wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2024 – 02:10 PM JST

PDB ID	:	8Y9X
Title	:	Crystal structure of the complex of lactoperoxidase with four inorganic substrates, SCN, I, Br and Cl
Authors	:	Viswanathan, V.; Singh, A.K.; Pandey, N.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2024-02-07
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

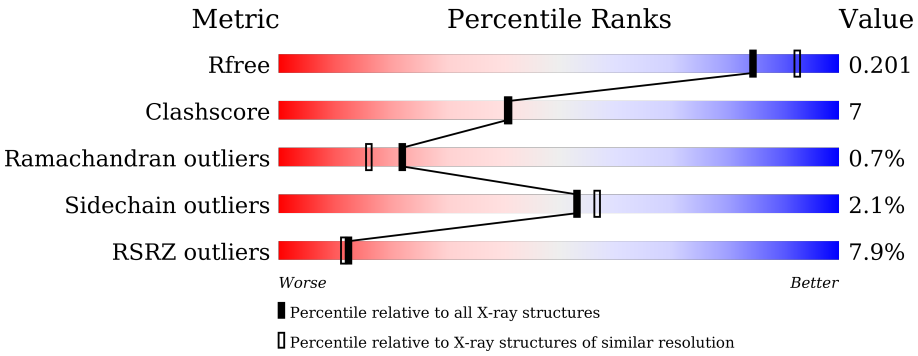
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	595	8% 86% 12%

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	603[A]	-	-	X	-

2 Entry composition (i)

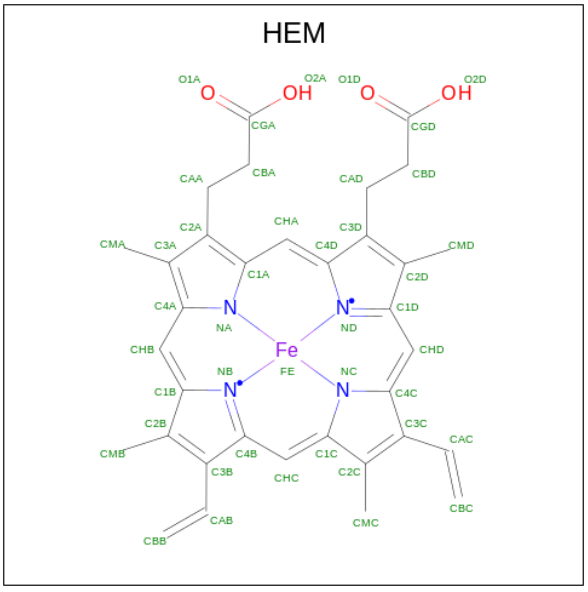
There are 10 unique types of molecules in this entry. The entry contains 5377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	592	4758	3033	841	855	29	0	3	0

- Molecule 2 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
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- 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	11	Total I 17 17	0	6

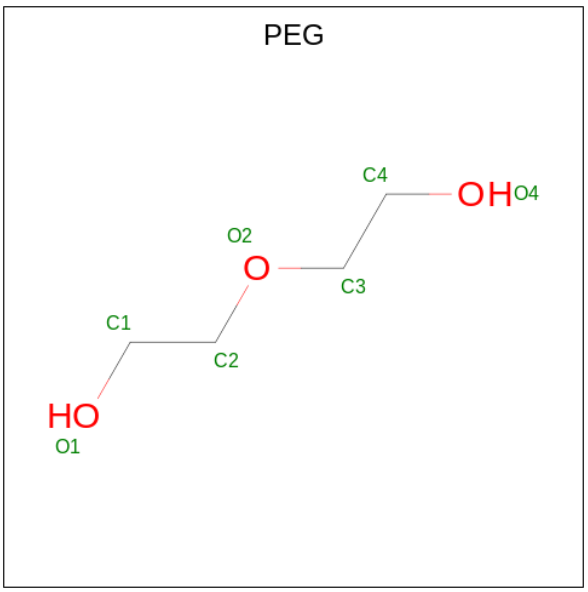
- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Br 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0

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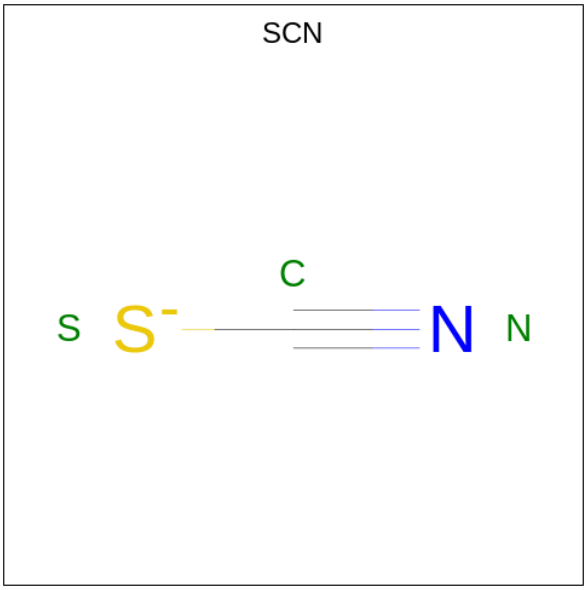
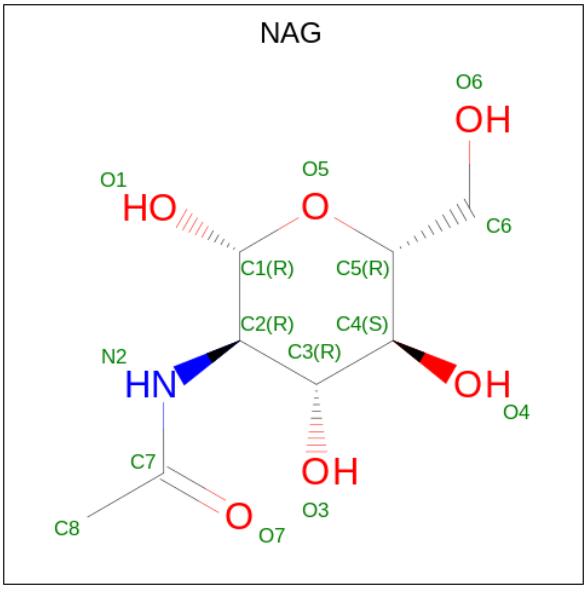
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 7 4 3	0	0

- Molecule 8 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 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
9	A	1	Total C N O 14 8 1 5	0	0
9	A	1	Total C N O 13 8 1 4	0	0
9	A	1	Total C N O 15 8 1 6	0	0
9	A	1	Total C N O 14 8 1 5	0	0
9	A	1	Total C N O 14 8 1 5	0	0
9	A	1	Total C N O 14 8 1 5	0	0

- Molecule 10 is water.

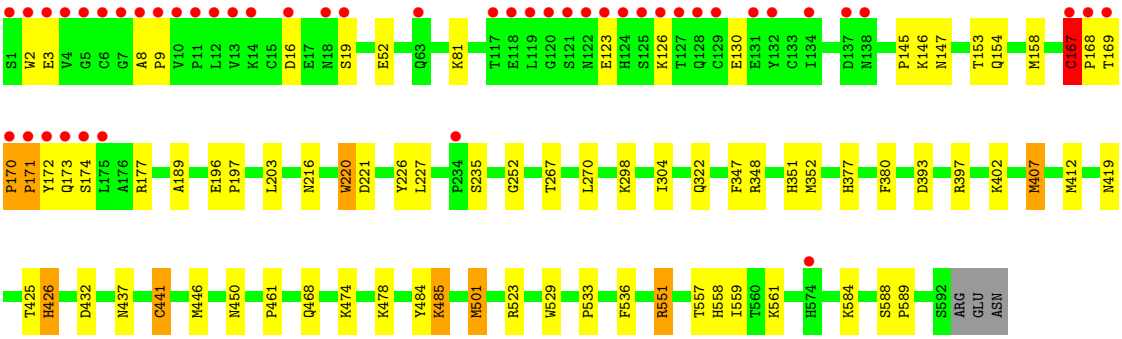
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	407	Total O 408 408	0	1

3 Residue-property plots (i)

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

- Molecule 1: Lactoperoxidase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.35Å 80.33Å 73.39Å 90.00° 103.94° 90.00°	Depositor
Resolution (Å)	43.52 – 2.00 43.52 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.52-2.00) 96.5 (43.52-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.42 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.151 , 0.195 0.160 , 0.201	Depositor DCC
R_{free} test set	1971 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 64.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5377	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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, BR, HEM, NAG, PEG, CL, SCN, IOD

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	0.43	0/4892	0.85	7/6636 (0.1%)

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

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

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	501	MET	CG-SD-CE	-9.42	85.13	100.20
1	A	348	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	A	177	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	A	426	HIS	CB-CA-C	5.90	122.20	110.40
1	A	407[A]	MET	CG-SD-CE	5.45	108.92	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	397	ARG	Sidechain

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	4758	0	4685	60	0
2	A	43	0	30	1	0
3	A	1	0	0	0	0
4	A	17	0	0	9	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	49	0	70	4	0
8	A	15	0	0	1	0
9	A	84	0	78	7	0
10	A	408	0	0	11	0
All	All	5377	0	4863	70	0

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

The worst 5 of 70 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)
9:A:626:NAG:C4	9:A:627:NAG:O1	1.77	1.31
4:A:604:IOD:I	10:A:1029:HOH:O	2.59	0.90
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.57	0.84
9:A:629:NAG:O4	9:A:630:NAG:C1	2.34	0.75
4:A:610:IOD:I	10:A:858:HOH:O	2.74	0.74

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	593/595 (100%)	573 (97%)	16 (3%)	4 (1%)	22 16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	174	SER
1	A	171	PRO
1	A	170	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	518/518 (100%)	506 (98%)	12 (2%)	50 53

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	347	PHE
1	A	441[A]	CYS
1	A	533	PRO
1	A	441[B]	CYS
1	A	19	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 20 are monoatomic - leaving 19 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	PEG	A	615	-	6,6,6	0.15	0	5,5,5	0.14	0
7	PEG	A	614	-	6,6,6	0.35	0	5,5,5	0.49	0
9	NAG	A	627	-	15,15,15	0.17	0	21,21,21	1.04	2 (9%)
2	HEM	A	601	1	41,50,50	1.56	7 (17%)	45,82,82	1.79	15 (33%)
9	NAG	A	630	-	14,14,15	0.42	0	17,19,21	2.19	2 (11%)
9	NAG	A	626	1	13,13,15	0.52	0	14,17,21	1.31	1 (7%)
9	NAG	A	629	1	14,14,15	0.41	0	17,19,21	1.05	0
7	PEG	A	617	-	6,6,6	0.19	0	5,5,5	0.16	0
7	PEG	A	619	-	6,6,6	0.18	0	5,5,5	0.19	0
7	PEG	A	616	-	6,6,6	0.15	0	5,5,5	0.19	0
8	SCN	A	622	-	1,2,2	0.42	0	0,1,1	-	-
9	NAG	A	628	1	14,14,15	0.37	0	17,19,21	0.99	1 (5%)
8	SCN	A	621	-	1,2,2	1.78	0	0,1,1	-	-
9	NAG	A	625	1	14,14,15	0.41	0	17,19,21	1.30	2 (11%)
8	SCN	A	631	-	1,2,2	0.31	0	0,1,1	-	-
8	SCN	A	624	-	1,2,2	0.00	0	0,1,1	-	-
7	PEG	A	620	-	6,6,6	0.20	0	5,5,5	0.16	0
7	PEG	A	618	-	6,6,6	0.21	0	5,5,5	0.25	0
8	SCN	A	623	-	1,2,2	0.06	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
7	PEG	A	615	-	-	1/4/4/4	-
9	NAG	A	628	1	-	0/6/23/26	0/1/1/1
9	NAG	A	630	-	-	0/6/23/26	0/1/1/1
7	PEG	A	614	-	-	1/4/4/4	-
9	NAG	A	626	1	-	2/6/19/26	0/1/1/1
9	NAG	A	627	-	-	0/6/26/26	0/1/1/1
2	HEM	A	601	1	-	4/12/54/54	-
9	NAG	A	629	1	-	0/6/23/26	0/1/1/1
7	PEG	A	617	-	-	1/4/4/4	-
7	PEG	A	620	-	-	4/4/4/4	-
9	NAG	A	625	1	-	2/6/23/26	0/1/1/1
7	PEG	A	618	-	-	0/4/4/4	-
7	PEG	A	619	-	-	3/4/4/4	-
7	PEG	A	616	-	-	2/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C1B-NB	-4.36	1.32	1.40
2	A	601	HEM	C4D-ND	-4.02	1.33	1.40
2	A	601	HEM	FE-NB	2.87	2.11	1.96
2	A	601	HEM	C4B-NB	-2.82	1.33	1.38
2	A	601	HEM	CHA-C4D	2.63	1.41	1.35

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	630	NAG	O5-C1-C2	-8.26	98.25	111.29
2	A	601	HEM	C1B-NB-C4B	4.68	109.91	105.07
2	A	601	HEM	C4B-CHC-C1C	4.45	128.43	122.56
2	A	601	HEM	CMC-C2C-C3C	3.69	131.58	124.68
9	A	625	NAG	C1-O5-C5	3.60	117.06	112.19

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	626	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	A	625	NAG	C8-C7-N2-C2
9	A	625	NAG	O7-C7-N2-C2
7	A	619	PEG	O1-C1-C2-O2
7	A	614	PEG	O1-C1-C2-O2

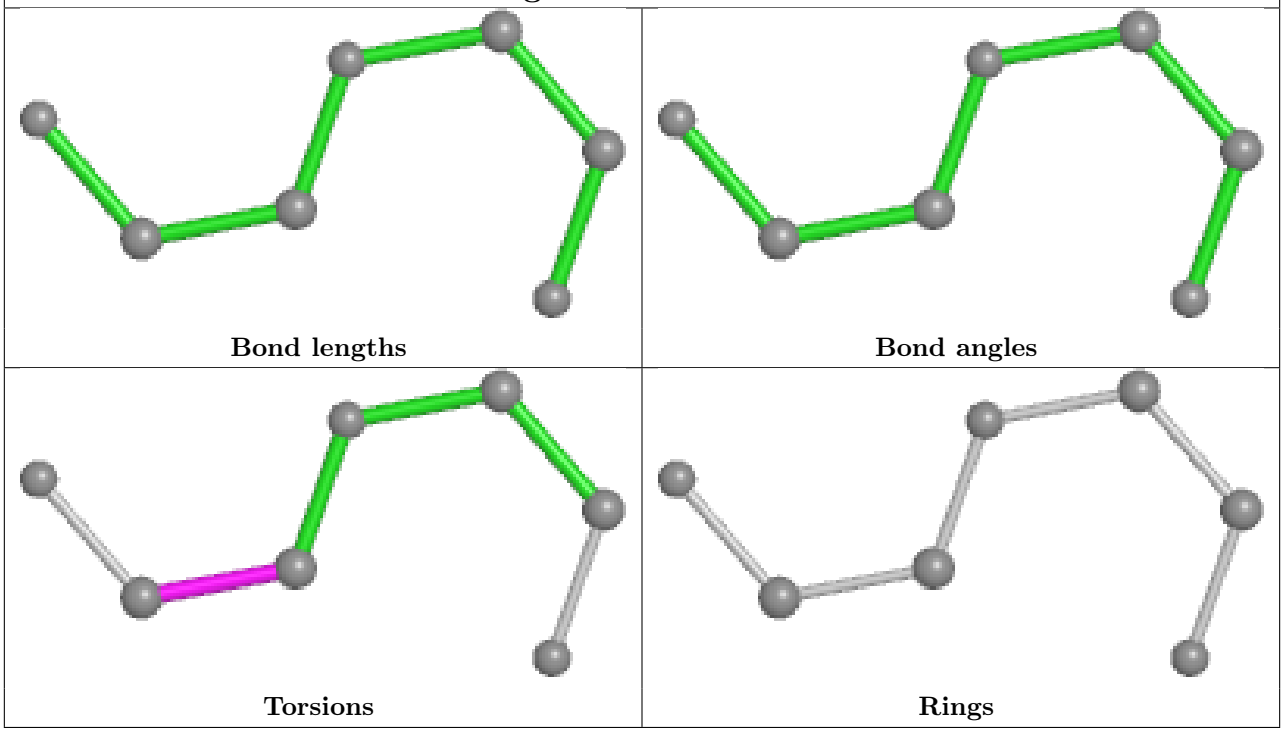
There are no ring outliers.

9 monomers are involved in 13 short contacts:

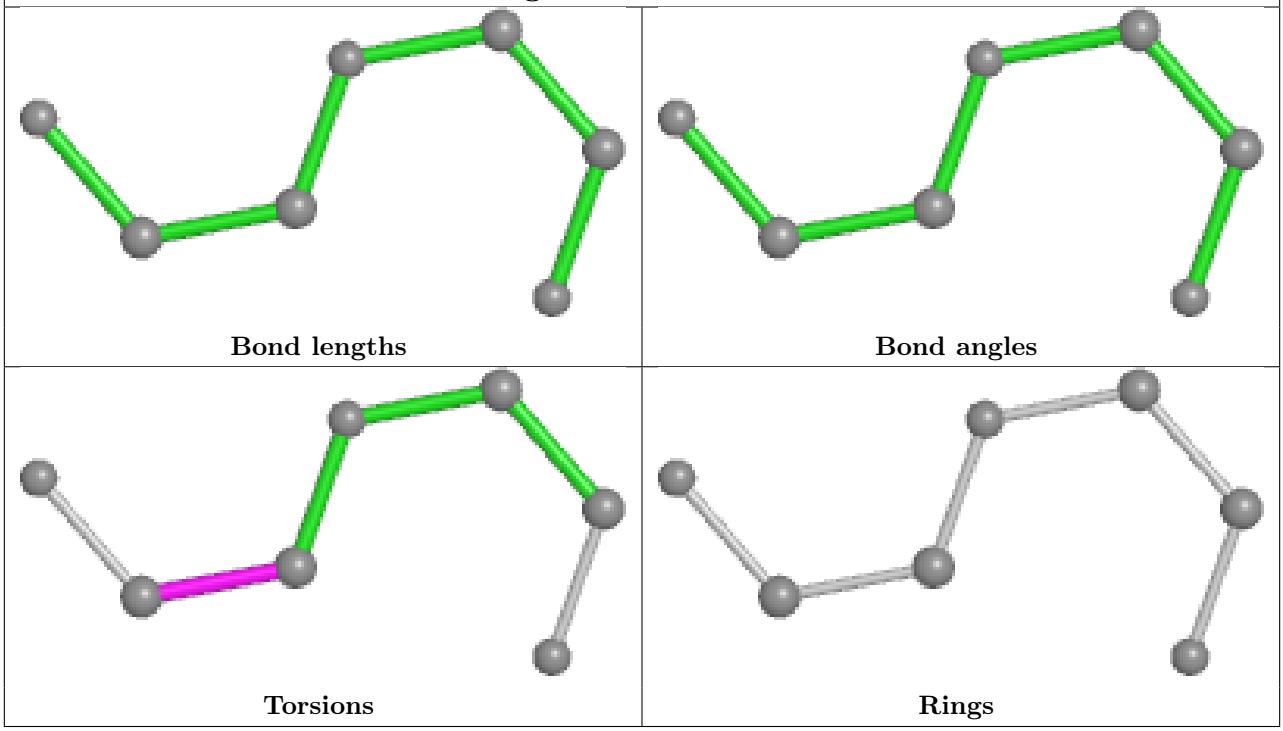
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	614	PEG	1	0
9	A	627	NAG	2	0
2	A	601	HEM	1	0
9	A	630	NAG	4	0
9	A	626	NAG	2	0
9	A	629	NAG	4	0
9	A	625	NAG	1	0
7	A	618	PEG	3	0
8	A	623	SCN	1	0

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.

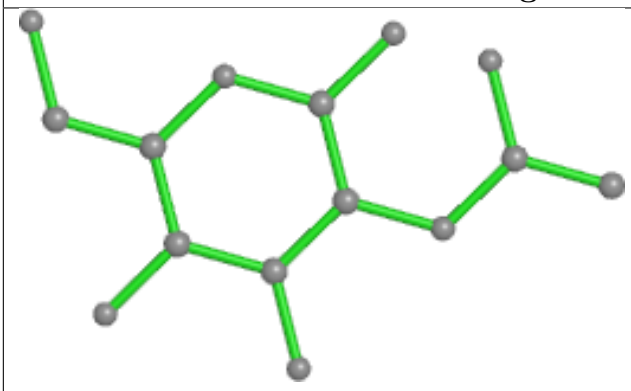
Ligand PEG A 615



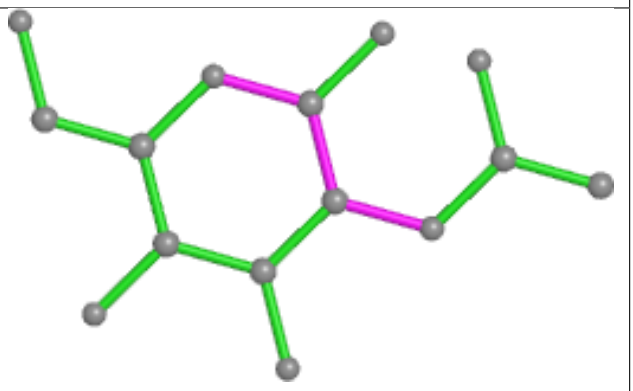
Ligand PEG A 614



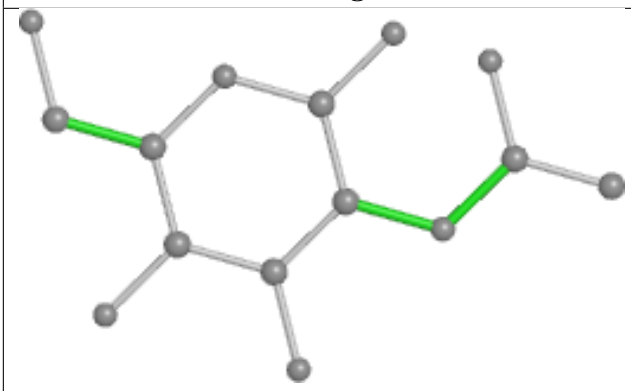
Ligand NAG A 627



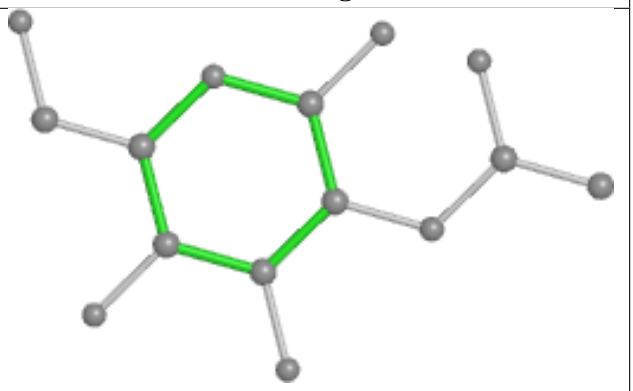
Bond lengths



Bond angles

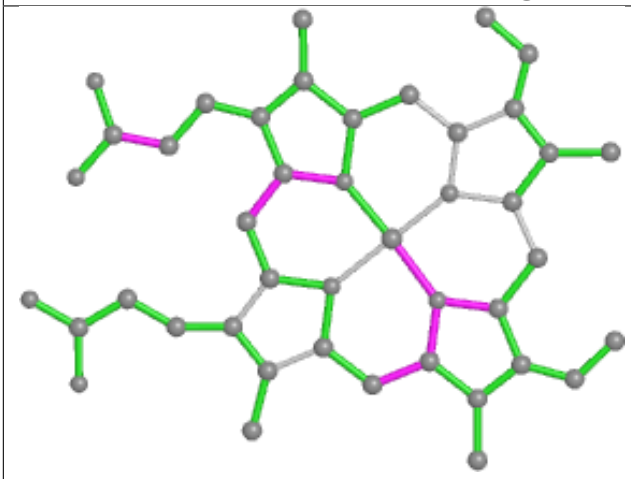


Torsions

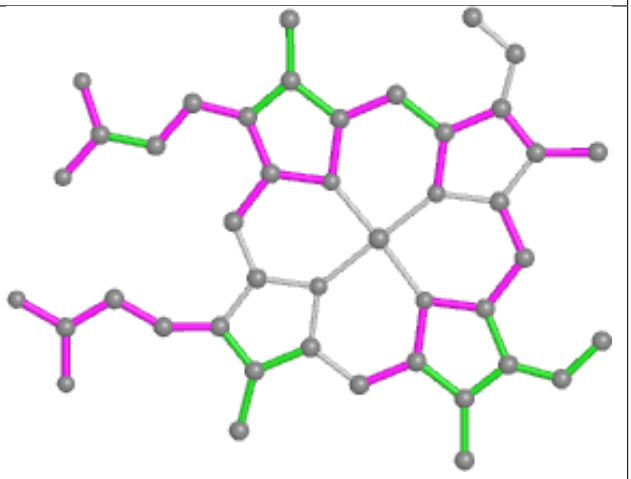


Rings

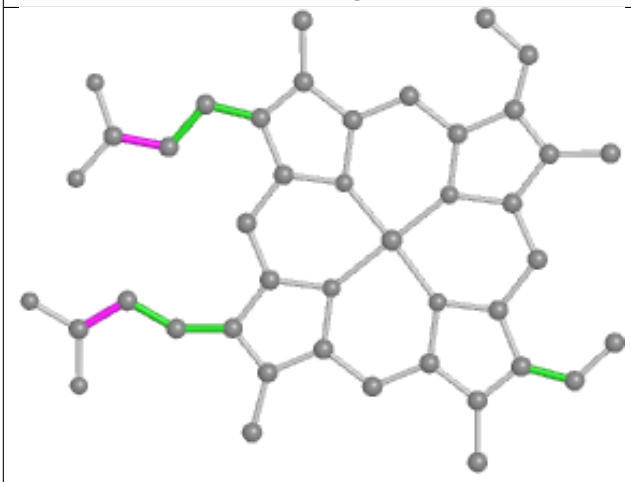
Ligand HEM A 601



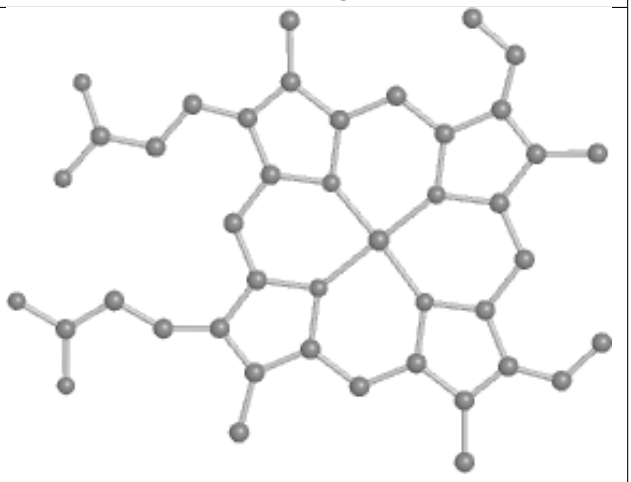
Bond lengths



Bond angles

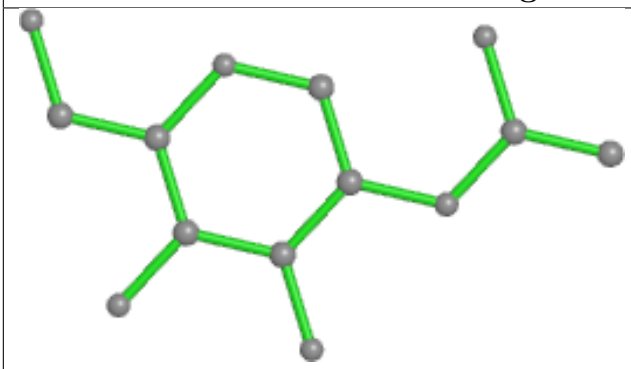


Torsions

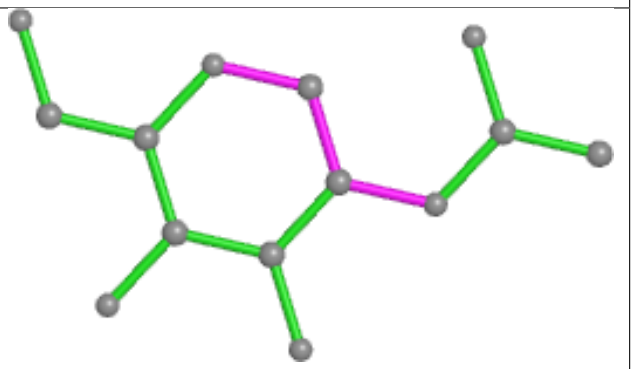


Rings

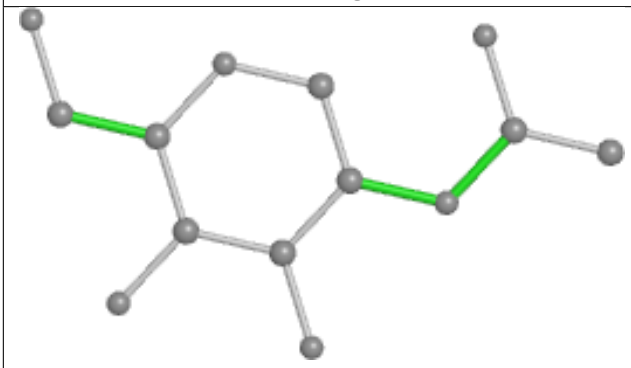
Ligand NAG A 630



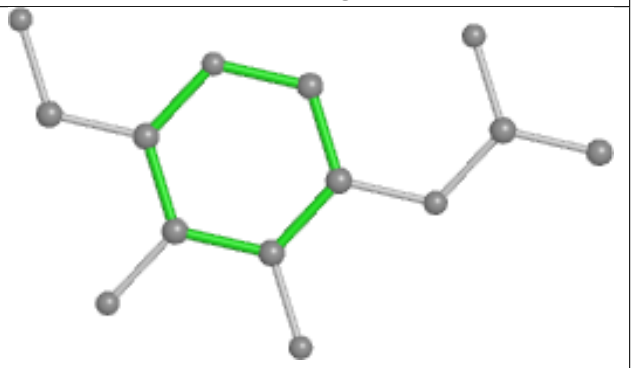
Bond lengths



Bond angles

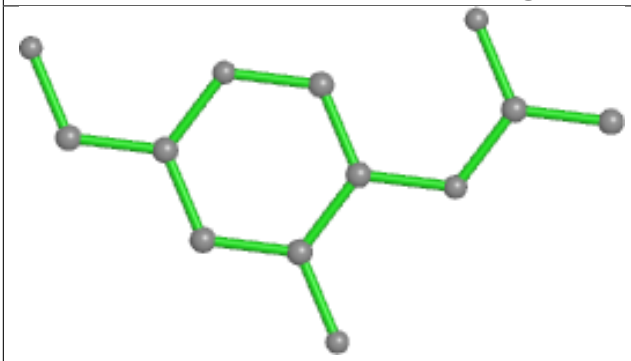


Torsions

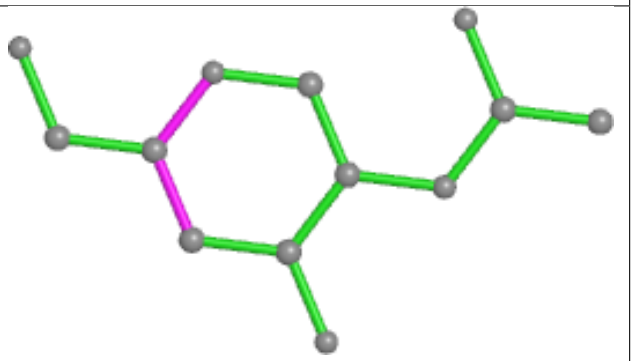


Rings

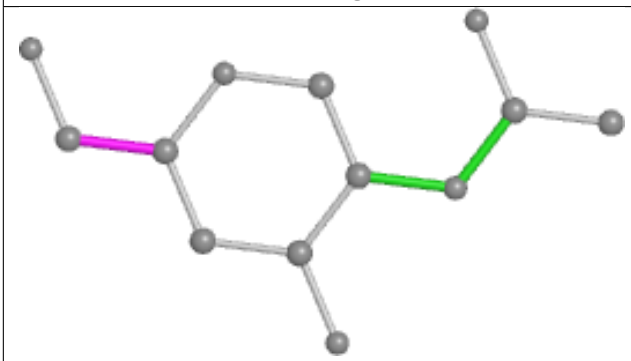
Ligand NAG A 626



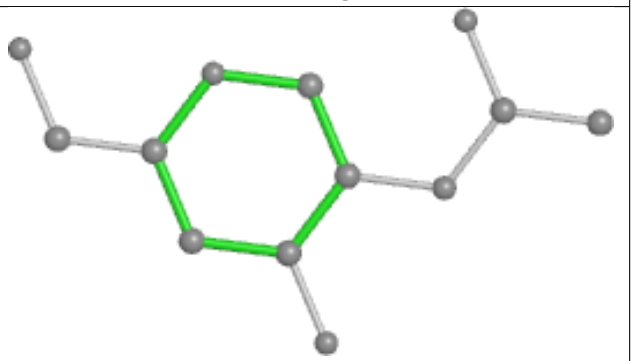
Bond lengths



Bond angles

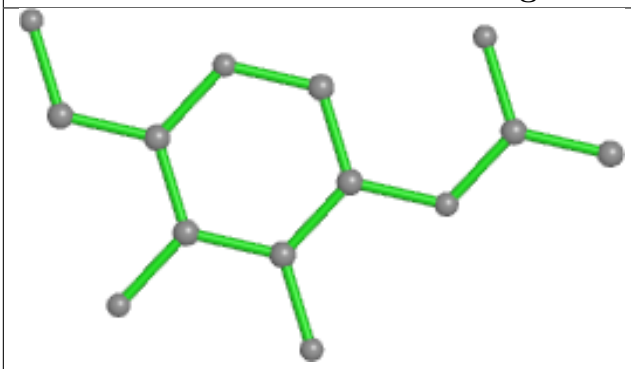


Torsions

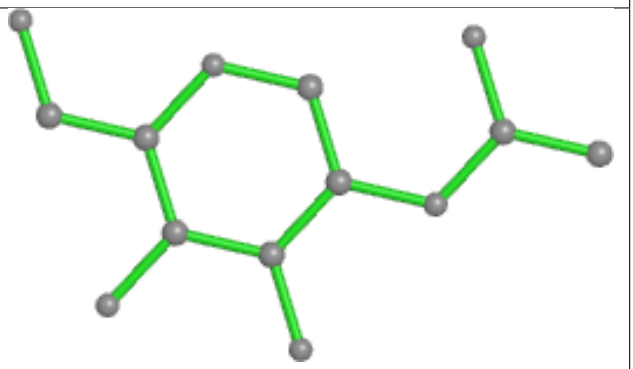


Rings

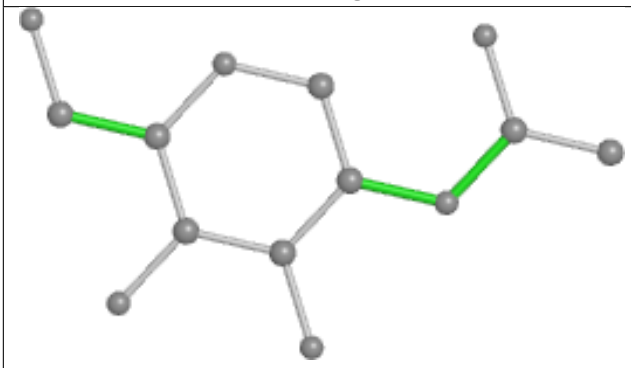
Ligand NAG A 629



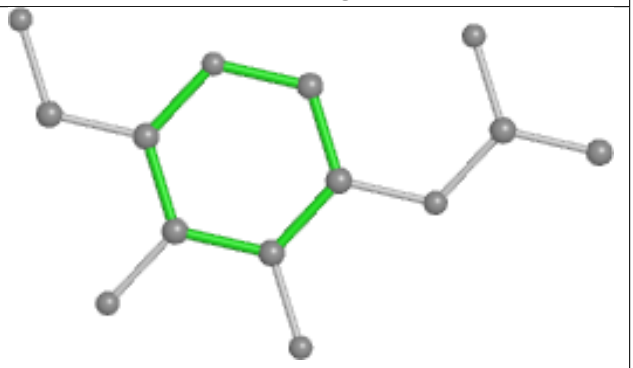
Bond lengths



Bond angles

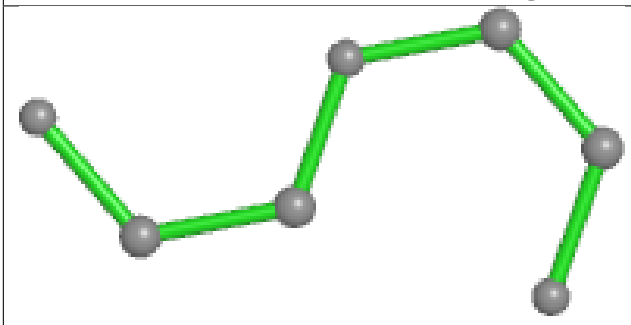


Torsions

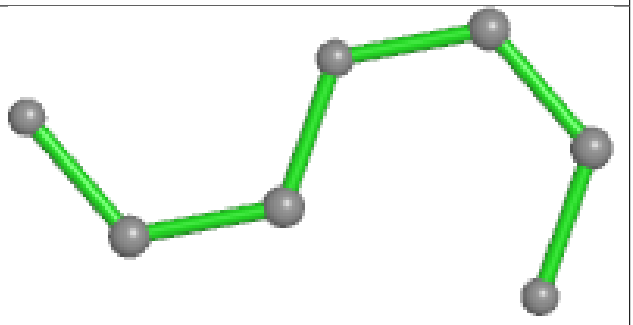


Rings

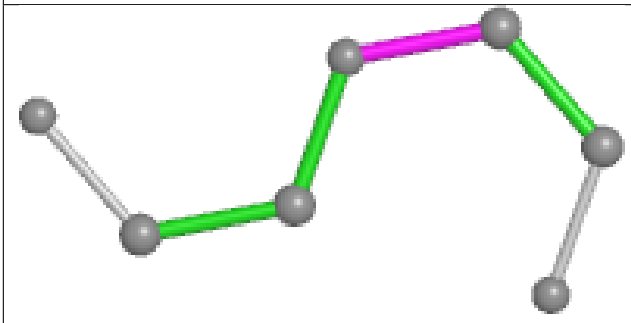
Ligand PEG A 617



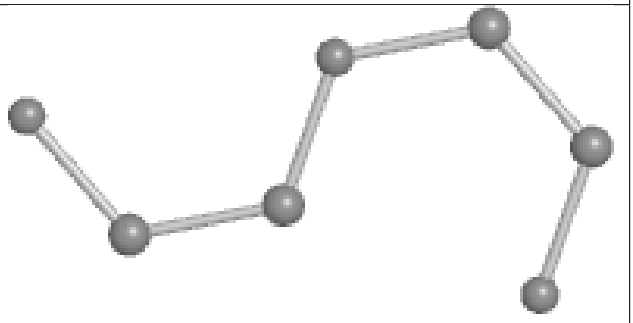
Bond lengths



Bond angles

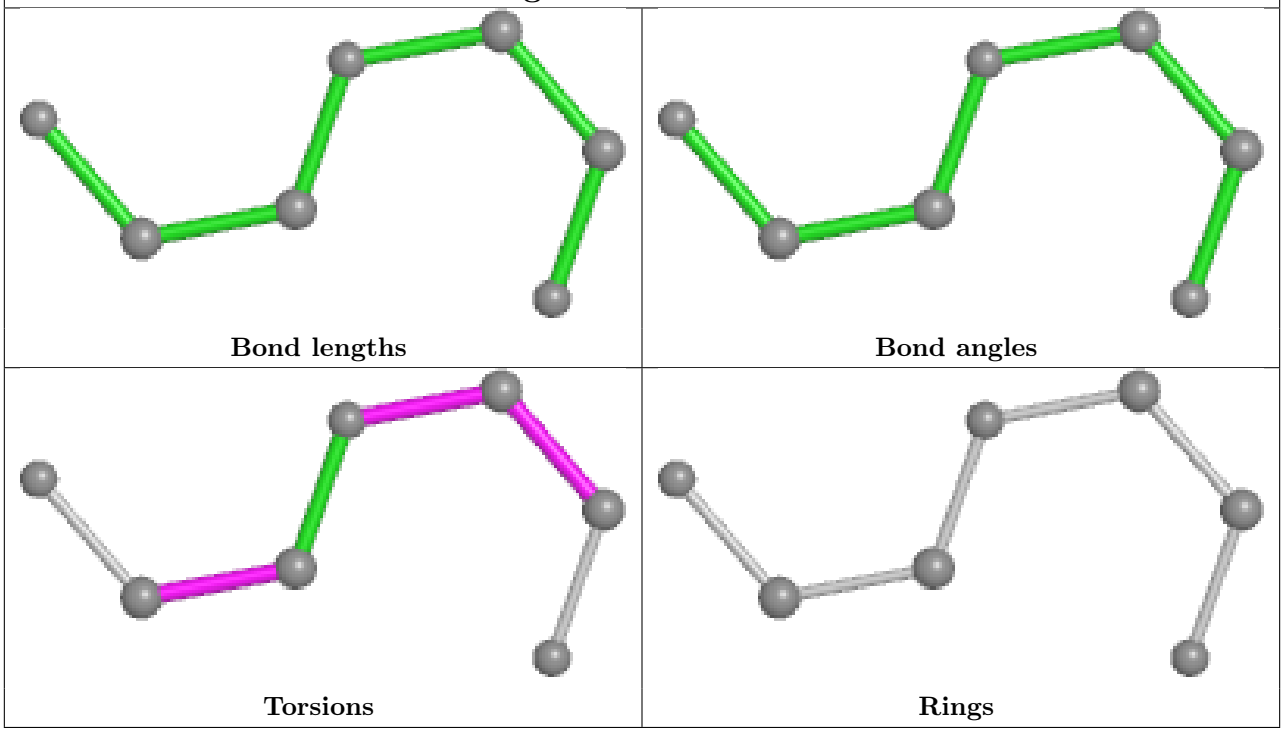


Torsions

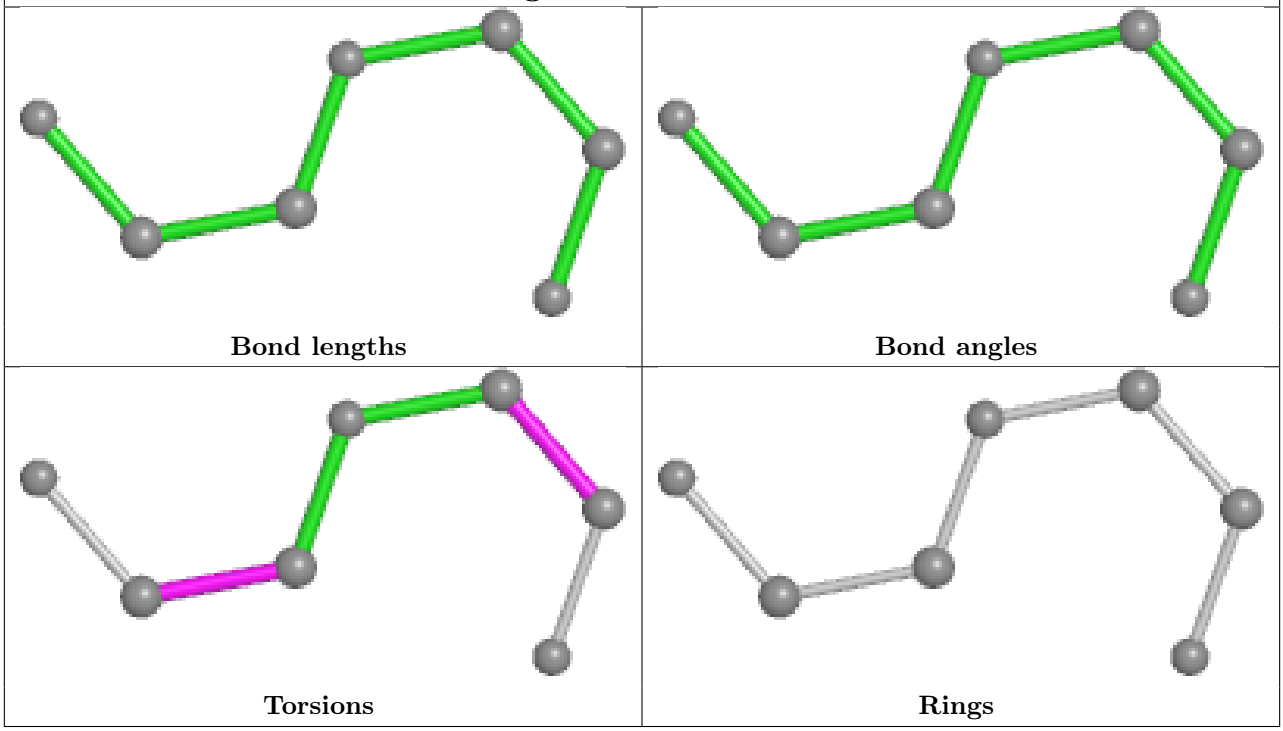


Rings

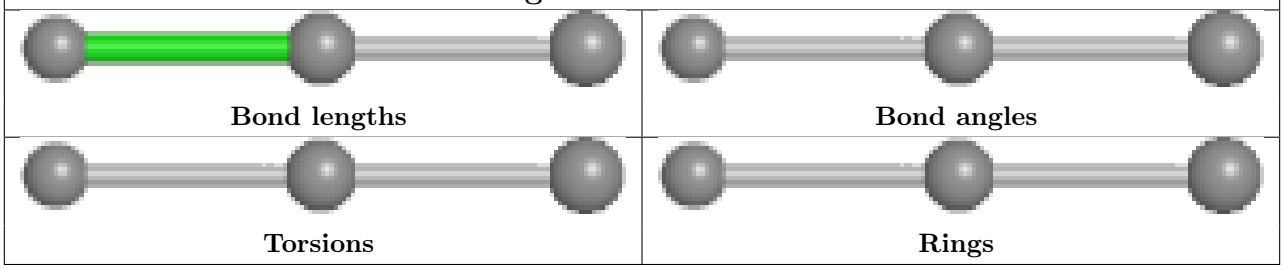
Ligand PEG A 619



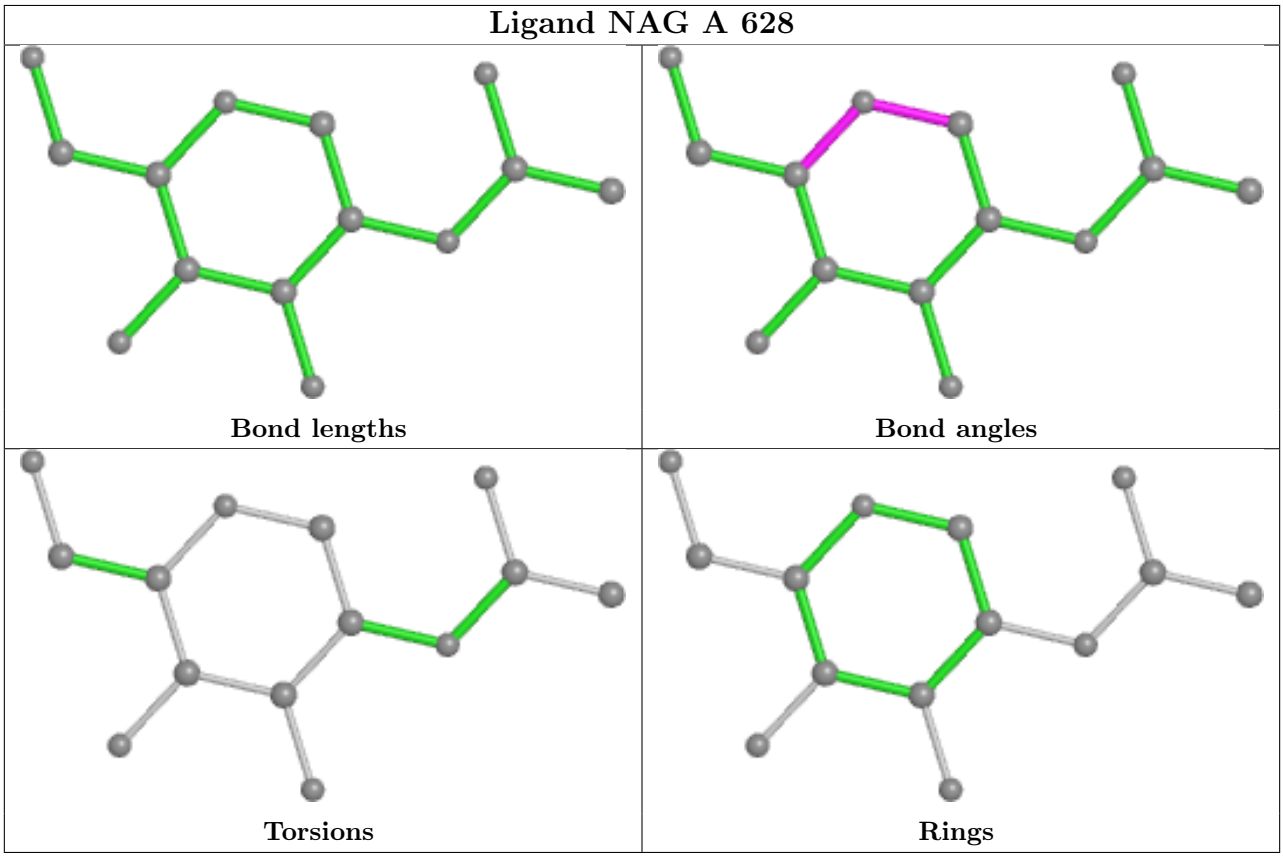
Ligand PEG A 616



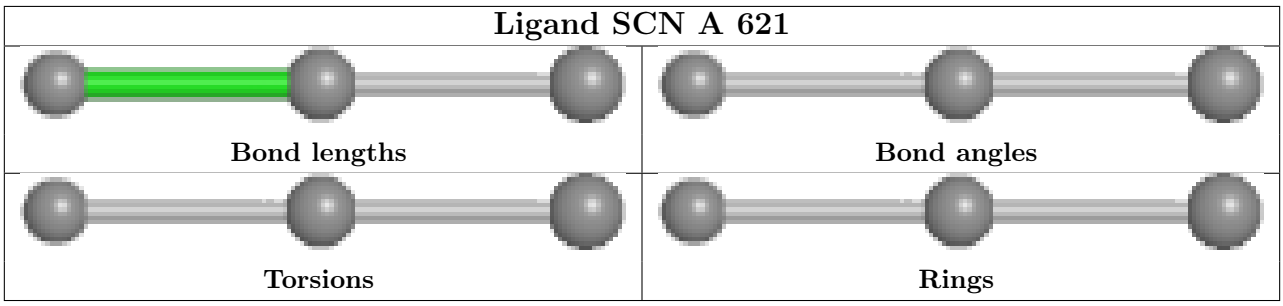
Ligand SCN A 622



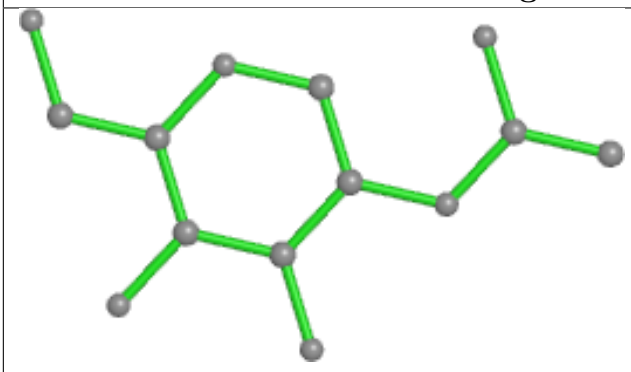
Ligand NAG A 628



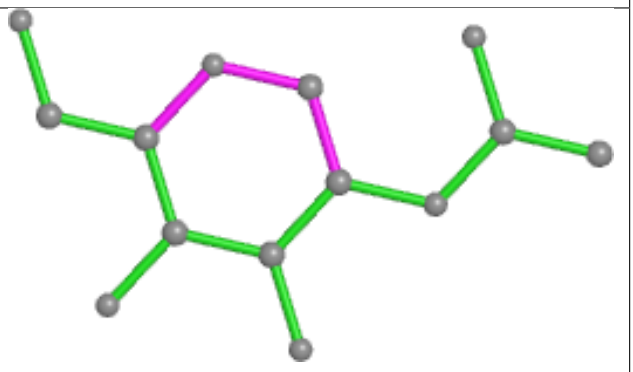
Ligand SCN A 621



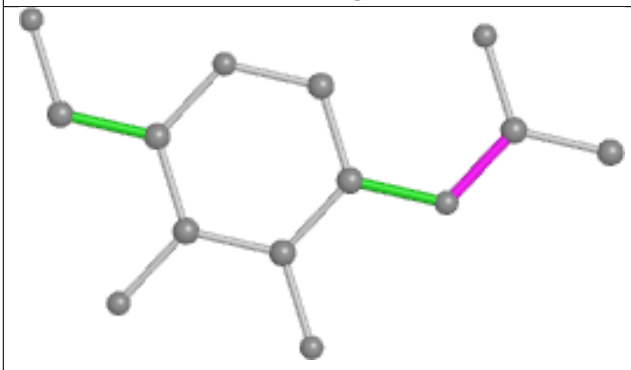
Ligand NAG A 625



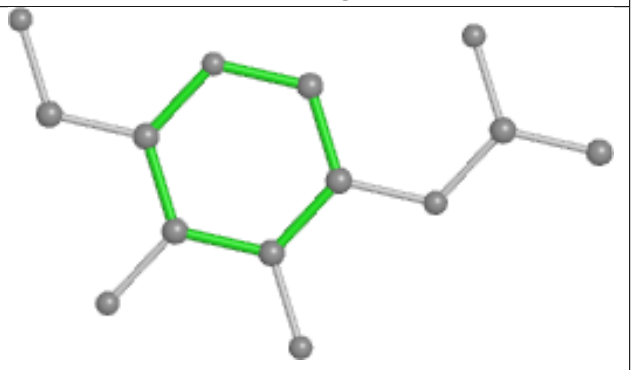
Bond lengths



Bond angles

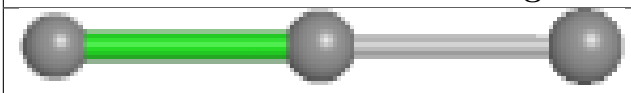


Torsions

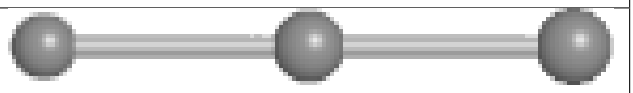


Rings

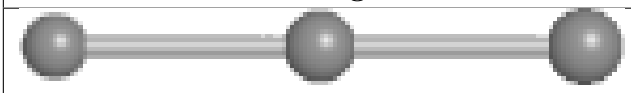
Ligand SCN A 631



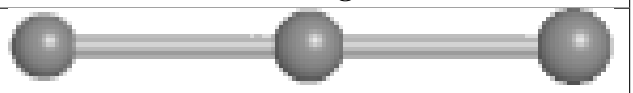
Bond lengths



Bond angles

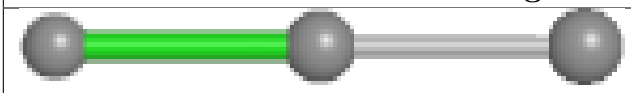


Torsions

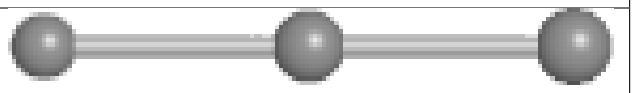


Rings

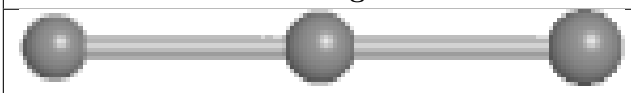
Ligand SCN A 624



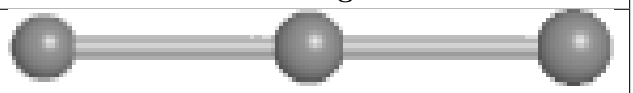
Bond lengths



Bond angles

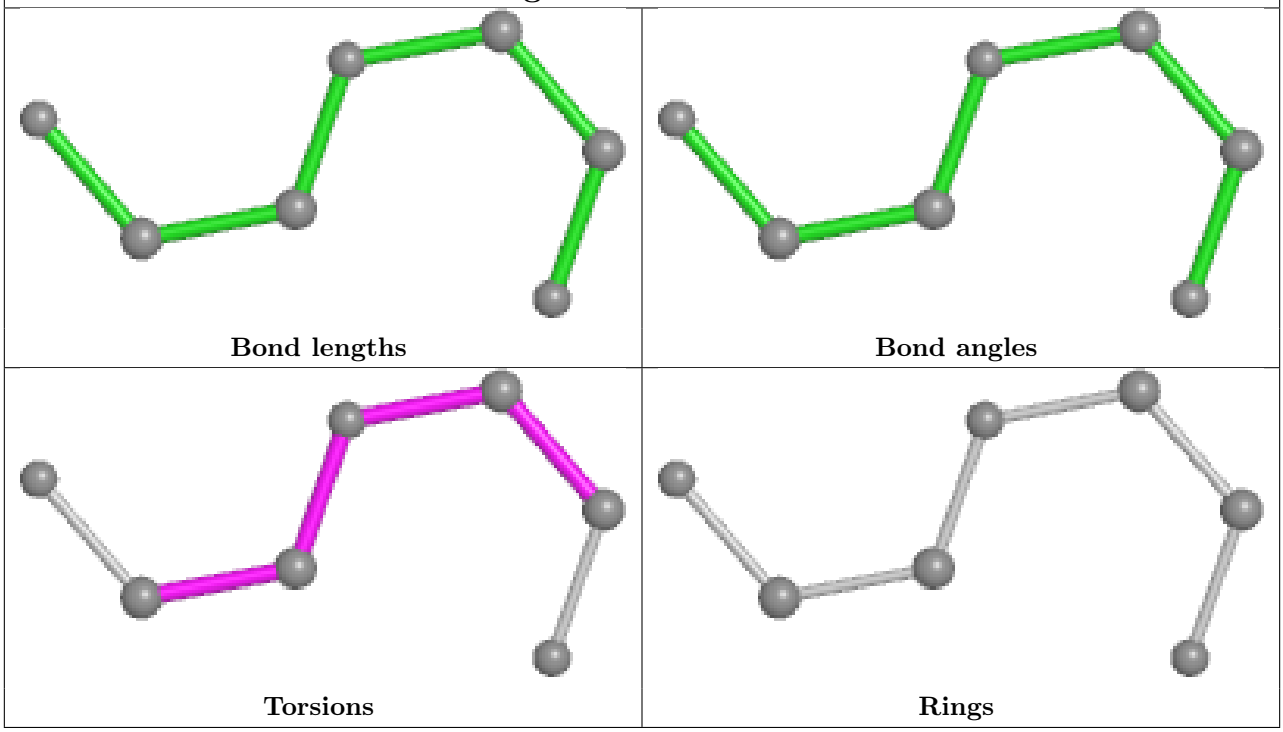


Torsions

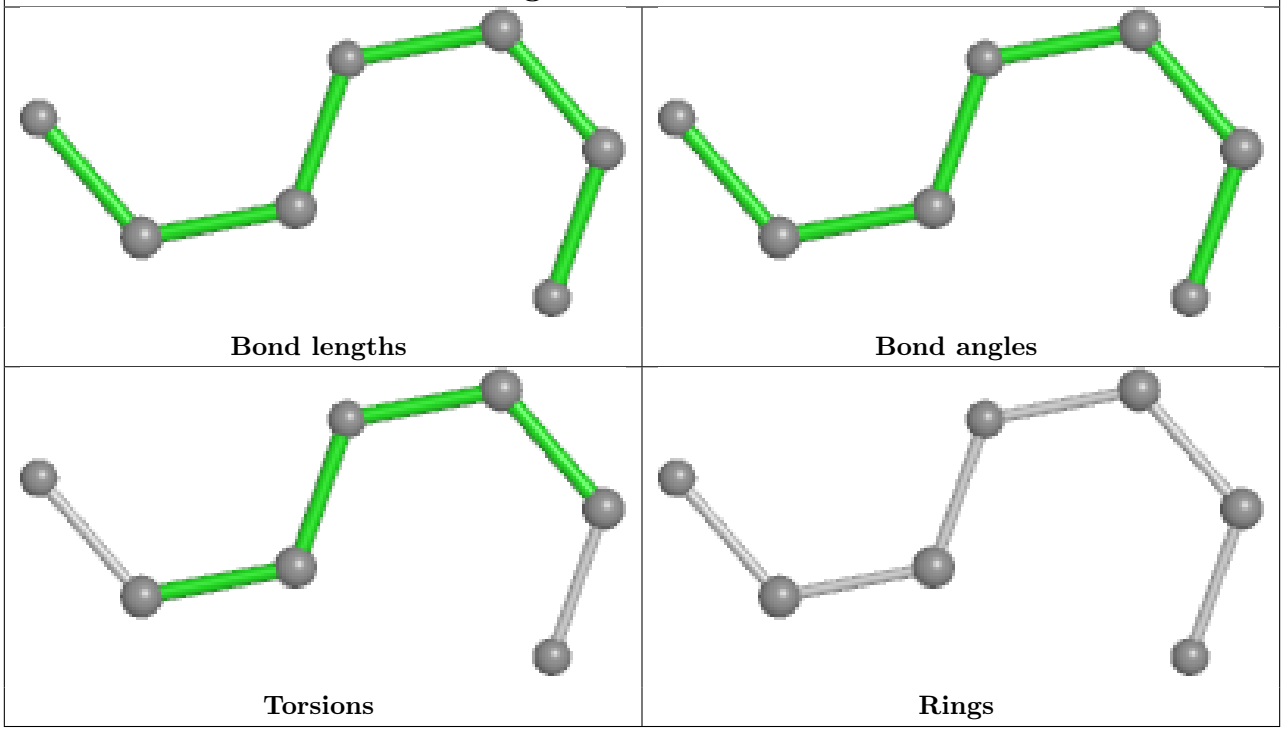


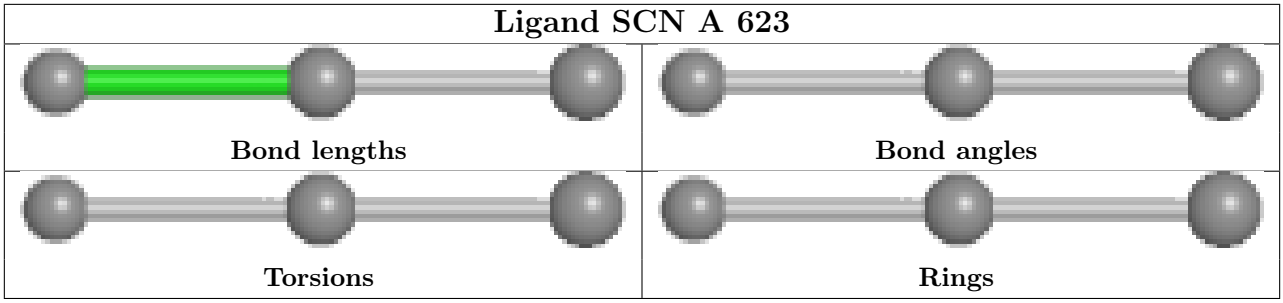
Rings

Ligand PEG A 620



Ligand PEG A 618





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	592/595 (99%)	0.19	47 (7%)	12	11	12, 23, 99, 199	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	GLY	22.2
1	A	120	GLY	20.3
1	A	1	SER	15.4
1	A	121	SER	13.9
1	A	2	TRP	13.4

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	A	630	14/15	0.78	0.20	57,77,81,81	0
9	NAG	A	627	15/15	0.79	0.25	49,67,71,74	0

Continued on next page...

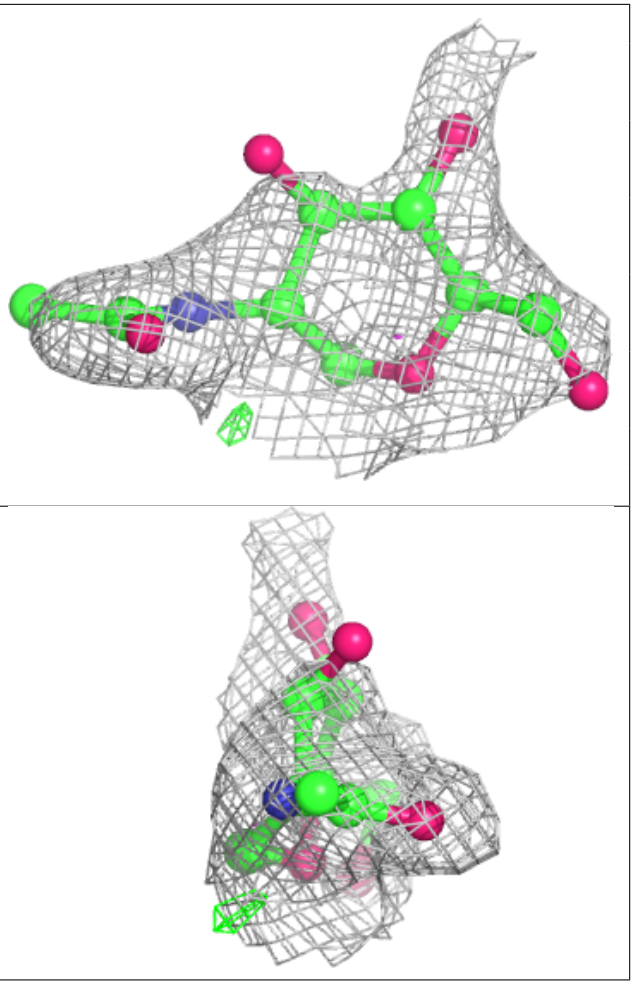
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PEG	A	616	7/7	0.84	0.13	48,49,55,58	0
7	PEG	A	615	7/7	0.85	0.12	49,50,52,53	0
9	NAG	A	625	14/15	0.86	0.24	42,47,52,56	0
7	PEG	A	619	7/7	0.86	0.12	45,45,53,58	0
7	PEG	A	620	7/7	0.86	0.13	48,49,51,55	0
9	NAG	A	628	14/15	0.89	0.17	45,56,63,72	0
7	PEG	A	618	7/7	0.89	0.17	37,41,47,55	0
7	PEG	A	617	7/7	0.90	0.15	51,52,54,55	0
7	PEG	A	614	7/7	0.94	0.11	20,24,29,33	0
9	NAG	A	626	13/15	0.95	0.10	30,36,41,41	0
8	SCN	A	621	3/3	0.96	0.11	23,23,24,26	0
4	IOD	A	633	1/1	0.96	0.05	51,51,51,51	1
9	NAG	A	629	14/15	0.96	0.09	22,30,40,41	0
4	IOD	A	608	1/1	0.96	0.05	66,66,66,66	1
8	SCN	A	623	3/3	0.97	0.07	31,31,36,37	0
8	SCN	A	624	3/3	0.97	0.08	34,34,37,38	0
2	HEM	A	601	43/43	0.98	0.14	11,13,17,19	0
4	IOD	A	604	1/1	0.98	0.12	61,61,61,61	1
8	SCN	A	631	3/3	0.98	0.14	24,24,24,25	3
4	IOD	A	603[A]	1/1	0.99	0.03	34,34,34,34	1
5	BR	A	611	1/1	0.99	0.05	26,26,26,26	1
4	IOD	A	603[B]	1/1	0.99	0.03	26,26,26,26	1
4	IOD	A	610	1/1	0.99	0.04	37,37,37,37	1
8	SCN	A	622	3/3	0.99	0.14	29,29,35,39	0
4	IOD	A	613[A]	1/1	0.99	0.03	48,48,48,48	1
4	IOD	A	613[B]	1/1	0.99	0.03	37,37,37,37	1
4	IOD	A	632[B]	1/1	1.00	0.05	19,19,19,19	1
4	IOD	A	607[A]	1/1	1.00	0.05	21,21,21,21	1
4	IOD	A	607[B]	1/1	1.00	0.05	16,16,16,16	1
6	CL	A	612	1/1	1.00	0.08	18,18,18,18	1
3	CA	A	602	1/1	1.00	0.12	16,16,16,16	0
4	IOD	A	609[A]	1/1	1.00	0.04	29,29,29,29	1
4	IOD	A	609[B]	1/1	1.00	0.04	24,24,24,24	1
4	IOD	A	605[A]	1/1	1.00	0.05	16,16,16,16	1
4	IOD	A	605[B]	1/1	1.00	0.05	30,30,30,30	1
4	IOD	A	606	1/1	1.00	0.06	22,22,22,22	1
4	IOD	A	632[A]	1/1	1.00	0.05	19,19,19,19	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.

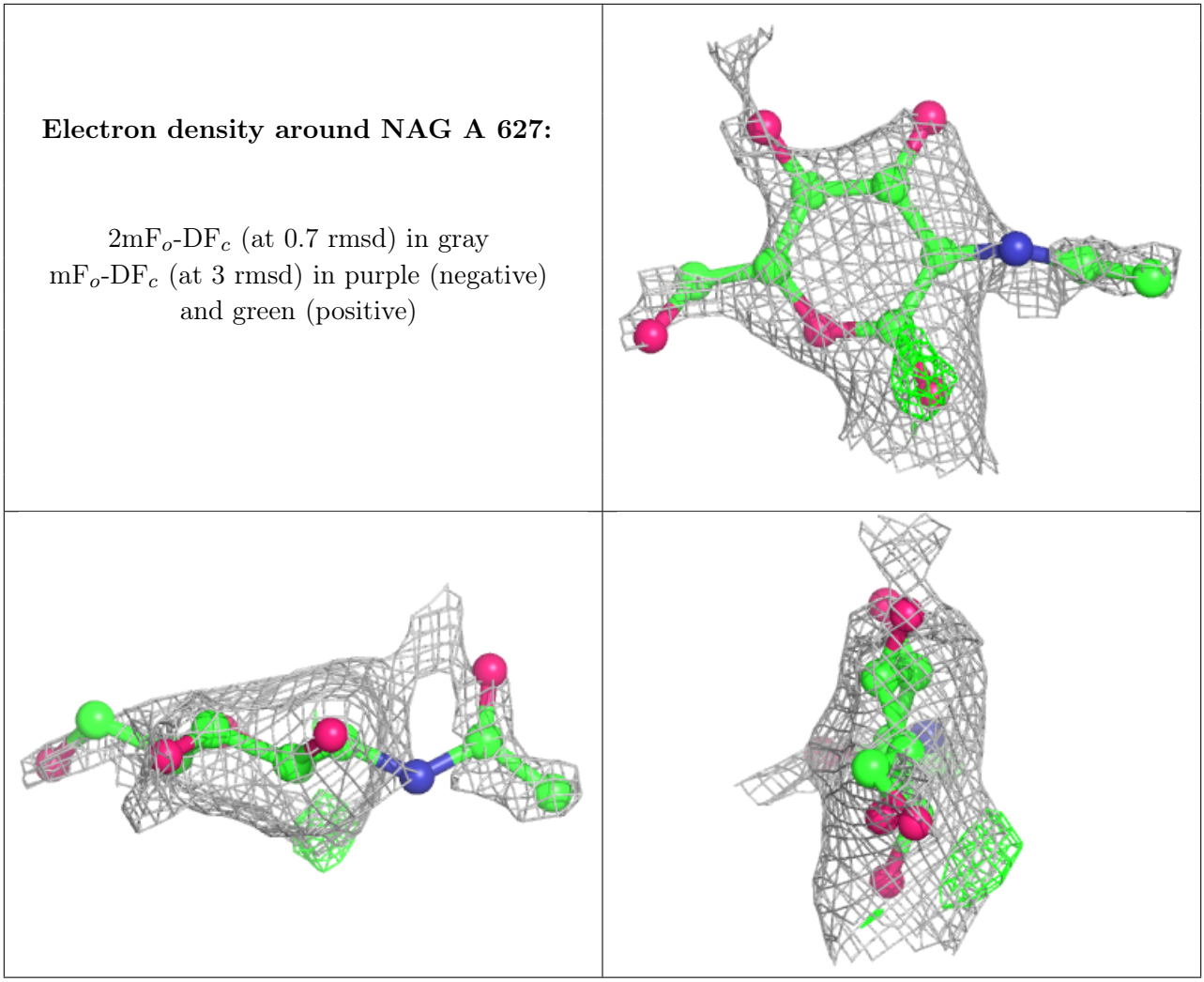
Electron density around NAG A 630:

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



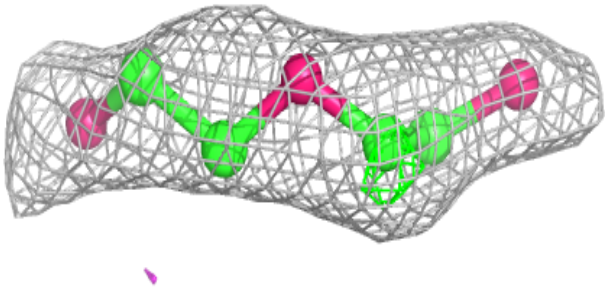
Electron density around NAG A 627:

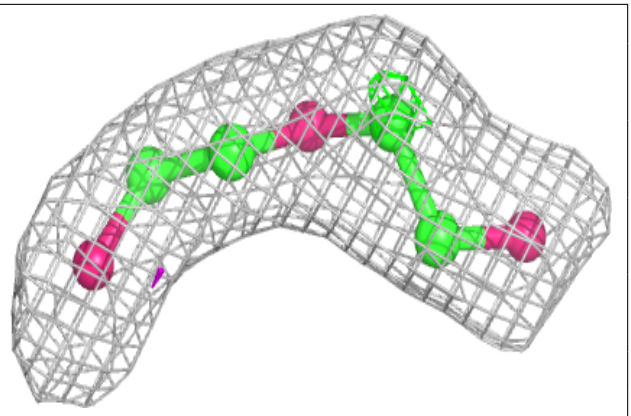
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

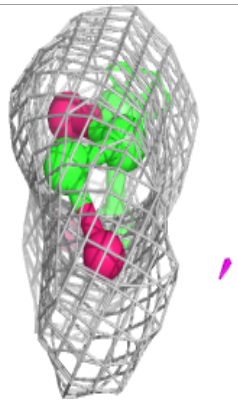


Electron density around PEG A 616:

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

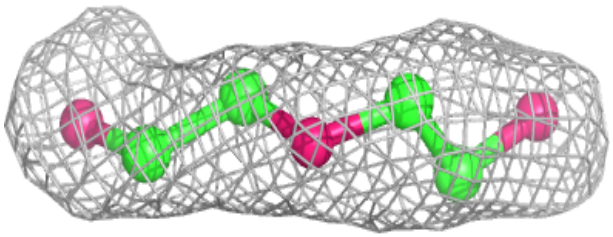


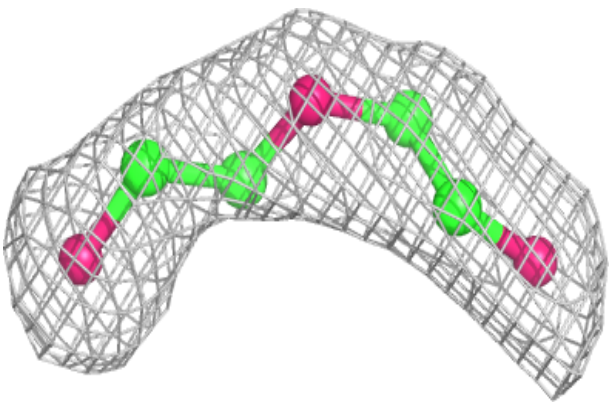


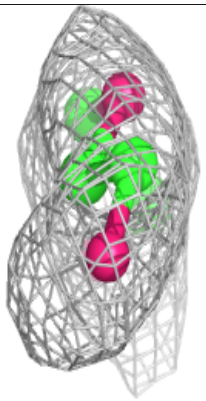


Electron density around PEG A 615:

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

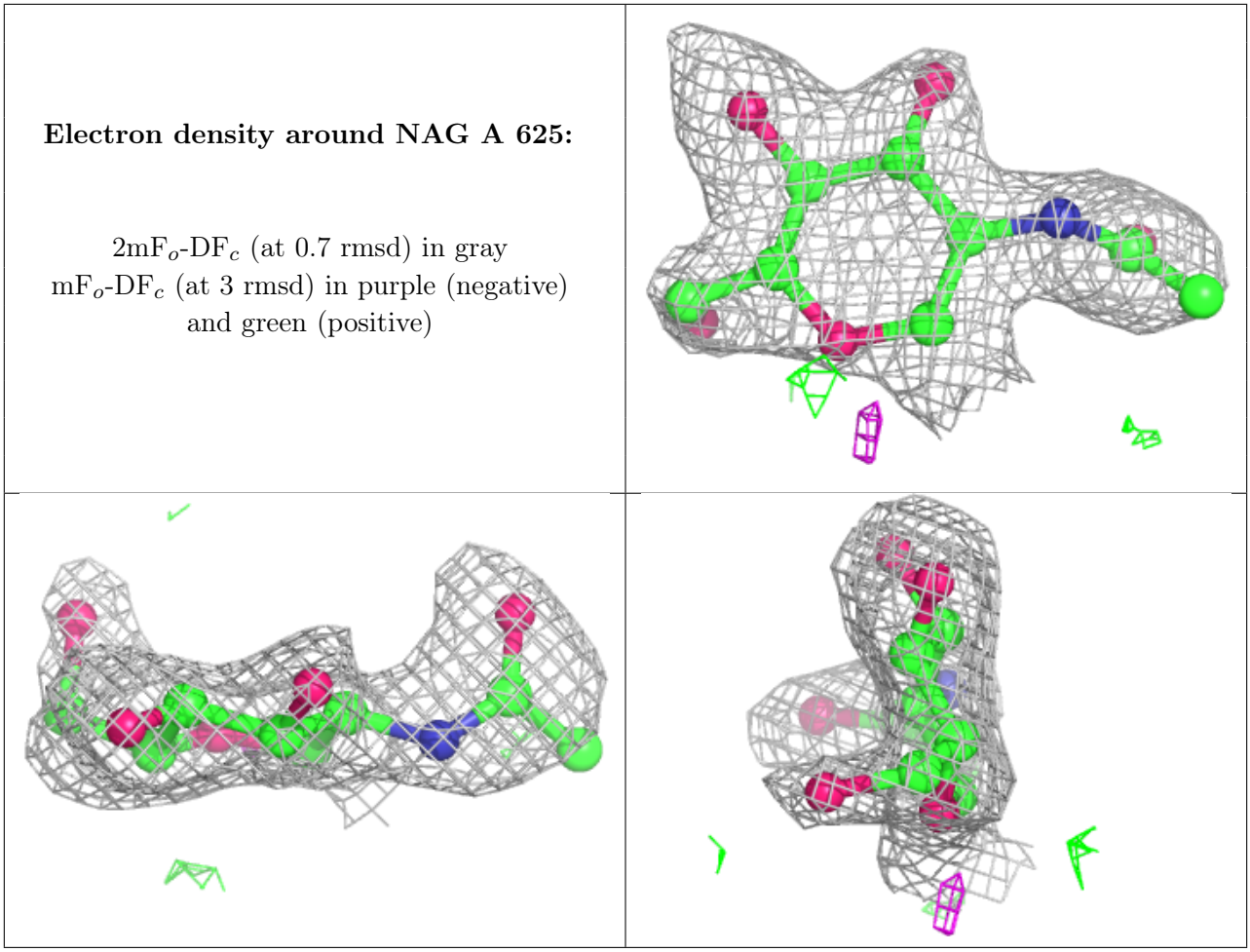






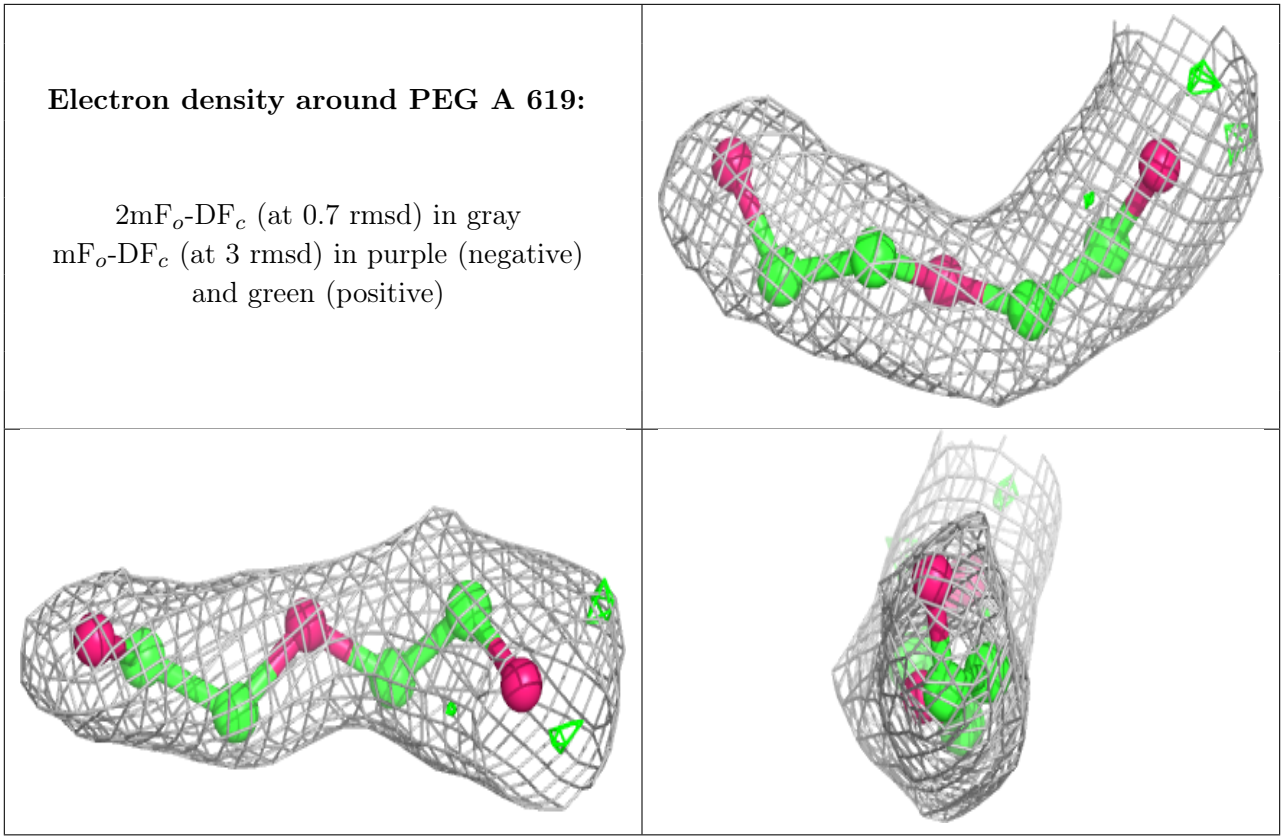
Electron density around NAG A 625:

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



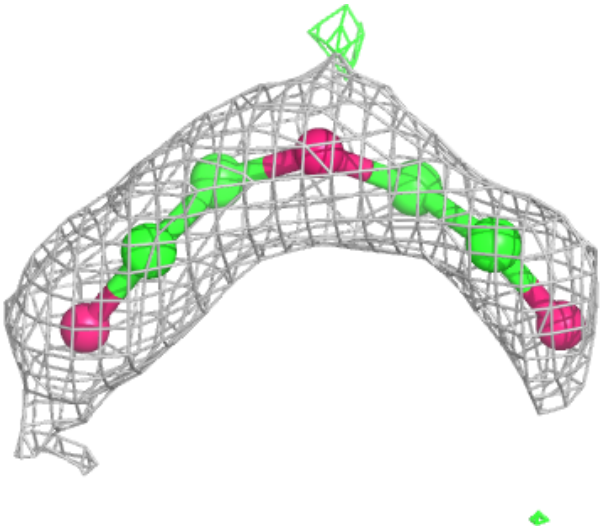
Electron density around PEG A 619:

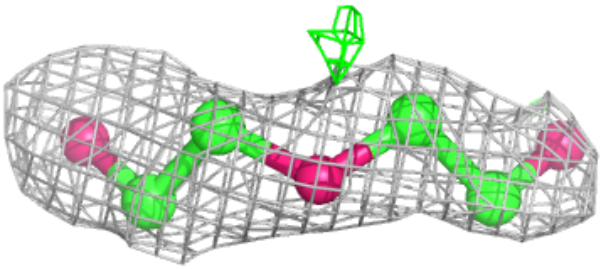
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

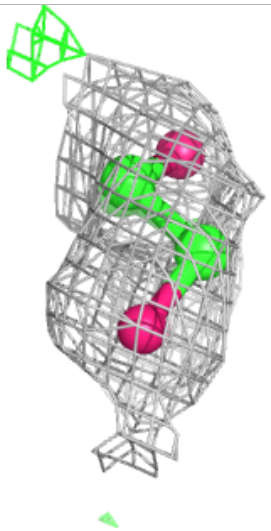


Electron density around PEG A 620:

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

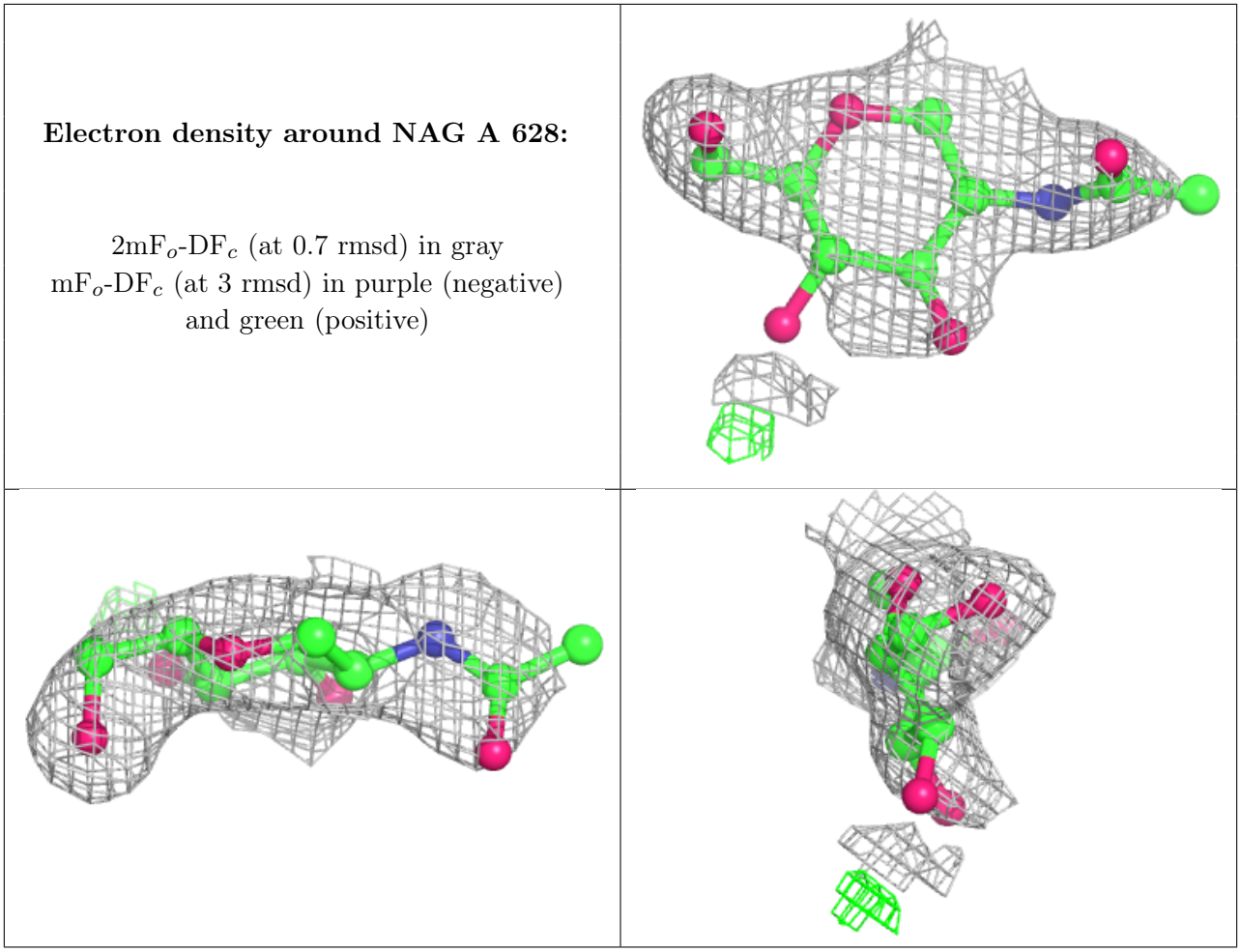






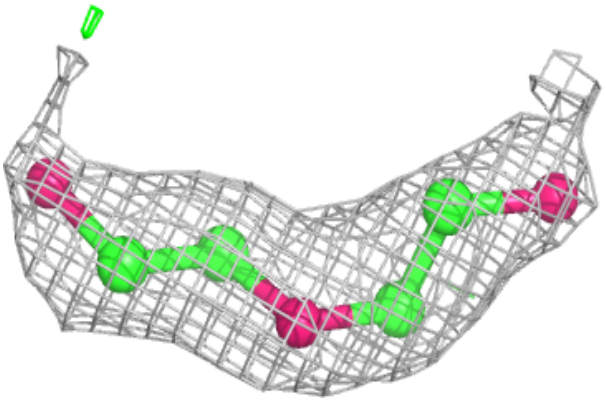
Electron density around NAG A 628:

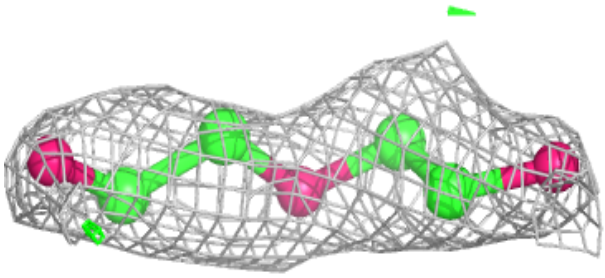
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

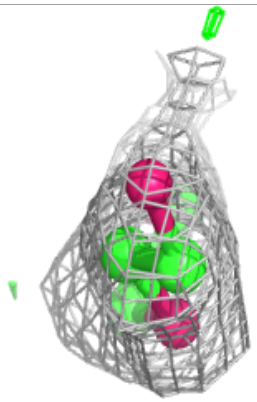


Electron density around PEG A 618:

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

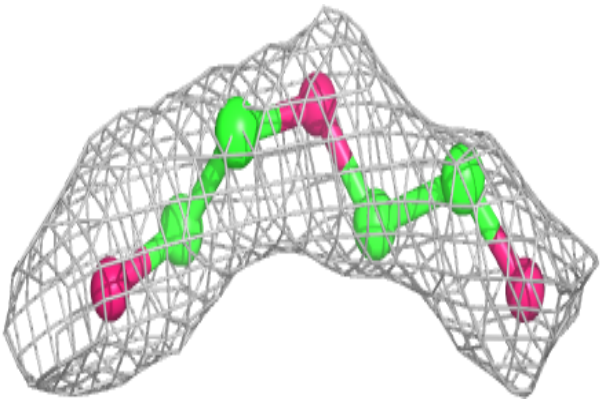


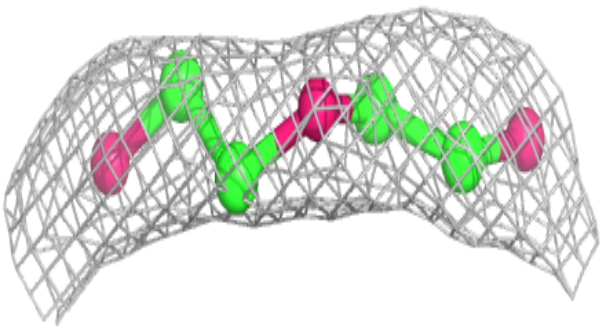


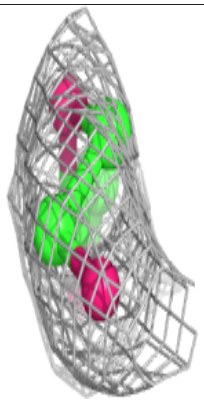


Electron density around PEG A 617:

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

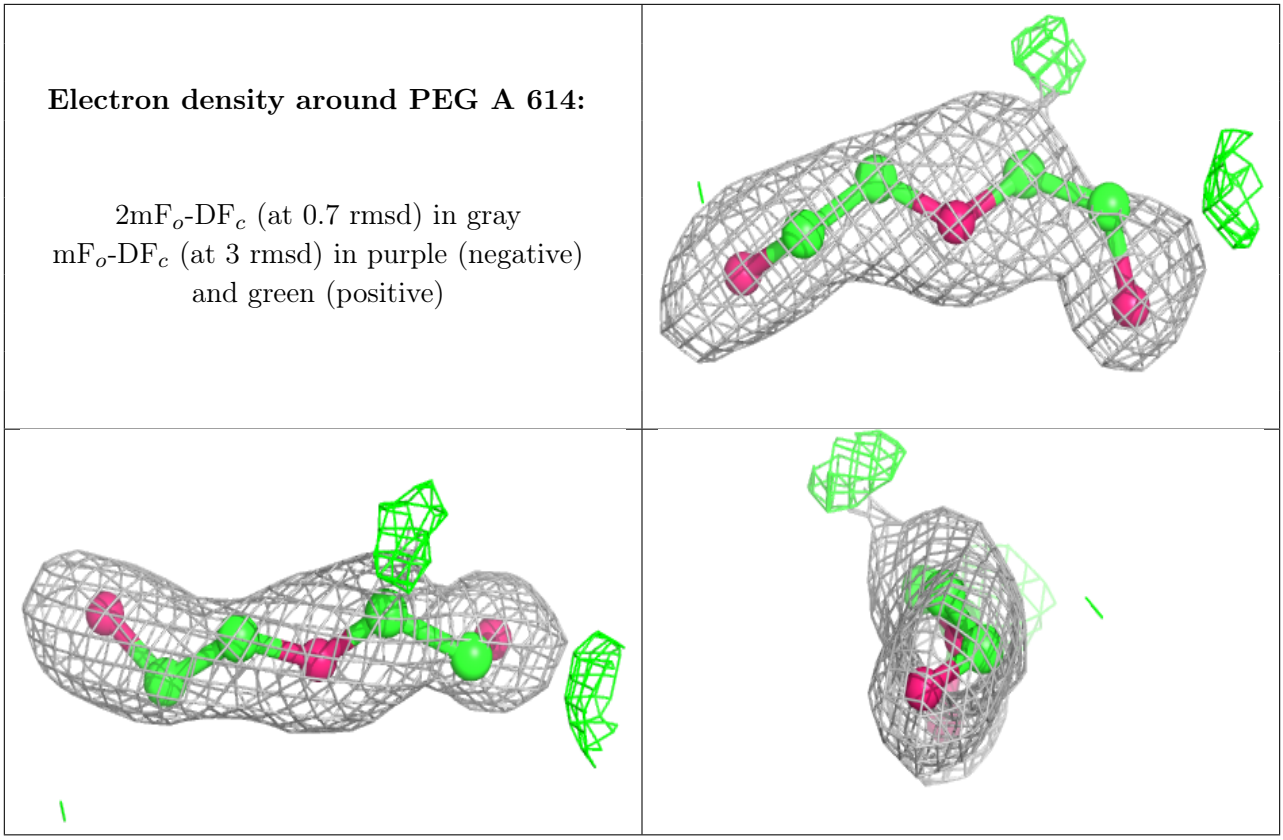






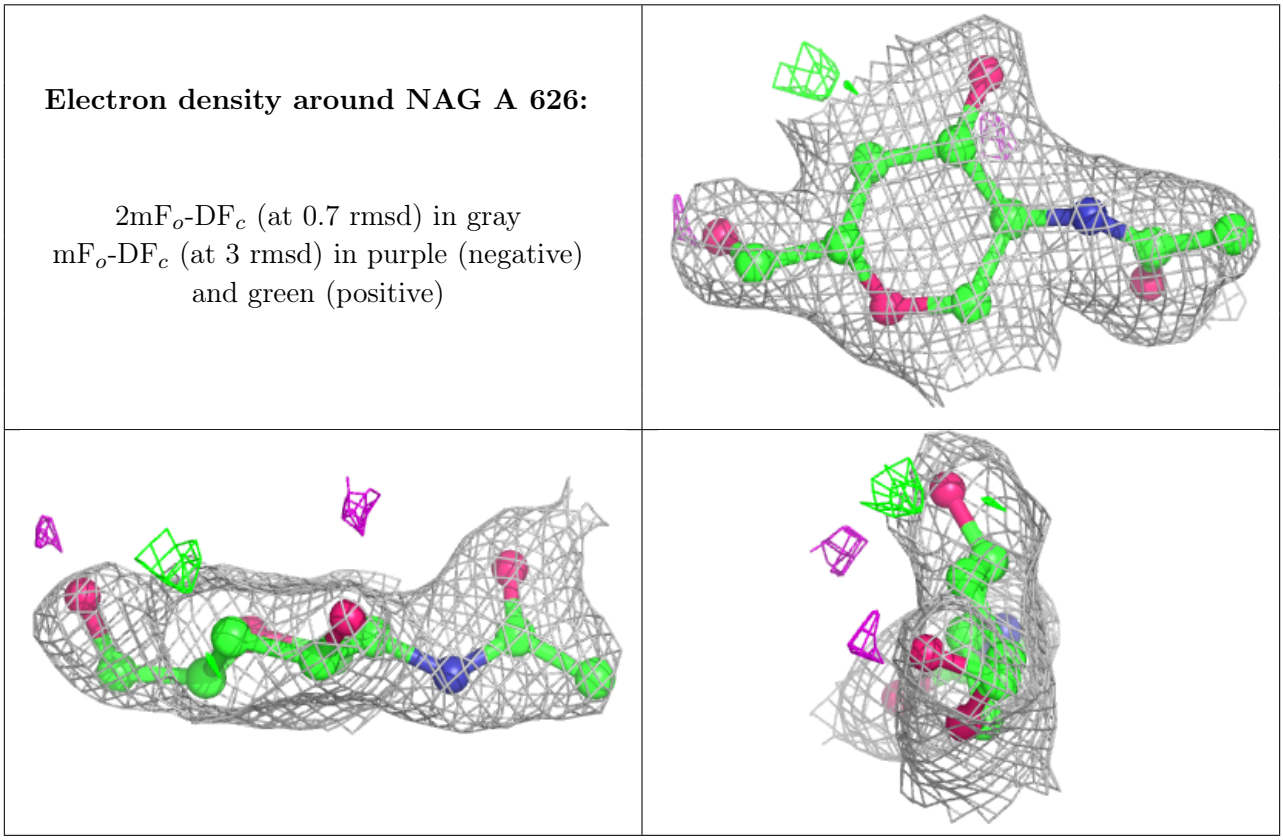
Electron density around PEG A 614:

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



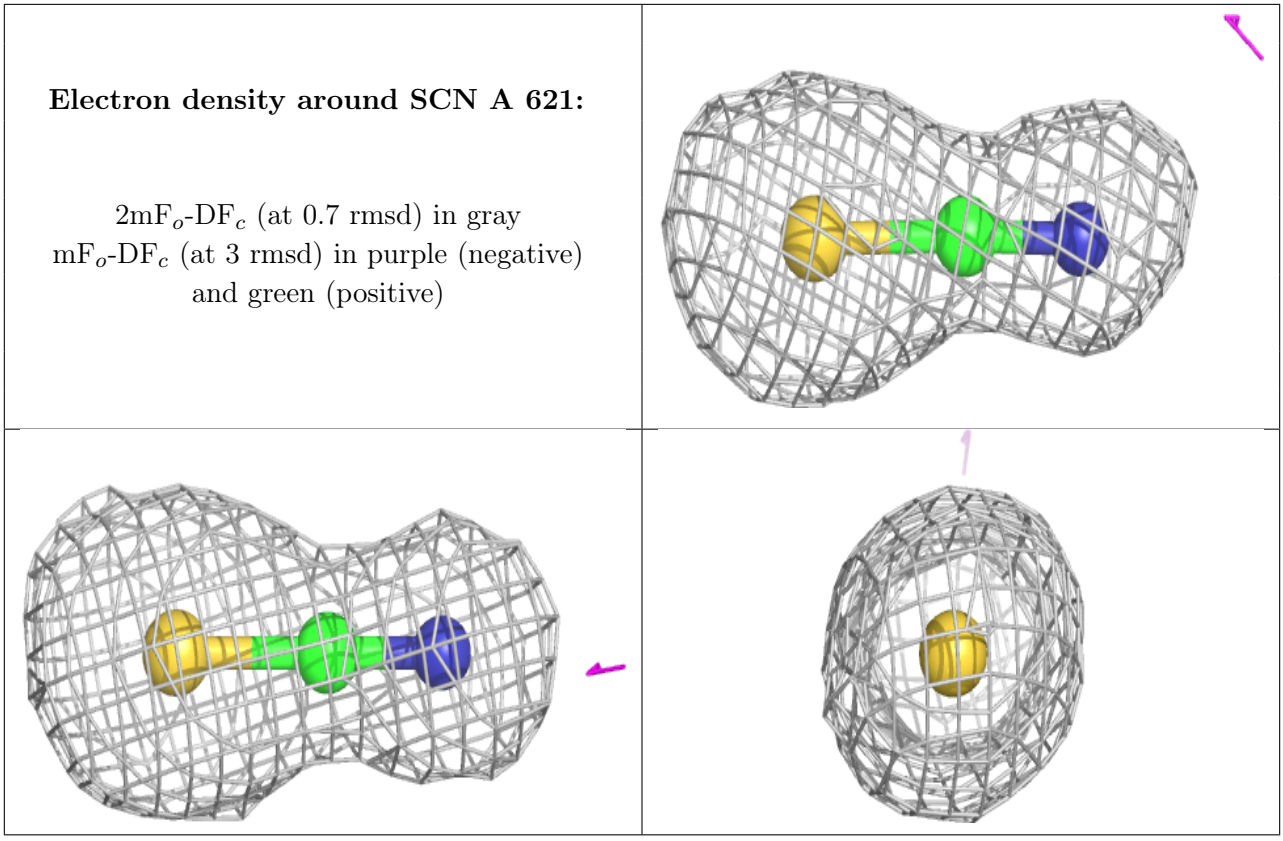
Electron density around NAG A 626:

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



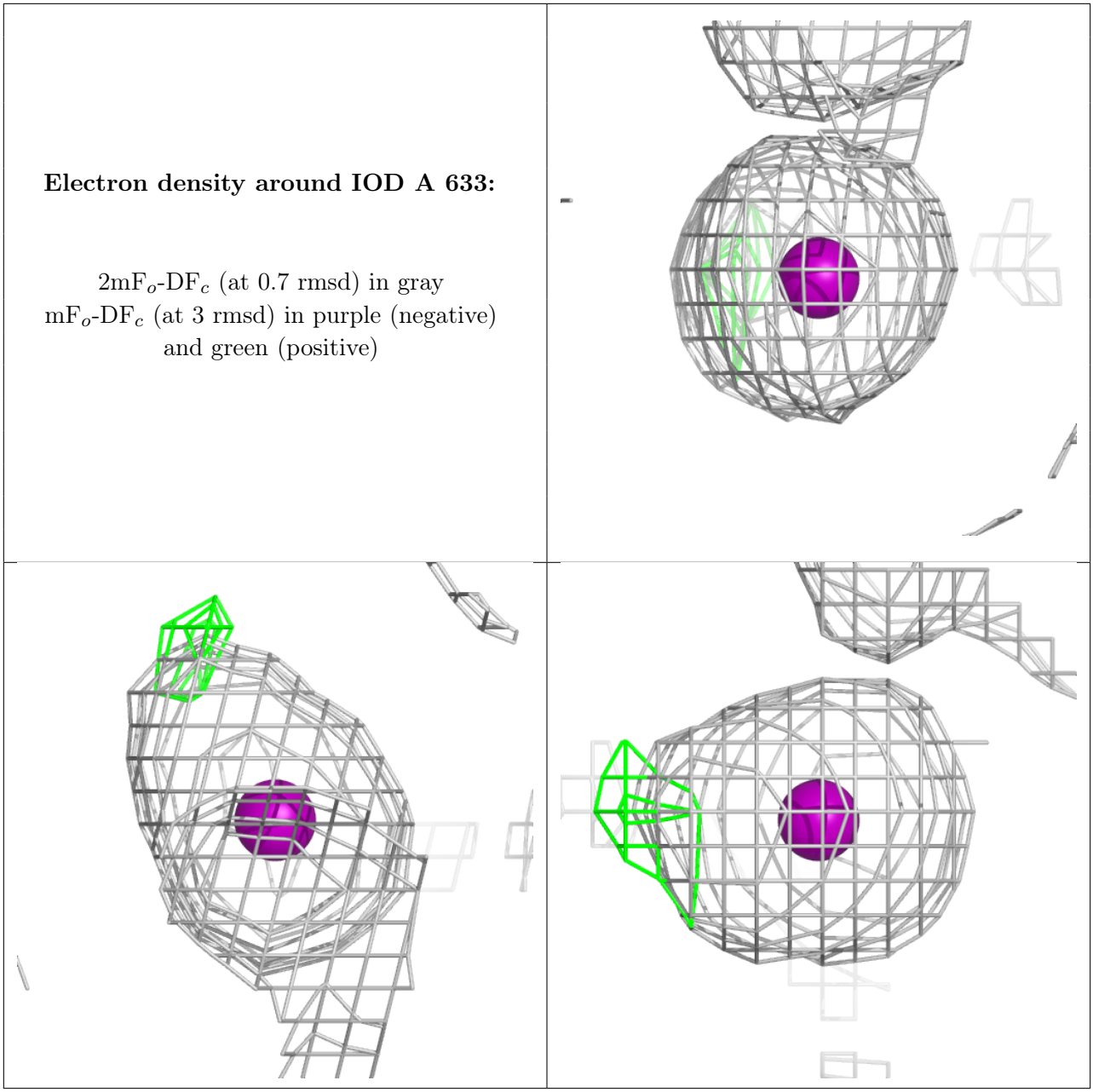
Electron density around SCN A 621:

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



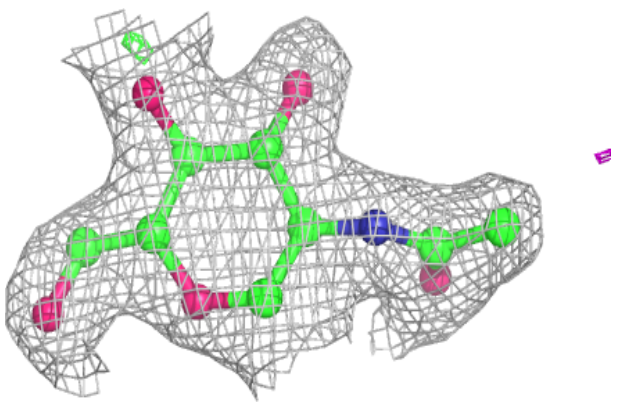
Electron density around IOD A 633:

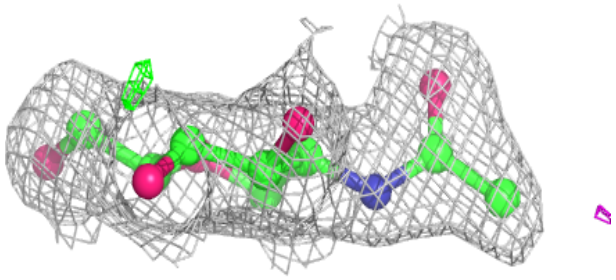
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

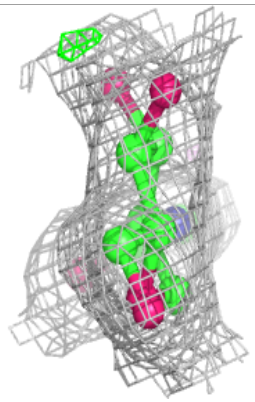


Electron density around NAG A 629:

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

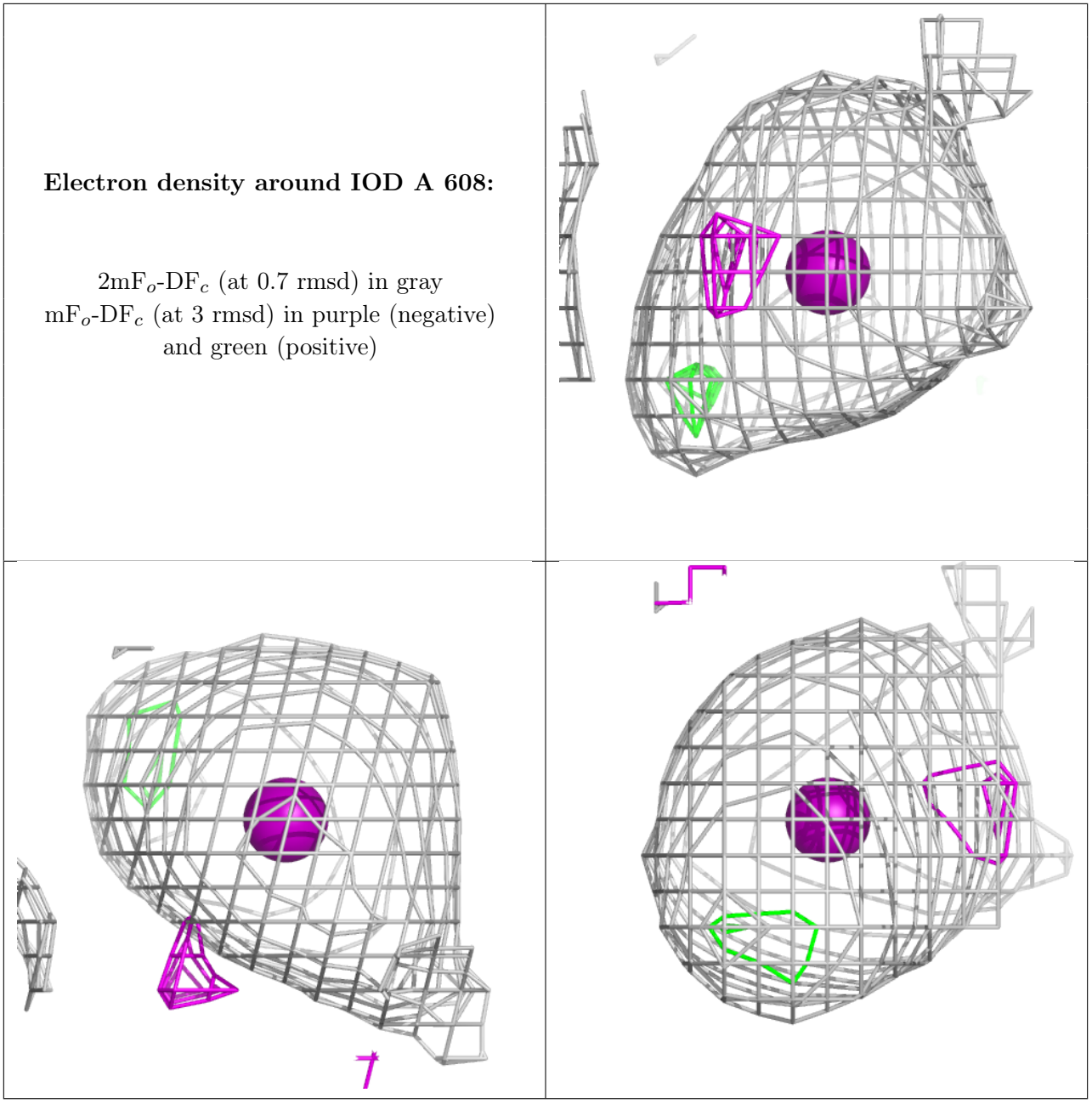






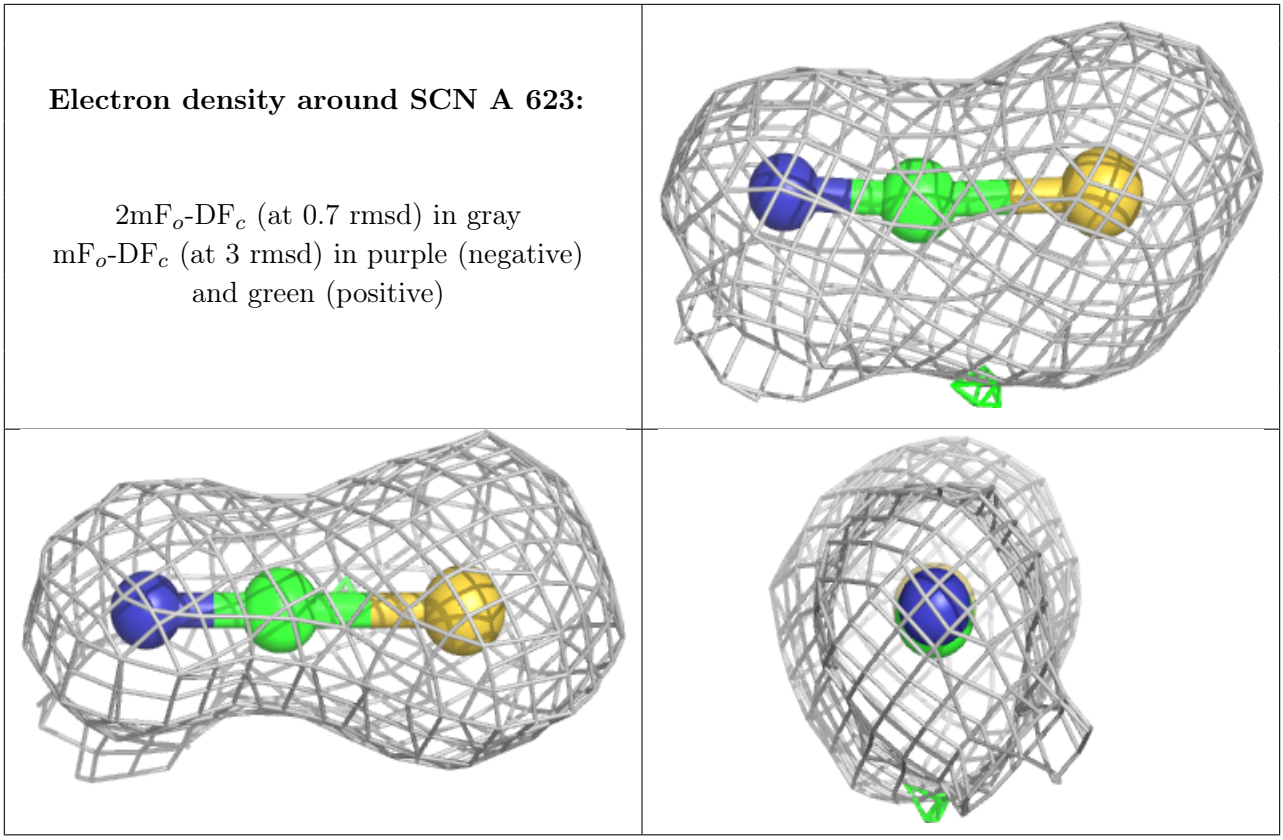
Electron density around IOD A 608:

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



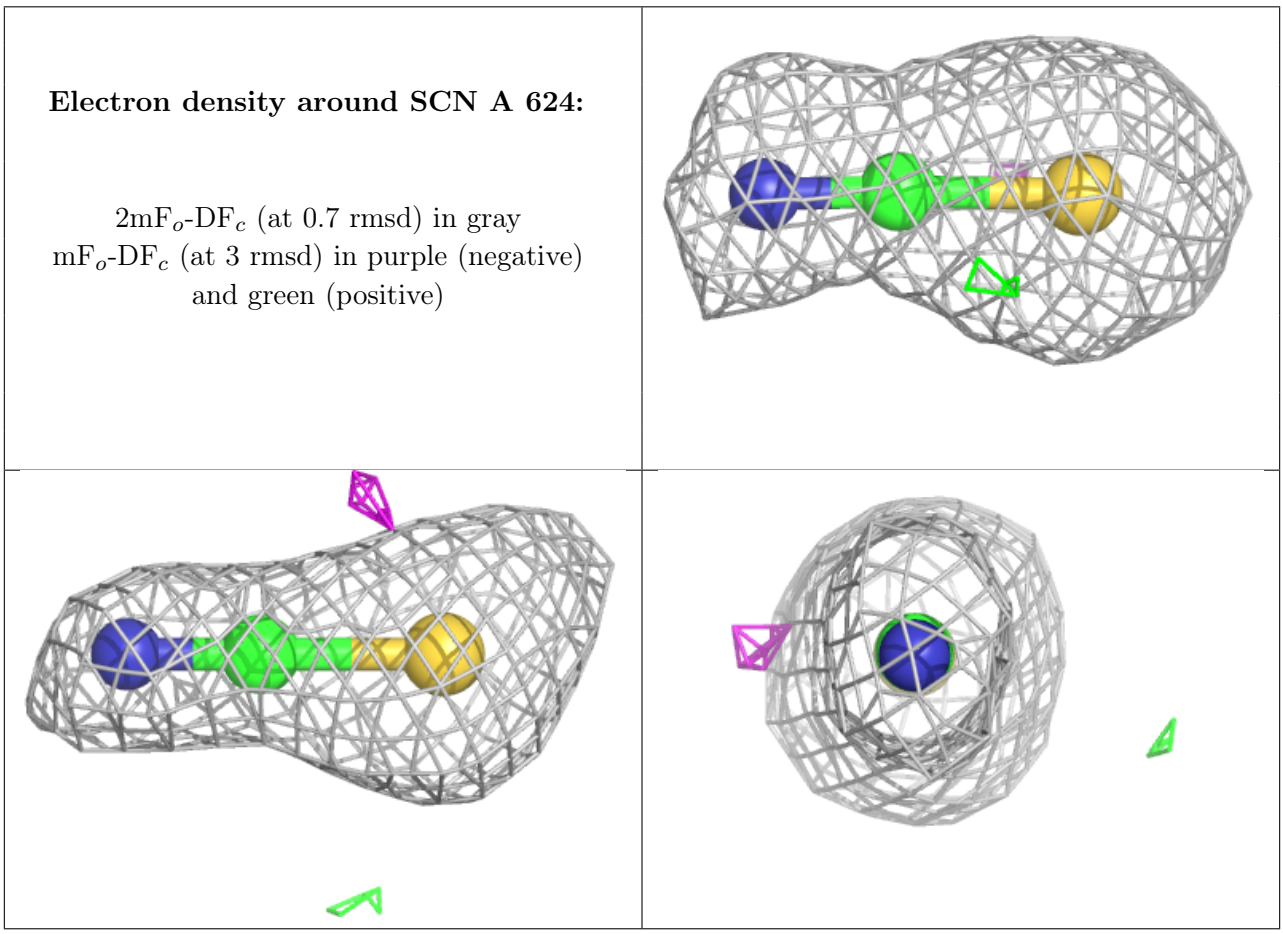
Electron density around SCN A 623:

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



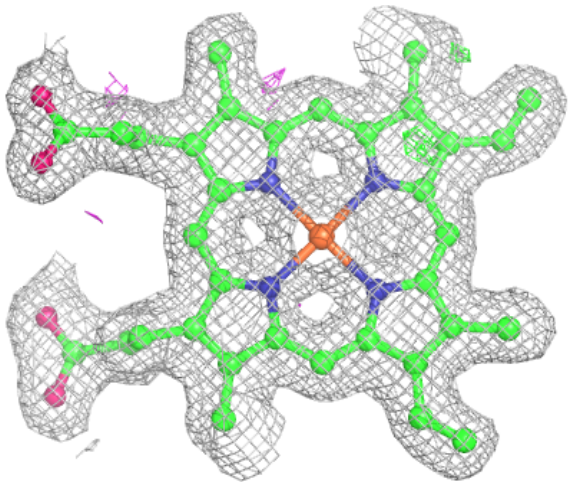
Electron density around SCN A 624:

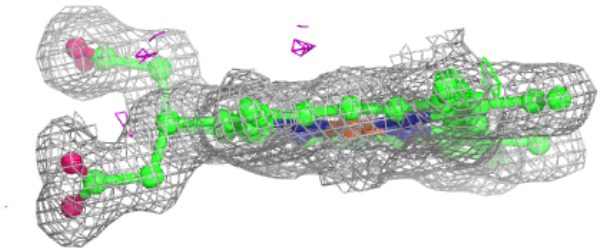
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

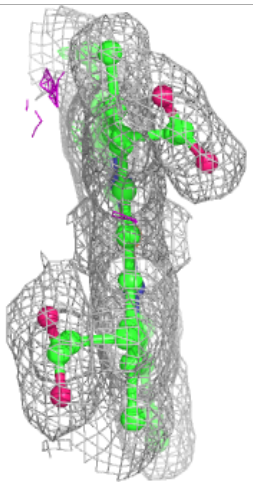


Electron density around HEM A 601:

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

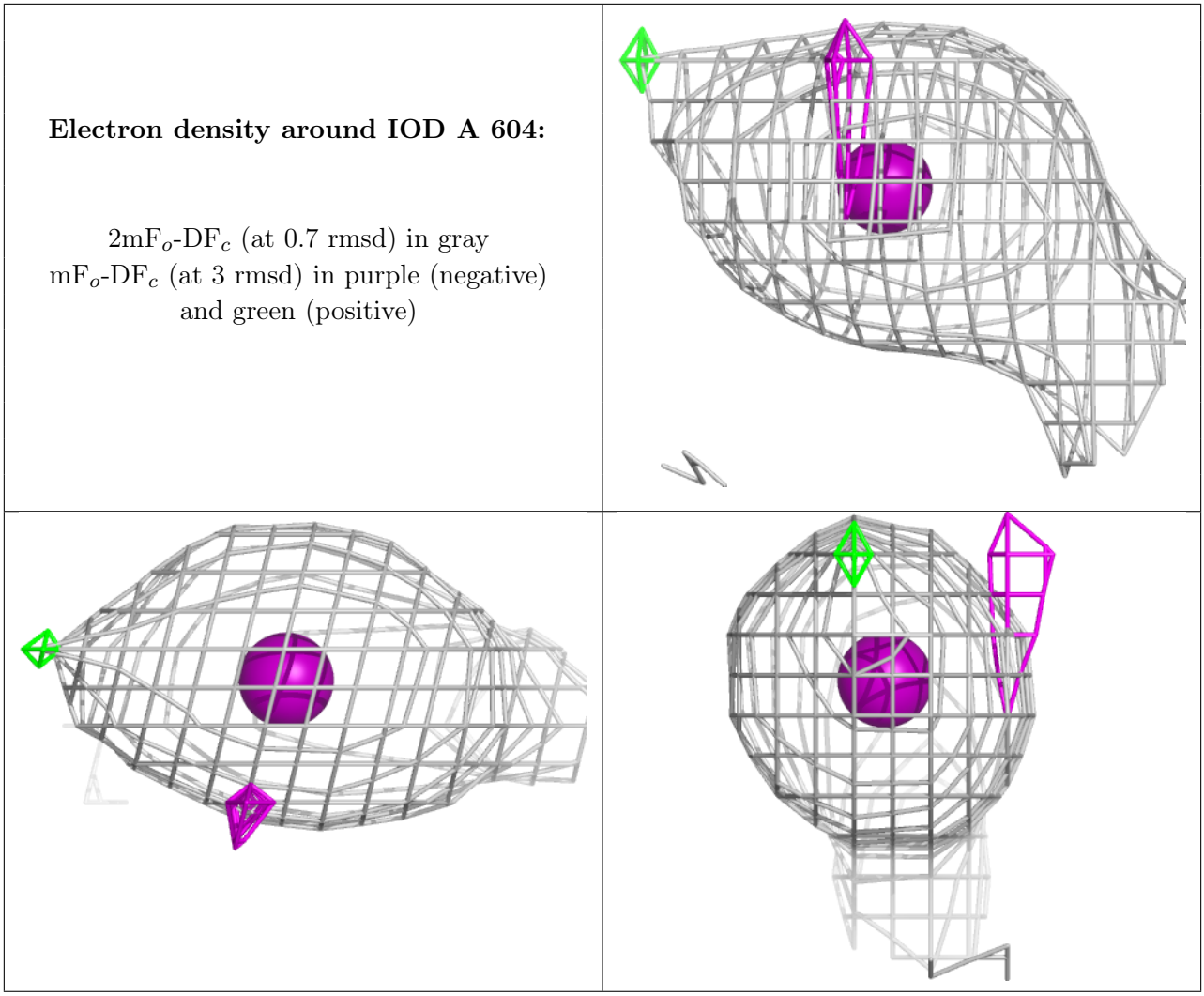






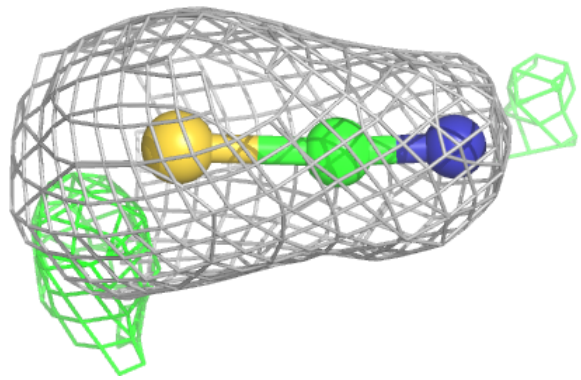
Electron density around IOD A 604:

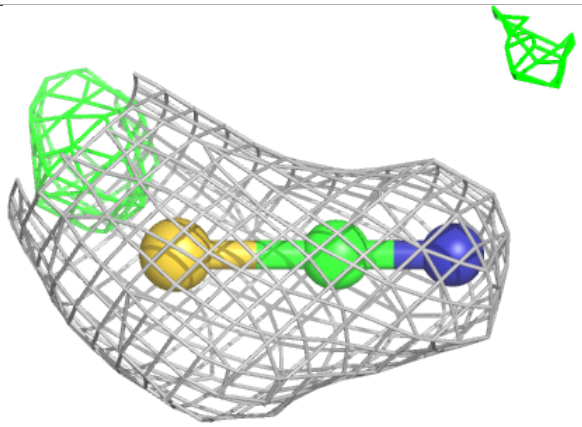
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

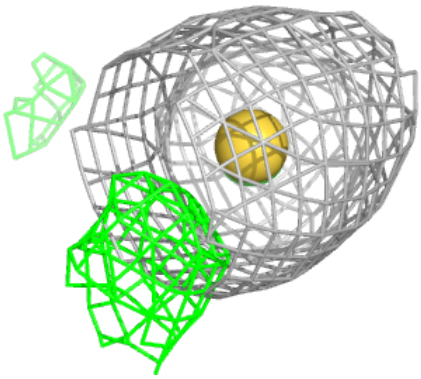


Electron density around SCN A 631:

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

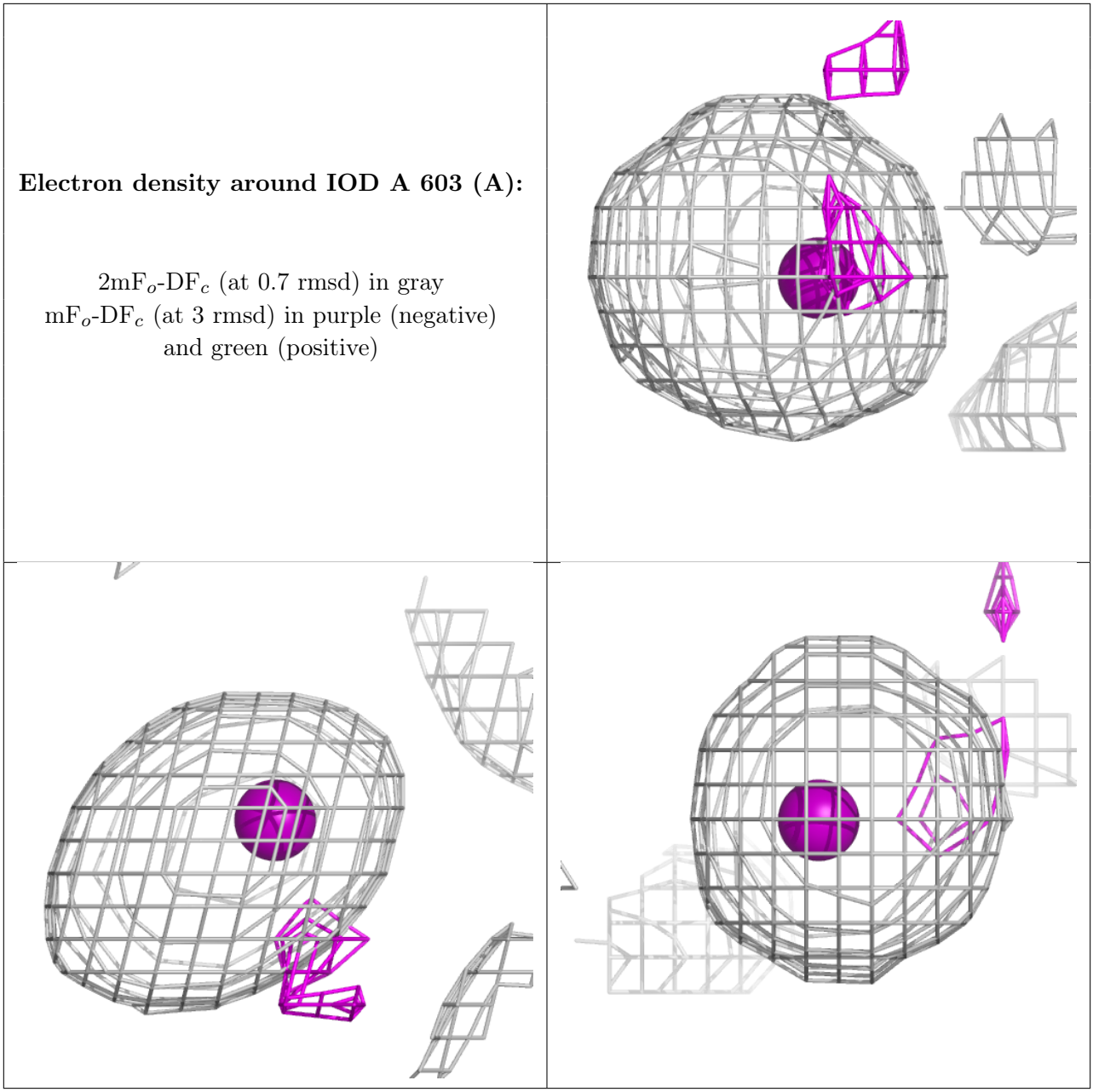






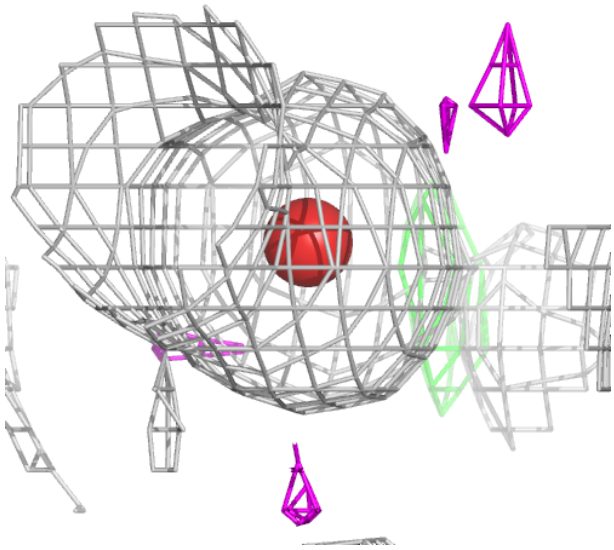
Electron density around IOD A 603 (A):

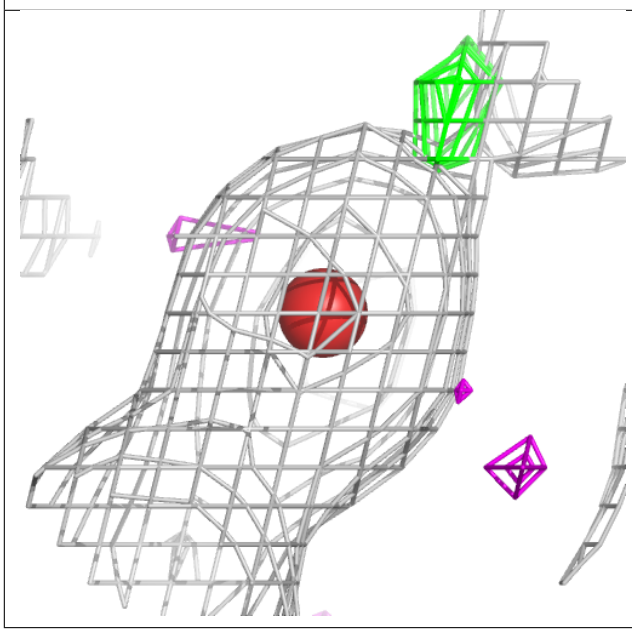
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

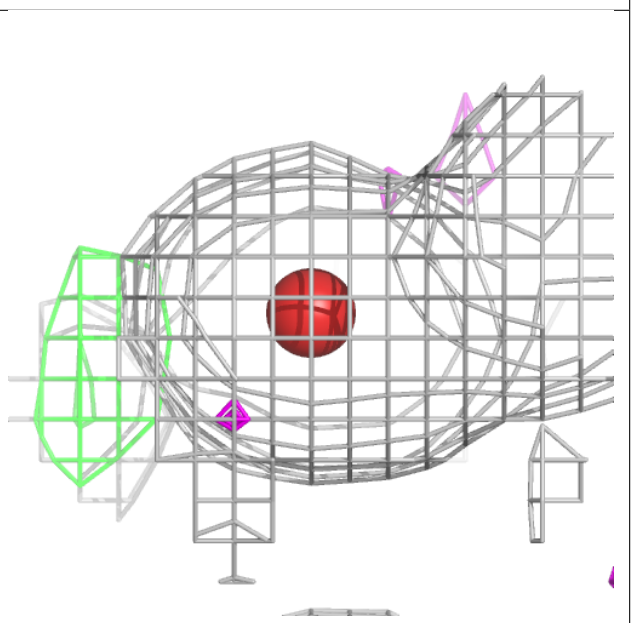


Electron density around BR A 611:

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

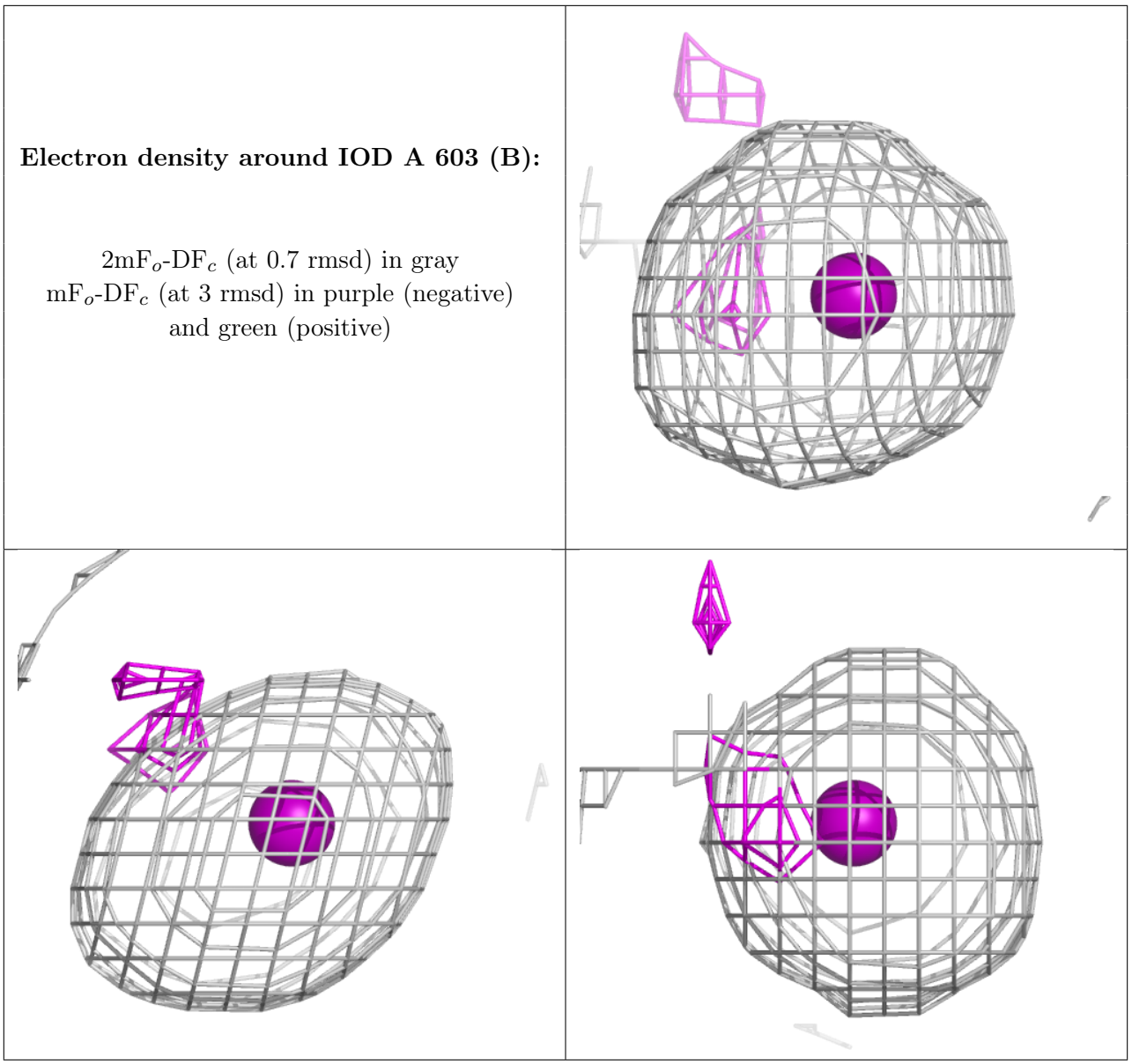






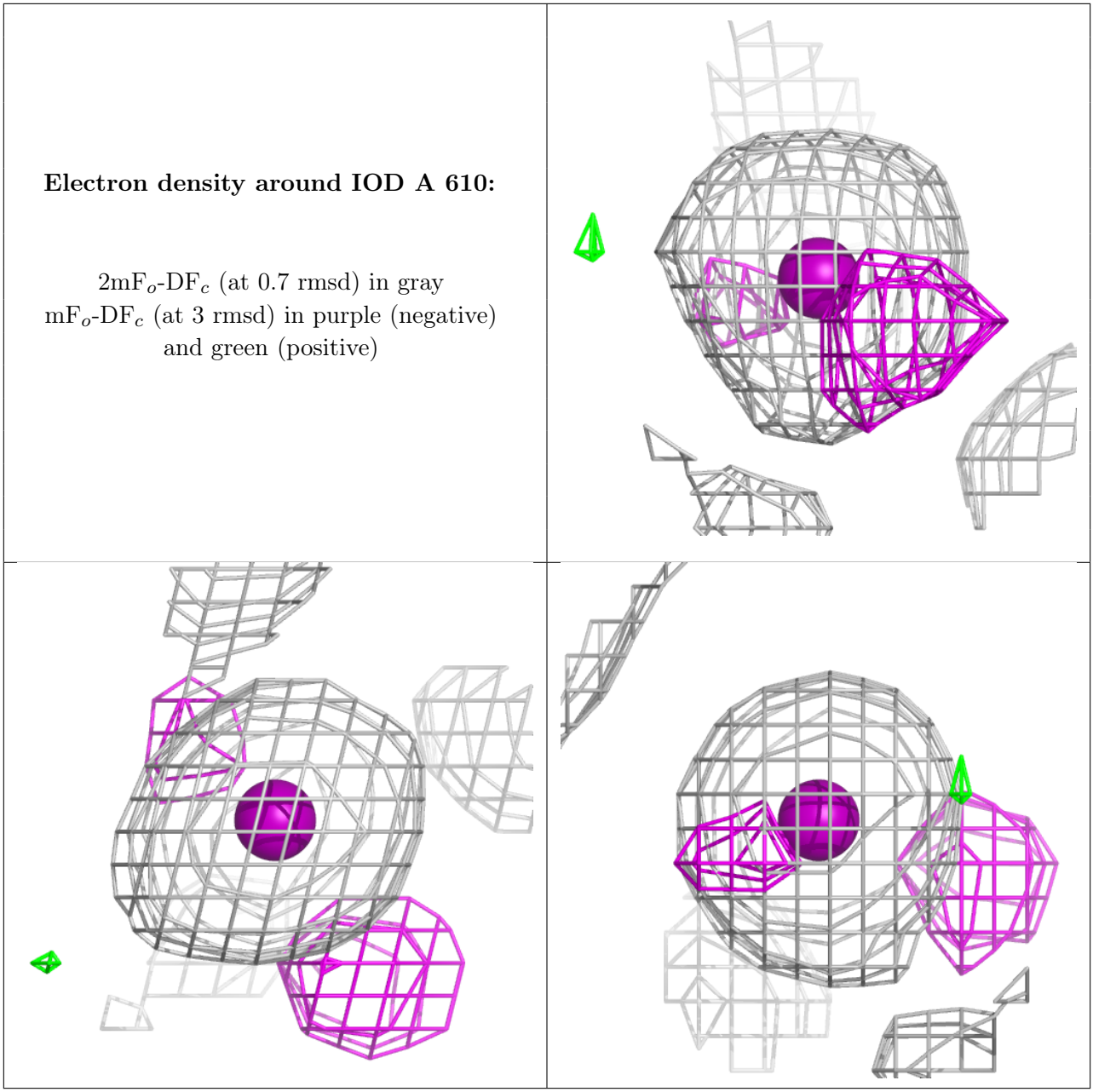
Electron density around IOD A 603 (B):

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



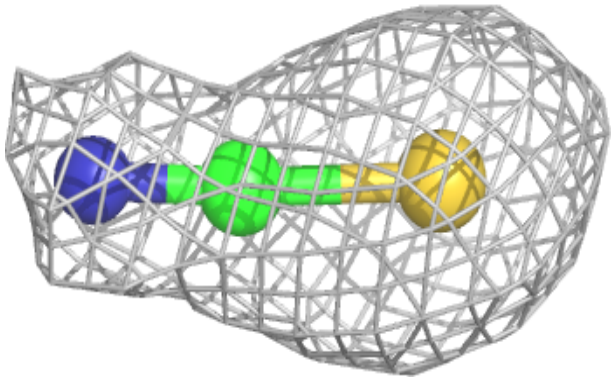
Electron density around IOD A 610:

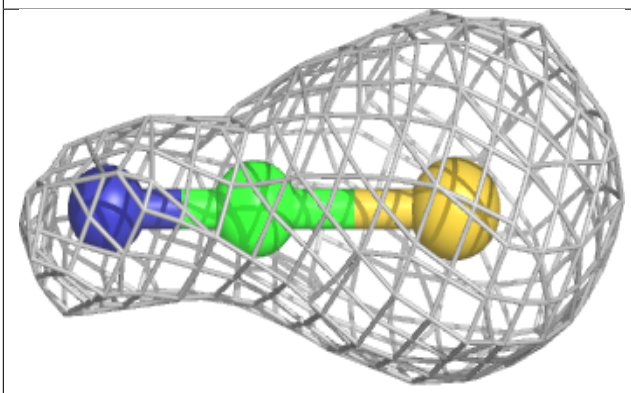
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

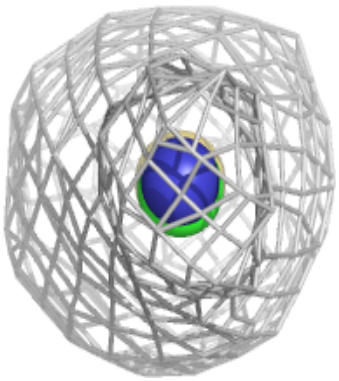


Electron density around SCN A 622:

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

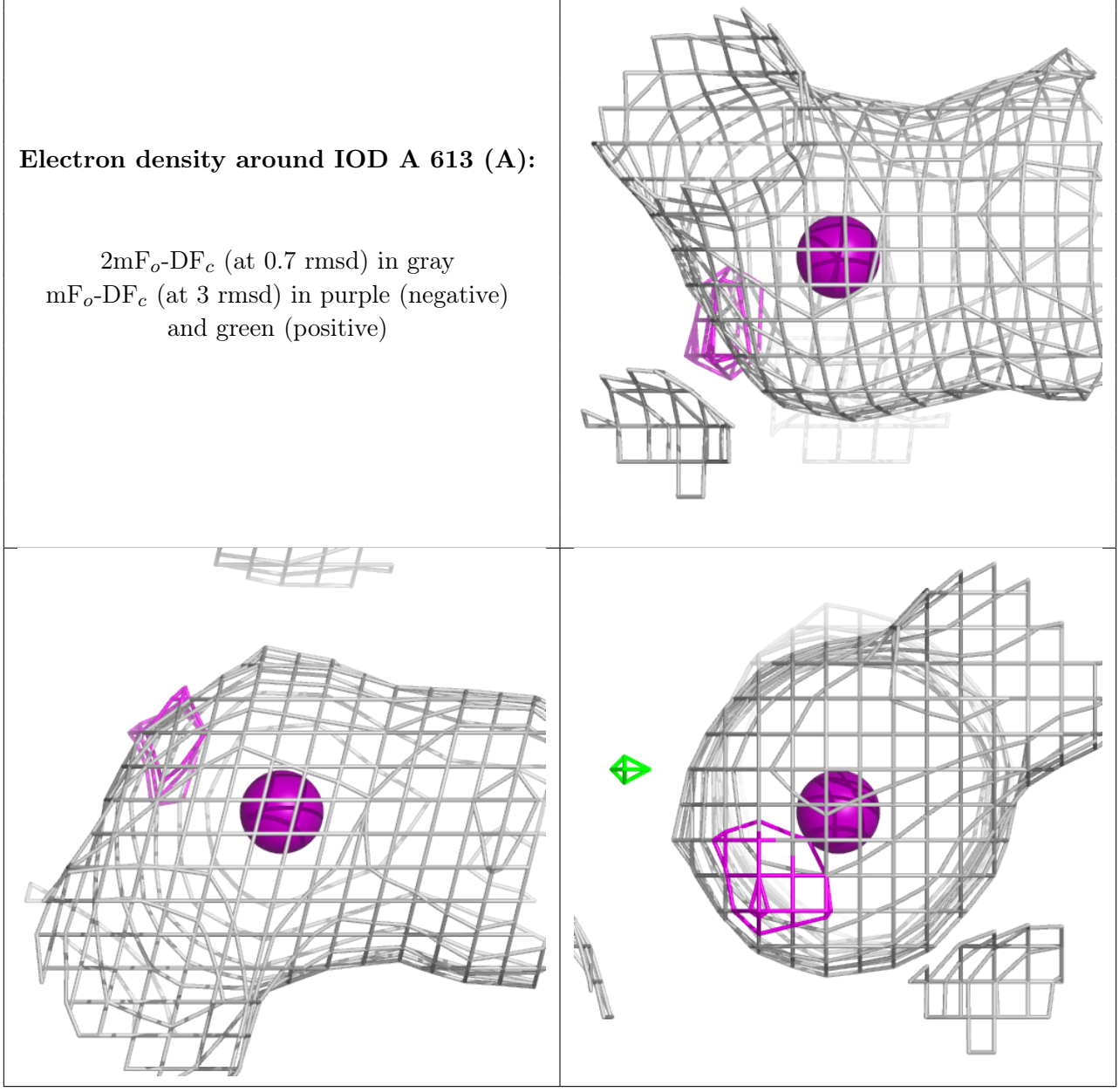






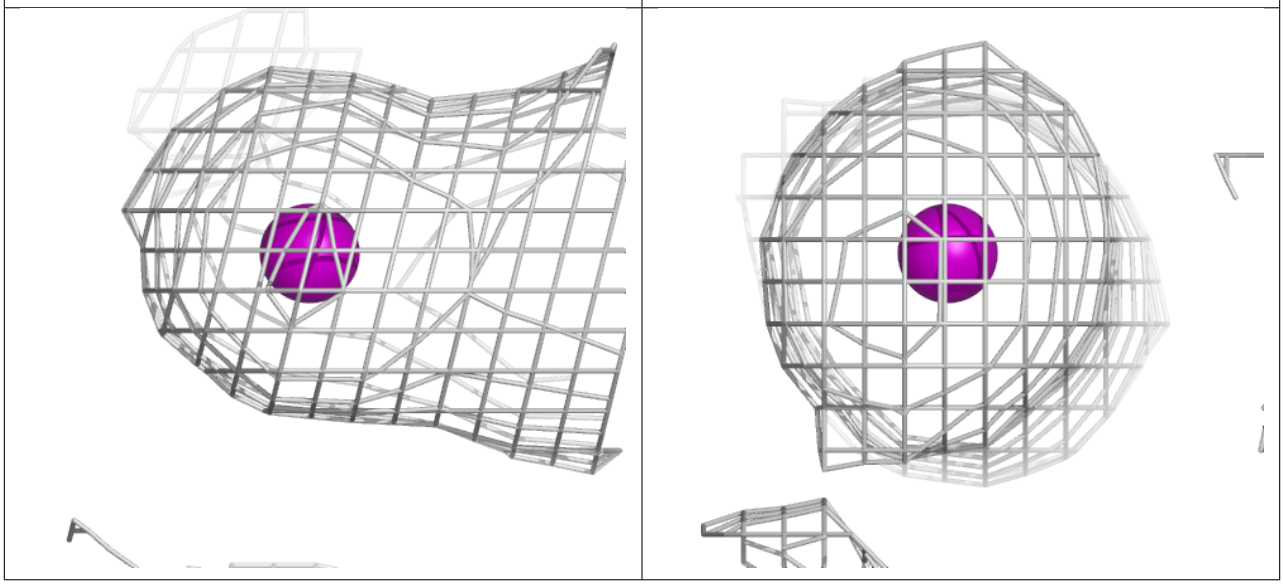
Electron density around IOD A 613 (A):

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



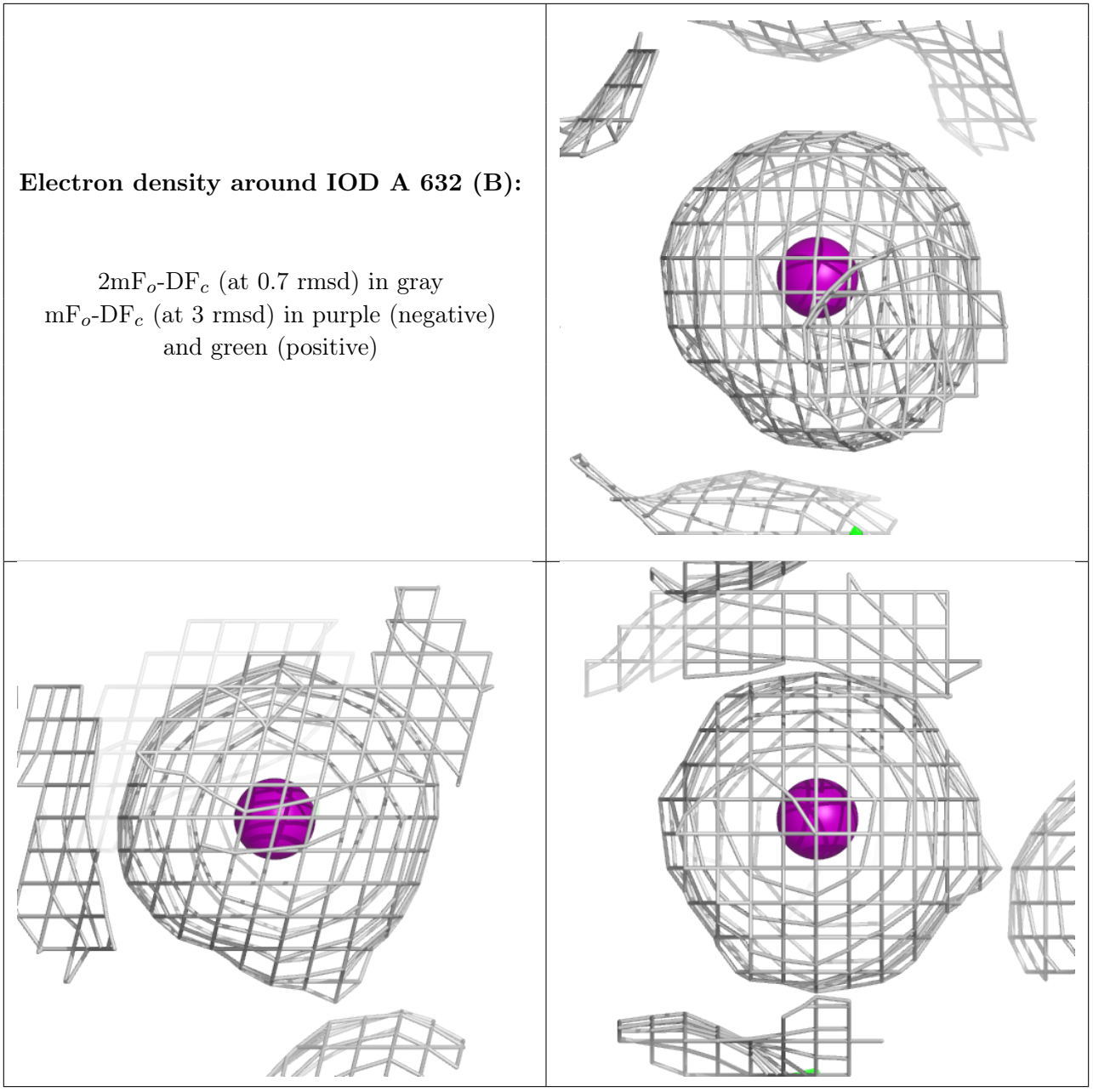
Electron density around IOD A 613 (B):

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



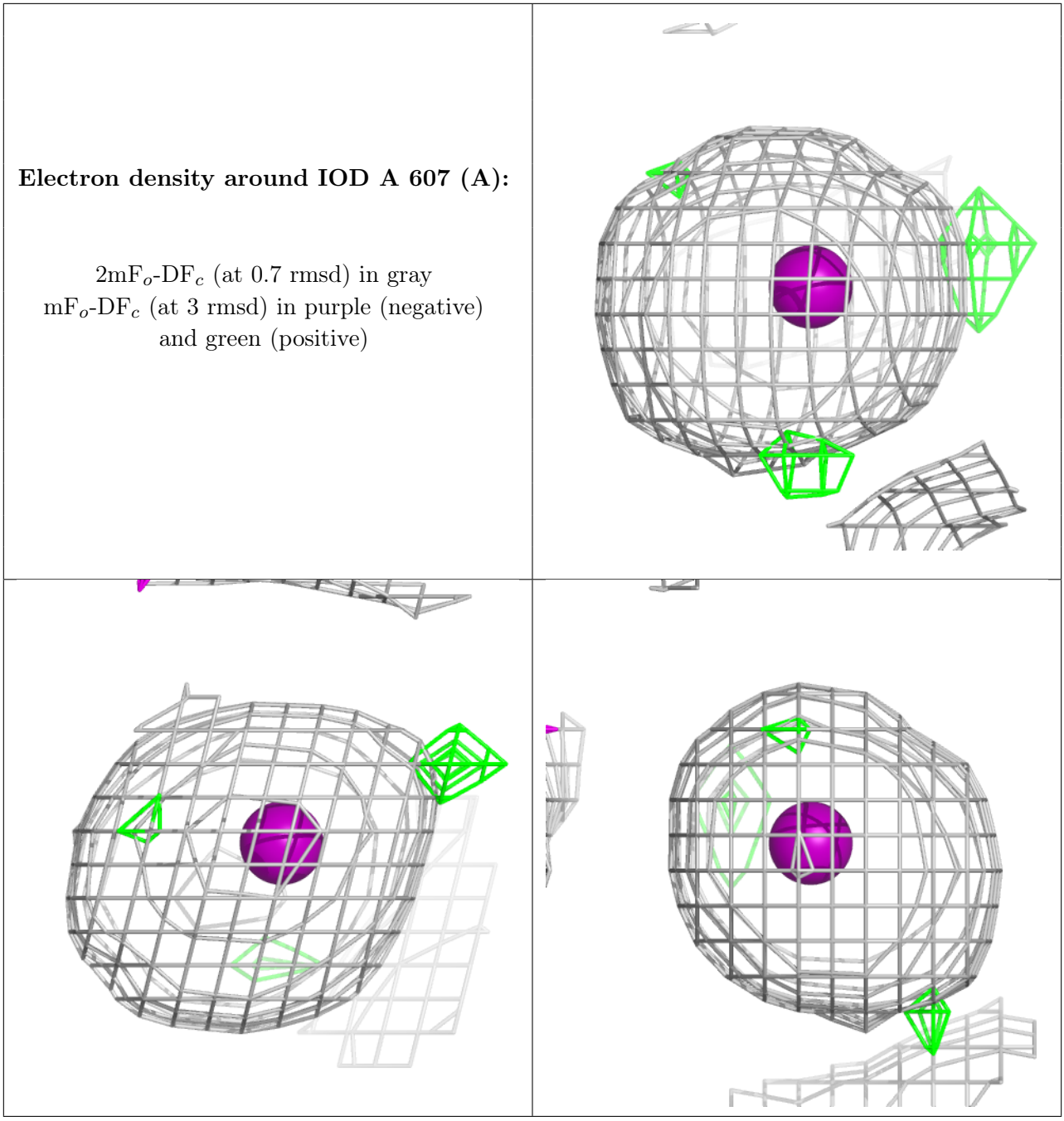
Electron density around IOD A 632 (B):

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



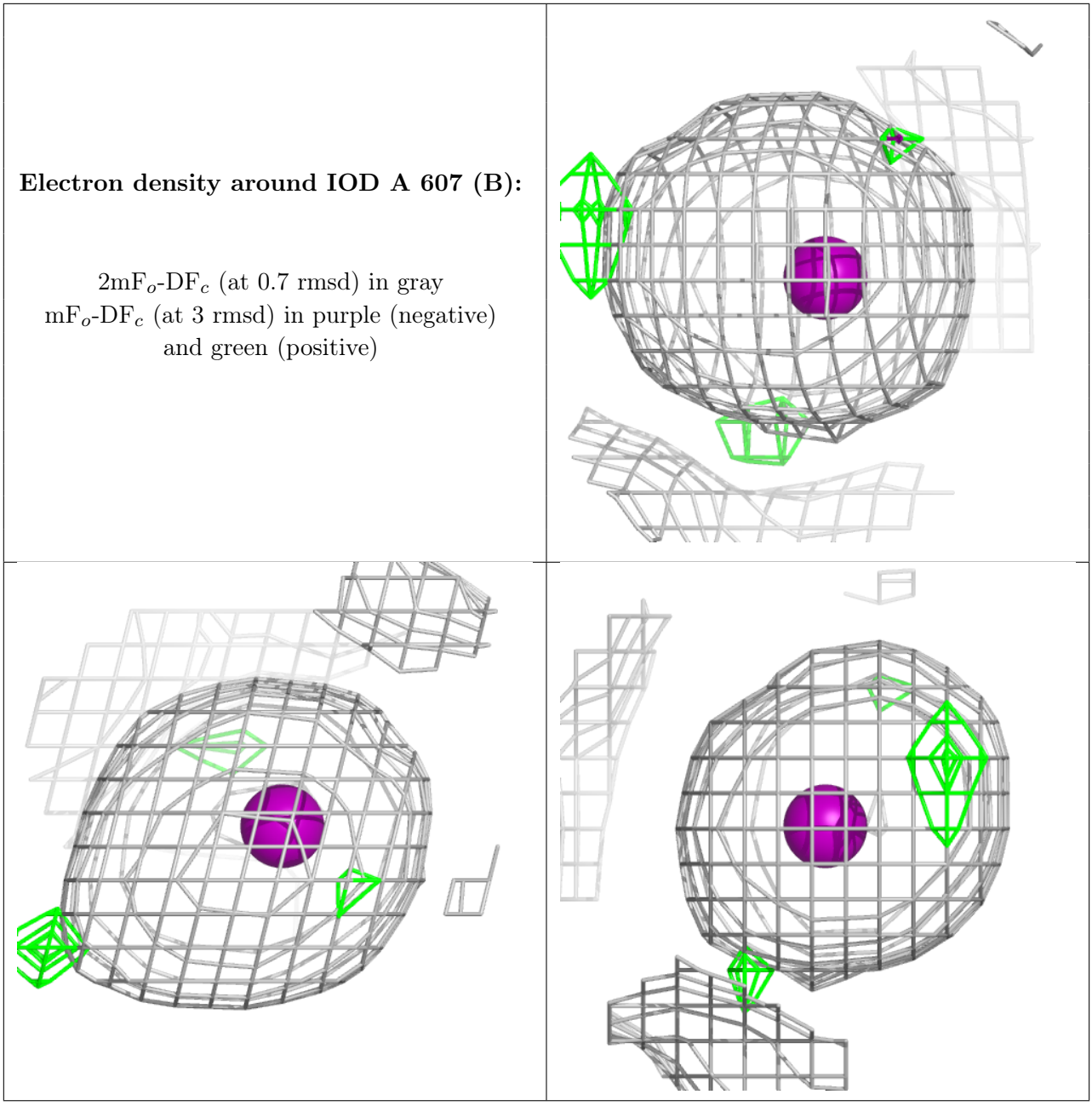
Electron density around IOD A 607 (A):

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



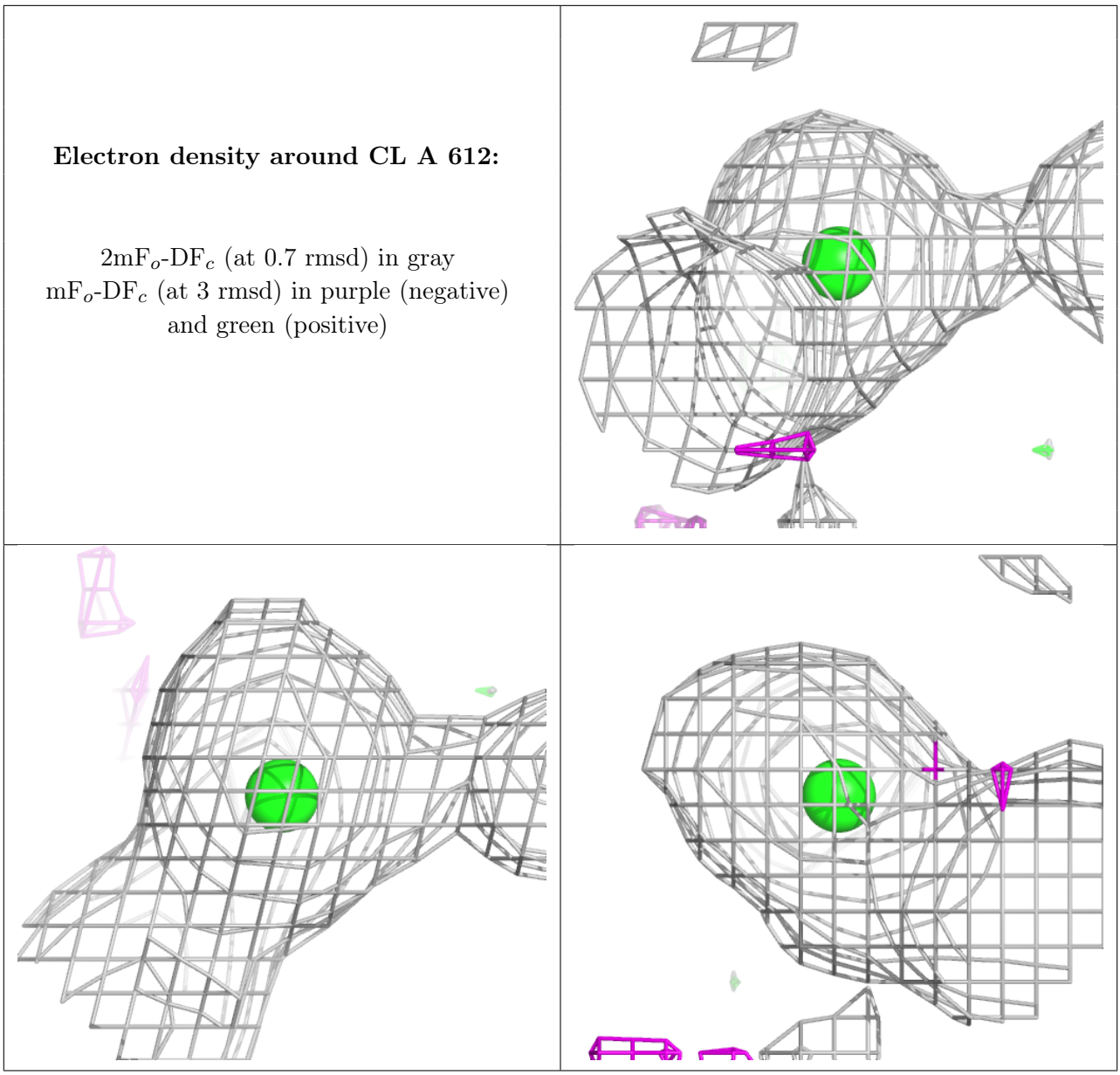
Electron density around IOD A 607 (B):

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



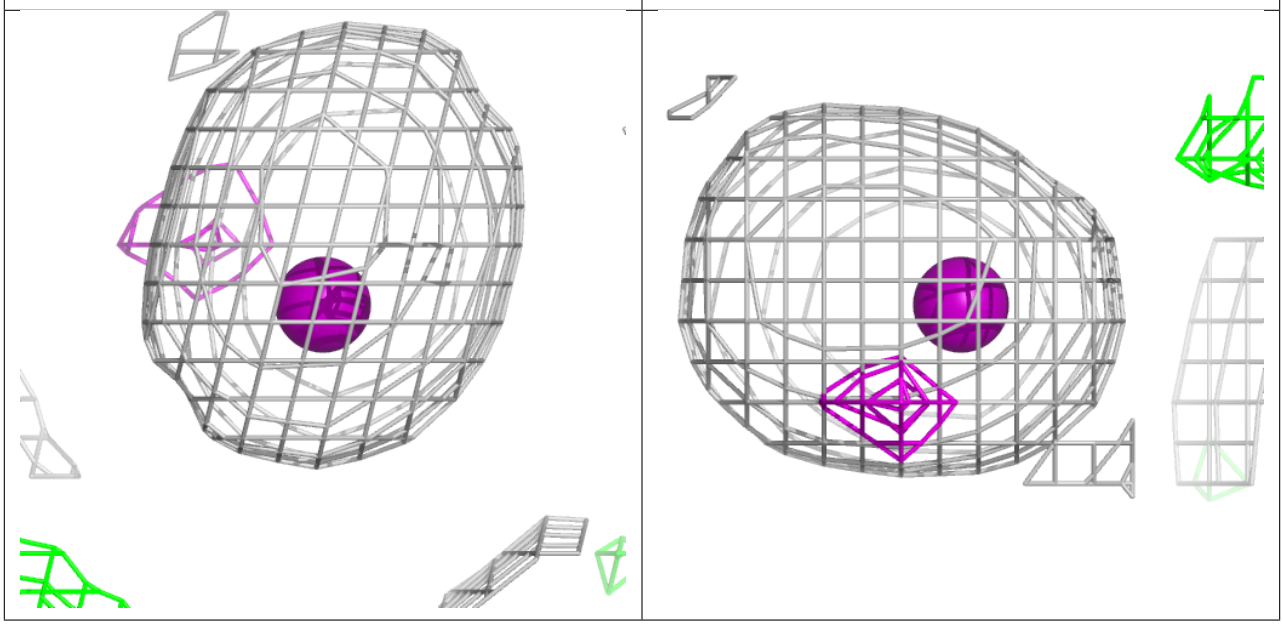
Electron density around CL A 612:

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



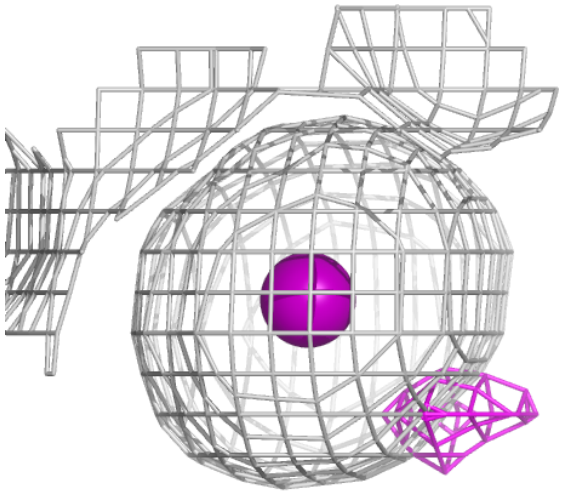
Electron density around IOD A 609 (A):

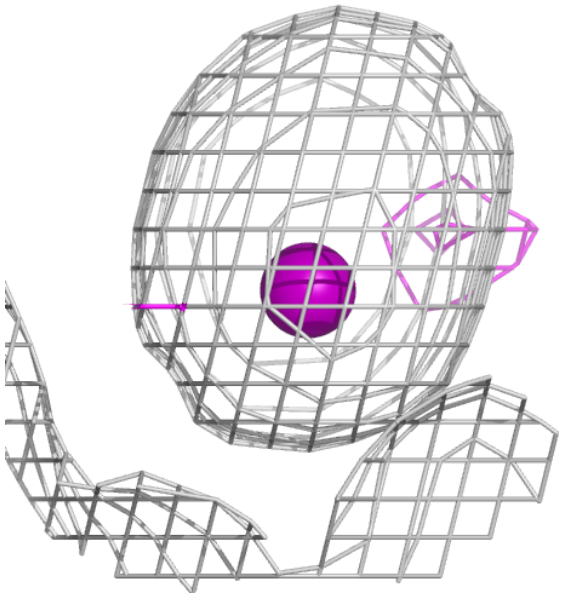
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

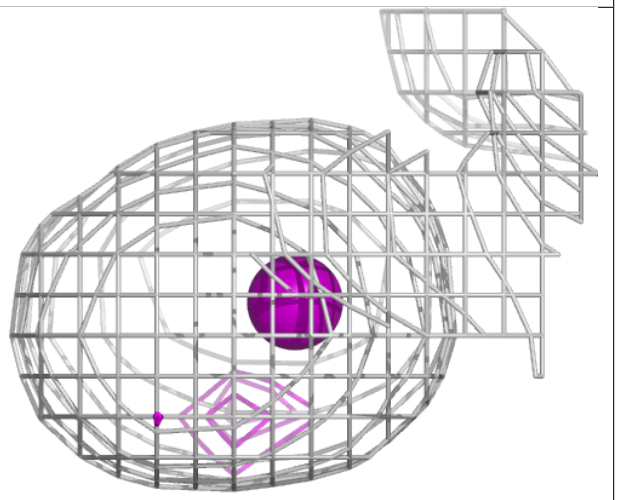


Electron density around IOD A 609 (B):

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

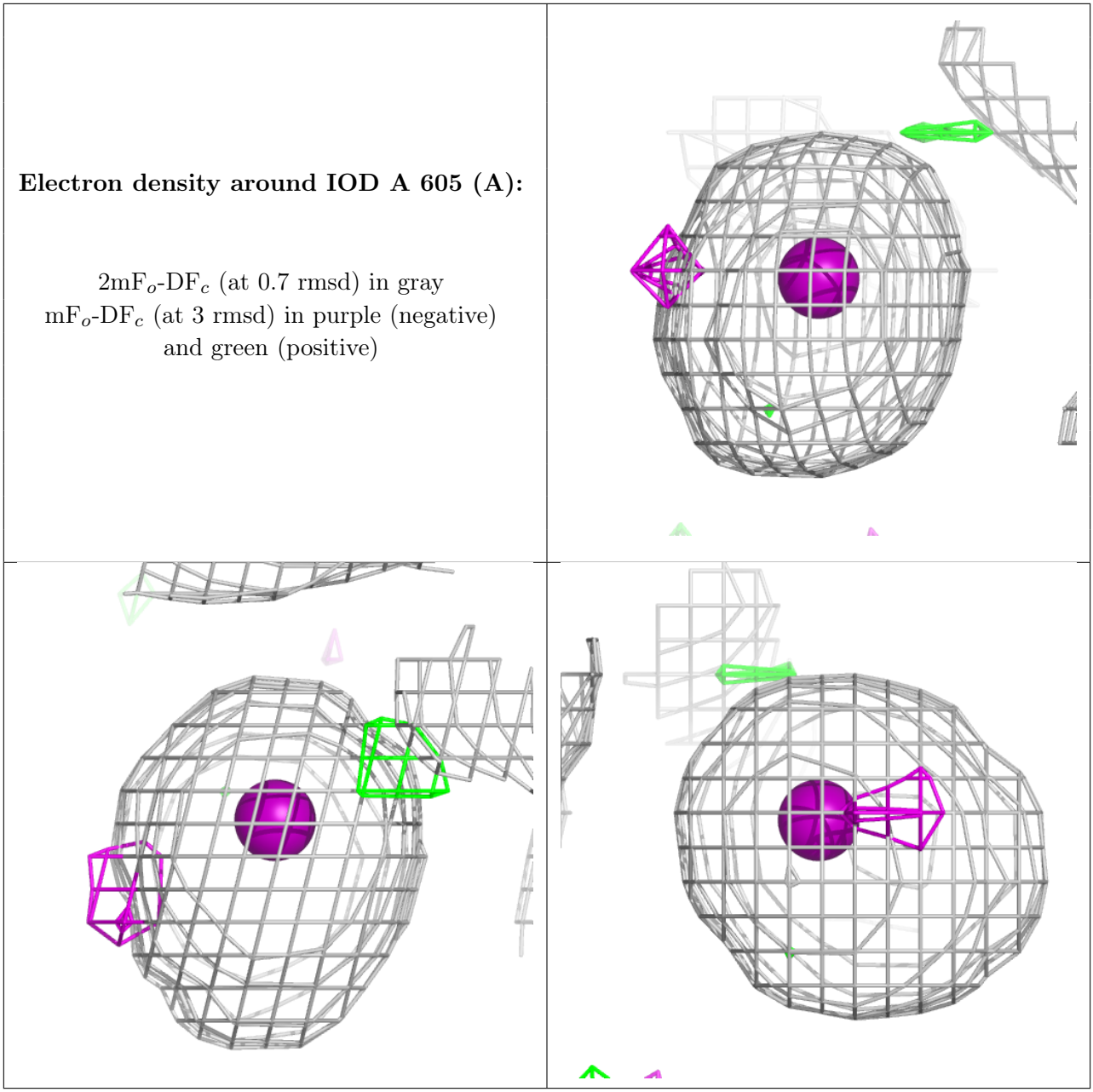






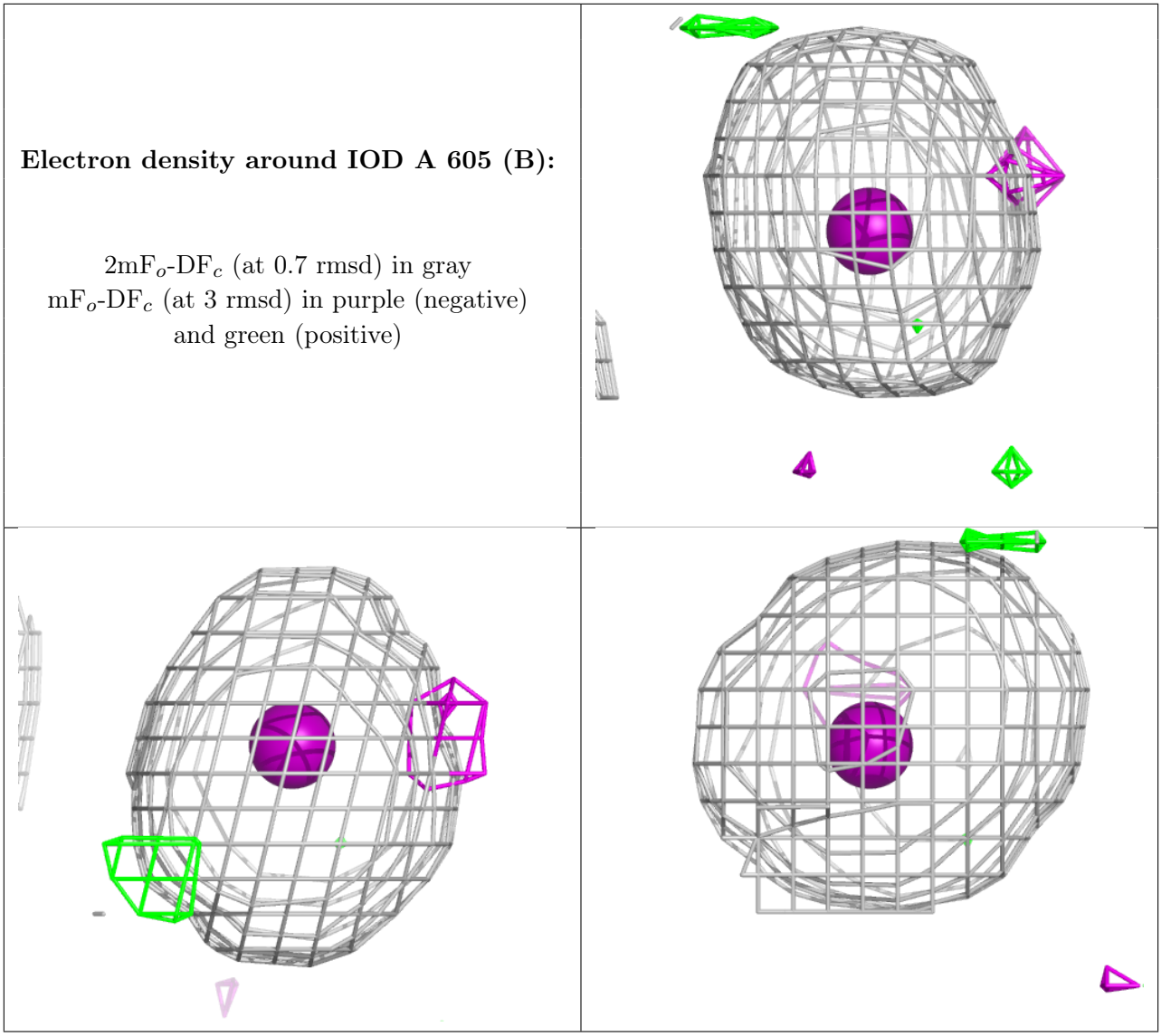
Electron density around IOD A 605 (A):

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



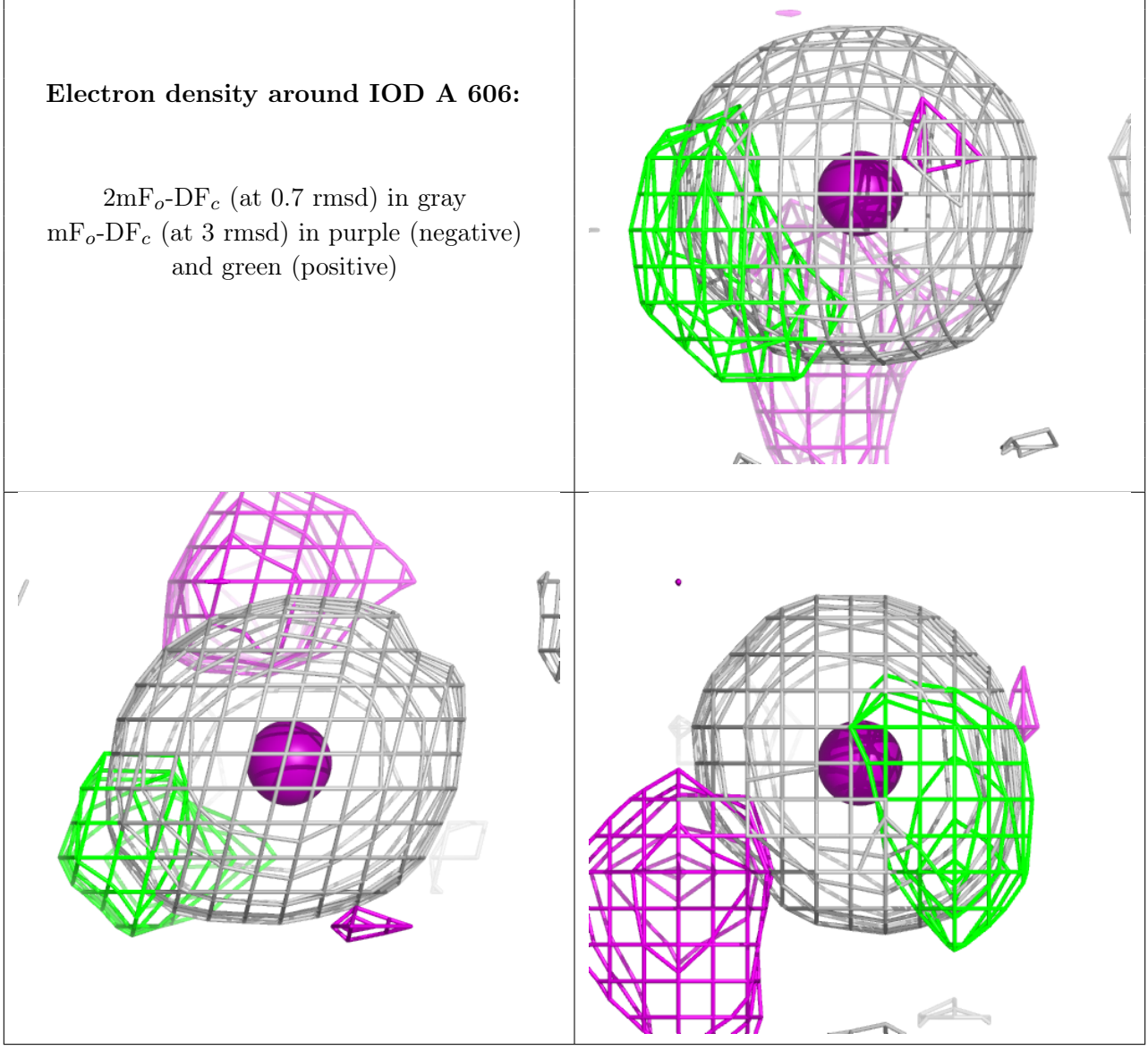
Electron density around IOD A 605 (B):

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



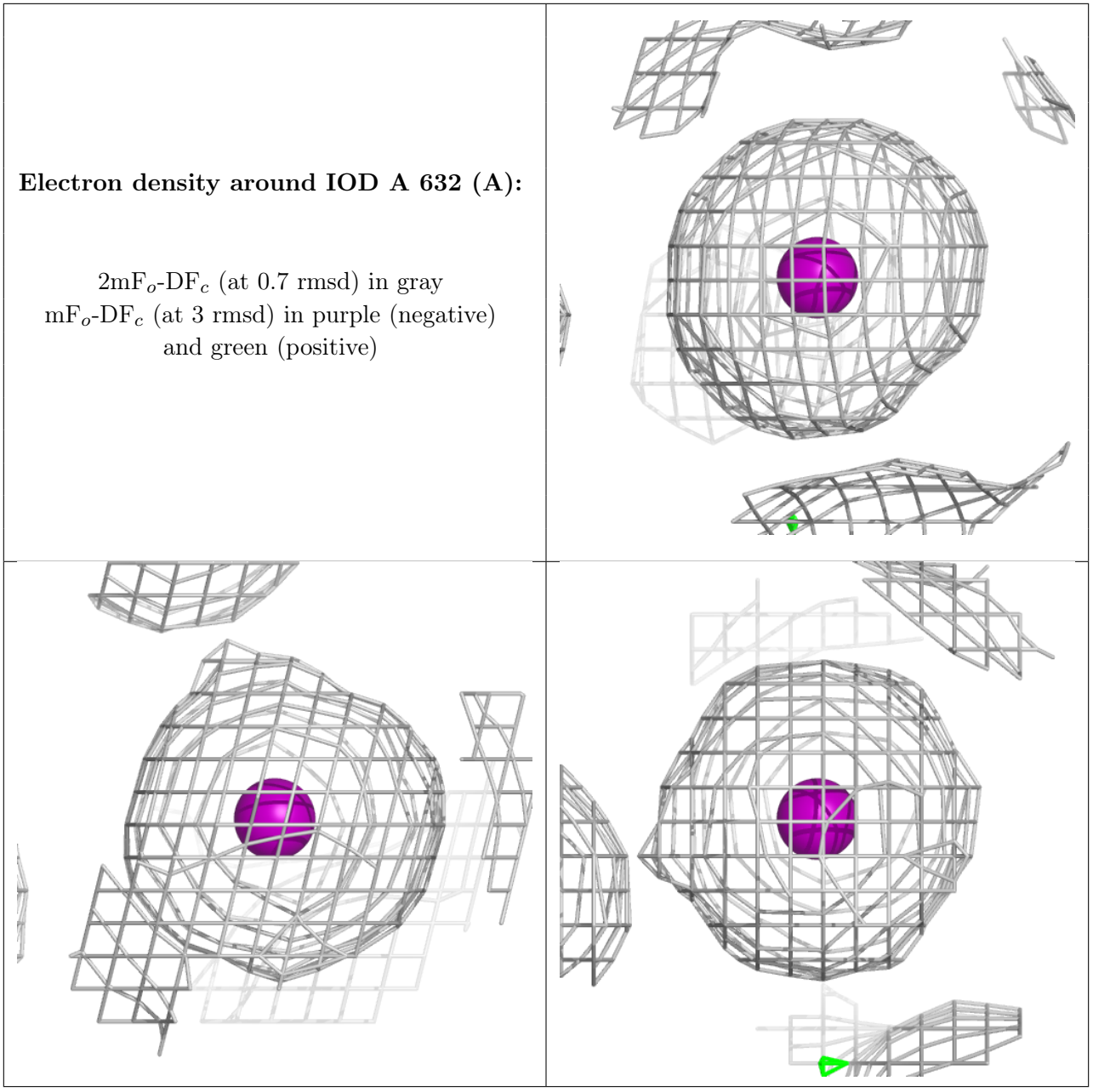
Electron density around IOD A 606:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.