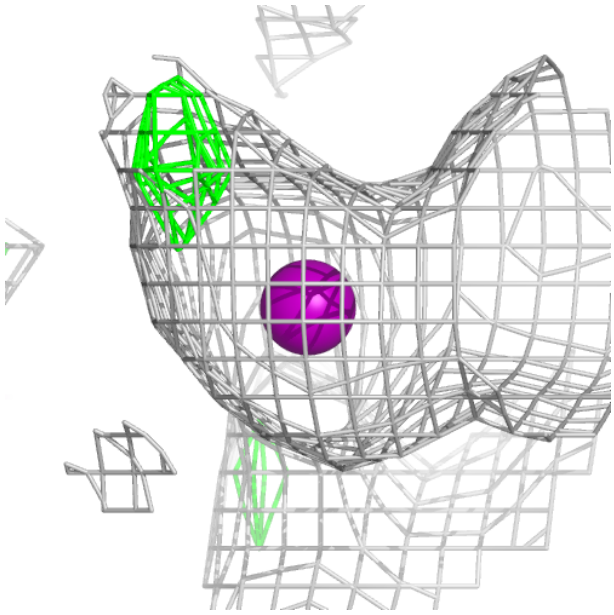
Electron density around IOD A 622 (A):

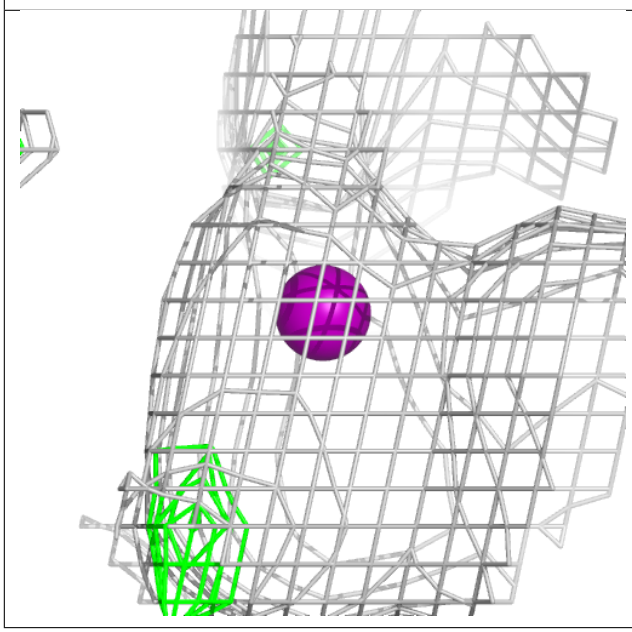
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

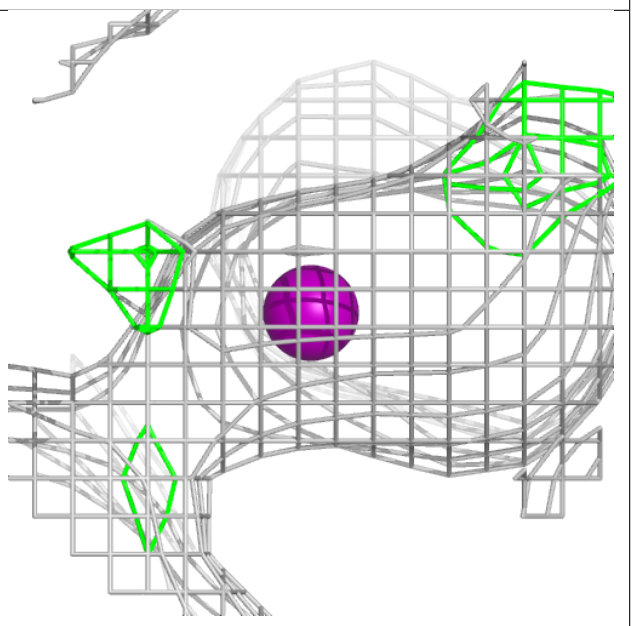


Electron density around IOD A 622 (B):

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

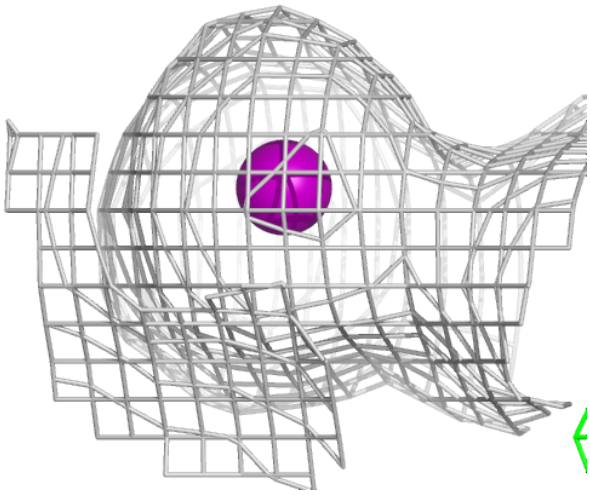


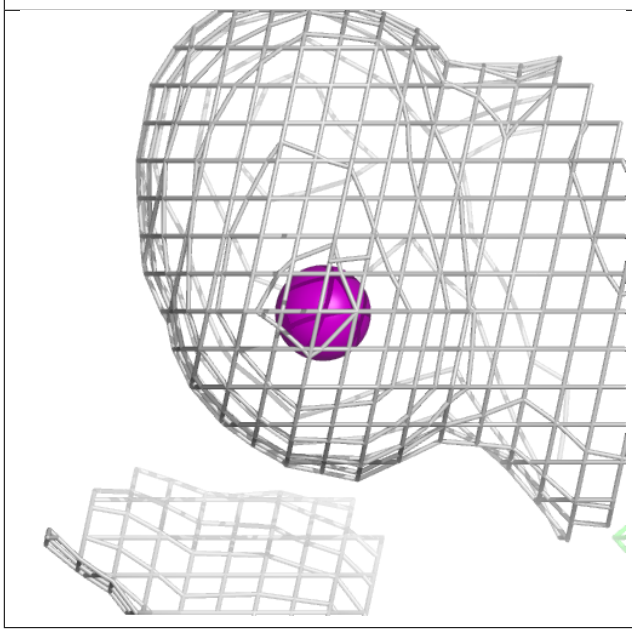


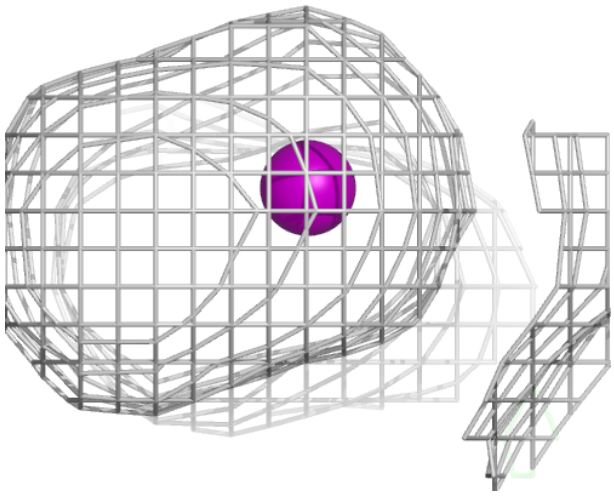


Electron density around IOD A 622 (C):

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

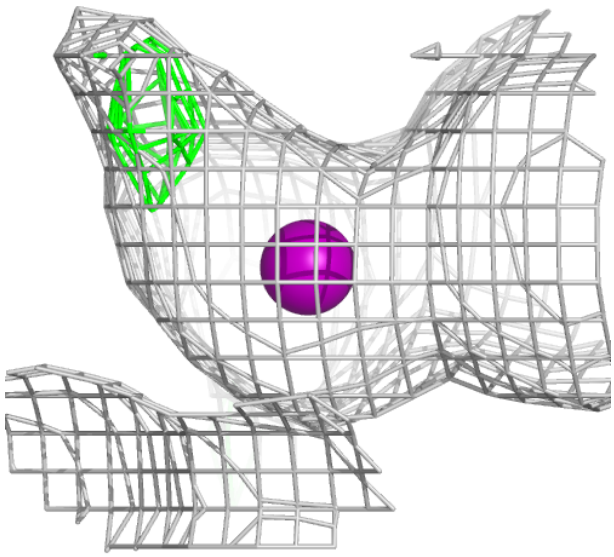


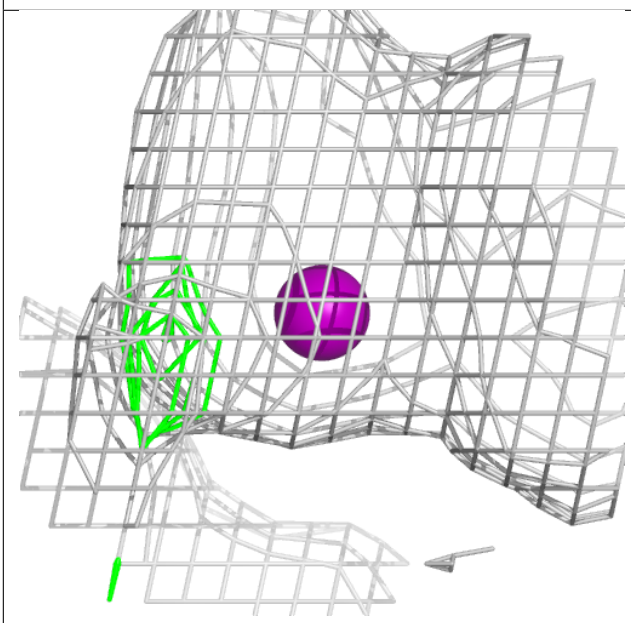


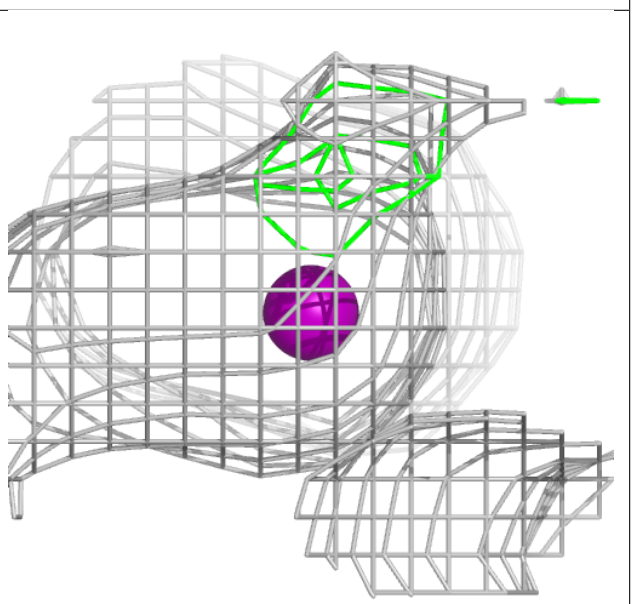


Electron density around IOD A 622 (D):

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

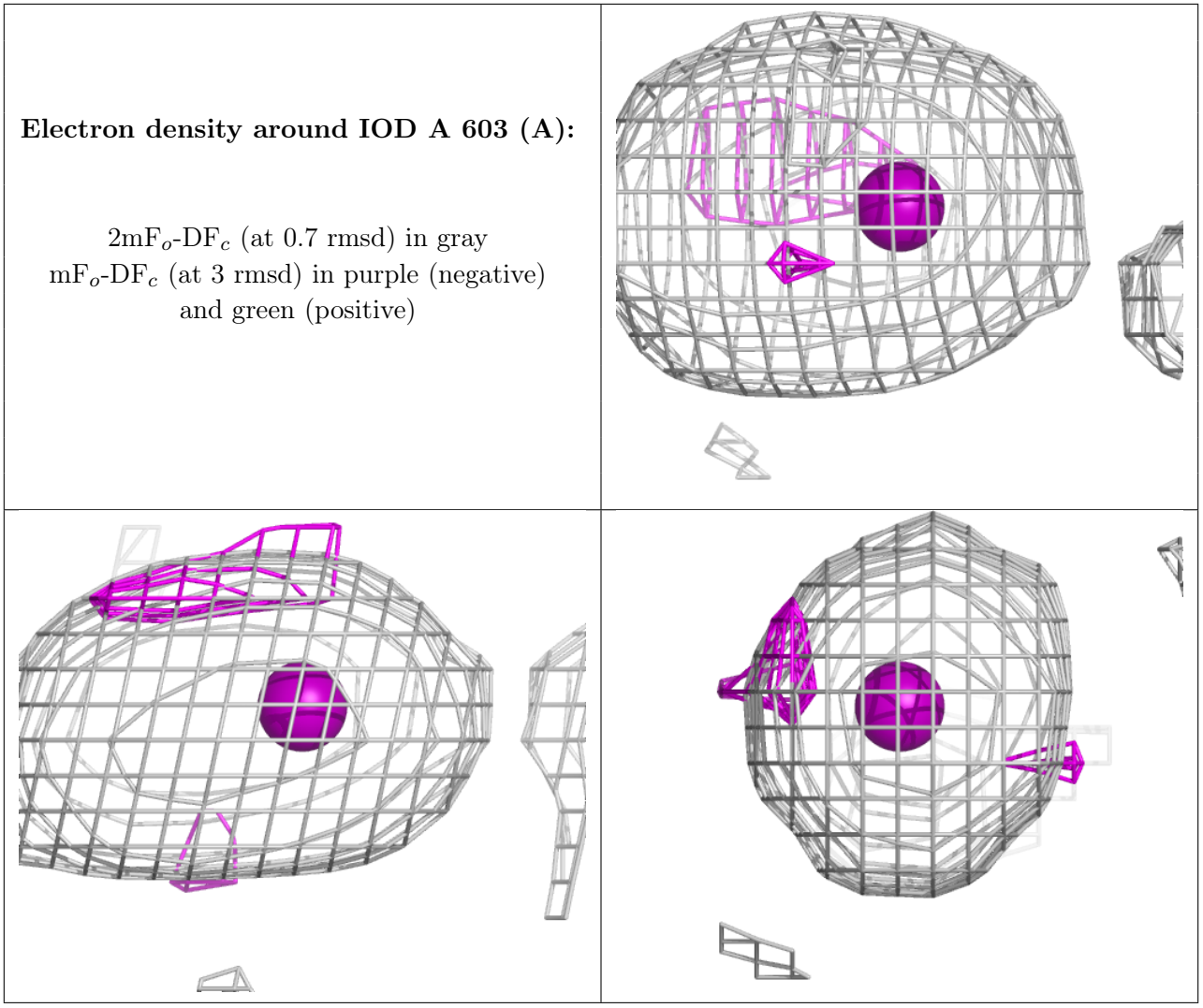






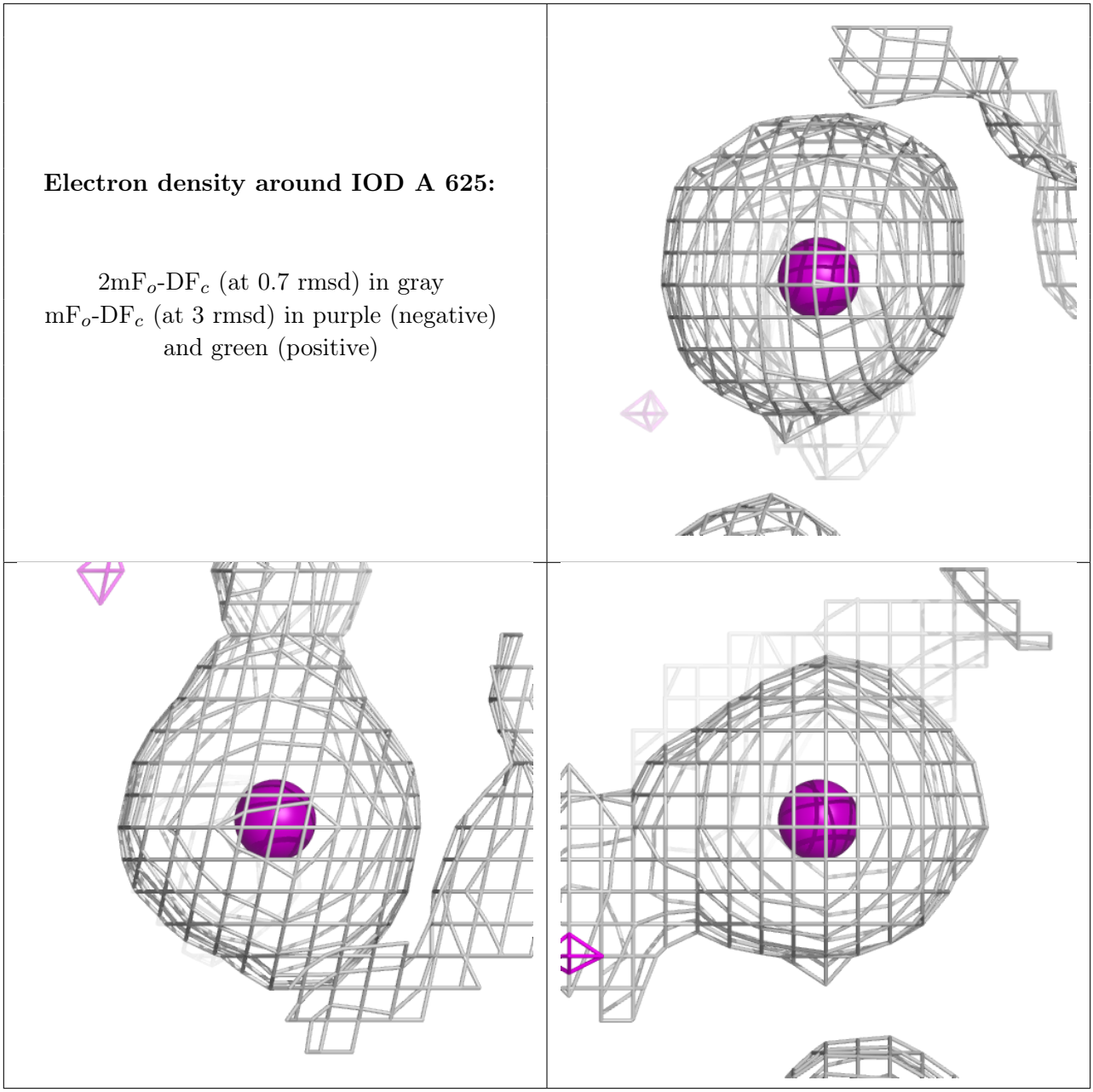
Electron density around IOD A 603 (A):

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



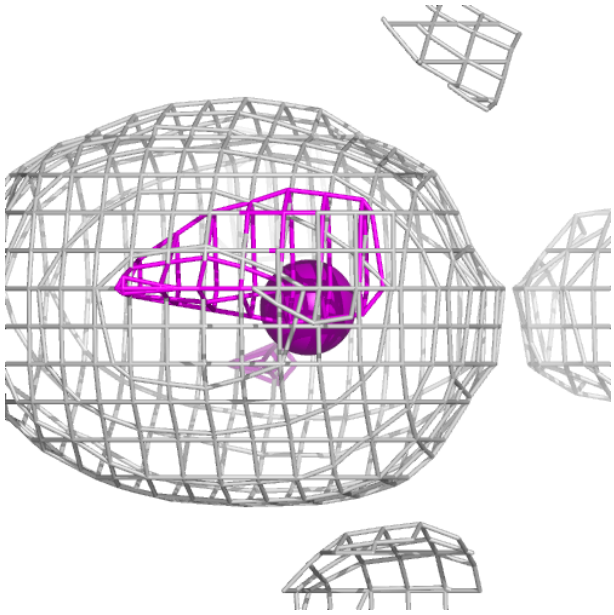
Electron density around IOD A 625:

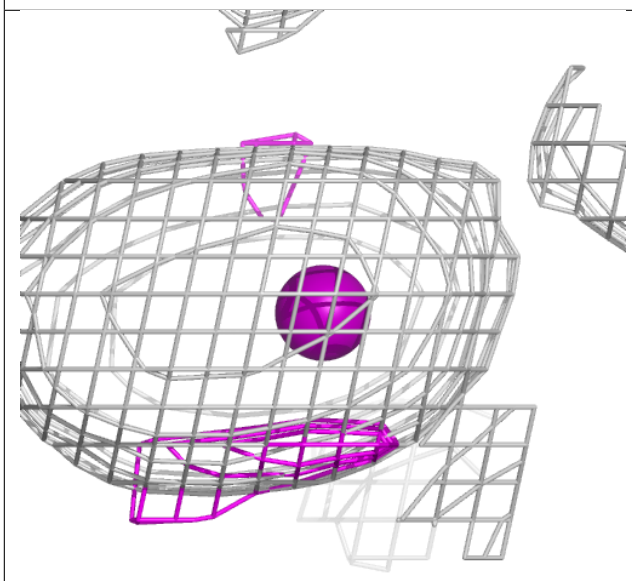
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

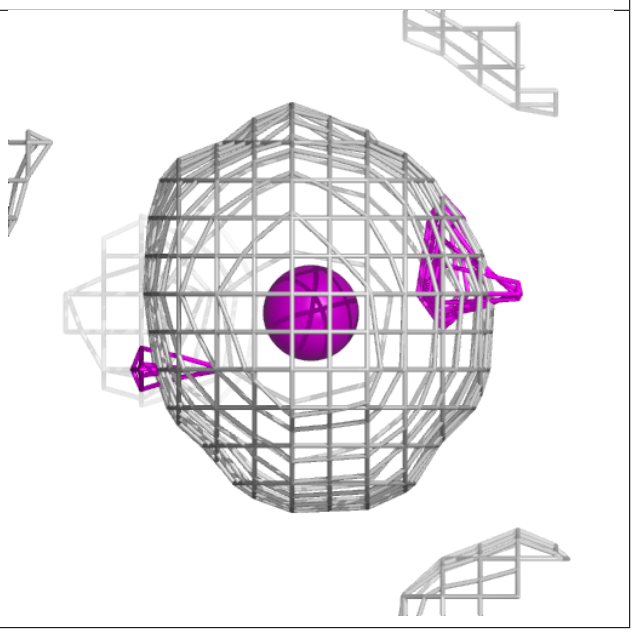


Electron density around IOD A 603 (B):

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

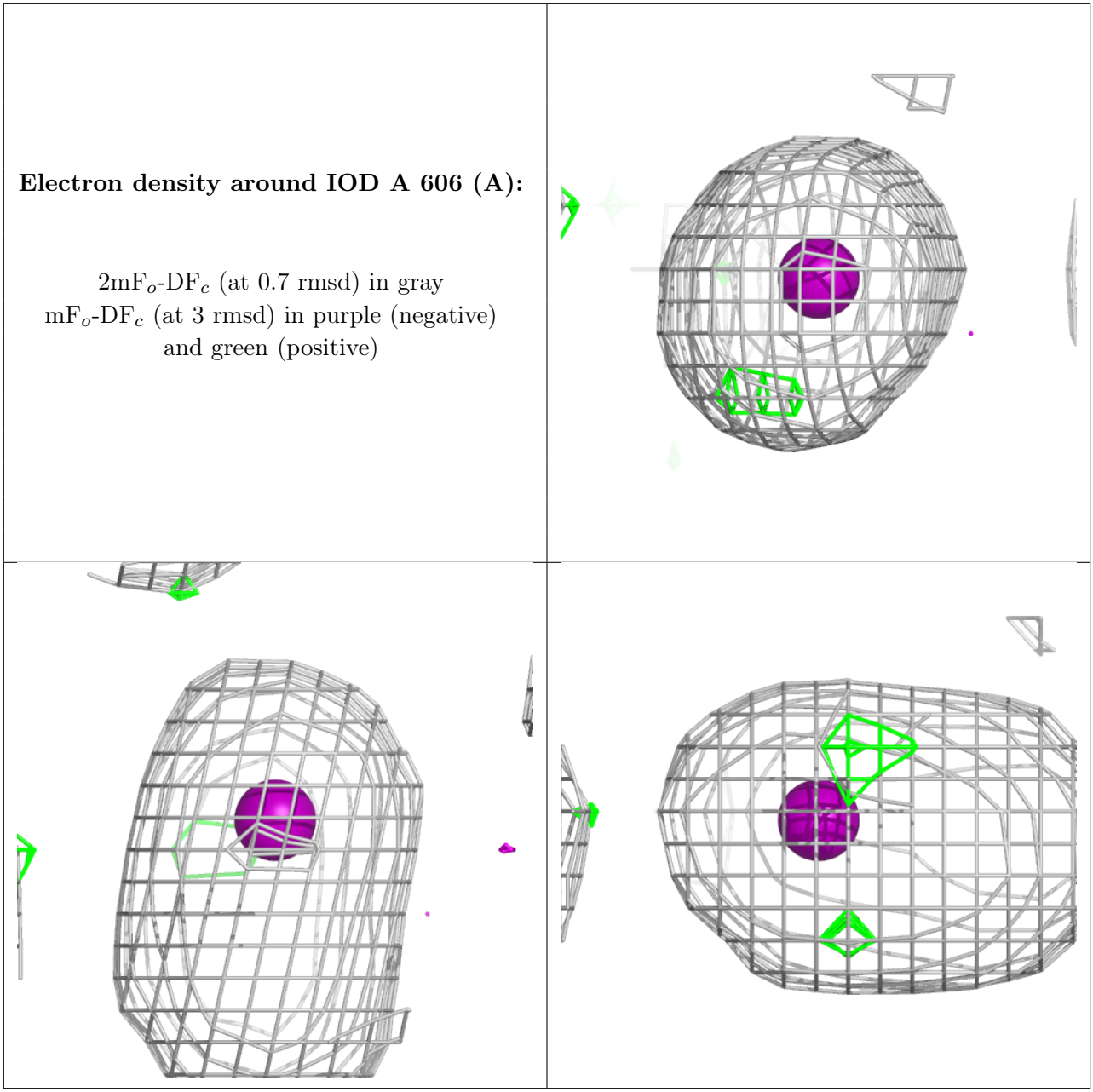






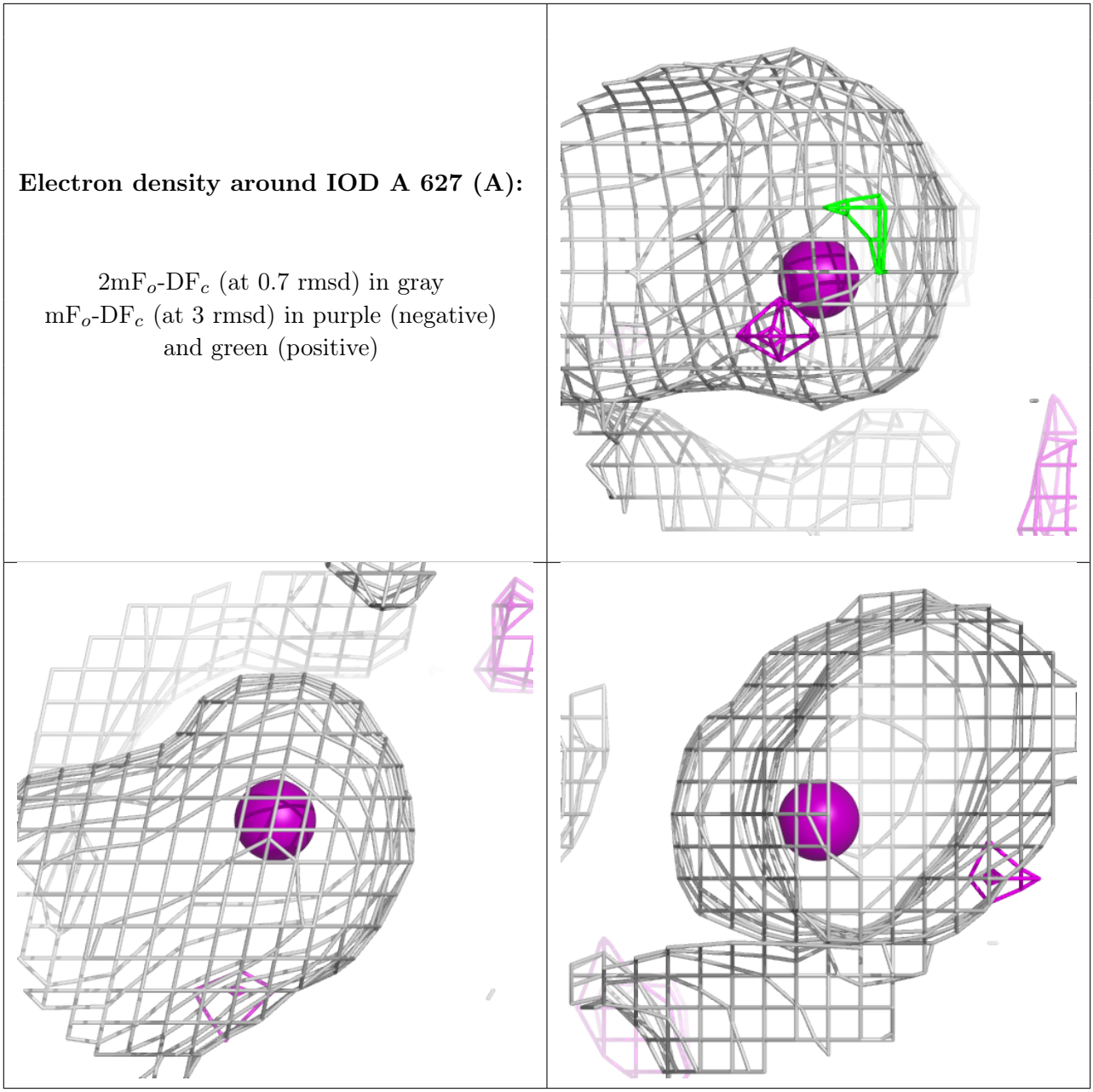
Electron density around IOD A 606 (A):

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



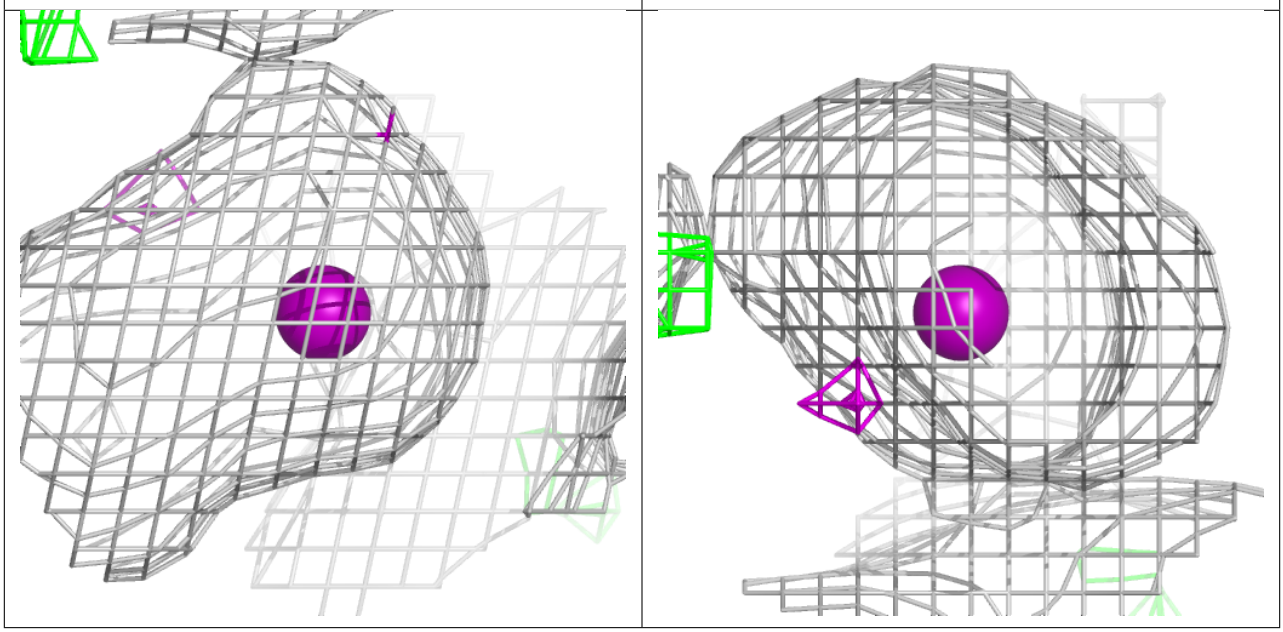
Electron density around IOD A 627 (A):

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



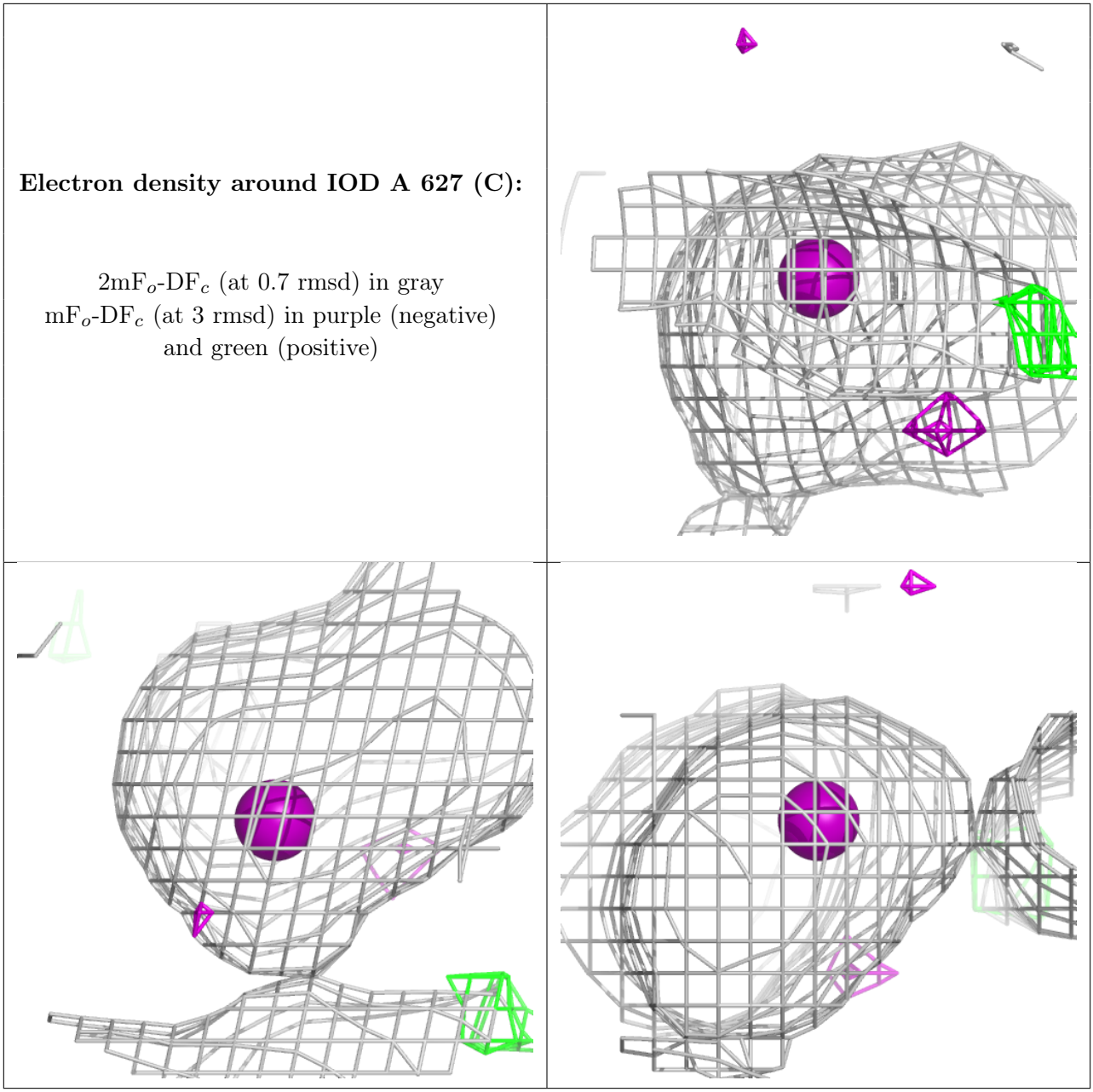
Electron density around IOD A 627 (B):

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



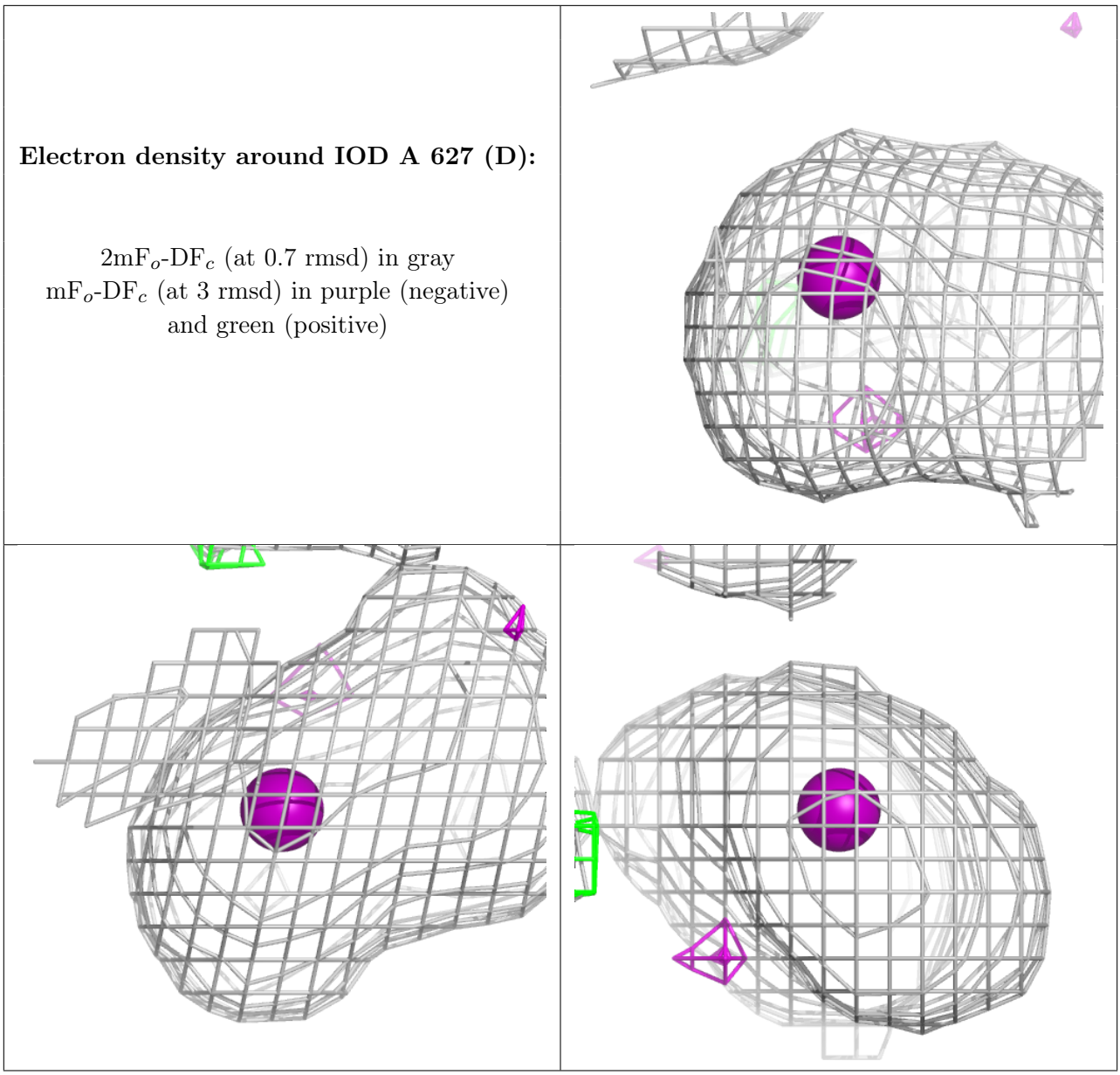
Electron density around IOD A 627 (C):

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



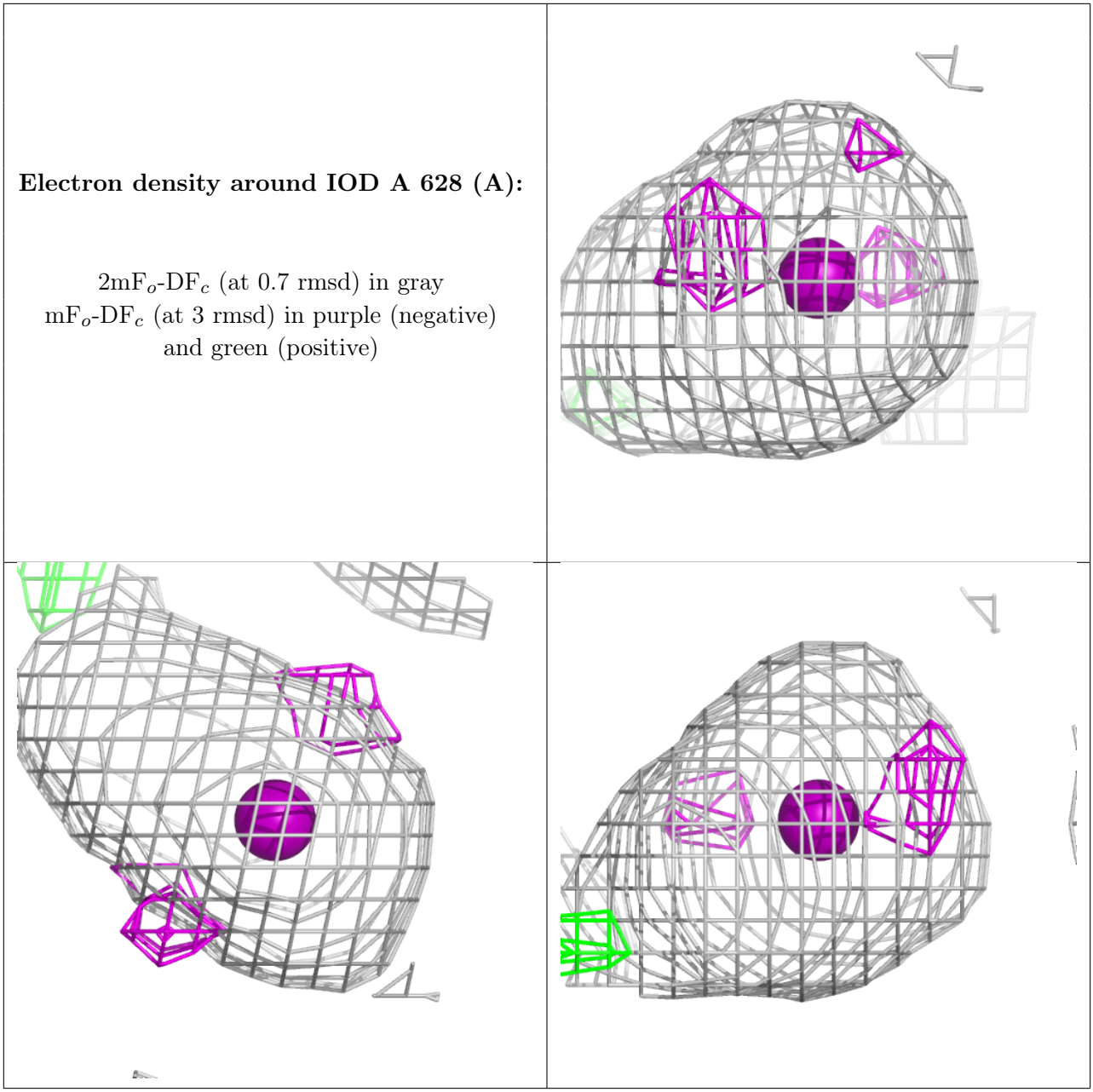
Electron density around IOD A 627 (D):

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



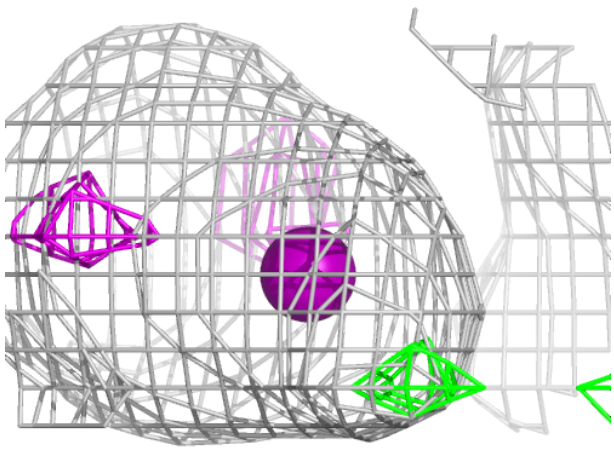
Electron density around IOD A 628 (A):

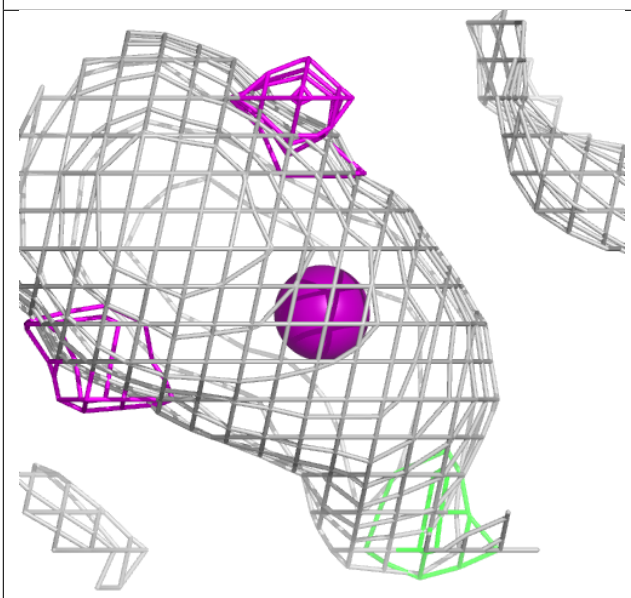
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

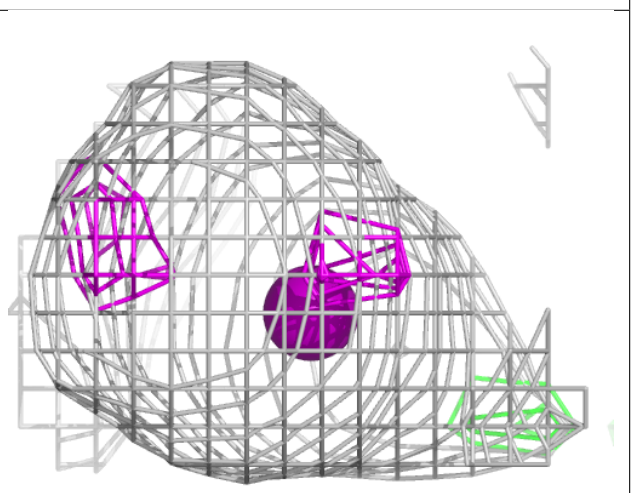


Electron density around IOD A 628 (B):

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

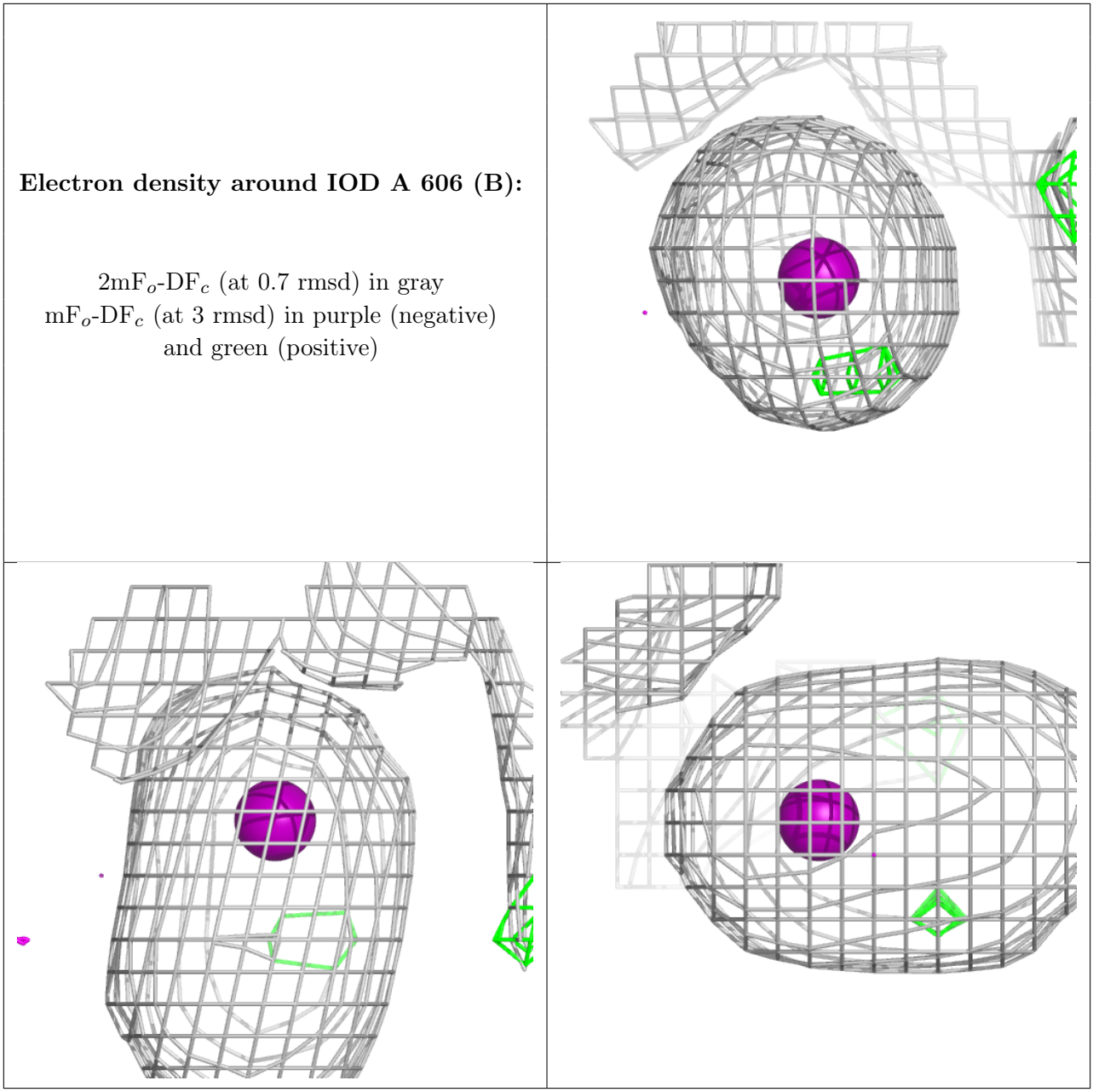






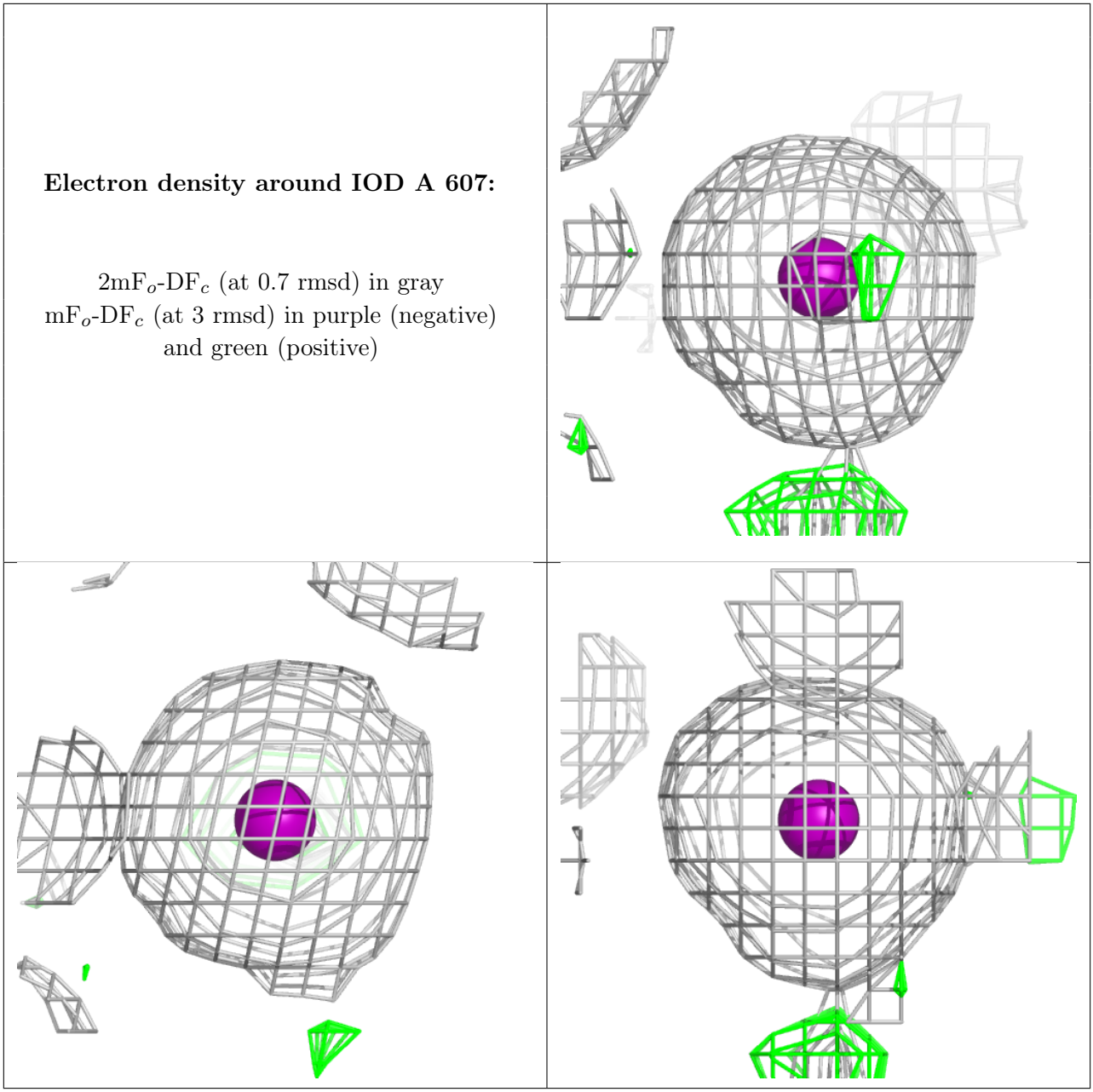
Electron density around IOD A 606 (B):

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



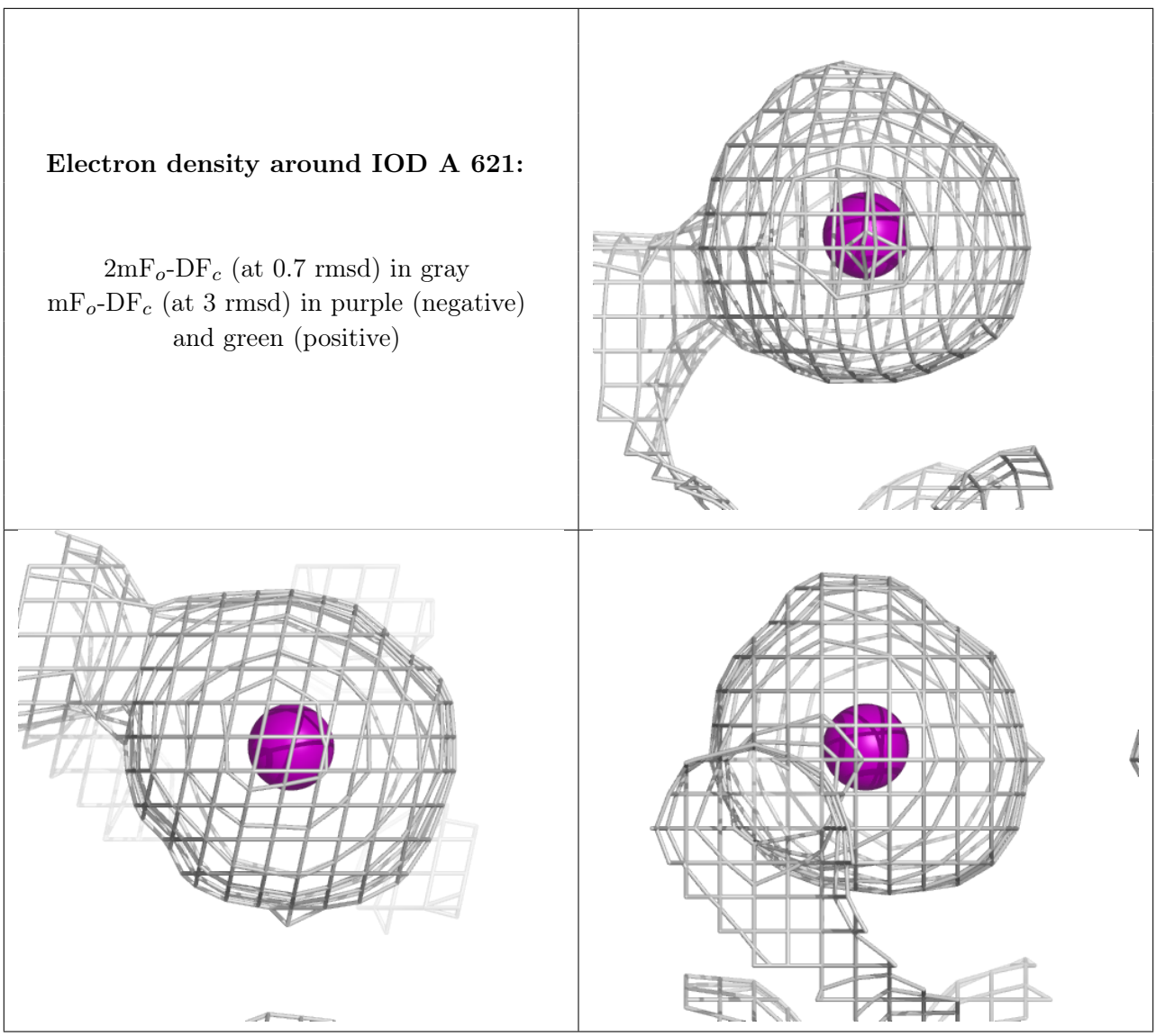
Electron density around IOD A 607:

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



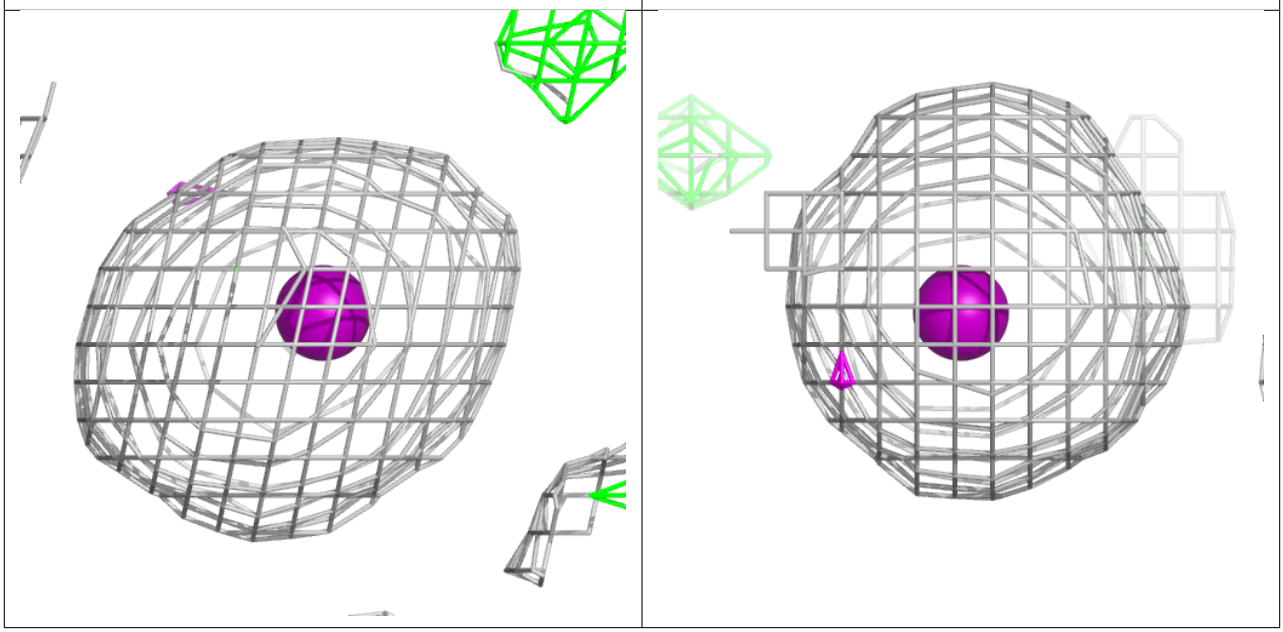
Electron density around IOD A 621:

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



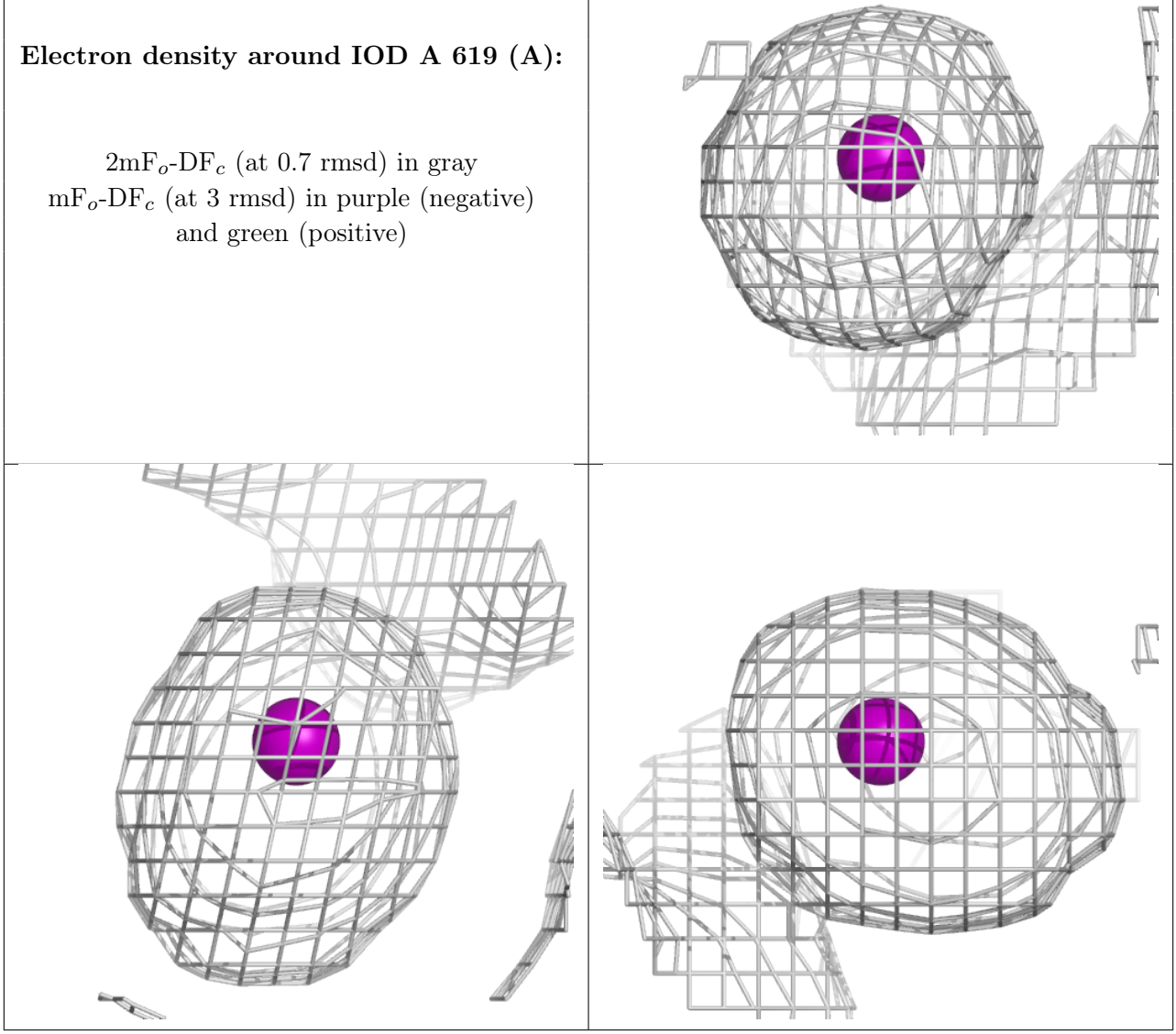
Electron density around IOD A 602 (B):

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



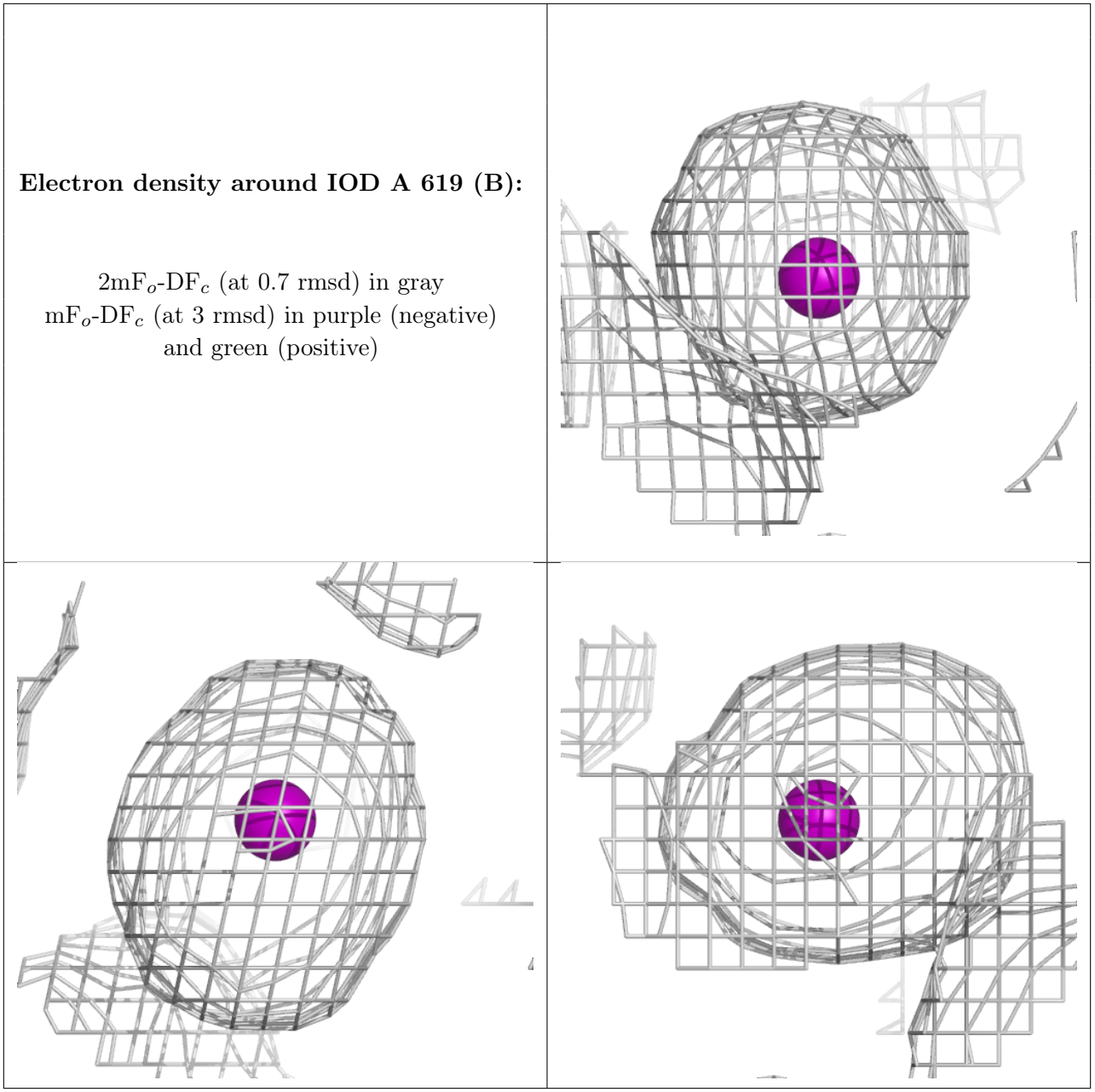
Electron density around IOD A 619 (A):

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



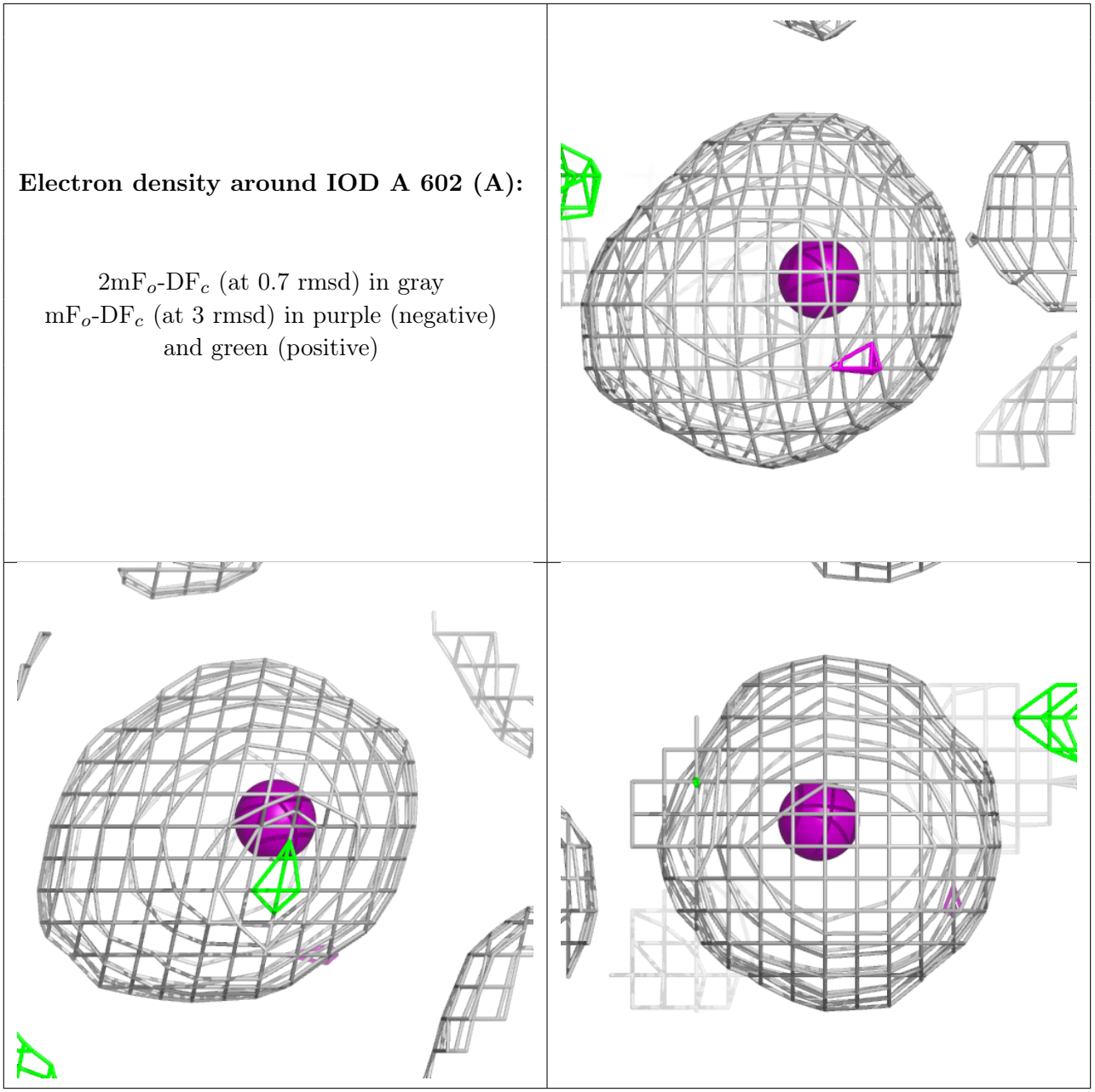
Electron density around IOD A 619 (B):

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



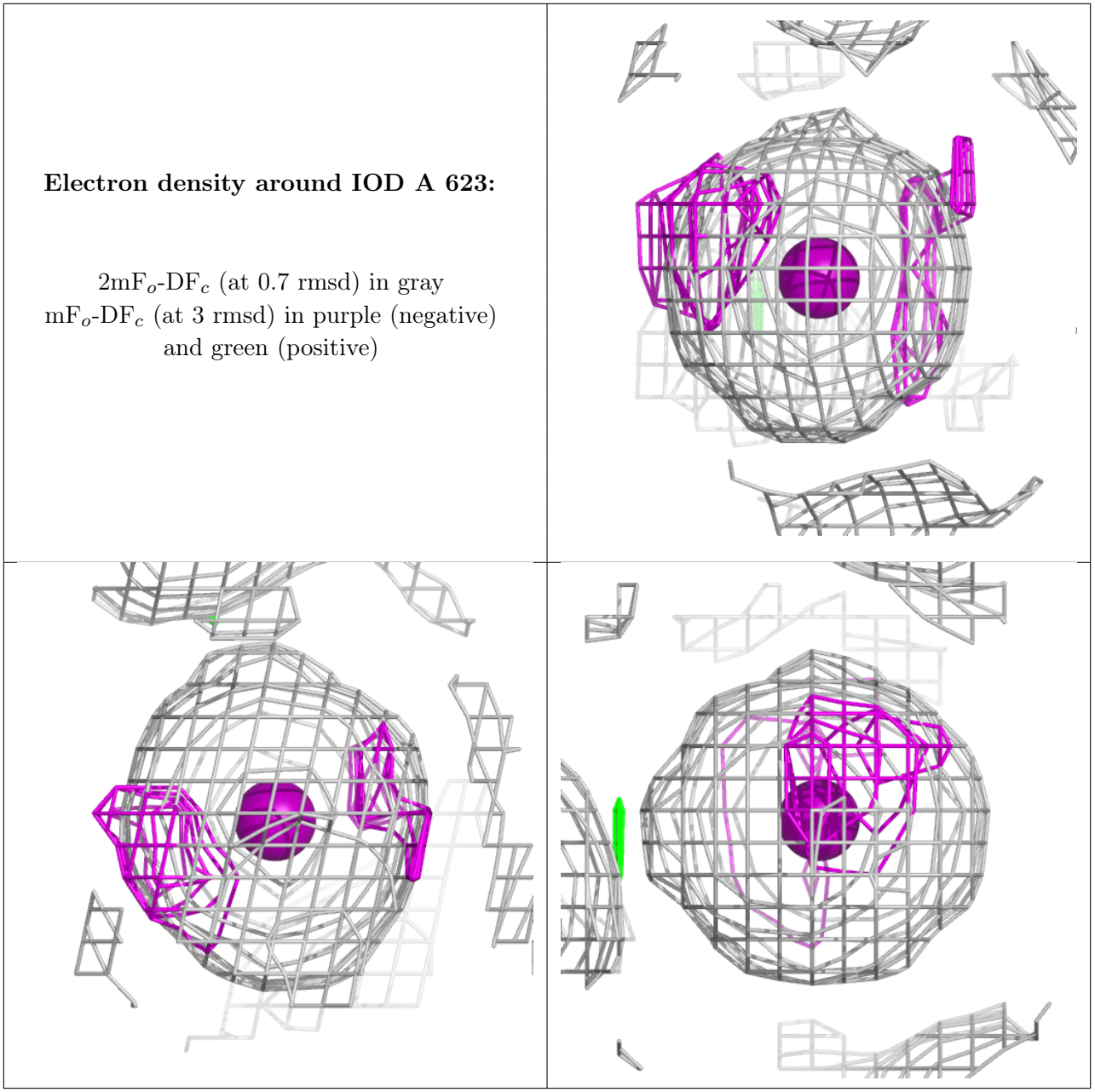
Electron density around IOD A 602 (A):

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



Electron density around IOD A 623:

$2mF_o$-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.