Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 07:17 AM JST

PDB ID	:	6L2J
Title	:	Crystal structure of yak lactoperoxidase at 1.93 A resolution.
Authors	:	Viswanathan, V.; Sharma, P.; Rani, C.; Sharma, S.; Singh, T.P.
Deposited on	:	2019-10-04
Resolution	:	1.93 Å(reported)

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

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

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

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

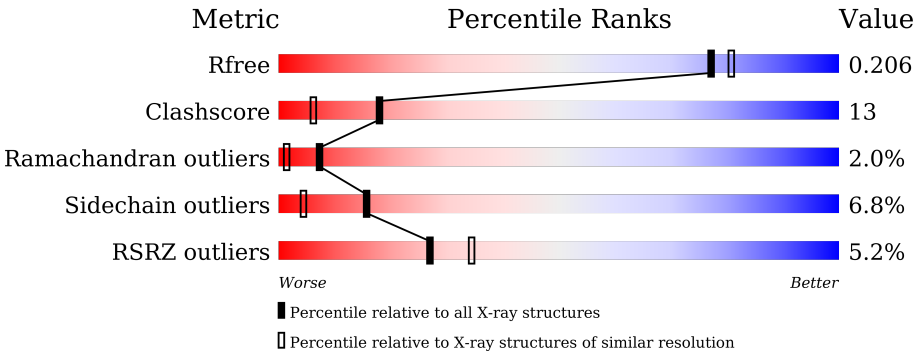
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	5%, 79%, 17%, • •
2	B	6	33%, 67%
3	C	2	50%, 50%

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
6	IOD	A	620	-	-	X	-
6	IOD	A	627	-	-	X	-
7	SCN	A	629	-	-	X	-
7	SCN	A	635	-	-	X	-
7	SCN	A	636	-	-	X	-
7	SCN	A	638	-	-	X	-
7	SCN	A	640	-	-	X	-
8	OSM	A	643	-	-	X	-
8	OSM	A	644[A]	-	-	X	-
8	OSM	A	644[B]	-	-	X	-
8	OSM	A	646	-	-	X	-
9	PEO	A	648	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 5800 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.

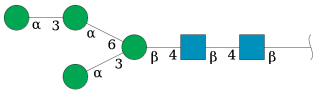
- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	595	4875	3122	858	865	30	0	20	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	SER	PHE	conflict	UNP L8ICE9
A	254	SER	PHE	conflict	UNP L8ICE9

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

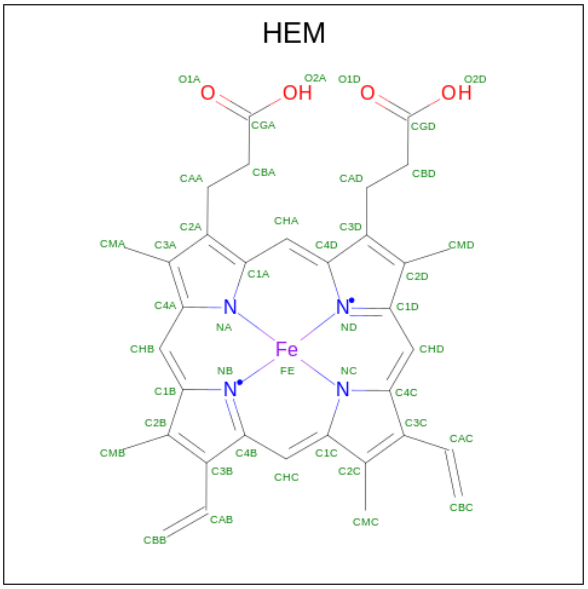


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	72	40	2	30	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

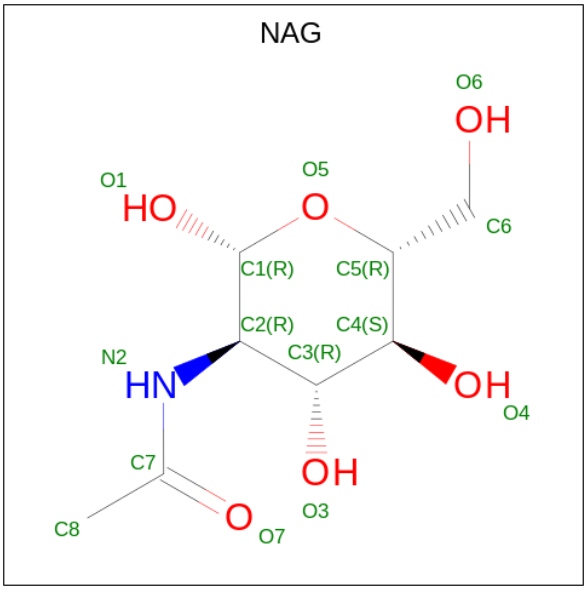
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0

- Molecule 4 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
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 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
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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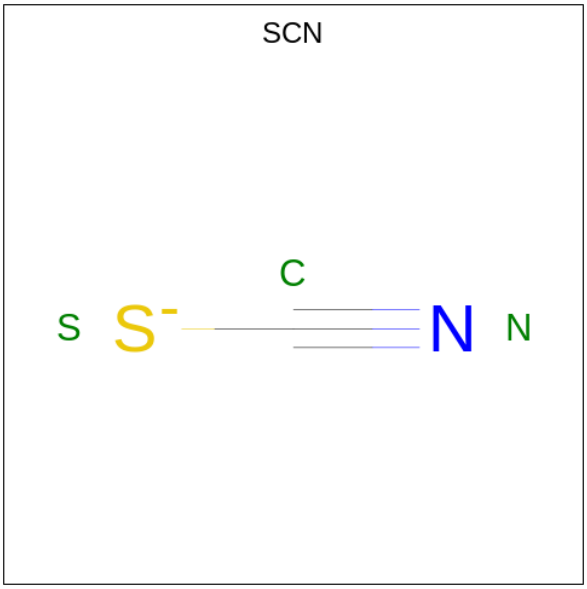
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	26	Total I 26 26	0	0

- Molecule 7 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS) (labeled as "Ligand of Interest" by depositor).



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

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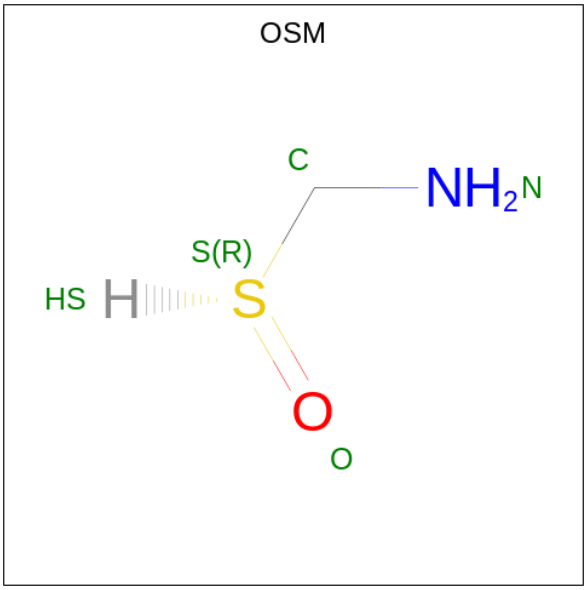
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N S 3 1 1 1	0	0
7	A	1	Total C N S 3 1 1 1	0	0
7	A	1	Total C N S 3 1 1 1	0	0
7	A	1	Total C N S 3 1 1 1	0	0
7	A	1	Total C N S 3 1 1 1	0	0
7	A	1	Total C N S 3 1 1 1	0	0

- Molecule 8 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH_5NOS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O S 4 1 1 1 1	0	0
8	A	1	Total C N O S 8 2 2 2 2	0	1
8	A	1	Total C N O S 4 1 1 1 1	0	0
8	A	1	Total C N O S 8 2 2 2 2	0	1
8	A	1	Total C N O S 4 1 1 1 1	0	0

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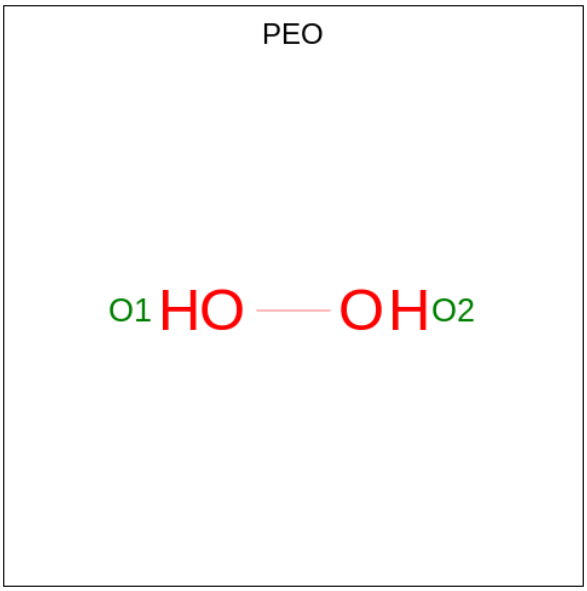
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O S 4 1 1 1 1	0	0
8	A	1	Total C N O S 4 1 1 1 1	0	0
8	A	1	Total C N O S 4 1 1 1 1	0	0

- Molecule 9 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H_2O_2) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	5	Total Ca 5 5	0	0

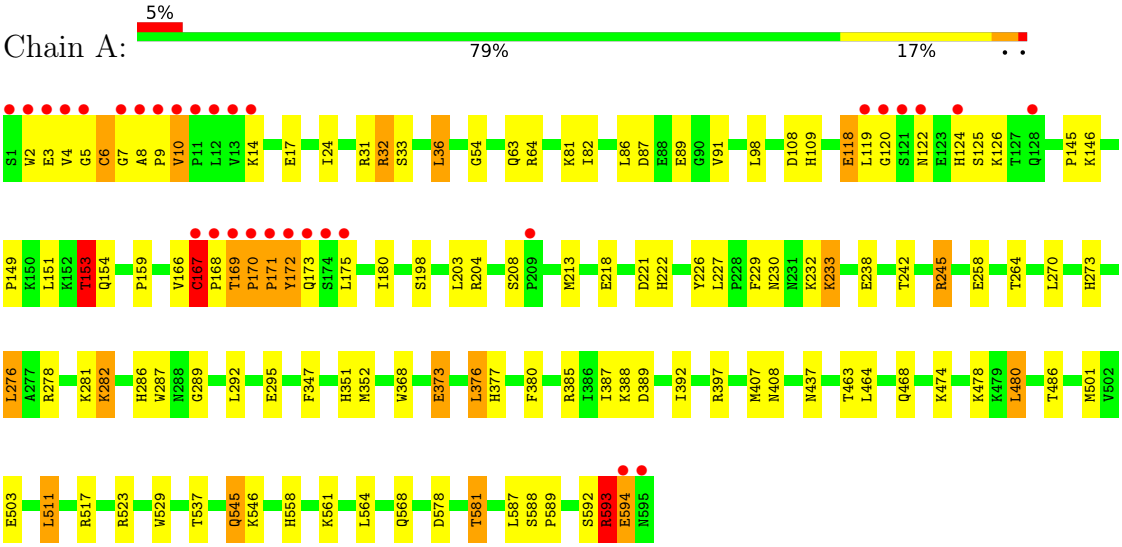
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	637	Total O 637 637	0	0

3 Residue-property plots (i)

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

• Molecule 1: Lactoperoxidase



• Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.85Å 78.92Å 67.75Å 90.00° 92.95° 90.00°	Depositor
Resolution (Å)	53.84 – 1.93 53.78 – 1.93	Depositor EDS
% Data completeness (in resolution range)	100.0 (53.84-1.93) 100.0 (53.78-1.93)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.44 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.145 , 0.198 0.155 , 0.206	Depositor DCC
R_{free} test set	1503 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å^2)	14.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5800	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, OSM, SCN, PEO, IOD, NAG, MAN, HEM, BMA

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	0.71	1/5063 (0.0%)	0.84	3/6865 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	373	GLU	CD-OE1	-5.10	1.20	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	CYS	CB-CA-C	5.21	120.82	110.40
1	A	153	THR	N-CA-CB	-5.17	100.48	110.30
1	A	397	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	CYS	Peptide
1	A	593	ARG	Peptide
1	A	594	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4875	0	4888	110	0
2	B	72	0	61	0	0
3	C	28	0	25	1	0
4	A	43	0	30	14	0
5	A	28	0	26	0	0
6	A	26	0	0	15	0
7	A	36	0	0	15	0
8	A	40	0	49	19	0
9	A	10	0	0	3	0
10	A	5	0	0	0	0
11	A	637	0	0	41	1
All	All	5800	0	5079	138	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (138) 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)
6:A:620:IOD:I	8:A:644[B]:OSM:N	1.12	1.66
6:A:620:IOD:I	8:A:644[A]:OSM:S	1.52	1.65
6:A:620:IOD:I	8:A:644[A]:OSM:O	1.00	1.62
1:A:108:ASP:OD2	4:A:601:HEM:CMD	1.70	1.38
1:A:258:GLU:OE2	4:A:601:HEM:CMB	1.73	1.35
6:A:620:IOD:I	8:A:644[B]:OSM:C	2.47	1.33
8:A:644[B]:OSM:H1	11:A:1145:HOH:O	1.38	1.24
8:A:644[B]:OSM:C	11:A:1145:HOH:O	1.91	1.14
6:A:613:IOD:I	8:A:644[B]:OSM:S	2.79	1.11
1:A:87:ASP:OD1	11:A:701:HOH:O	1.73	1.07
1:A:258:GLU:OE2	4:A:601:HEM:HMB1	0.89	1.06
8:A:644[A]:OSM:H2	11:A:1145:HOH:O	1.56	1.03
6:A:620:IOD:I	9:A:648:PEO:O1	2.52	0.97
1:A:108:ASP:CG	4:A:601:HEM:HMD1	1.83	0.97
1:A:145:PRO:HG2	7:A:635:SCN:N	1.80	0.97
6:A:665:IOD:I	11:A:1166:HOH:O	2.53	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASP:OD2	4:A:601:HEM:HMD1	0.75	0.93
8:A:644[A]:OSM:C	11:A:1145:HOH:O	2.17	0.91
6:A:659:IOD:I	11:A:907:HOH:O	2.61	0.88
7:A:637:SCN:N	11:A:702:HOH:O	2.08	0.85
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.25	0.83
1:A:368[A]:TRP:HZ3	1:A:389:ASP:OD1	1.63	0.80
1:A:407[A]:MET:HE1	11:A:993:HOH:O	1.81	0.79
1:A:32[A]:ARG:HG2	11:A:885:HOH:O	1.82	0.78
7:A:629:SCN:N	9:A:649:PEO:O1	2.20	0.74
7:A:640:SCN:S	11:A:1050:HOH:O	2.47	0.72
1:A:238:GLU:OE2	6:A:627:IOD:I	2.78	0.72
8:A:644[B]:OSM:H2	11:A:1145:HOH:O	1.72	0.71
1:A:368[A]:TRP:CZ3	1:A:389:ASP:OD1	2.44	0.69
1:A:159:PRO:O	11:A:703:HOH:O	2.11	0.69
1:A:153:THR:HG23	11:A:747:HOH:O	1.93	0.68
1:A:407[A]:MET:CE	11:A:993:HOH:O	2.38	0.67
7:A:629:SCN:N	11:A:709:HOH:O	2.29	0.66
1:A:86:LEU:O	11:A:704:HOH:O	2.13	0.66
1:A:282:LYS:HA	1:A:282:LYS:HE3	1.79	0.65
1:A:153:THR:HG21	11:A:1209:HOH:O	1.96	0.63
1:A:230:ASN:HD21	1:A:232:LYS:HE3	1.64	0.61
4:A:601:HEM:HMC2	4:A:601:HEM:HBC2	1.83	0.61
1:A:258:GLU:CD	4:A:601:HEM:CMB	2.64	0.61
7:A:638:SCN:S	11:A:714:HOH:O	2.51	0.61
1:A:31:ARG:HD2	6:A:666:IOD:I	2.70	0.61
1:A:352[A]:MET:CB	1:A:407[A]:MET:HG2	2.29	0.61
1:A:352[A]:MET:SD	1:A:407[A]:MET:SD	2.99	0.60
1:A:108:ASP:CG	4:A:601:HEM:CMD	2.56	0.60
1:A:537:THR:HG21	1:A:593:ARG:HH22	1.67	0.60
1:A:258:GLU:OE2	4:A:601:HEM:C2B	2.54	0.60
1:A:153:THR:CG2	11:A:747:HOH:O	2.50	0.59
1:A:289:GLY:HA3	8:A:643:OSM:H1	1.84	0.59
1:A:517:ARG:NE	11:A:710:HOH:O	2.32	0.59
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.83	0.58
8:A:643:OSM:H2	11:A:886:HOH:O	2.03	0.58
1:A:64:ARG:HG2	11:A:1009:HOH:O	2.03	0.58
1:A:82:ILE:HD13	1:A:480[A]:LEU:CD1	2.34	0.58
1:A:546:LYS:HE2	11:A:783:HOH:O	2.05	0.57
1:A:407[A]:MET:HE3	1:A:408:ASN:N	2.21	0.56
1:A:568:GLN:NE2	11:A:708:HOH:O	2.28	0.56
1:A:286:HIS:HB2	6:A:624:IOD:I	2.77	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.87	0.55
1:A:230:ASN:HD21	1:A:232:LYS:CE	2.21	0.54
6:A:621:IOD:I	11:A:895:HOH:O	2.89	0.54
1:A:561:LYS:HB2	7:A:631:SCN:N	2.23	0.53
1:A:592:SER:O	1:A:593:ARG:HB2	2.09	0.53
1:A:145:PRO:CG	7:A:635:SCN:N	2.65	0.53
1:A:352[A]:MET:HB2	1:A:407[A]:MET:HG2	1.89	0.52
1:A:278:ARG:NH1	11:A:720:HOH:O	2.42	0.52
1:A:352[A]:MET:HB3	1:A:407[A]:MET:HG2	1.90	0.52
7:A:632:SCN:S	7:A:636:SCN:N	2.82	0.52
1:A:118:GLU:C	1:A:120:GLY:H	2.13	0.51
1:A:169:THR:N	1:A:170:PRO:CD	2.74	0.51
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.40	0.51
1:A:171:PRO:O	1:A:172:TYR:CB	2.58	0.51
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.46	0.51
1:A:407[B]:MET:HE1	11:A:993:HOH:O	2.11	0.50
1:A:388:LYS:HE2	3:C:1:NAG:O6	2.11	0.50
1:A:463:THR:HG23	7:A:636:SCN:S	2.52	0.50
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.47	0.50
1:A:578:ASP:O	1:A:581:THR:HB	2.11	0.50
1:A:109:HIS:NE2	9:A:648:PEO:O1	2.41	0.50
1:A:503:GLU:HG2	11:A:1166:HOH:O	2.13	0.49
1:A:17:GLU:N	7:A:630:SCN:S	2.82	0.49
1:A:81:LYS:HE3	7:A:635:SCN:S	2.53	0.49
1:A:170:PRO:HD2	1:A:171:PRO:HD2	1.95	0.49
1:A:227:LEU:HD12	1:A:270:LEU:HD22	1.95	0.49
1:A:408:ASN:HB2	11:A:924:HOH:O	2.12	0.49
1:A:9:PRO:CD	11:A:797:HOH:O	2.61	0.48
1:A:503:GLU:CG	11:A:1166:HOH:O	2.61	0.48
1:A:588:SER:N	1:A:589:PRO:CD	2.77	0.48
1:A:6:CYS:HB3	11:A:1251:HOH:O	2.14	0.48
1:A:218:GLU:HG2	7:A:640:SCN:N	2.29	0.48
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.96	0.47
4:A:601:HEM:HBB2	4:A:601:HEM:HMB2	1.96	0.47
1:A:281:LYS:HD2	11:A:721:HOH:O	2.14	0.47
1:A:222:HIS:O	1:A:558:HIS:HE1	1.98	0.47
1:A:108:ASP:OD2	4:A:601:HEM:C2D	2.58	0.46
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.51	0.46
1:A:233:LYS:HE2	6:A:627:IOD:I	2.84	0.46
1:A:32[A]:ARG:CG	11:A:885:HOH:O	2.52	0.46
8:A:646:OSM:N	8:A:667:OSM:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLU:O	7:A:638:SCN:N	2.49	0.46
1:A:82:ILE:HD13	1:A:480[A]:LEU:HD12	1.97	0.46
1:A:198:SER:HB2	8:A:645:OSM:O	2.16	0.46
4:A:601:HEM:CMB	4:A:601:HEM:HBB2	2.46	0.46
1:A:54:GLY:HA2	11:A:1112:HOH:O	2.15	0.45
1:A:545:GLN:HG2	11:A:1133:HOH:O	2.16	0.45
1:A:208:SER:O	8:A:643:OSM:O	2.35	0.45
1:A:287:TRP:CZ3	1:A:295:GLU:HG3	2.52	0.44
1:A:166:VAL:HG12	1:A:180:ILE:HG12	1.99	0.44
1:A:33:SER:HB3	1:A:36:LEU:HD22	1.98	0.44
4:A:601:HEM:HMA1	8:A:644[A]:OSM:H1	1.99	0.44
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.53	0.43
6:A:653:IOD:I	11:A:1282:HOH:O	2.92	0.43
1:A:385:ARG:O	1:A:389:ASP:HB3	2.19	0.43
1:A:171:PRO:O	1:A:172:TYR:HB2	2.17	0.43
1:A:537:THR:HG21	1:A:593:ARG:NH2	2.31	0.42
1:A:581:THR:HG23	11:A:1279:HOH:O	2.19	0.42
4:A:601:HEM:HBC2	4:A:601:HEM:CMC	2.49	0.42
1:A:166:VAL:CG1	1:A:180:ILE:HG12	2.50	0.42
1:A:204:ARG:HH21	8:A:643:OSM:HS	1.67	0.42
1:A:407[A]:MET:CE	1:A:408:ASN:N	2.82	0.42
1:A:593:ARG:HD2	1:A:594:GLU:CD	2.40	0.42
1:A:226:TYR:CE2	1:A:387:ILE:HD12	2.55	0.42
1:A:276:LEU:HD12	1:A:587:LEU:HD11	2.01	0.42
1:A:24:ILE:H	8:A:646:OSM:HN1	1.68	0.41
1:A:407[B]:MET:HB2	1:A:407[B]:MET:HE3	1.42	0.41
1:A:258:GLU:HG3	6:A:620:IOD:I	2.90	0.41
1:A:478[A]:LYS:HD3	11:A:1054:HOH:O	2.21	0.41
1:A:149:PRO:HG2	8:A:641:OSM:H1	2.02	0.41
1:A:242:THR:O	1:A:245[B]:ARG:CZ	2.69	0.41
1:A:511[A]:LEU:HD12	1:A:511[A]:LEU:HA	1.85	0.41
1:A:4:VAL:O	1:A:4:VAL:HG12	2.21	0.41
1:A:501[B]:MET:HE2	1:A:501[B]:MET:HB2	1.93	0.41
1:A:581:THR:CG2	11:A:1279:HOH:O	2.68	0.41
1:A:229:PHE:CD2	7:A:640:SCN:N	2.89	0.41
1:A:173:GLN:HE21	1:A:173:GLN:HA	1.85	0.40
1:A:230:ASN:ND2	1:A:232:LYS:HE3	2.35	0.40
1:A:264:THR:HG23	1:A:392:ILE:HB	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1107:HOH:O	11:A:1185:HOH:O[1_655]	2.08	0.12

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	613/595 (103%)	579 (94%)	22 (4%)	12 (2%)	7 1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	170	PRO
1	A	172	TYR
1	A	5	GLY
1	A	7	GLY
1	A	124	HIS
1	A	593	ARG
1	A	10	VAL
1	A	118	GLU
1	A	125	SER
1	A	171	PRO
1	A	119	LEU

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	538/518 (104%)	494 (92%)	44 (8%)	11 2

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	3	GLU
1	A	6	CYS
1	A	10	VAL
1	A	14	LYS
1	A	32[A]	ARG
1	A	32[B]	ARG
1	A	36	LEU
1	A	63	GLN
1	A	89[A]	GLU
1	A	89[B]	GLU
1	A	91	VAL
1	A	98[A]	LEU
1	A	98[B]	LEU
1	A	122	ASN
1	A	126	LYS
1	A	146	LYS
1	A	151	LEU
1	A	153	THR
1	A	154	GLN
1	A	169	THR
1	A	175	LEU
1	A	203[A]	LEU
1	A	203[B]	LEU
1	A	233	LYS
1	A	245[A]	ARG
1	A	245[B]	ARG
1	A	276	LEU
1	A	282	LYS
1	A	292	LEU
1	A	347	PHE
1	A	376[A]	LEU
1	A	376[B]	LEU
1	A	464[A]	LEU
1	A	464[B]	LEU
1	A	480[A]	LEU
1	A	480[B]	LEU
1	A	486	THR

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Mol	Chain	Res	Type
1	A	511[A]	LEU
1	A	511[B]	LEU
1	A	545	GLN
1	A	564	LEU
1	A	581	THR
1	A	593	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	124	HIS
1	A	173	GLN
1	A	217	GLN
1	A	222	HIS
1	A	329	GLN

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)

8 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	0.64	0	17,19,21	1.59	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	2	2	14,14,15	0.37	0	17,19,21	1.47	3 (17%)
2	BMA	B	3	2	11,11,12	0.70	0	15,15,17	1.27	2 (13%)
2	MAN	B	4	2	11,11,12	0.60	0	15,15,17	0.85	0
2	MAN	B	5	2	11,11,12	0.66	0	15,15,17	1.03	0
2	MAN	B	6	2	11,11,12	0.78	0	15,15,17	1.41	3 (20%)
3	NAG	C	1	3,1	14,14,15	0.40	0	17,19,21	0.73	1 (5%)
3	NAG	C	2	3	14,14,15	0.60	0	17,19,21	1.80	3 (17%)

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	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	1/2/19/22	0/1/1/1
2	MAN	B	6	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	NAG	C1-O5-C5	4.62	118.45	112.19
2	B	2	NAG	C1-O5-C5	4.22	117.90	112.19
2	B	1	NAG	C1-C2-N2	3.98	117.29	110.49
3	C	2	NAG	O5-C5-C6	2.85	111.68	107.20
2	B	6	MAN	C2-C3-C4	-2.81	106.04	110.89
3	C	2	NAG	O3-C3-C4	-2.60	104.34	110.35
2	B	2	NAG	C6-C5-C4	-2.51	107.14	113.00
2	B	1	NAG	O5-C5-C6	2.44	111.03	107.20
2	B	6	MAN	O3-C3-C2	2.43	114.64	109.99
2	B	3	BMA	C1-O5-C5	2.24	115.23	112.19
2	B	3	BMA	O3-C3-C2	2.20	114.20	109.99
2	B	1	NAG	O4-C4-C3	-2.19	105.28	110.35
2	B	6	MAN	O5-C1-C2	-2.10	107.54	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	C1-O5-C5	-2.06	109.40	112.19
3	C	1	NAG	O4-C4-C3	-2.04	105.64	110.35
2	B	2	NAG	C3-C4-C5	2.01	113.82	110.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	6	MAN	C4-C5-C6-O6
2	B	6	MAN	O5-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6

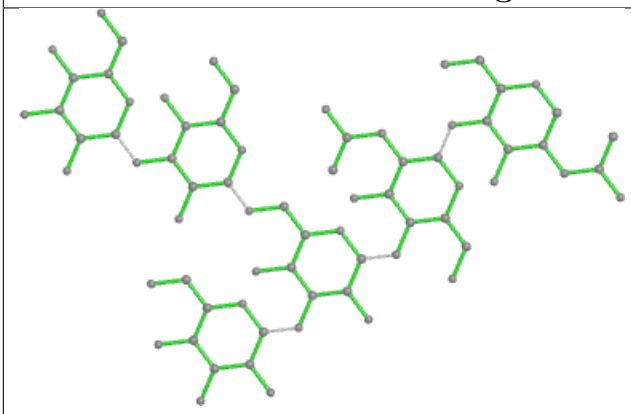
There are no ring outliers.

1 monomer is involved in 1 short contact:

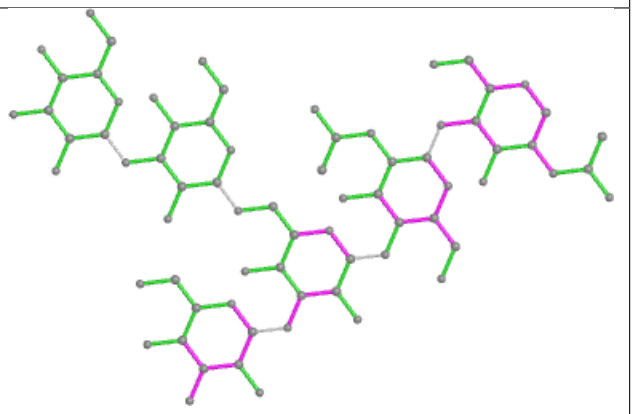
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0

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

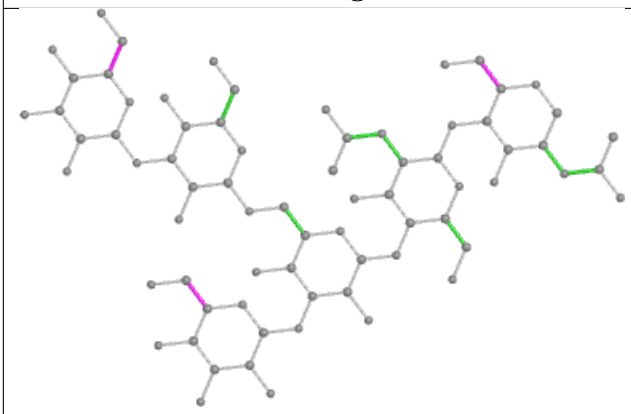
Oligosaccharide Chain B



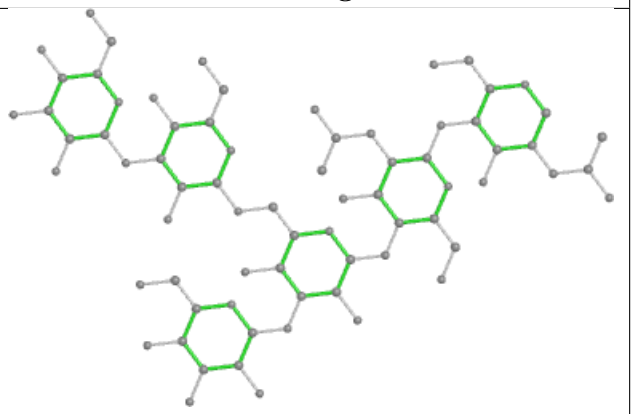
Bond lengths



Bond angles

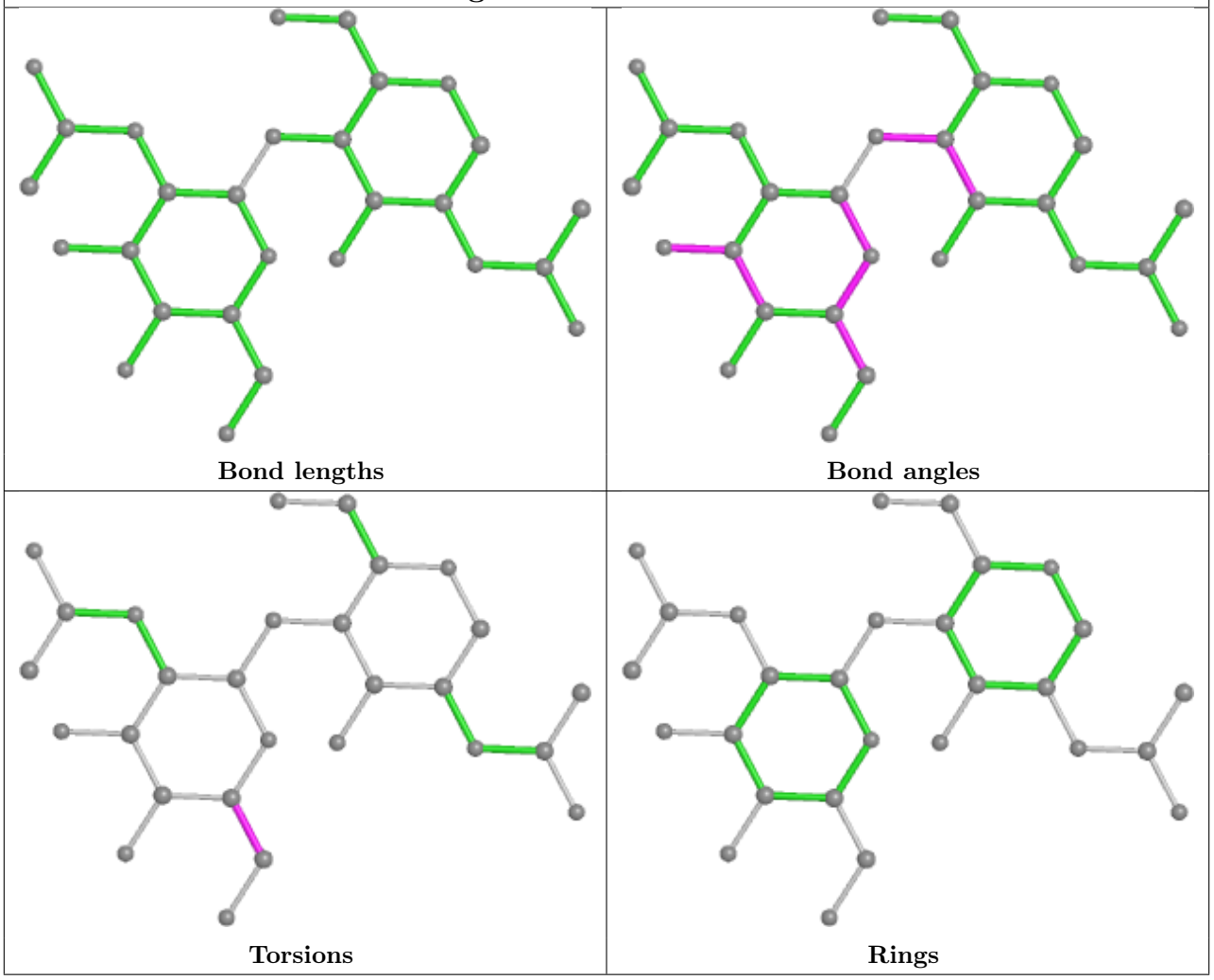


Torsions



Rings

Oligosaccharide Chain C



5.6 Ligand geometry (i)

Of 61 ligands modelled in this entry, 31 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
7	SCN	A	640	-	1,2,2	0.42	0	0,1,1	-	-
9	PEO	A	648	4	1,1,1	0.47	0	-		
9	PEO	A	650	-	1,1,1	0.78	0	-		
7	SCN	A	638	-	1,2,2	0.44	0	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	SCN	A	639	-	1,2,2	0.22	0	0,1,1	-	-
8	OSM	A	645	-	1,3,3	0.04	0	0,2,2	-	-
9	PEO	A	652	-	1,1,1	0.43	0	-		
8	OSM	A	644[A]	-	1,3,3	0.04	0	0,2,2	-	-
8	OSM	A	643	-	1,3,3	0.03	0	0,2,2	-	-
5	NAG	A	602	1	14,14,15	0.53	0	17,19,21	1.45	1 (5%)
7	SCN	A	629	-	1,2,2	0.25	0	0,1,1	-	-
7	SCN	A	635	-	1,2,2	0.45	0	0,1,1	-	-
8	OSM	A	642[B]	-	1,3,3	0.03	0	0,2,2	-	-
4	HEM	A	601	9,1	41,50,50	1.48	9 (21%)	45,82,82	2.12	16 (35%)
7	SCN	A	634	-	1,2,2	0.50	0	0,1,1	-	-
7	SCN	A	636	-	1,2,2	0.21	0	0,1,1	-	-
8	OSM	A	646	-	1,3,3	0.03	0	0,2,2	-	-
9	PEO	A	649	-	1,1,1	0.18	0	-		
8	OSM	A	667	-	1,3,3	0.05	0	0,2,2	-	-
7	SCN	A	637	-	1,2,2	0.10	0	0,1,1	-	-
8	OSM	A	644[B]	-	1,3,3	0.02	0	0,2,2	-	-
8	OSM	A	647	-	1,3,3	0.02	0	0,2,2	-	-
7	SCN	A	633	-	1,2,2	0.17	0	0,1,1	-	-
8	OSM	A	641	-	1,3,3	0.04	0	0,2,2	-	-
5	NAG	A	603	1	14,14,15	0.60	0	17,19,21	1.57	3 (17%)
7	SCN	A	630	-	1,2,2	0.14	0	0,1,1	-	-
8	OSM	A	642[A]	-	1,3,3	0.02	0	0,2,2	-	-
9	PEO	A	651	-	1,1,1	0.46	0	-		
7	SCN	A	631	-	1,2,2	0.06	0	0,1,1	-	-
7	SCN	A	632	-	1,2,2	0.76	0	0,1,1	-	-

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	OSM	A	642[A]	-	-	0/0/1/1	-
8	OSM	A	667	-	-	0/0/1/1	-
8	OSM	A	641	-	-	0/0/1/1	-
8	OSM	A	642[B]	-	-	0/0/1/1	-
4	HEM	A	601	9,1	-	4/12/54/54	-
8	OSM	A	645	-	-	0/0/1/1	-
8	OSM	A	644[A]	-	-	0/0/1/1	-
8	OSM	A	643	-	-	0/0/1/1	-
8	OSM	A	646	-	-	0/0/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OSM	A	644[B]	-	-	0/0/1/1	-
8	OSM	A	647	-	-	0/0/1/1	-
5	NAG	A	602	1	-	0/6/23/26	0/1/1/1
5	NAG	A	603	1	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	HEM	C1B-NB	-4.14	1.33	1.40
4	A	601	HEM	FE-NB	2.80	2.10	1.96
4	A	601	HEM	C1D-ND	-2.60	1.33	1.38
4	A	601	HEM	C1D-C2D	2.49	1.49	1.44
4	A	601	HEM	C4B-NB	-2.34	1.34	1.38
4	A	601	HEM	C3D-C2D	-2.32	1.31	1.36
4	A	601	HEM	C4D-ND	-2.24	1.36	1.40
4	A	601	HEM	CHA-C4D	2.21	1.40	1.35
4	A	601	HEM	CHB-C1B	2.20	1.40	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	601	HEM	C1B-NB-C4B	5.09	110.33	105.07
4	A	601	HEM	CHC-C4B-NB	4.96	129.82	124.43
4	A	601	HEM	CHA-C4D-ND	4.62	130.09	124.38
4	A	601	HEM	CMD-C2D-C1D	4.24	131.50	125.04
5	A	603	NAG	C1-O5-C5	3.75	117.28	112.19
5	A	602	NAG	O5-C1-C2	-3.49	105.78	111.29
4	A	601	HEM	CHA-C4D-C3D	-3.38	118.98	125.33
4	A	601	HEM	CAD-C3D-C4D	2.99	129.88	124.66
4	A	601	HEM	C4B-CHC-C1C	2.92	126.41	122.56
5	A	603	NAG	C8-C7-N2	2.65	120.58	116.10
4	A	601	HEM	CHB-C1B-NB	2.60	127.60	124.38
4	A	601	HEM	O2D-CGD-CBD	2.55	122.24	114.03
4	A	601	HEM	CBA-CAA-C2A	-2.46	108.42	112.62
4	A	601	HEM	CMC-C2C-C3C	2.42	129.20	124.68
4	A	601	HEM	O2D-CGD-O1D	-2.38	117.38	123.30
5	A	603	NAG	C1-C2-N2	-2.26	106.62	110.49
4	A	601	HEM	C3C-C4C-NC	-2.09	106.99	110.94
4	A	601	HEM	C4B-C3B-C2B	-2.08	105.47	107.11
4	A	601	HEM	CAD-C3D-C2D	-2.06	124.05	127.88
4	A	601	HEM	CMB-C2B-C1B	2.05	128.17	125.04

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	603	NAG	C8-C7-N2-C2
5	A	603	NAG	O7-C7-N2-C2
4	A	601	HEM	CAA-CBA-CGA-O1A
4	A	601	HEM	CAA-CBA-CGA-O2A
4	A	601	HEM	CAD-CBD-CGD-O2D
4	A	601	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

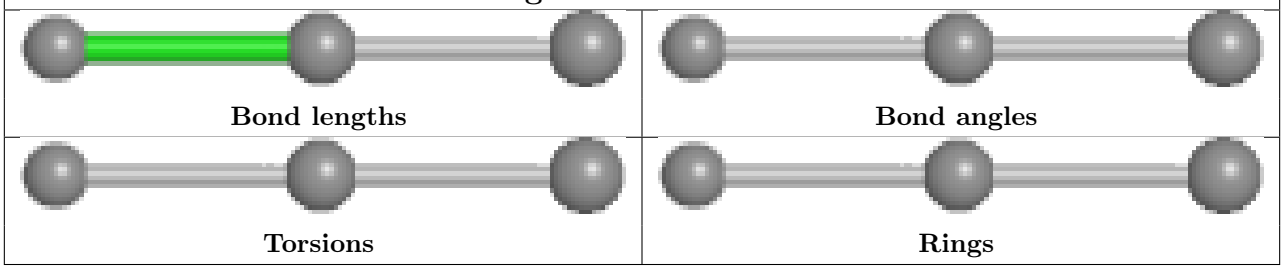
19 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	640	SCN	3	0
9	A	648	PEO	2	0
7	A	638	SCN	2	0
8	A	645	OSM	1	0
8	A	644[A]	OSM	5	0
8	A	643	OSM	4	0
7	A	629	SCN	2	0
7	A	635	SCN	3	0
4	A	601	HEM	14	0
7	A	636	SCN	2	0
8	A	646	OSM	2	0
9	A	649	PEO	1	0
8	A	667	OSM	1	0
7	A	637	SCN	1	0
8	A	644[B]	OSM	6	0
8	A	641	OSM	1	0
7	A	630	SCN	1	0
7	A	631	SCN	1	0
7	A	632	SCN	1	0

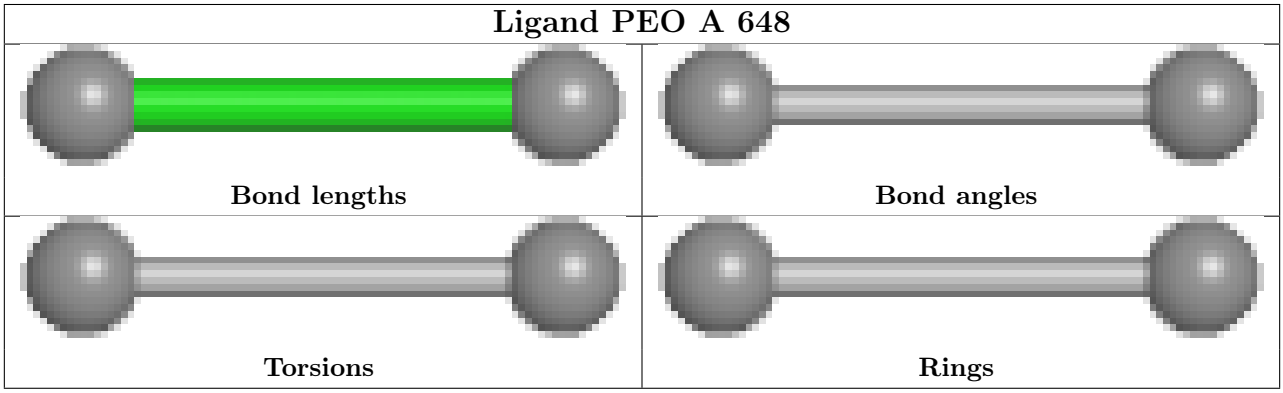
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

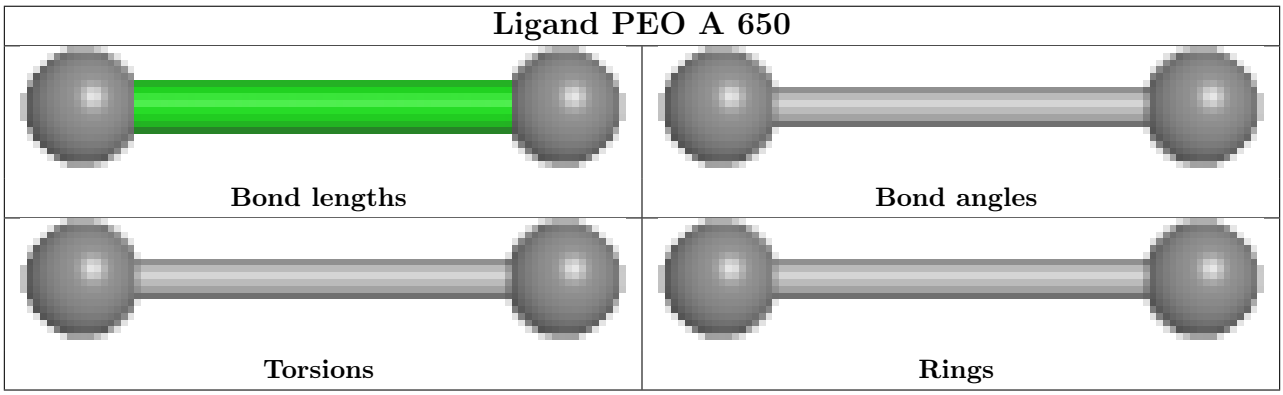
Ligand SCN A 640



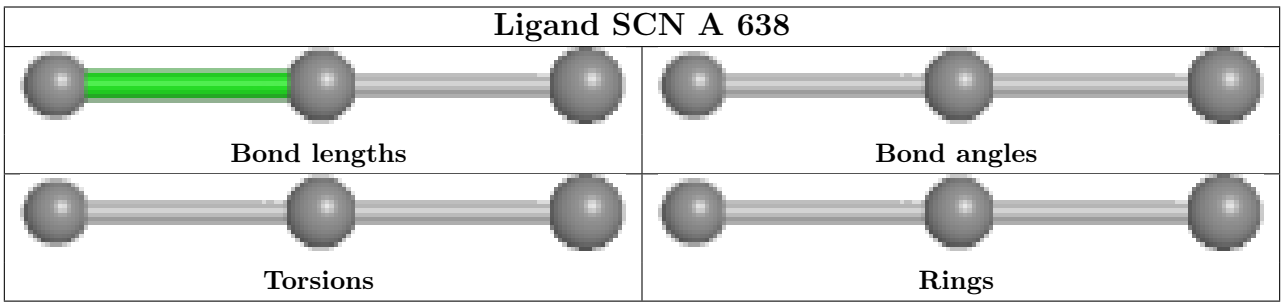
Ligand PEO A 648



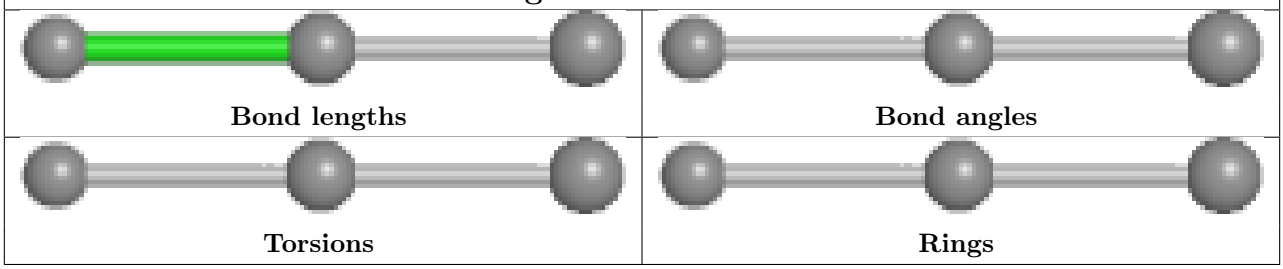
Ligand PEO A 650



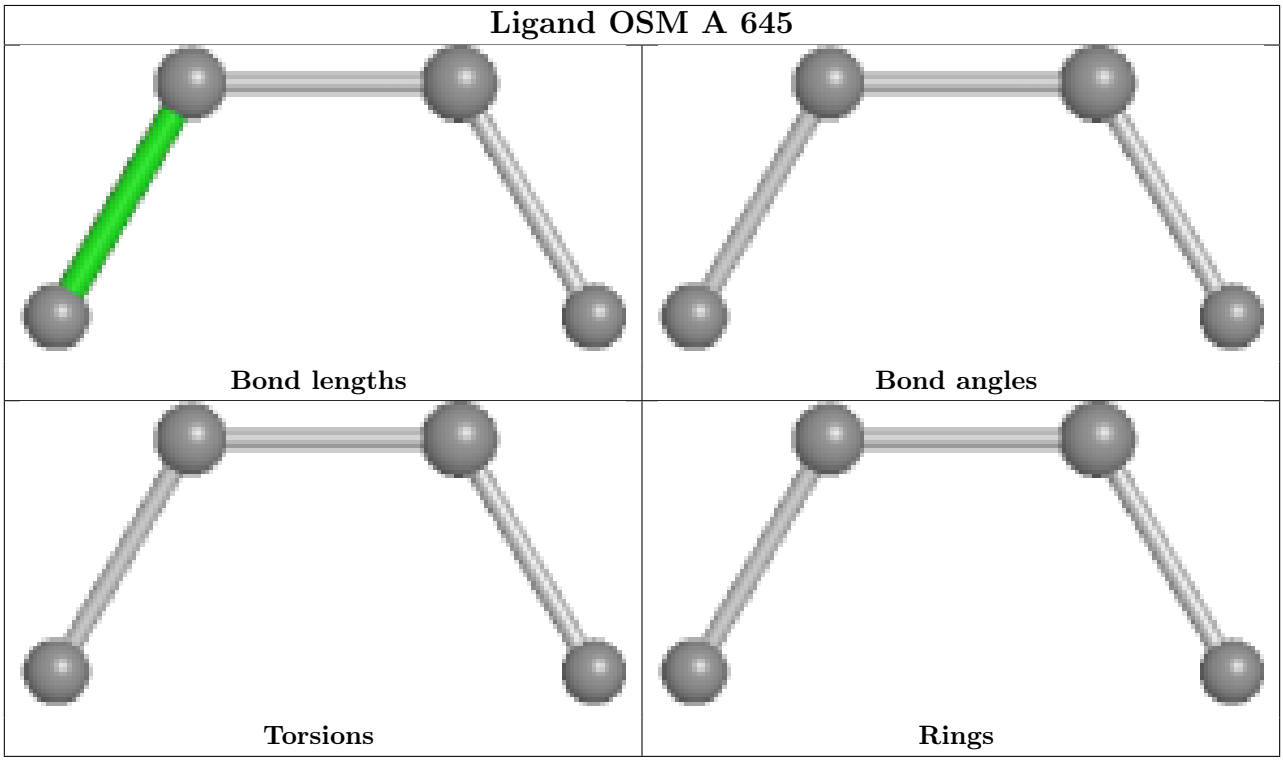
Ligand SCN A 638



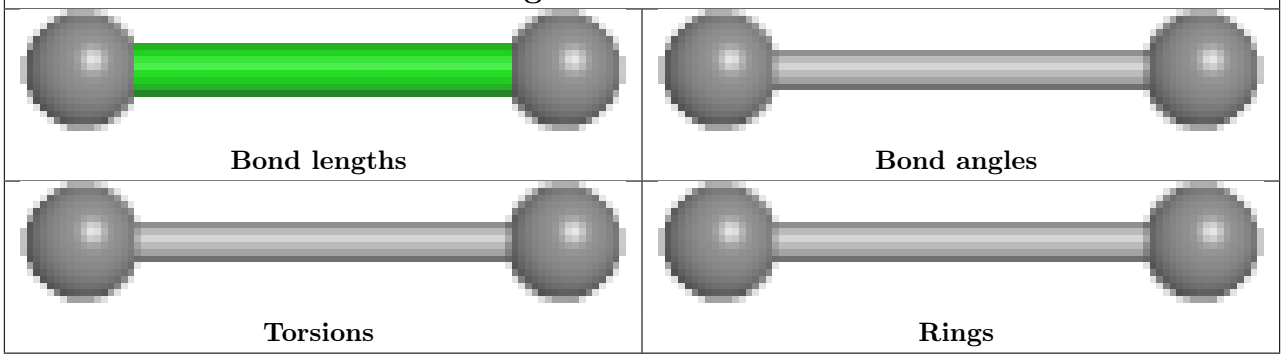
Ligand SCN A 639



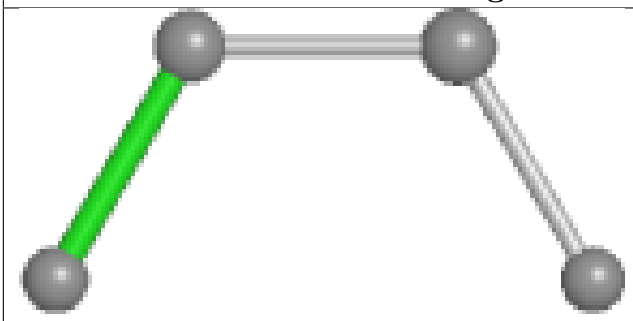
Ligand OSM A 645



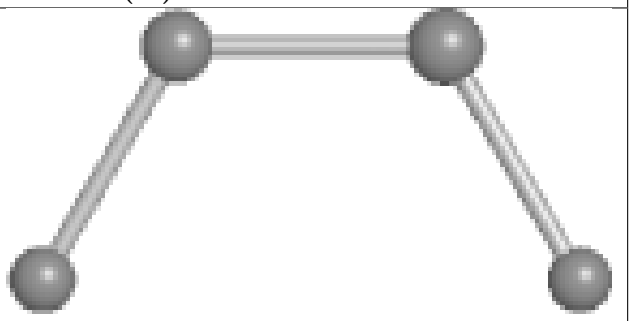
Ligand PEO A 652



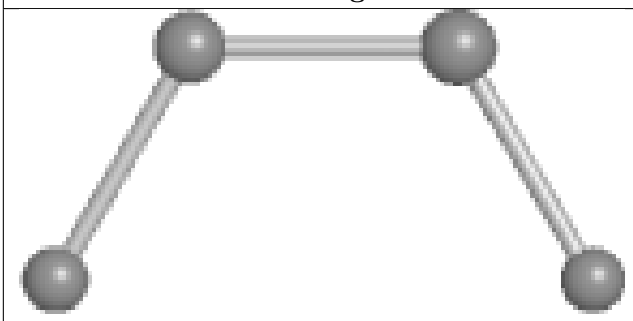
Ligand OSM A 644 (A)



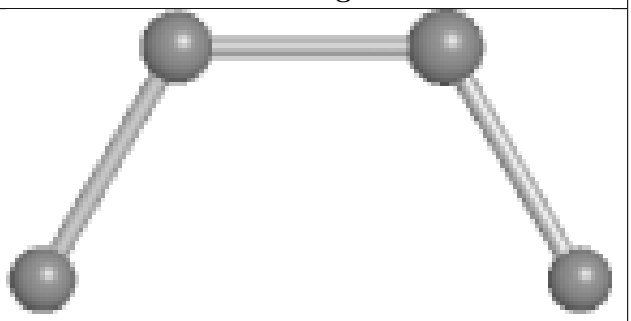
Bond lengths



Bond angles

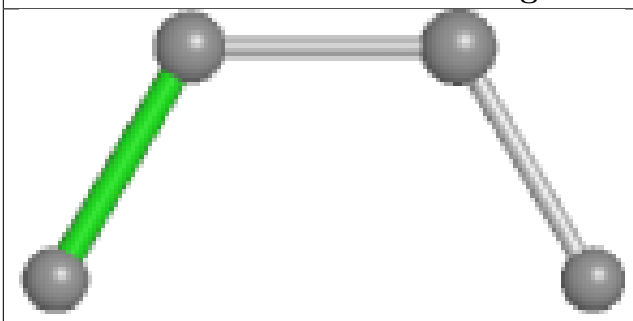


Torsions

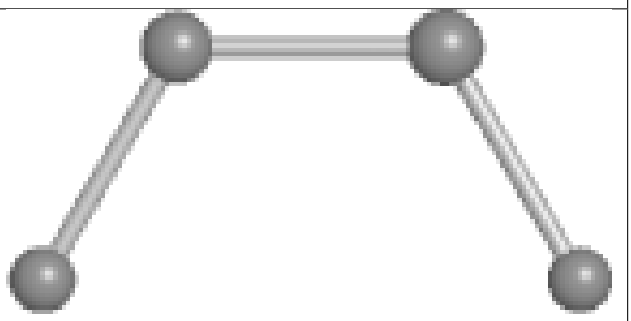


Rings

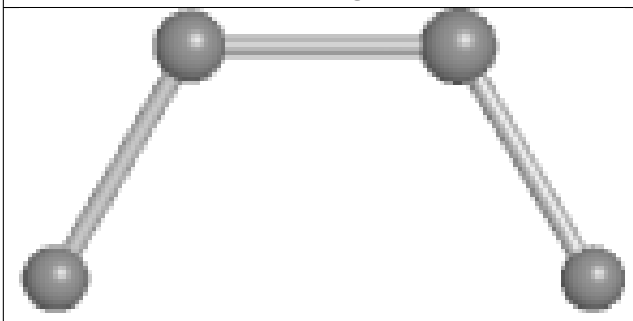
Ligand OSM A 643



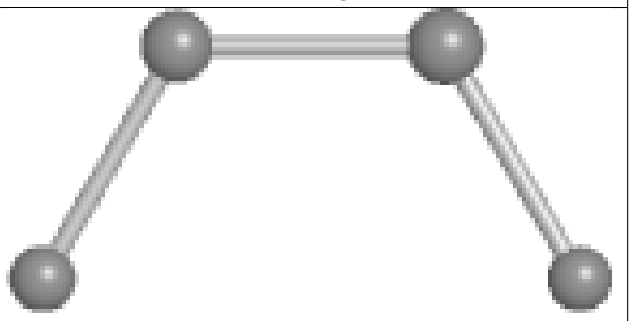
Bond lengths



Bond angles

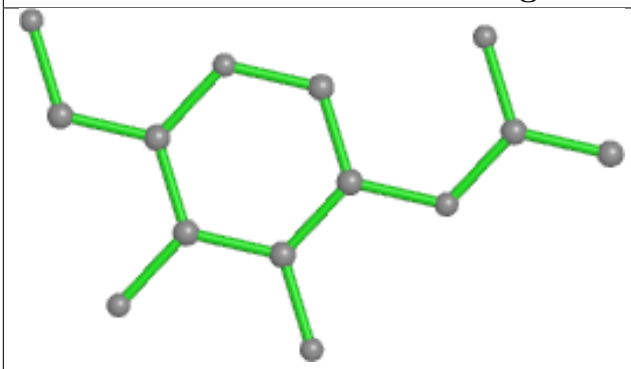


Torsions

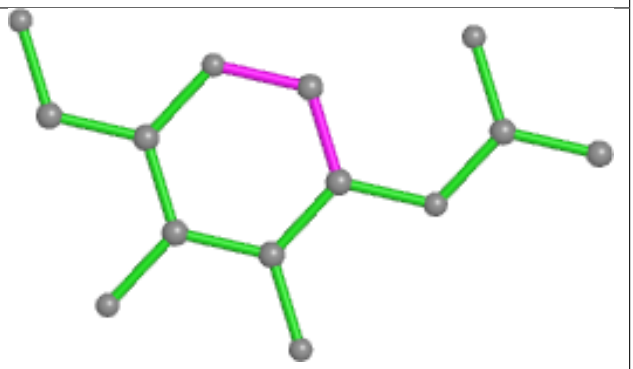


Rings

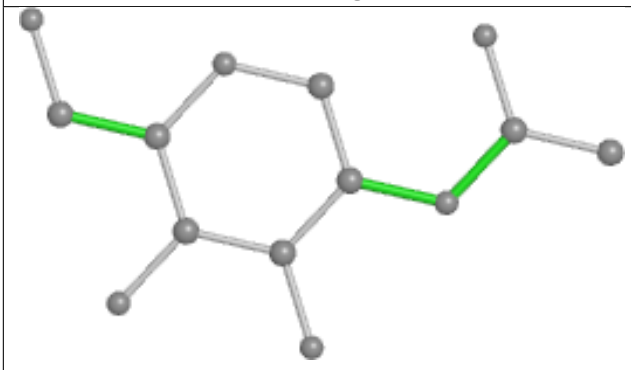
Ligand NAG A 602



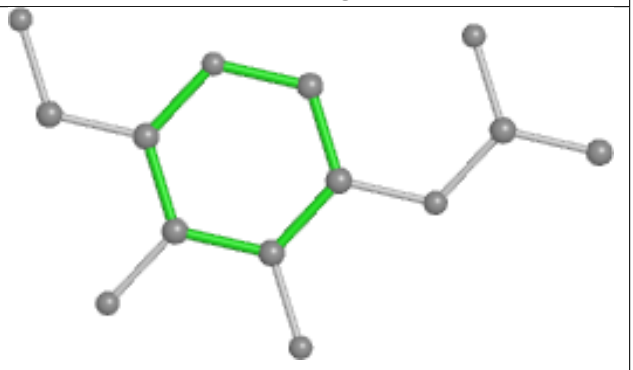
Bond lengths



Bond angles

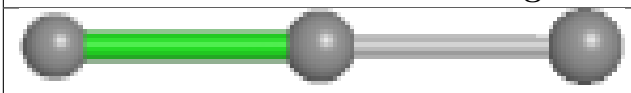


Torsions

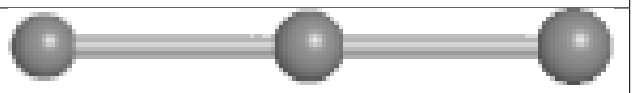


Rings

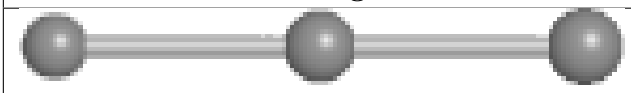
Ligand SCN A 629



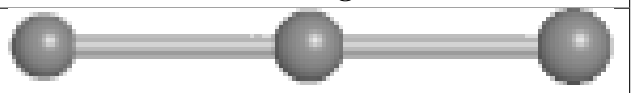
Bond lengths



Bond angles

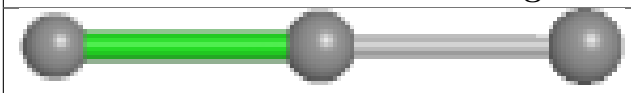


Torsions

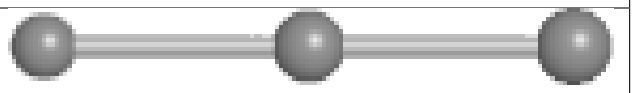


Rings

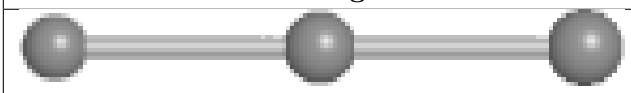
Ligand SCN A 635



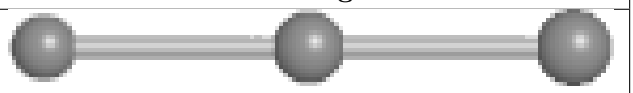
Bond lengths



Bond angles

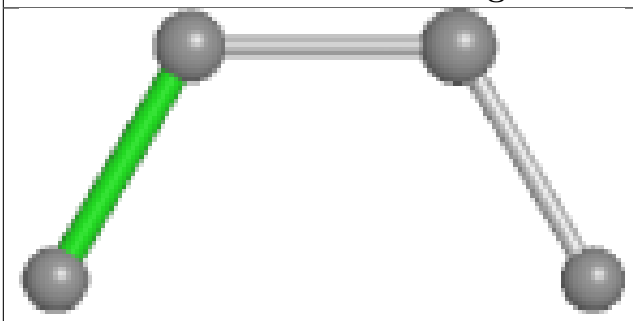


Torsions

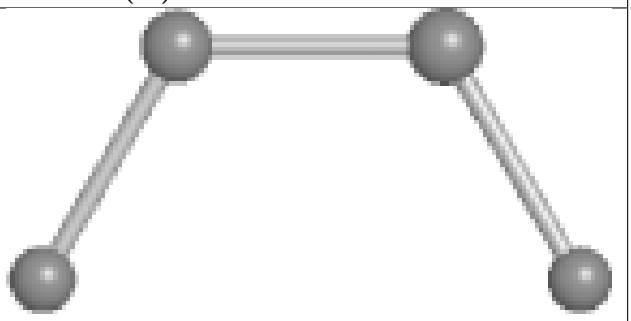


Rings

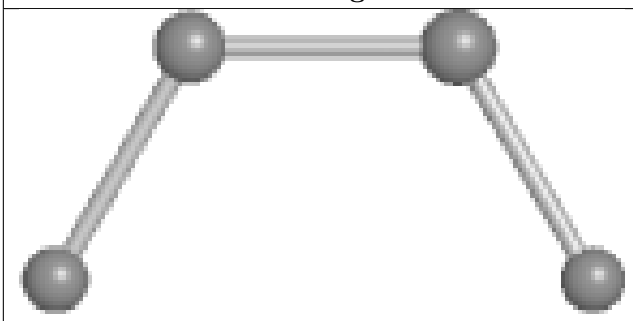
Ligand OSM A 642 (B)



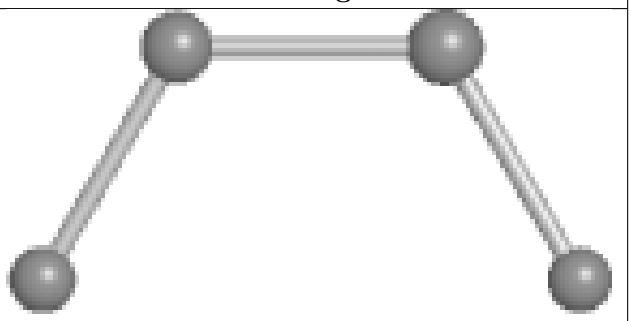
Bond lengths



Bond angles

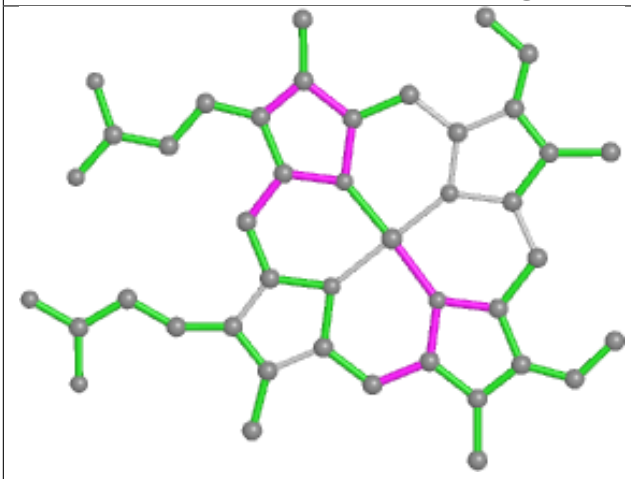


Torsions

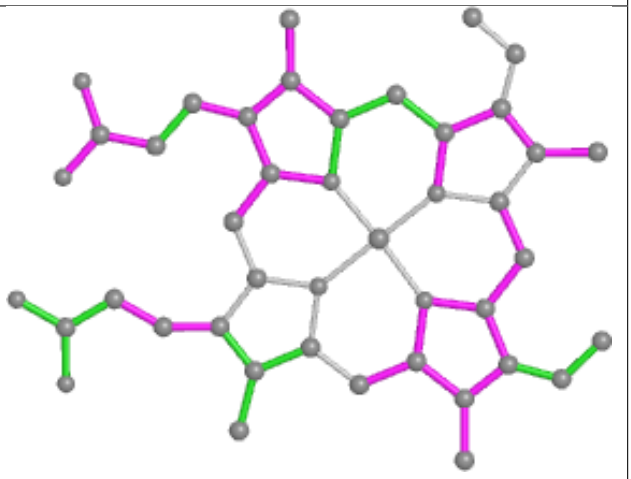


Rings

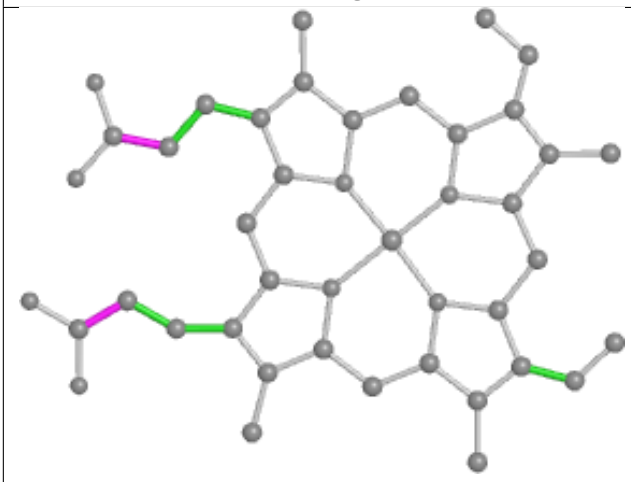
Ligand HEM A 601



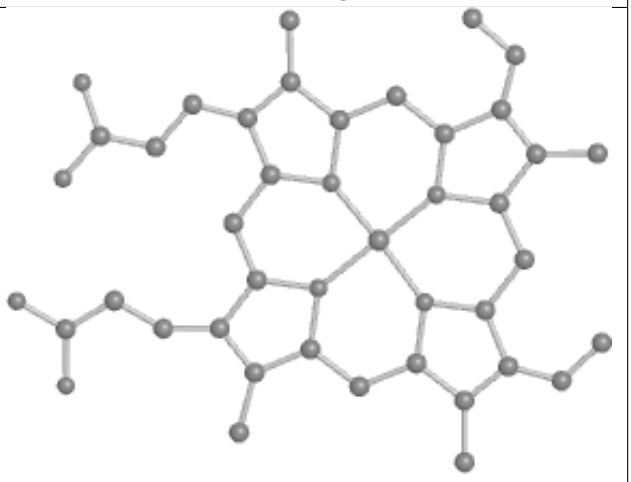
Bond lengths



Bond angles

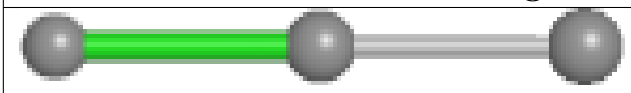


Torsions

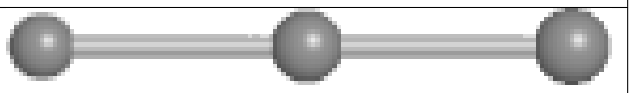


Rings

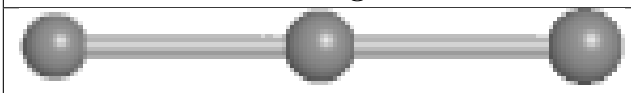
Ligand SCN A 634



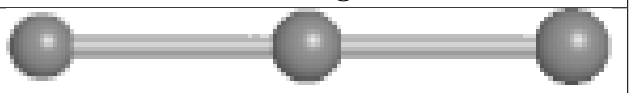
Bond lengths



Bond angles

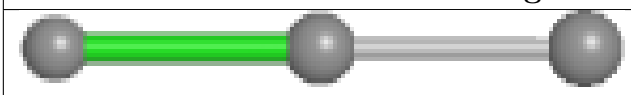


Torsions

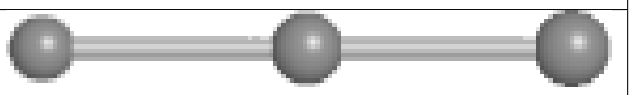


Rings

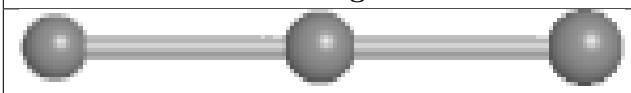
Ligand SCN A 636



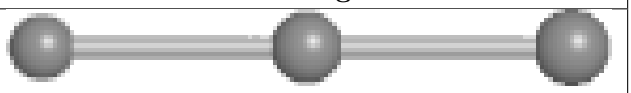
Bond lengths



Bond angles

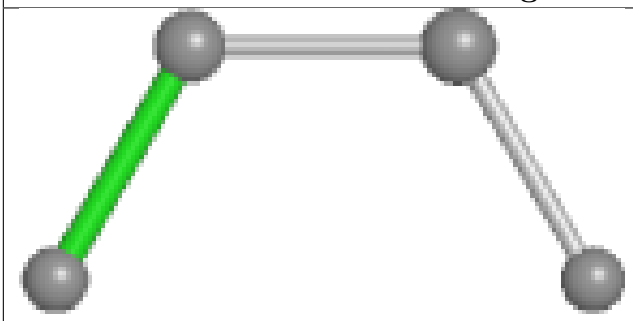


Torsions

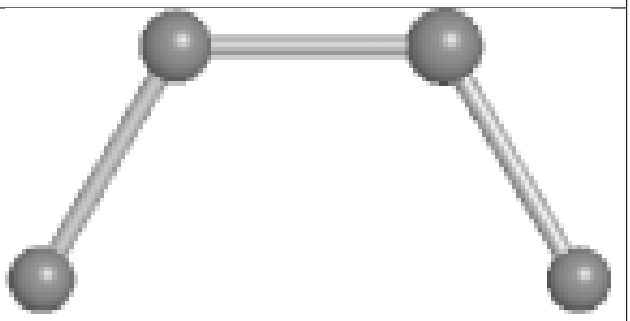


Rings

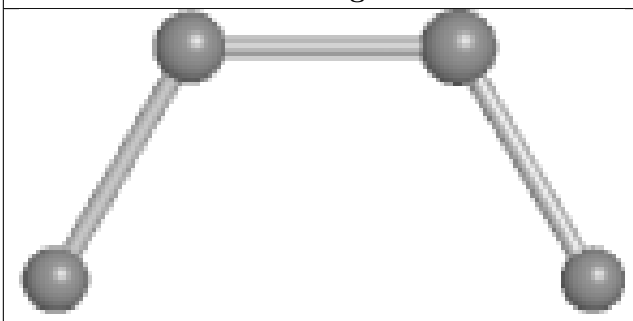
Ligand OSM A 646



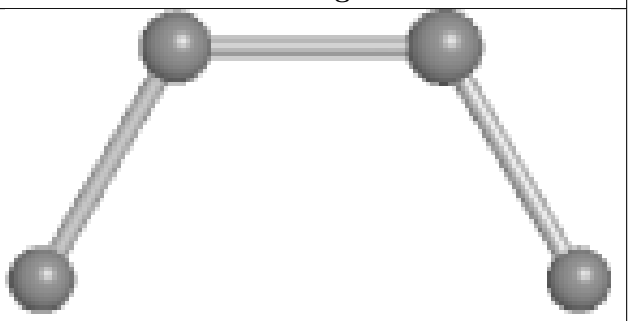
Bond lengths



Bond angles

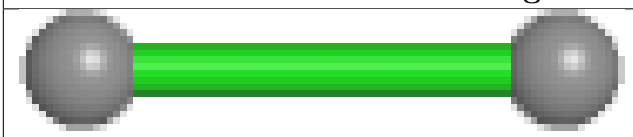


Torsions

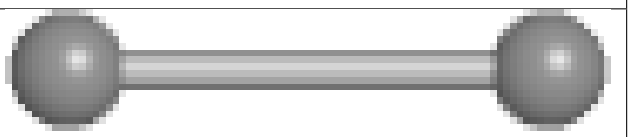


Rings

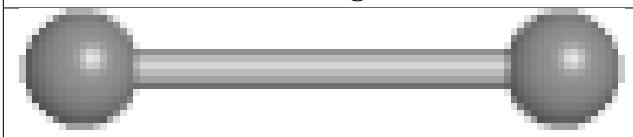
Ligand PEO A 649



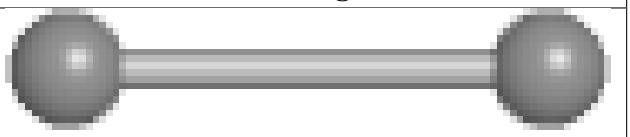
Bond lengths



Bond angles

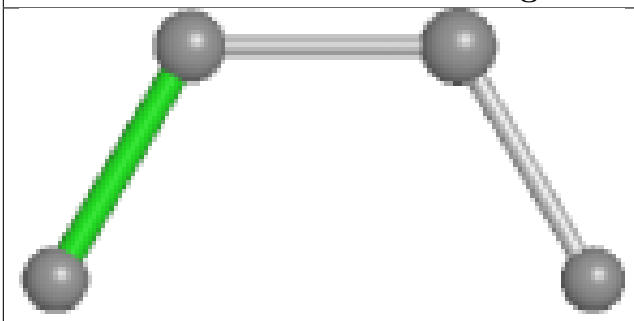


Torsions

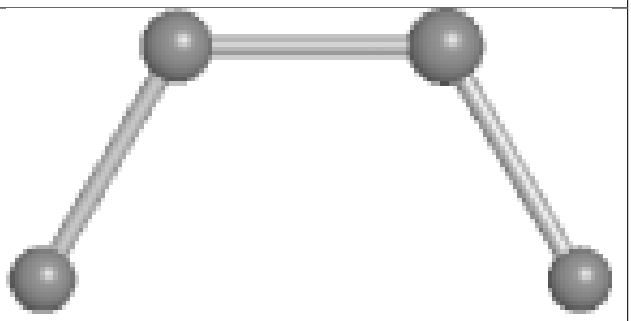


Rings

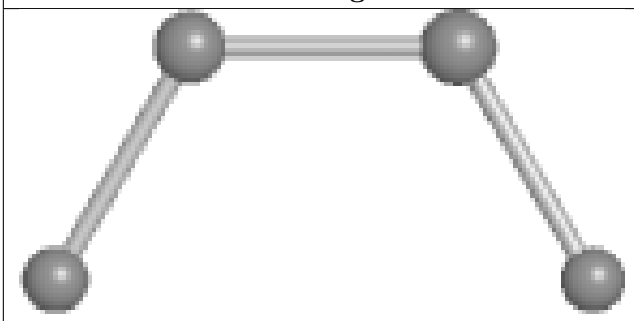
Ligand OSM A 667



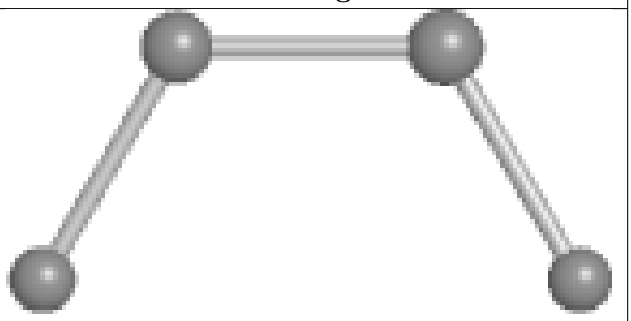
Bond lengths



Bond angles

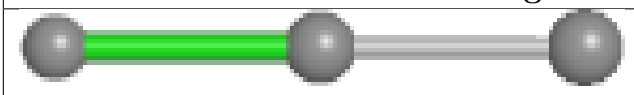


Torsions

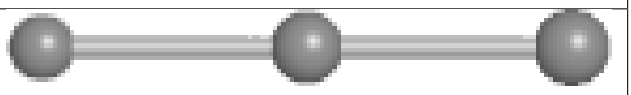


Rings

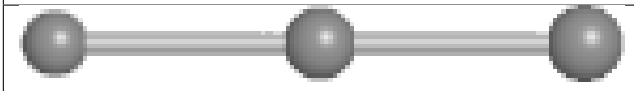
Ligand SCN A 637



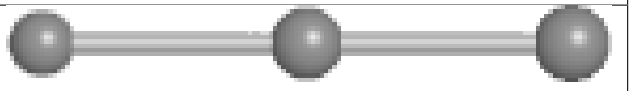
Bond lengths



Bond angles

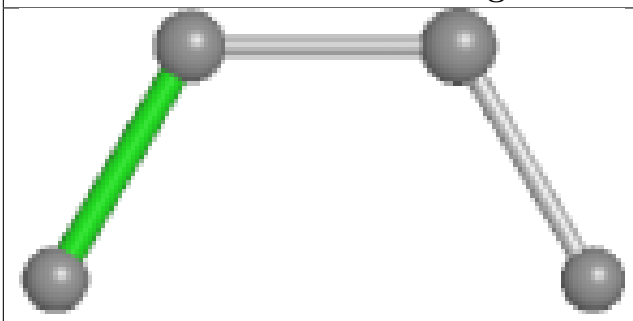


Torsions

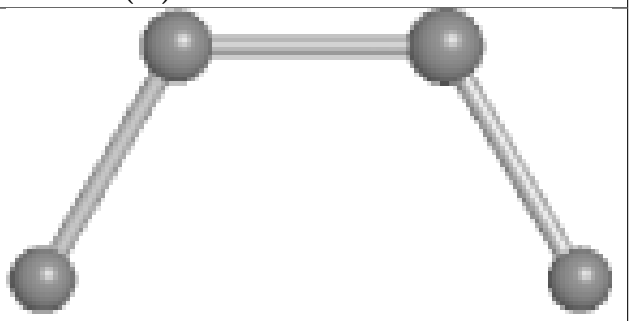


Rings

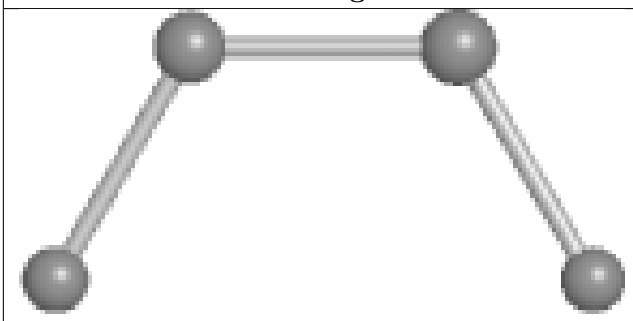
Ligand OSM A 644 (B)



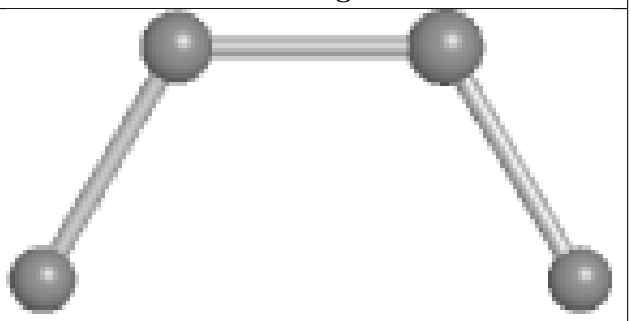
Bond lengths



Bond angles

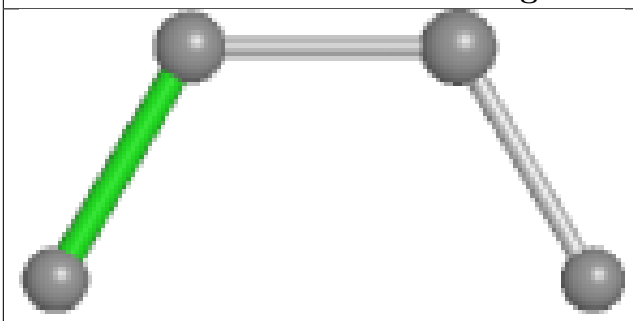


Torsions

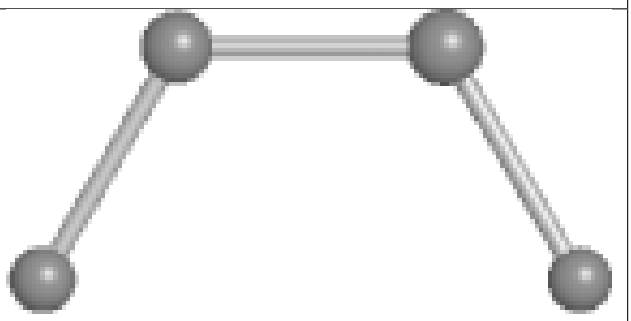


Rings

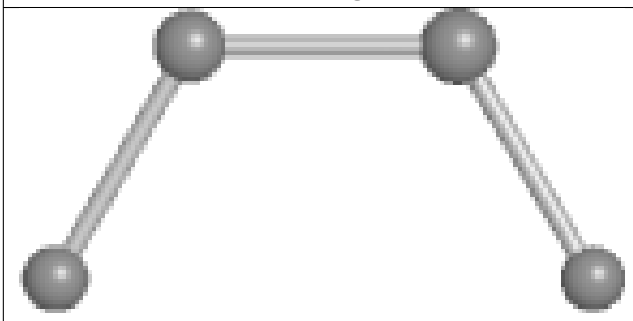
Ligand OSM A 647



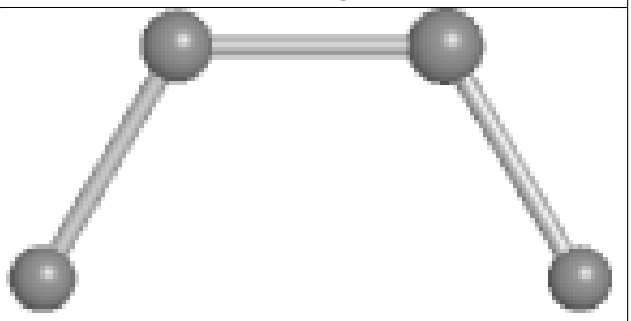
Bond lengths



Bond angles

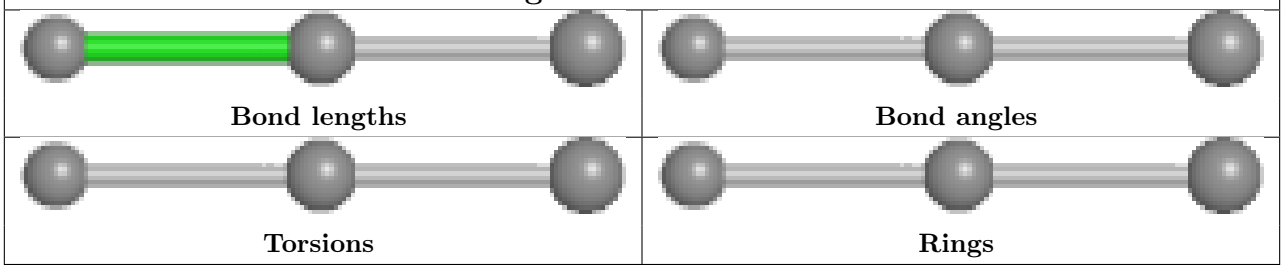


Torsions

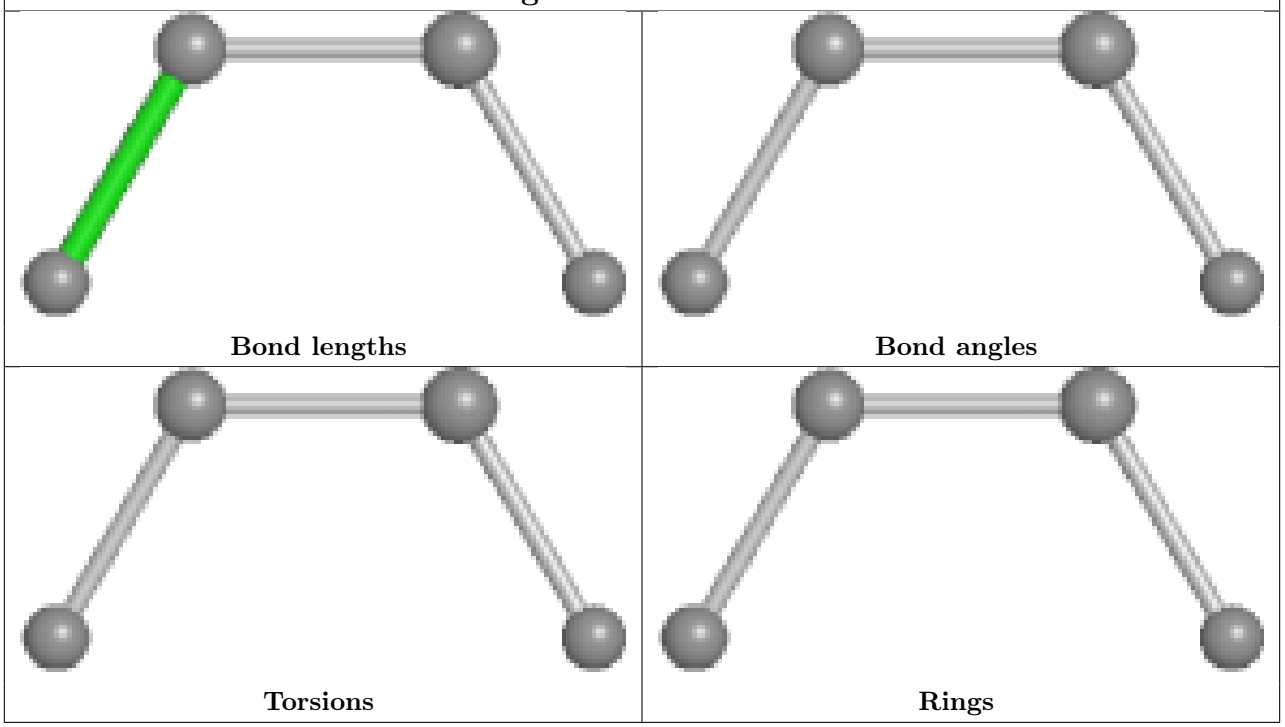


Rings

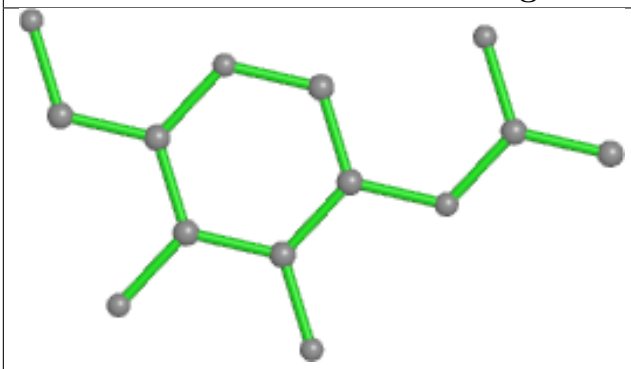
Ligand SCN A 633



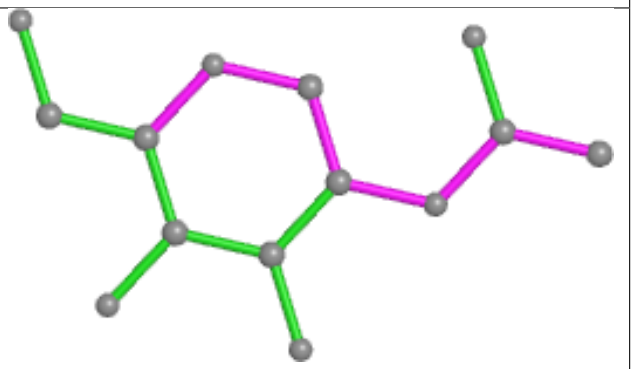
Ligand OSM A 641



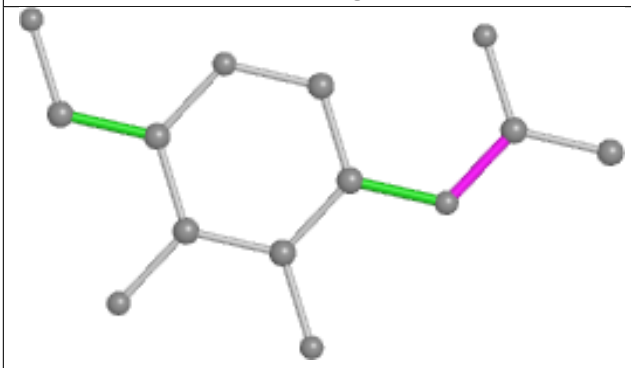
Ligand NAG A 603



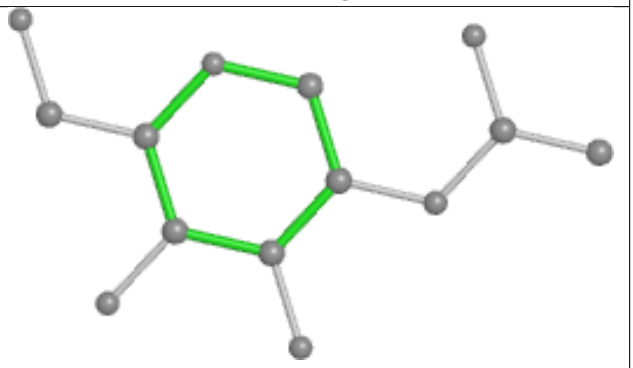
Bond lengths



Bond angles

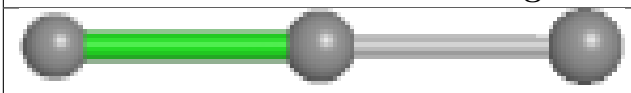


Torsions

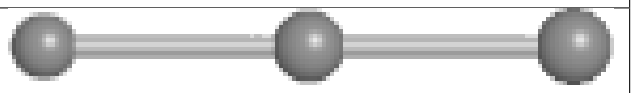


Rings

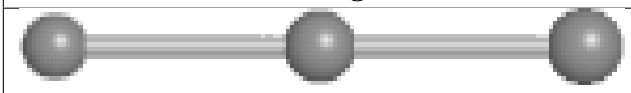
Ligand SCN A 630



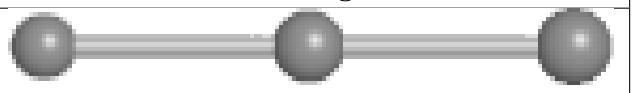
Bond lengths



Bond angles

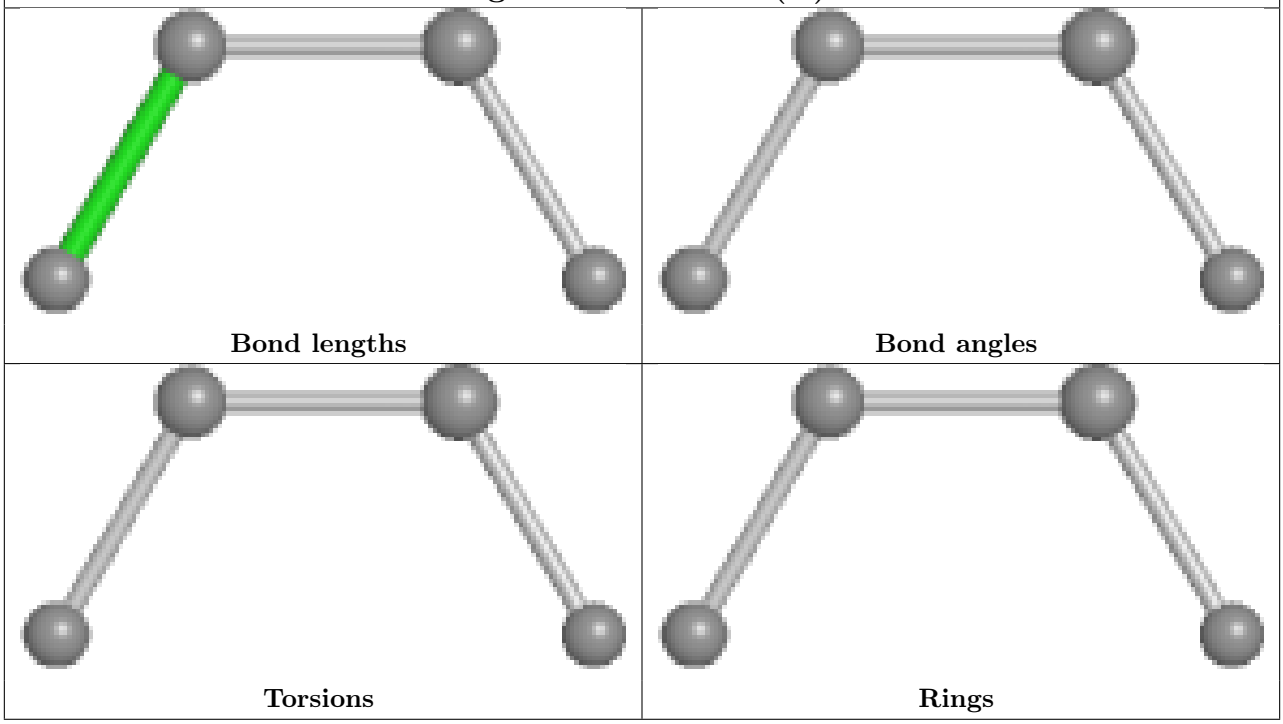


Torsions

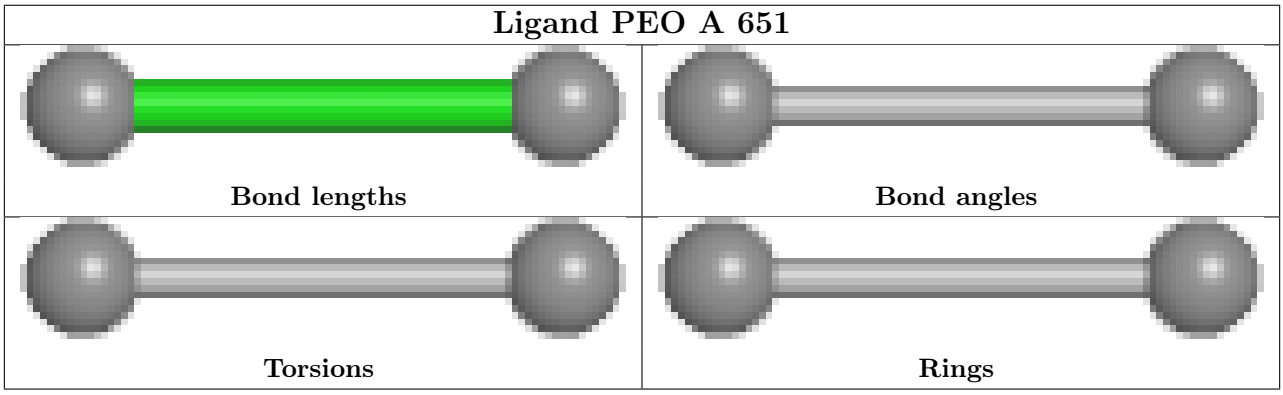


Rings

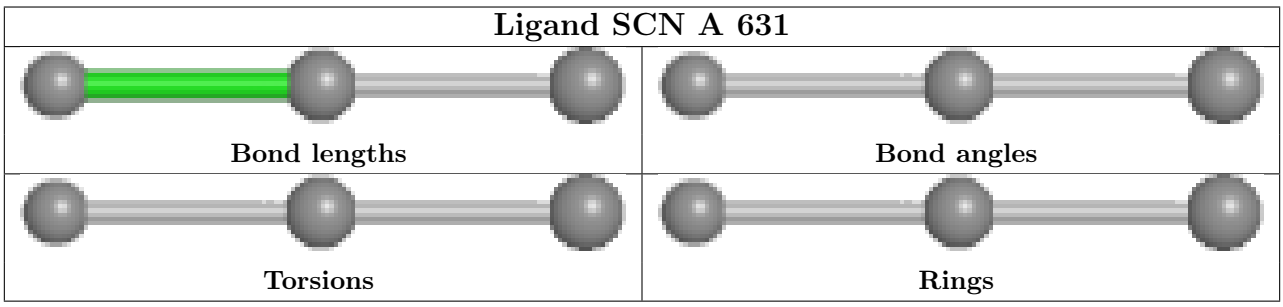
Ligand OSM A 642 (A)



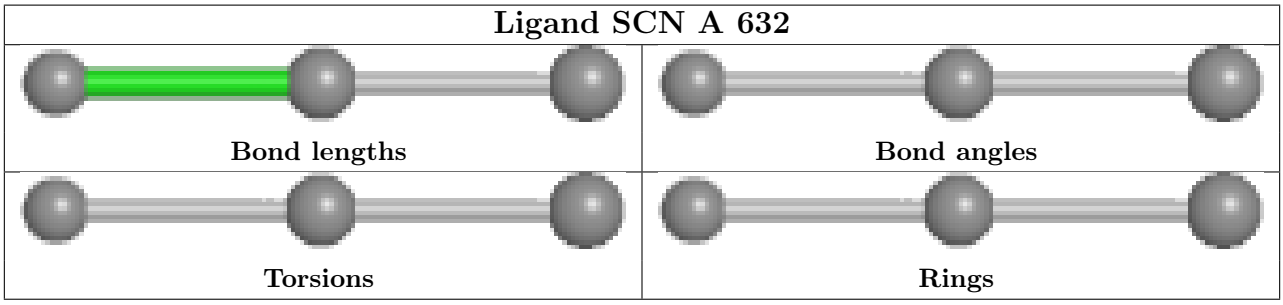
Ligand PEO A 651



Ligand SCN A 631



Ligand SCN A 632



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%)	-0.13	31 (5%) 27 34	7, 15, 58, 145	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	25.0
1	A	1	SER	17.4
1	A	7	GLY	17.0
1	A	121	SER	12.8
1	A	11	PRO	11.8
1	A	122	ASN	10.7
1	A	120	GLY	10.3
1	A	10	VAL	9.1
1	A	124	HIS	8.2
1	A	9	PRO	7.6
1	A	12	LEU	7.5
1	A	169	THR	6.8
1	A	172	TYR	6.6
1	A	174	SER	6.5
1	A	171	PRO	5.7
1	A	8	ALA	5.1
1	A	119	LEU	5.1
1	A	4	VAL	4.7
1	A	173	GLN	4.6
1	A	13	VAL	4.6
1	A	170	PRO	4.2
1	A	595	ASN	3.9
1	A	5	GLY	3.3
1	A	14	LYS	2.6
1	A	3	GLU	2.4
1	A	128	GLN	2.3
1	A	167	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	168	PRO	2.1
1	A	209	PRO	2.1
1	A	175	LEU	2.1
1	A	594	GLU	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)

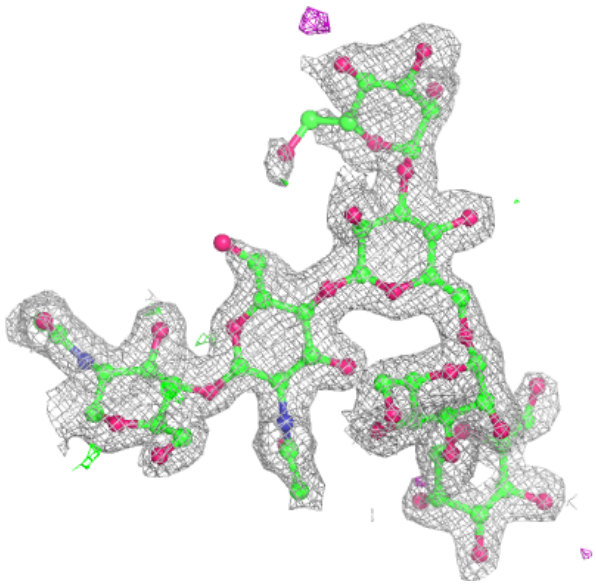
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

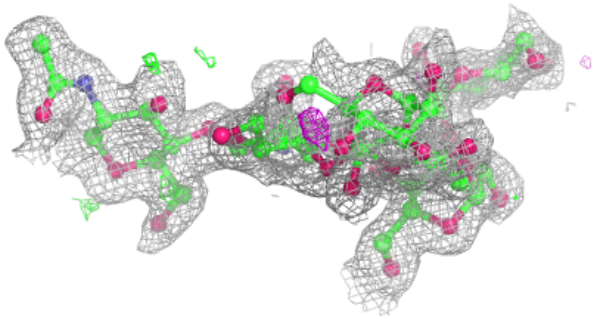
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	C	2	14/15	0.79	0.18	36,46,51,51	0
2	MAN	B	6	11/12	0.83	0.16	36,41,48,49	0
2	NAG	B	1	14/15	0.90	0.11	19,23,28,36	0
2	MAN	B	5	11/12	0.90	0.20	30,33,37,42	0
2	NAG	B	2	14/15	0.92	0.13	26,29,35,42	0
2	BMA	B	3	11/12	0.93	0.12	24,29,32,33	0
2	MAN	B	4	11/12	0.94	0.12	24,26,27,28	0
3	NAG	C	1	14/15	0.95	0.09	17,20,27,28	0

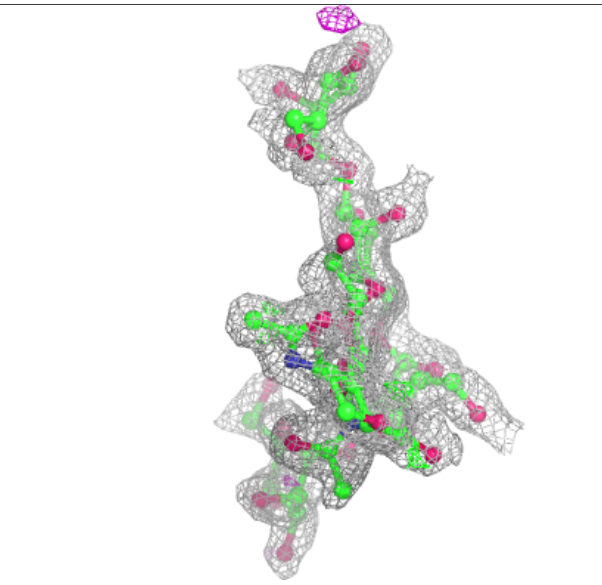
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

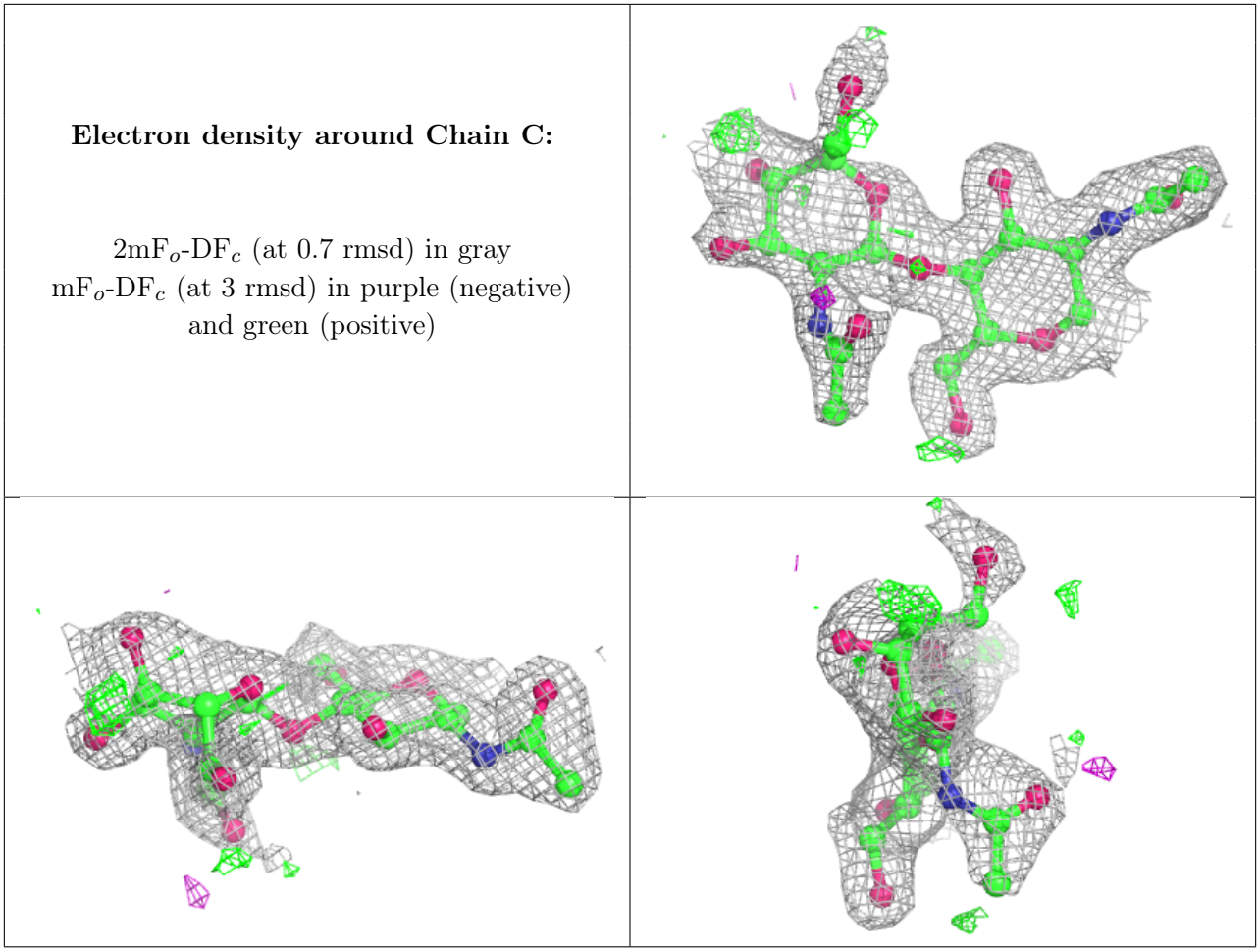






Electron density around Chain C:

$2mF_o$-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
8	OSM	A	647	4/4	0.73	0.20	37,37,41,44	0
8	OSM	A	646	4/4	0.86	0.14	36,37,39,40	0
8	OSM	A	643	4/4	0.90	0.14	25,26,26,30	0
9	PEO	A	650	2/2	0.90	0.12	23,23,23,23	0
5	NAG	A	602	14/15	0.91	0.15	32,37,43,44	0
6	IOD	A	664	1/1	0.91	0.07	47,47,47,47	1
5	NAG	A	603	14/15	0.92	0.10	31,35,38,43	0
9	PEO	A	651	2/2	0.92	0.08	32,32,32,36	0
6	IOD	A	661	1/1	0.94	0.08	55,55,55,55	1
8	OSM	A	645	4/4	0.94	0.16	21,24,25,33	0
9	PEO	A	652	2/2	0.94	0.12	26,26,26,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SCN	A	632	3/3	0.95	0.12	30,30,32,40	0
7	SCN	A	639	3/3	0.97	0.11	26,26,27,37	0
8	OSM	A	667	4/4	0.97	0.11	20,20,22,33	0
6	IOD	A	666	1/1	0.97	0.08	45,45,45,45	1
7	SCN	A	629	3/3	0.97	0.05	25,25,26,27	0
6	IOD	A	653	1/1	0.97	0.04	37,37,37,37	1
10	CA	A	655	1/1	0.97	0.07	38,38,38,38	0
8	OSM	A	642[B]	4/4	0.98	0.13	0,0,0,0	4
6	IOD	A	624	1/1	0.98	0.03	24,24,24,24	1
6	IOD	A	627	1/1	0.98	0.10	55,55,55,55	1
4	HEM	A	601	43/43	0.98	0.07	8,9,10,11	0
7	SCN	A	630	3/3	0.98	0.10	25,25,30,33	0
7	SCN	A	631	3/3	0.98	0.10	23,23,26,29	0
9	PEO	A	649	2/2	0.98	0.14	18,18,18,20	0
6	IOD	A	616	1/1	0.98	0.04	30,30,30,30	1
6	IOD	A	662	1/1	0.98	0.08	39,39,39,39	1
8	OSM	A	641	4/4	0.98	0.10	15,18,19,26	0
8	OSM	A	642[A]	4/4	0.98	0.13	9,11,12,13	4
10	CA	A	658	1/1	0.98	0.09	34,34,34,34	0
6	IOD	A	659	1/1	0.99	0.04	35,35,35,35	1
6	IOD	A	660	1/1	0.99	0.06	42,42,42,42	1
6	IOD	A	619	1/1	0.99	0.04	21,21,21,21	1
6	IOD	A	614	1/1	0.99	0.03	24,24,24,24	1
9	PEO	A	648	2/2	0.99	0.17	22,22,22,24	0
6	IOD	A	626	1/1	0.99	0.03	28,28,28,28	1
6	IOD	A	665	1/1	0.99	0.09	43,43,43,43	1
6	IOD	A	615	1/1	0.99	0.04	25,25,25,25	1
6	IOD	A	613	1/1	0.99	0.04	32,32,32,32	1
10	CA	A	654	1/1	0.99	0.06	24,24,24,24	0
8	OSM	A	644[A]	4/4	0.99	0.10	10,11,11,11	4
10	CA	A	657	1/1	0.99	0.08	31,31,31,31	0
8	OSM	A	644[B]	4/4	0.99	0.10	12,12,12,12	4
6	IOD	A	625	1/1	1.00	0.03	19,19,19,19	1
6	IOD	A	618	1/1	1.00	0.04	14,14,14,14	1
6	IOD	A	612	1/1	1.00	0.03	11,11,11,11	0
6	IOD	A	628	1/1	1.00	0.02	17,17,17,17	1
6	IOD	A	620	1/1	1.00	0.04	12,12,12,12	1
6	IOD	A	621	1/1	1.00	0.02	20,20,20,20	1
6	IOD	A	622	1/1	1.00	0.01	21,21,21,21	1
7	SCN	A	633	3/3	1.00	0.05	5,5,5,5	3
7	SCN	A	634	3/3	1.00	0.07	6,6,6,6	3
7	SCN	A	635	3/3	1.00	0.06	2,2,2,2	3

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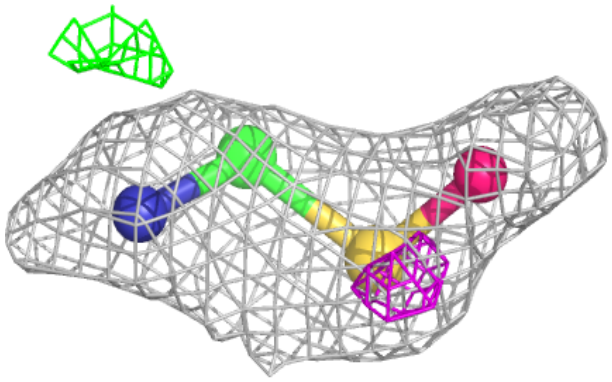
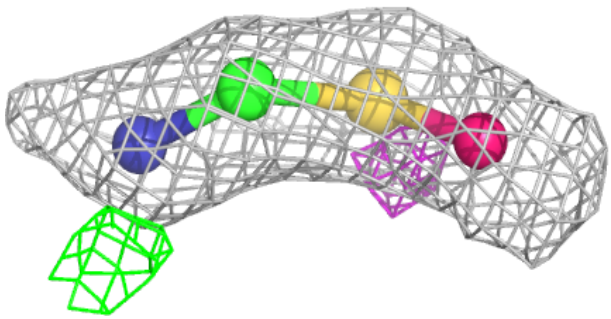
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SCN	A	636	3/3	1.00	0.08	25,25,26,26	3
7	SCN	A	637	3/3	1.00	0.05	5,5,5,5	3
7	SCN	A	638	3/3	1.00	0.09	12,12,12,13	3
6	IOD	A	623	1/1	1.00	0.03	12,12,12,12	1
7	SCN	A	640	3/3	1.00	0.04	12,12,12,12	3
10	CA	A	656	1/1	1.00	0.04	10,10,10,10	0
6	IOD	A	617	1/1	1.00	0.03	12,12,12,12	1
6	IOD	A	663	1/1	1.00	0.06	12,12,12,12	1

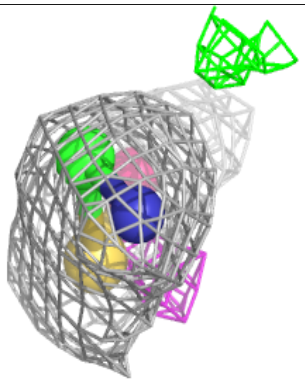
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OSM A 647:

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

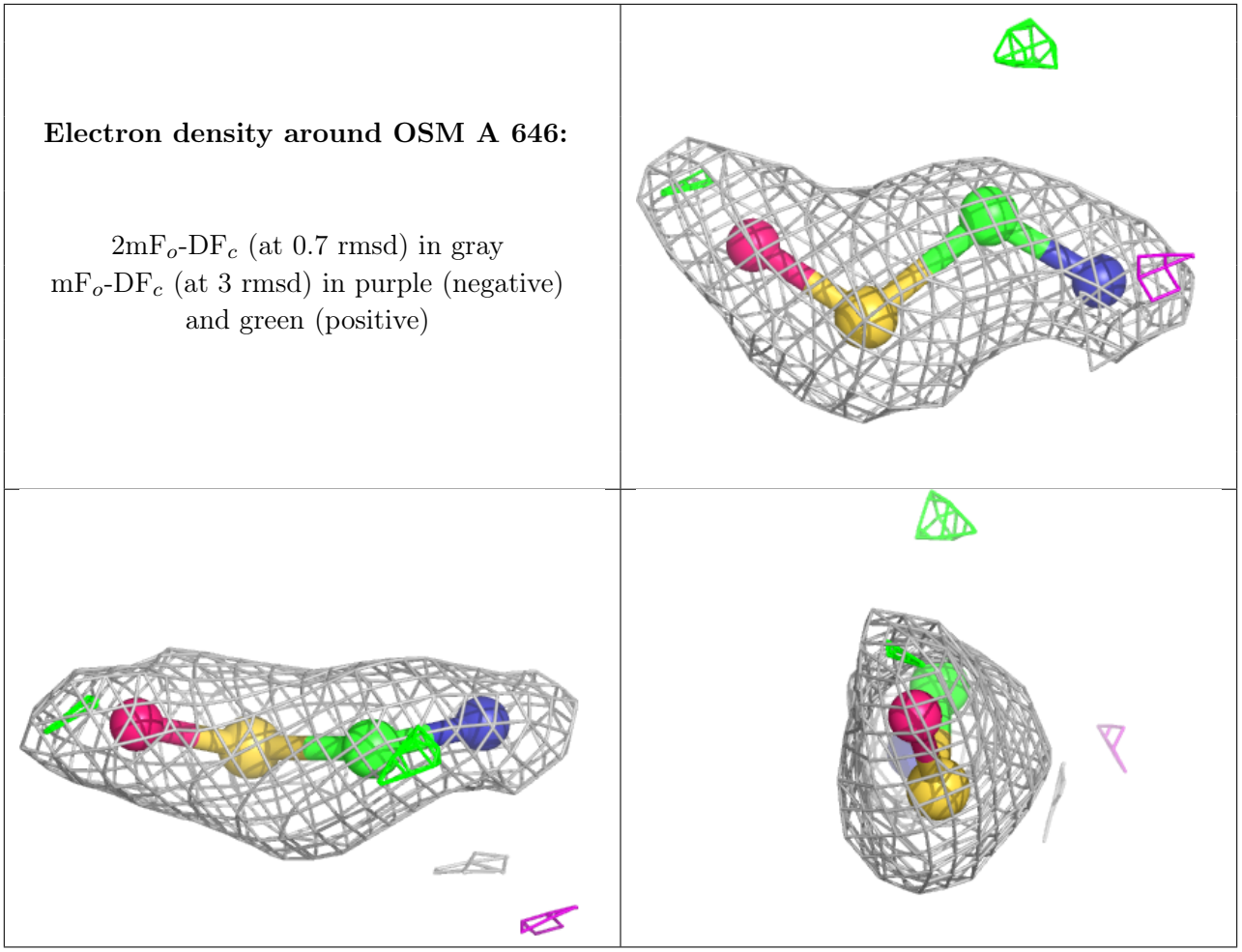






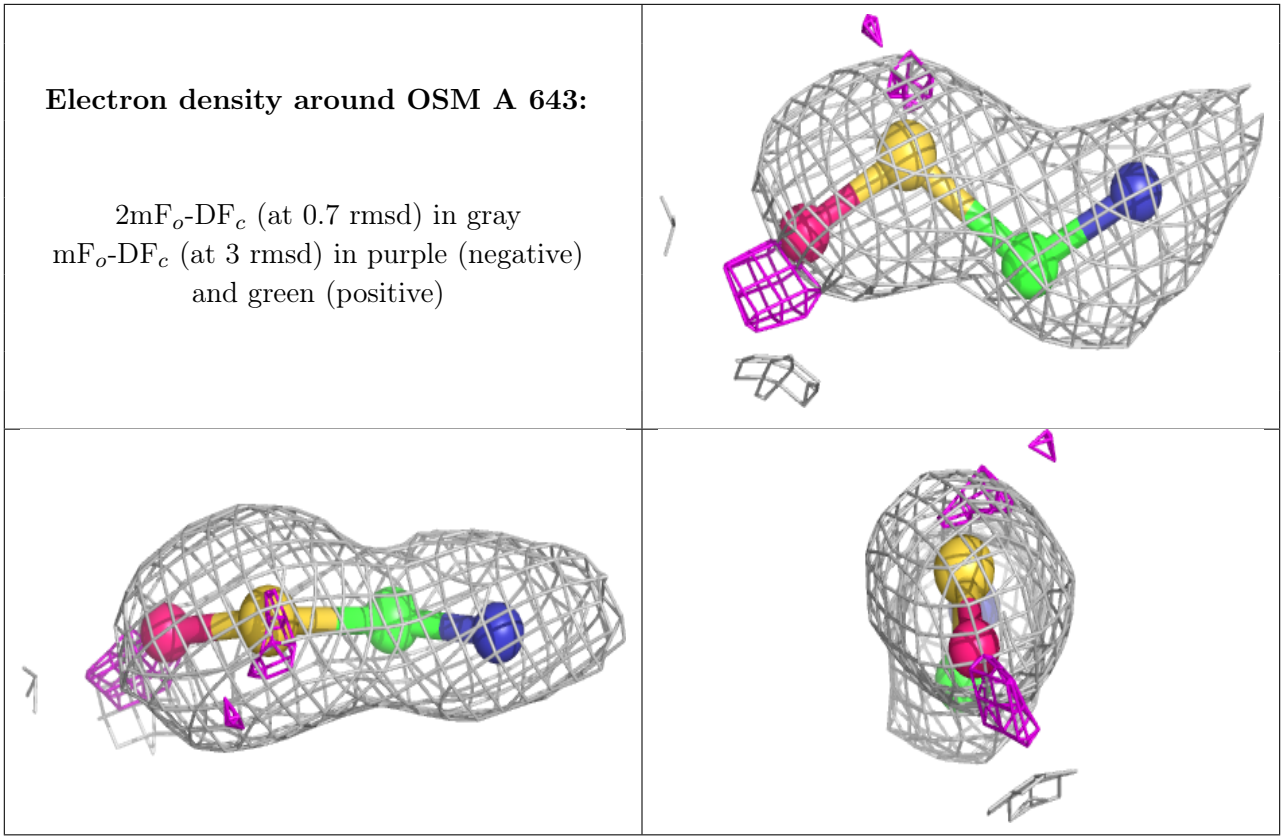
Electron density around OSM A 646:

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



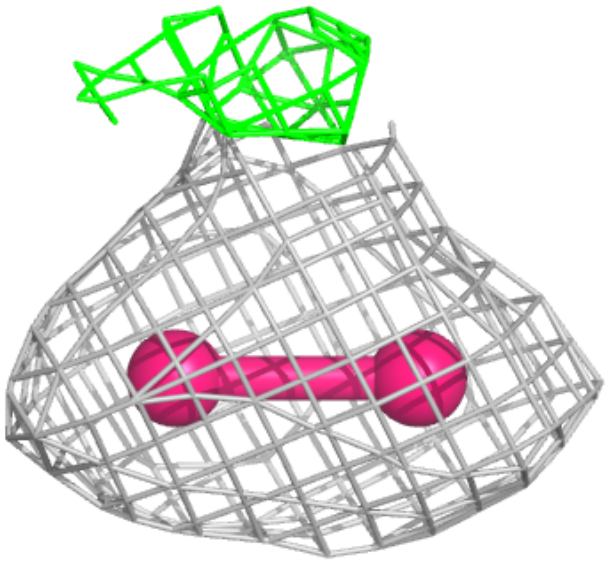
Electron density around OSM A 643:

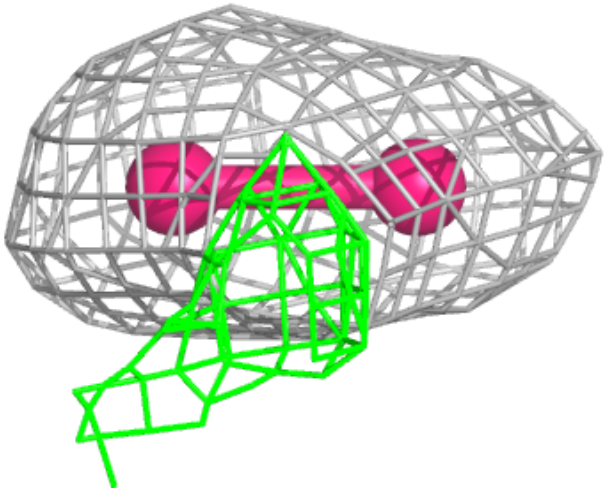
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

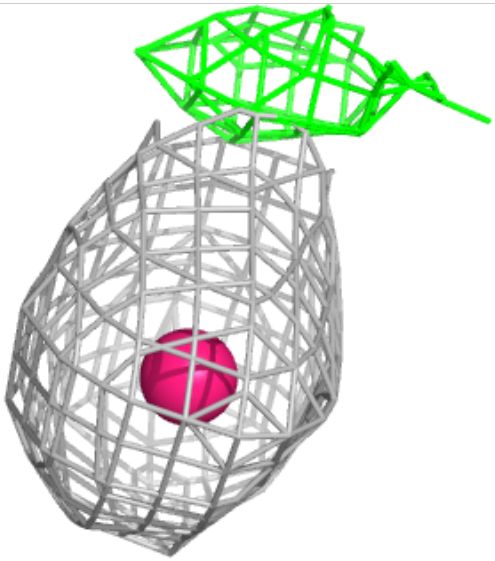


Electron density around PEO A 650:

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

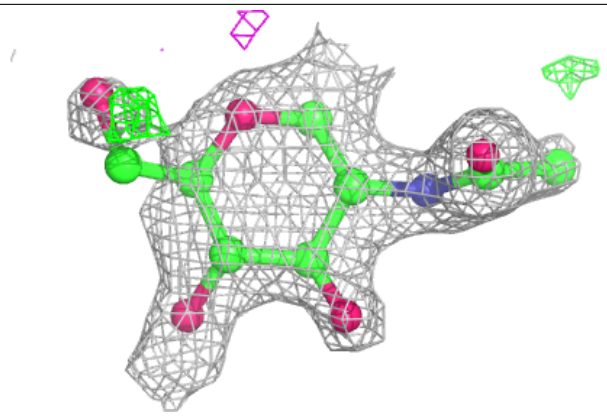


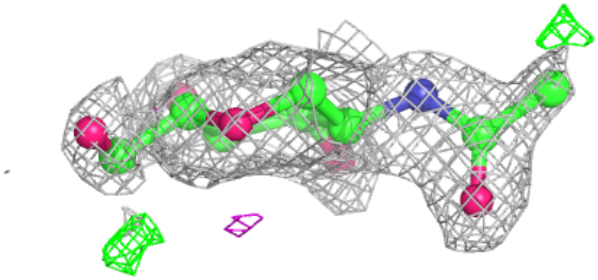


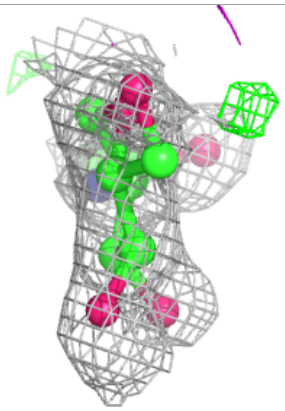


Electron density around NAG A 602:

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

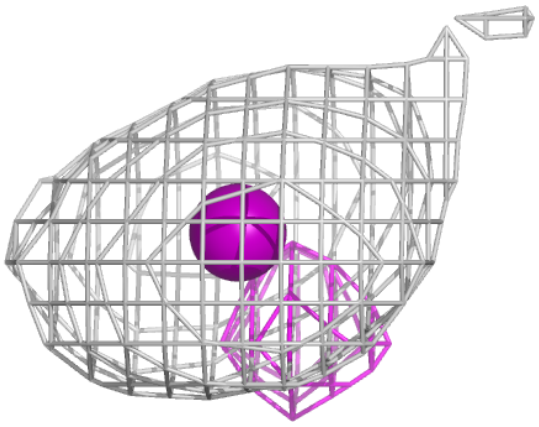


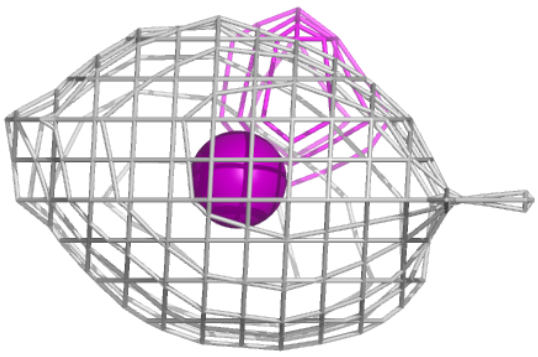


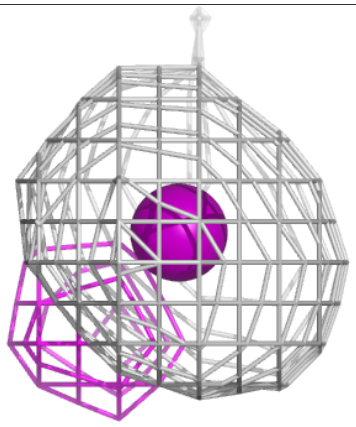


Electron density around IOD A 664:

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

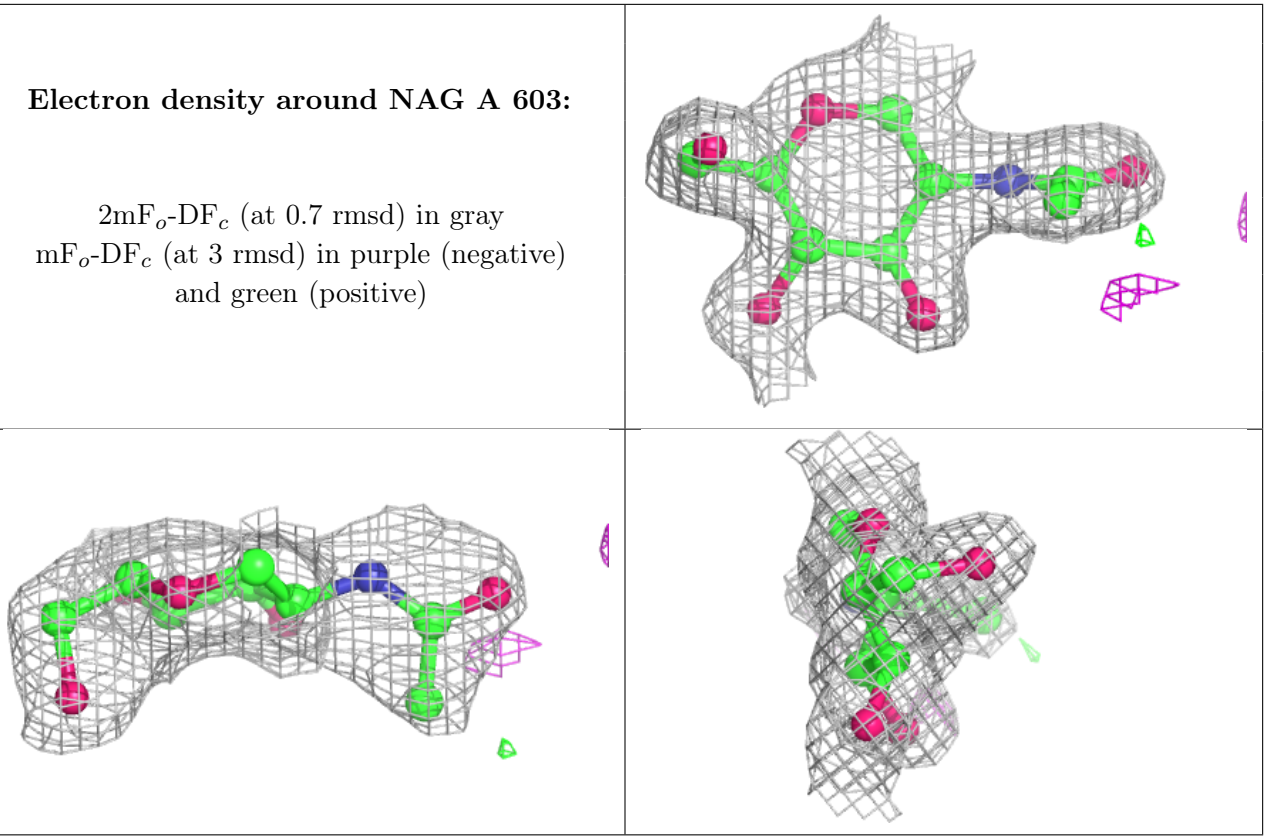






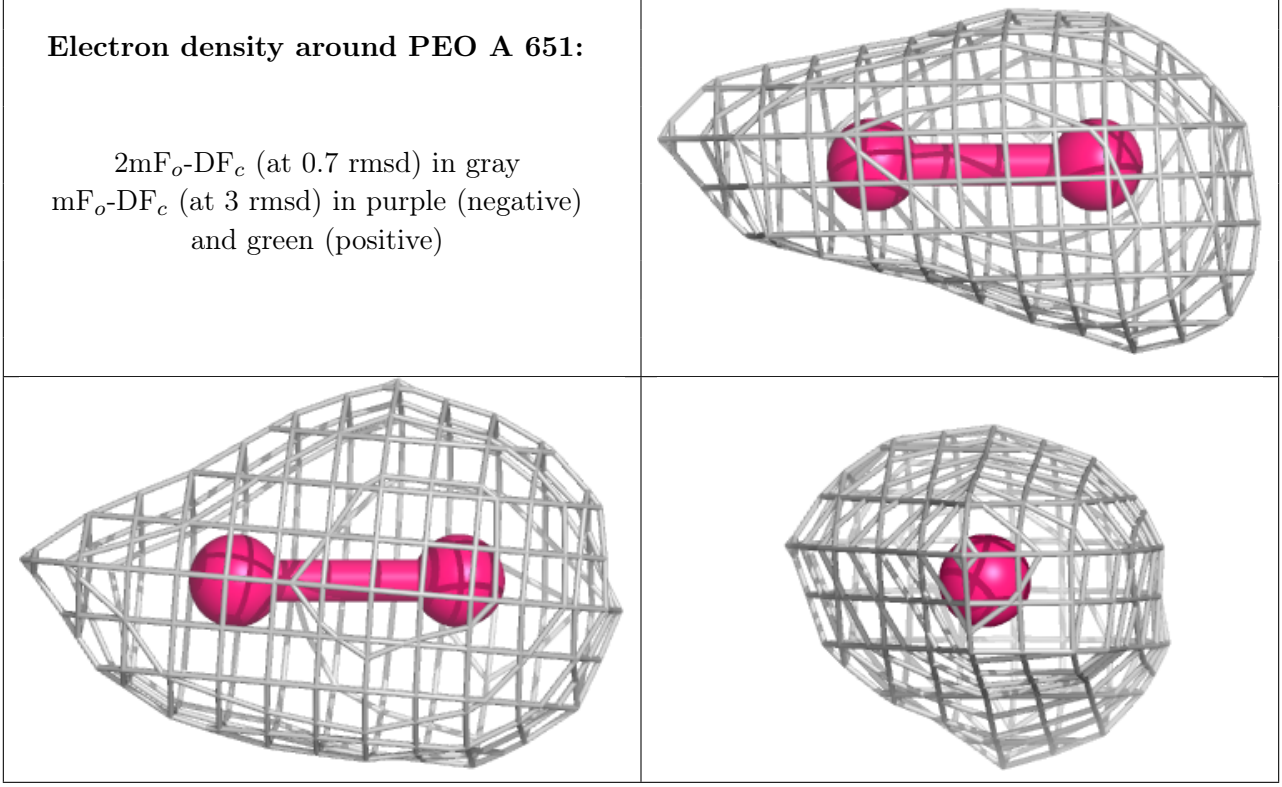
Electron density around NAG A 603:

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



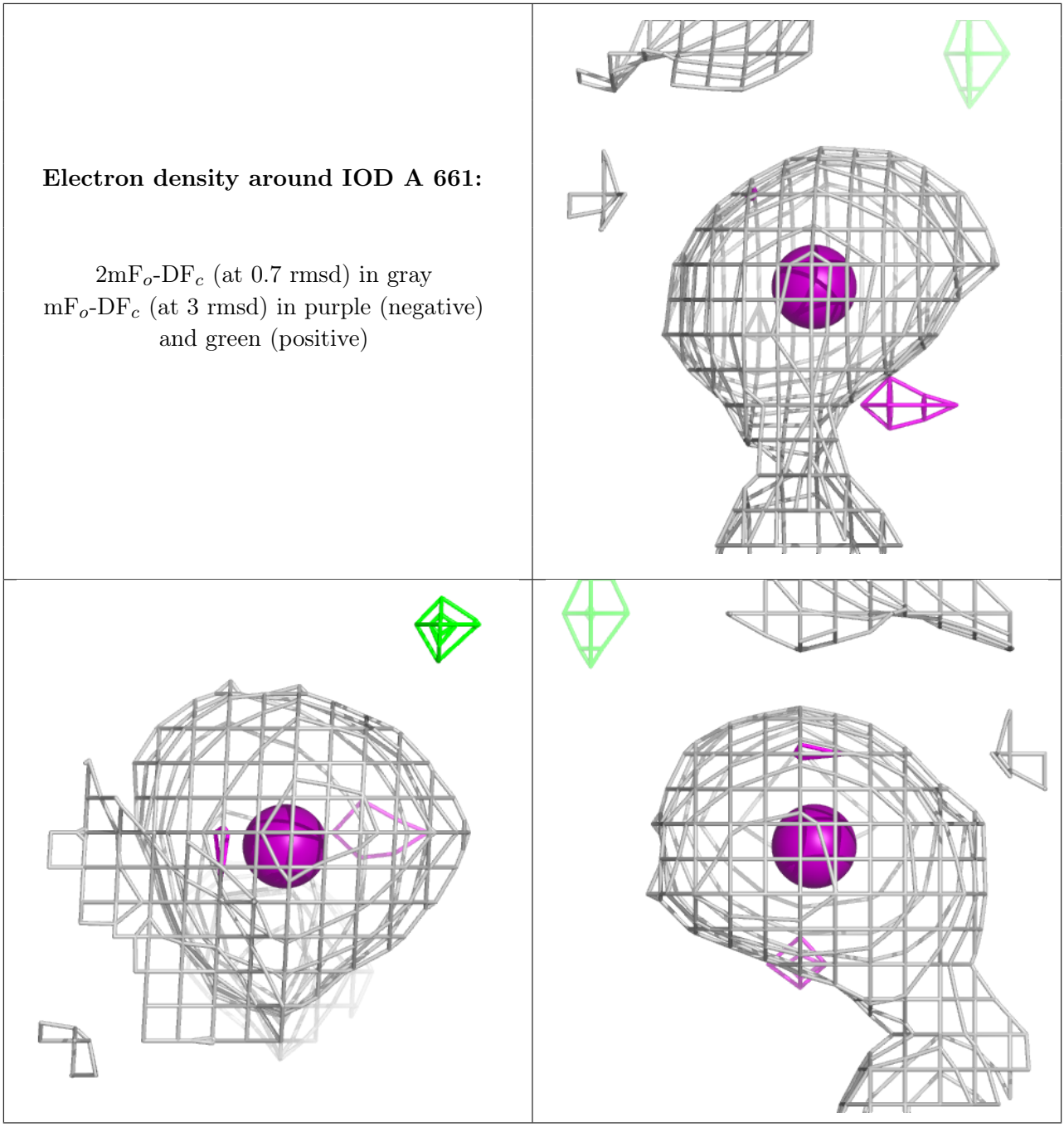
Electron density around PEO A 651:

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



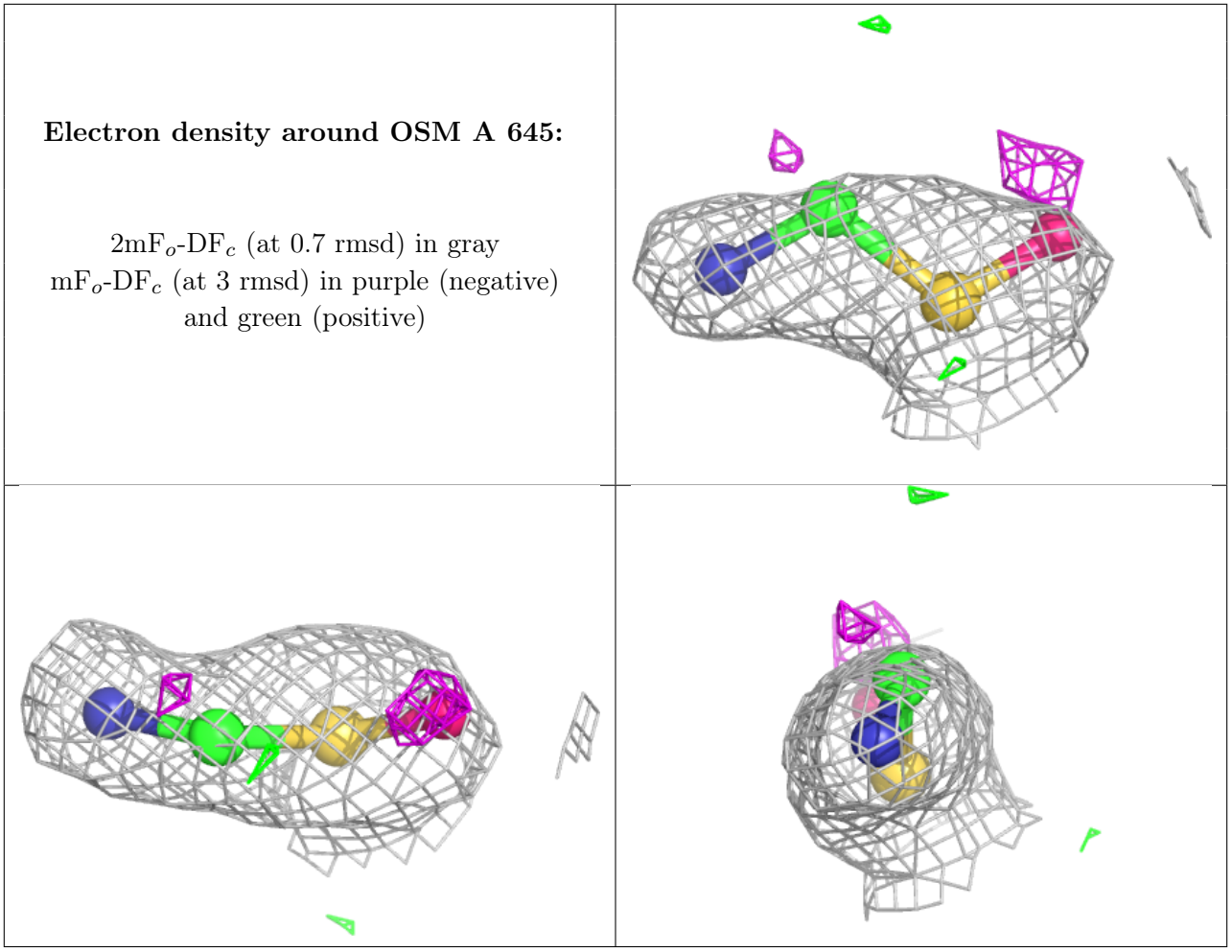
Electron density around IOD A 661:

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



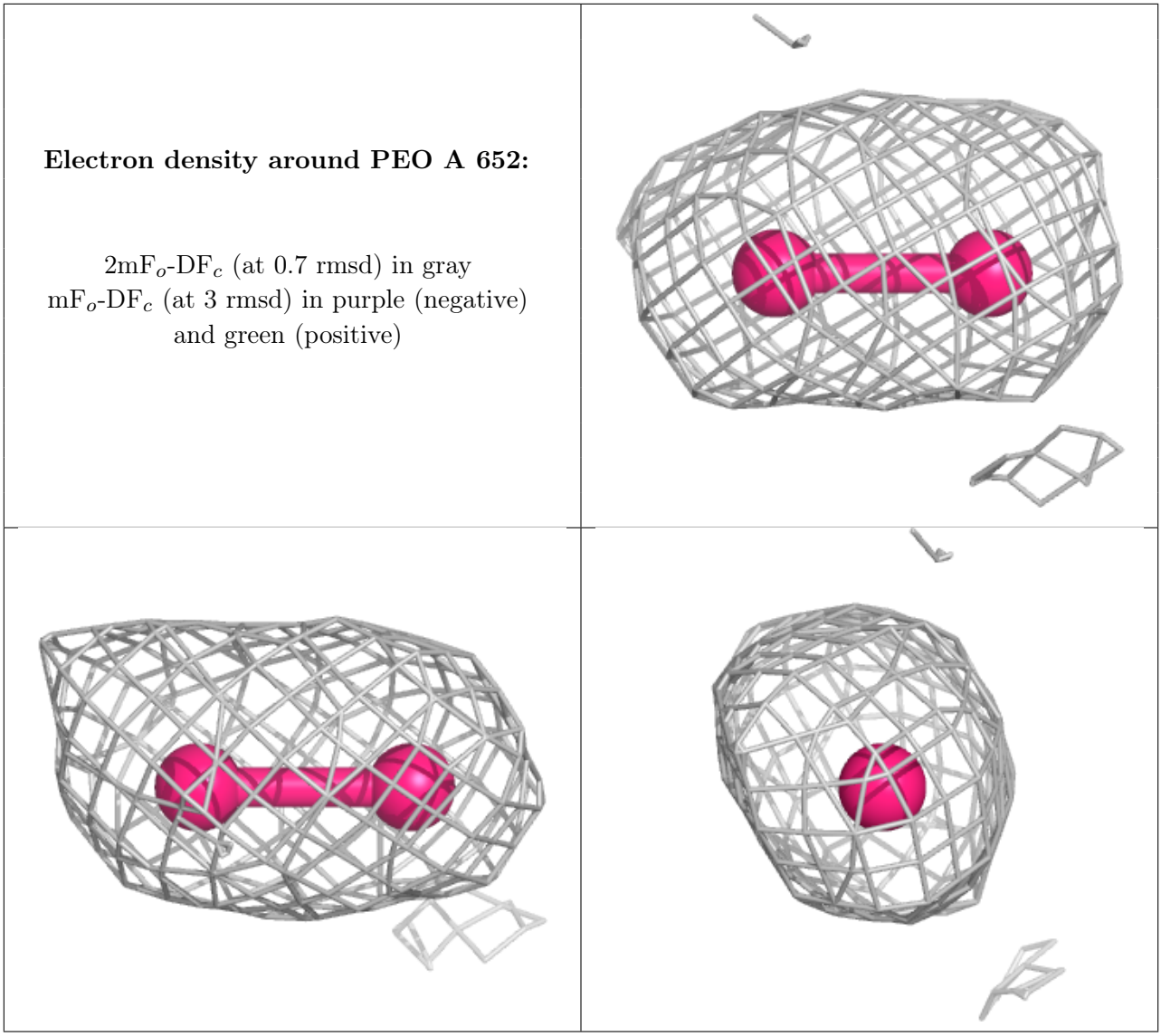
Electron density around OSM A 645:

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



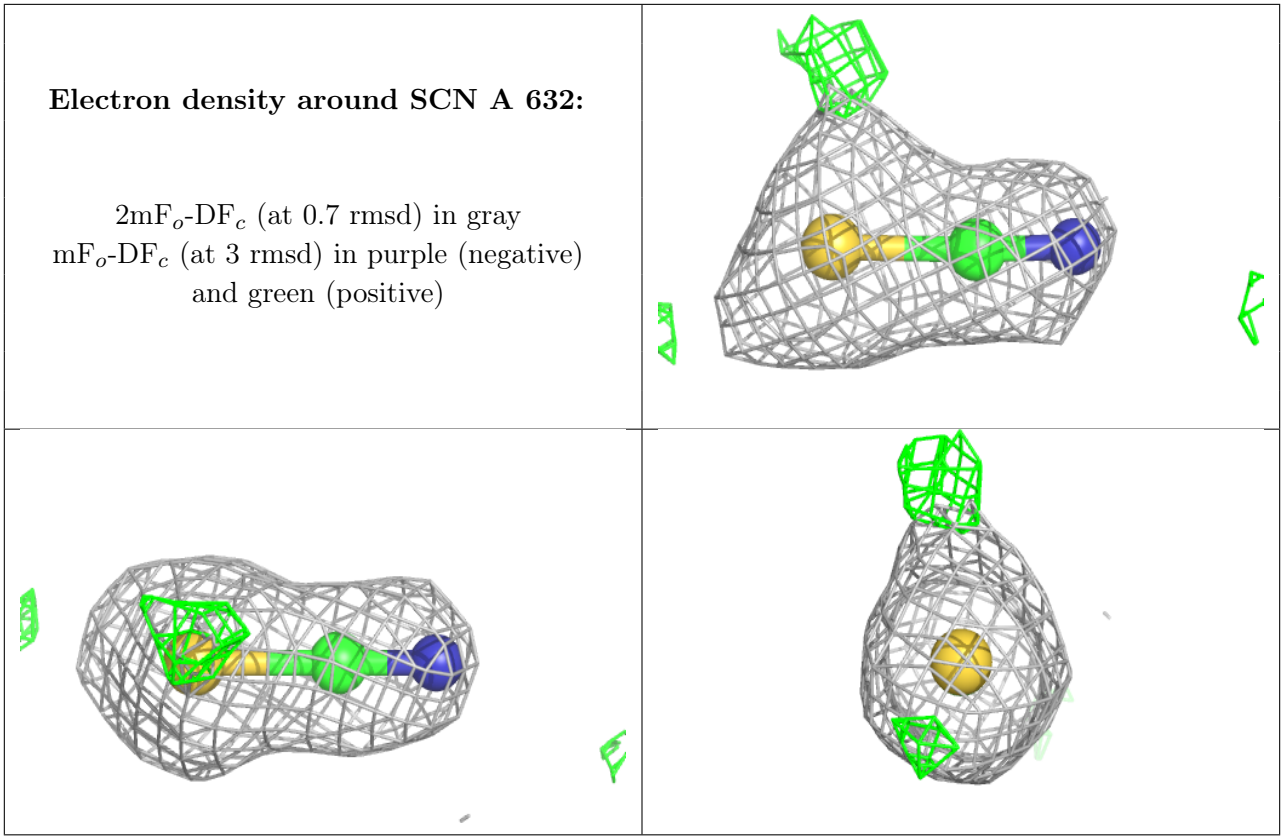
Electron density around PEO A 652:

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



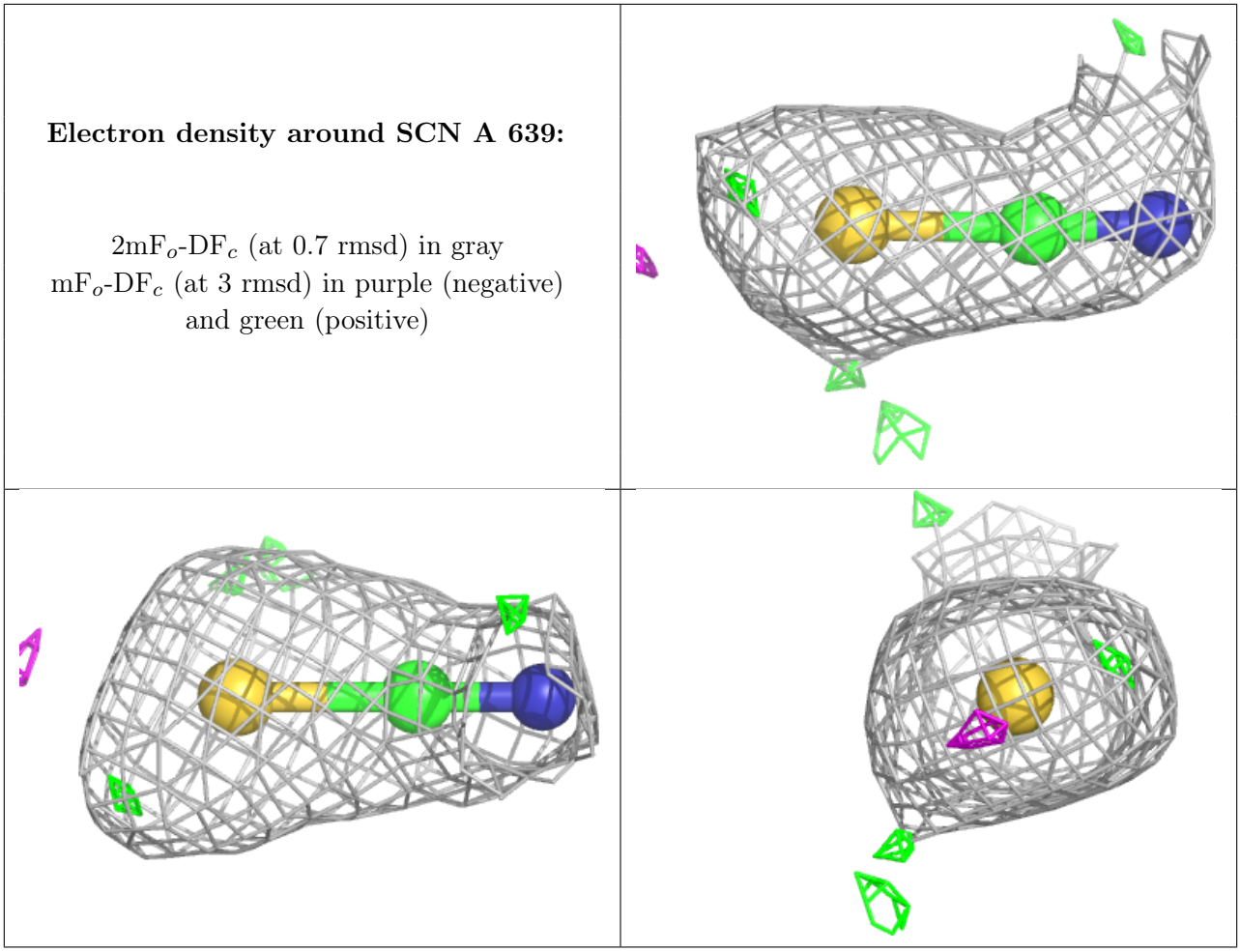
Electron density around SCN A 632:

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



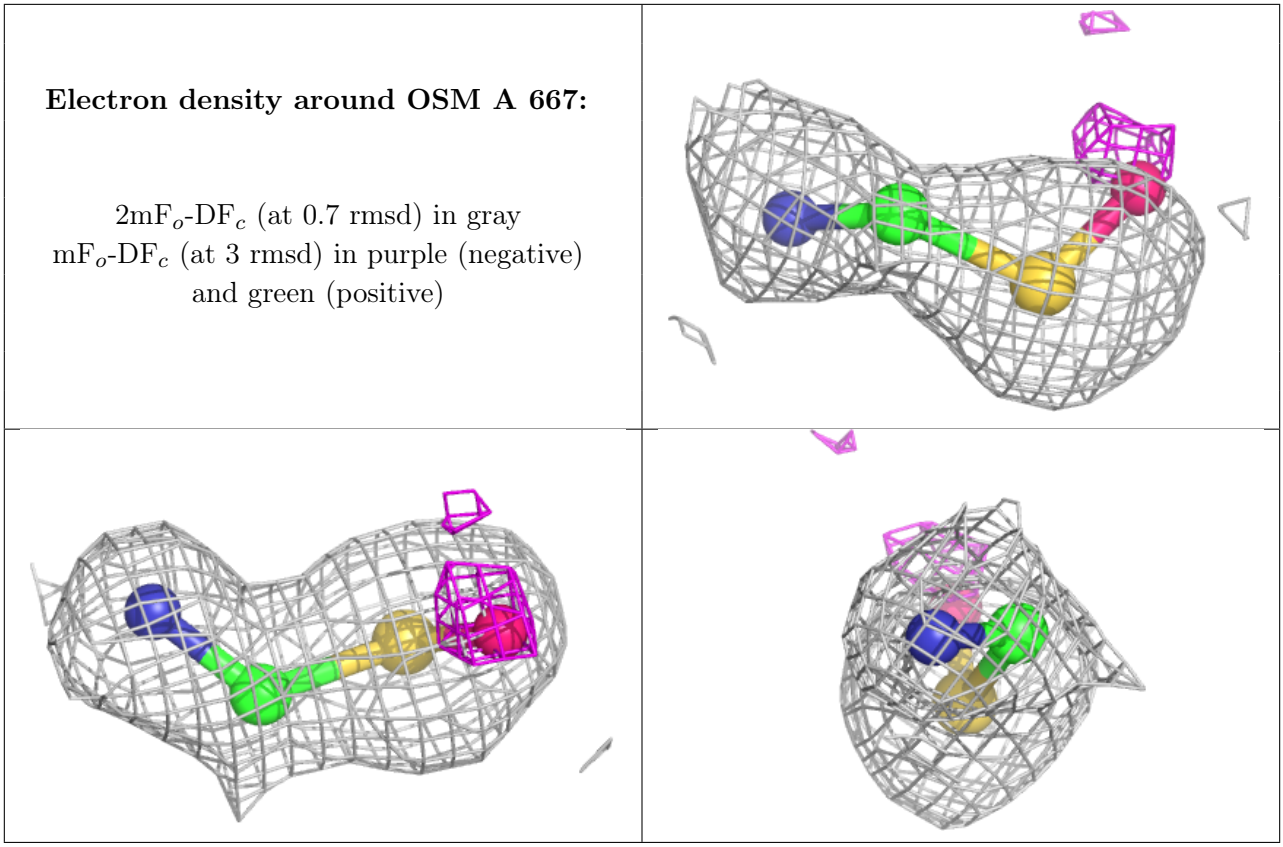
Electron density around SCN A 639:

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



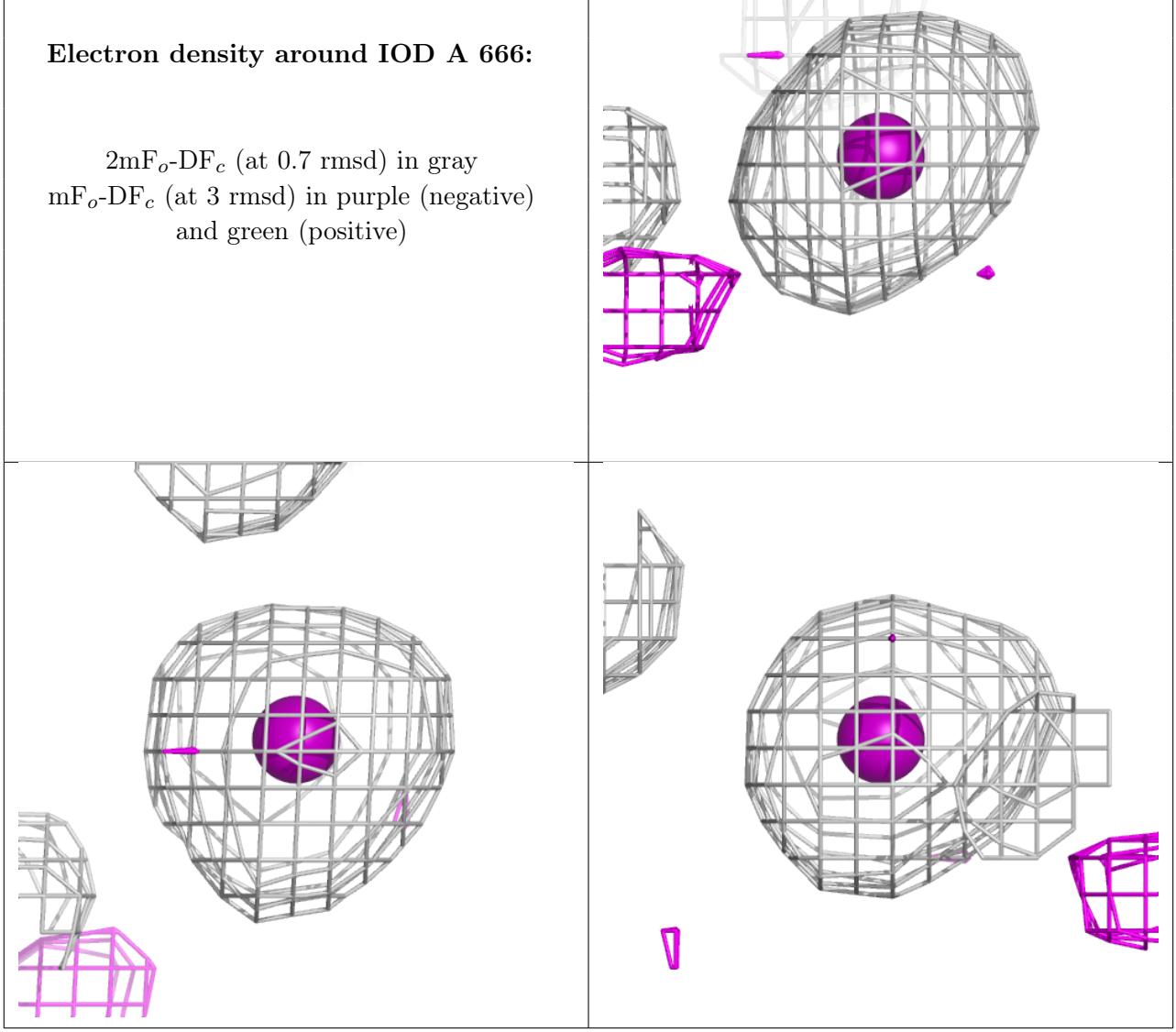
Electron density around OSM A 667:

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



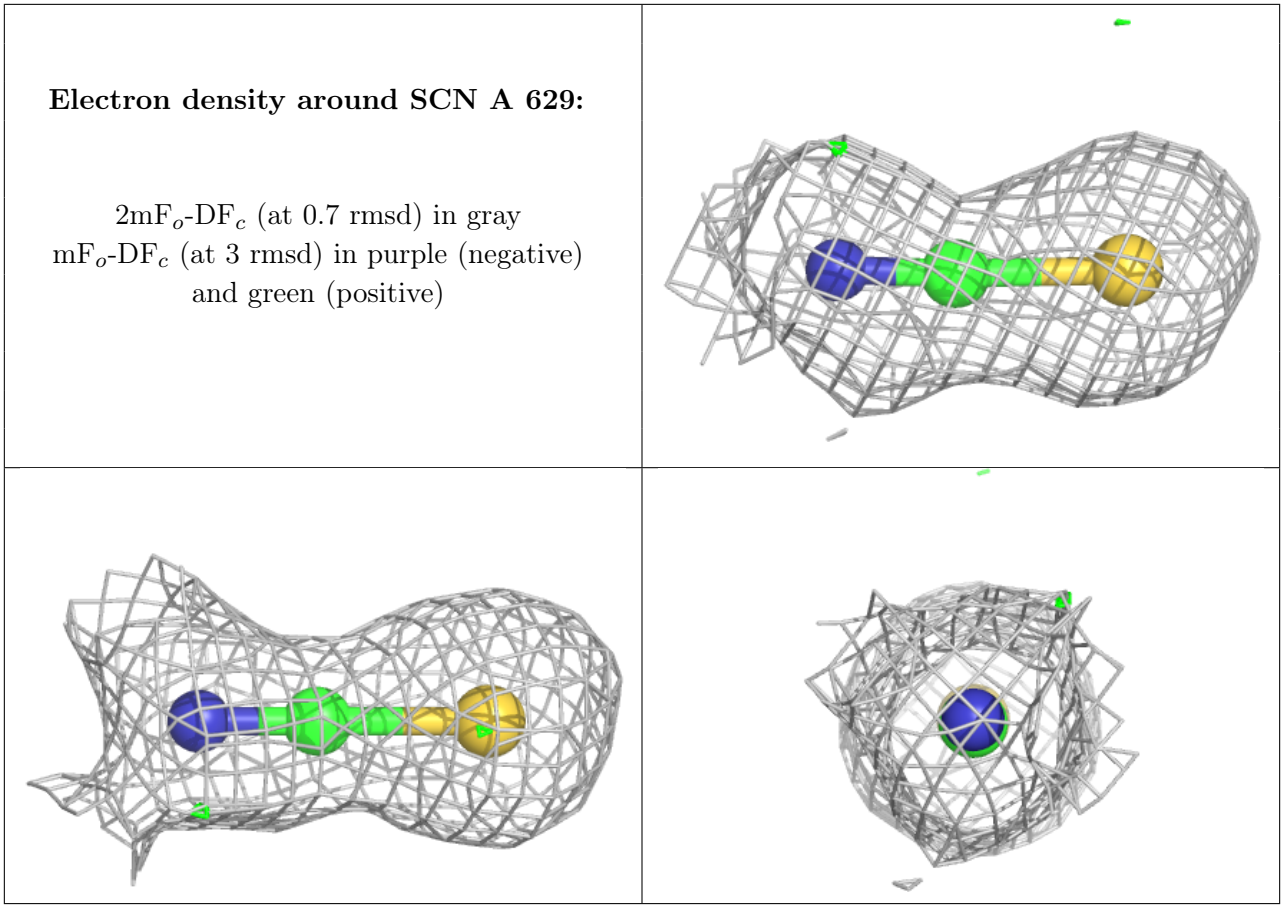
Electron density around IOD A 666:

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



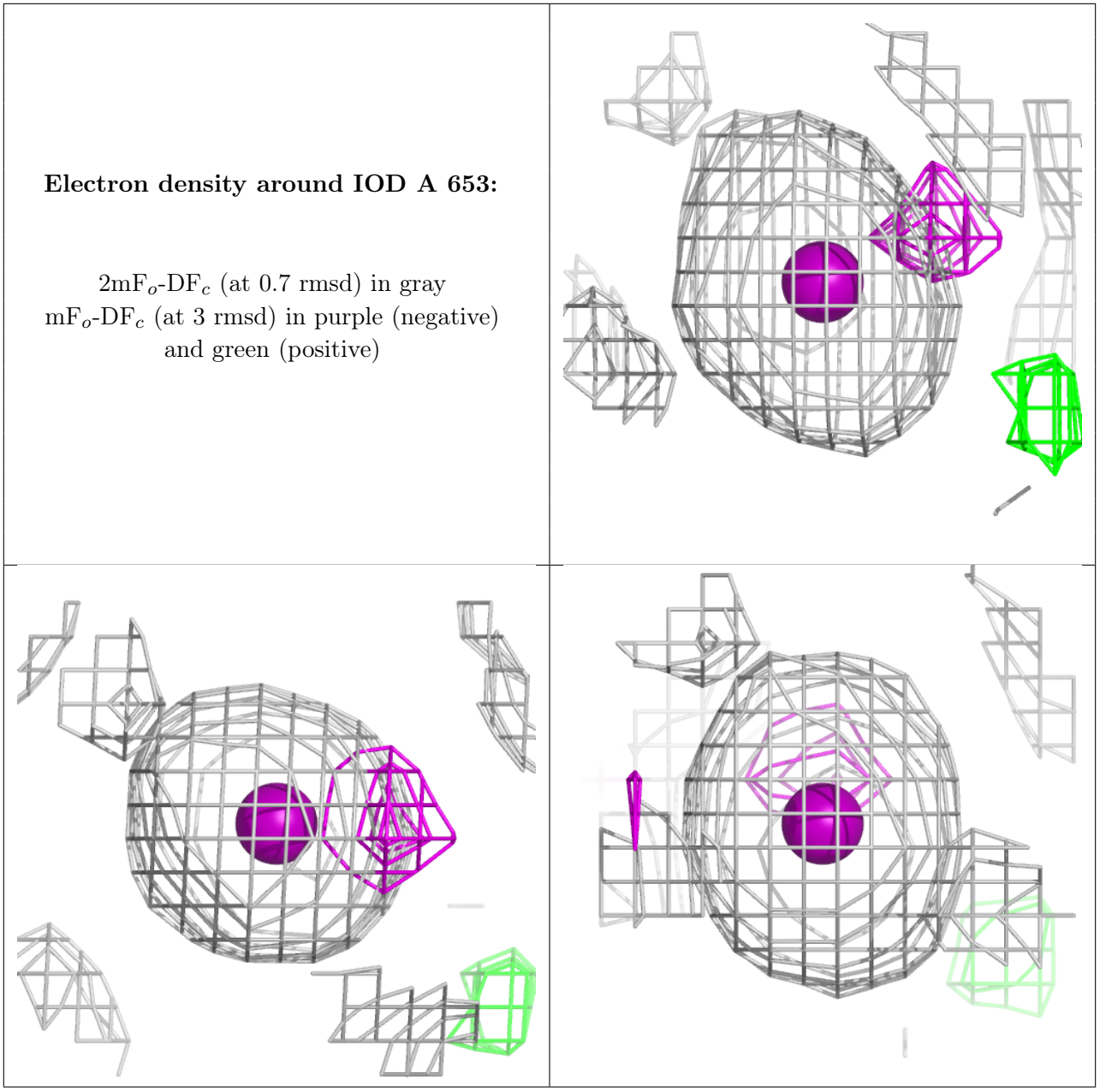
Electron density around SCN A 629:

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



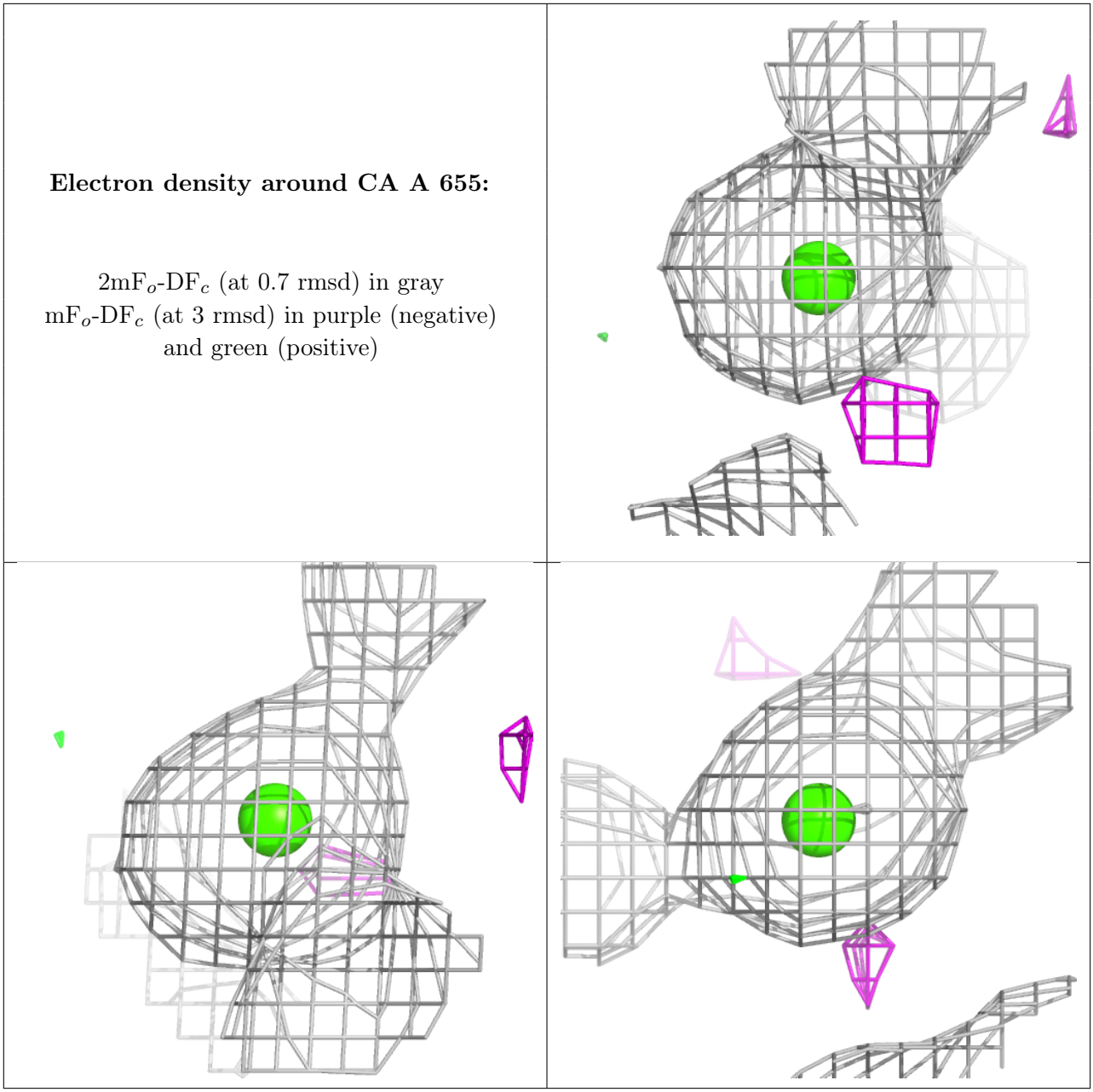
Electron density around IOD A 653:

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



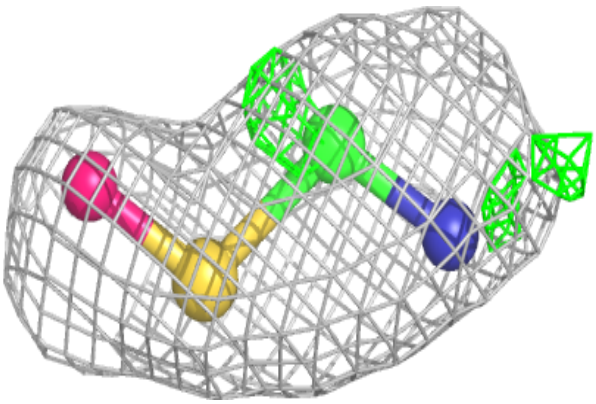
Electron density around CA A 655:

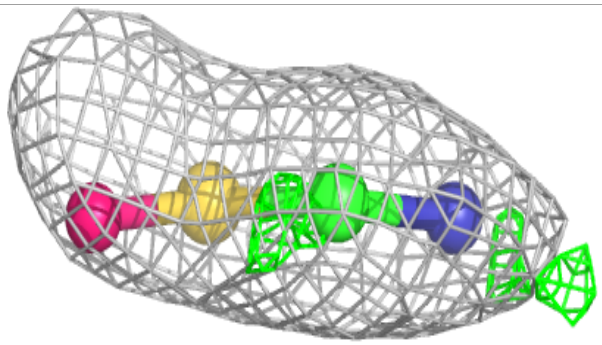
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

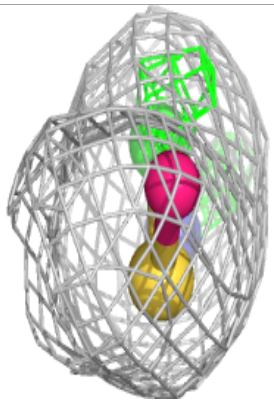


Electron density around OSM A 642 (B):

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

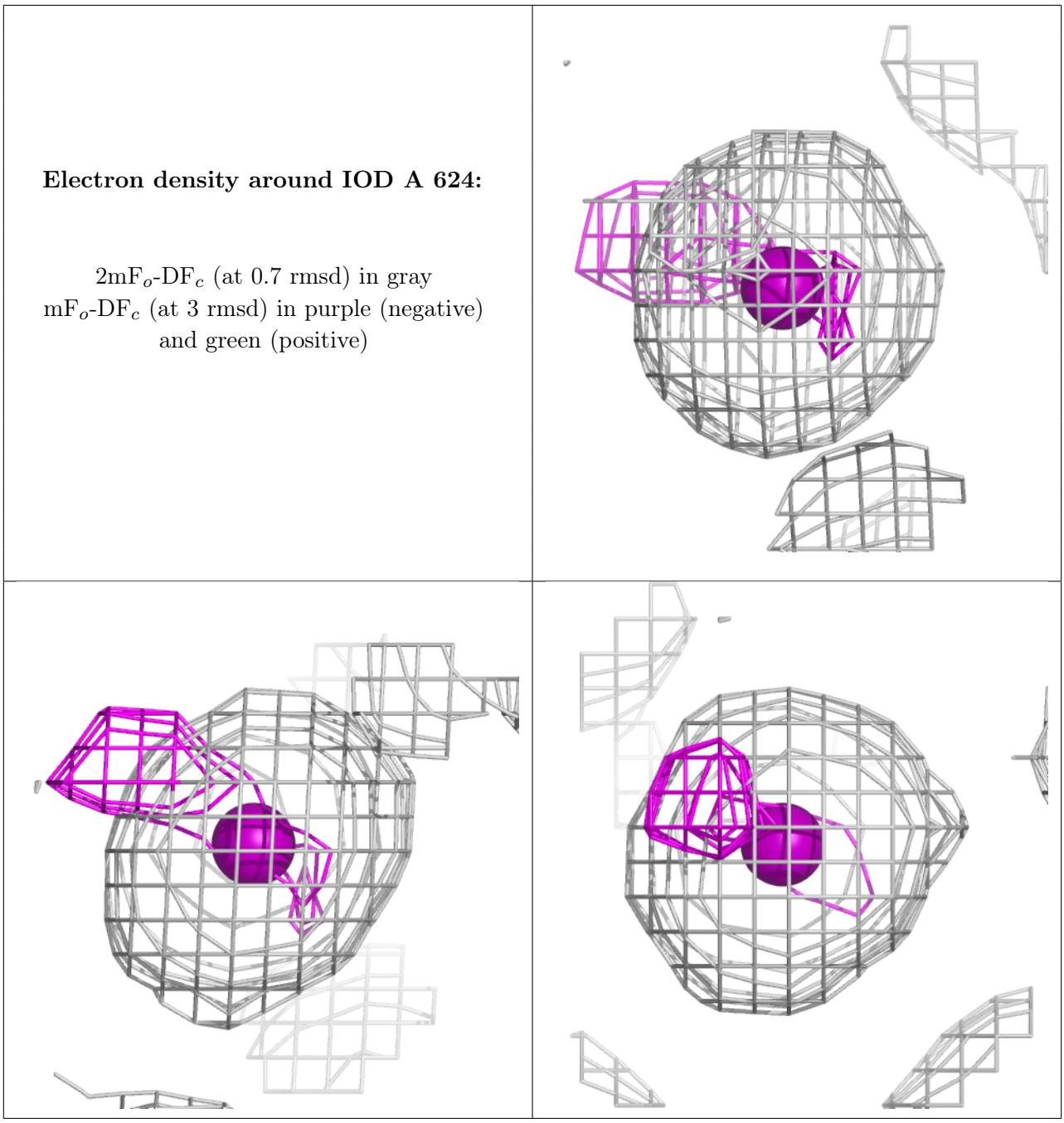






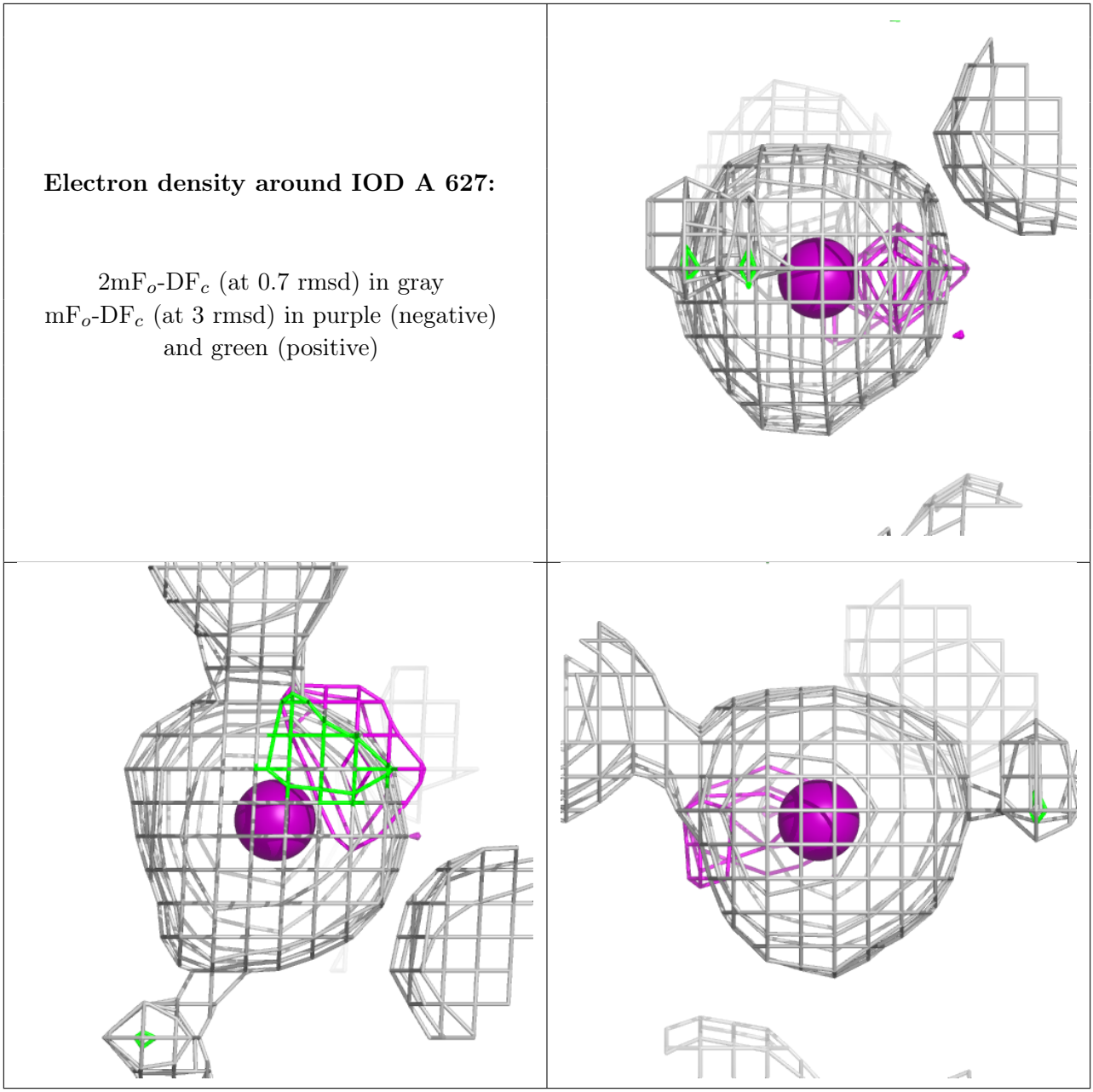
Electron density around IOD A 624:

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



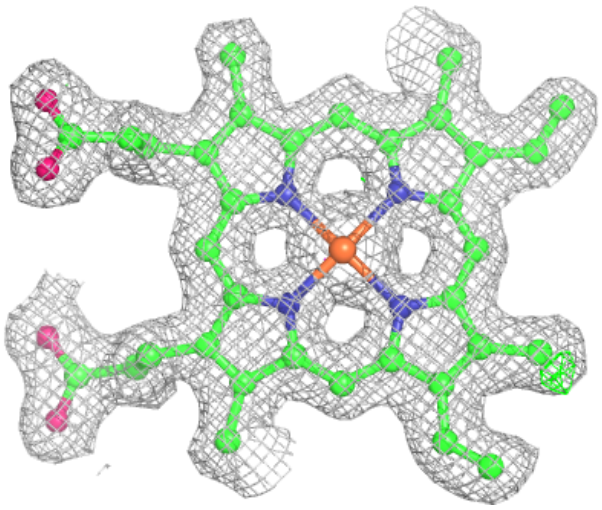
Electron density around IOD A 627:

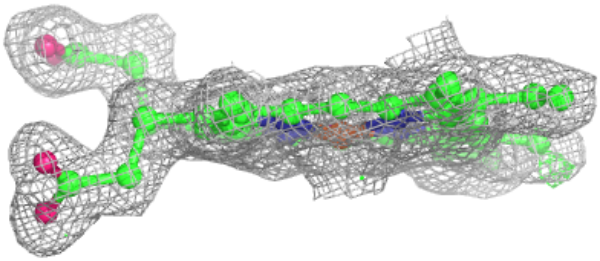
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

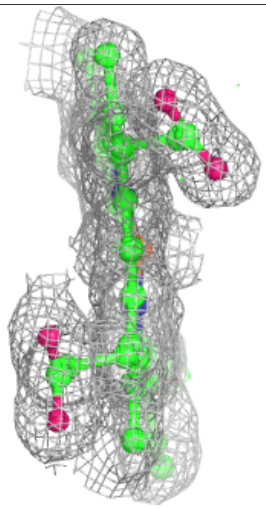


Electron density around HEM A 601:

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

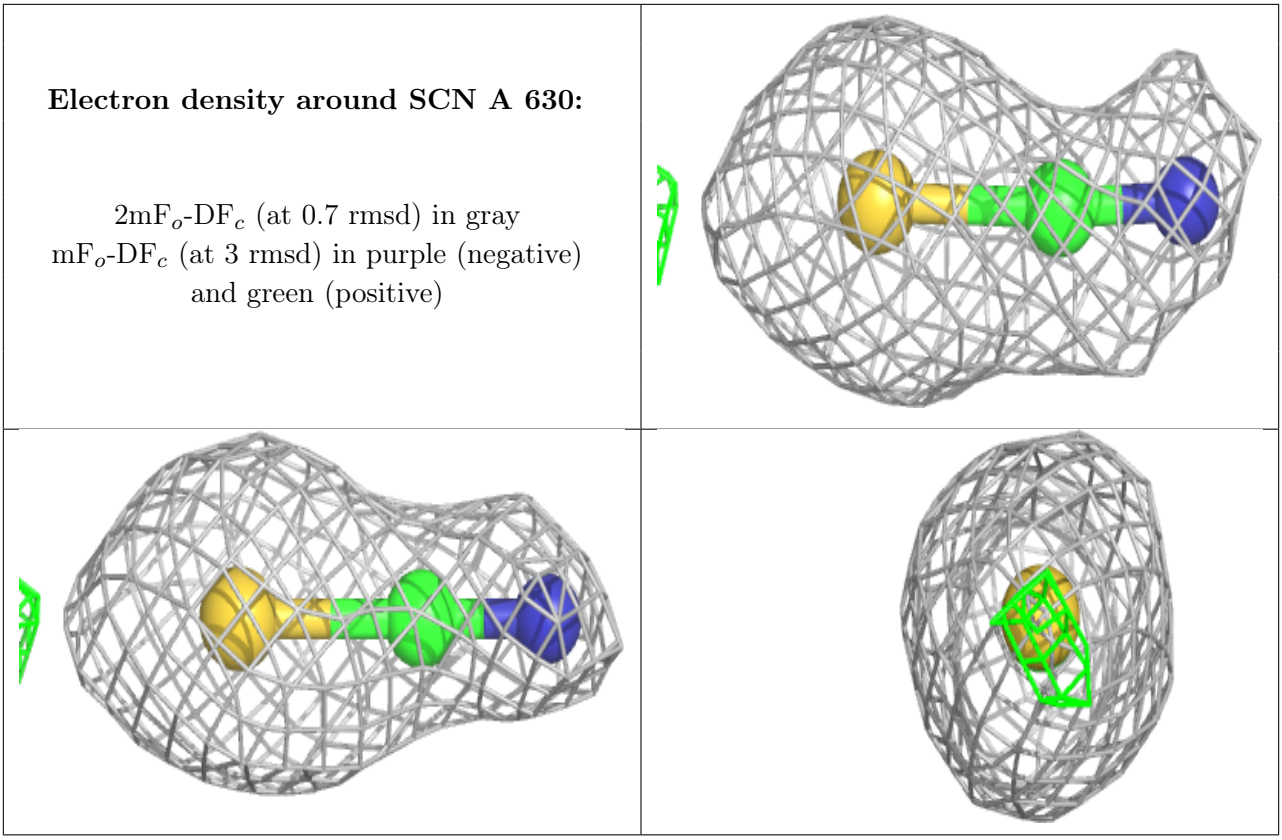






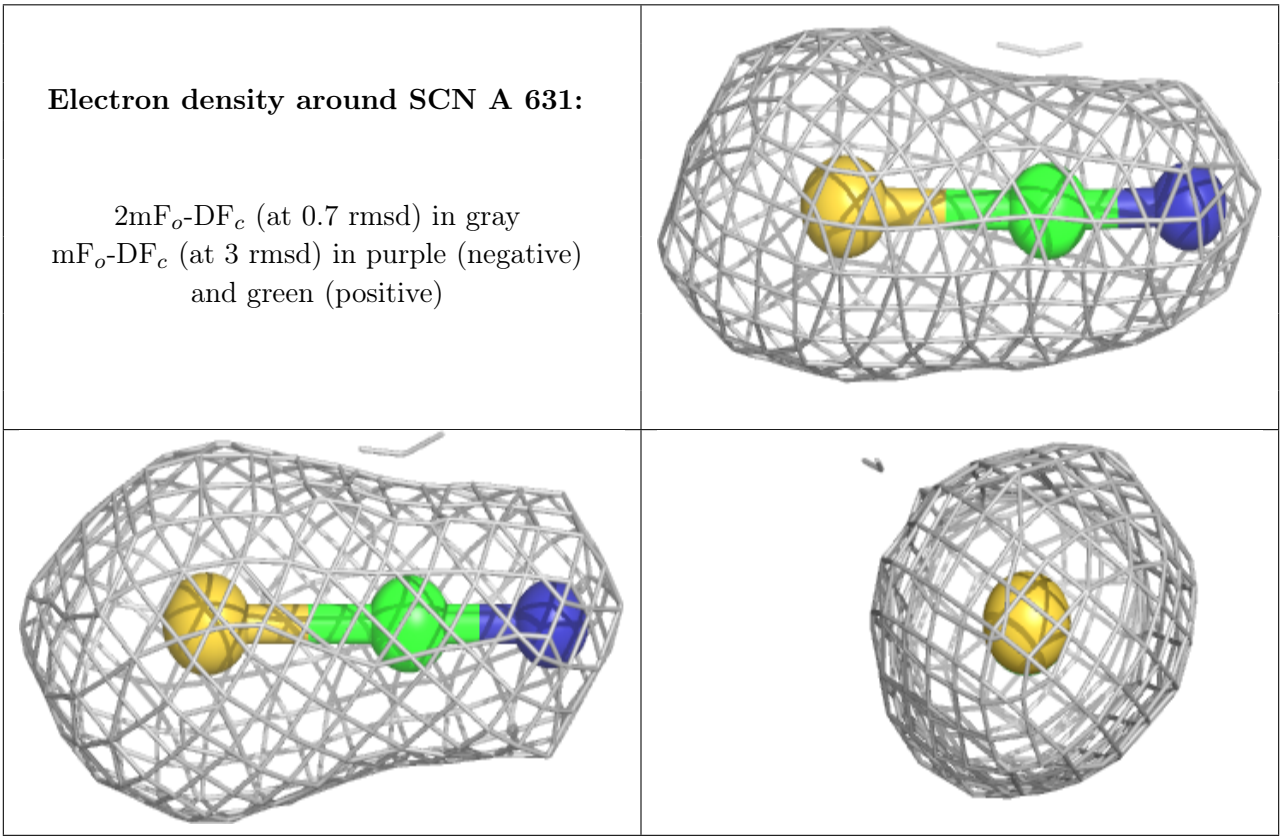
Electron density around SCN A 630:

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



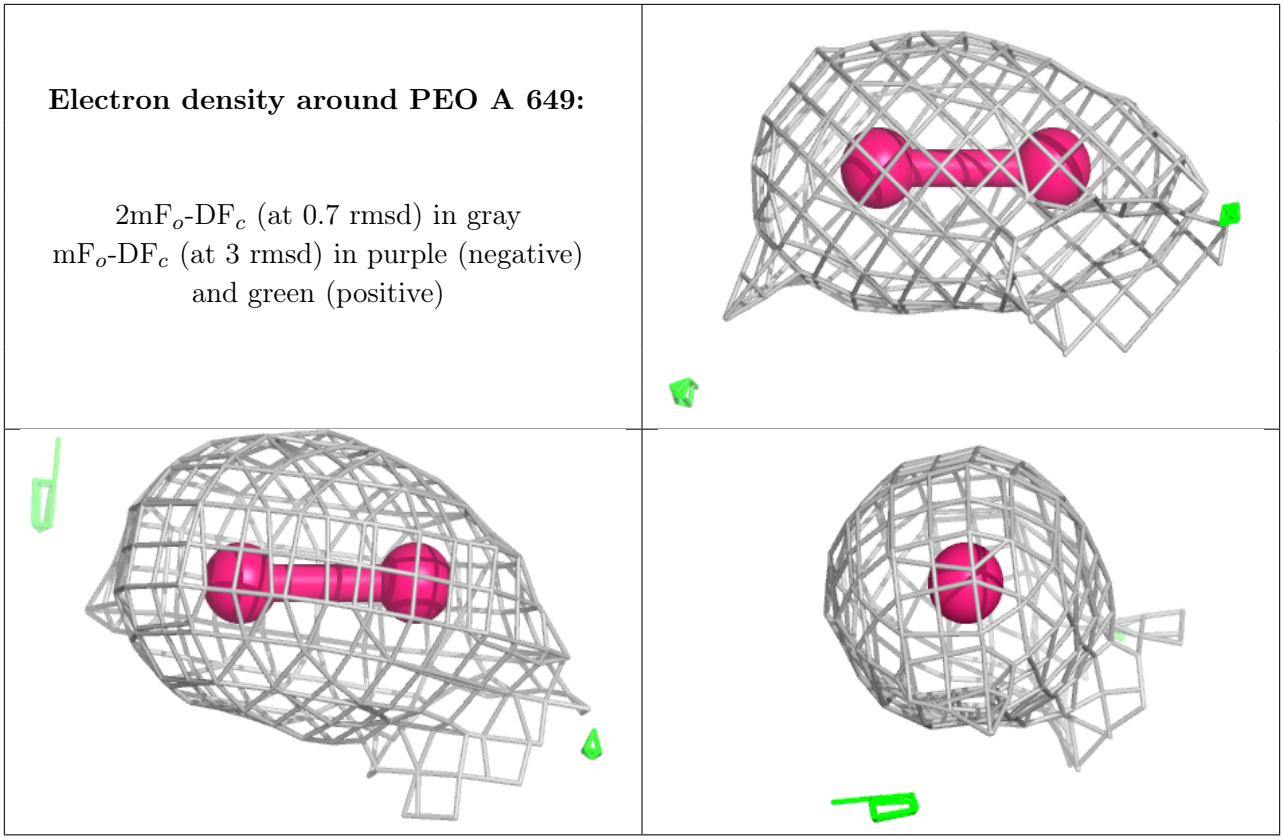
Electron density around SCN A 631:

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



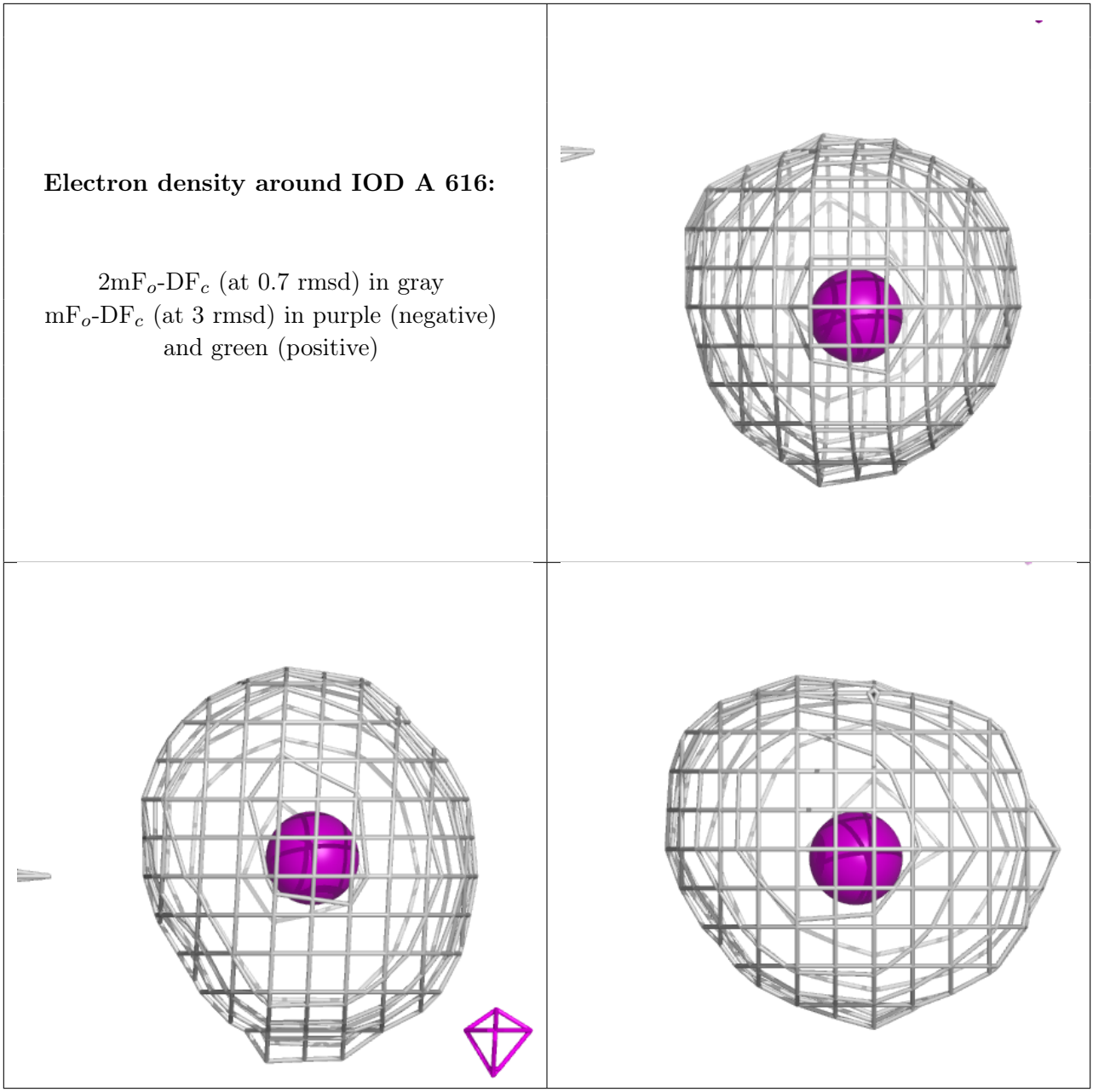
Electron density around PEO A 649:

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



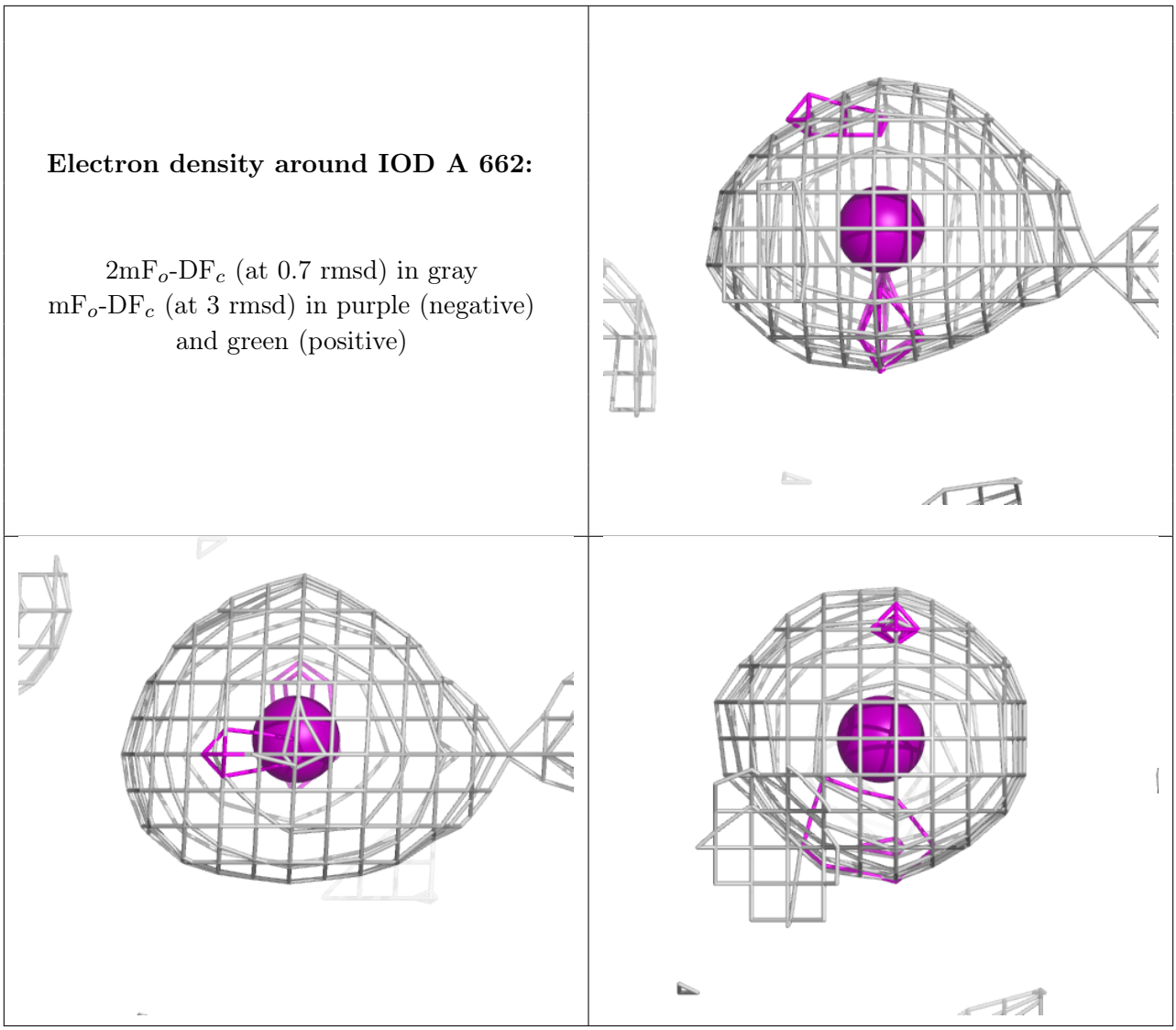
Electron density around IOD A 616:

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



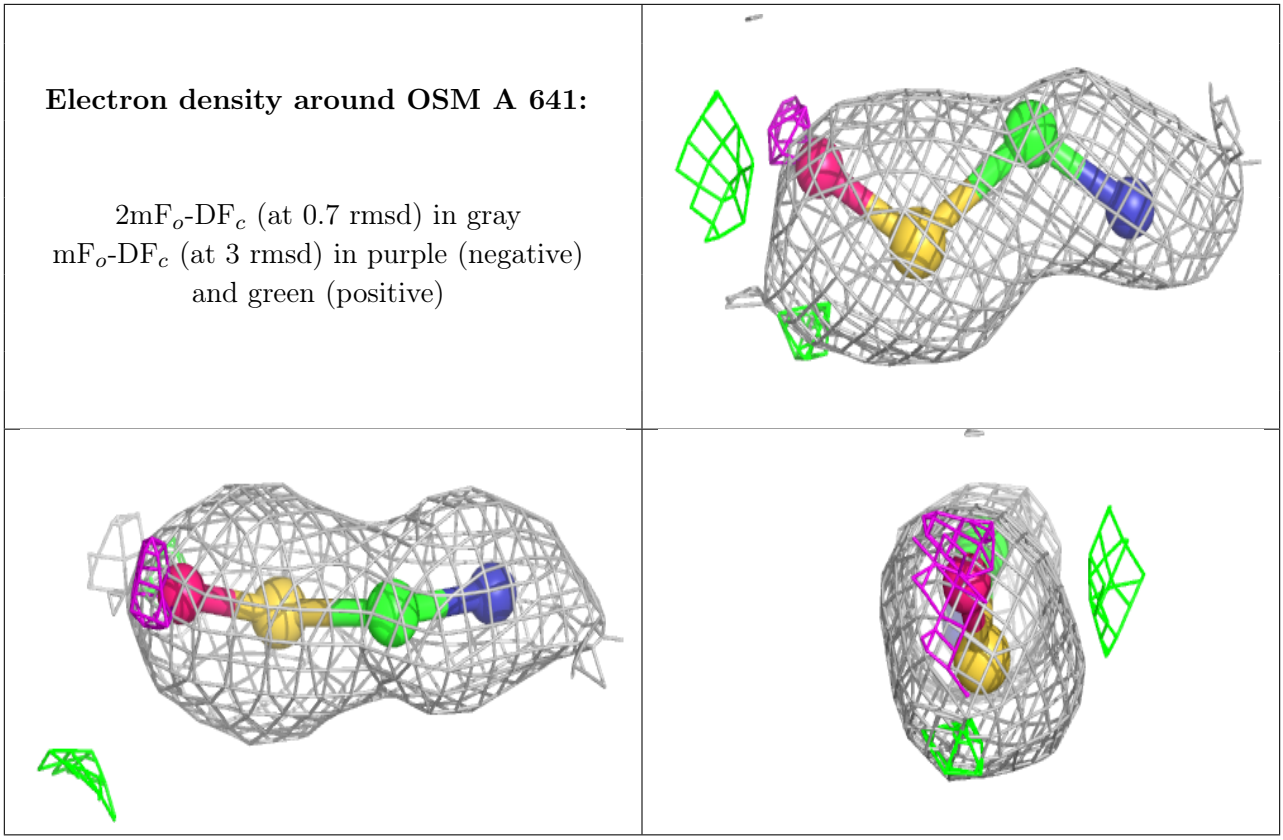
Electron density around IOD A 662:

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



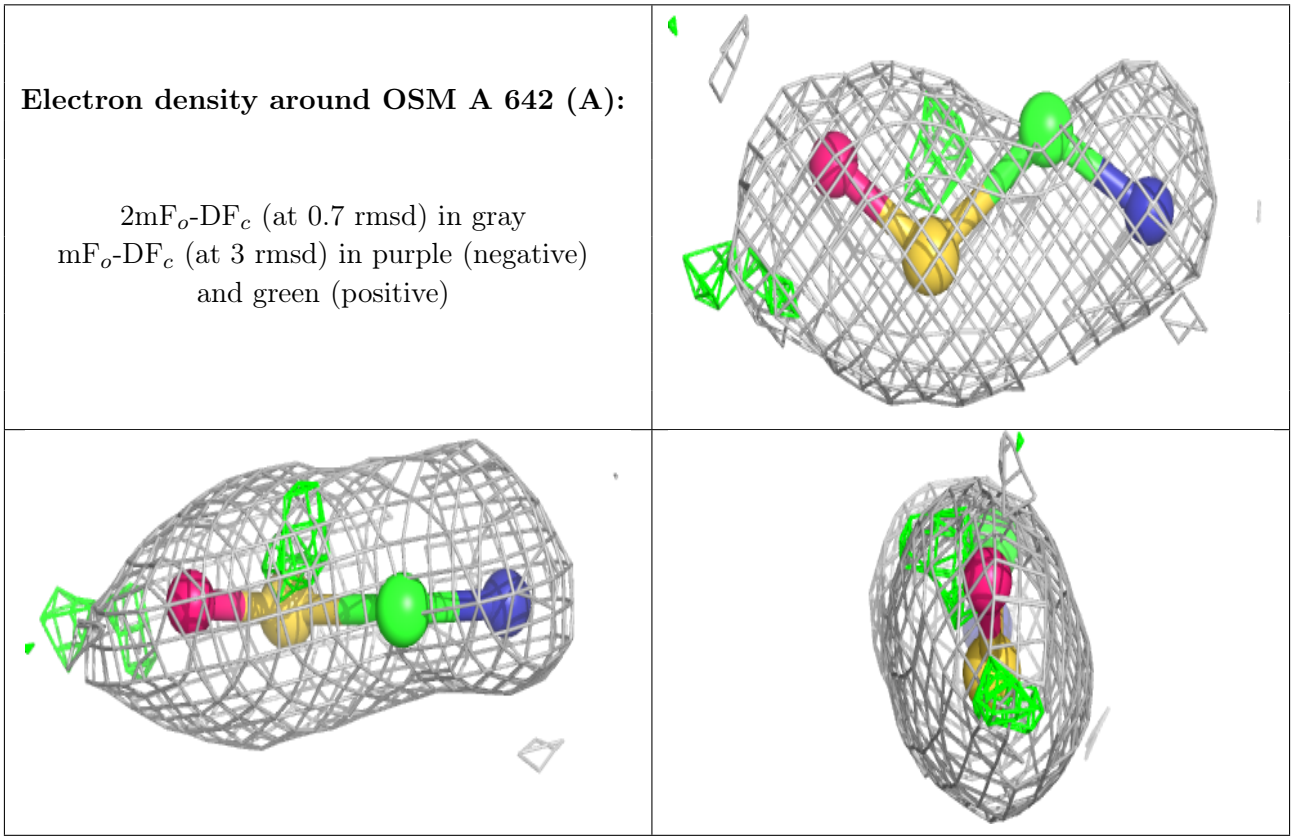
Electron density around OSM A 641:

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



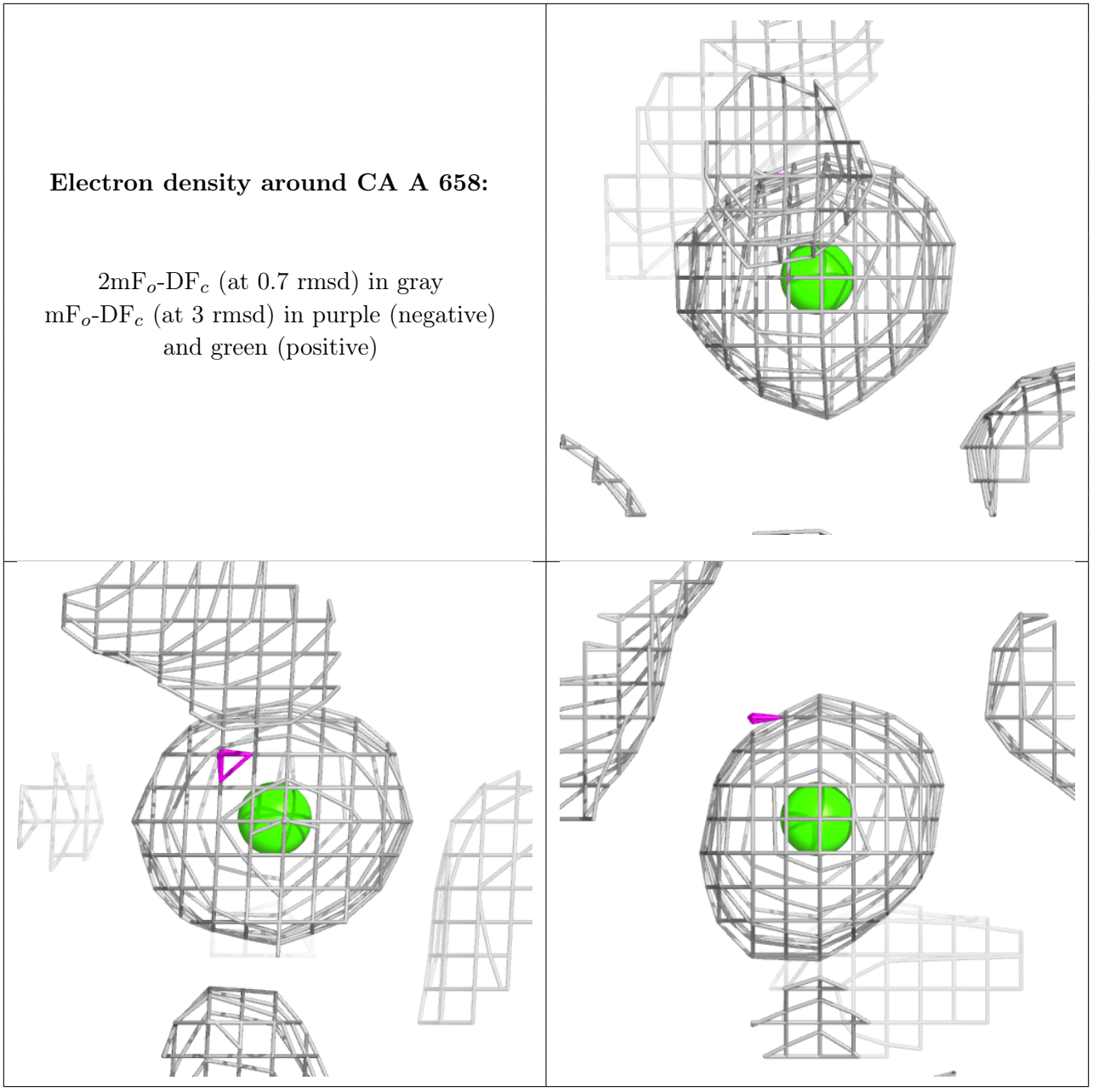
Electron density around OSM A 642 (A):

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



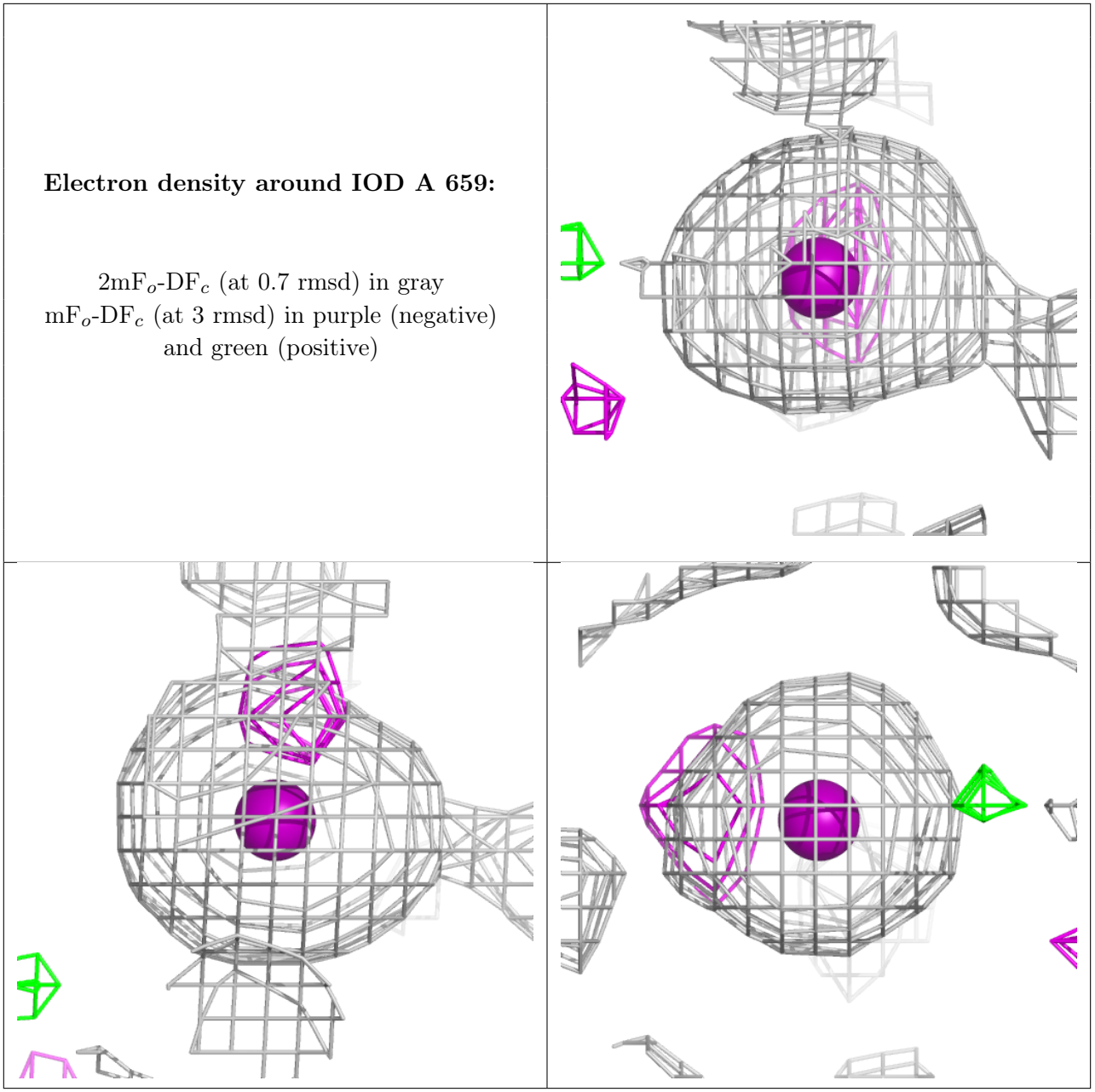
Electron density around CA A 658:

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



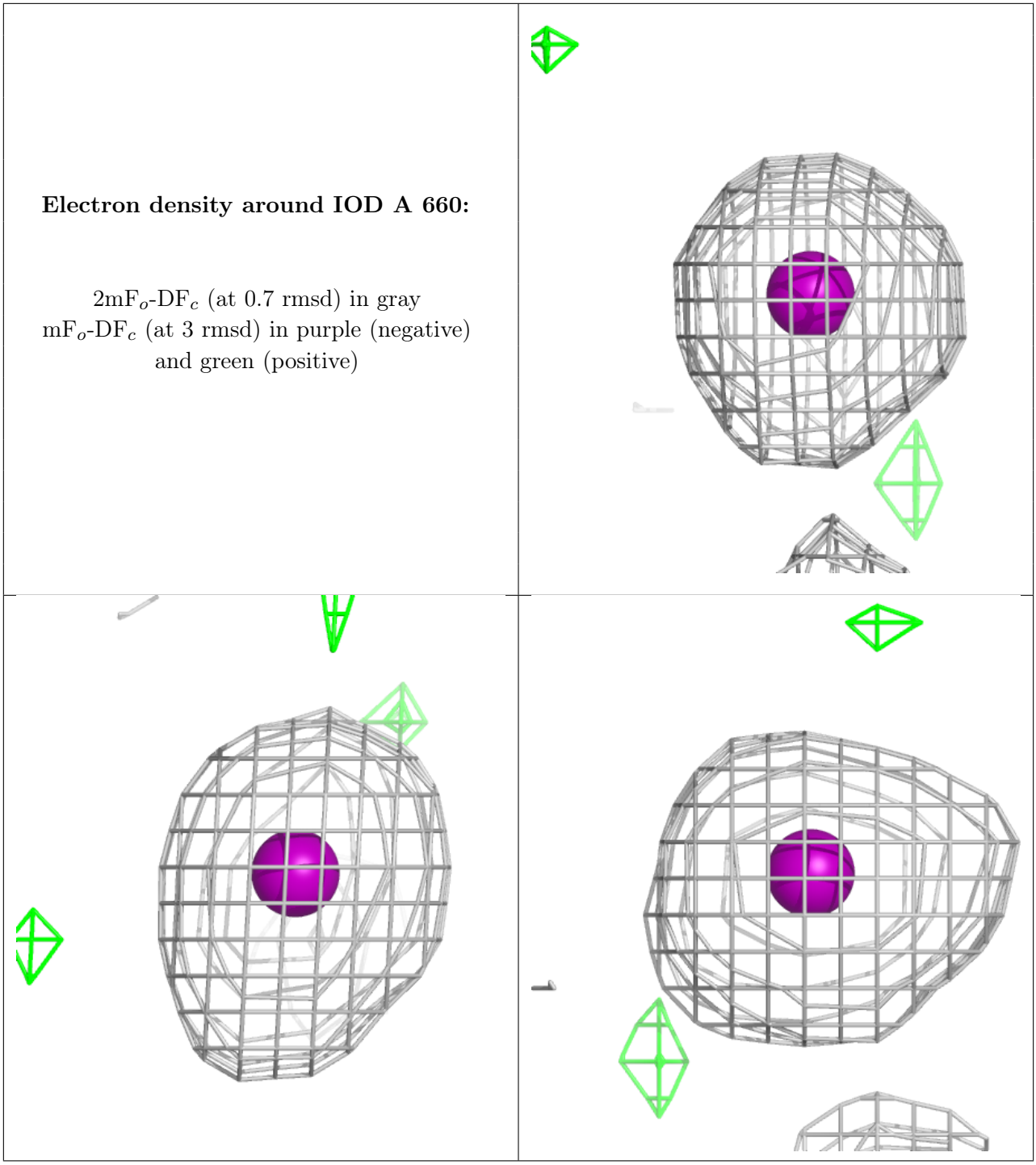
Electron density around IOD A 659:

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



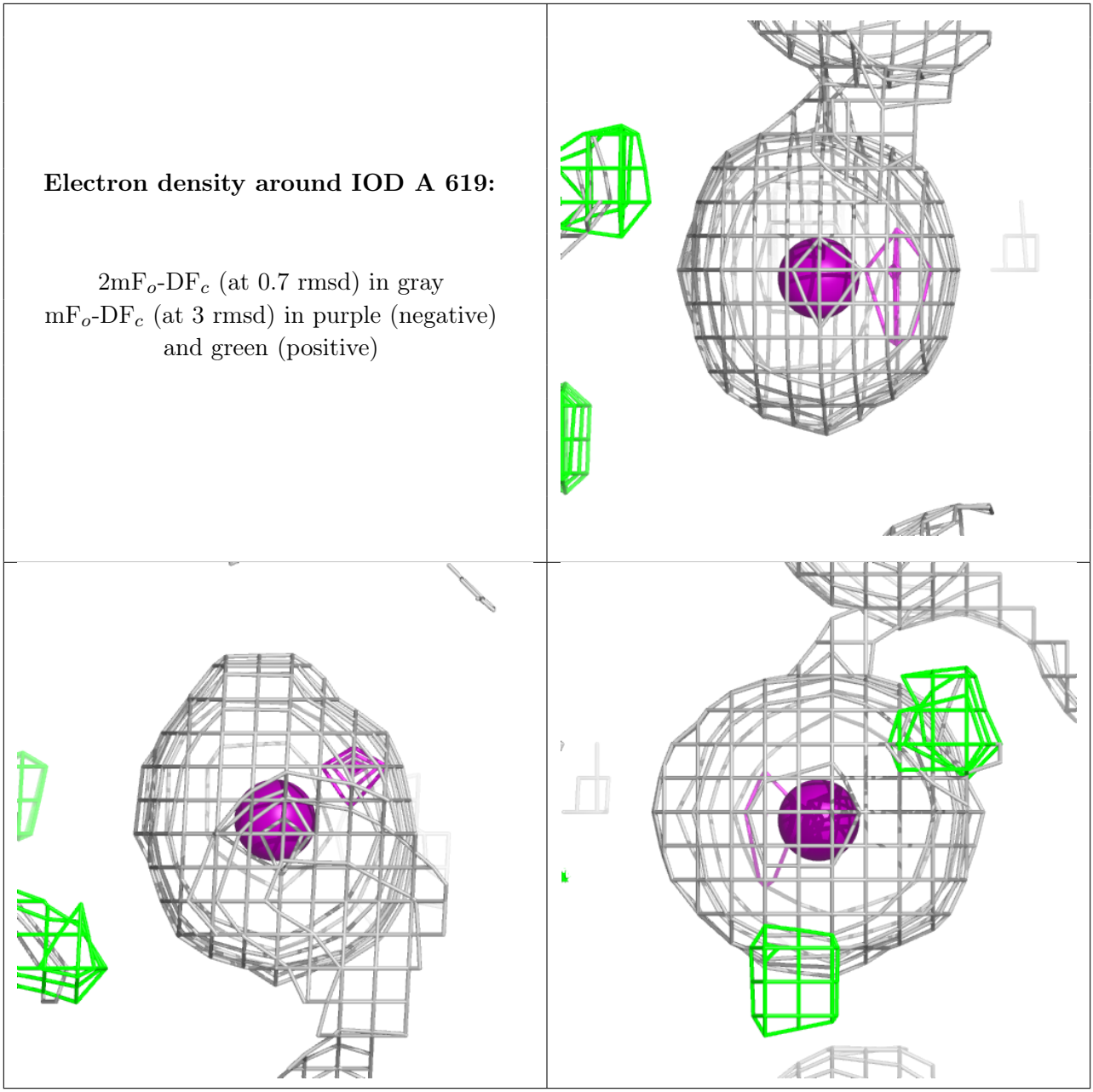
Electron density around IOD A 660:

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



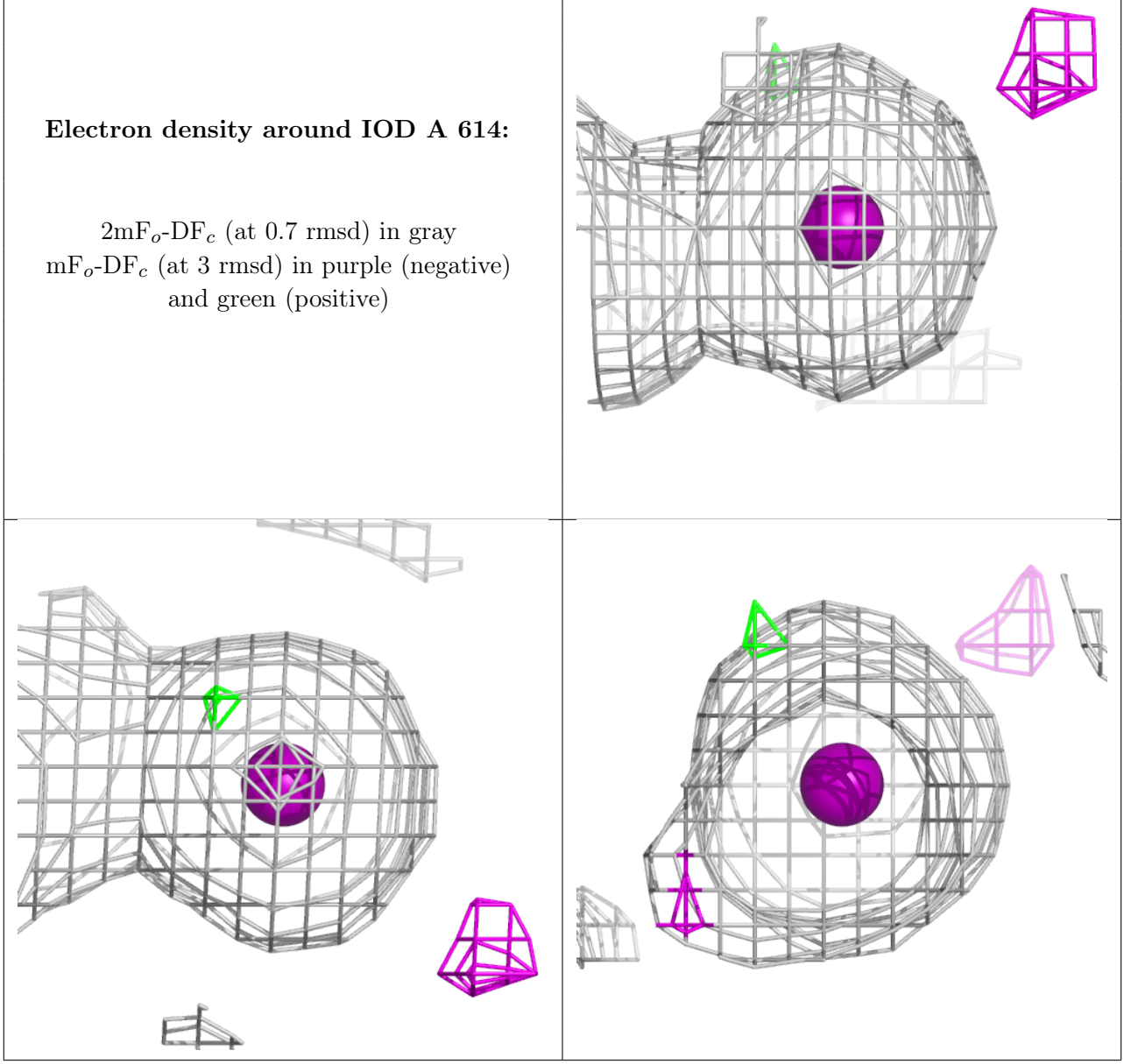
Electron density around IOD A 619:

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



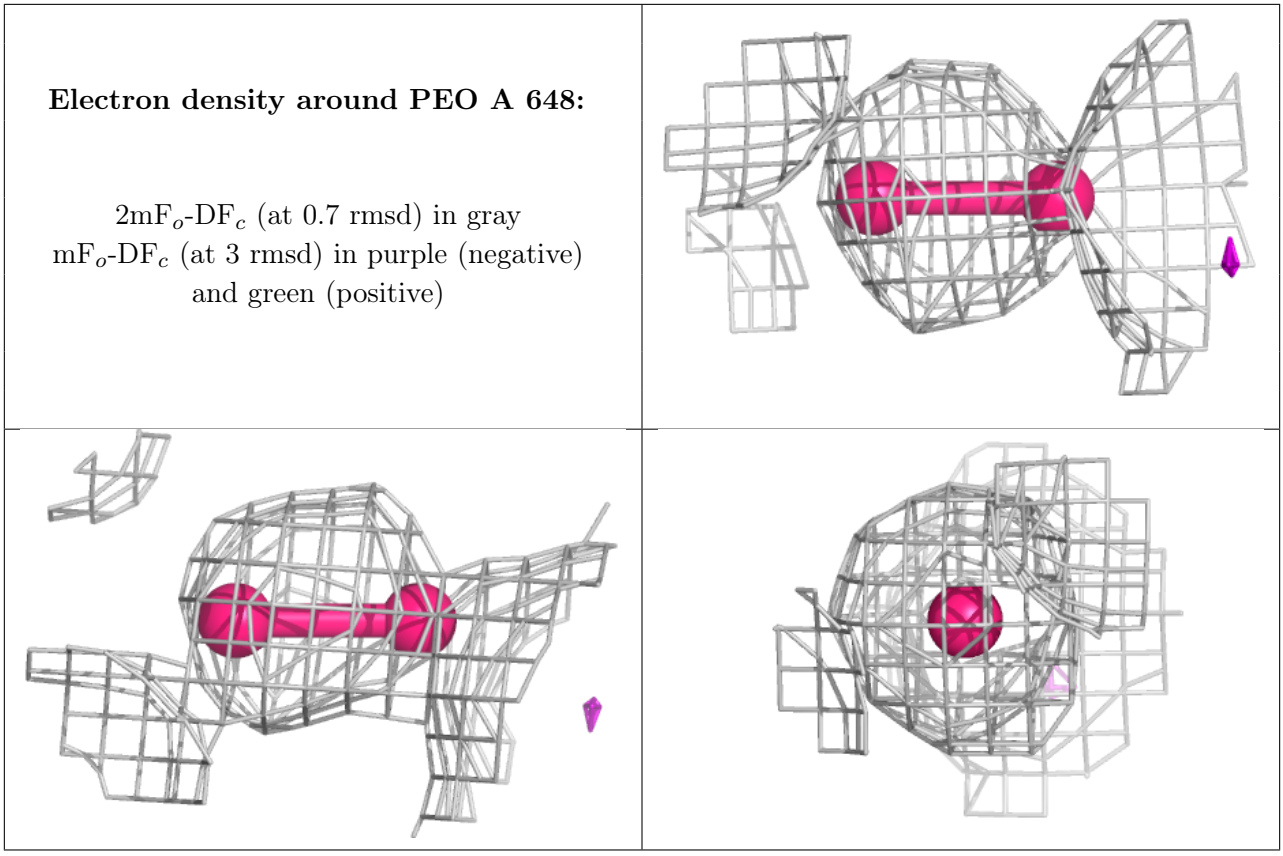
Electron density around IOD A 614:

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



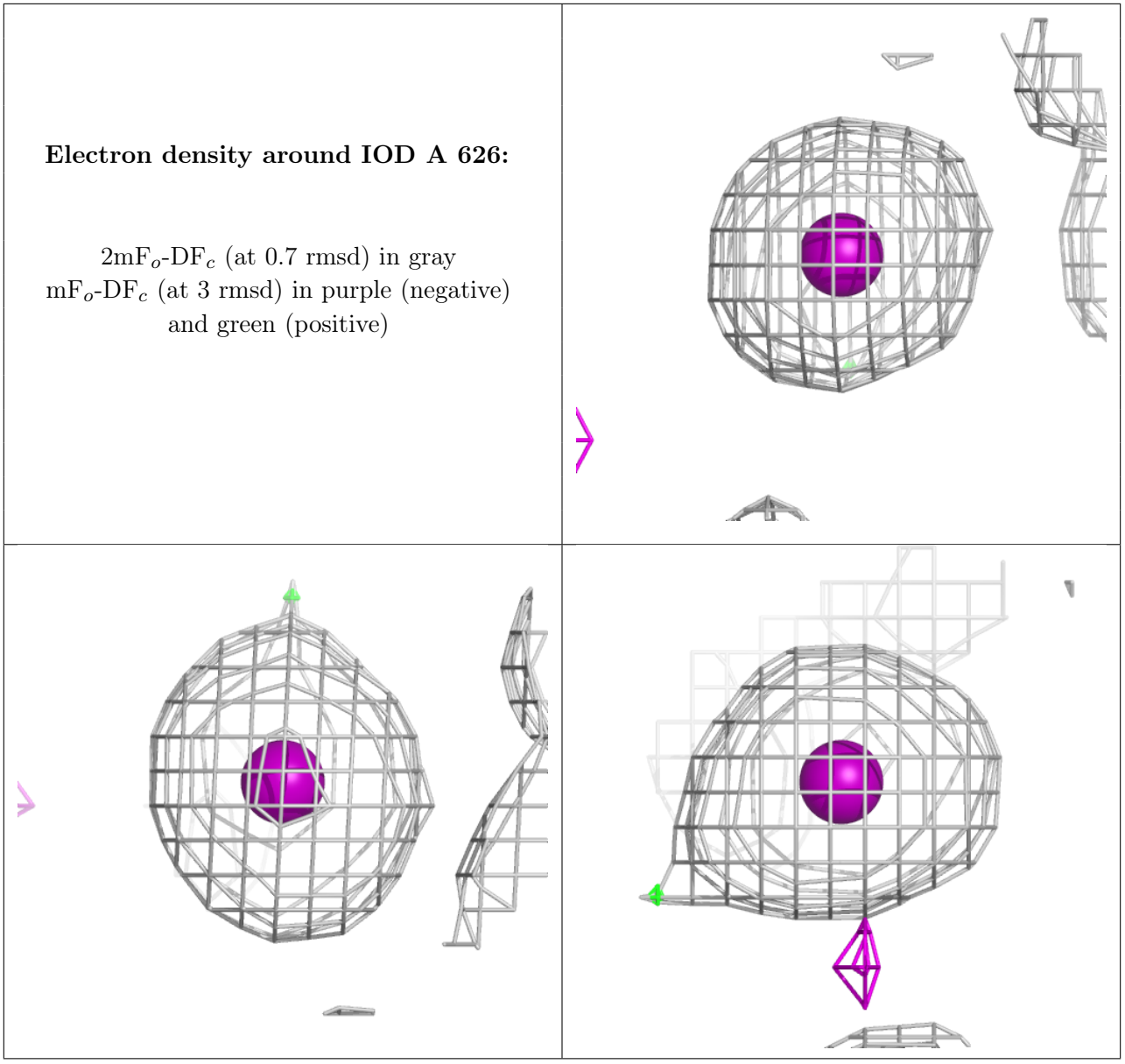
Electron density around PEO A 648:

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



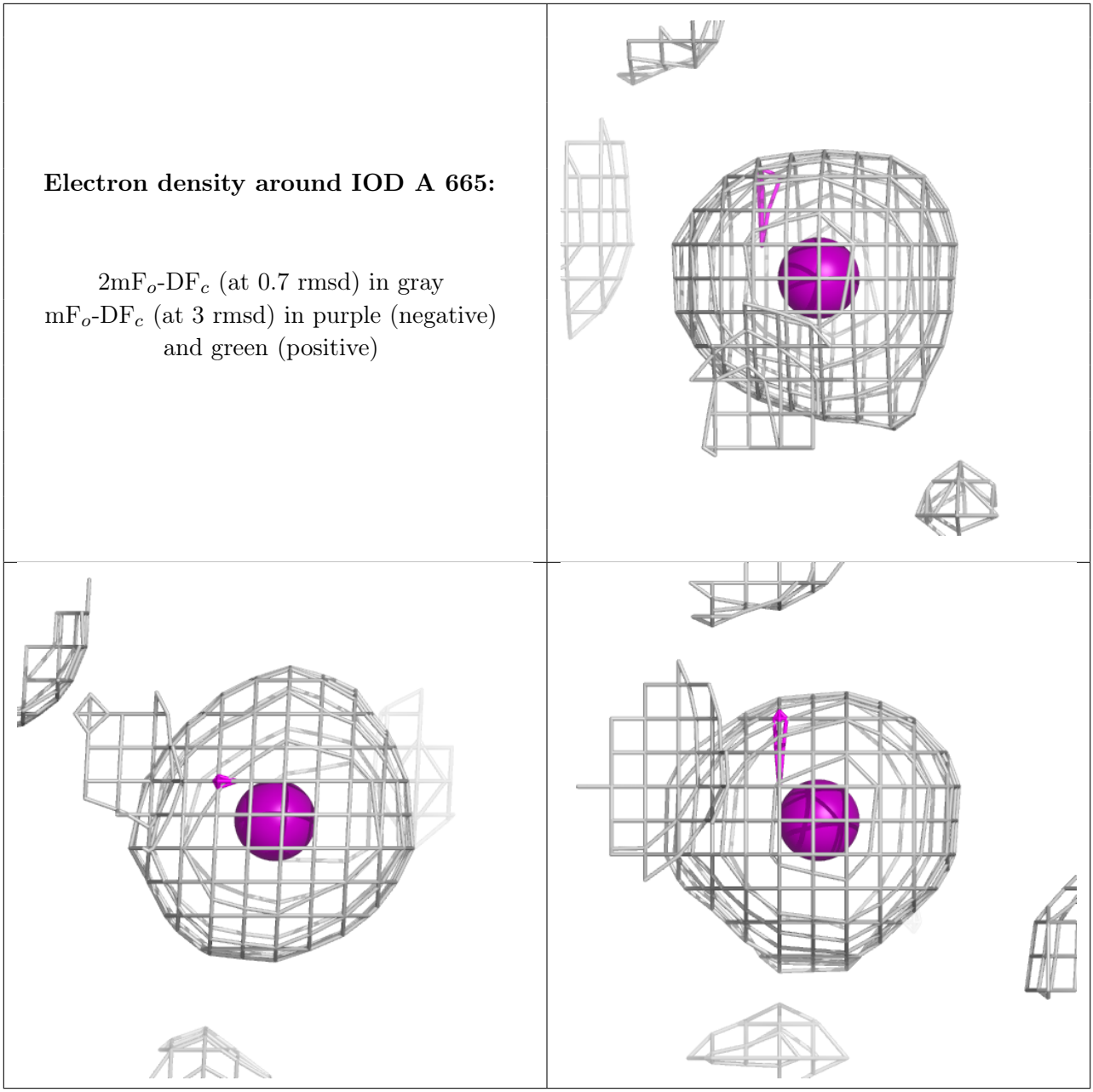
Electron density around IOD A 626:

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



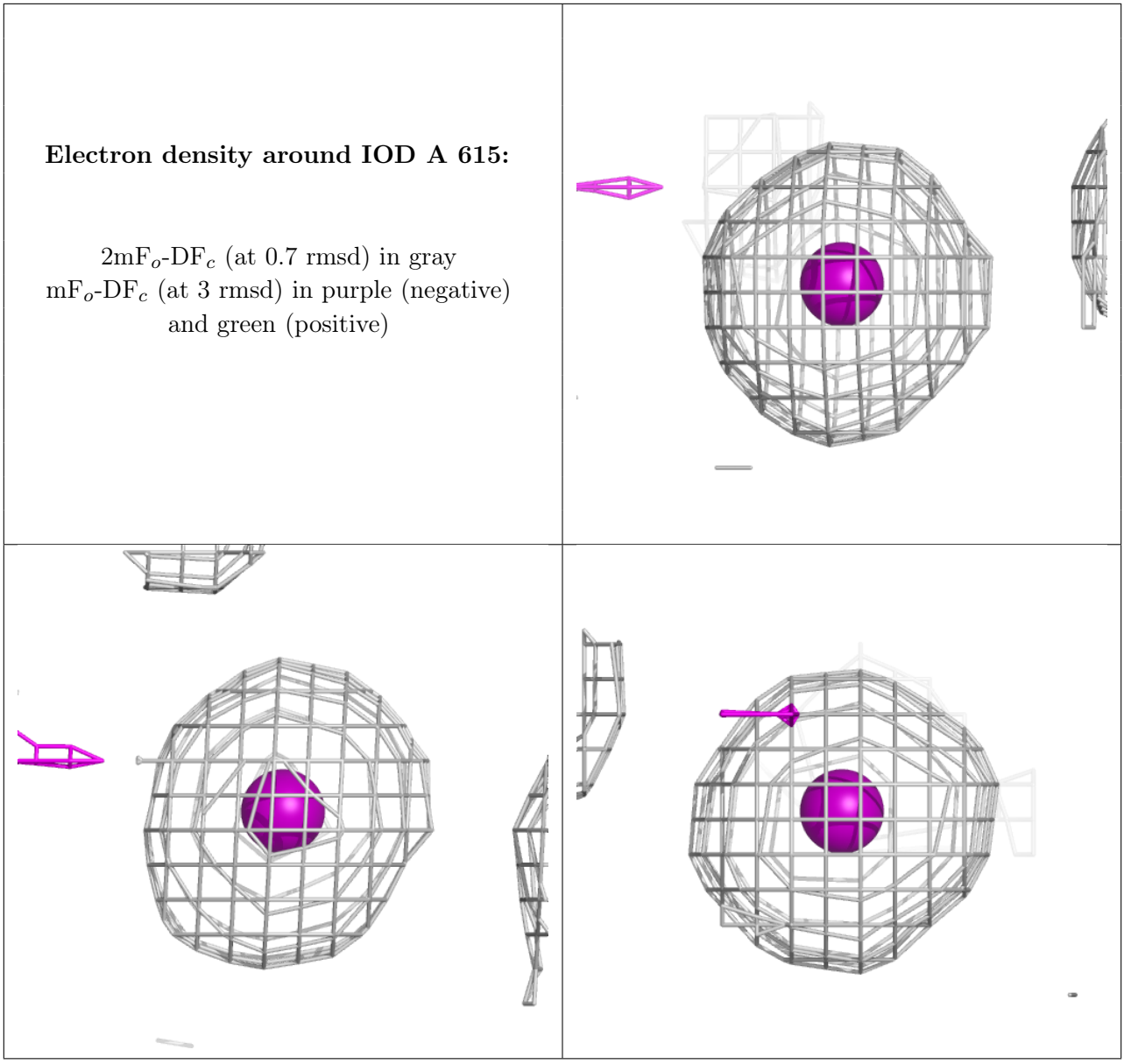
Electron density around IOD A 665:

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



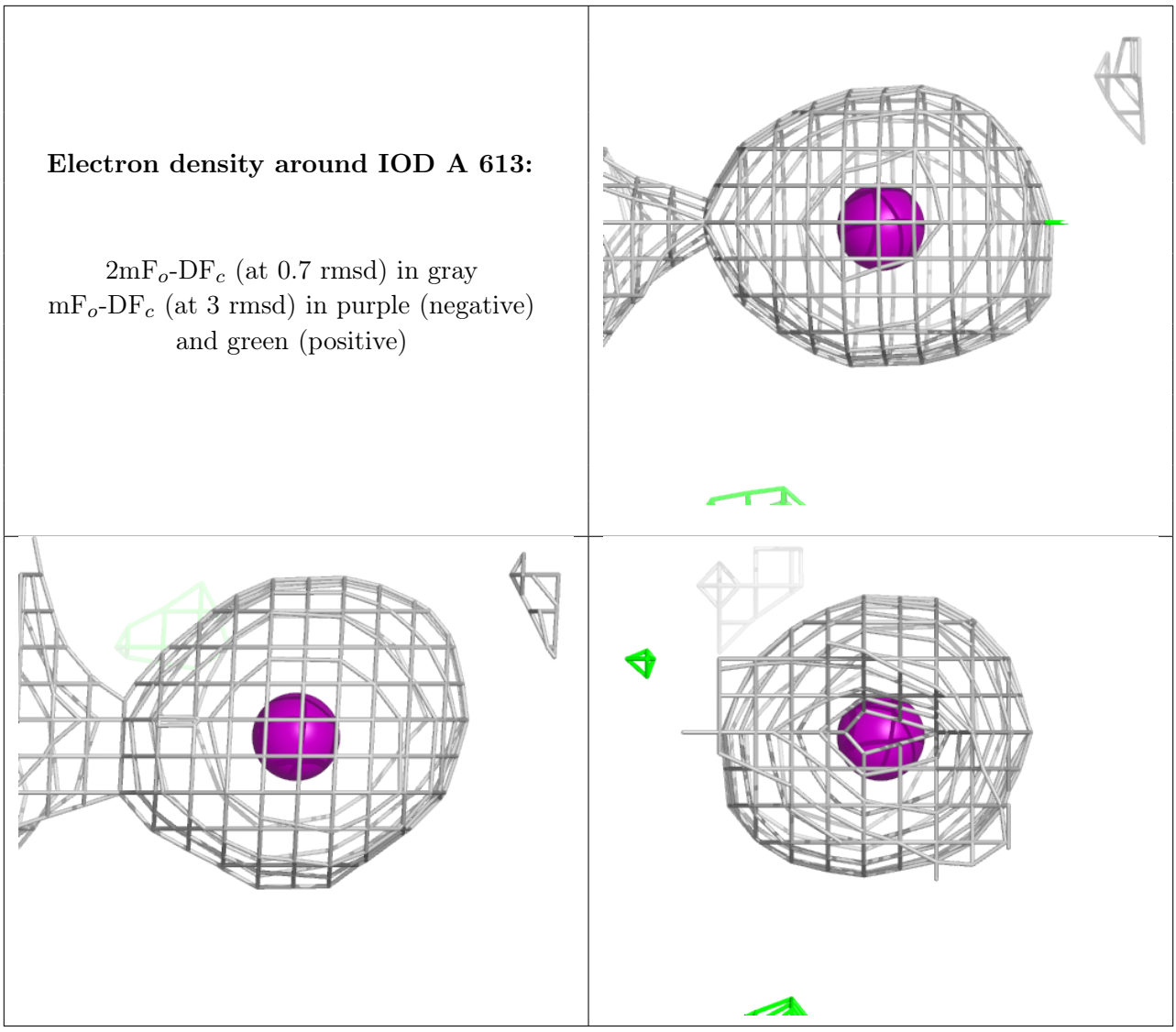
Electron density around IOD A 615:

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



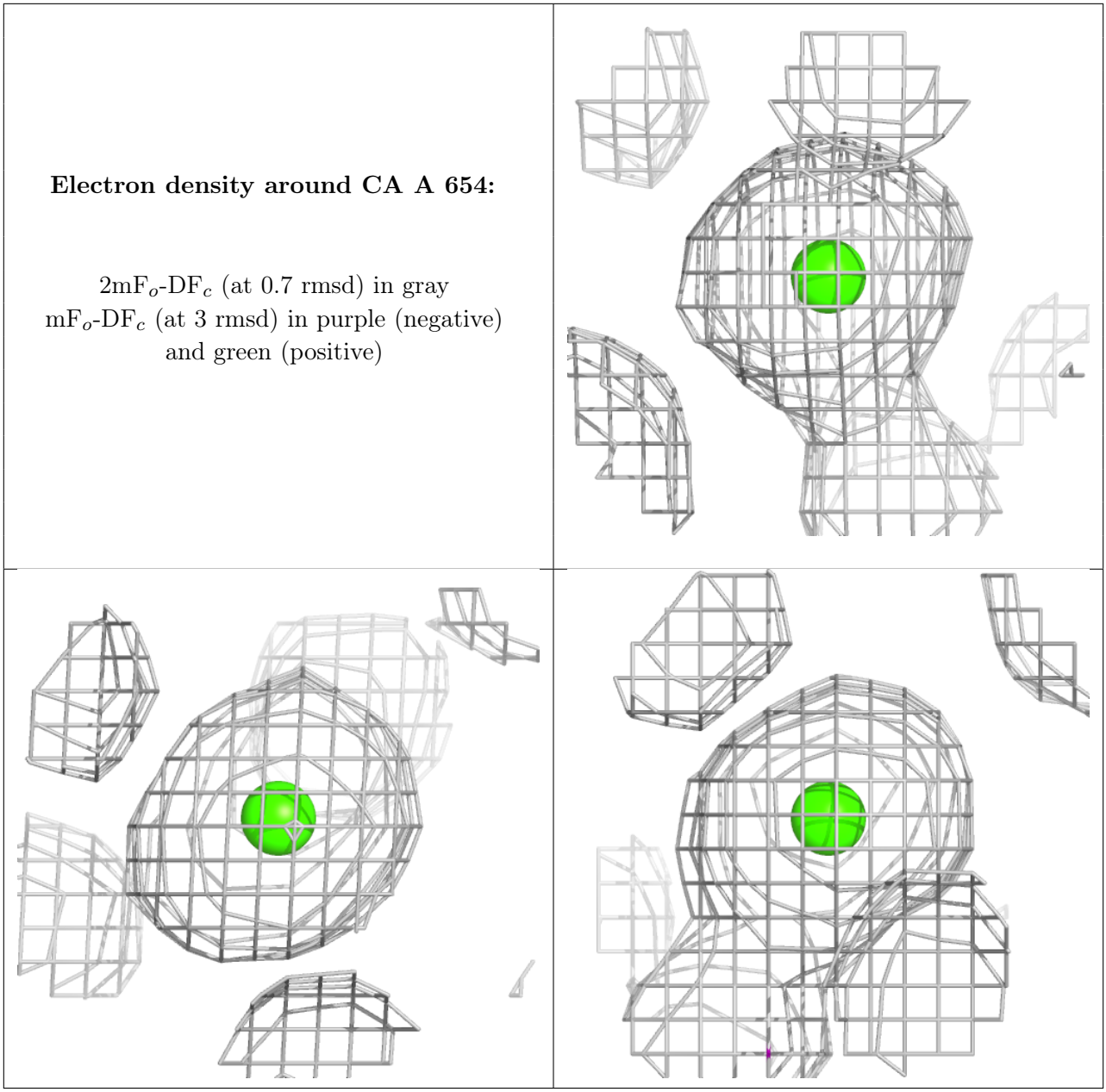
Electron density around IOD A 613:

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



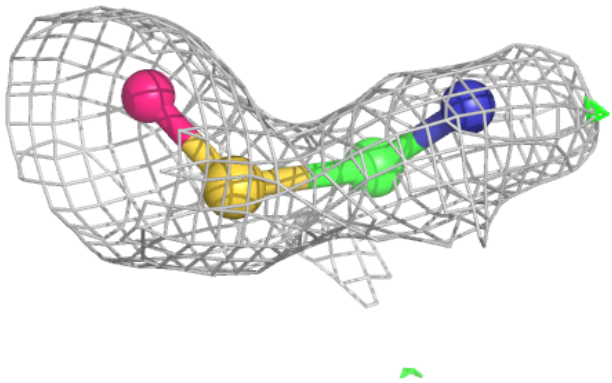
Electron density around CA A 654:

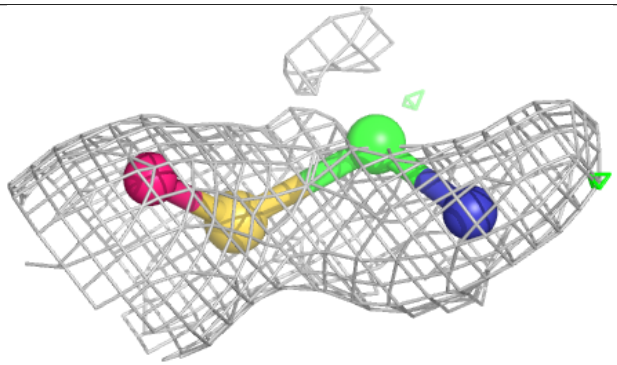
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

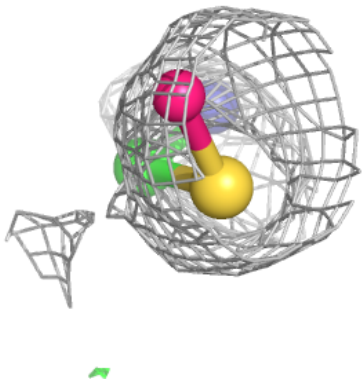


Electron density around OSM A 644 (A):

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

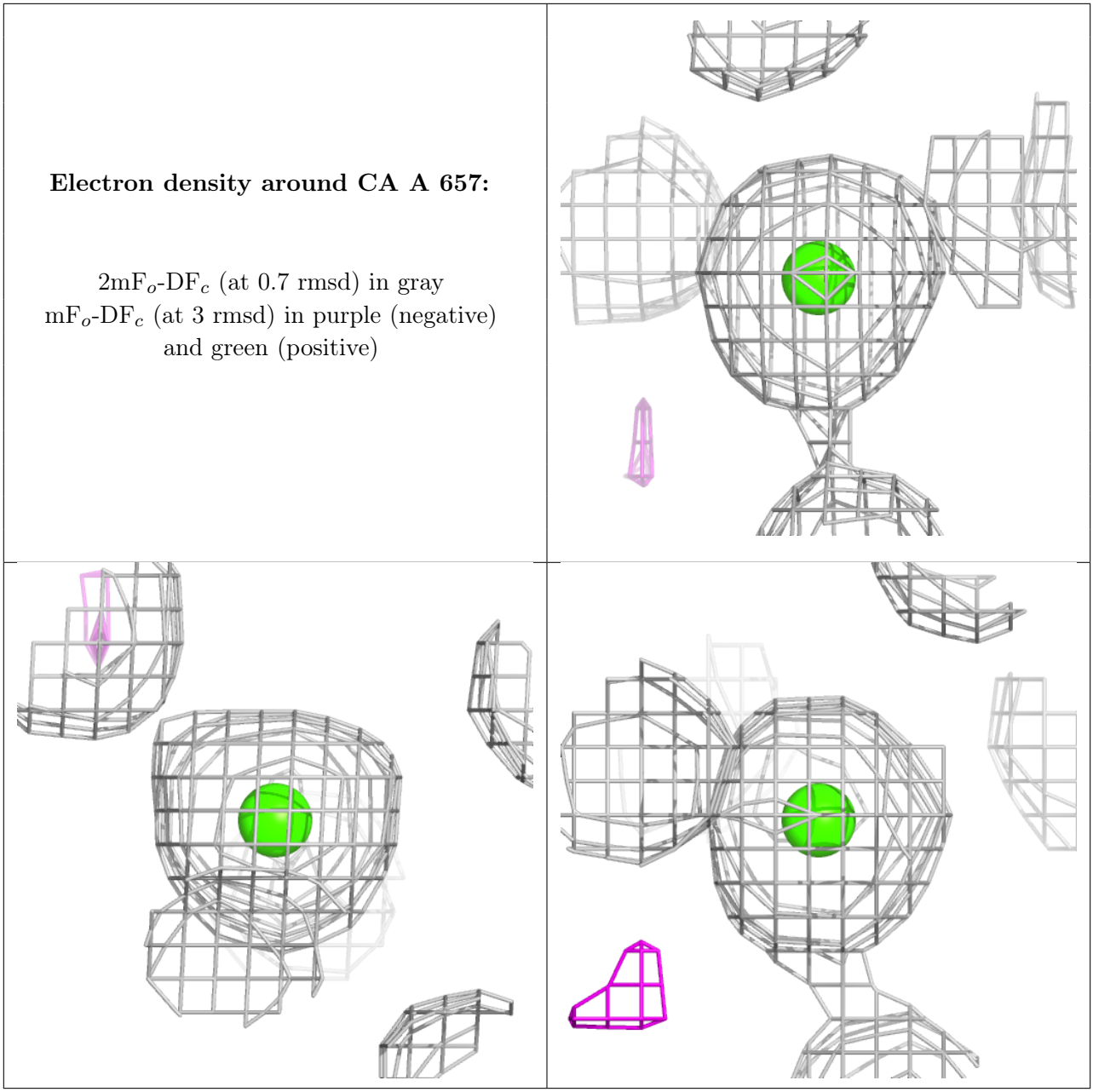






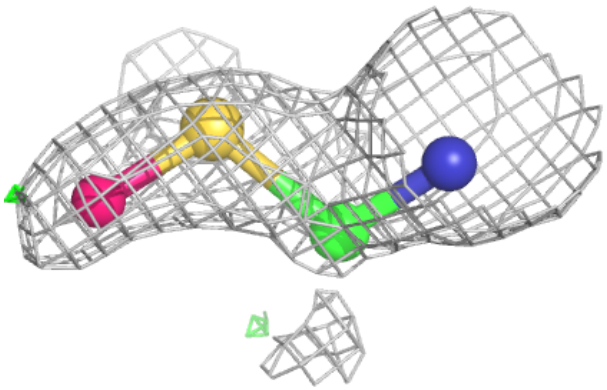
Electron density around CA A 657:

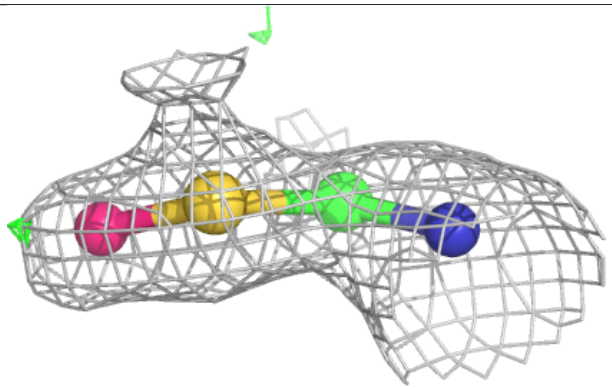
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

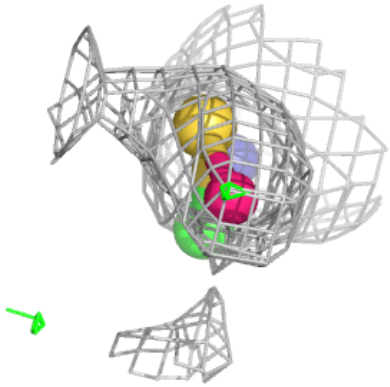


Electron density around OSM A 644 (B):

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

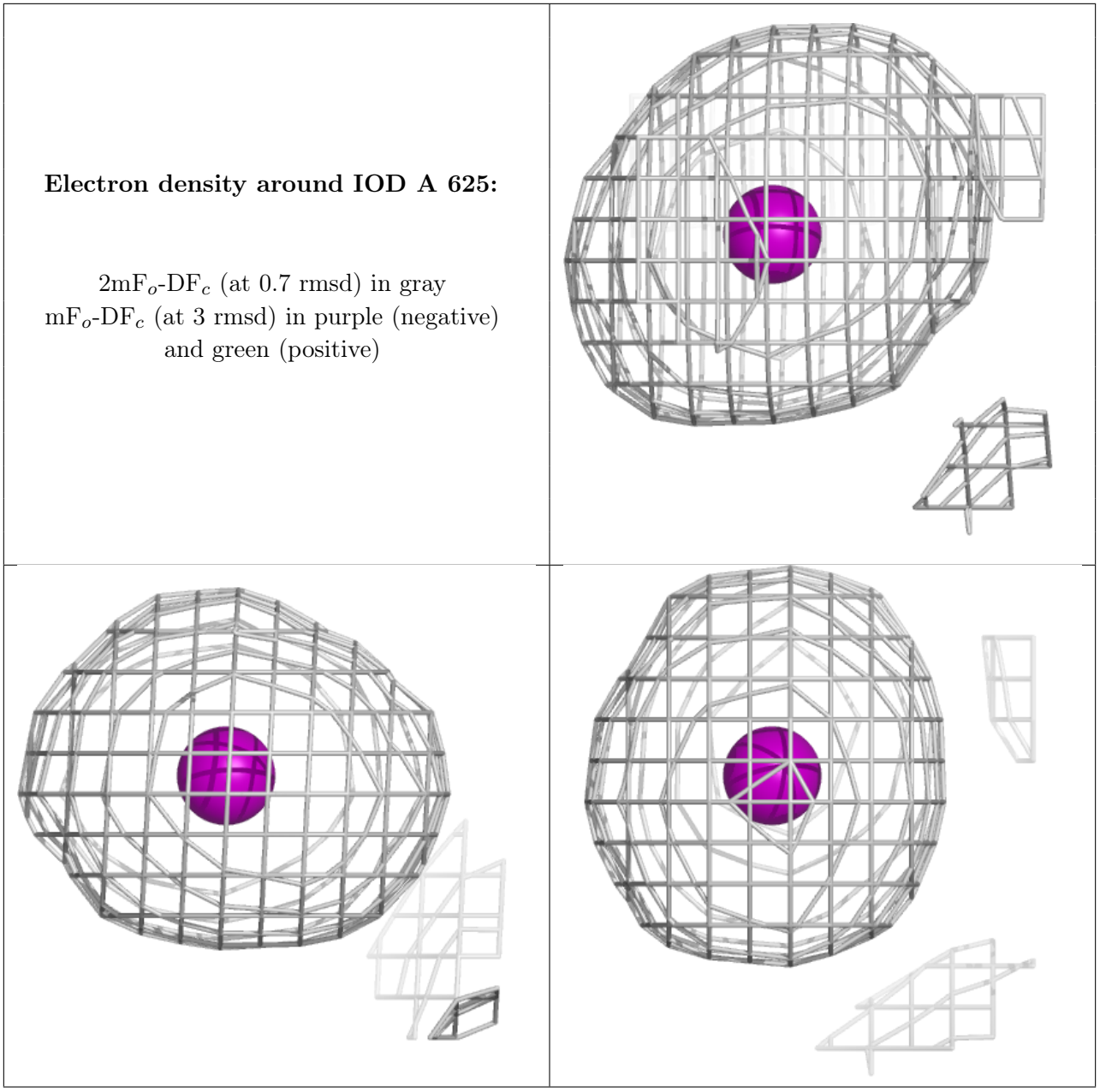






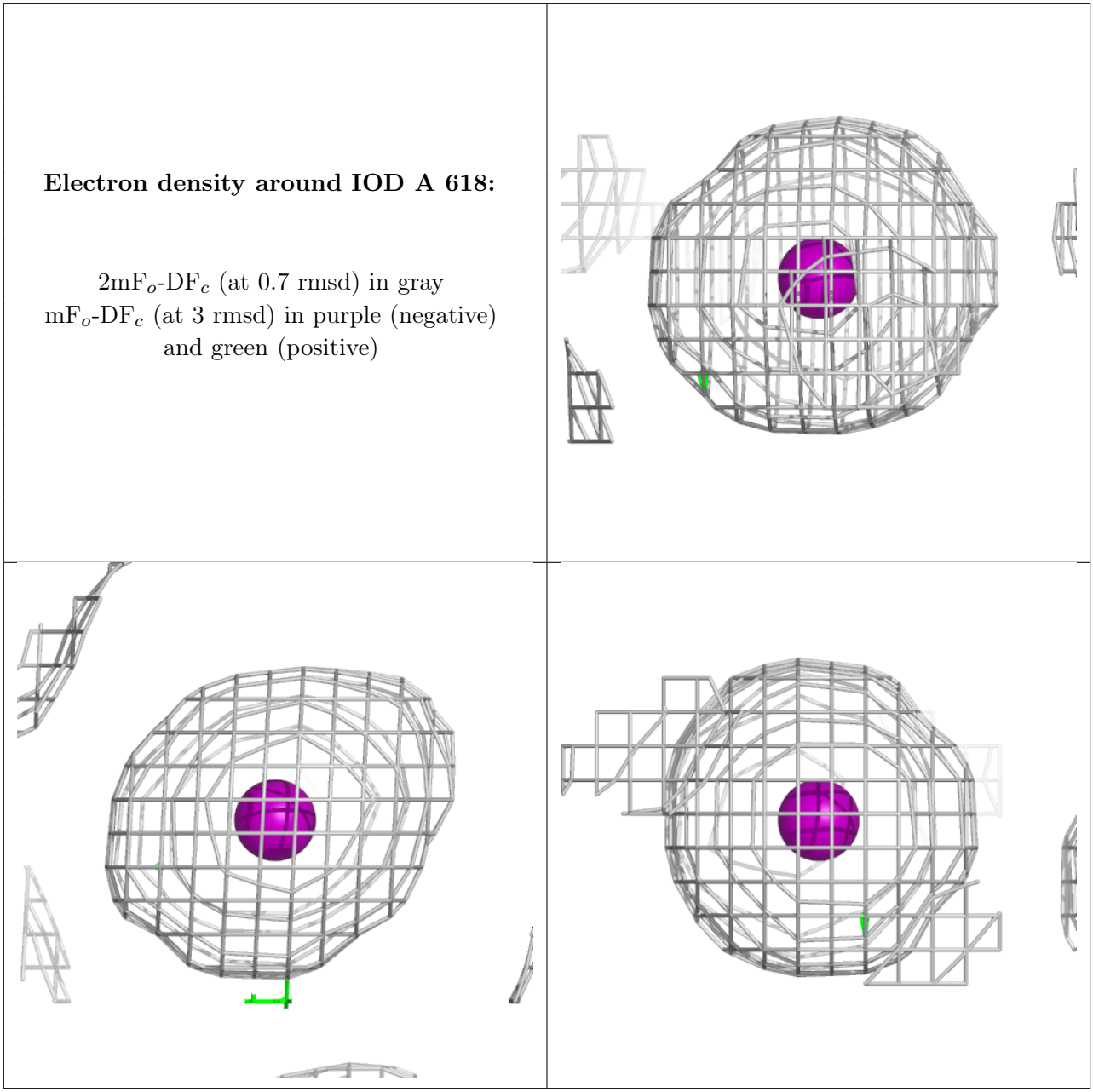
Electron density around IOD A 625:

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



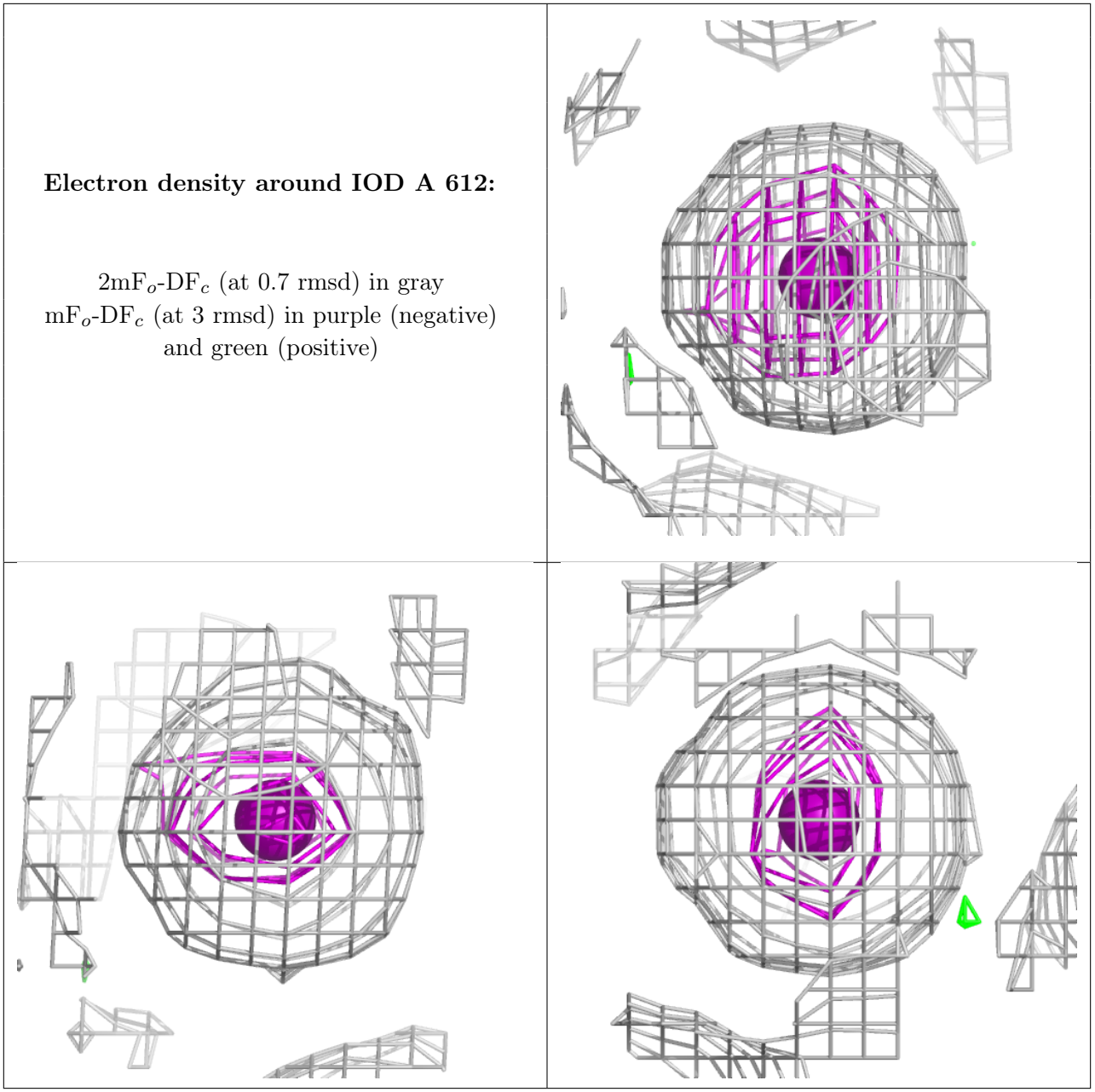
Electron density around IOD A 618:

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



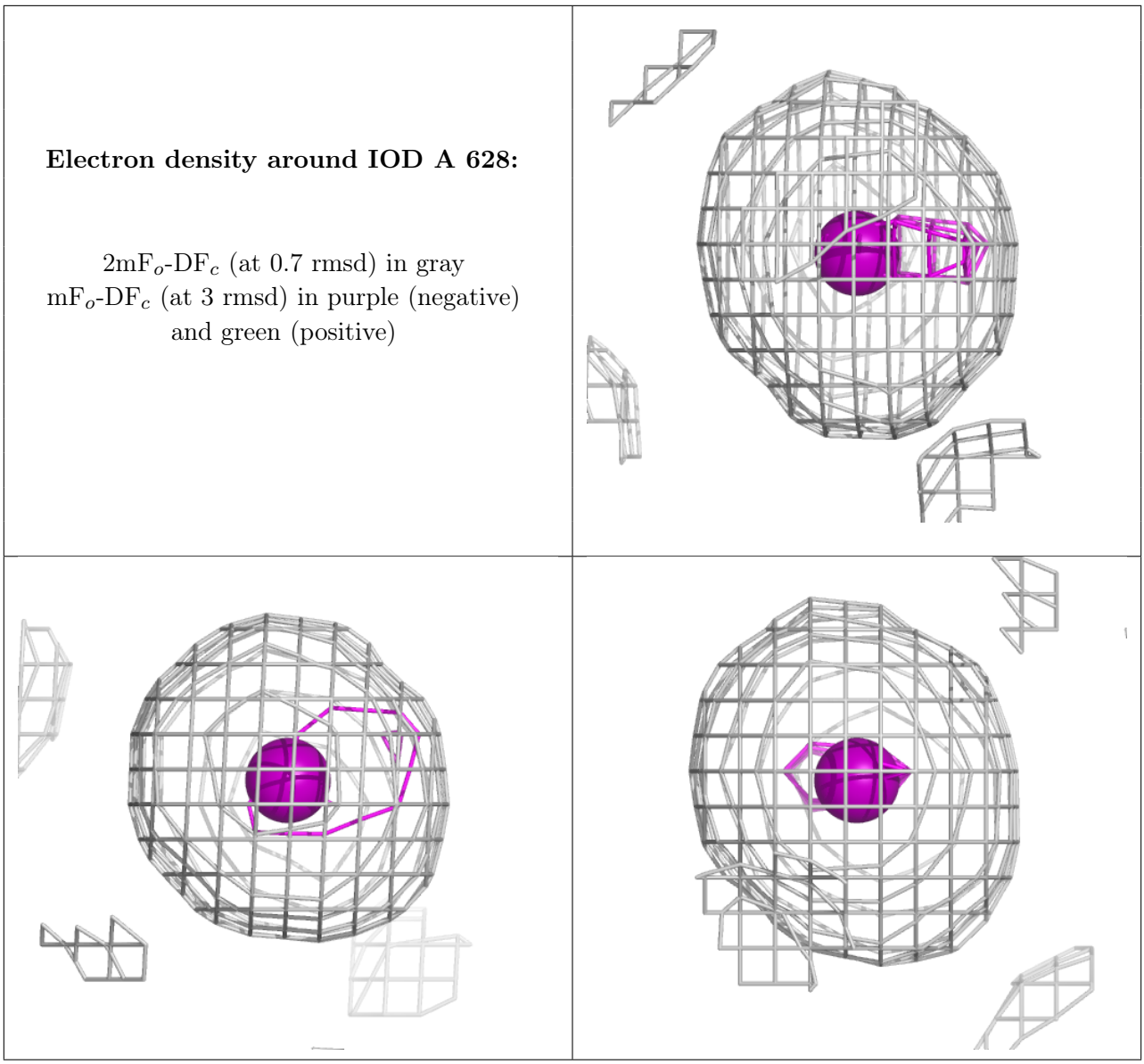
Electron density around IOD A 612:

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



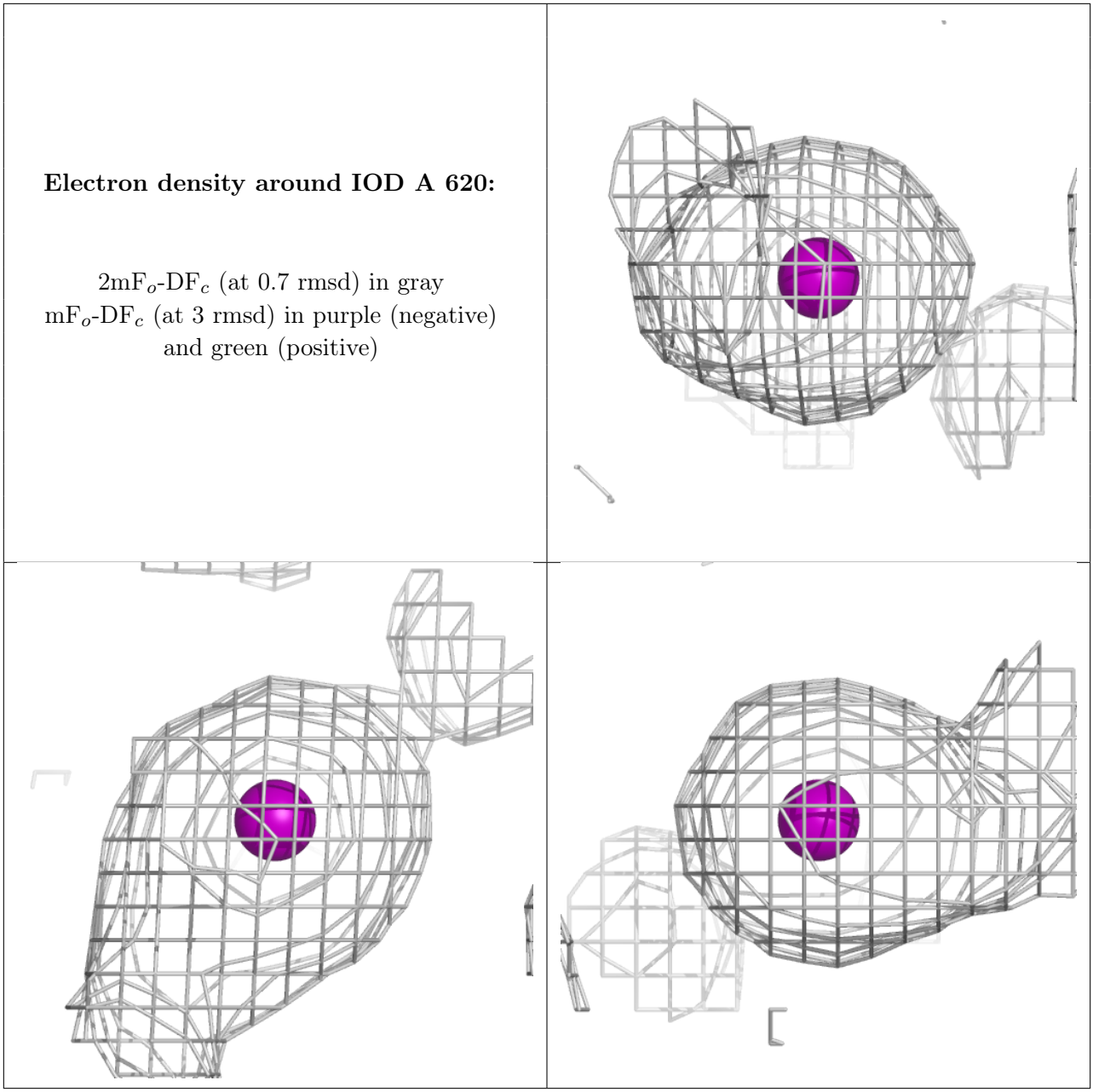
Electron density around IOD A 628:

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



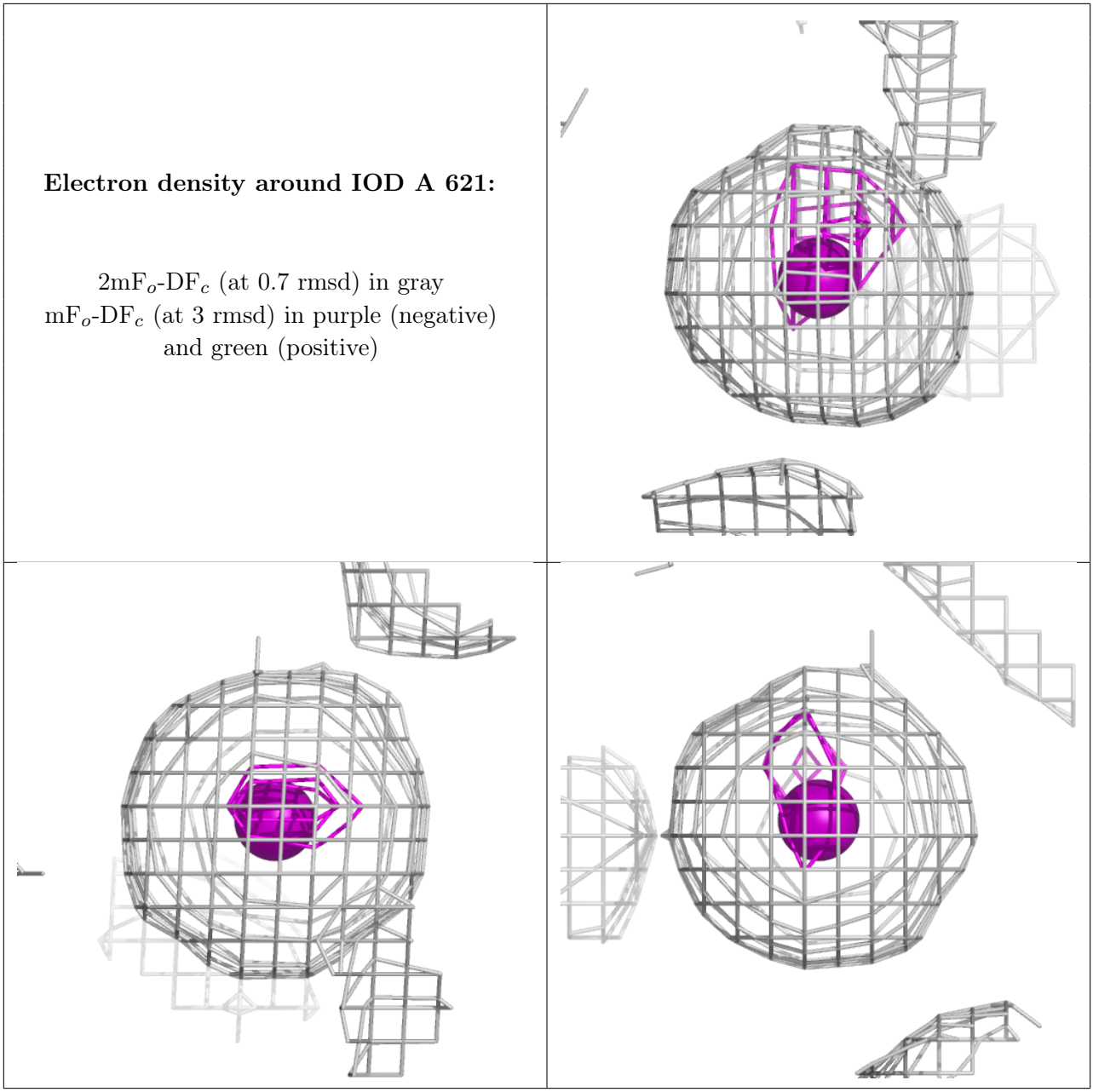
Electron density around IOD A 620:

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



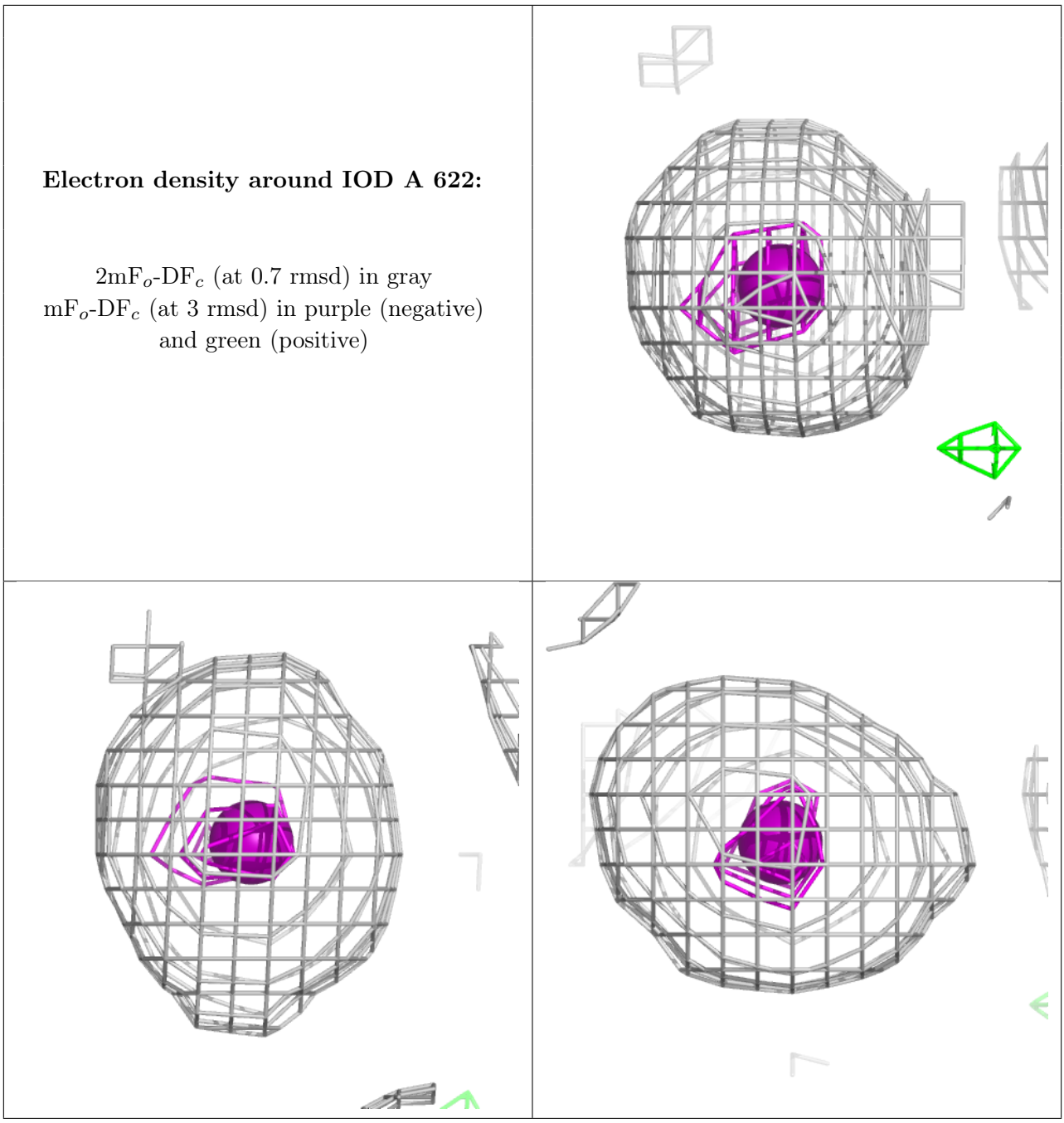
Electron density around IOD A 621:

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



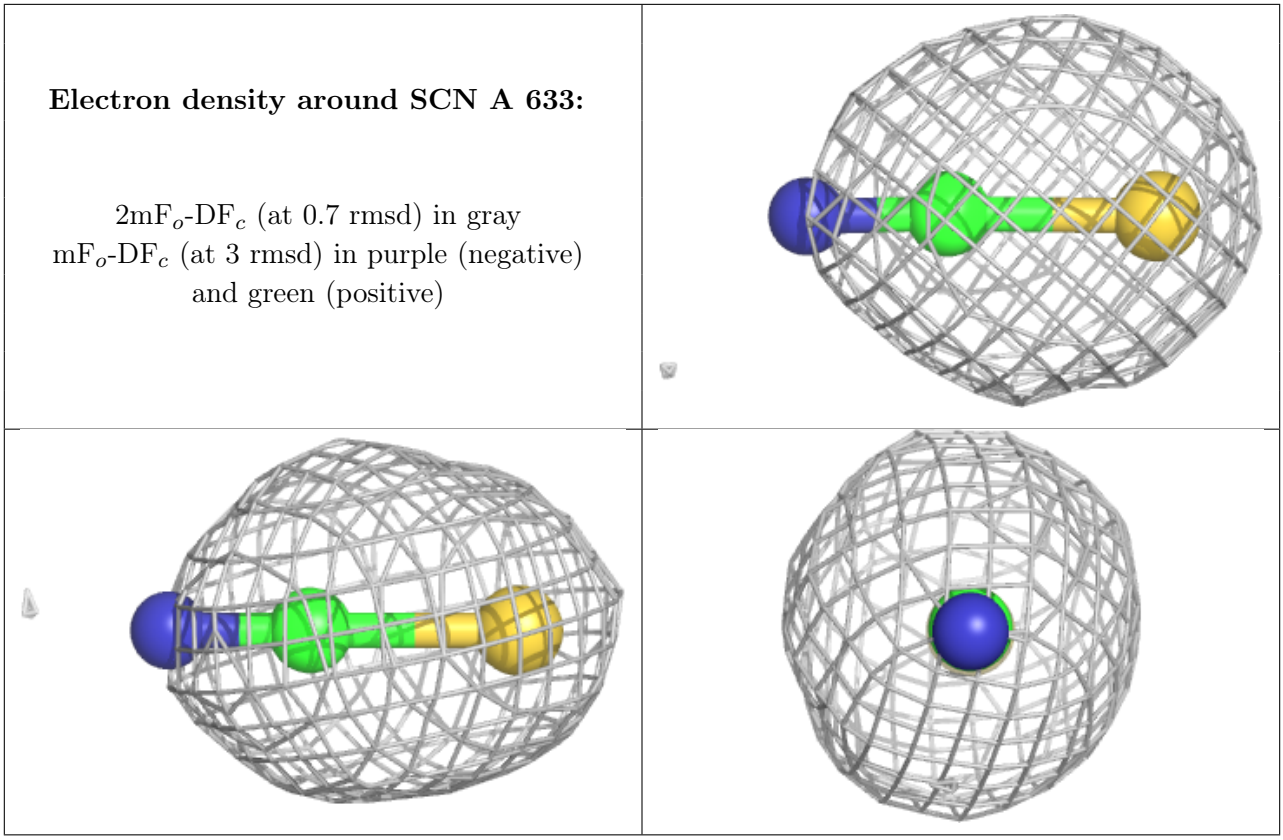
Electron density around IOD A 622:

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



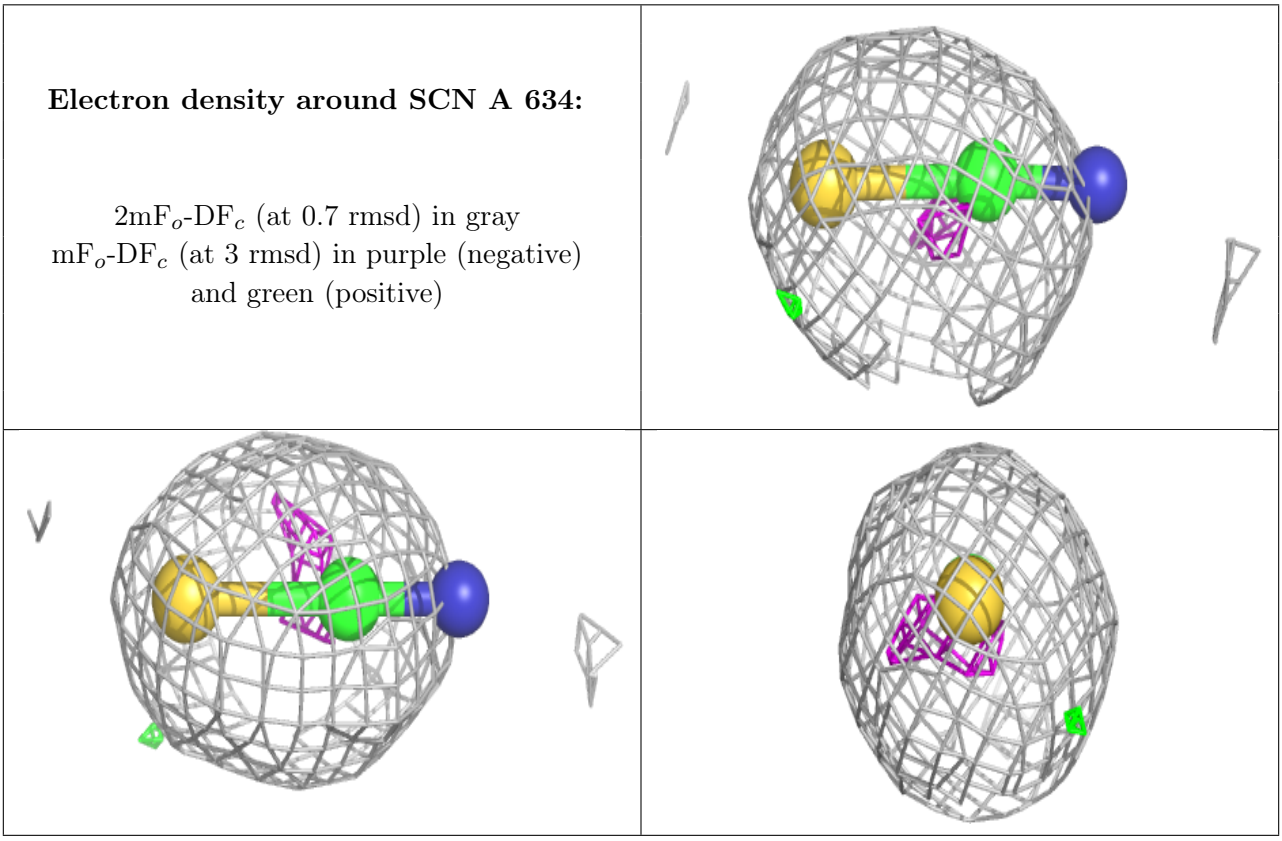
Electron density around SCN A 633:

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



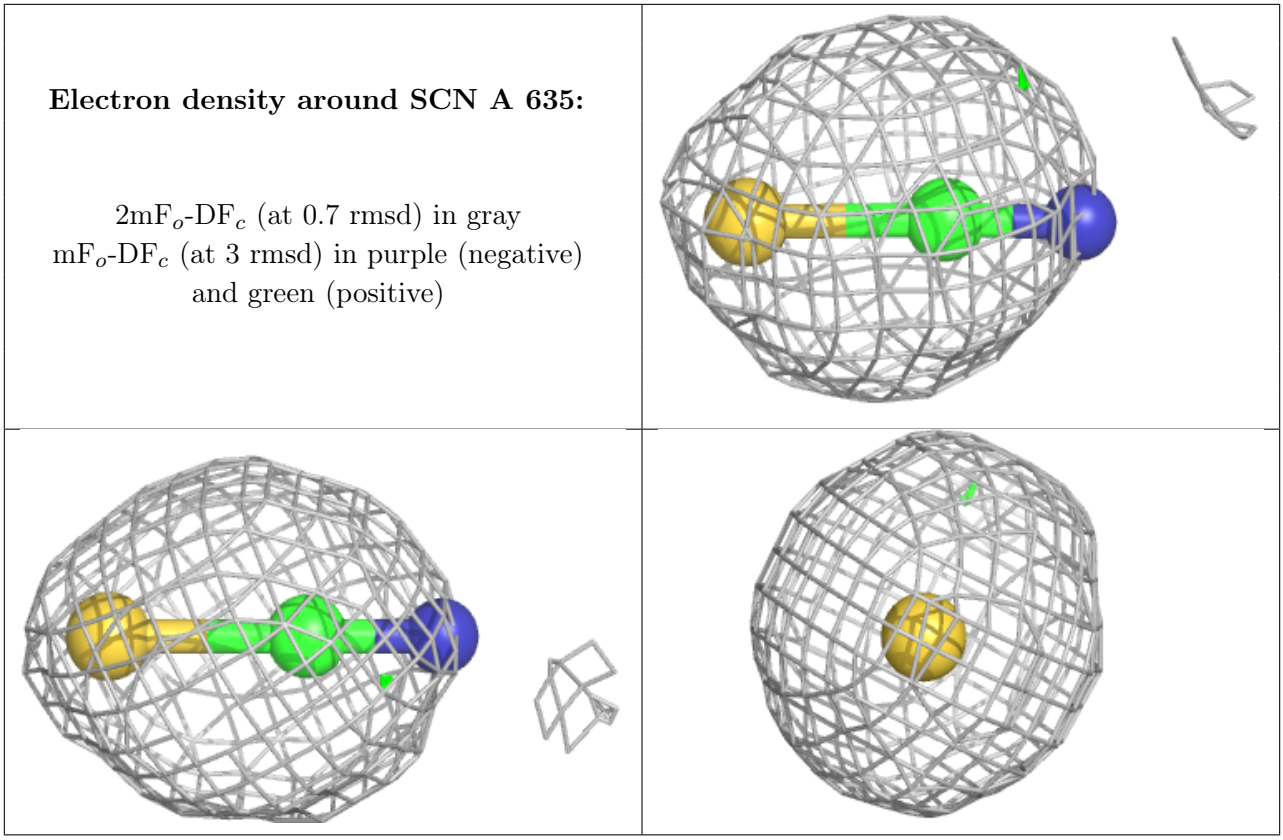
Electron density around SCN A 634:

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



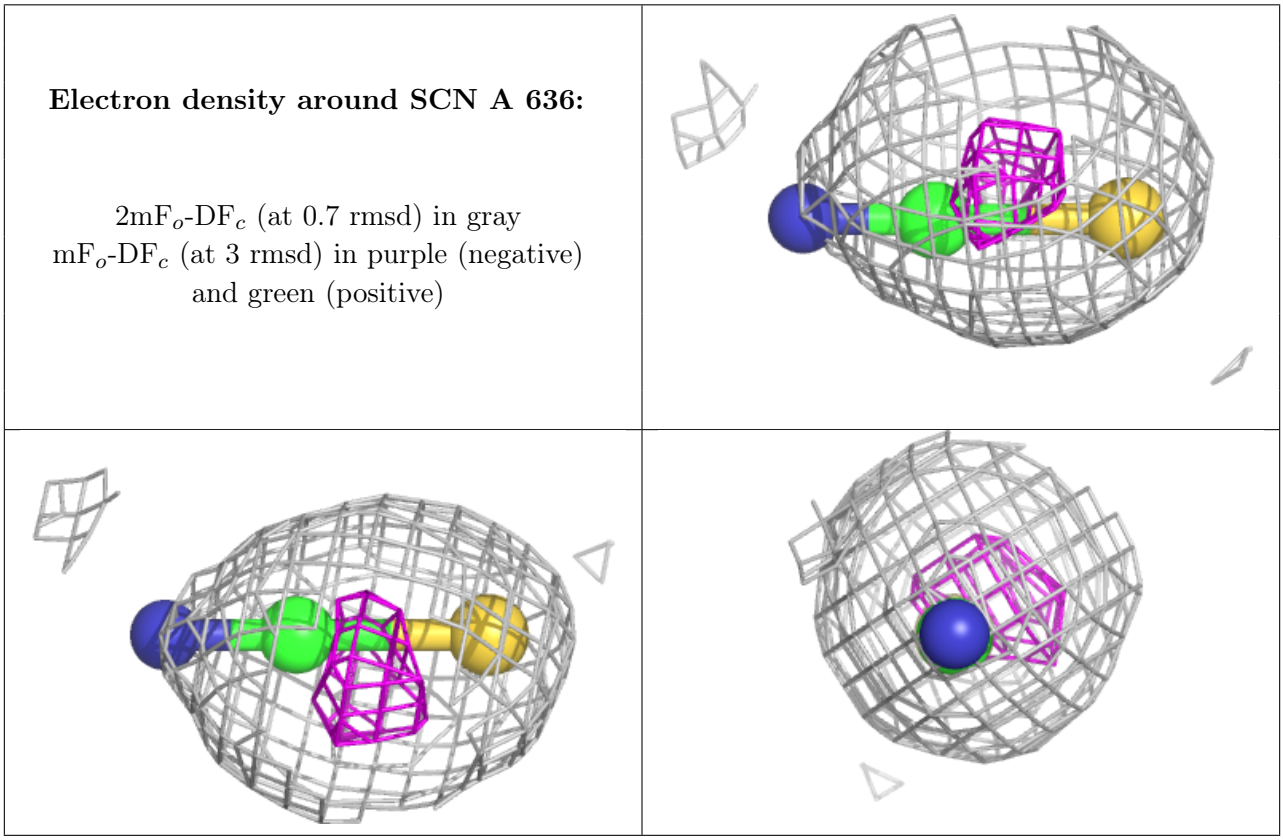
Electron density around SCN A 635:

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



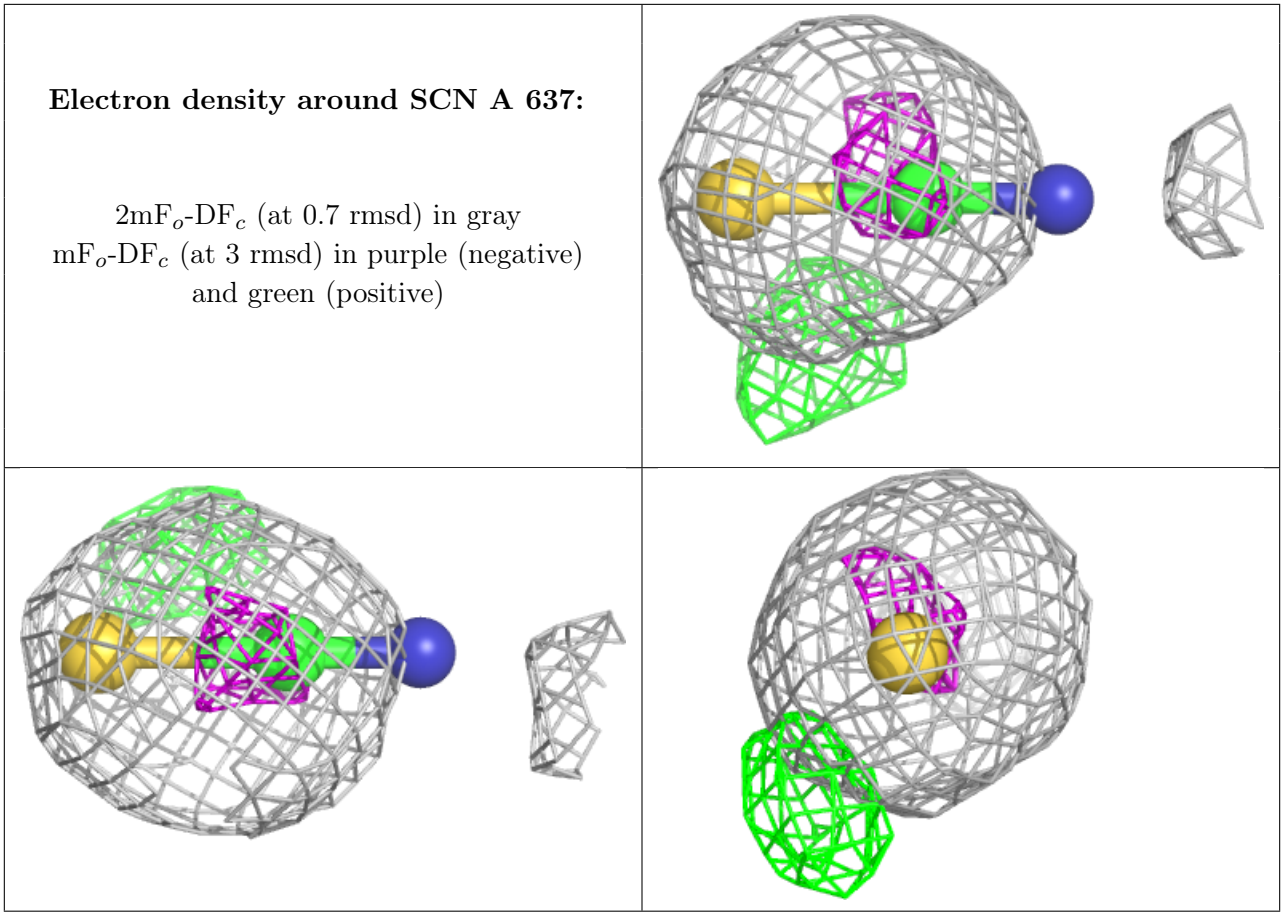
Electron density around SCN A 636:

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



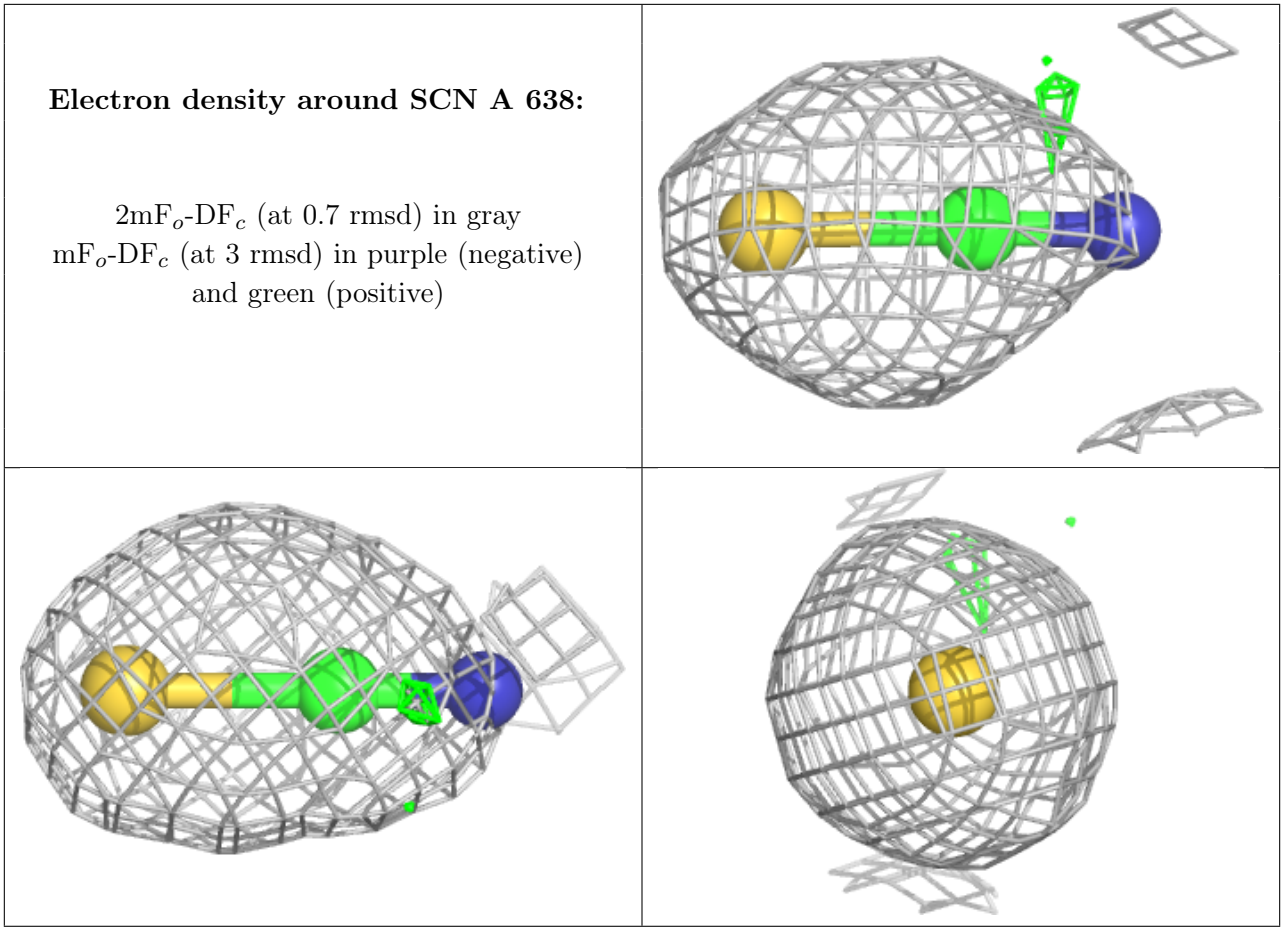
Electron density around SCN A 637:

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



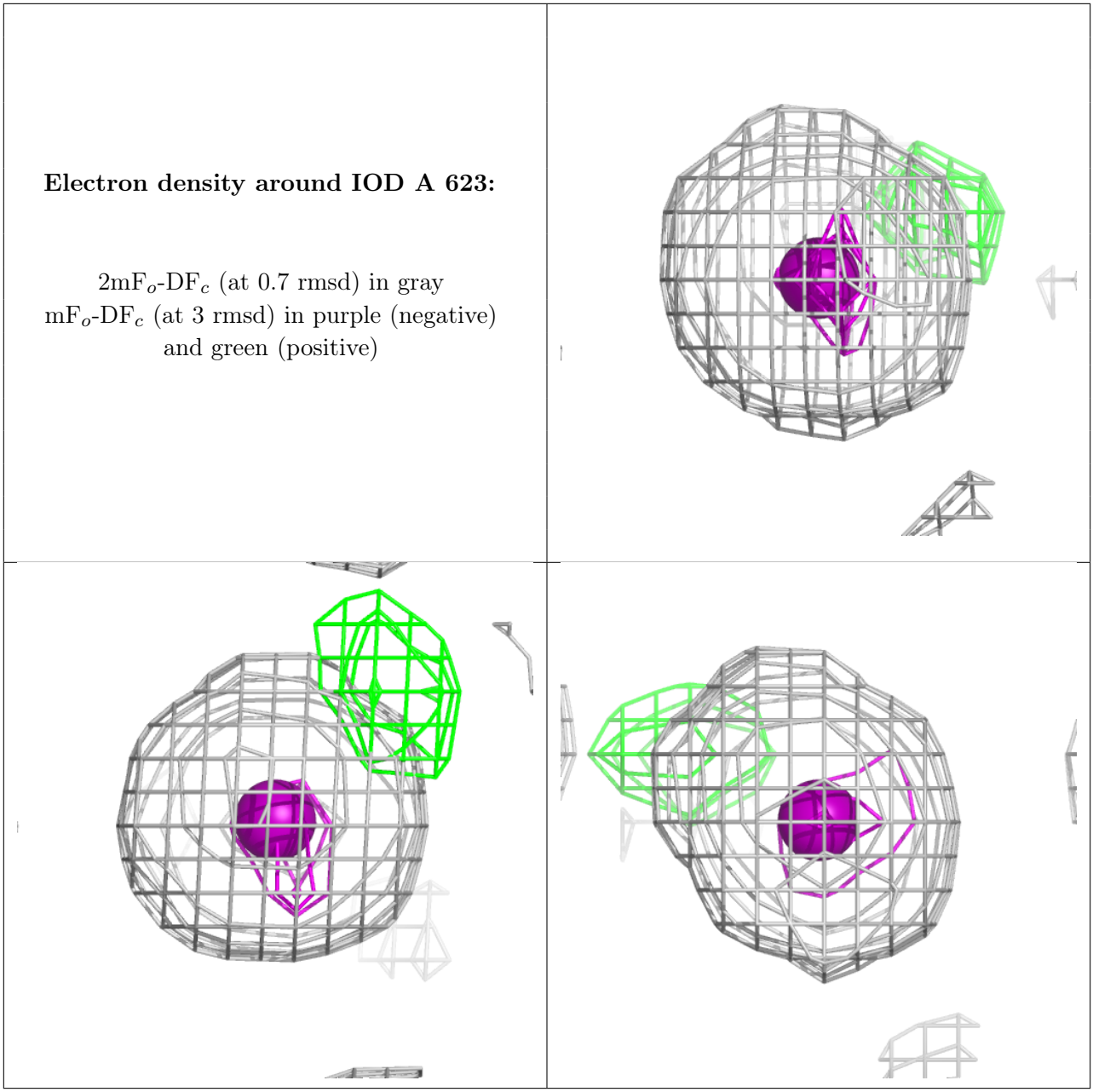
Electron density around SCN A 638:

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



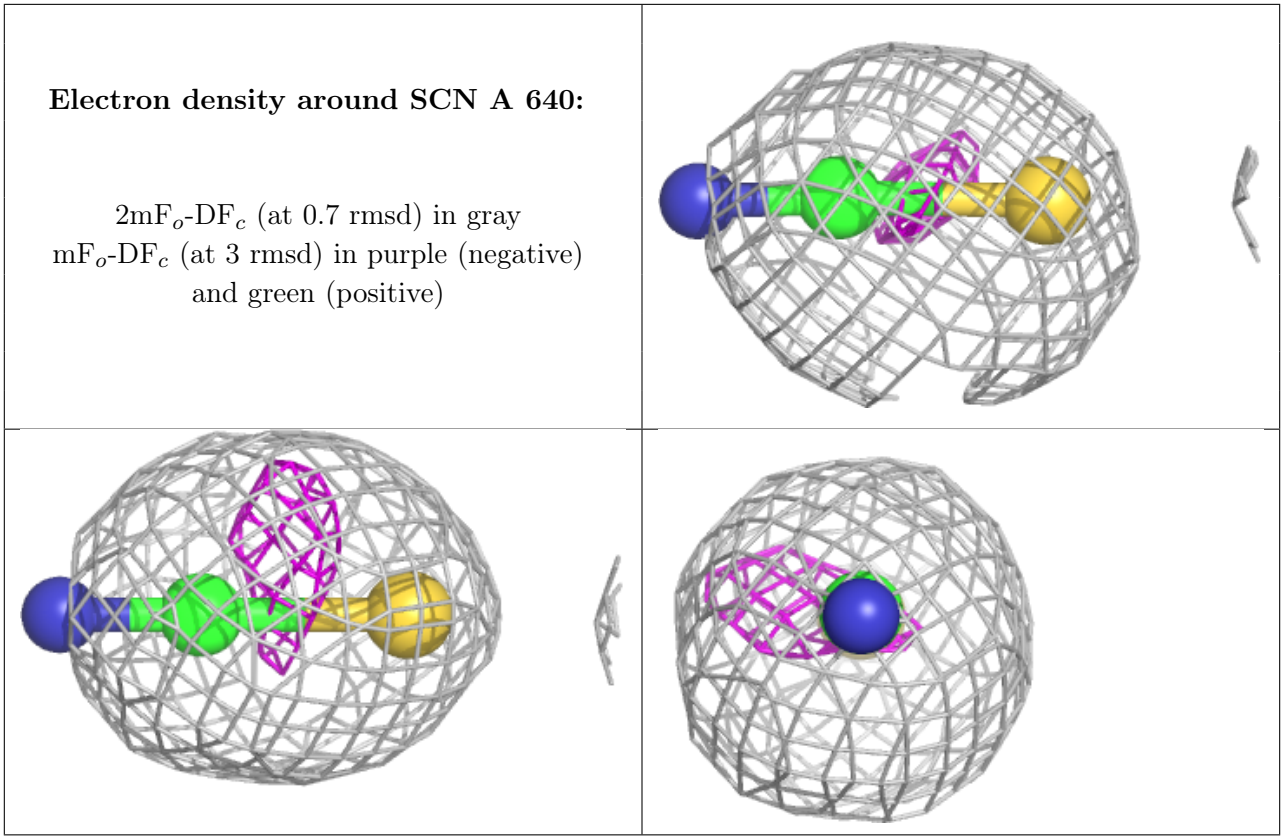
Electron density around IOD A 623:

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



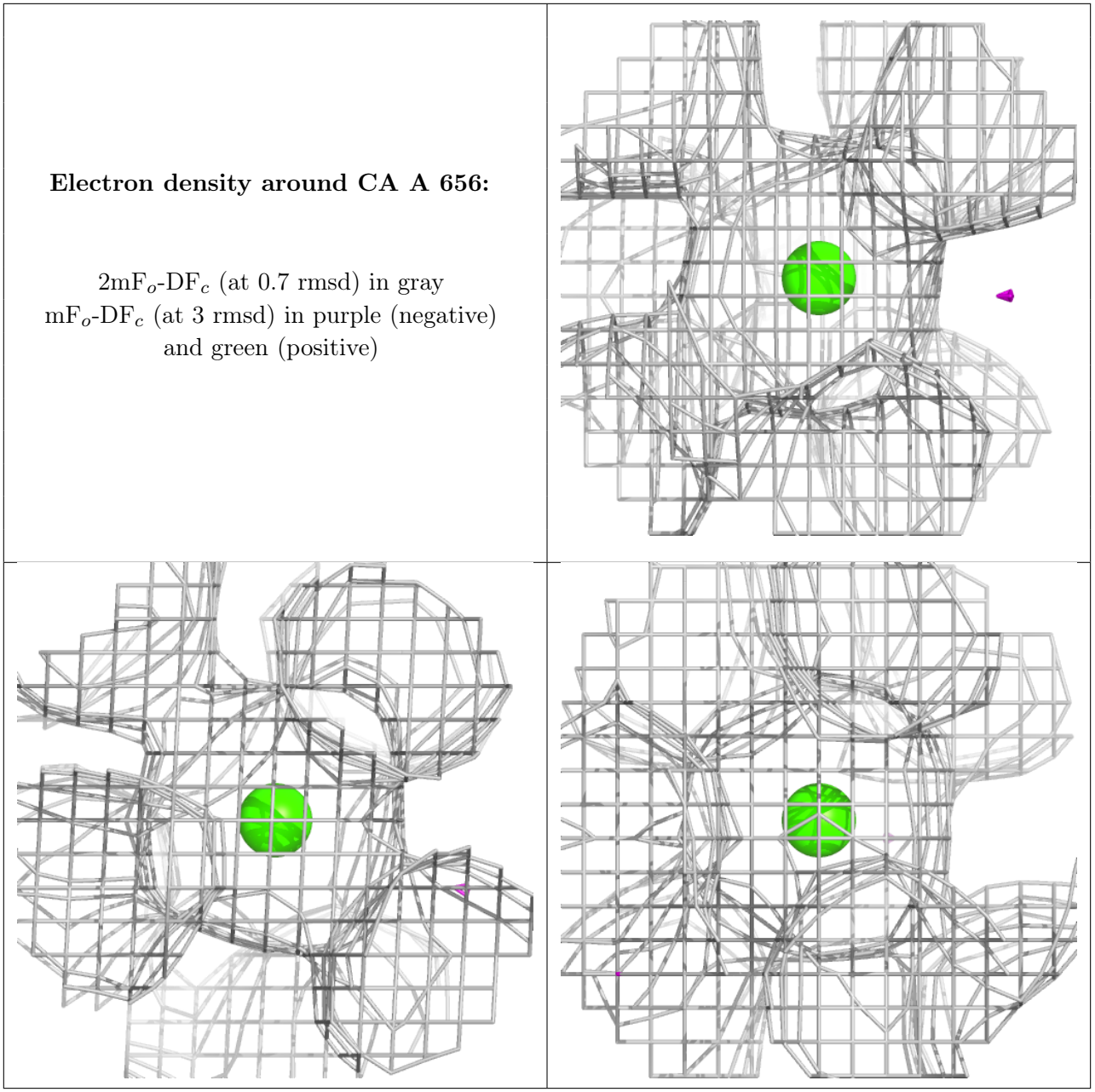
Electron density around SCN A 640:

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



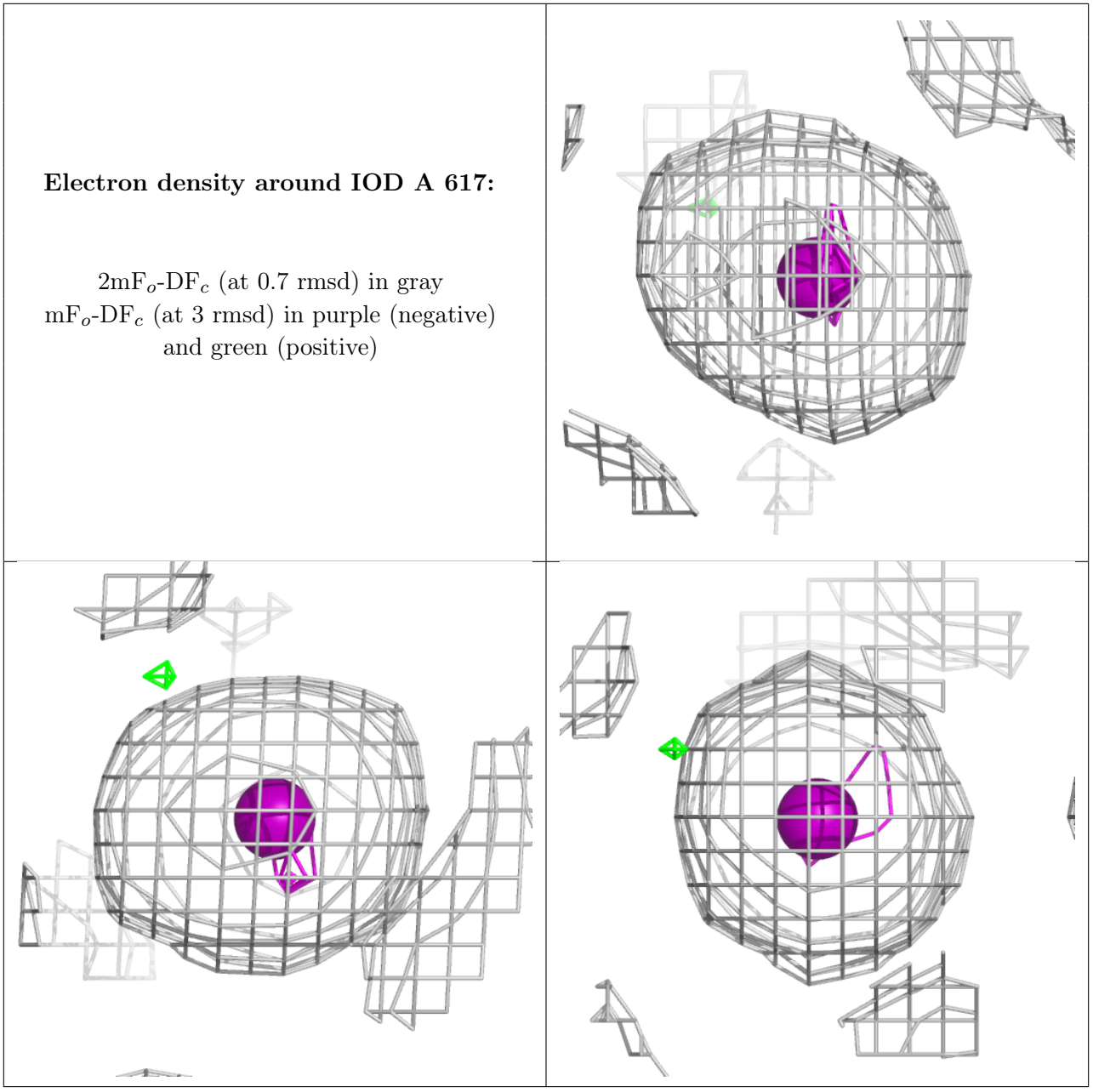
Electron density around CA A 656:

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



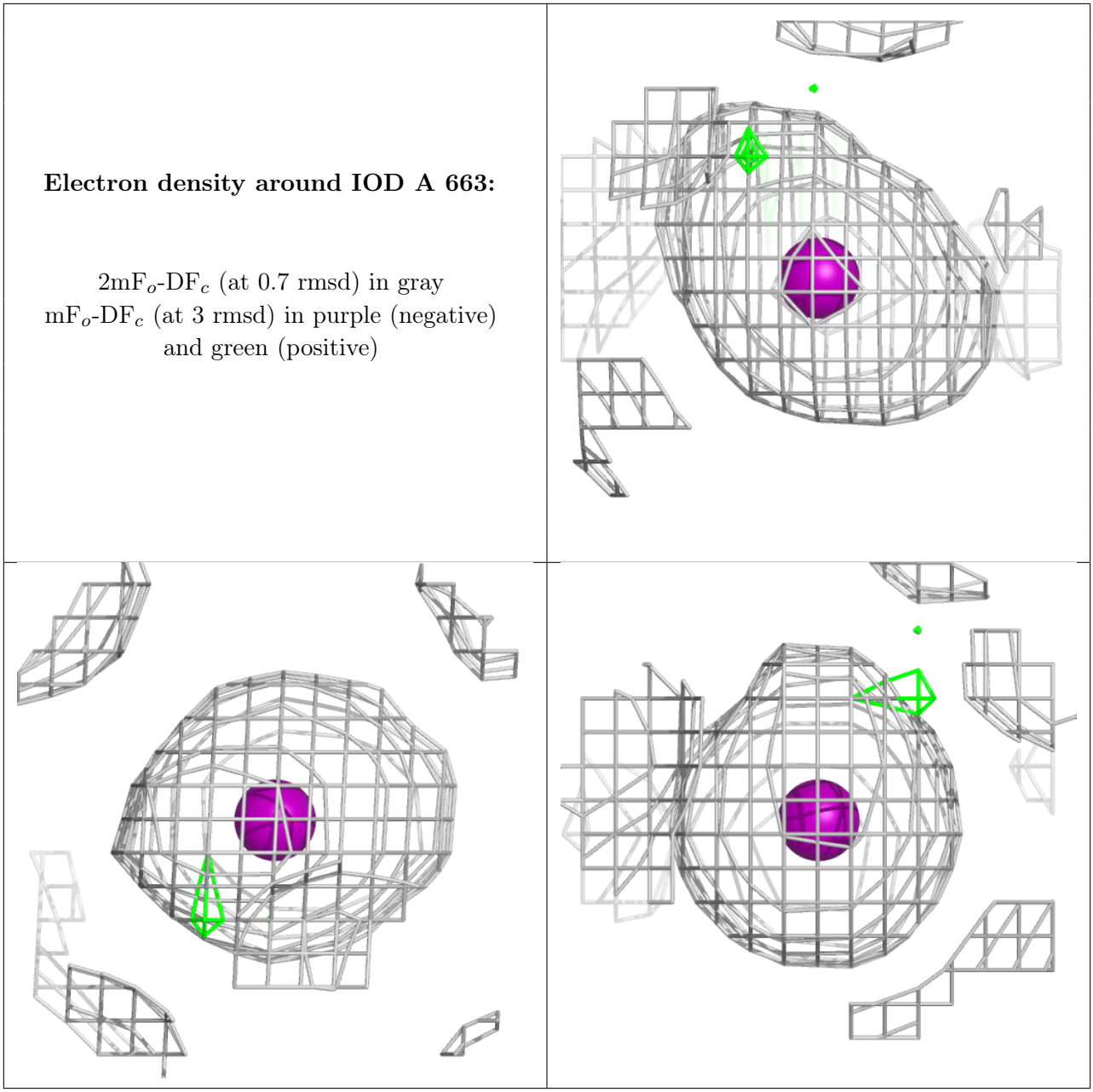
Electron density around IOD A 617:

$2mF_o$-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 663:

$2mF_o$-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.