



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:30 PM UTC

PDB ID : 9IT8 / pdb_00009it8
Title : Crystal structure of the ternary complex of lactoperoxidase with nitric oxide and nitrite ion at 1.95 Å resolution
Authors : Maurya, A.; Ahmad, N.; Sharma, P.; Sharma, S.; Singh, T.P.
Deposited on : 2024-07-19
Resolution : 1.95 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

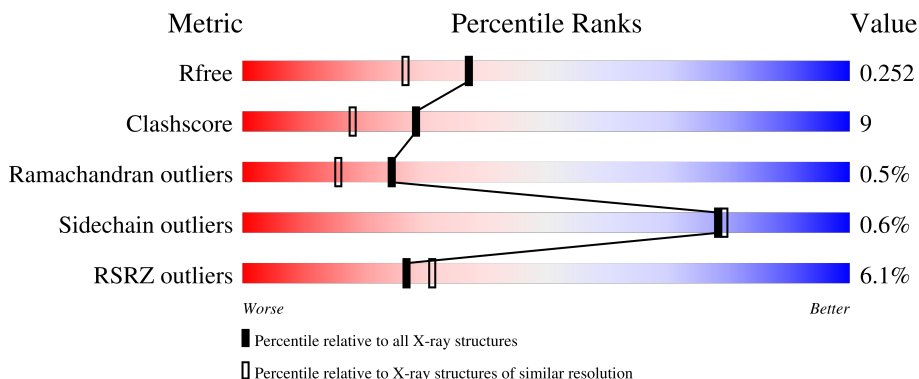
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

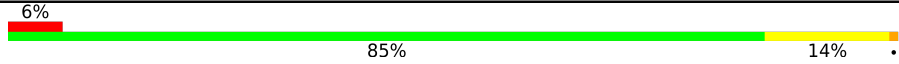
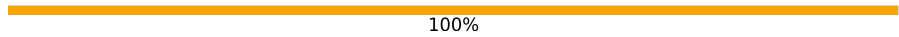
The reported resolution of this entry is 1.95 Å.

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. 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	
2	B	2	

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	NO3	A	613	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 5322 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.

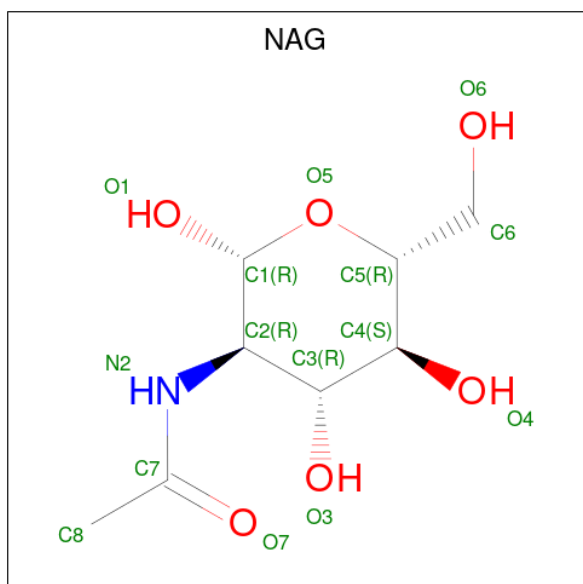
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	595	4784	3047	850	861	26	0	2	0

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



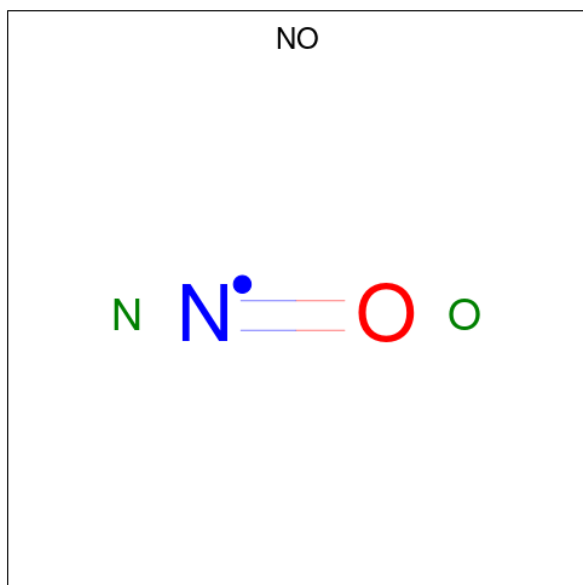
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



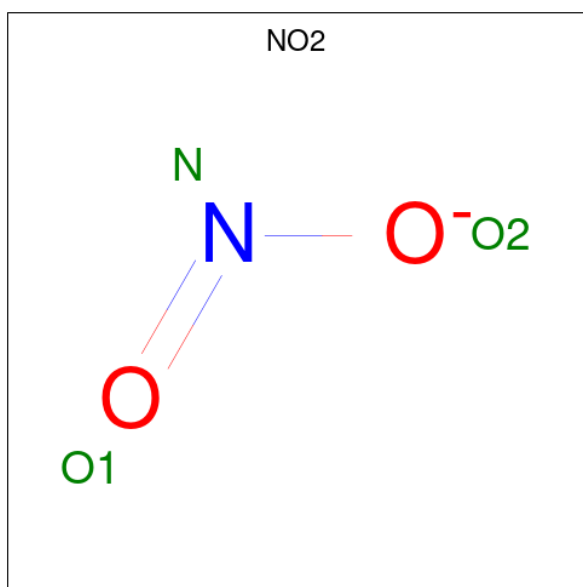
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is NITRIC OXIDE (CCD ID: NO) (formula: NO) (labeled as "Ligand of Interest" by depositor).



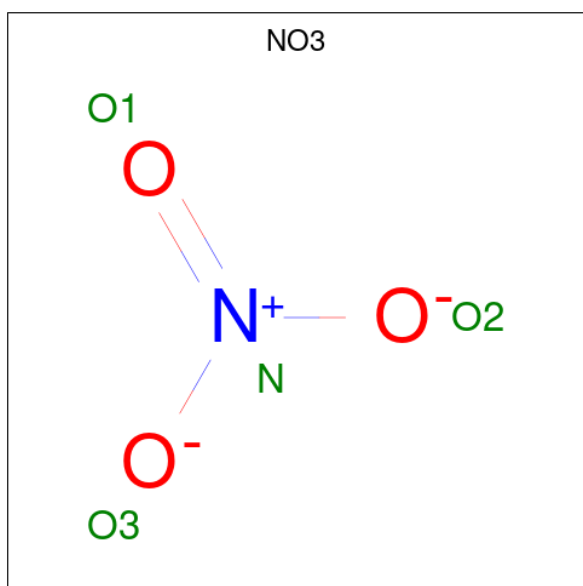
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			2	1	1		
4	A	1	Total	N	O	0	0
			2	1	1		

- Molecule 5 is NITRITE ION (CCD ID: NO₂) (formula: NO₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is NITRATE ION (CCD ID: NO3) (formula: NO_3) (labeled as "Ligand of Interest" by depositor).



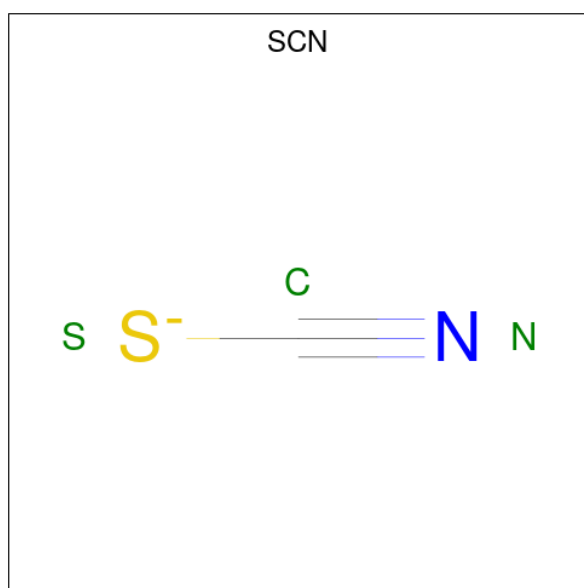
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		

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



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

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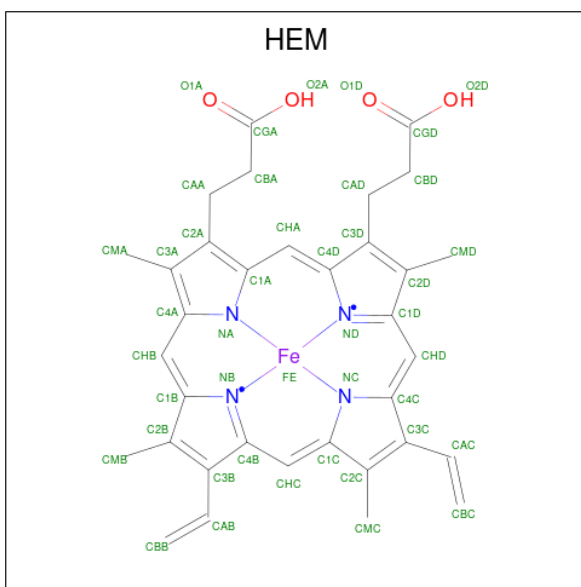
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	S	0	0
			3	1	1	1		
7	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 8 is IODIDE ION (CCD ID: IOD) (formula: I) (labeled as "Ligand of Interest" by depositor).

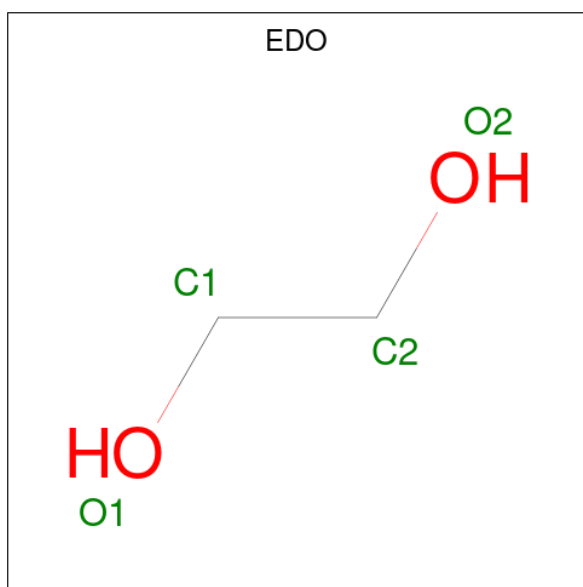
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	17	Total	I	0	0
			17	17		

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).

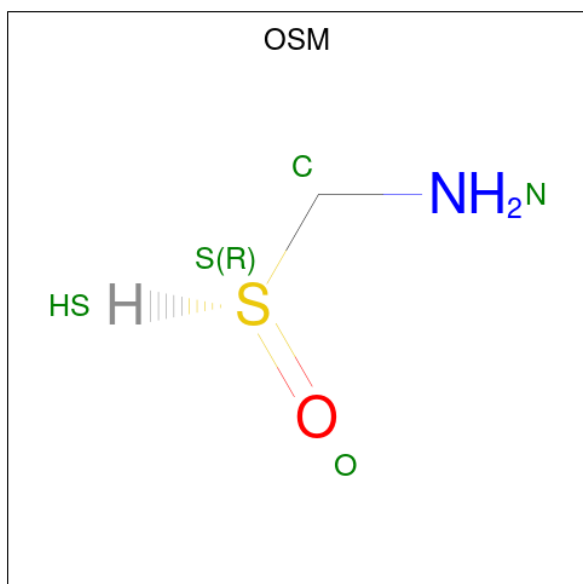


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 2 2	0	0

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 12 is 1-(OXIDOSULFANYL)METHANAMINE (CCD ID: OSM) (formula: CH₅NOS) (labeled as "Ligand of Interest" by depositor).



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

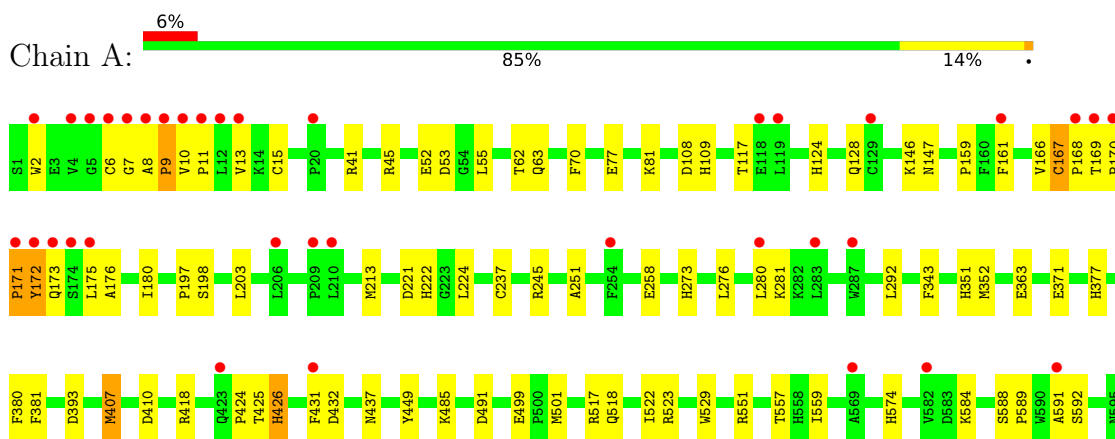
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	338	339	339	0	1

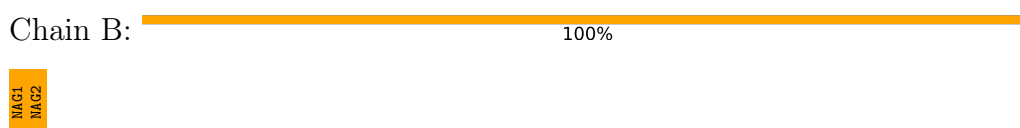
3 Residue-property plots [i](#)

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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.05Å 80.50Å 75.95Å 90.00° 102.85° 90.00°	Depositor
Resolution (Å)	74.05 – 1.95 74.05 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (74.05-1.95) 99.5 (74.05-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.188 , 0.247 0.198 , 0.252	Depositor DCC
R_{free} test set	1357 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtrriage
Anisotropy	0.111	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5322	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CA, NO, NAG, NO3, IOD, HEM, NO2, OSM, SCN

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	0.53	0/4918	1.00	8/6670 (0.1%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TYR	N-CA-CB	-12.05	92.18	111.22
1	A	591	ALA	N-CA-C	-8.32	98.02	110.24
1	A	426	HIS	CB-CA-C	6.56	120.57	109.55
1	A	591	ALA	CB-CA-C	6.51	119.61	109.84
1	A	592	SER	N-CA-C	-6.01	97.35	107.99

There are no chirality outliers.

There are no planarity outliers.

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	4784	0	4712	76	0
2	B	28	0	25	4	0
3	A	42	0	39	0	0
4	A	4	0	0	1	0
5	A	6	0	0	0	0
6	A	32	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	18	0	0	1	0
8	A	17	0	0	6	0
9	A	43	0	30	11	0
10	A	4	0	5	0	0
11	A	1	0	0	0	0
12	A	4	0	5	0	0
13	A	339	0	0	15	0
All	All	5322	0	4816	86	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 9.

The worst 5 of 86 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASP:OD2	9:A:624:HEM:CMD	1.76	1.31
1:A:258:GLU:OE2	9:A:624:HEM:CMB	1.85	1.22
1:A:258:GLU:OE2	9:A:624:HEM:HMB1	1.03	1.20
1:A:198:SER:OG	8:A:639:IOD:I	2.32	1.17
1:A:108:ASP:OD2	9:A:624:HEM:HMD1	0.82	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	595/595 (100%)	571 (96%)	21 (4%)	3 (0%)	24 16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	170	PRO
1	A	9	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	520/518 (100%)	517 (99%)	3 (1%)	78 79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	ARG
1	A	371	GLU
1	A	407	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	ASN
1	A	489	ASN
1	A	565	HIS
1	A	94	GLN
1	A	68	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates i

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1	1,2	14,14,15	0.49	0	17,19,21	1.71	3 (17%)
2	NAG	B	2	2	14,14,15	0.43	0	17,19,21	2.25	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	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	7.79	122.63	112.19
2	B	1	NAG	C1-C2-N2	4.87	118.10	110.43
2	B	2	NAG	C1-C2-N2	-3.54	104.86	110.43
2	B	2	NAG	O5-C1-C2	-2.97	106.69	111.29
2	B	1	NAG	O4-C4-C5	2.97	116.64	109.32

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2

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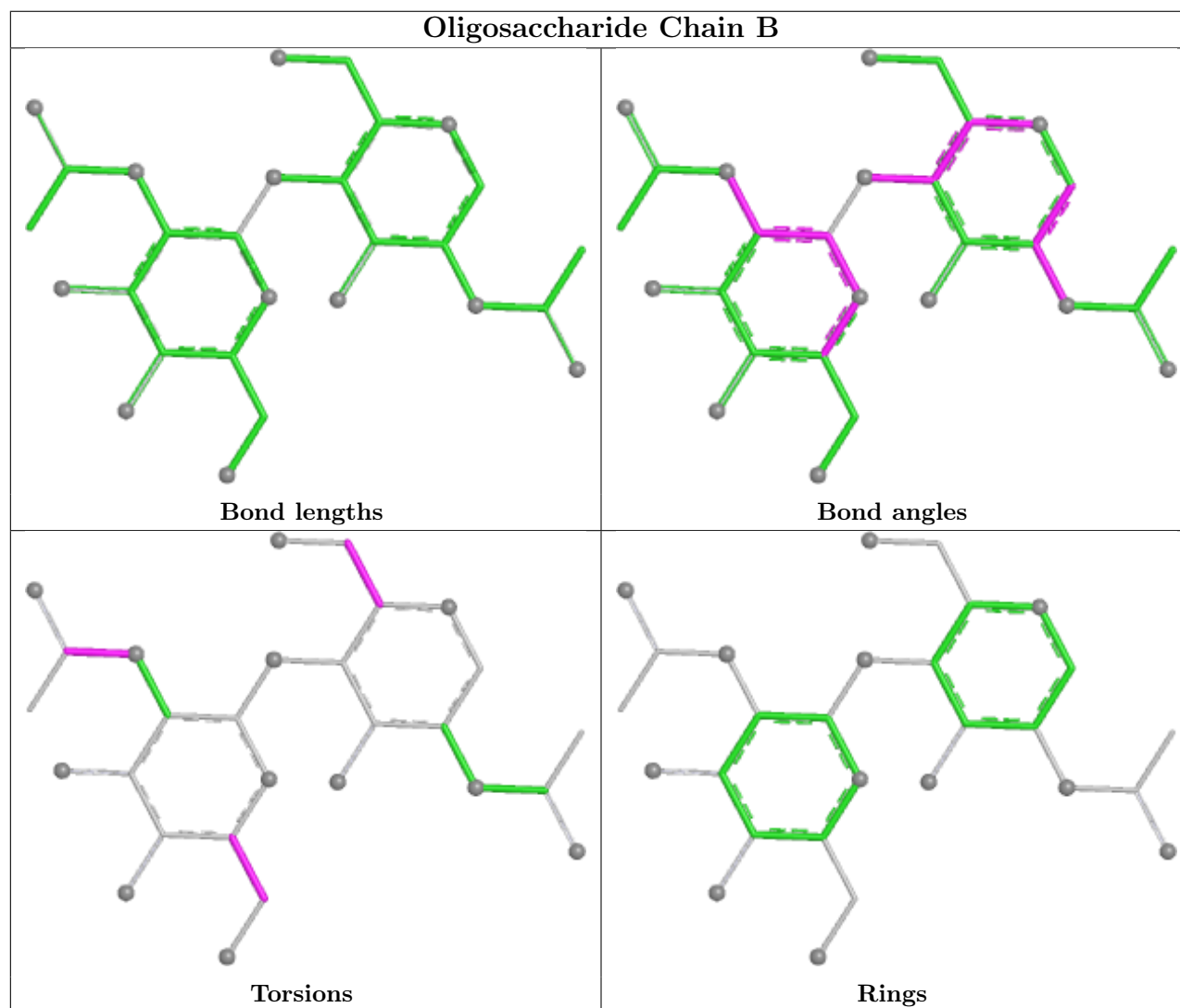
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	4	0
2	B	1	NAG	2	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.



5.6 Ligand geometry

Of 42 ligands modelled in this entry, 18 are monoatomic - leaving 24 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
6	NO3	A	606	-	1,3,3	0.27	0	0,3,3	-	-
3	NAG	A	602	1	14,14,15	0.47	0	17,19,21	1.37	2 (11%)
6	NO3	A	613	-	1,3,3	0.11	0	0,3,3	-	-
6	NO3	A	611	-	1,3,3	0.62	0	0,3,3	-	-
3	NAG	A	601	1	14,14,15	0.44	0	17,19,21	1.60	2 (11%)
6	NO3	A	614	-	1,3,3	0.33	0	0,3,3	-	-
9	HEM	A	624	4,1	50,50,50	1.69	9 (18%)	67,82,82	1.66	14 (20%)
12	OSM	A	628	-	1,3,3	0.29	0	0,2,2	-	-
7	SCN	A	636	-	1,2,2	0.86	0	0,1,1	-	-
7	SCN	A	637	-	1,2,2	0.24	0	0,1,1	-	-
6	NO3	A	633	-	1,3,3	0.23	0	0,3,3	-	-
7	SCN	A	609	-	1,2,2	0.74	0	0,1,1	-	-
7	SCN	A	610	-	1,2,2	0.73	0	0,1,1	-	-
4	NO	A	634	-	0,1,1	-	-	-	-	-
5	NO2	A	635	-	1,2,2	0.64	0	0,1,1	-	-
7	SCN	A	627	-	1,2,2	1.00	0	0,1,1	-	-
6	NO3	A	607	-	1,3,3	0.31	0	0,3,3	-	-
6	NO3	A	615	-	1,3,3	0.25	0	0,3,3	-	-
4	NO	A	604	9	0,1,1	-	-	-	-	-
3	NAG	A	603	1	14,14,15	0.41	0	17,19,21	1.34	3 (17%)
10	EDO	A	625	-	3,3,3	0.64	0	2,2,2	0.27	0
5	NO2	A	605	-	1,2,2	0.57	0	0,1,1	-	-
6	NO3	A	612	8	1,3,3	0.42	0	0,3,3	-	-
7	SCN	A	608	-	1,2,2	0.12	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
10	EDO	A	625	-	-	0/1/1/1	-
3	NAG	A	603	1	-	2/6/23/26	0/1/1/1
9	HEM	A	624	4,1	-	4/14/54/54	-
12	OSM	A	628	-	-	0/0/1/1	-
3	NAG	A	602	1	-	4/6/23/26	0/1/1/1
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	624	HEM	FE-NB	4.82	2.09	1.94
9	A	624	HEM	C1B-NB	-4.58	1.32	1.40
9	A	624	HEM	FE-NC	4.33	2.09	1.95
9	A	624	HEM	C4C-NC	-3.06	1.33	1.39
9	A	624	HEM	C4D-ND	-2.80	1.35	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAG	O5-C1-C2	5.09	119.16	111.29
9	A	624	HEM	C1B-NB-C4B	3.93	109.86	105.21
9	A	624	HEM	C4B-C3B-C2B	-3.92	103.68	107.28
9	A	624	HEM	CHA-C4D-ND	3.90	129.19	124.37
9	A	624	HEM	C3B-C2B-C1B	3.71	109.19	106.41

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	NAG	O5-C5-C6-O6
3	A	601	NAG	C8-C7-N2-C2
3	A	602	NAG	O5-C5-C6-O6
3	A	601	NAG	O7-C7-N2-C2
3	A	602	NAG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 17 short contacts:

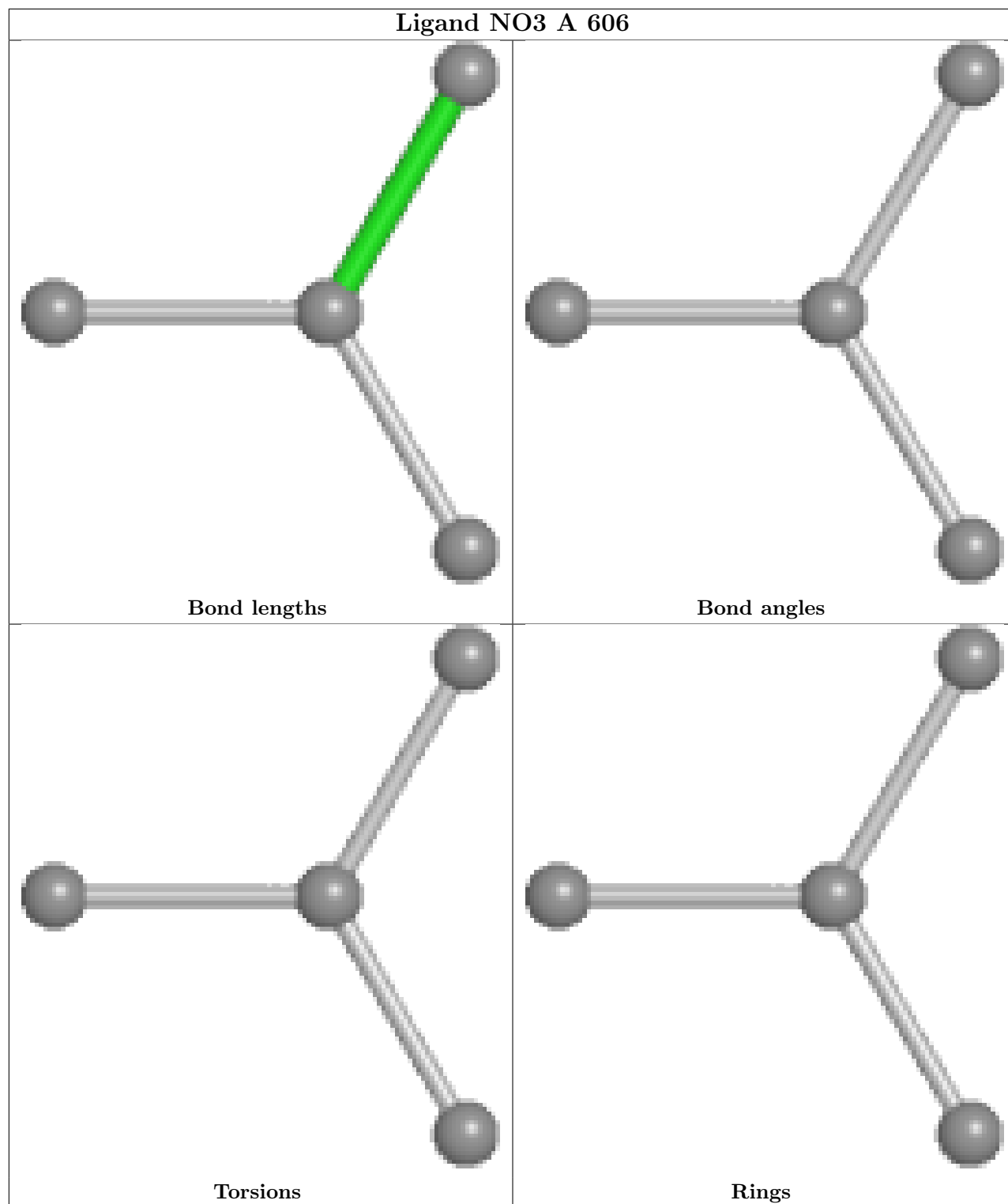
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	613	NO3	2	0
6	A	611	NO3	1	0

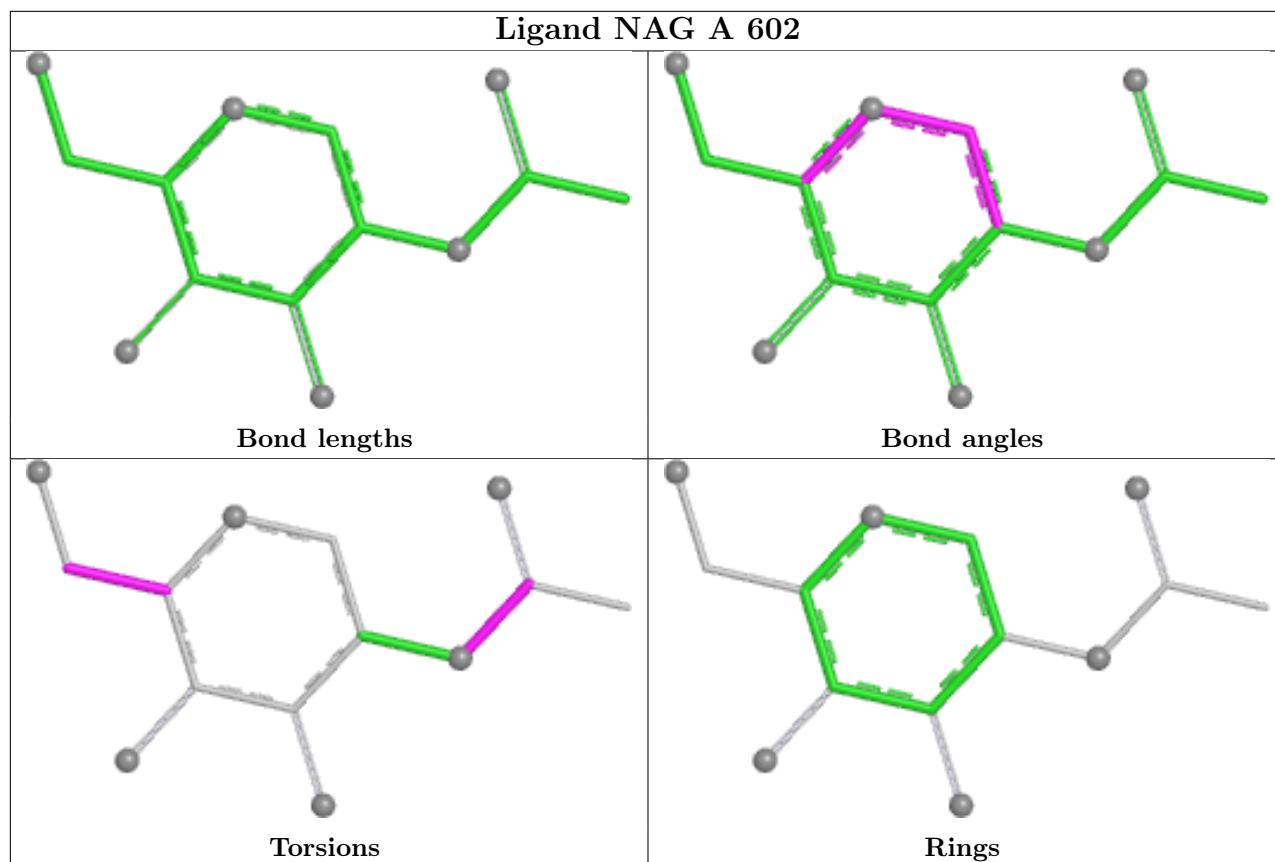
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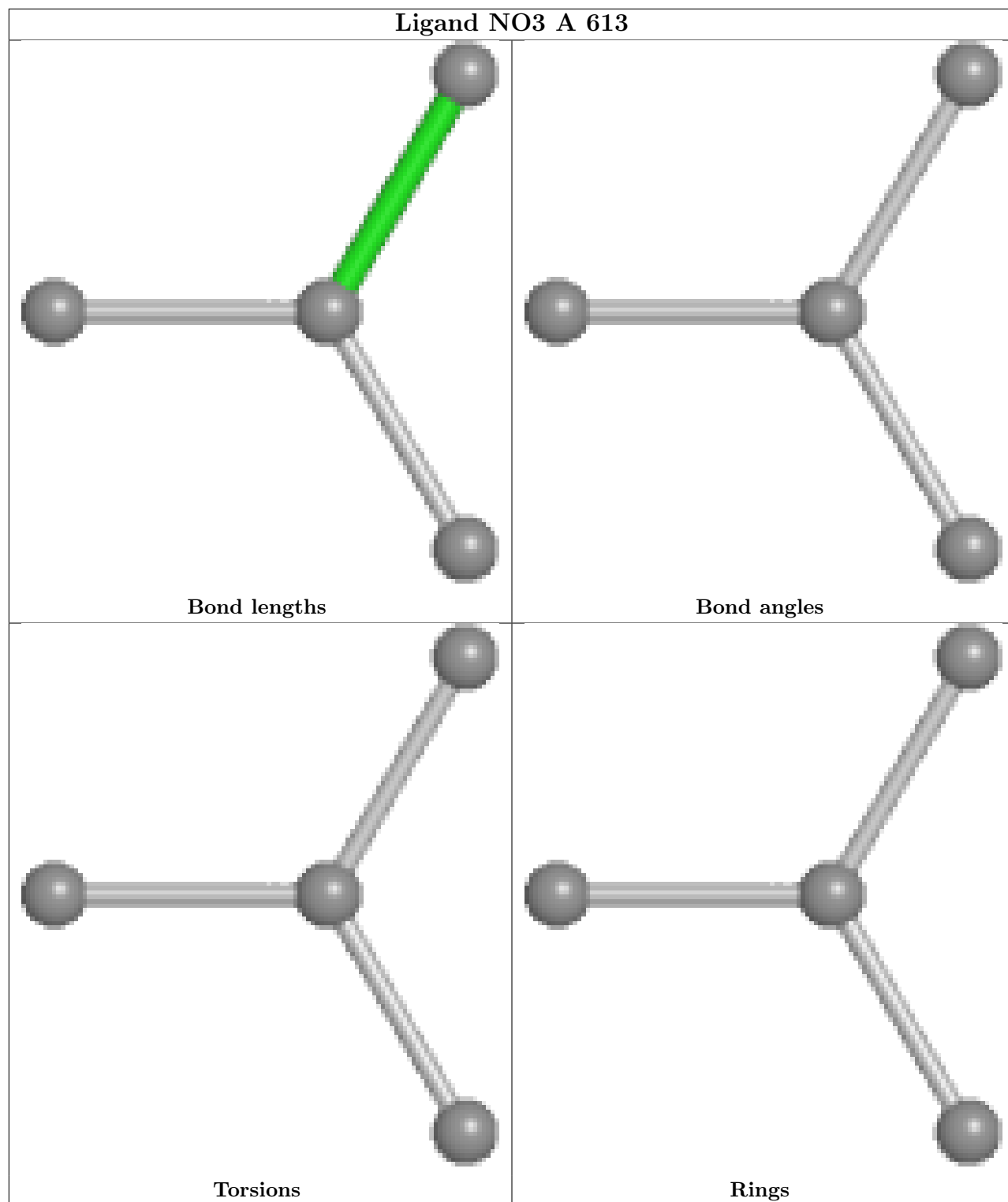
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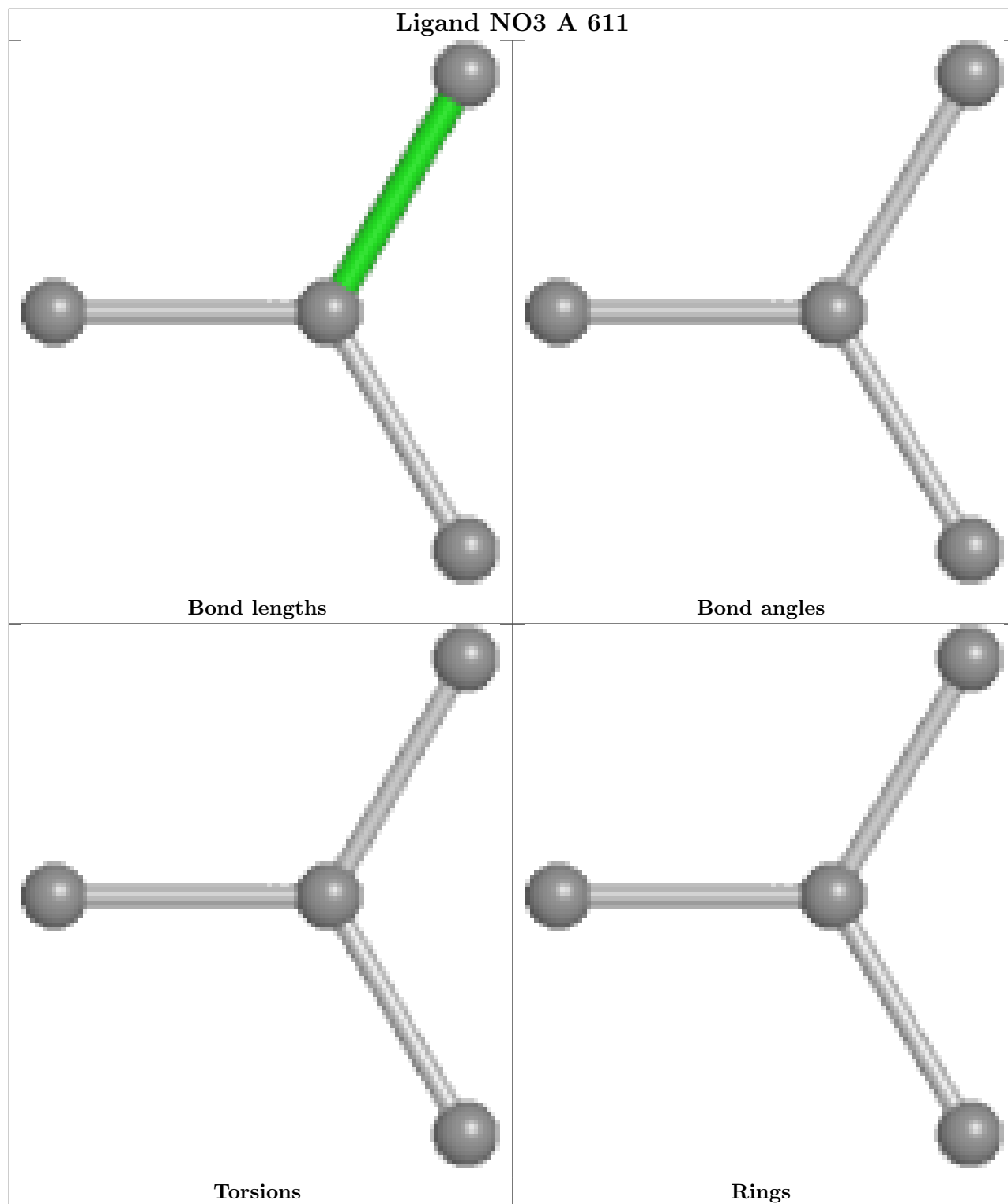
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	624	HEM	11	0
7	A	637	SCN	1	0
6	A	633	NO3	1	0
4	A	604	NO	1	0

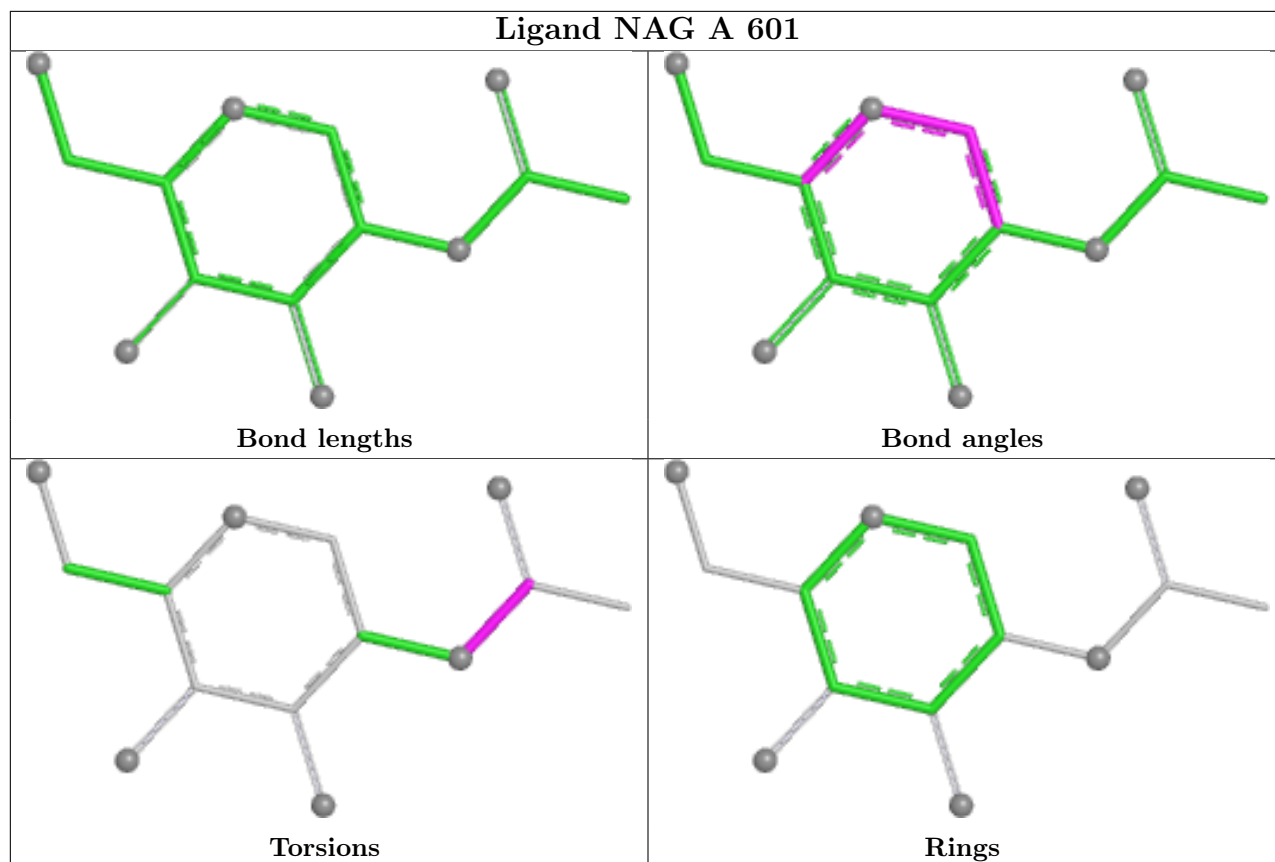
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

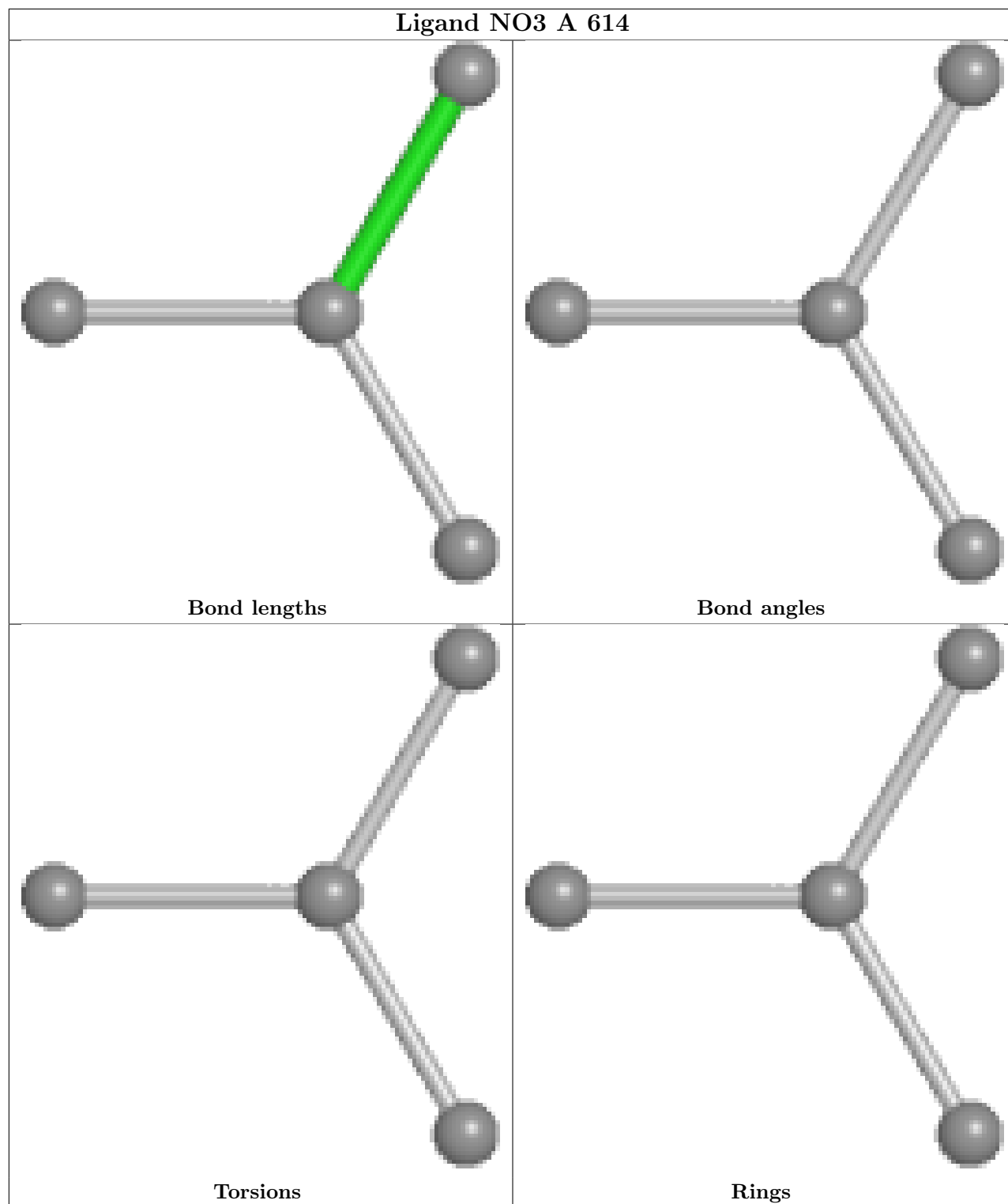


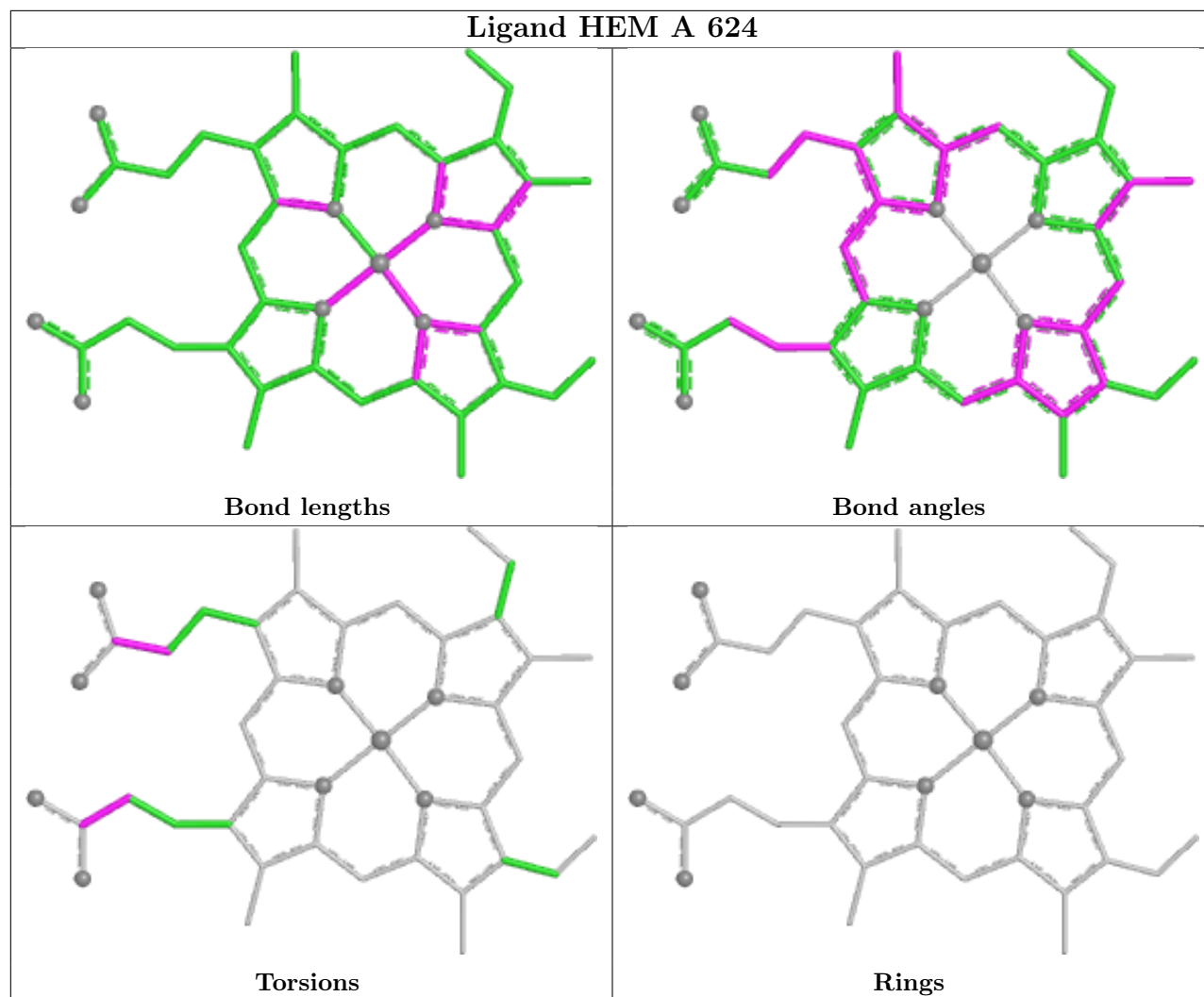


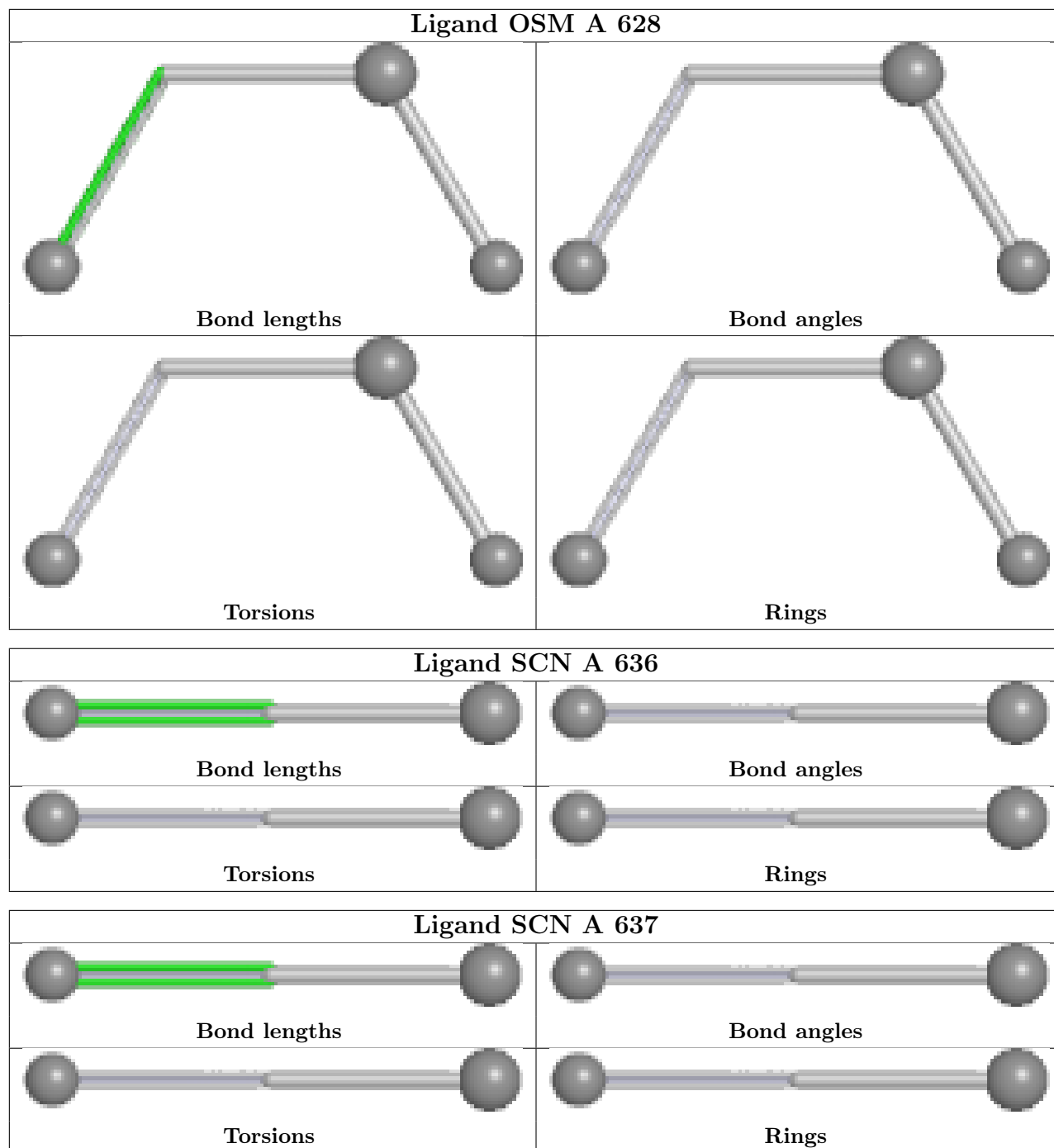


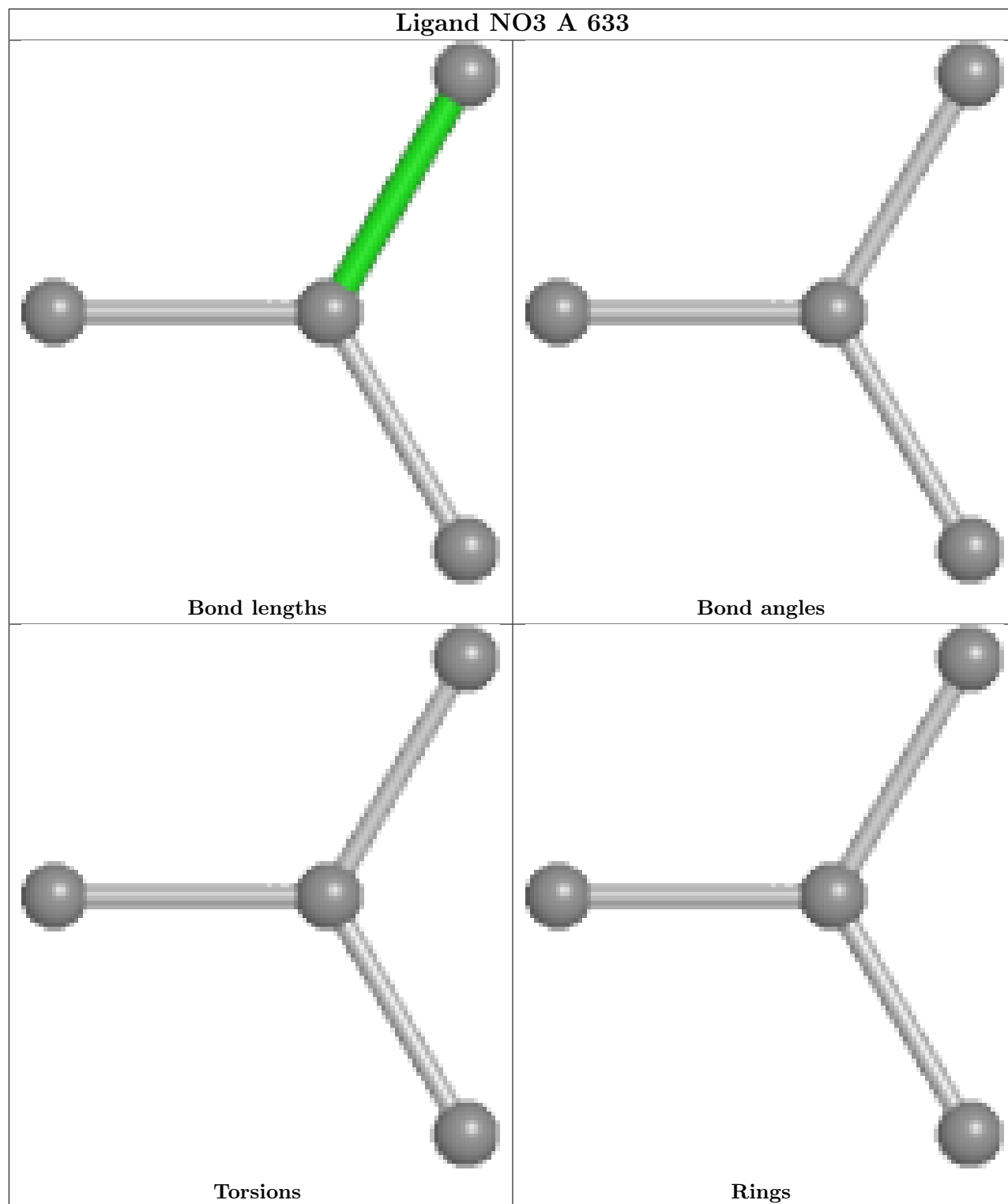


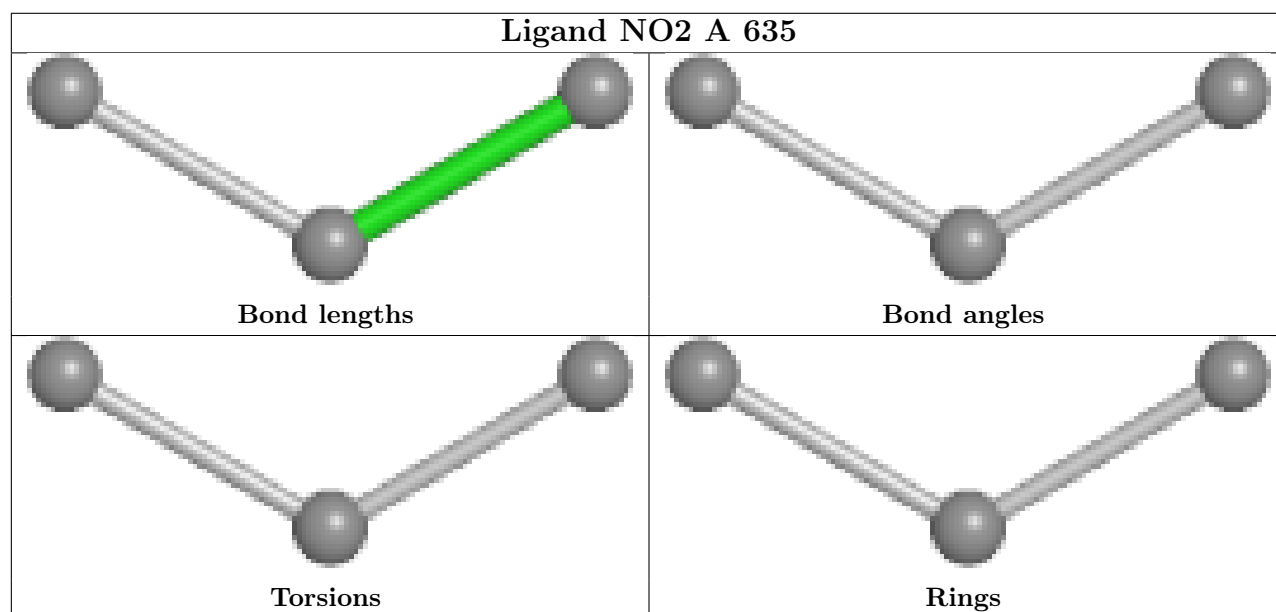
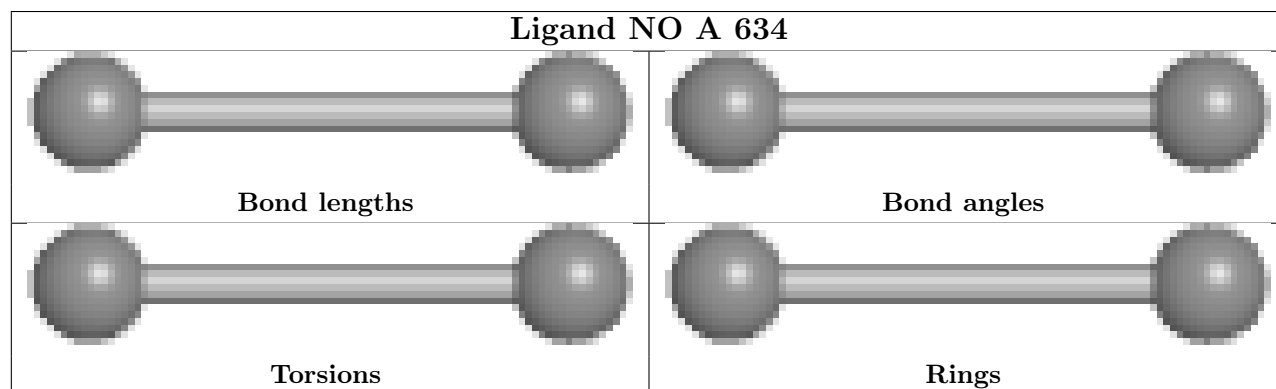
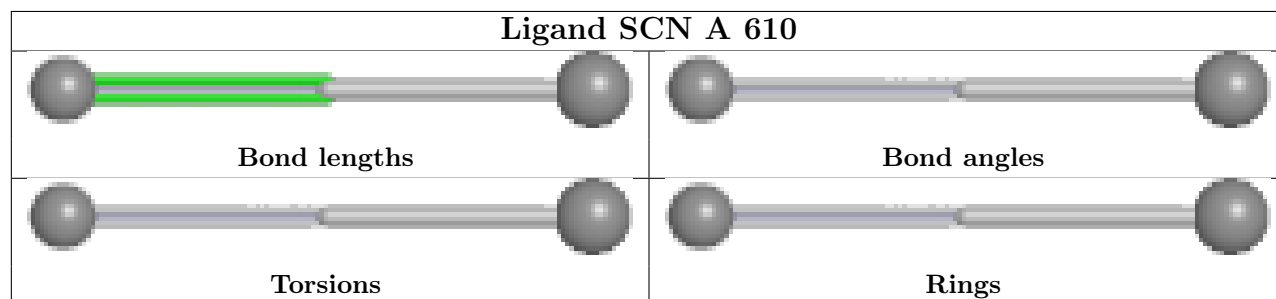
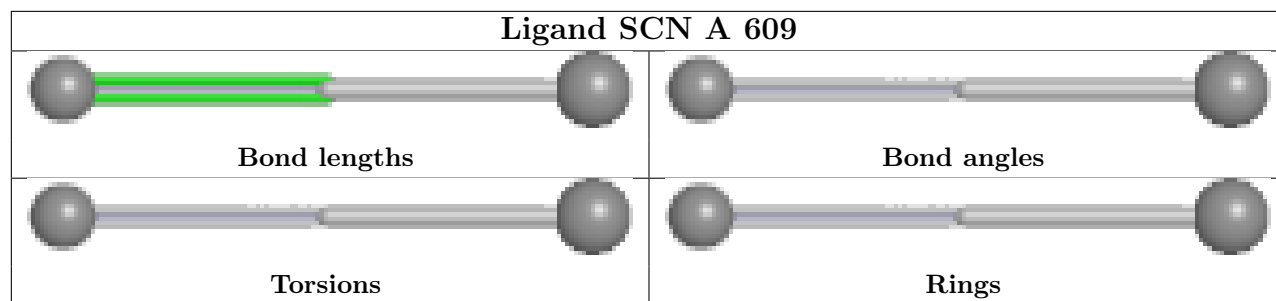


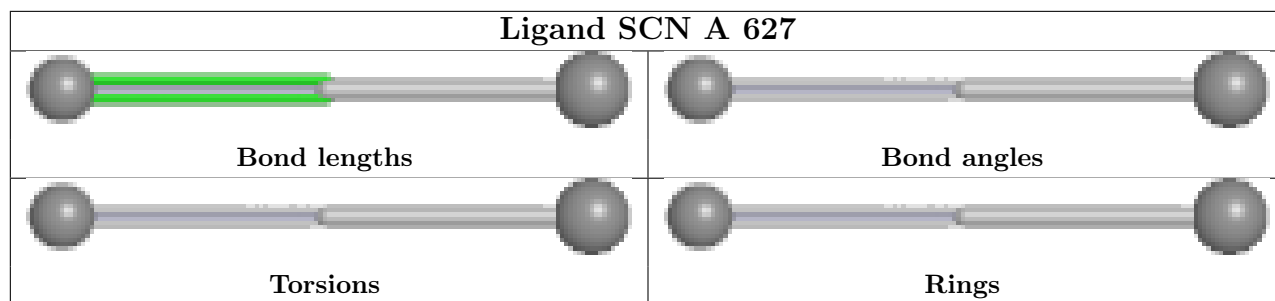


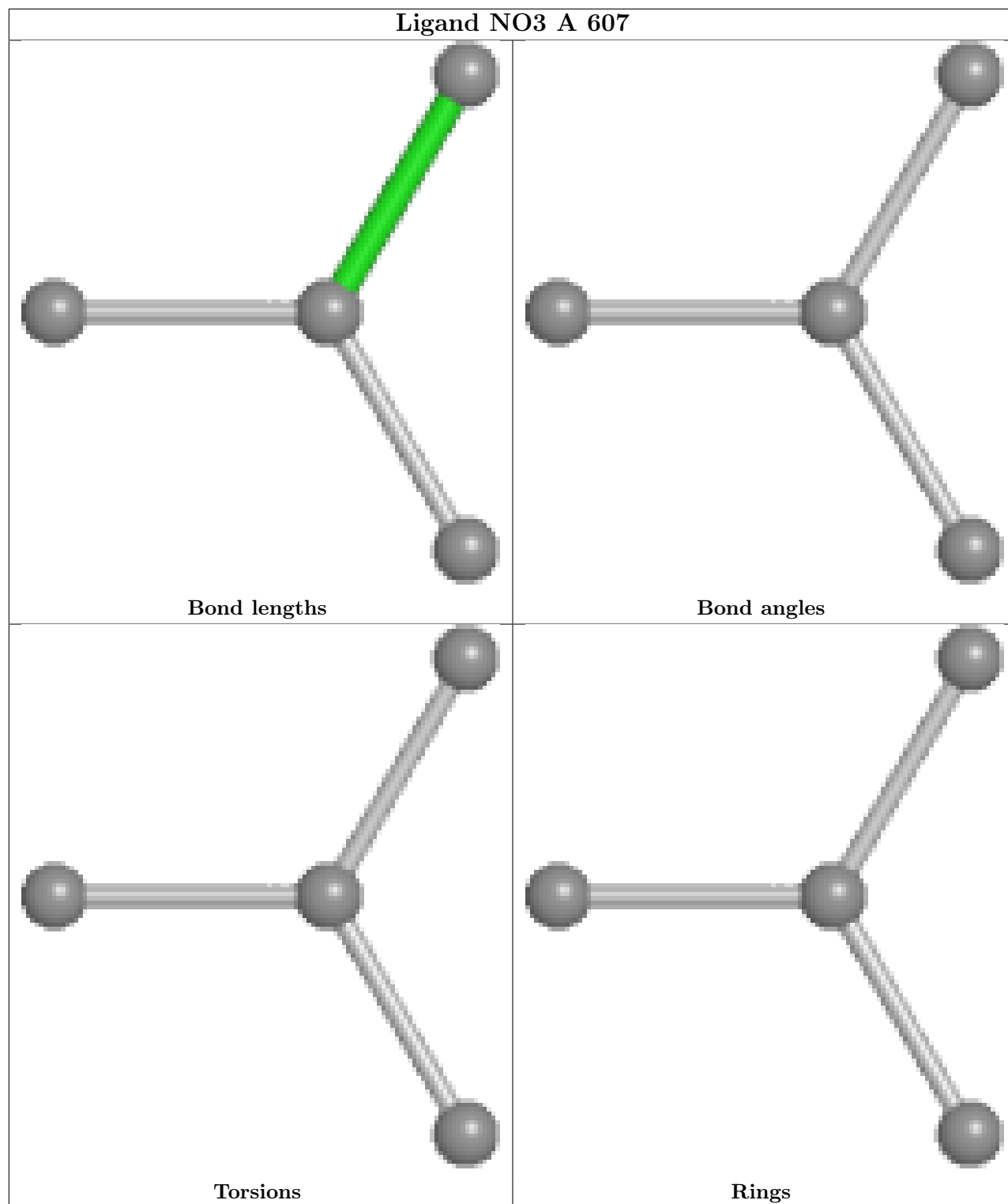


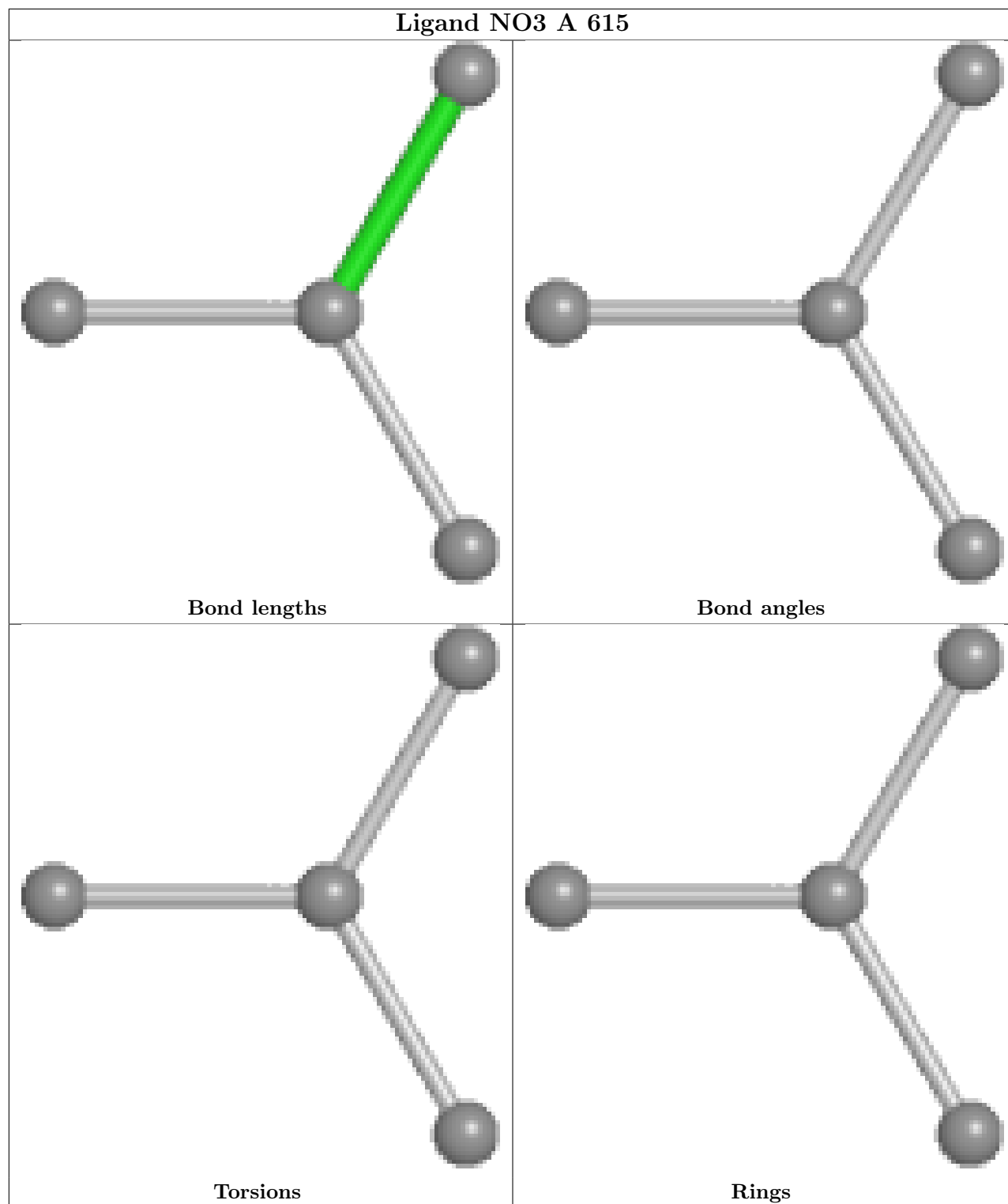


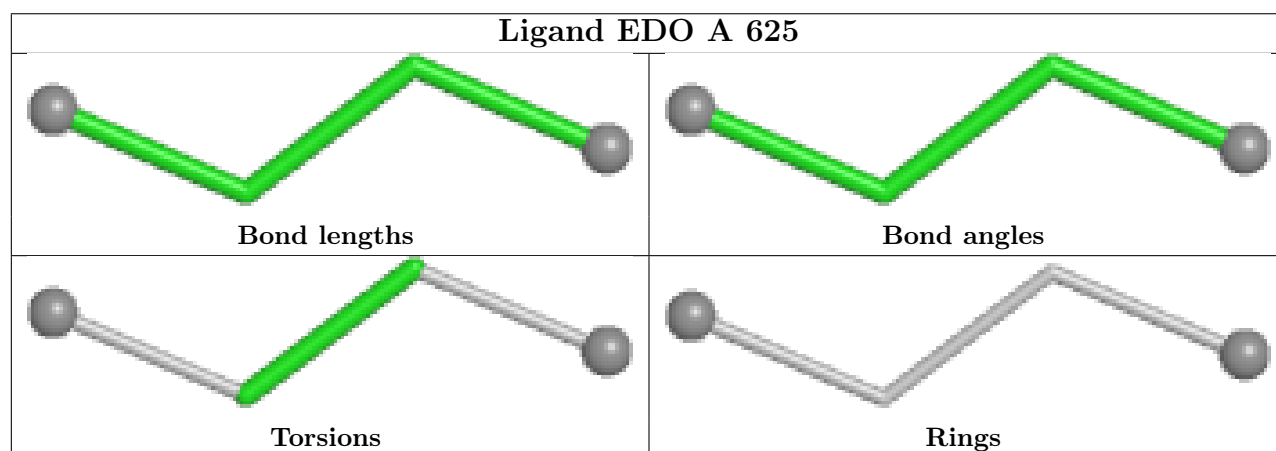
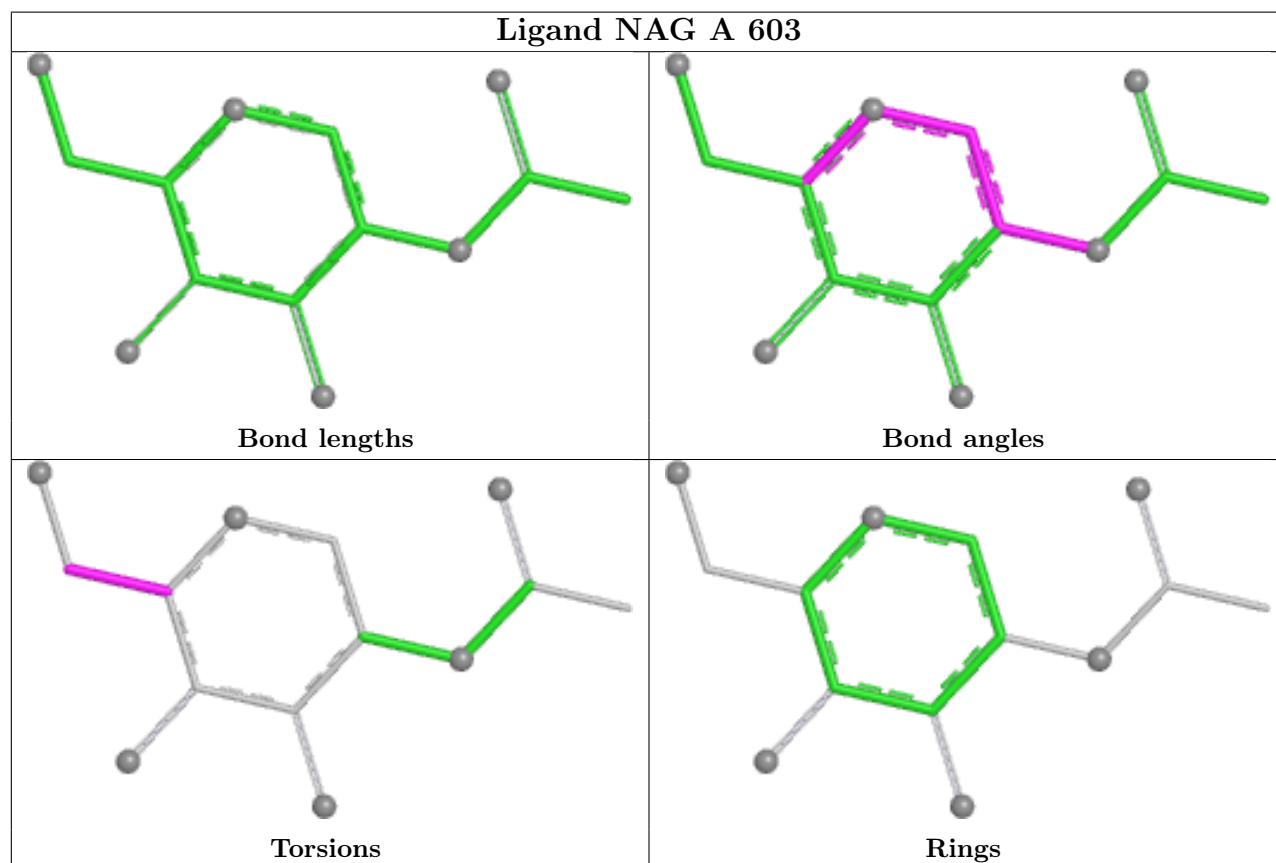
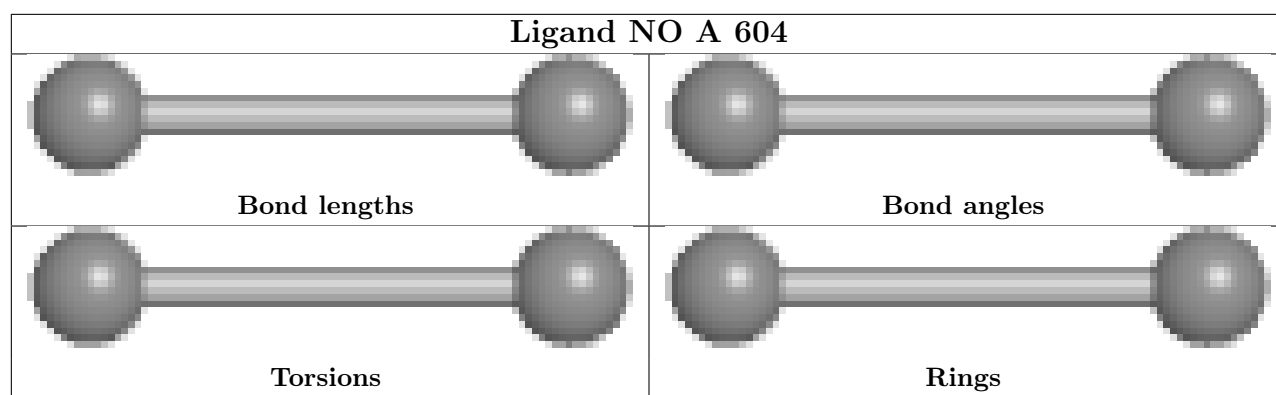


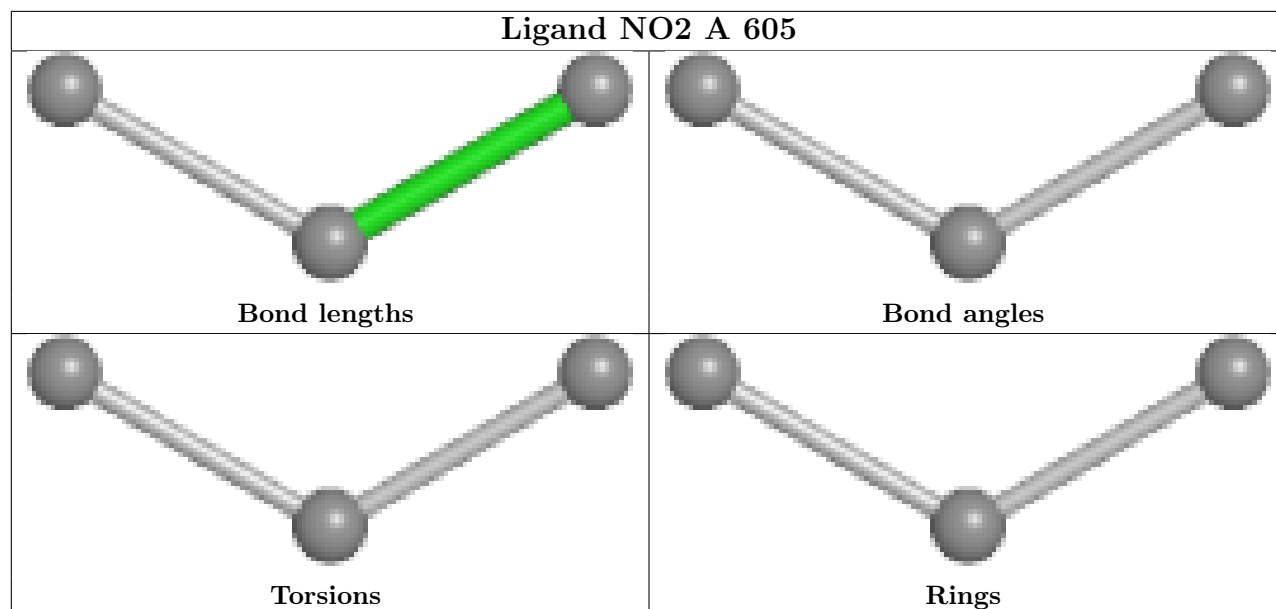


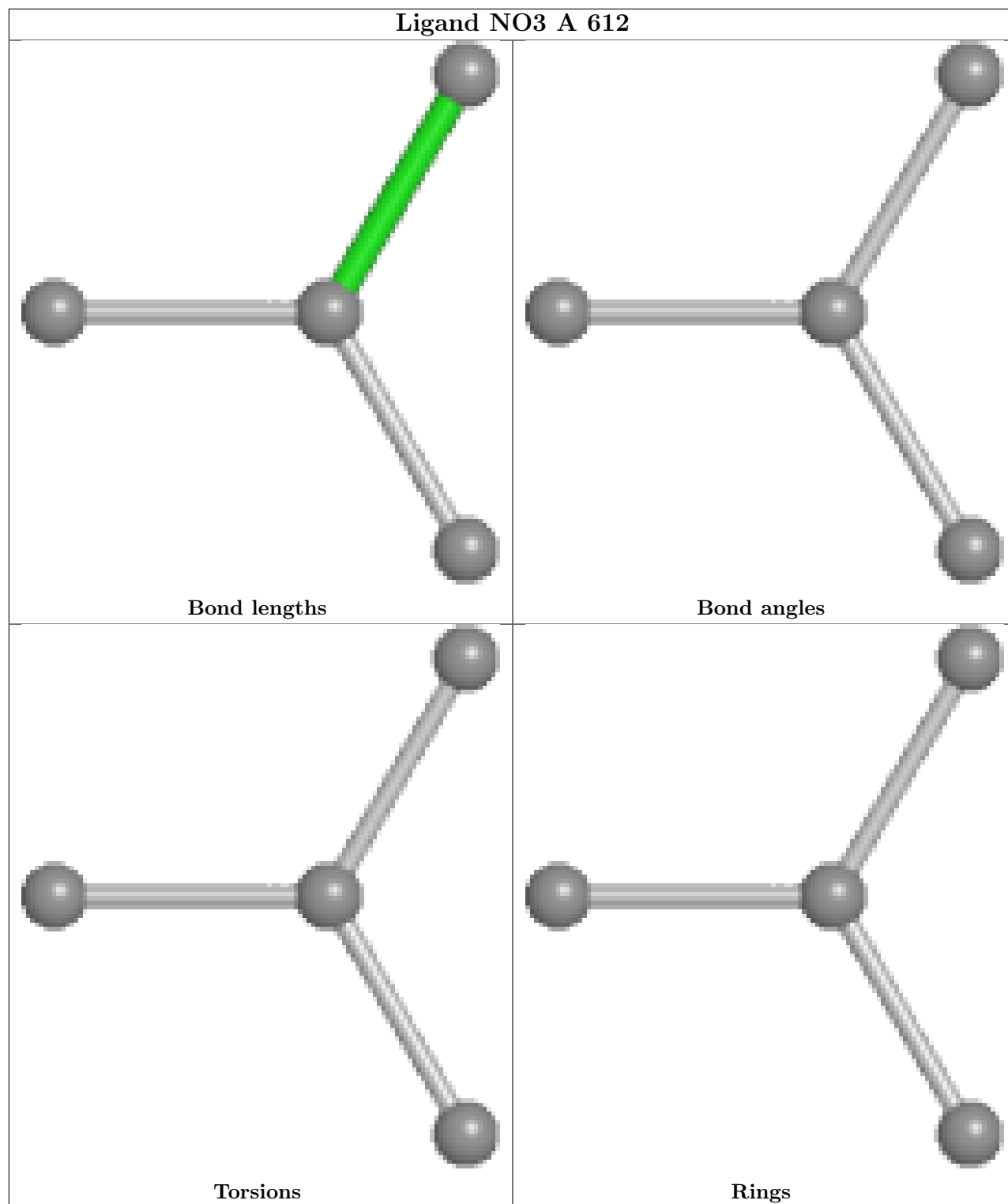


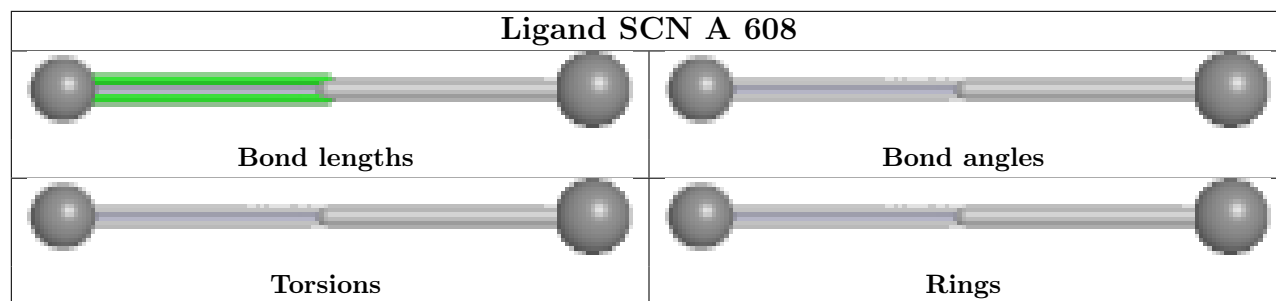












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	0.51	36 (6%) 27 31	24, 50, 119, 226	2 (0%)

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	ALA	5.0
1	A	10	VAL	4.5
1	A	119	LEU	4.3
1	A	172	TYR	4.2
1	A	2	TRP	4.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

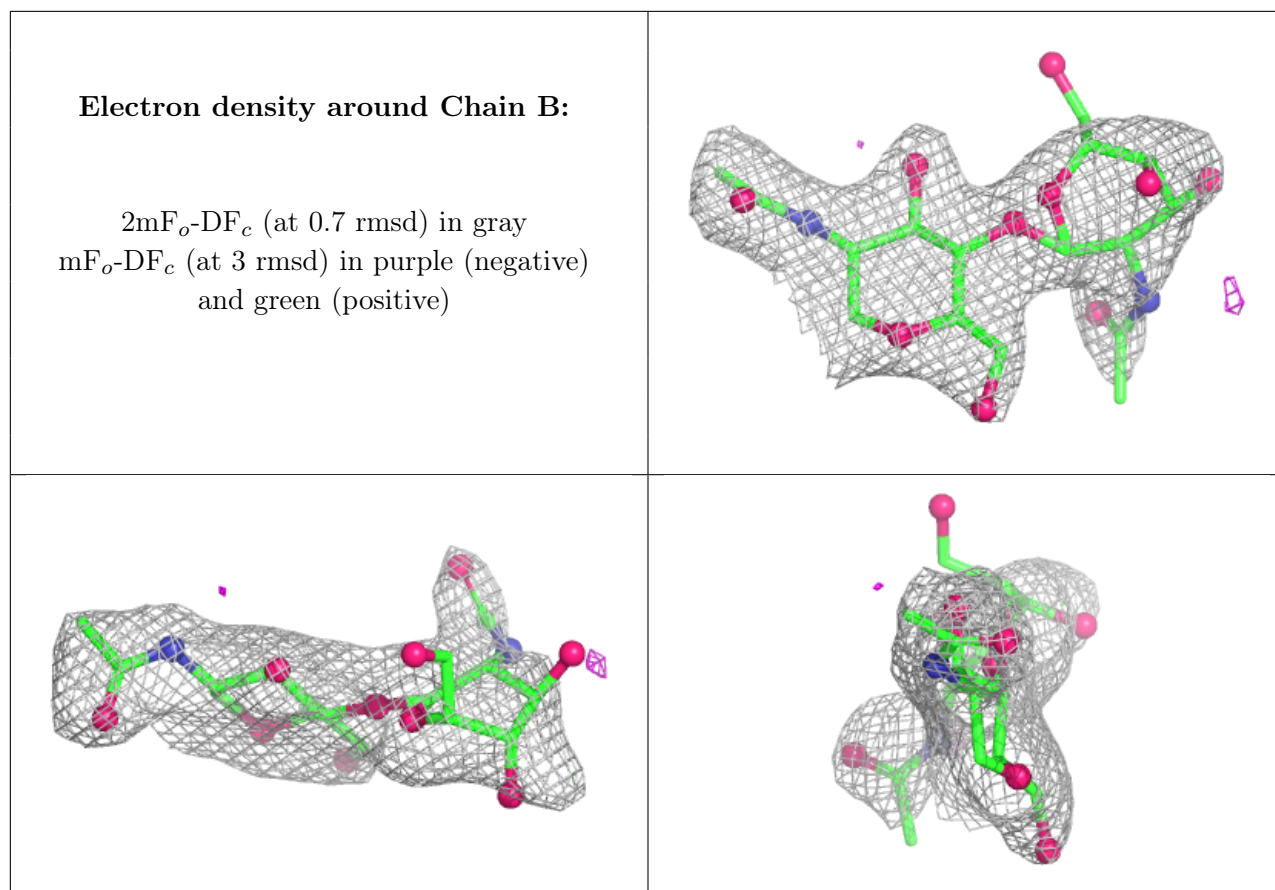
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.78	0.14	67,76,84,84	14
2	NAG	B	1	14/15	0.92	0.09	50,56,64,71	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.



6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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	A	601	14/15	0.67	0.15	76,92,101,102	0
3	NAG	A	603	14/15	0.80	0.13	71,76,80,81	14
5	NO2	A	635	3/3	0.85	0.11	57,57,62,68	0
10	EDO	A	625	4/4	0.86	0.13	39,43,48,53	0
3	NAG	A	602	14/15	0.87	0.11	66,72,79,80	0
12	OSM	A	628	4/4	0.87	0.14	58,62,63,71	4
6	NO3	A	613	4/4	0.89	0.09	25,28,28,31	4
7	SCN	A	608	3/3	0.89	0.13	52,52,58,62	3
6	NO3	A	607	4/4	0.91	0.13	32,35,38,58	4
7	SCN	A	636	3/3	0.91	0.11	54,54,62,67	0
4	NO	A	634	2/2	0.92	0.09	40,40,40,49	0
8	IOD	A	640	1/1	0.92	0.10	56,56,56,56	1
6	NO3	A	615	4/4	0.93	0.11	38,49,52,62	0

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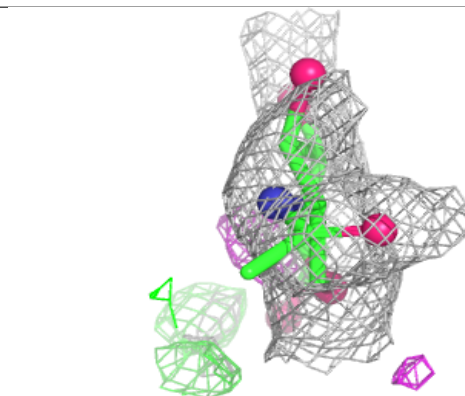
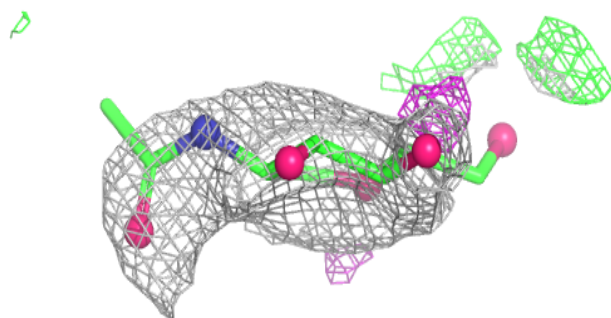
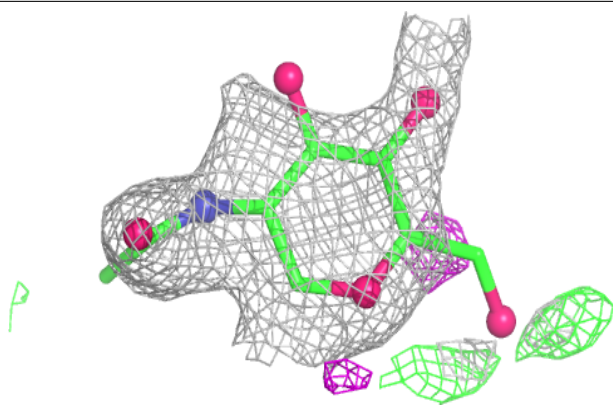
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NO3	A	611	4/4	0.93	0.08	26,26,28,29	4
4	NO	A	604	2/2	0.94	0.09	41,41,41,55	0
6	NO3	A	614	4/4	0.94	0.06	24,30,33,34	4
8	IOD	A	632	1/1	0.95	0.09	66,66,66,66	1
8	IOD	A	639	1/1	0.95	0.10	56,56,56,56	1
6	NO3	A	612	4/4	0.95	0.08	30,34,36,37	4
7	SCN	A	627	3/3	0.95	0.09	43,43,48,54	0
6	NO3	A	606	4/4	0.95	0.09	38,39,53,54	0
8	IOD	A	641	1/1	0.96	0.05	53,53,53,53	1
7	SCN	A	610	3/3	0.96	0.10	48,48,49,49	0
6	NO3	A	633	4/4	0.96	0.09	21,21,25,33	4
7	SCN	A	609	3/3	0.97	0.09	45,45,57,59	0
9	HEM	A	624	43/43	0.97	0.06	28,32,38,40	0
8	IOD	A	623	1/1	0.97	0.12	56,56,56,56	1
8	IOD	A	631	1/1	0.97	0.07	60,60,60,60	1
8	IOD	A	617	1/1	0.98	0.06	59,59,59,59	0
8	IOD	A	642	1/1	0.98	0.04	51,51,51,51	1
8	IOD	A	638	1/1	0.98	0.04	46,46,46,46	1
5	NO2	A	605	3/3	0.98	0.04	32,32,36,38	3
7	SCN	A	637	3/3	0.98	0.08	45,45,50,51	3
8	IOD	A	622	1/1	0.99	0.05	62,62,62,62	1
8	IOD	A	616	1/1	0.99	0.02	36,36,36,36	1
8	IOD	A	629	1/1	0.99	0.05	48,48,48,48	1
8	IOD	A	630	1/1	0.99	0.04	47,47,47,47	1
8	IOD	A	618	1/1	0.99	0.06	43,43,43,43	1
8	IOD	A	619	1/1	0.99	0.04	52,52,52,52	1
11	CA	A	626	1/1	0.99	0.03	39,39,39,39	0
8	IOD	A	620	1/1	0.99	0.06	55,55,55,55	1
8	IOD	A	621	1/1	1.00	0.02	50,50,50,50	1

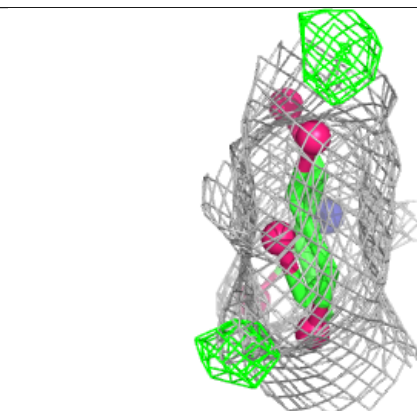
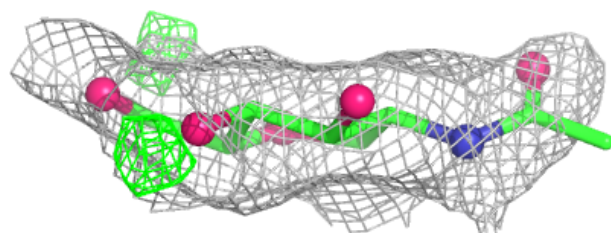
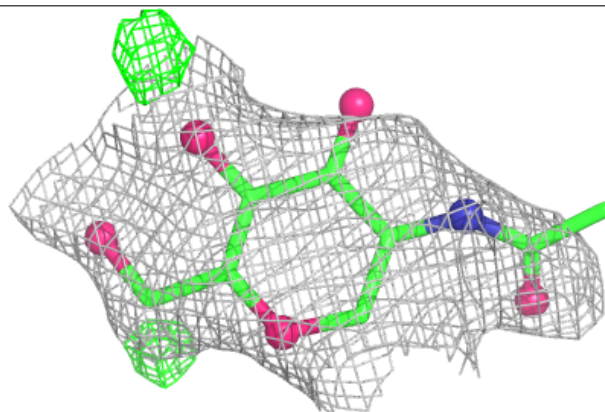
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 601:

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

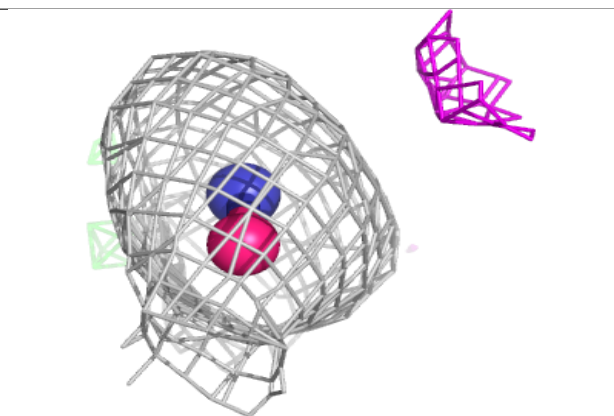
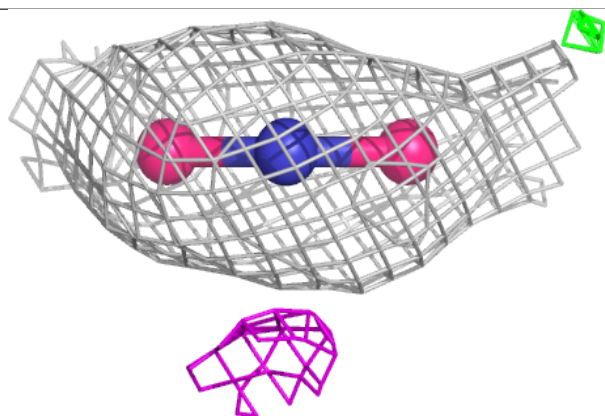
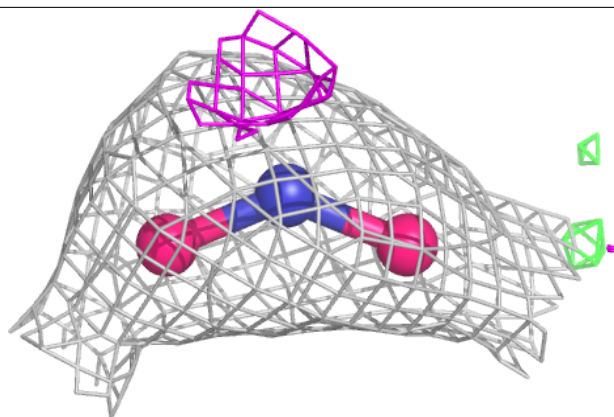
**Electron density around NAG A 603:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

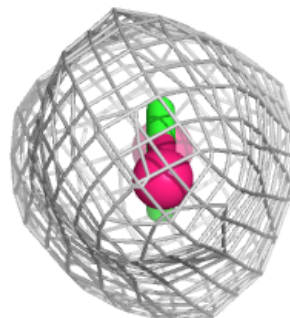
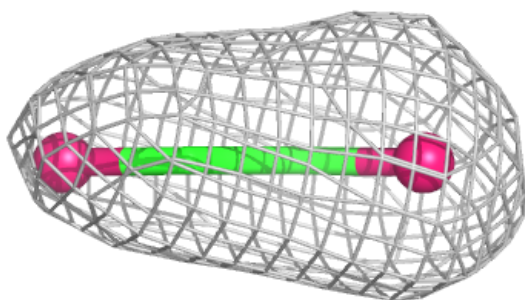
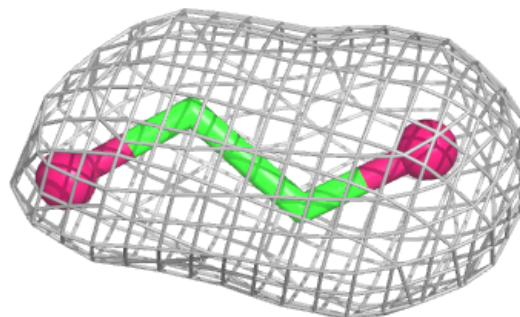


Electron density around NO2 A 635:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

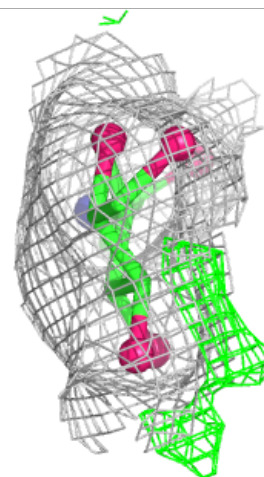
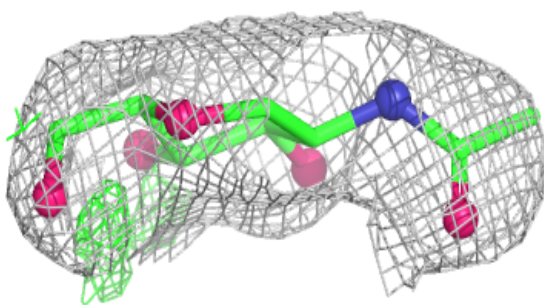
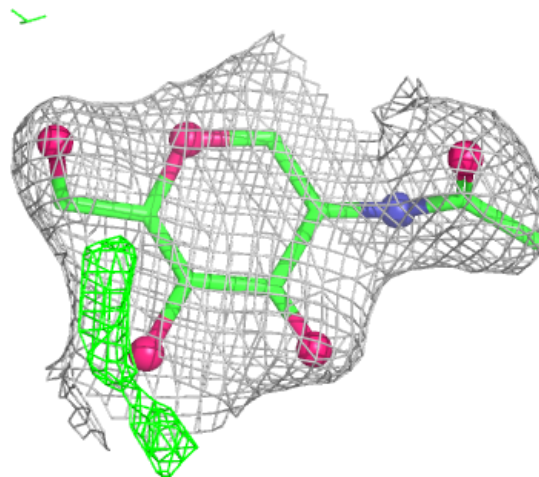
**Electron density around EDO A 625:**

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and green (positive)



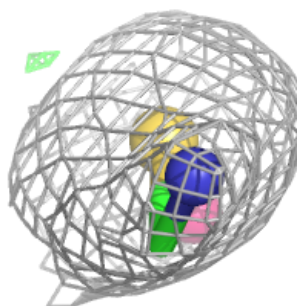
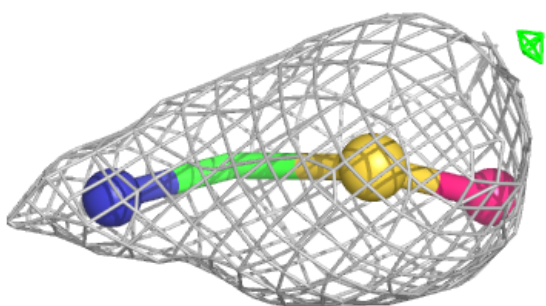
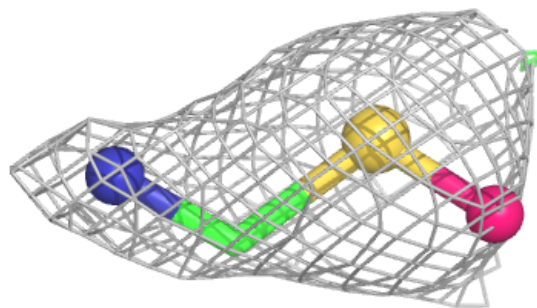
Electron density around NAG A 602:

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and green (positive)



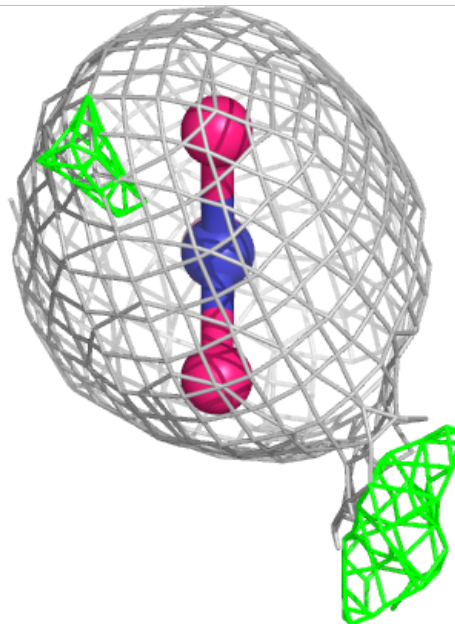
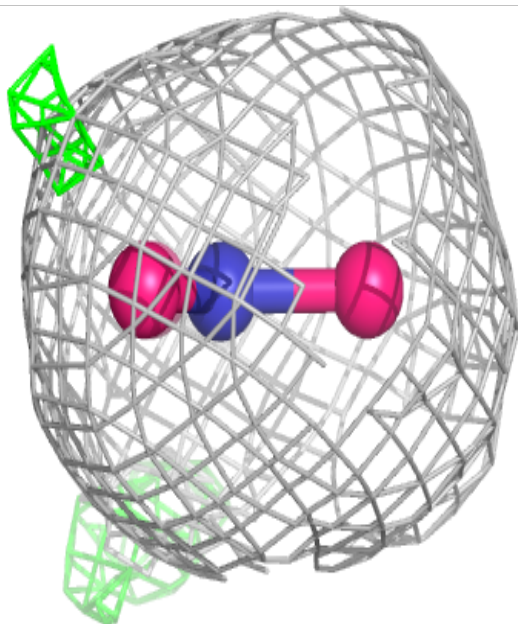
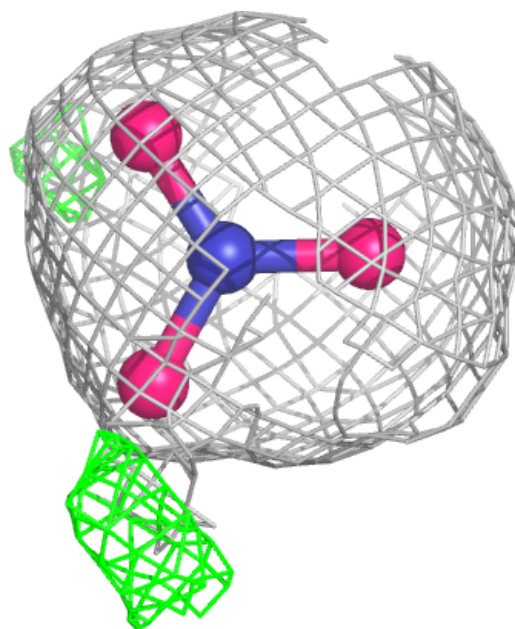
Electron density around OSM A 628:

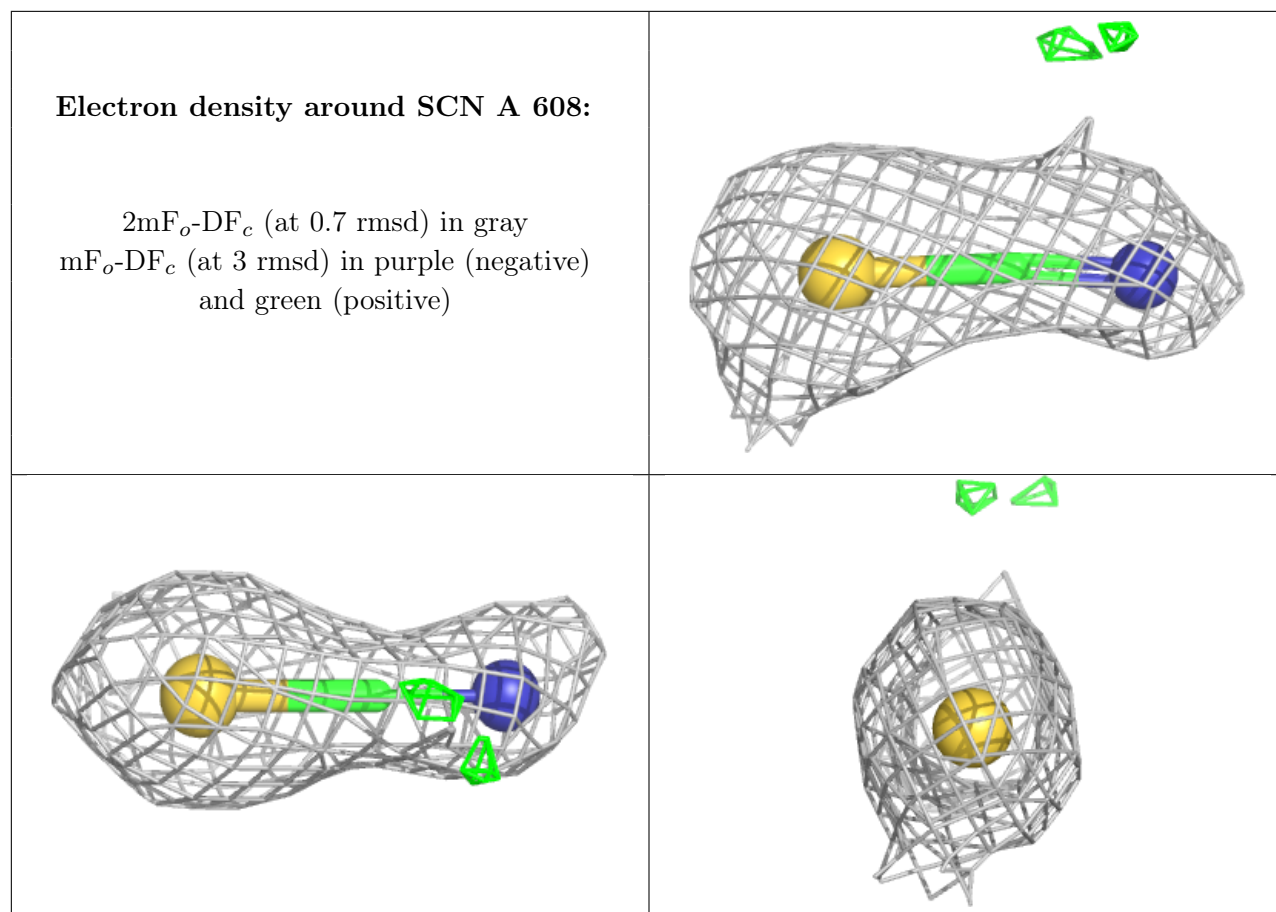
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)



Electron density around NO3 A 613:

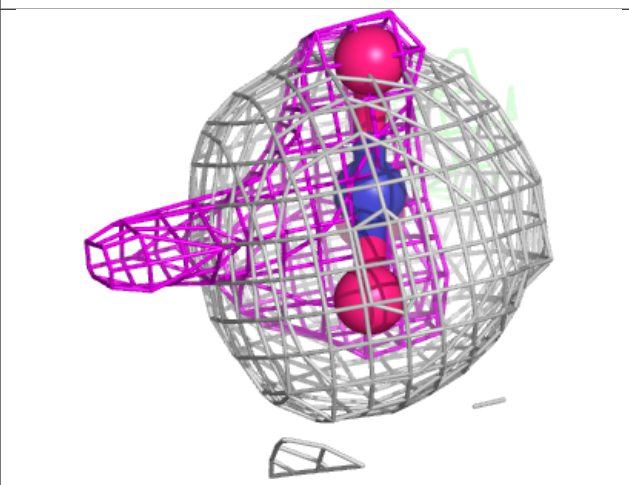
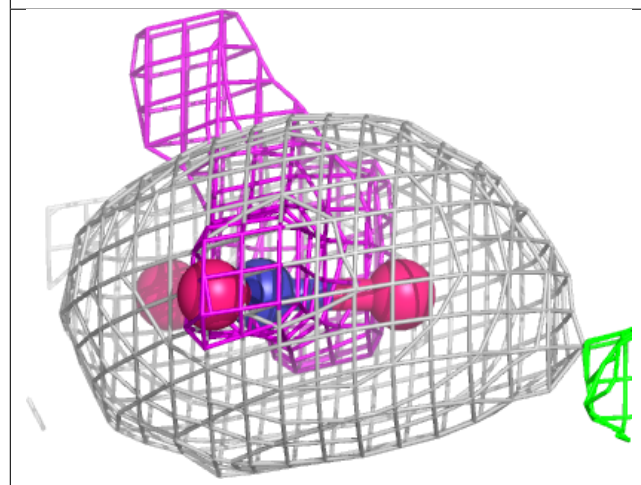
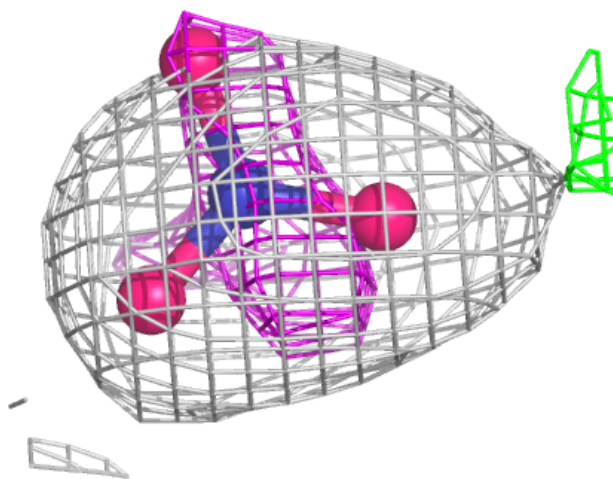
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

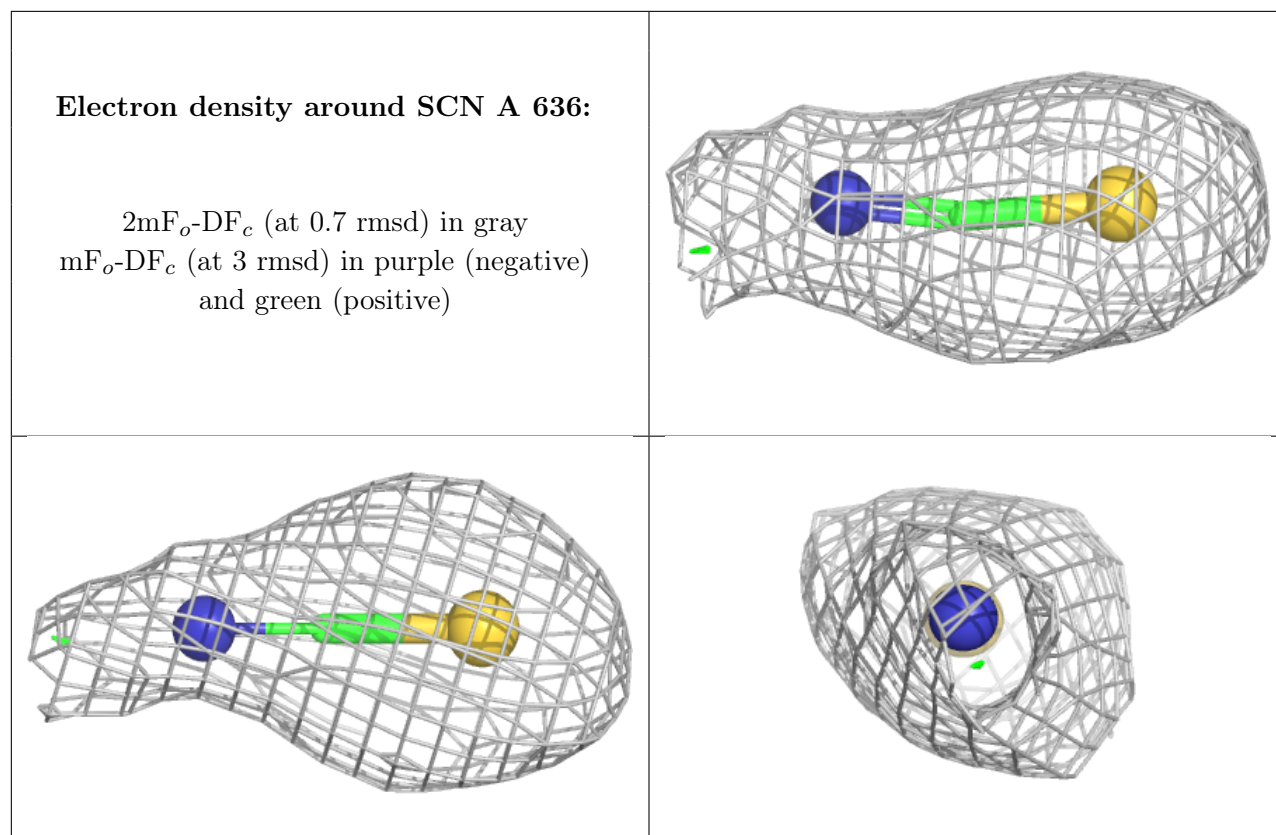




Electron density around NO3 A 607:

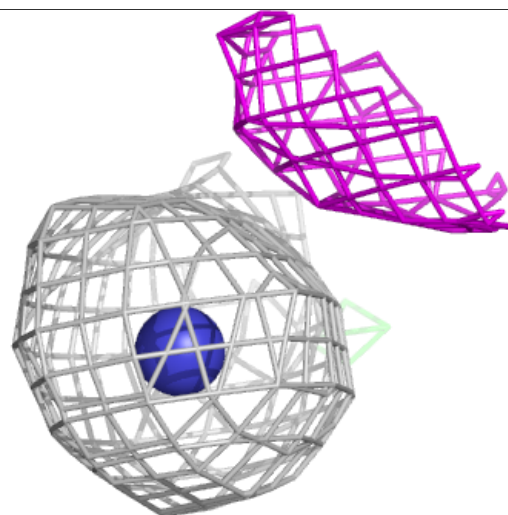
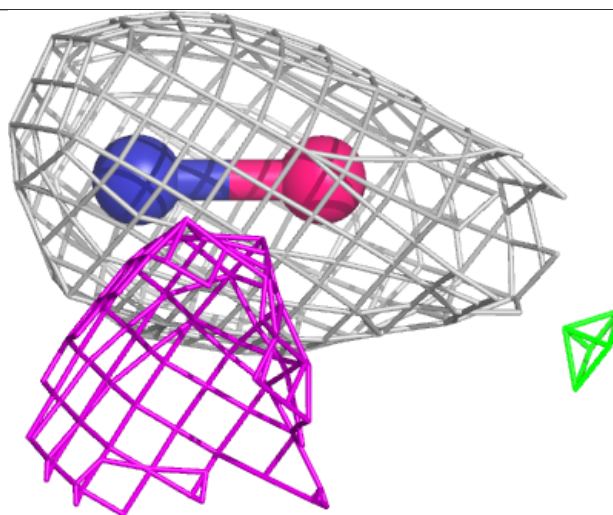
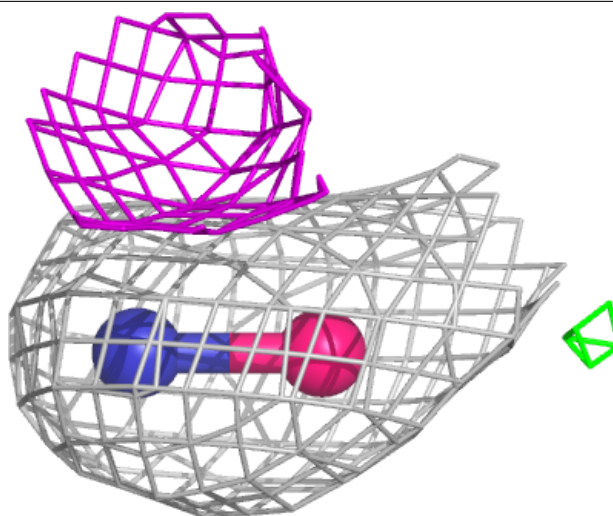
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





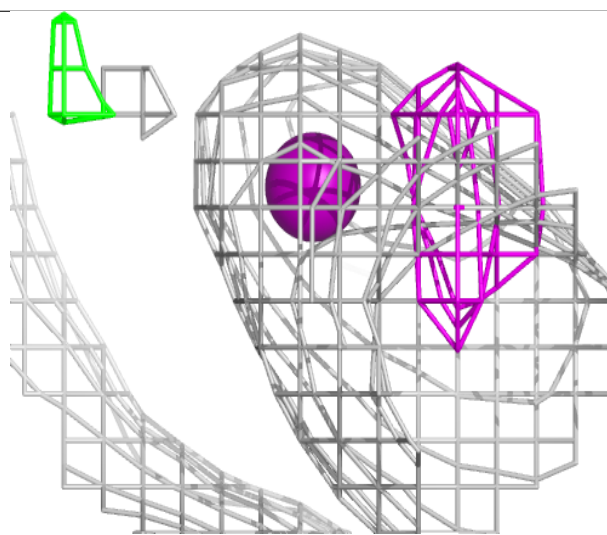
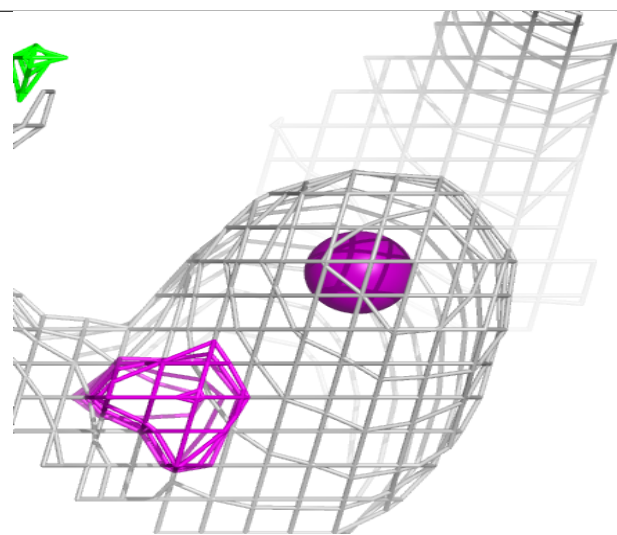
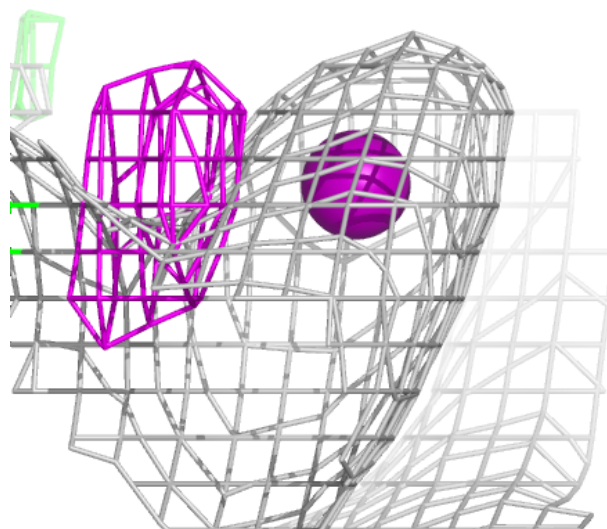
Electron density around NO A 634:

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



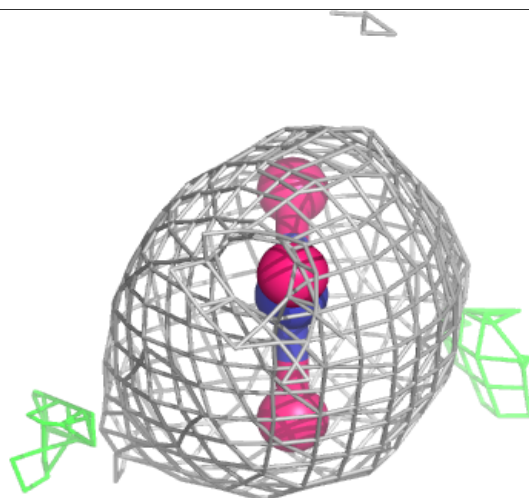
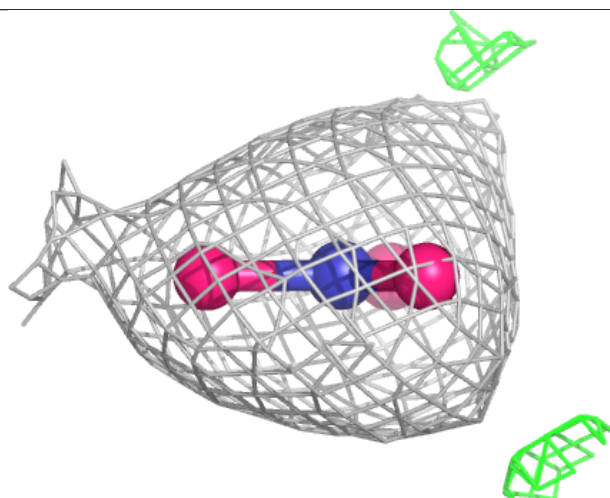
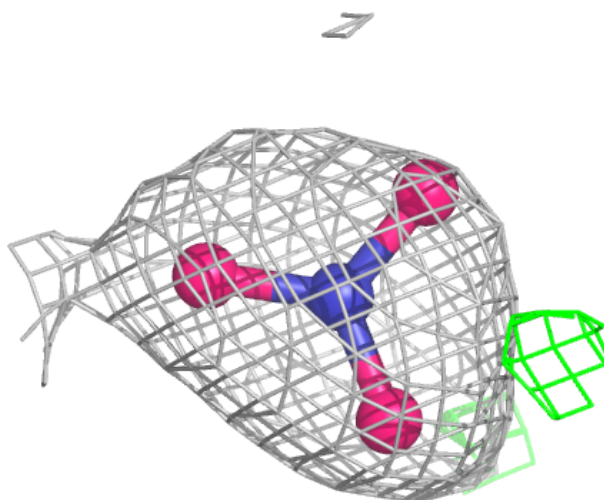
Electron density around IOD A 640:

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



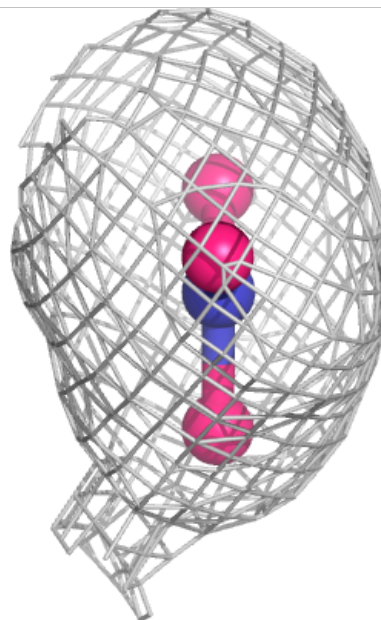
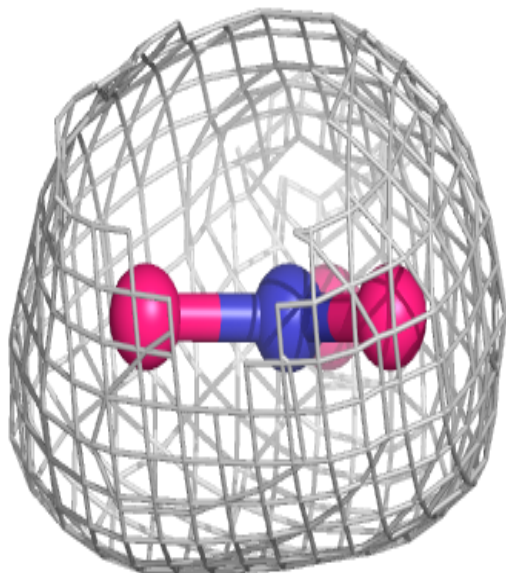
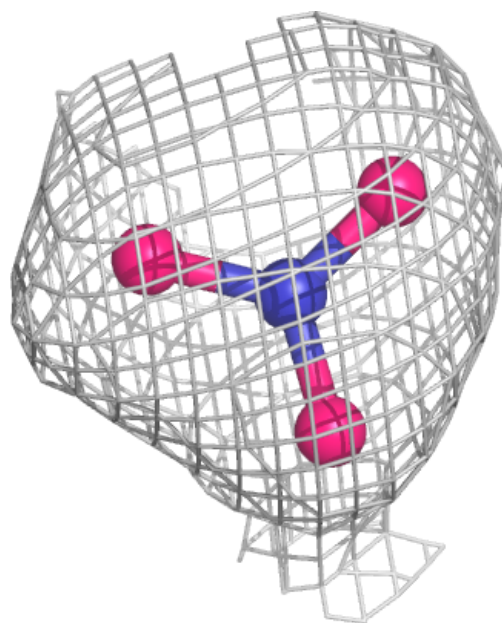
Electron density around NO3 A 615:

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



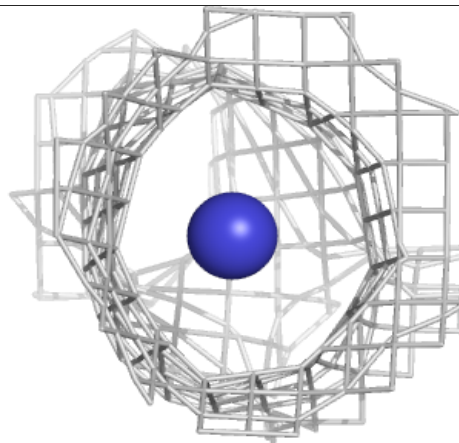
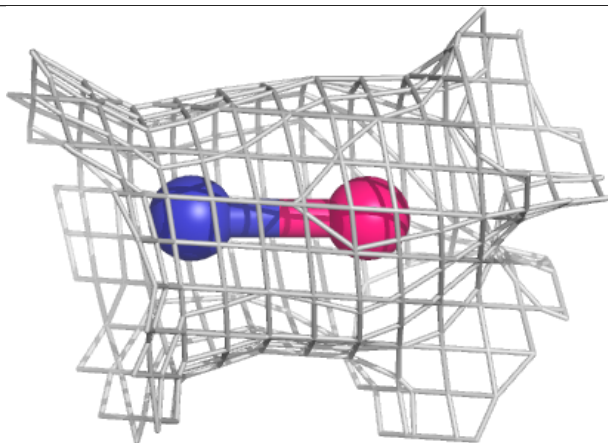
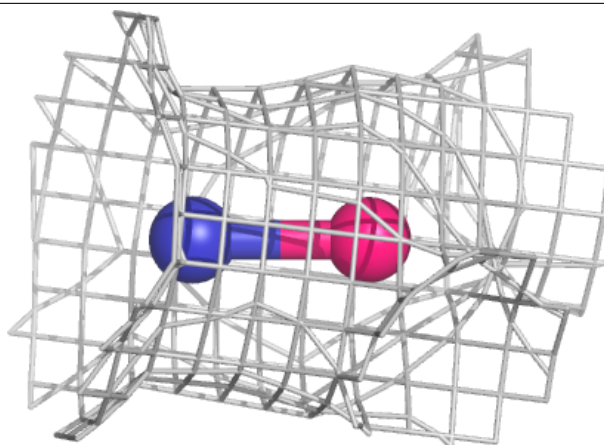
Electron density around NO3 A 611:

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



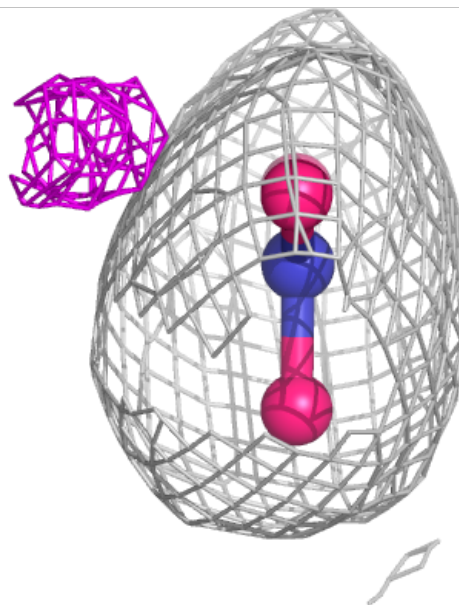
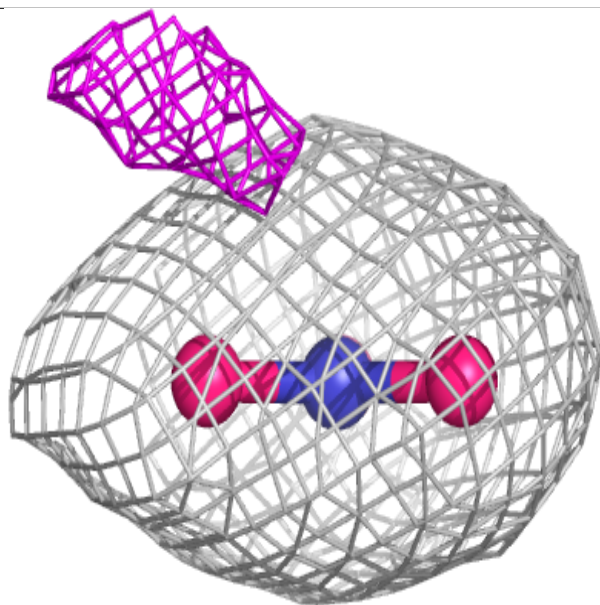
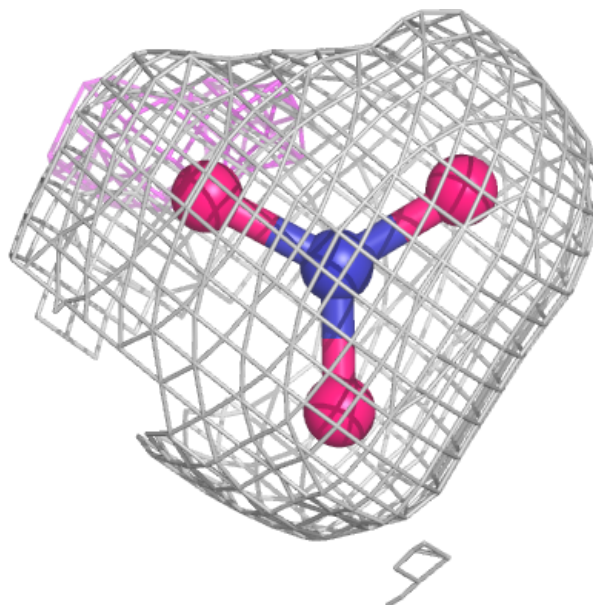
Electron density around NO A 604:

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



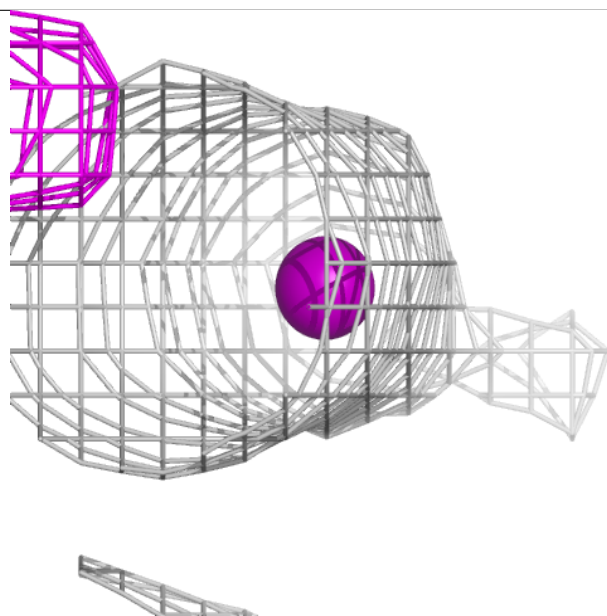
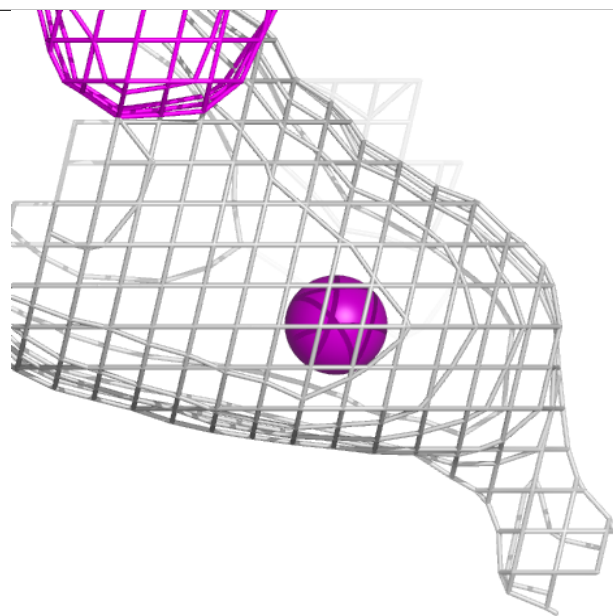
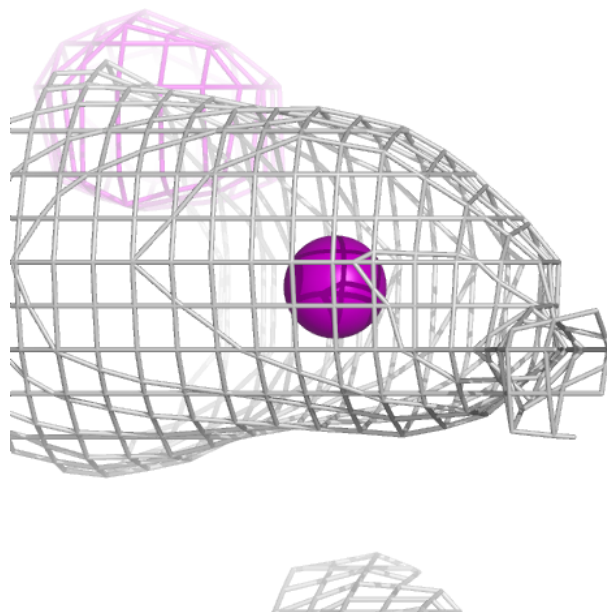
Electron density around NO3 A 614:

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



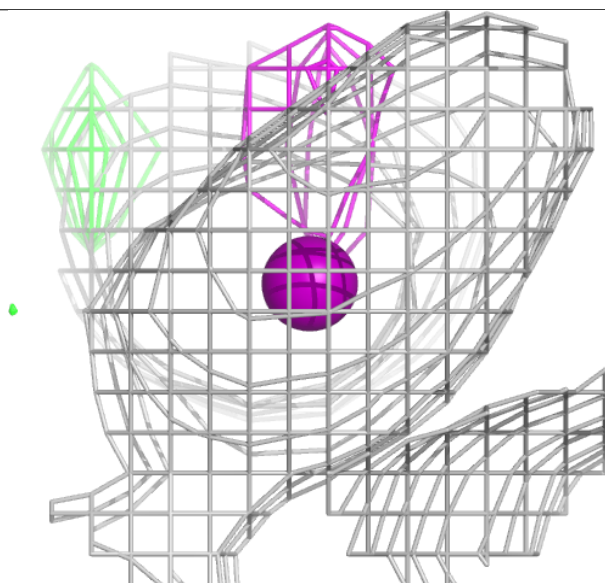
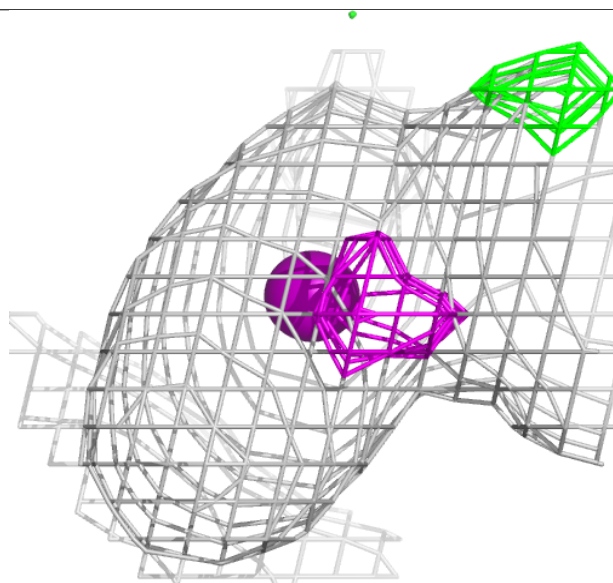
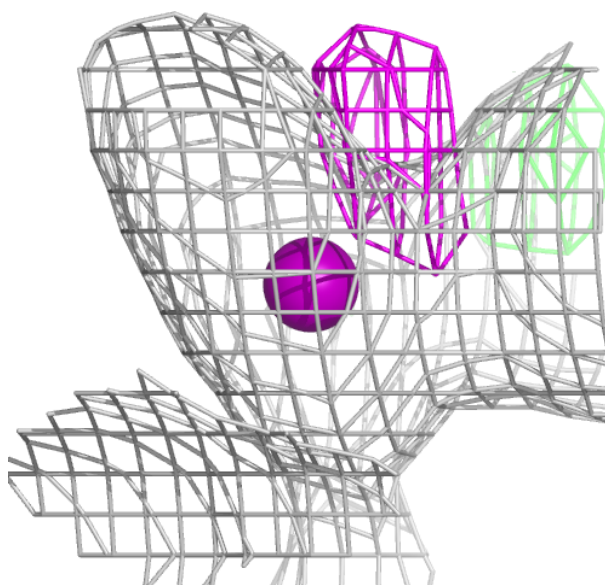
Electron density around IOD A 632:

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



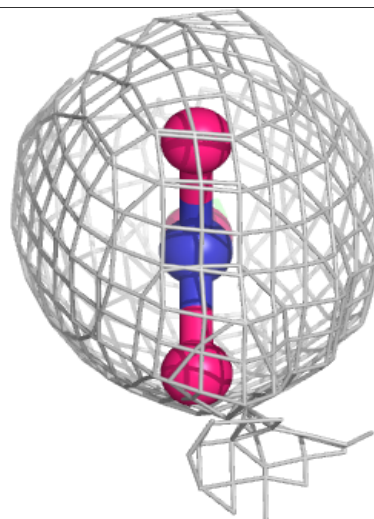
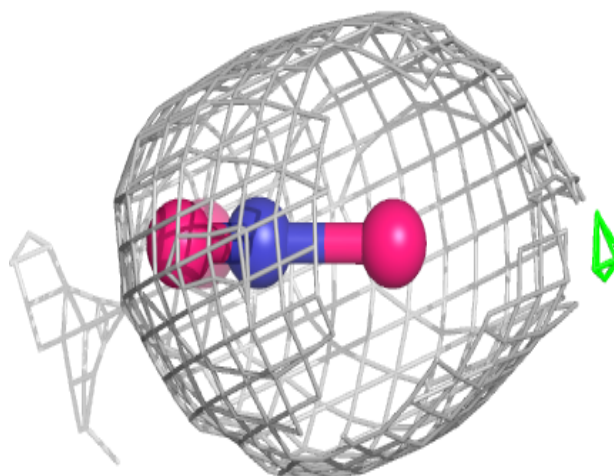
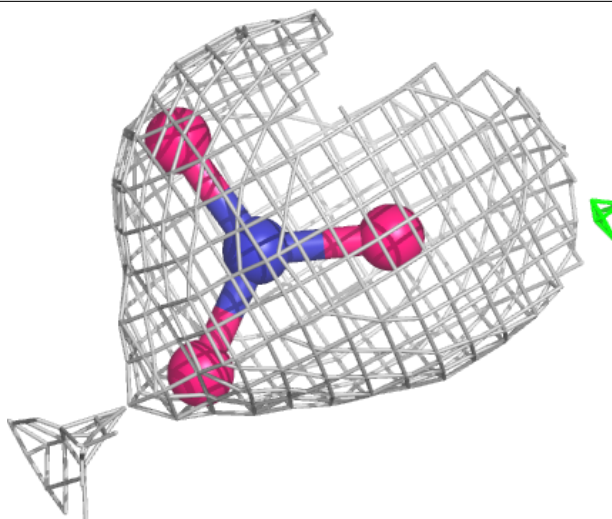
Electron density around IOD A 639:

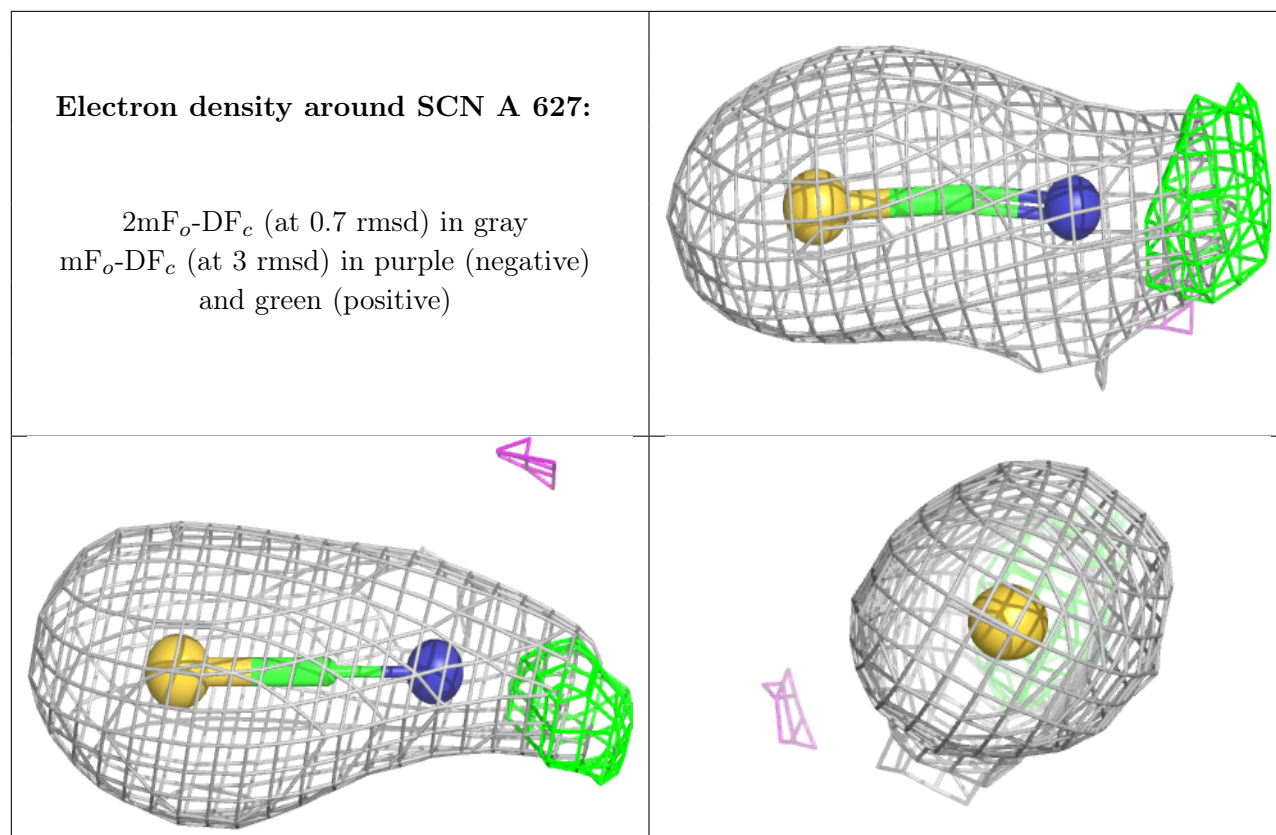
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NO3 A 612:

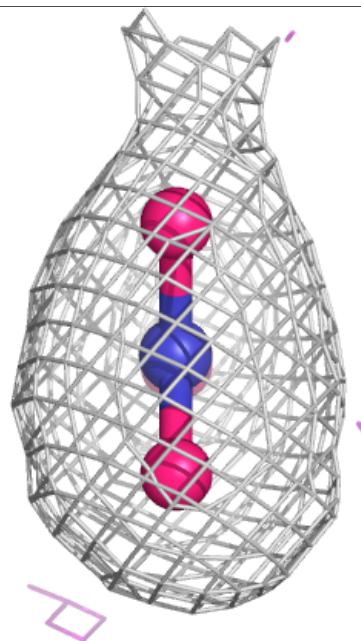
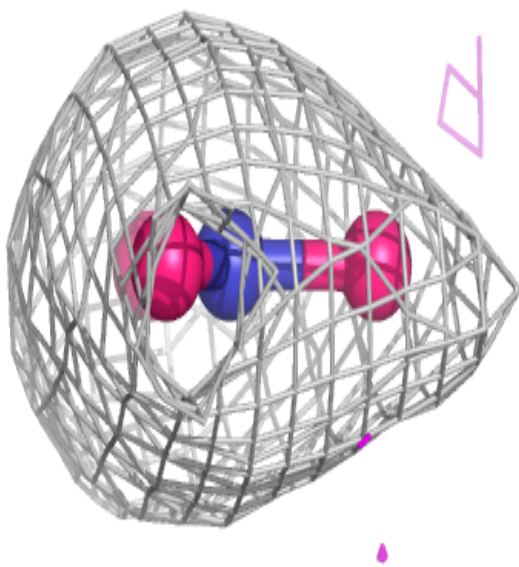
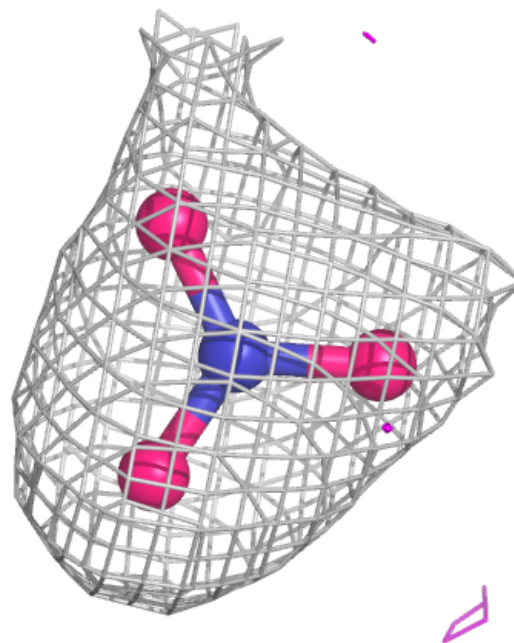
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





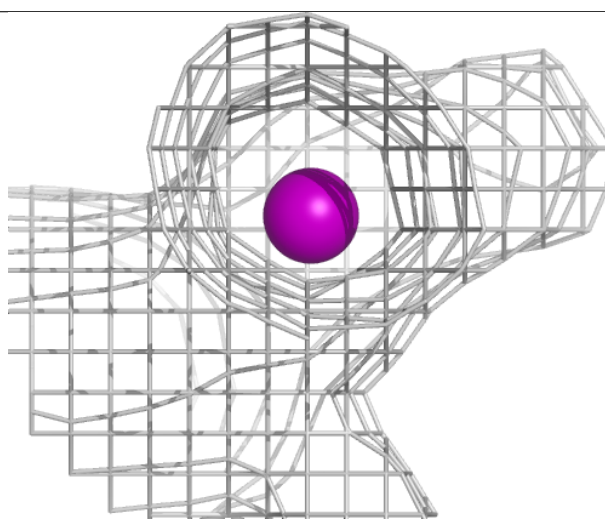
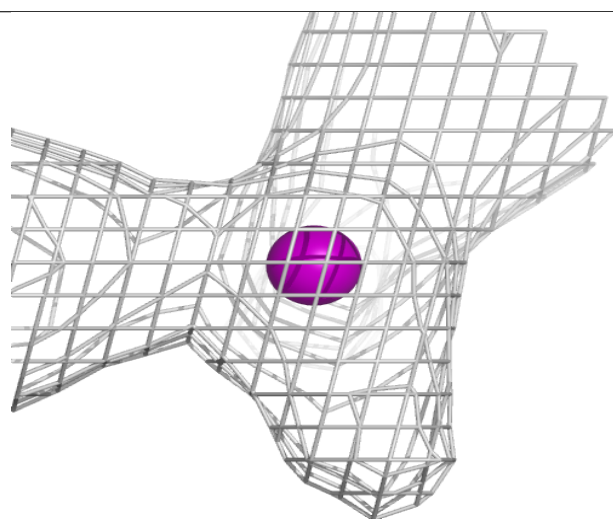
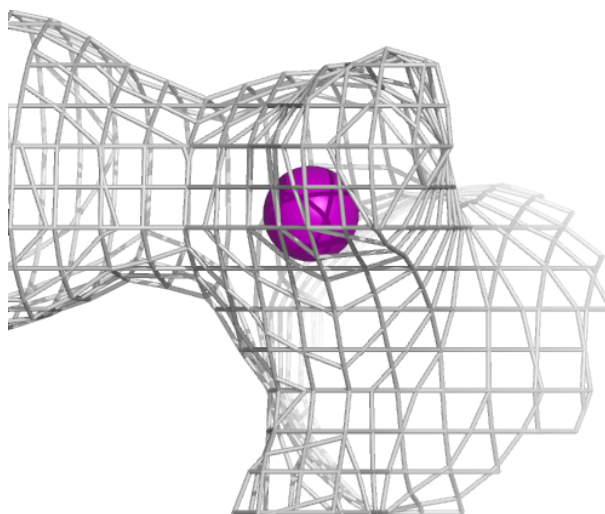
Electron density around NO3 A 606:

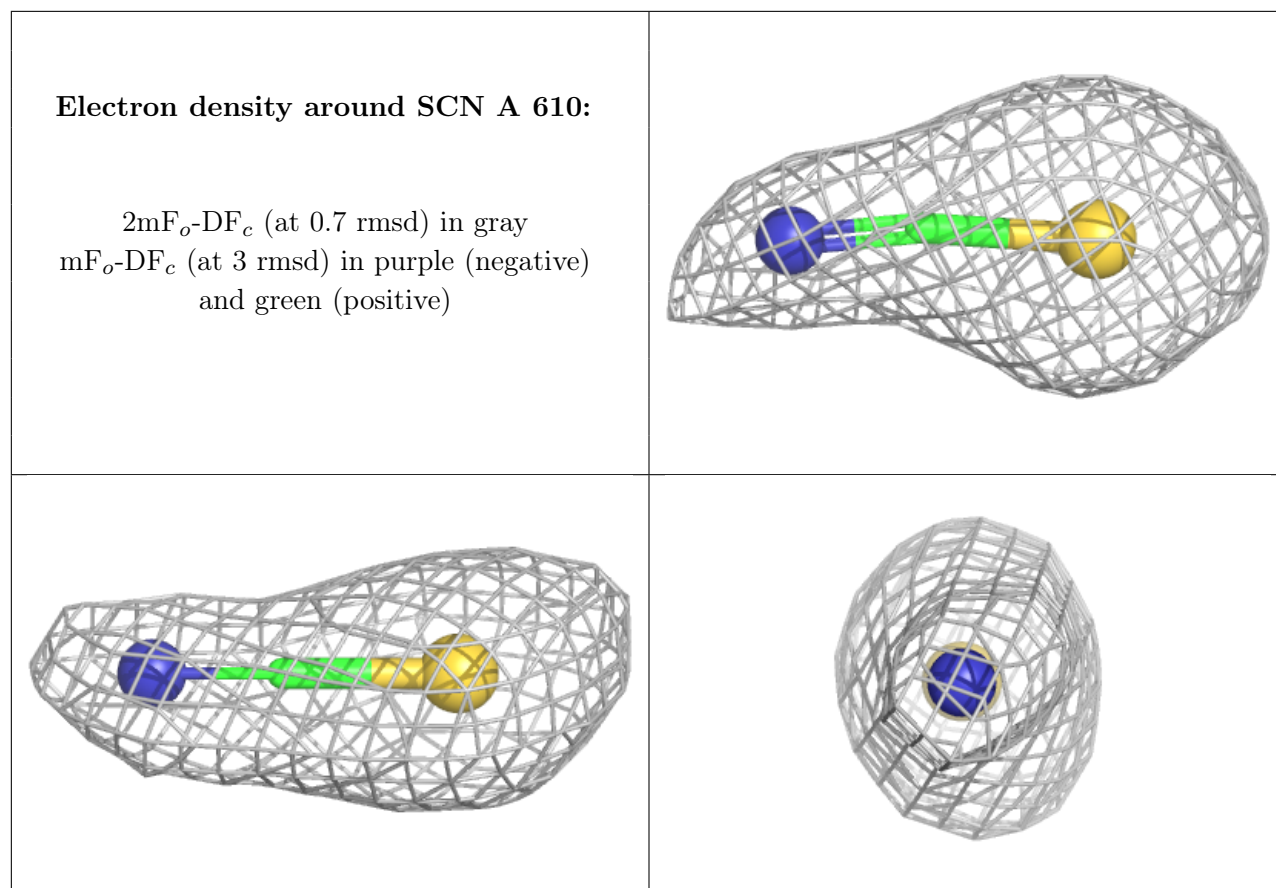
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around IOD A 641:

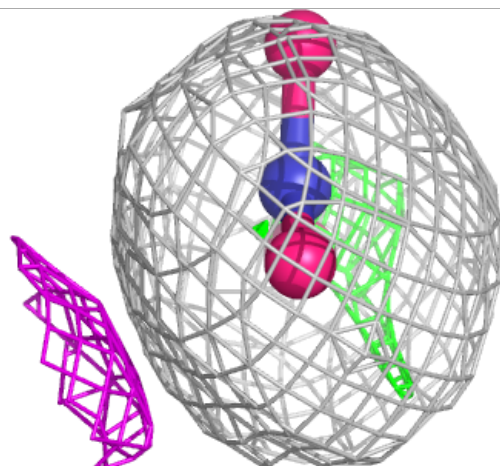
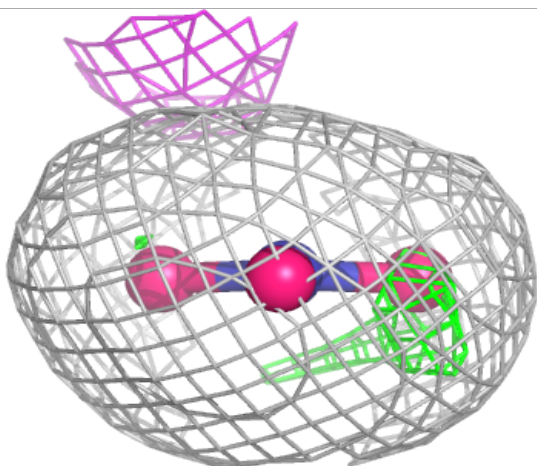
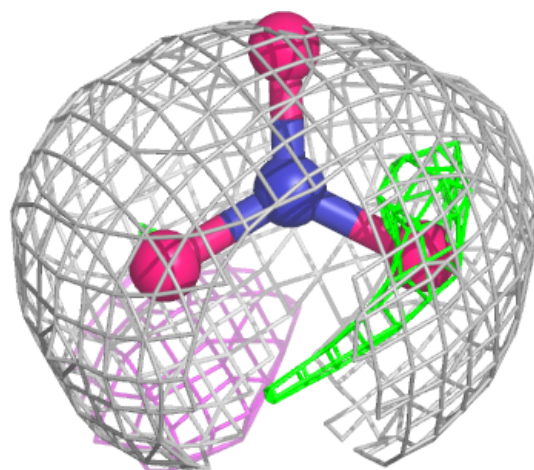
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





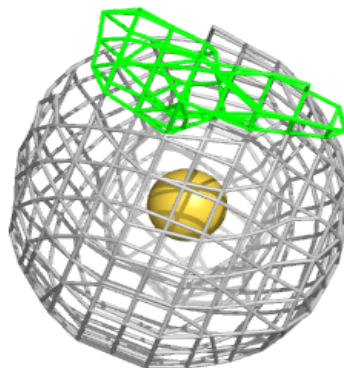
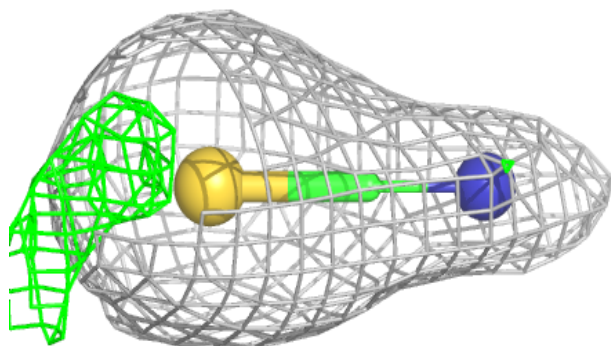
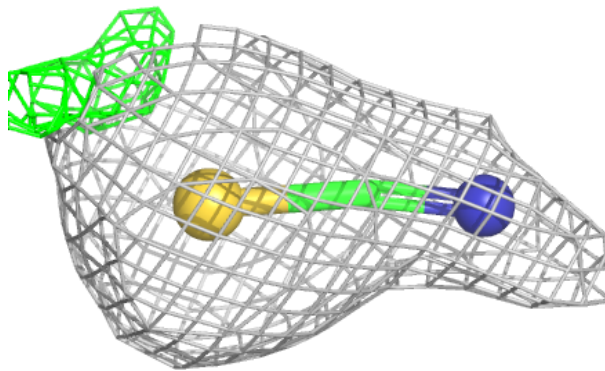
Electron density around NO3 A 633:

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



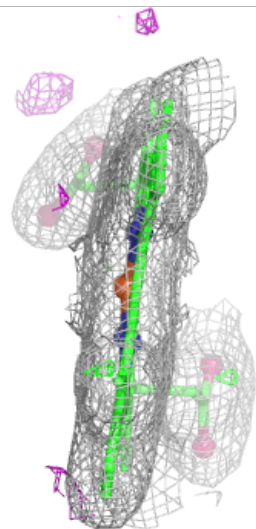
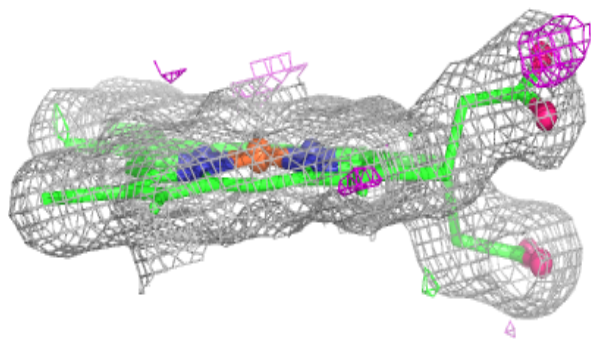
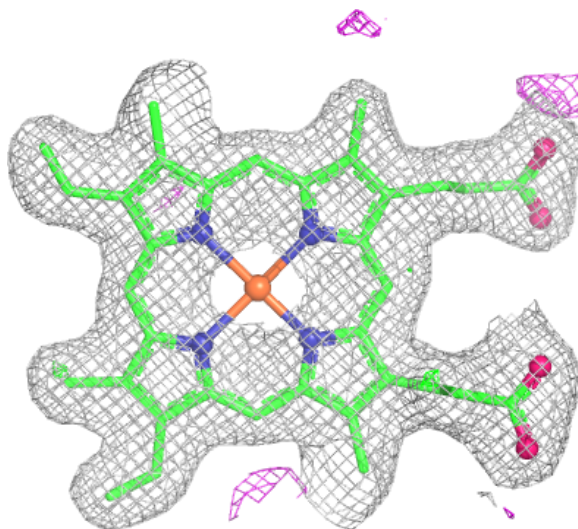
Electron density around SCN A 609:

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



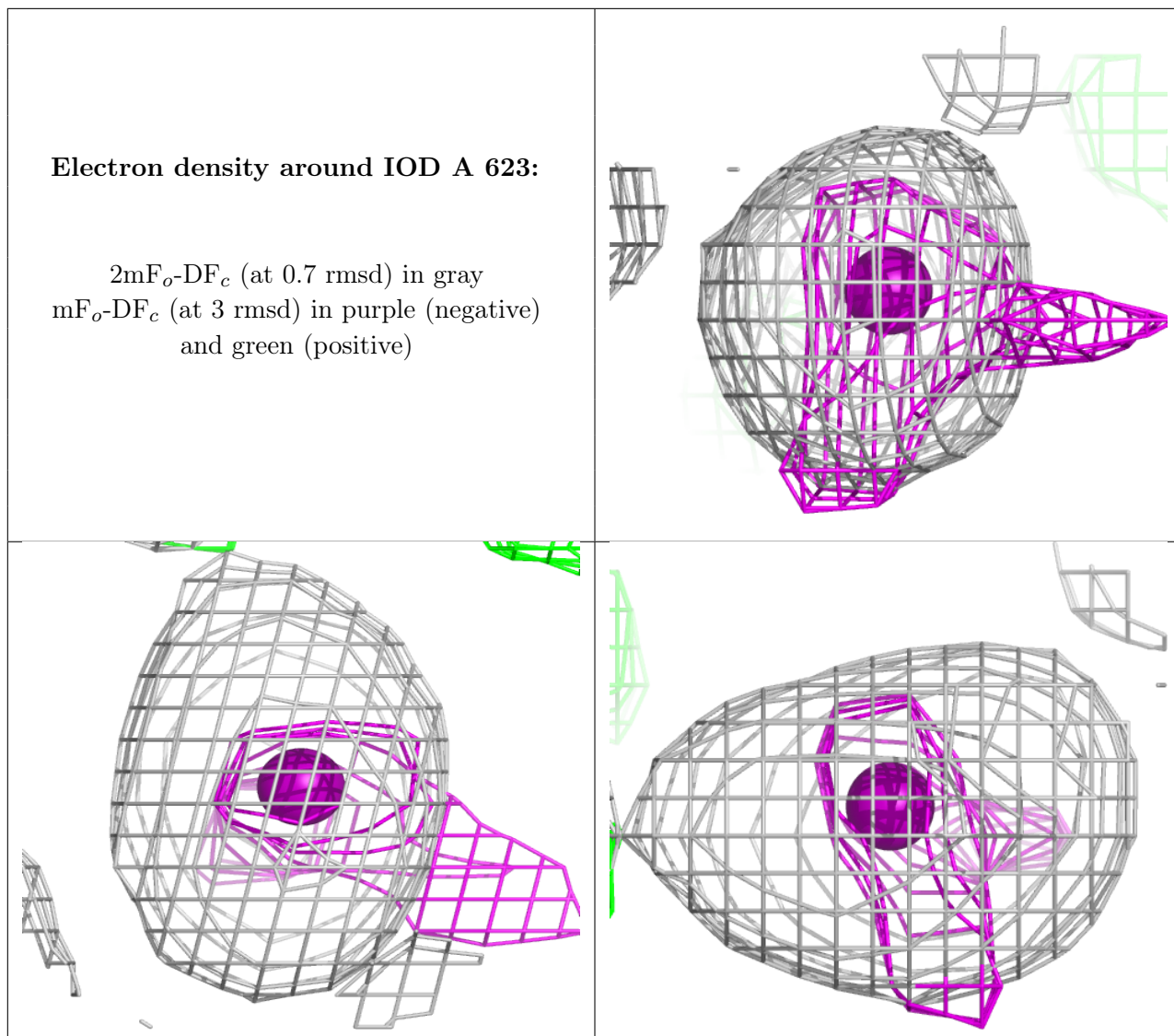
Electron density around HEM A 624:

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



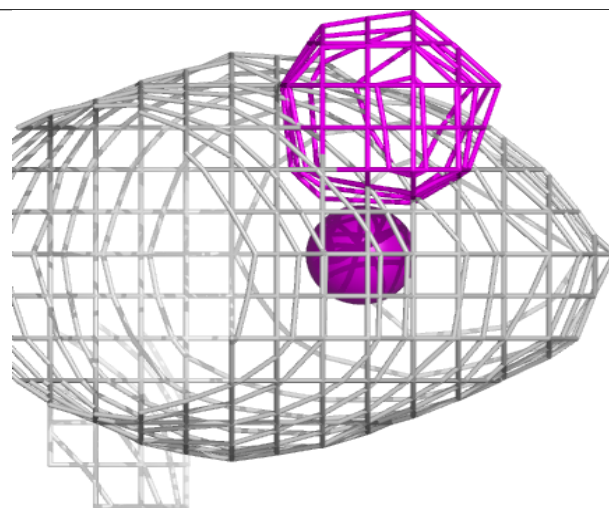
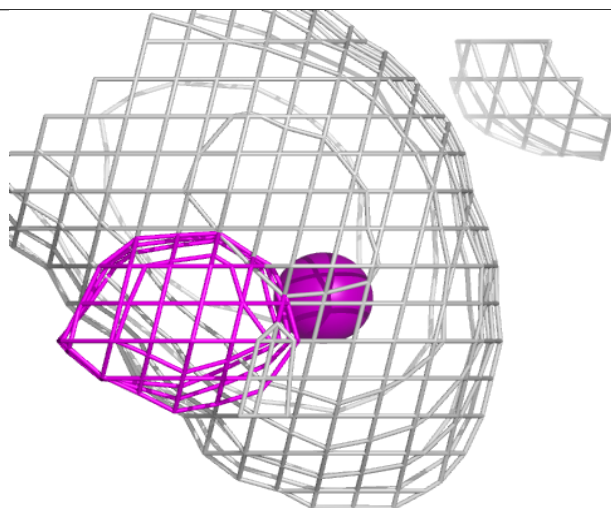
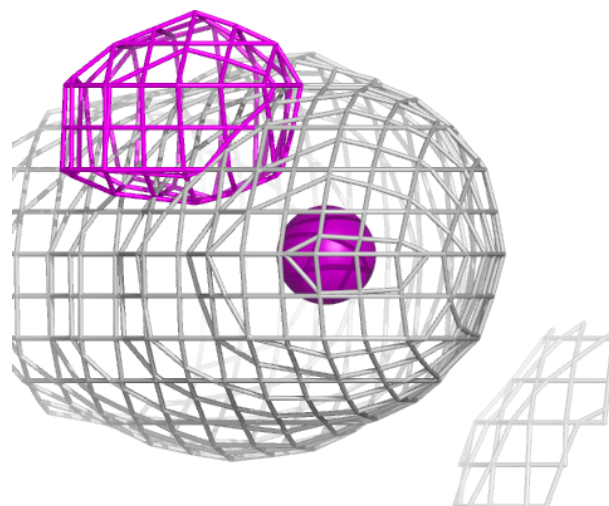
Electron density around IOD A 623:

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



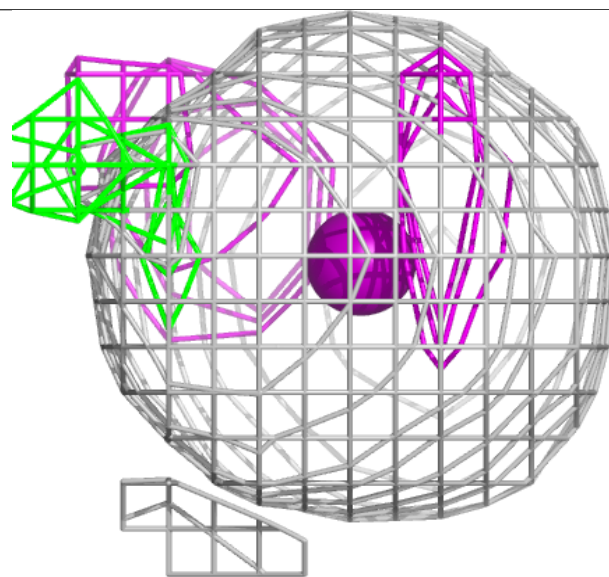
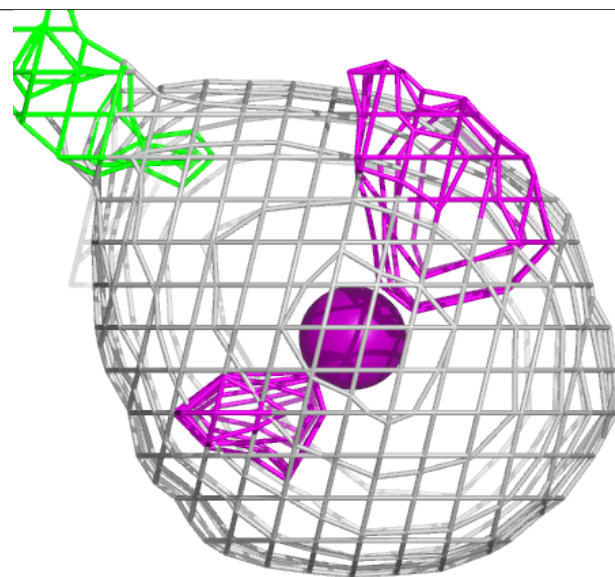
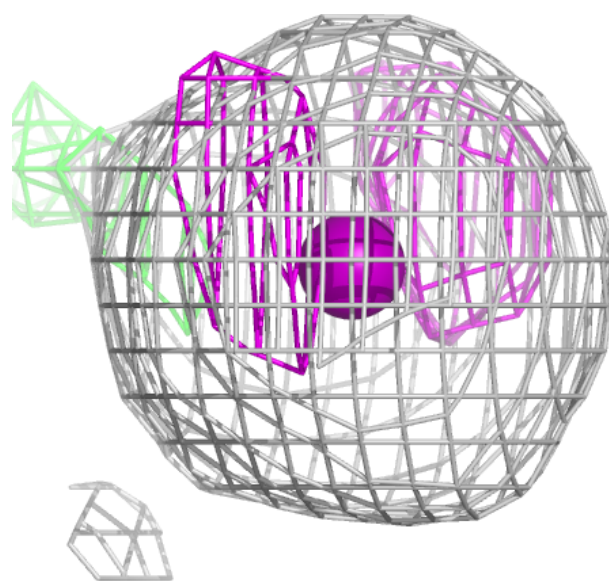
Electron density around IOD A 631:

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



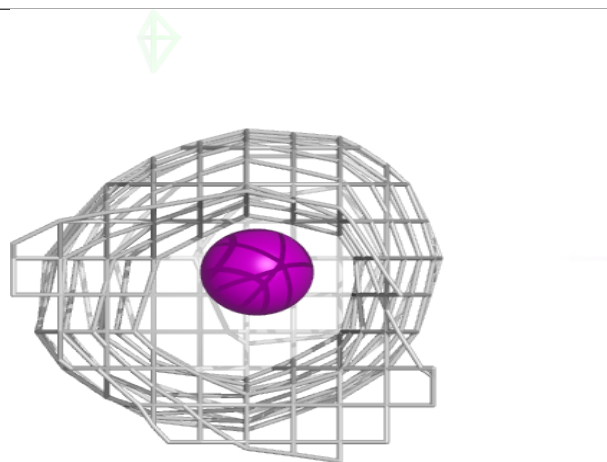
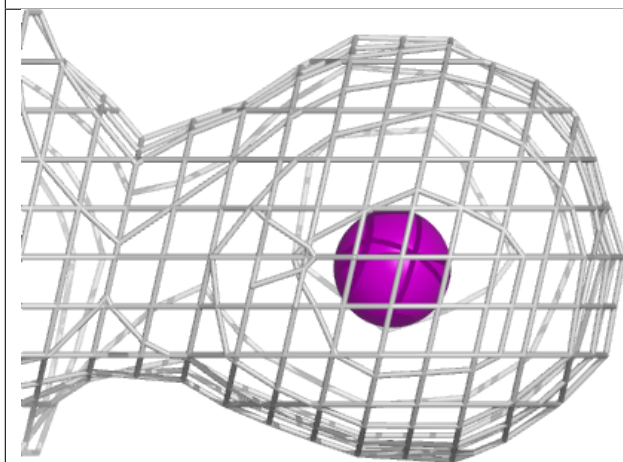
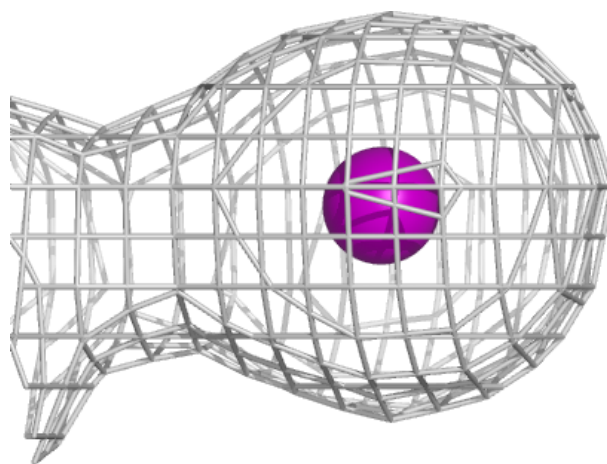
Electron density around IOD A 617:

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



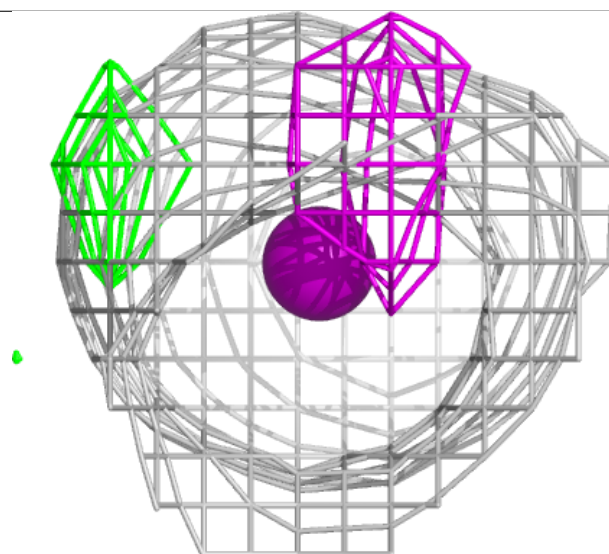
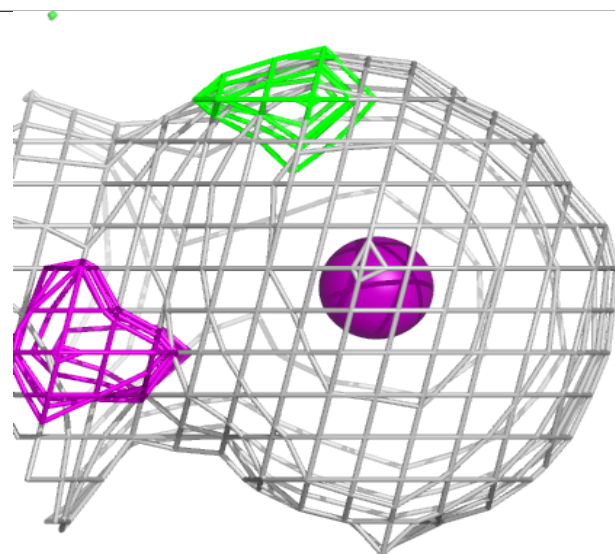
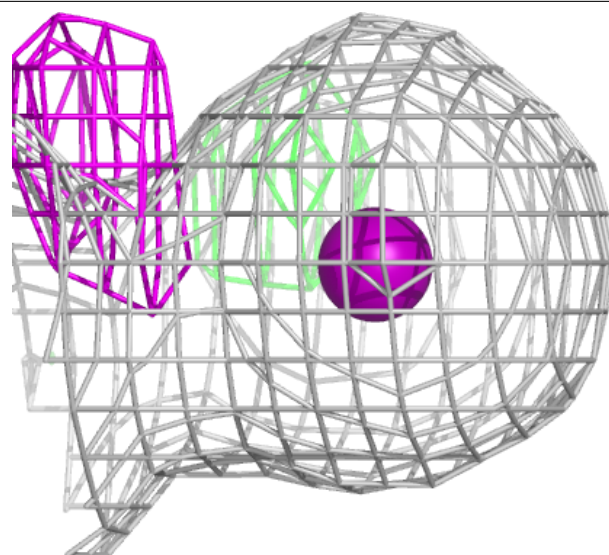
Electron density around IOD A 642:

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



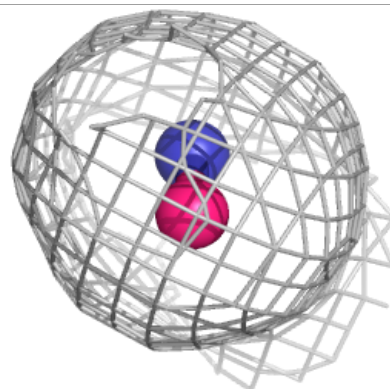
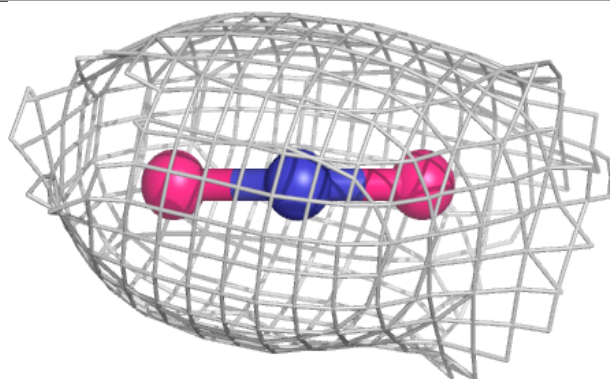
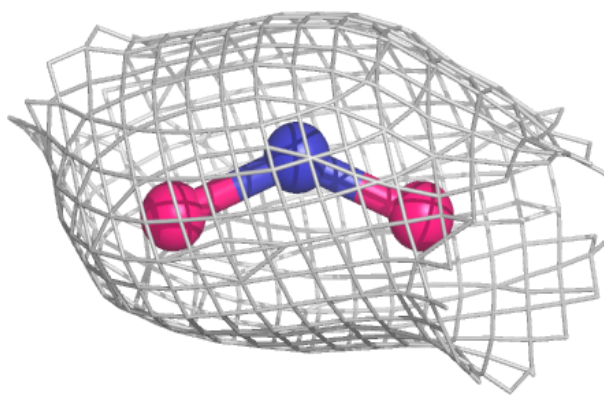
Electron density around IOD A 638:

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

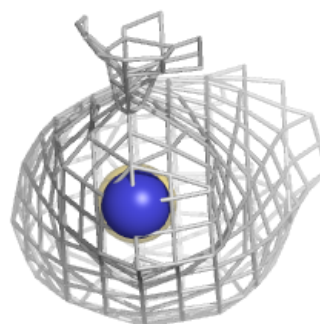
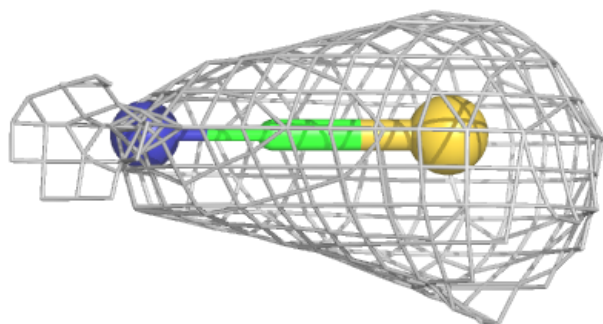
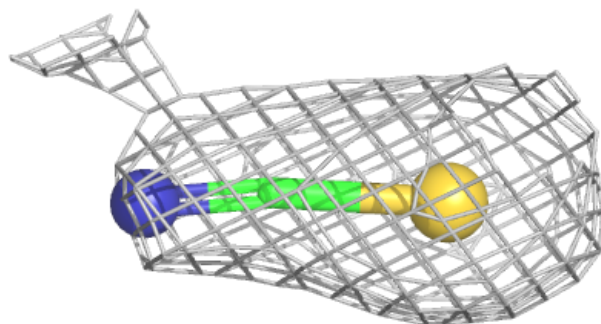


Electron density around NO2 A 605:

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

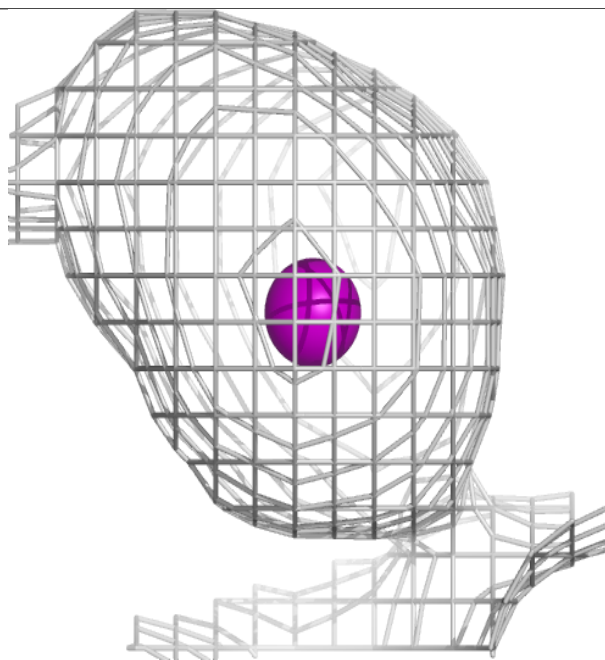
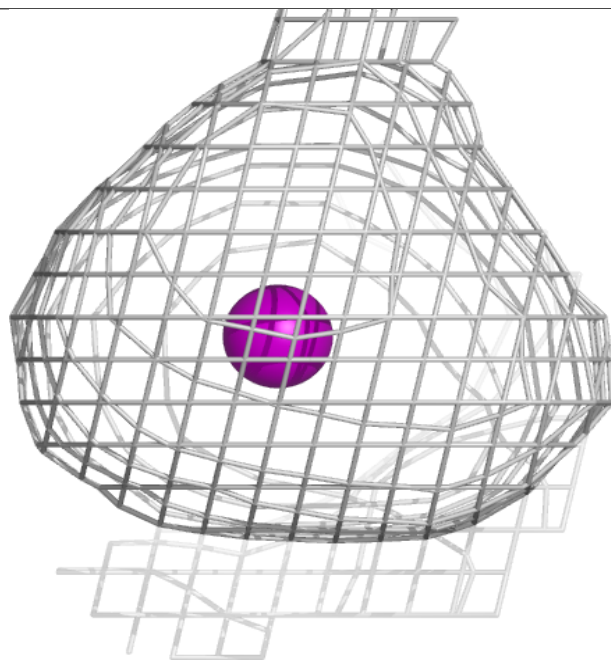
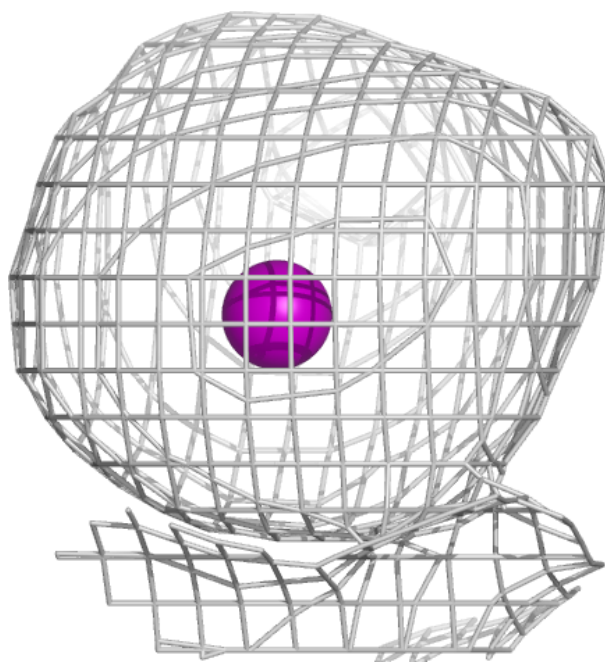
**Electron density around SCN A 637:**

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



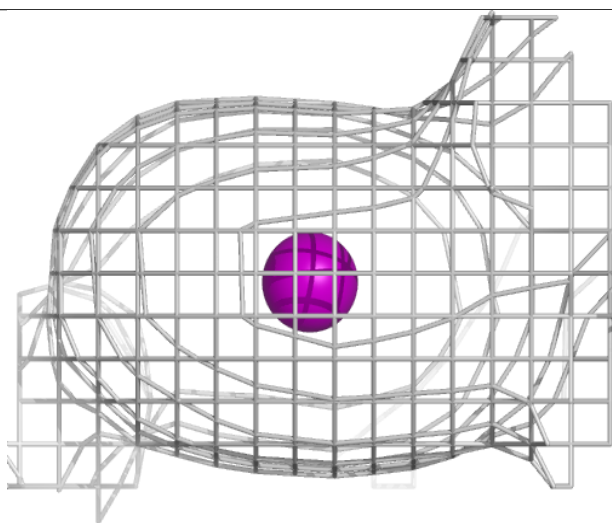
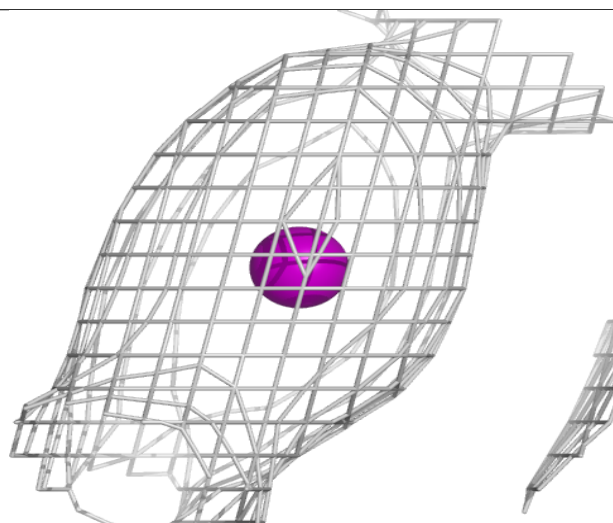
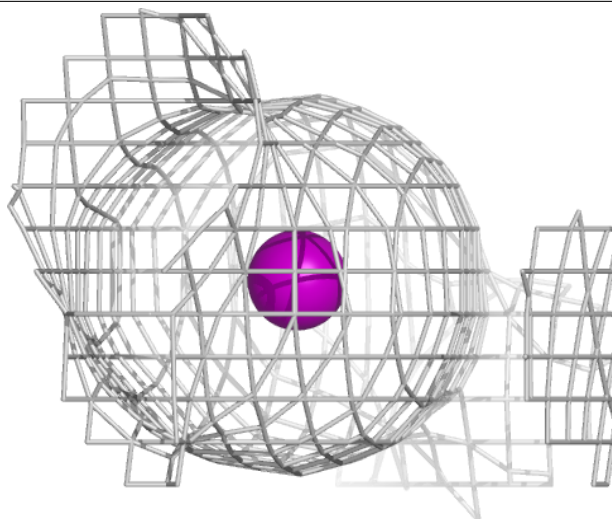
Electron density around IOD A 622:

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



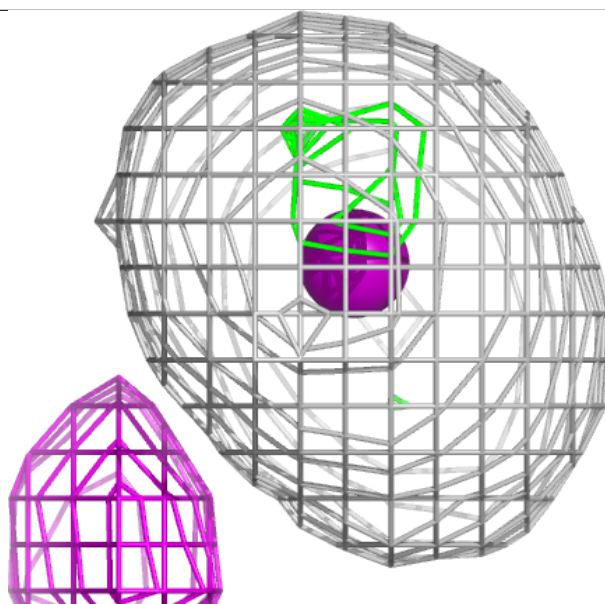
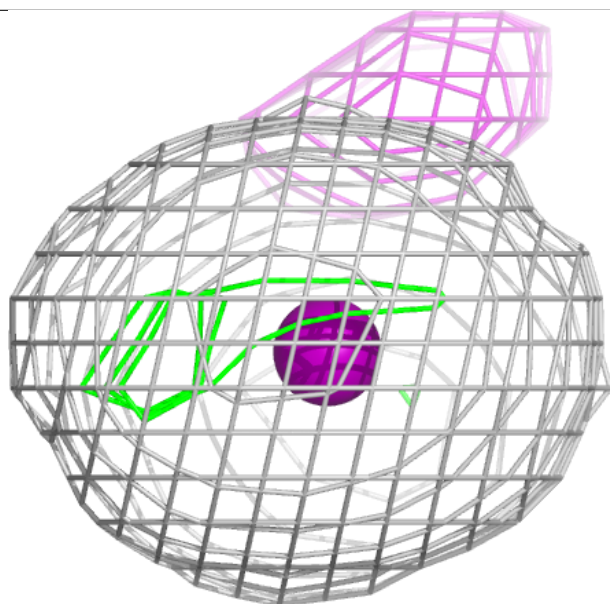
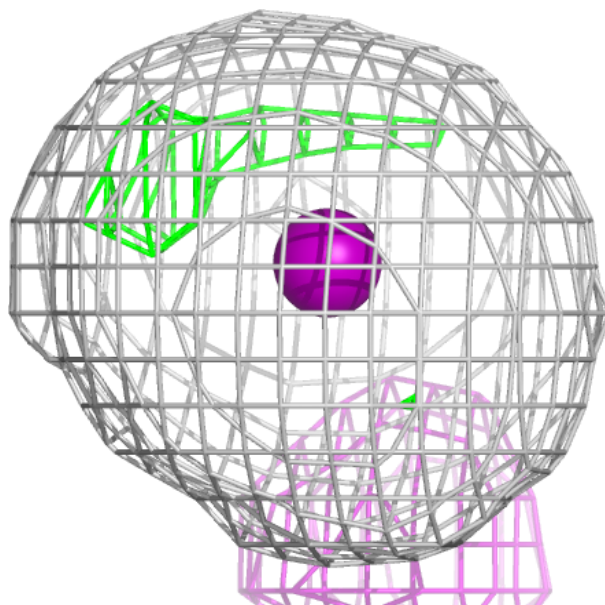
Electron density around IOD A 616:

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



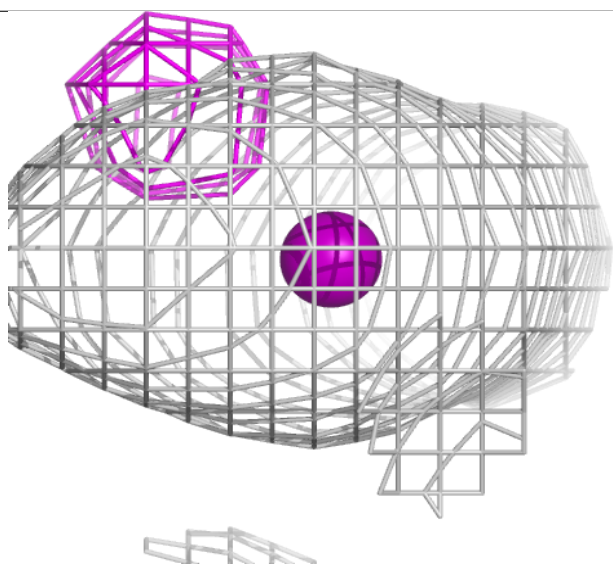
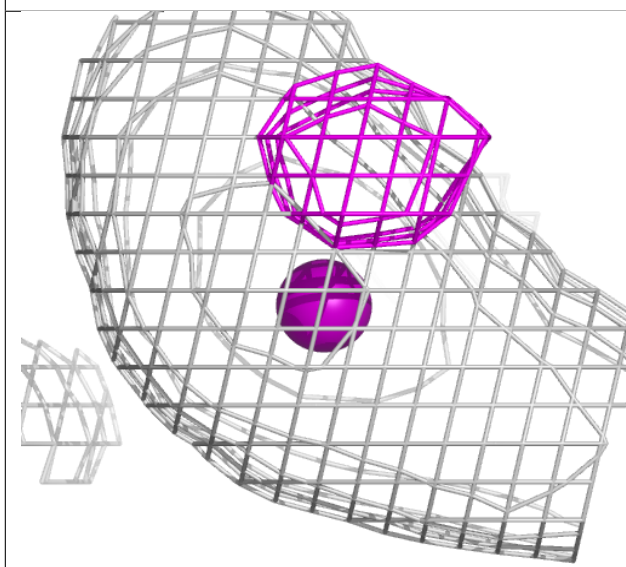
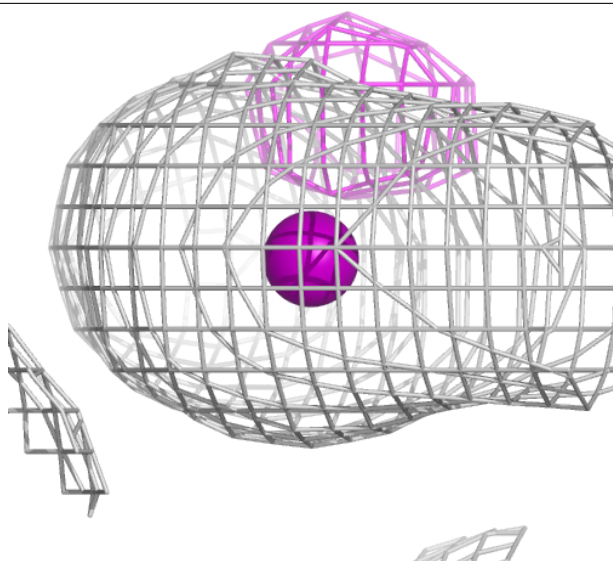
Electron density around IOD A 629:

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



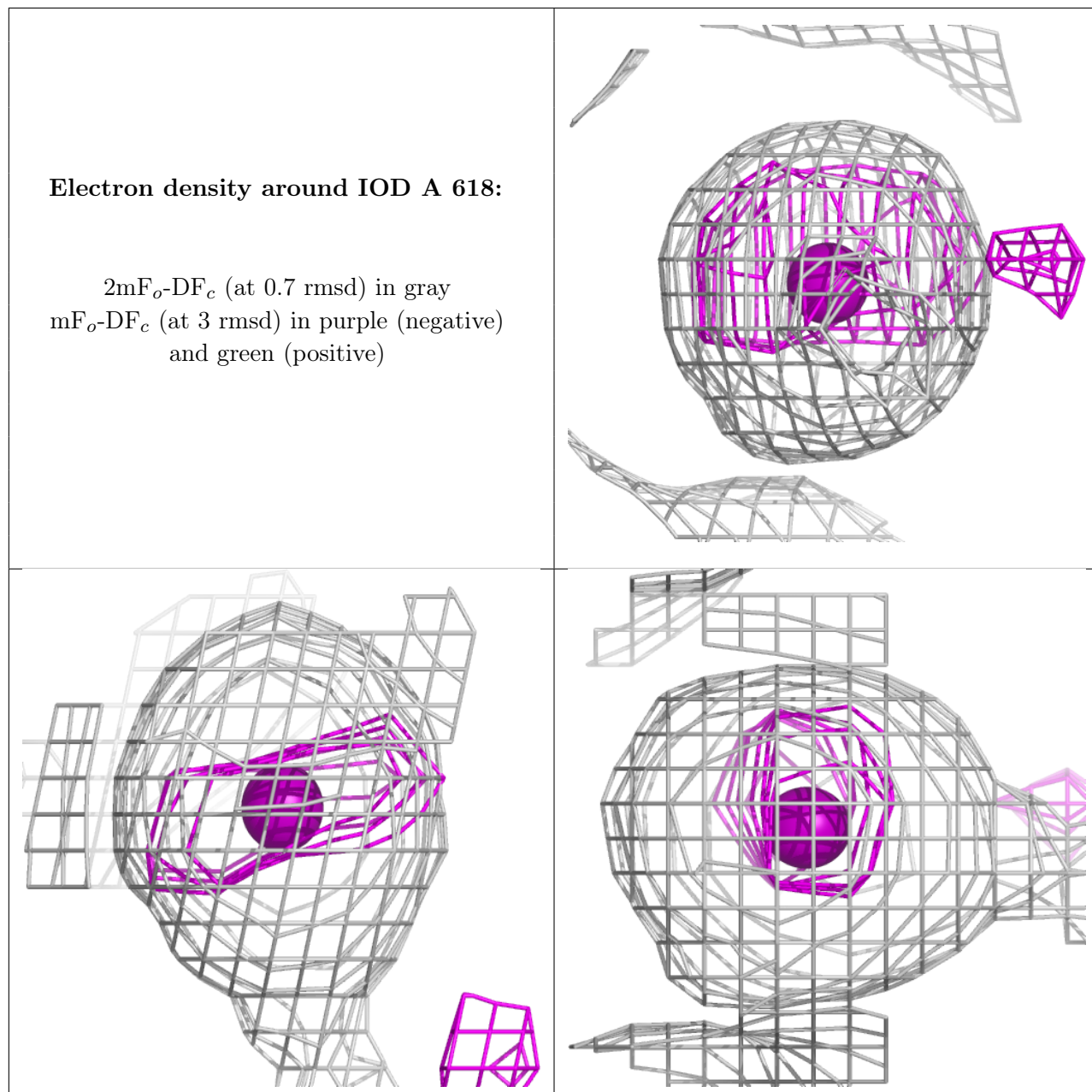
Electron density around IOD A 630:

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



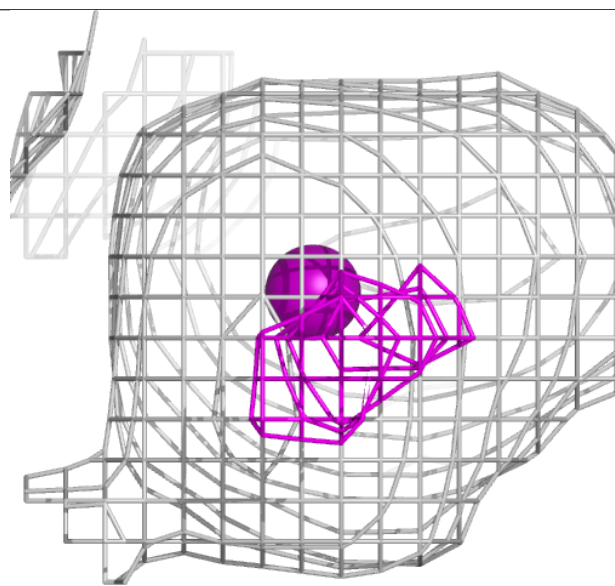
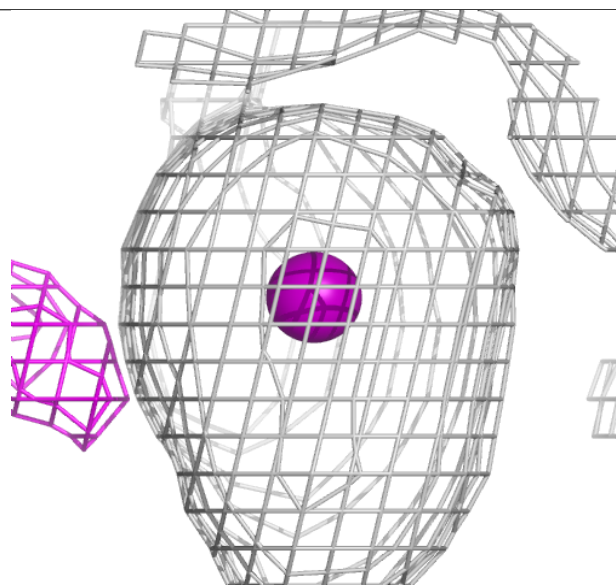
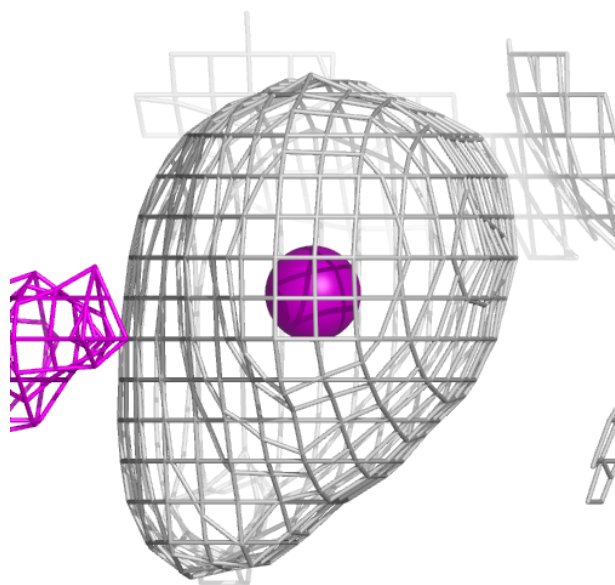
Electron density around IOD A 618:

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



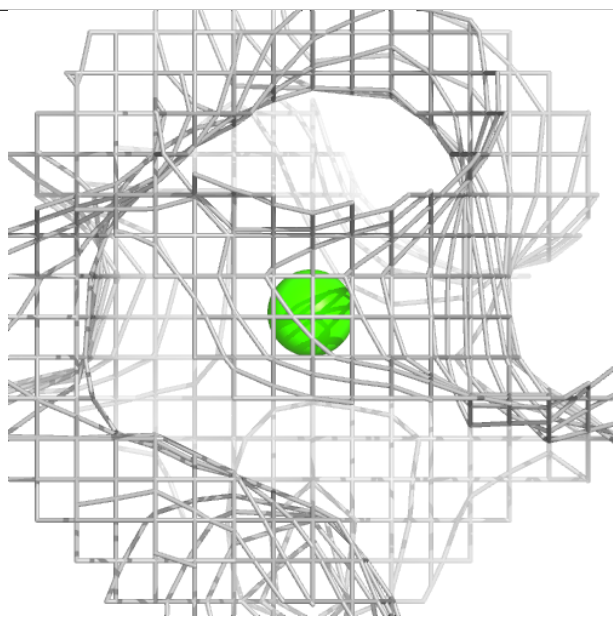
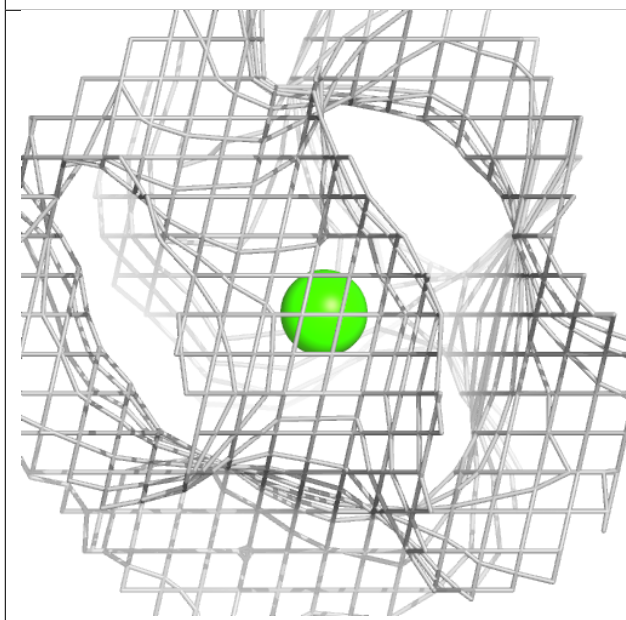
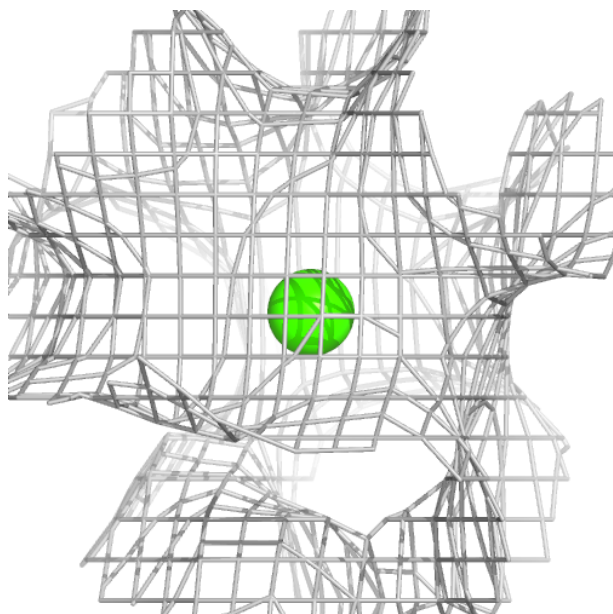
Electron density around IOD A 619:

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



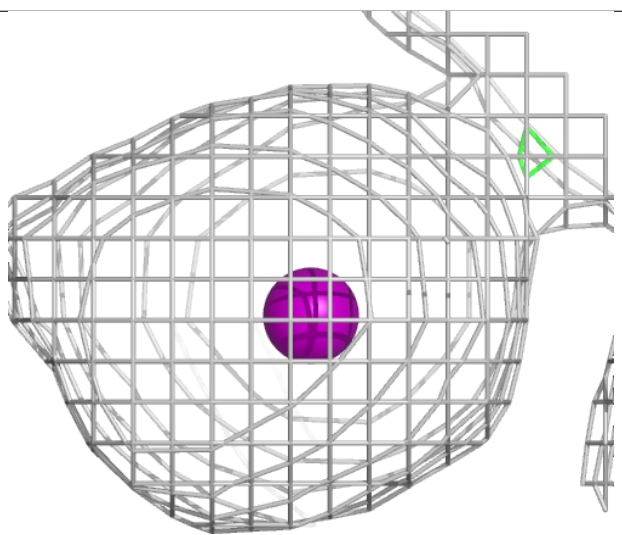
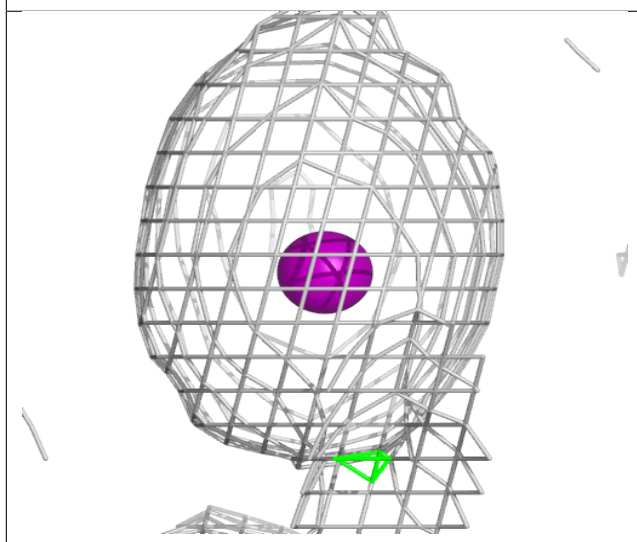
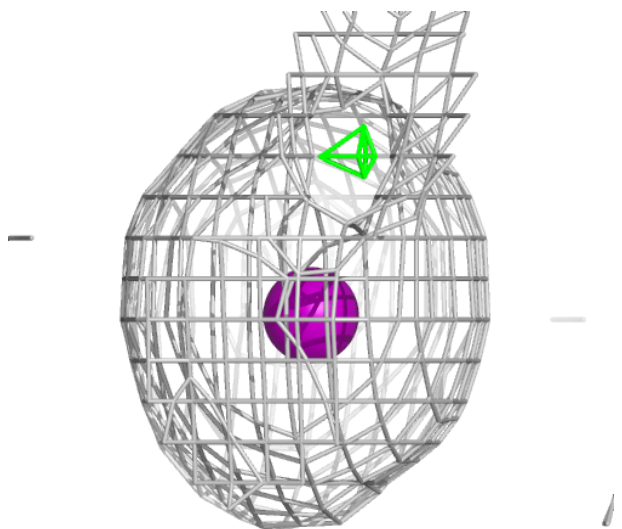
Electron density around CA A 626:

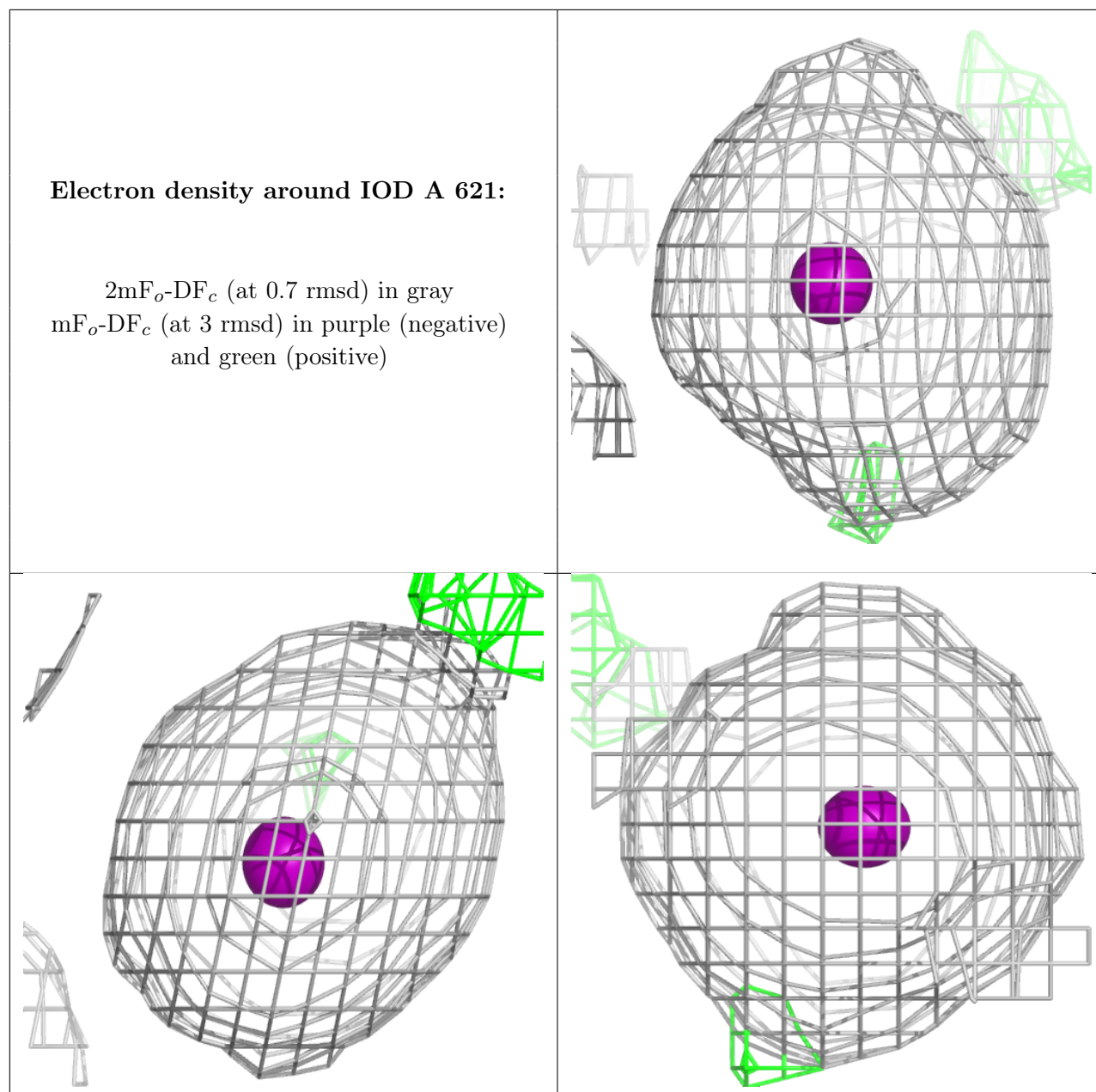
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around IOD A 620:

$2mF_o-DF_c$ (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.