



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 27, 2019 – 12:52 PM EST

PDB ID : 6LCO
Title : Crystal structure of bovine lactoperoxidase with substrates thiocynate and iodide bound at the distal heme side at 1.99 Å resolution.
Authors : Viswanathan, V.; Sirohi, H.V.; Kushwaha, G.S.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2019-11-19
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

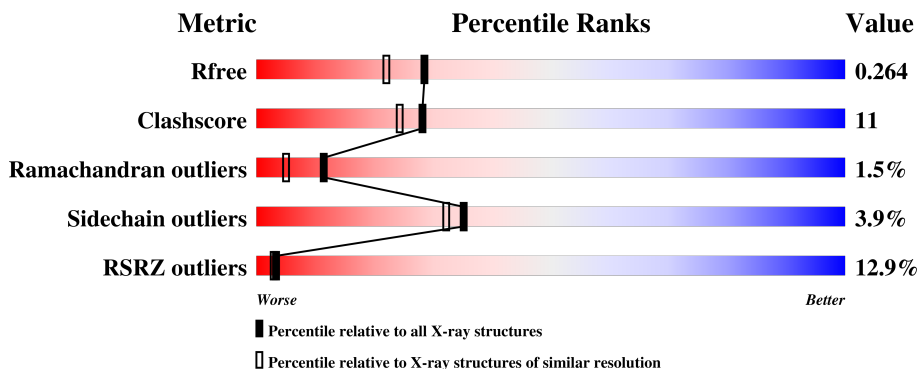
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	

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:

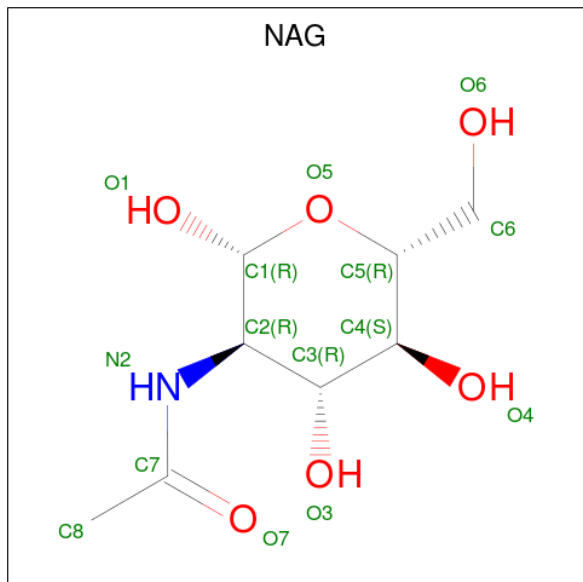
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	IOD	A	612	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	IOD	A	613	-	-	X	-
5	IOD	A	615	-	-	X	-
5	IOD	A	617	-	-	X	-
5	IOD	A	618	-	-	X	-
7	SCN	A	624	-	-	X	-
7	SCN	A	625	-	-	X	-
7	SCN	A	626	-	-	X	-
7	SCN	A	629	-	-	X	-
7	SCN	A	630	-	-	X	-

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by author).

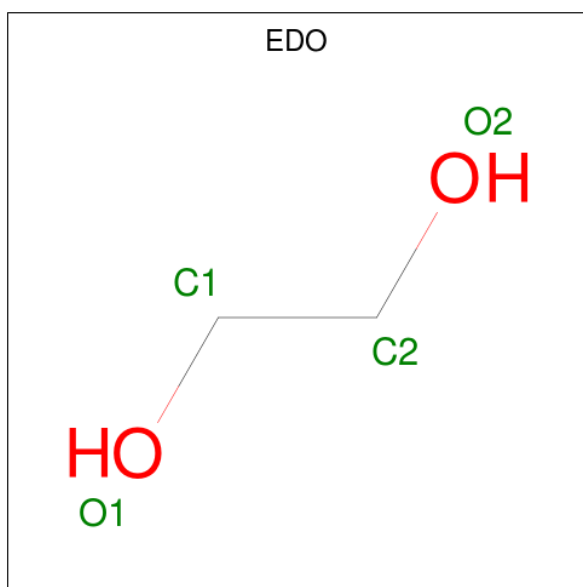


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I) (labeled as "Ligand of Interest" by author).

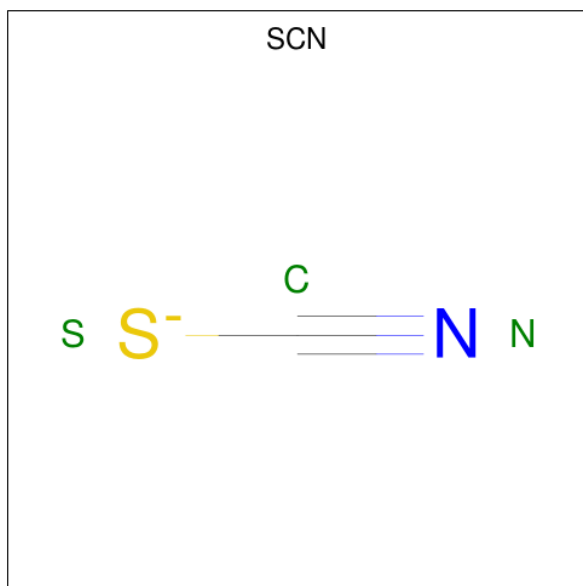
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	I	0	0
			16	16		

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



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

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



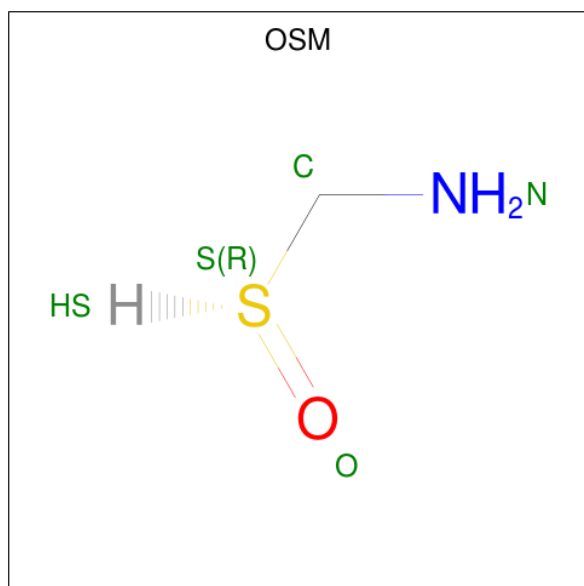
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	S	0	0
			3	1	1	1		
7	A	1	Total	C	N	S	0	0
			3	1	1	1		

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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		
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		

- Molecule 8 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH₅NOS) (labeled as "Ligand of Interest" by author).



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

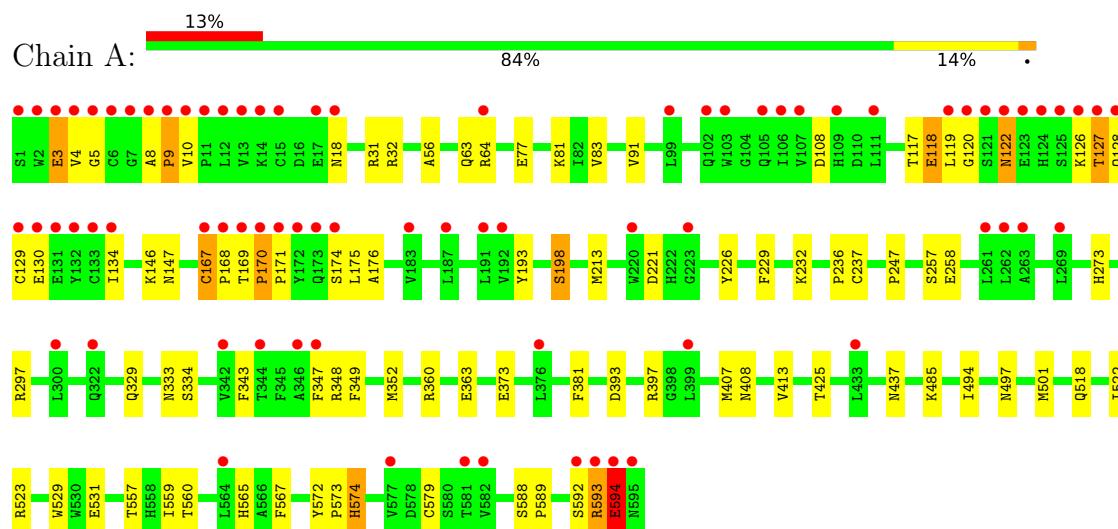
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	393	Total	O	0	0
			393	393		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.27Å 80.44Å 76.60Å 90.00° 103.20° 90.00°	Depositor
Resolution (Å)	39.10 – 2.00 39.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.6 (39.10-2.00) 92.6 (39.11-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.207 , 0.261 0.214 , 0.264	Depositor DCC
R_{free} test set	2014 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5344	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SCN, NAG, CA, EDO, OSM, HEM, 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	0.67	0/4921	0.79	0/6676

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4784	0	4709	84	0
2	A	43	0	30	13	0
3	A	1	0	0	0	0
4	A	70	0	64	3	0
5	A	16	0	0	19	0
6	A	4	0	6	3	0
7	A	21	0	0	16	0
8	A	12	0	15	1	0
9	A	393	0	0	14	0
All	All	5344	0	4824	104	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 11.

All (104) 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)
5:A:615:IOD:I	7:A:625:SCN:C	2.33	1.44
1:A:363[B]:GLU:CG	5:A:613:IOD:I	2.32	1.43
1:A:258:GLU:OE2	2:A:601:HEM:CMB	1.75	1.30
1:A:363[B]:GLU:CD	5:A:613:IOD:I	0.81	1.29
1:A:108:ASP:OD2	2:A:601:HEM:CMD	1.77	1.28
5:A:617:IOD:I	7:A:629:SCN:S	1.54	1.24
1:A:258:GLU:OE2	2:A:601:HEM:HMB1	1.05	1.23
1:A:363[B]:GLU:OE1	5:A:613:IOD:I	1.06	1.22
1:A:363[B]:GLU:OE2	5:A:613:IOD:I	1.21	1.22
5:A:612:IOD:I	7:A:626:SCN:S	2.67	1.21
5:A:615:IOD:I	7:A:625:SCN:S	0.80	1.09
5:A:619:IOD:I	6:A:623:EDO:O2	2.42	1.07
1:A:108:ASP:OD2	2:A:601:HEM:HMD1	0.86	1.02
1:A:198[B]:SER:OG	7:A:626:SCN:S	2.24	0.95
1:A:108:ASP:CG	2:A:601:HEM:HMD1	1.97	0.84
5:A:622:IOD:I	9:A:996:HOH:O	2.67	0.82
5:A:617:IOD:I	7:A:629:SCN:N	1.35	0.80
6:A:623:EDO:O2	7:A:624:SCN:N	2.16	0.77
1:A:407:MET:HB3	1:A:501:MET:CE	2.18	0.74
1:A:593:ARG:HG3	1:A:593:ARG:HH11	1.55	0.72
1:A:128:GLN:HE22	1:A:134:ILE:HB	1.55	0.69
4:A:607:NAG:H4	9:A:1022:HOH:O	1.93	0.68
5:A:617:IOD:I	7:A:629:SCN:C	0.28	0.68
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.31	0.66
1:A:408:ASN:HB2	9:A:932:HOH:O	1.95	0.66
1:A:574:HIS:C	1:A:574:HIS:HD1	2.00	0.65
7:A:625:SCN:N	9:A:706:HOH:O	2.29	0.65
1:A:531:GLU:OE2	9:A:702:HOH:O	2.14	0.65
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.79	0.63
1:A:352:MET:SD	1:A:407:MET:SD	2.97	0.63
7:A:624:SCN:S	9:A:848:HOH:O	2.53	0.62
1:A:258:GLU:OE2	2:A:601:HEM:HMB2	1.91	0.62
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.35	0.61
1:A:4:VAL:H	1:A:5:GLY:HA2	1.65	0.61
1:A:127:THR:N	1:A:128:GLN:HA	2.15	0.60
1:A:258:GLU:HG3	5:A:618:IOD:I	2.71	0.60
1:A:518:GLN:O	1:A:522[A]:ILE:HG13	2.02	0.60
1:A:128:GLN:NE2	1:A:134:ILE:HB	2.17	0.59
1:A:31:ARG:HD2	7:A:630:SCN:S	2.43	0.59
4:A:606:NAG:H62	9:A:701:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASP:HB2	1:A:226:TYR:CE1	2.38	0.58
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.85	0.58
1:A:258:GLU:OE2	2:A:601:HEM:C2B	2.56	0.57
1:A:126:LYS:N	1:A:127:THR:HA	2.20	0.57
1:A:126:LYS:HB3	1:A:127:THR:C	2.26	0.56
1:A:594:GLU:OE2	1:A:594:GLU:HA	2.07	0.54
1:A:237:CYS:HA	1:A:381:PHE:O	2.09	0.53
7:A:624:SCN:N	9:A:714:HOH:O	2.34	0.53
1:A:3:GLU:OE2	1:A:4:VAL:N	2.42	0.53
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.44	0.53
2:A:601:HEM:CMB	2:A:601:HEM:HBB2	2.40	0.52
1:A:594:GLU:HB2	9:A:734:HOH:O	2.10	0.52
1:A:363[B]:GLU:HG2	1:A:397:ARG:NH2	2.25	0.51
1:A:574:HIS:C	1:A:574:HIS:ND1	2.62	0.51
1:A:108:ASP:CG	2:A:601:HEM:CMD	2.66	0.51
1:A:4:VAL:N	1:A:5:GLY:HA2	2.26	0.50
1:A:32:ARG:NH1	9:A:725:HOH:O	2.45	0.50
1:A:363[B]:GLU:CB	5:A:613:IOD:I	3.27	0.49
1:A:560:THR:HA	1:A:579:CYS:SG	2.52	0.49
1:A:425:THR:N	7:A:628:SCN:S	2.78	0.49
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.95	0.49
1:A:567:PHE:HB2	7:A:629:SCN:S	2.53	0.49
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.33	0.48
1:A:393:ASP:OD1	1:A:557:THR:HB	2.13	0.48
5:A:618:IOD:I	6:A:623:EDO:O2	2.98	0.47
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.12	0.47
1:A:4:VAL:HG12	1:A:5:GLY:HA2	1.97	0.47
1:A:83:VAL:HG12	1:A:413:VAL:HB	1.97	0.47
1:A:258:GLU:CD	2:A:601:HEM:CMB	2.73	0.46
1:A:170:PRO:HD2	1:A:171:PRO:HD2	1.98	0.46
1:A:559:ILE:HG23	5:A:613:IOD:I	2.87	0.45
1:A:594:GLU:HB3	9:A:971:HOH:O	2.17	0.45
1:A:3:GLU:CD	1:A:4:VAL:H	2.19	0.45
1:A:572:TYR:CG	1:A:573:PRO:HA	2.52	0.45
1:A:373:GLU:HB2	8:A:632:OSM:O	2.16	0.45
1:A:128:GLN:O	1:A:130:GLU:N	2.50	0.44
1:A:3:GLU:HG3	1:A:175:LEU:HD22	1.99	0.44
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.83	0.44
1:A:594:GLU:OE2	1:A:594:GLU:CA	2.66	0.44
1:A:117:THR:C	1:A:118:GLU:HG2	2.37	0.44
1:A:127:THR:HG23	1:A:128:GLN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LYS:O	1:A:147:ASN:HB2	2.18	0.44
1:A:167:CYS:O	1:A:169:THR:N	2.50	0.44
1:A:18:ASN:HA	9:A:754:HOH:O	2.18	0.43
1:A:10:VAL:HG13	1:A:10:VAL:O	2.18	0.43
4:A:606:NAG:O4	9:A:701:HOH:O	2.12	0.43
1:A:193:TYR:CZ	1:A:297:ARG:HA	2.53	0.43
1:A:236:PRO:HA	5:A:608:IOD:I	2.89	0.43
1:A:122:ASN:ND2	1:A:122:ASN:O	2.52	0.42
1:A:363[B]:GLU:HG2	1:A:397:ARG:CZ	2.49	0.42
1:A:127:THR:N	1:A:128:GLN:CA	2.80	0.42
1:A:588:SER:N	1:A:589:PRO:CD	2.82	0.42
1:A:5:GLY:N	9:A:740:HOH:O	2.53	0.42
1:A:108:ASP:OD2	2:A:601:HEM:C2D	2.62	0.42
1:A:333:ASN:HD22	7:A:630:SCN:C	2.33	0.42
1:A:229:PHE:HB3	1:A:247:PRO:HG2	2.00	0.41
5:A:612:IOD:I	7:A:626:SCN:C	3.37	0.41
1:A:407:MET:HB3	1:A:501:MET:HE3	1.96	0.41
1:A:175:LEU:HG	1:A:176:ALA:N	2.34	0.41
1:A:565:HIS:HA	5:A:617:IOD:I	2.91	0.41
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.69	0.40
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.57	0.40
1:A:572:TYR:CD2	1:A:573:PRO:HA	2.57	0.40
1:A:257:SER:O	1:A:381:PHE:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	596/595 (100%)	557 (94%)	30 (5%)	9 (2%)	11 5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	CYS
1	A	174	SER
1	A	594	GLU
1	A	118	GLU
1	A	170	PRO
1	A	9	PRO
1	A	120	GLY
1	A	56	ALA
1	A	168	PRO

5.3.2 Protein sidechains ⓘ

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	521/518 (101%)	500 (96%)	21 (4%)	34	31

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	63	GLN
1	A	64	ARG
1	A	91	VAL
1	A	119	LEU
1	A	122	ASN
1	A	127	THR
1	A	167	CYS
1	A	198[A]	SER
1	A	198[B]	SER
1	A	232	LYS
1	A	329	GLN
1	A	334	SER
1	A	347	PHE
1	A	360	ARG
1	A	485	LYS
1	A	494	ILE
1	A	574	HIS

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Mol	Chain	Res	Type
1	A	592	SER
1	A	593	ARG
1	A	594	GLU

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

Mol	Chain	Res	Type
1	A	18	ASN
1	A	437	ASN
1	A	468	GLN
1	A	497	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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 17 are monoatomic - leaving 17 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	$\# Z > 2$
2	HEM	A	601	1,9	27,50,50	1.07	2 (7%)	17,82,82	1.68	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	603	1,4	14,14,15	0.53	0	17,19,21	1.27	3 (17%)
4	NAG	A	604	4	14,14,15	0.47	0	17,19,21	1.72	3 (17%)
4	NAG	A	605	1	14,14,15	0.57	0	17,19,21	2.05	4 (23%)
4	NAG	A	606	1	14,14,15	0.37	0	17,19,21	1.61	1 (5%)
4	NAG	A	607	1	14,14,15	0.53	0	17,19,21	2.02	4 (23%)
6	EDO	A	623	-	3,3,3	0.13	0	2,2,2	0.33	0
7	SCN	A	624	-	1,2,2	0.09	0	0,1,1	0.00	-
7	SCN	A	625	-	1,2,2	0.36	0	0,1,1	0.00	-
7	SCN	A	626	-	1,2,2	0.17	0	0,1,1	0.00	-
7	SCN	A	627	5	1,2,2	0.96	0	0,1,1	0.00	-
7	SCN	A	628	-	1,2,2	0.86	0	0,1,1	0.00	-
7	SCN	A	629	-	1,2,2	0.18	0	0,1,1	0.00	-
7	SCN	A	630	-	1,2,2	1.57	0	0,1,1	0.00	-
8	OSM	A	631	-	1,3,3	0.03	0	0,2,2	0.00	-
8	OSM	A	632	-	1,3,3	0.03	0	0,2,2	0.00	-
8	OSM	A	633	-	1,3,3	0.01	0	0,2,2	0.00	-

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	HEM	A	601	1,9	-	0/6/54/54	-
4	NAG	A	603	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	604	4	-	1/6/23/26	0/1/1/1
4	NAG	A	605	1	-	0/6/23/26	0/1/1/1
4	NAG	A	606	1	-	0/6/23/26	0/1/1/1
4	NAG	A	607	1	-	4/6/23/26	0/1/1/1
6	EDO	A	623	-	-	0/1/1/1	-
8	OSM	A	631	-	-	0/0/1/1	-
8	OSM	A	632	-	-	0/0/1/1	-
8	OSM	A	633	-	-	0/0/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3B-C2B	-3.27	1.35	1.40
2	A	601	HEM	C3D-C2D	-2.04	1.31	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	607	NAG	C1-O5-C5	6.18	120.60	112.20
4	A	605	NAG	C1-O5-C5	5.95	120.29	112.20
4	A	606	NAG	C1-O5-C5	5.45	119.61	112.20
4	A	604	NAG	C1-O5-C5	4.66	118.54	112.20
4	A	603	NAG	C4-C3-C2	-3.20	106.33	111.02
4	A	604	NAG	O5-C1-C2	3.06	116.16	111.36
4	A	607	NAG	C8-C7-N2	3.05	121.35	116.10
4	A	605	NAG	O7-C7-N2	3.02	127.58	121.95
2	A	601	HEM	CBD-CAD-C3D	-2.92	106.90	112.47
4	A	605	NAG	O4-C4-C5	2.75	116.16	109.29
4	A	607	NAG	C2-N2-C7	2.65	126.72	122.92
2	A	601	HEM	CMD-C2D-C3D	-2.60	120.04	124.94
2	A	601	HEM	CMC-C2C-C3C	2.52	129.52	124.80
4	A	607	NAG	O5-C5-C4	2.38	116.61	110.83
4	A	604	NAG	C3-C4-C5	2.38	114.50	110.23
2	A	601	HEM	CAA-CBA-CGA	2.31	116.61	112.66
2	A	601	HEM	CMD-C2D-C1D	2.31	132.01	128.46
4	A	605	NAG	C3-C4-C5	-2.28	106.13	110.23
2	A	601	HEM	CBA-CAA-C2A	-2.27	108.15	112.48
4	A	603	NAG	O5-C1-C2	-2.12	108.02	111.36
4	A	603	NAG	C2-N2-C7	-2.12	119.89	122.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

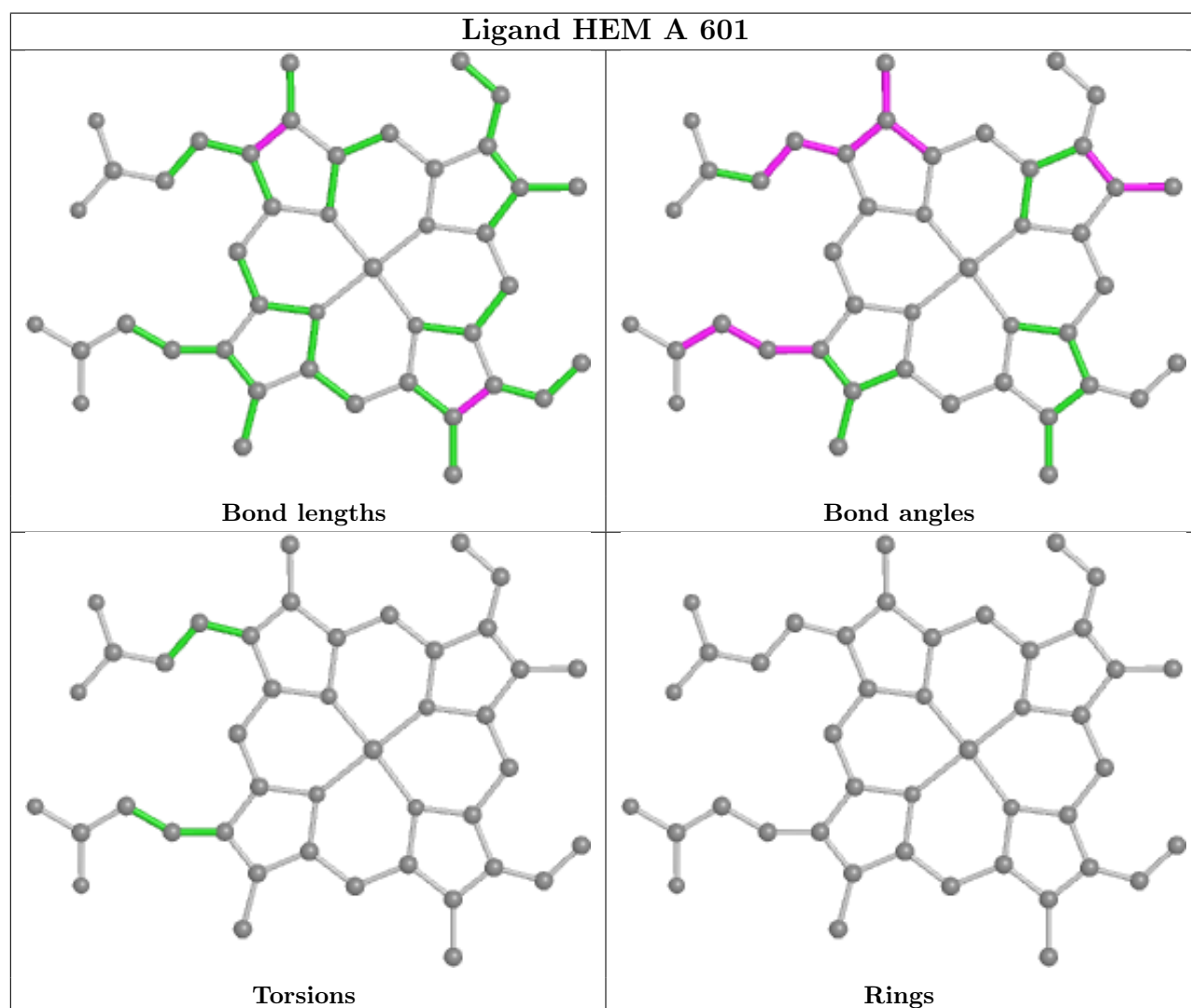
Mol	Chain	Res	Type	Atoms
4	A	607	NAG	O5-C5-C6-O6
4	A	607	NAG	C8-C7-N2-C2
4	A	607	NAG	O7-C7-N2-C2
4	A	607	NAG	C4-C5-C6-O6
4	A	604	NAG	O5-C5-C6-O6

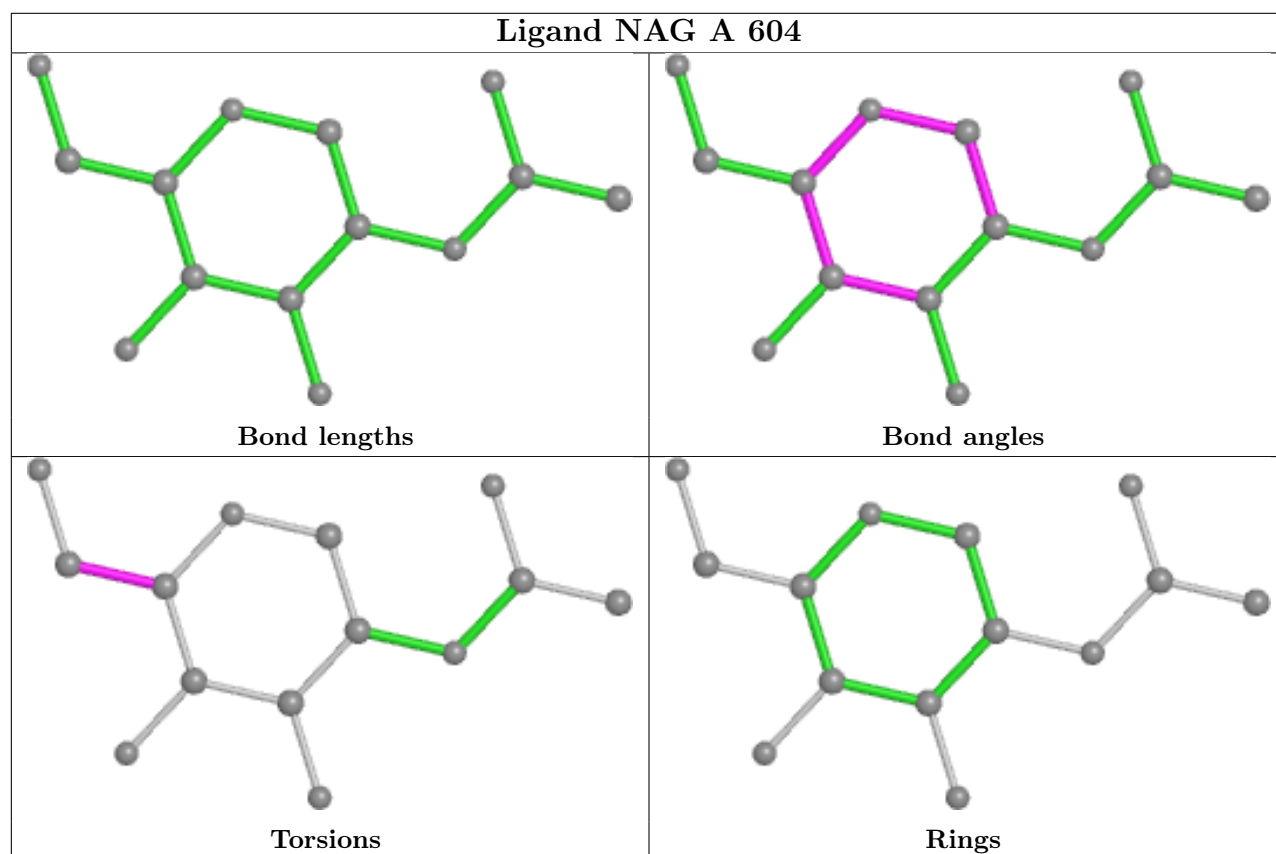
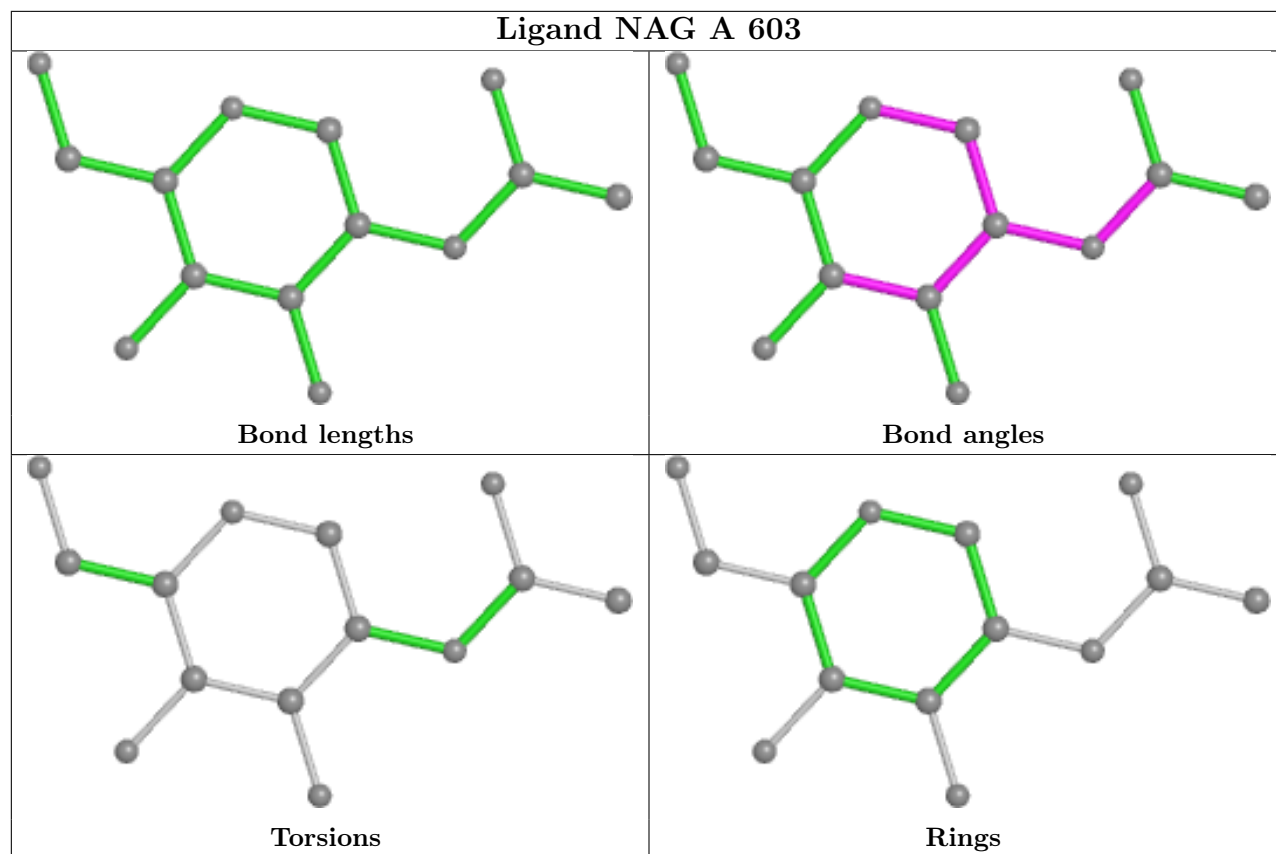
There are no ring outliers.

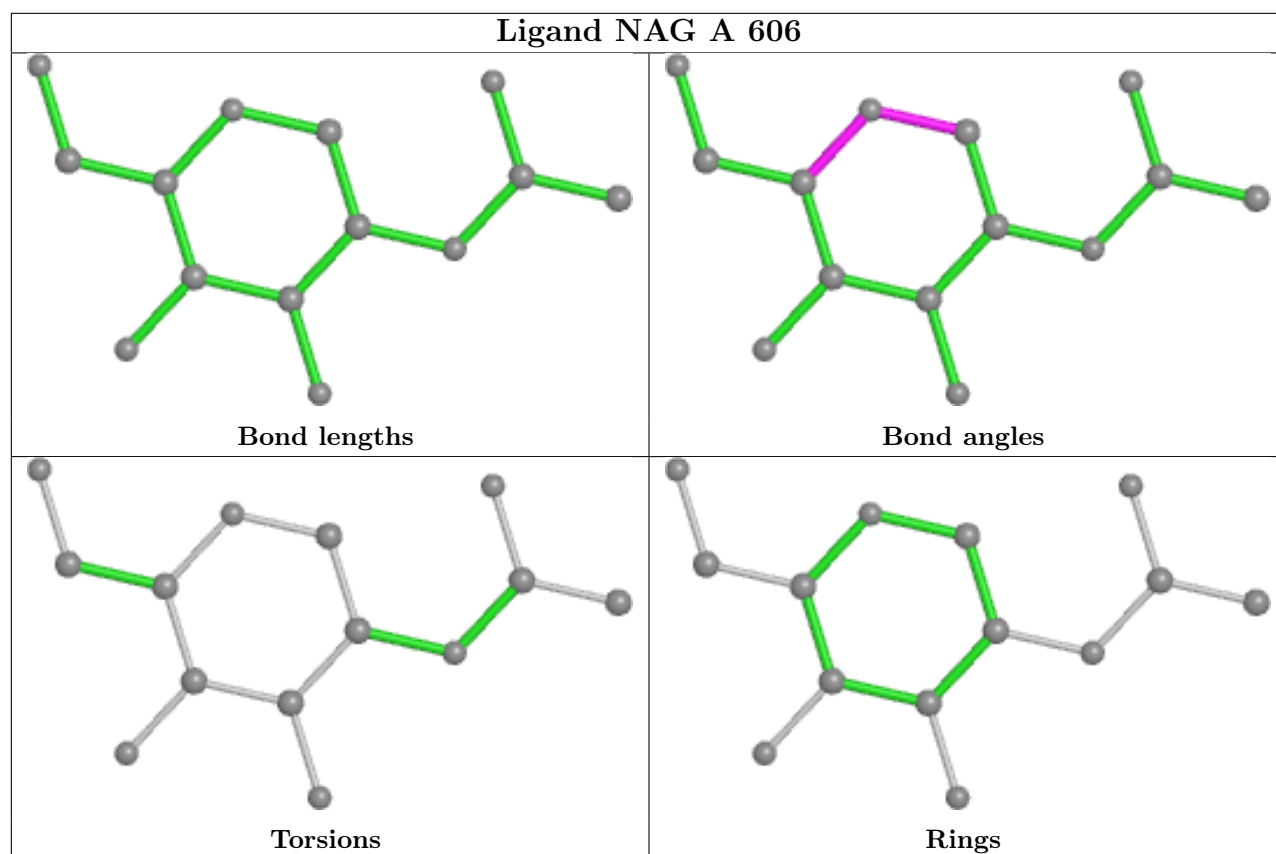
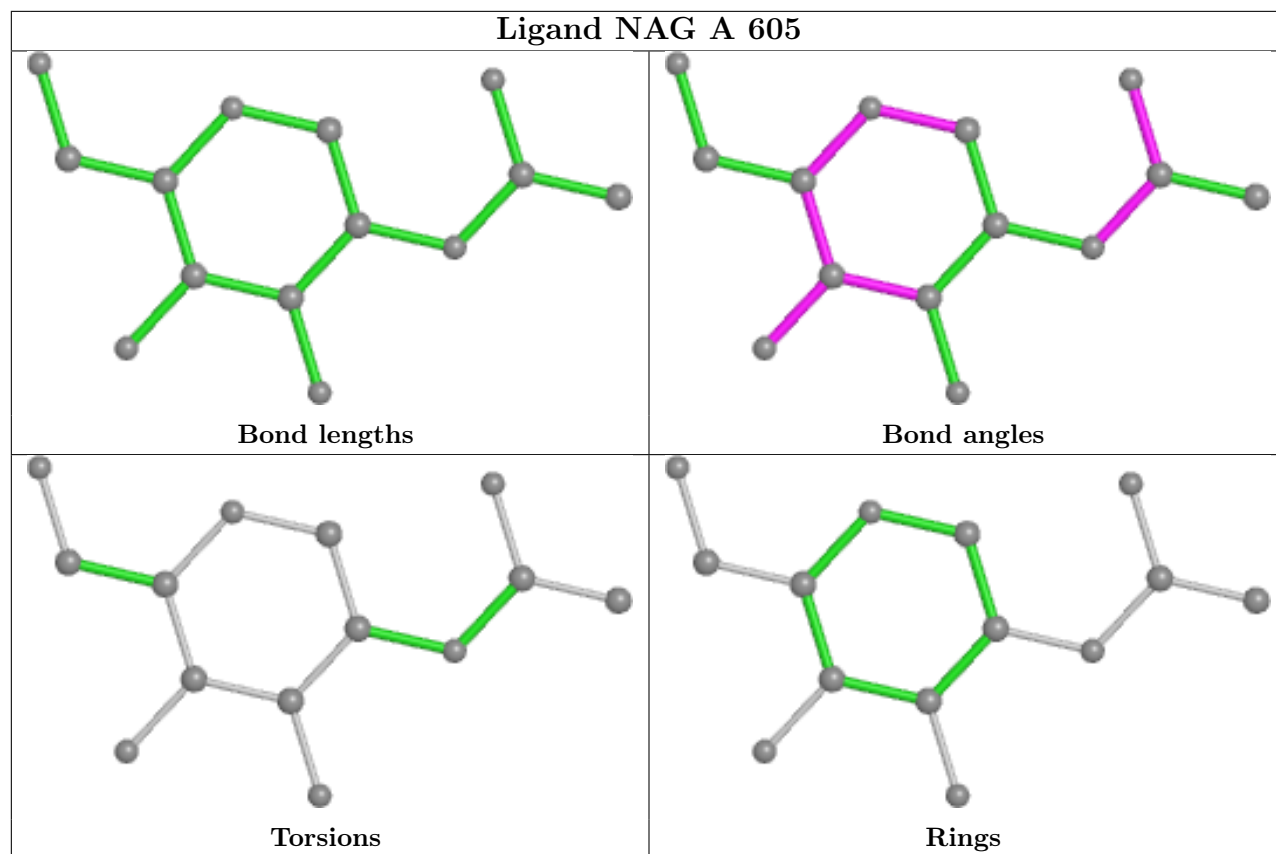
5 monomers are involved in 20 short contacts:

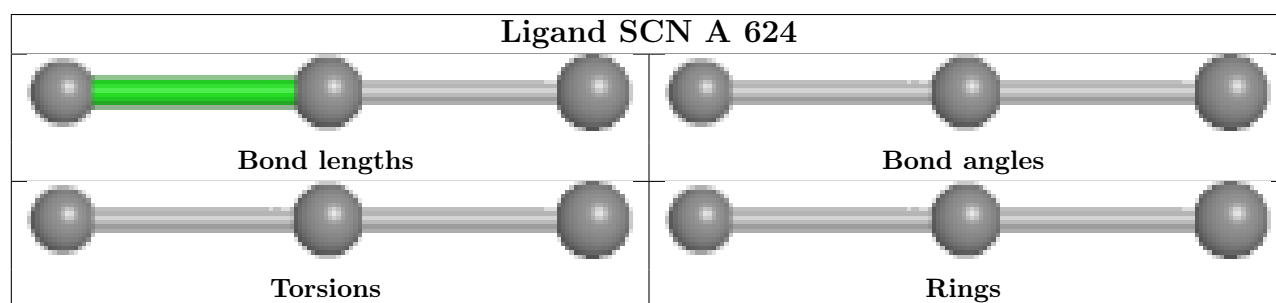
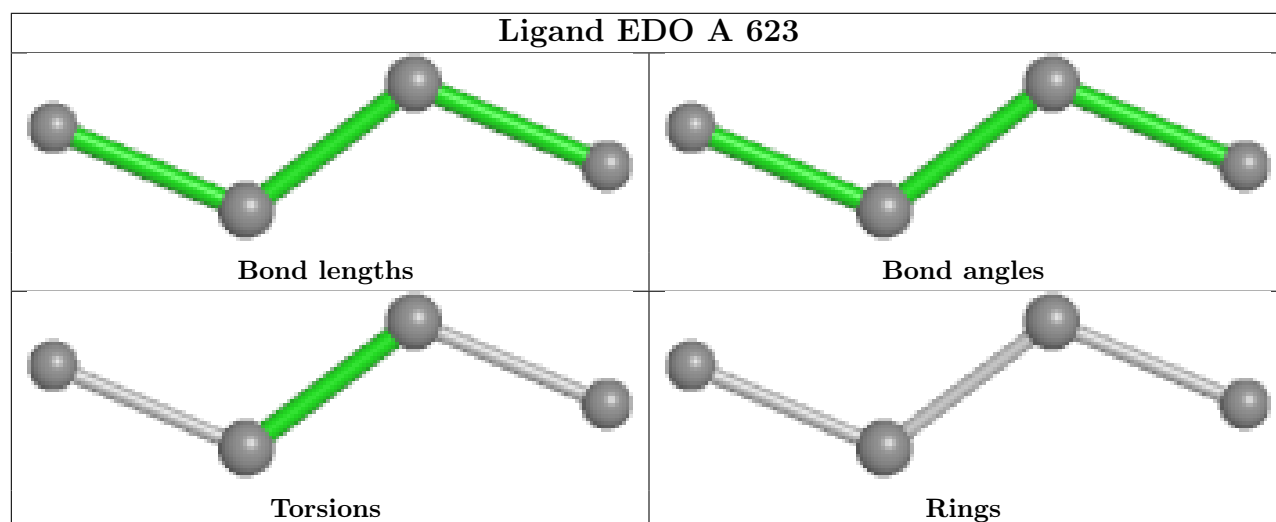
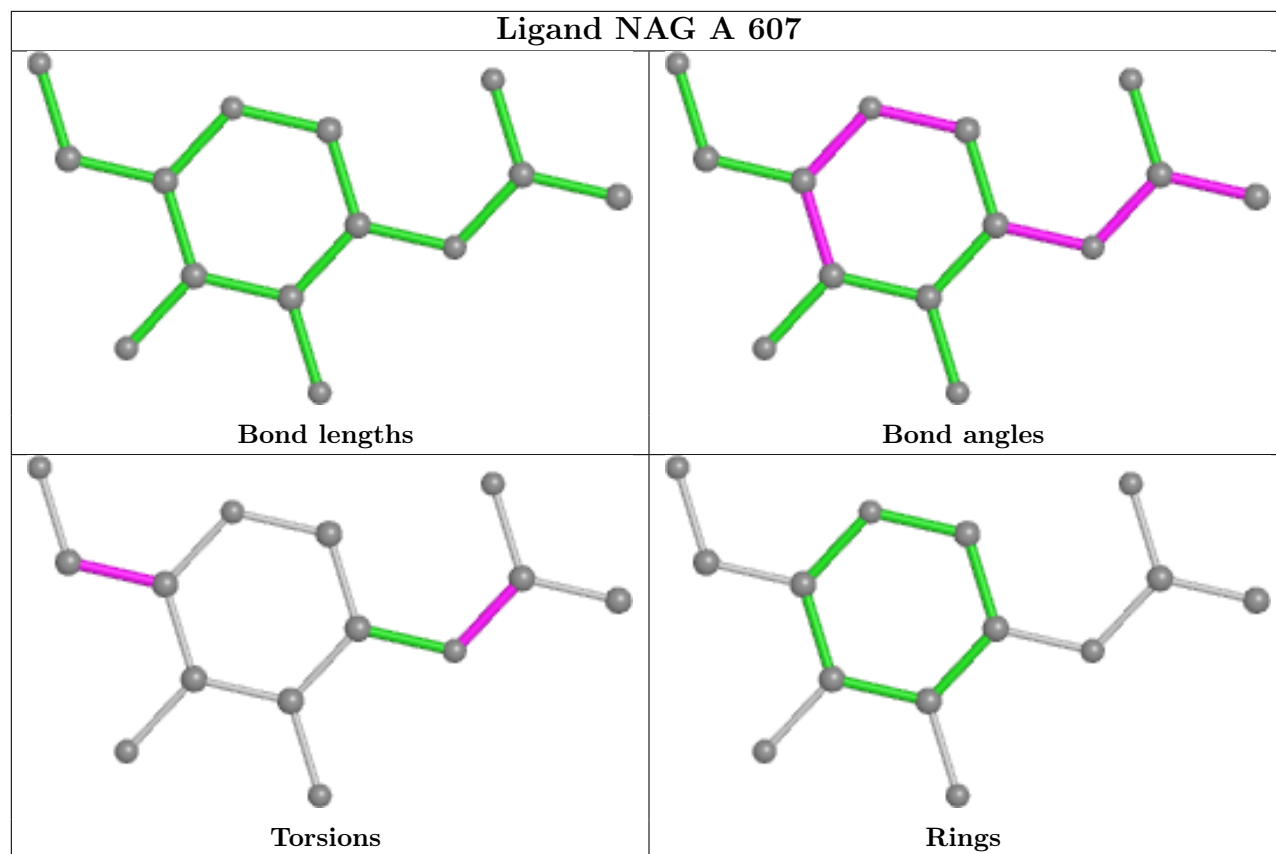
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	13	0
4	A	606	NAG	2	0
4	A	607	NAG	1	0
6	A	623	EDO	3	0
8	A	632	OSM	1	0

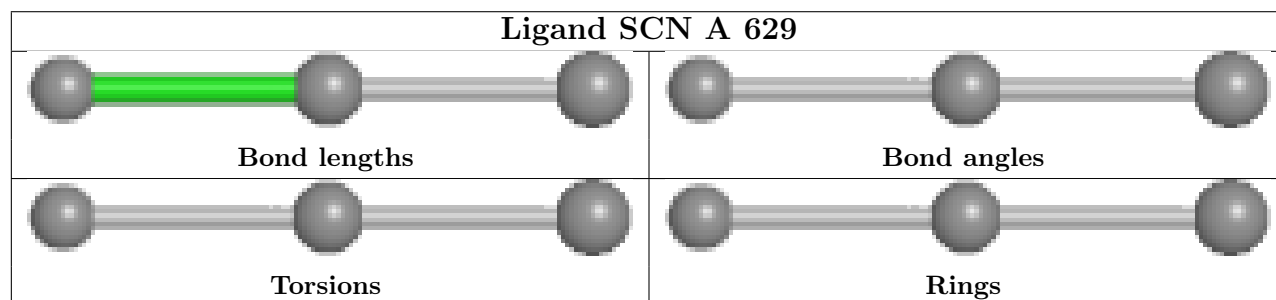
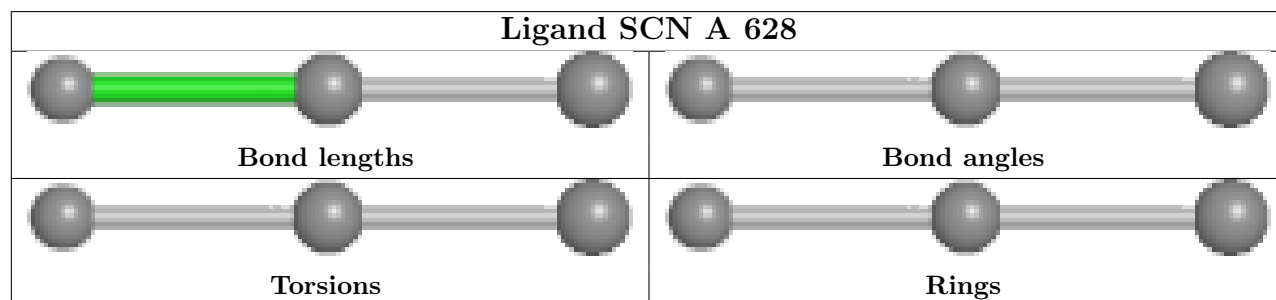
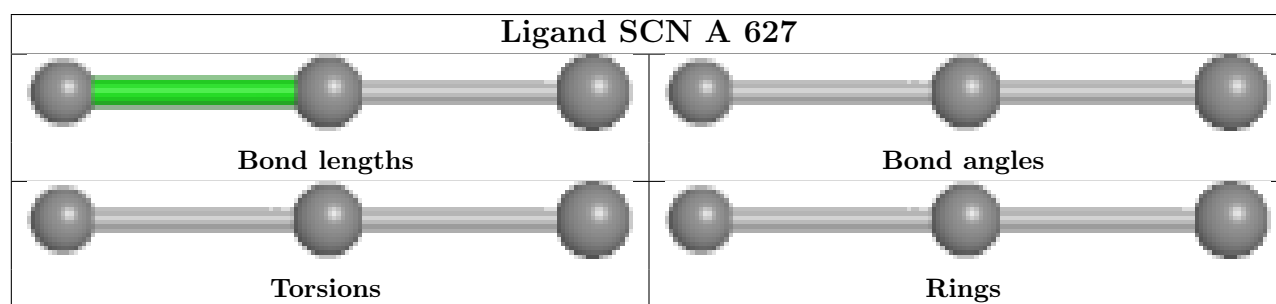
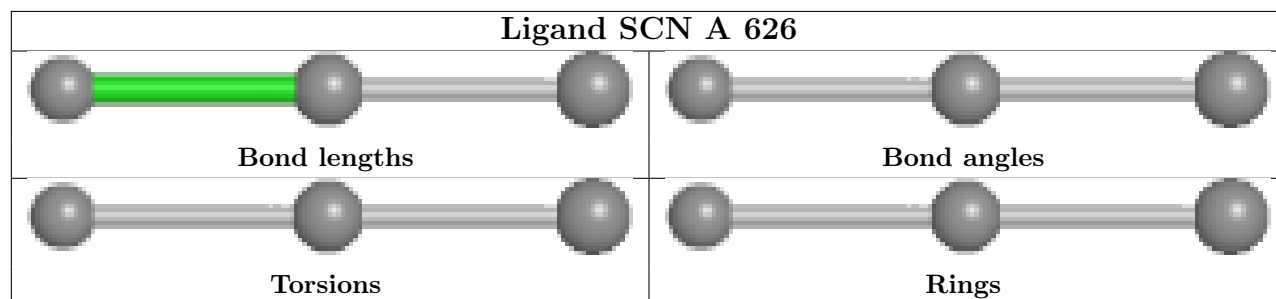
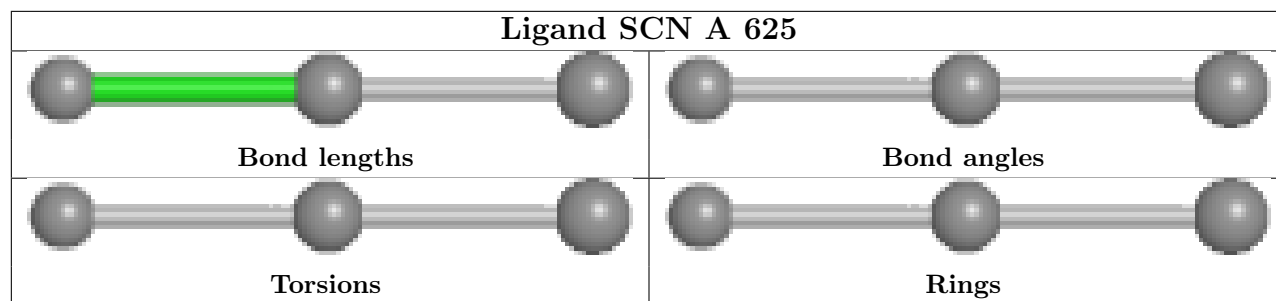
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

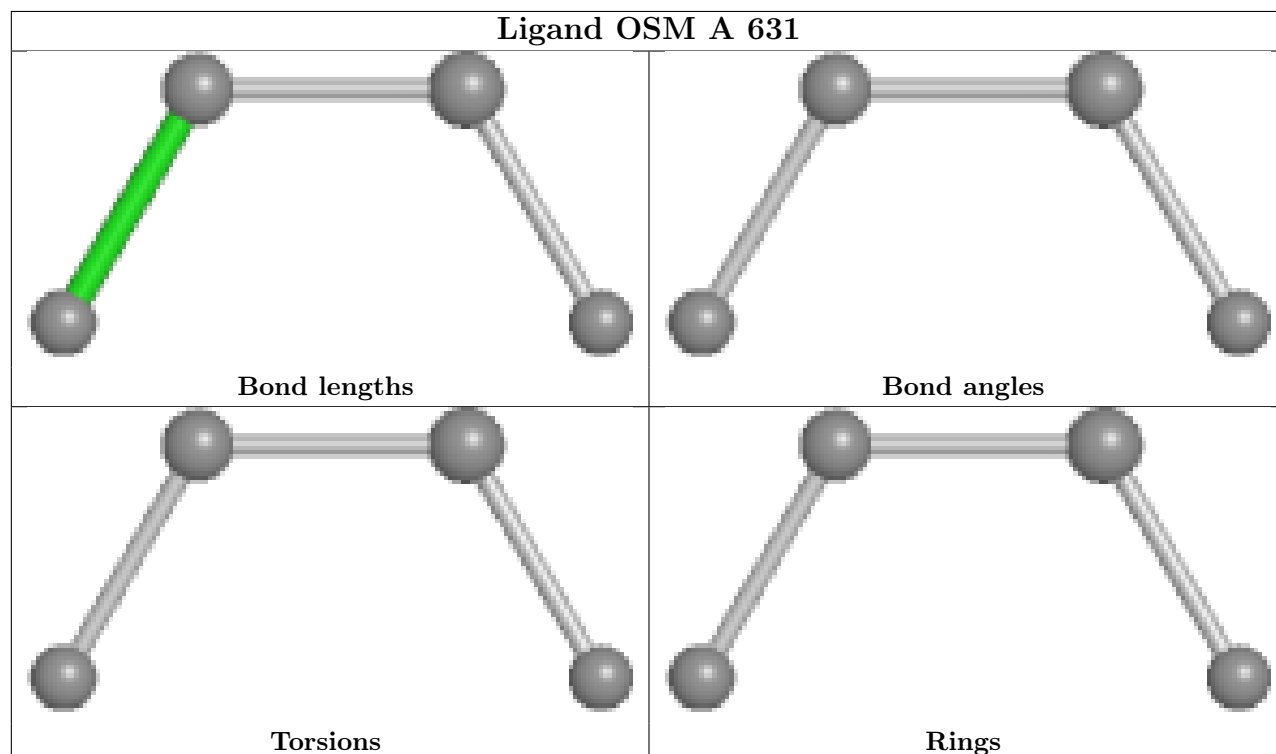
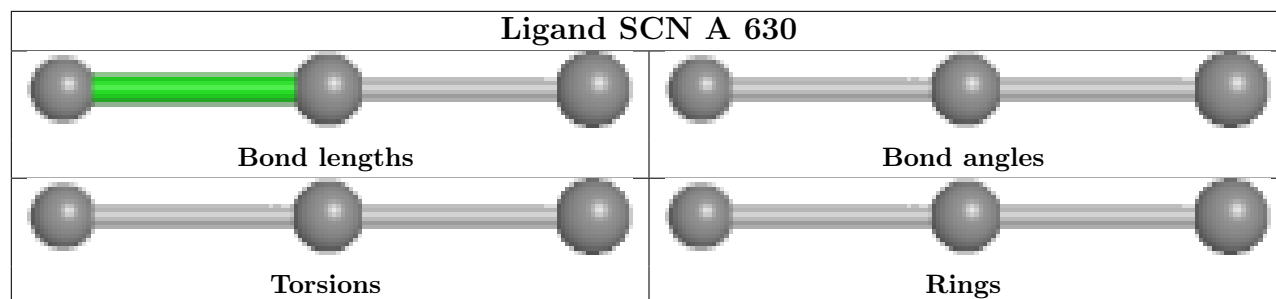


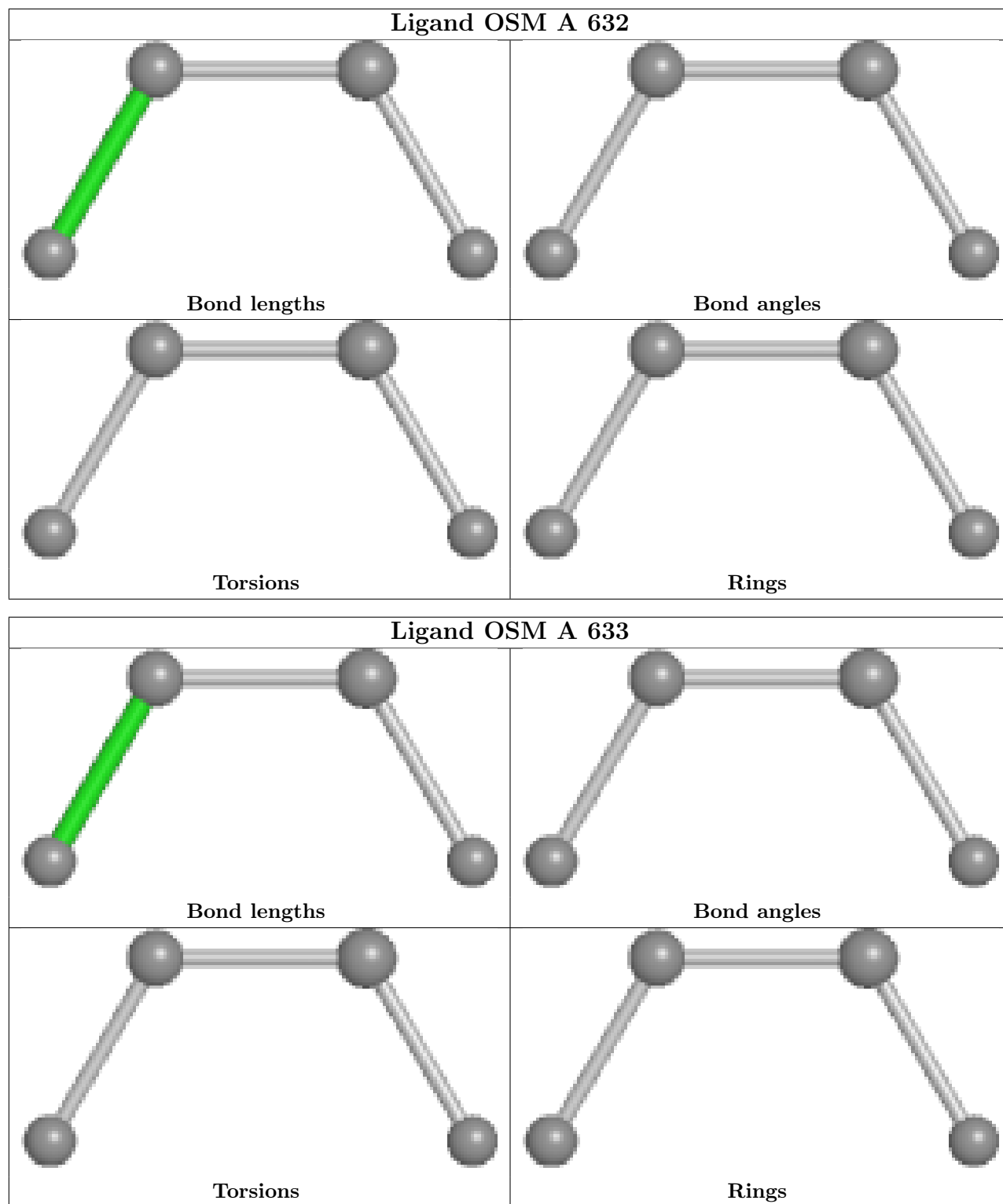












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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%)	0.88	77 (12%) 3 3	31, 48, 115, 178	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	28.2
1	A	120	GLY	22.7
1	A	172	TYR	20.1
1	A	119	LEU	15.8
1	A	1	SER	14.7
1	A	12	LEU	13.1
1	A	11	PRO	12.2
1	A	8	ALA	11.9
1	A	122	ASN	11.8
1	A	121	SER	11.0
1	A	174	SER	11.0
1	A	595	ASN	10.1
1	A	123	GLU	9.5
1	A	173	GLN	9.3
1	A	7	GLY	9.1
1	A	593	ARG	8.7
1	A	4	VAL	8.5
1	A	169	THR	7.9
1	A	171	PRO	7.2
1	A	9	PRO	7.0
1	A	10	VAL	6.8
1	A	124	HIS	6.7
1	A	594	GLU	5.6
1	A	13	VAL	5.4
1	A	170	PRO	4.8
1	A	125	SER	4.7
1	A	262	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	107	VAL	4.4
1	A	126	LYS	4.4
1	A	128	GLN	4.3
1	A	6	CYS	4.2
1	A	106	ILE	4.2
1	A	3	GLU	4.0
1	A	223	GLY	4.0
1	A	15	CYS	3.9
1	A	5	GLY	3.7
1	A	261	LEU	3.7
1	A	111	LEU	3.5
1	A	132	TYR	3.5
1	A	134	ILE	3.5
1	A	220	TRP	3.5
1	A	592	SER	3.4
1	A	376	LEU	3.4
1	A	17	GLU	3.2
1	A	399	LEU	3.2
1	A	64	ARG	3.1
1	A	131	GLU	3.1
1	A	14	LYS	2.9
1	A	127	THR	2.9
1	A	344	THR	2.9
1	A	130	GLU	2.7
1	A	342	VAL	2.7
1	A	167	CYS	2.7
1	A	109	HIS	2.7
1	A	168	PRO	2.6
1	A	346	ALA	2.5
1	A	582	VAL	2.5
1	A	129	CYS	2.5
1	A	103	TRP	2.5
1	A	300	LEU	2.4
1	A	269	LEU	2.4
1	A	564	LEU	2.4
1	A	18	ASN	2.3
1	A	322	GLN	2.3
1	A	133	CYS	2.3
1	A	105	GLN	2.3
1	A	192	VAL	2.2
1	A	263	ALA	2.2
1	A	347	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	183	VAL	2.2
1	A	99	LEU	2.2
1	A	187	LEU	2.2
1	A	433	LEU	2.1
1	A	102	GLN	2.1
1	A	577	VAL	2.1
1	A	581	THR	2.1
1	A	191	LEU	2.1

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 carbohydrates 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, 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
8	OSM	A	631	4/4	0.76	0.22	74,74,77,80	0
7	SCN	A	630	3/3	0.80	0.19	49,49,64,72	0
4	NAG	A	605	14/15	0.82	0.12	58,67,72,74	0
4	NAG	A	604	14/15	0.83	0.28	69,77,94,99	0
4	NAG	A	606	14/15	0.85	0.23	77,88,94,94	0
5	IOD	A	621	1/1	0.85	0.07	79,79,79,79	1
4	NAG	A	607	14/15	0.86	0.29	66,79,88,98	0
6	EDO	A	623	4/4	0.89	0.30	51,59,63,67	0
4	NAG	A	603	14/15	0.94	0.11	44,52,64,64	0
5	IOD	A	622	1/1	0.95	0.05	64,64,64,64	1
8	OSM	A	633	4/4	0.96	0.12	58,62,63,69	0
5	IOD	A	613	1/1	0.96	0.08	65,65,65,65	1
7	SCN	A	627	3/3	0.97	0.08	40,40,46,48	3
5	IOD	A	616	1/1	0.97	0.05	63,63,63,63	1
8	OSM	A	632	4/4	0.97	0.13	48,53,55,56	0

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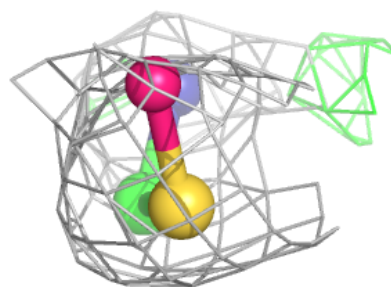
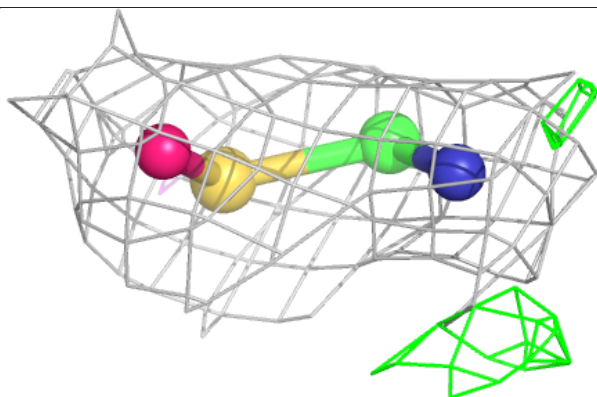
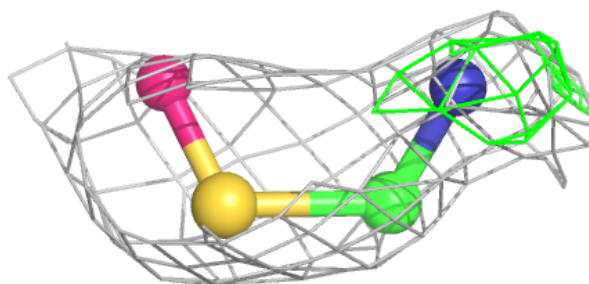
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	A	601	43/43	0.97	0.21	28,32,36,42	0
5	IOD	A	617	1/1	0.98	0.06	77,77,77,77	1
5	IOD	A	619	1/1	0.98	0.08	61,61,61,61	1
7	SCN	A	626	3/3	0.98	0.06	32,32,37,47	3
3	CA	A	602	1/1	0.98	0.08	36,36,36,36	0
5	IOD	A	610	1/1	0.99	0.08	50,50,50,50	0
5	IOD	A	608	1/1	0.99	0.07	54,54,54,54	1
7	SCN	A	624	3/3	0.99	0.18	35,35,43,53	3
7	SCN	A	625	3/3	0.99	0.08	31,31,33,35	3
5	IOD	A	634	1/1	0.99	0.05	51,51,51,51	1
5	IOD	A	612	1/1	0.99	0.06	53,53,53,53	1
5	IOD	A	611	1/1	0.99	0.05	57,57,57,57	1
5	IOD	A	615	1/1	0.99	0.05	74,74,74,74	1
5	IOD	A	620	1/1	0.99	0.05	88,88,88,88	1
7	SCN	A	628	3/3	0.99	0.08	23,23,24,24	3
7	SCN	A	629	3/3	0.99	0.15	35,35,36,48	3
5	IOD	A	614	1/1	0.99	0.04	49,49,49,49	1
5	IOD	A	618	1/1	0.99	0.11	42,42,42,42	1
5	IOD	A	609	1/1	1.00	0.07	38,38,38,38	0

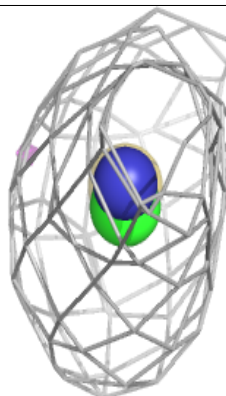
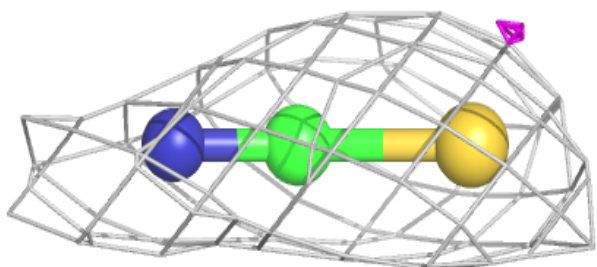
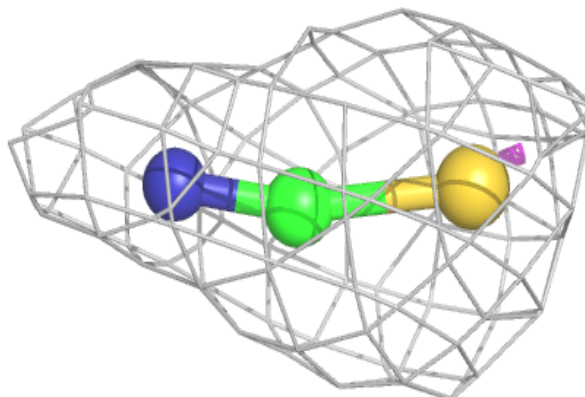
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OSM 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)

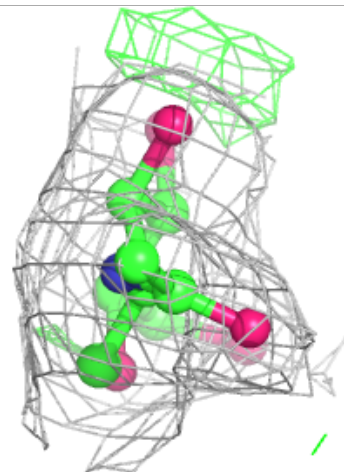
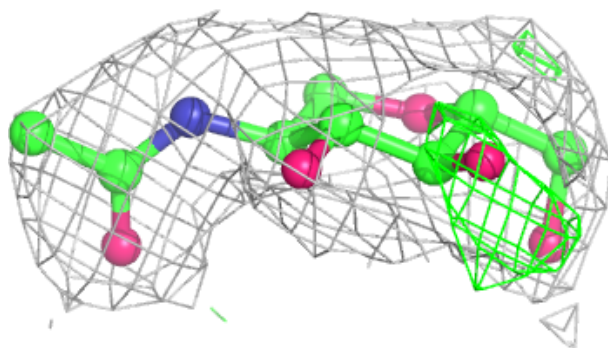
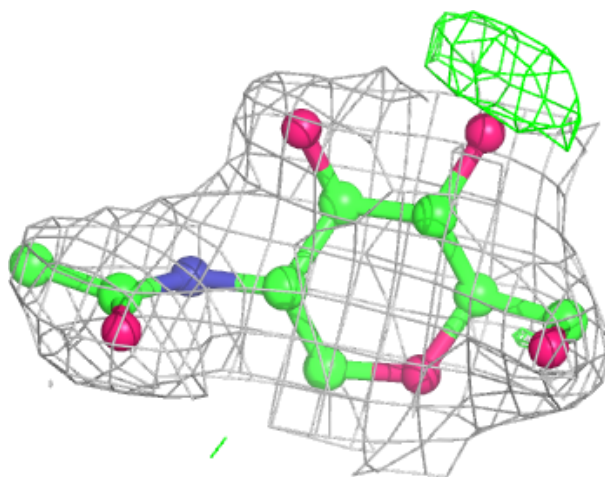
**Electron density around SCN A 630:**

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



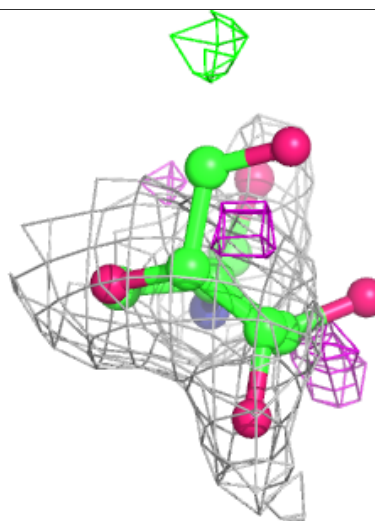
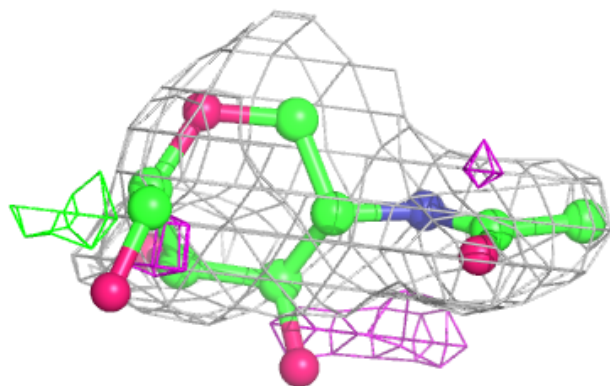
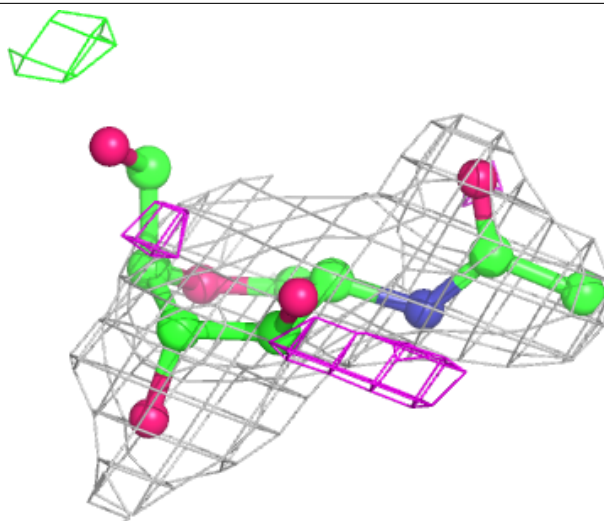
Electron density around NAG A 605:

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



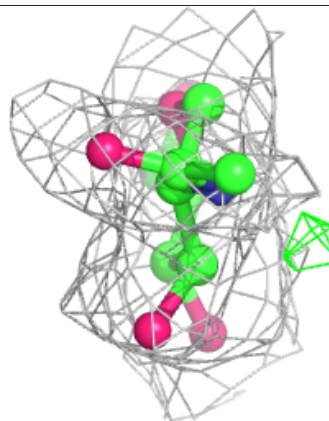
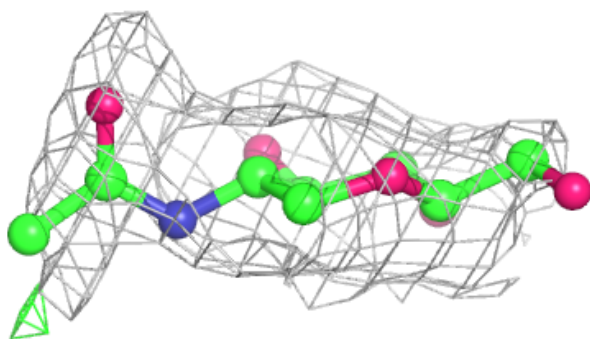
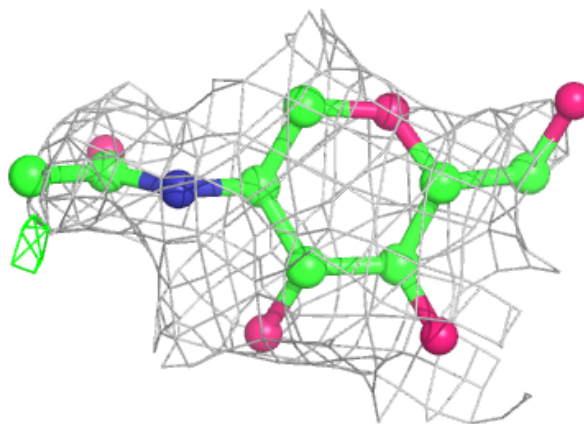
Electron density around NAG A 604:

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



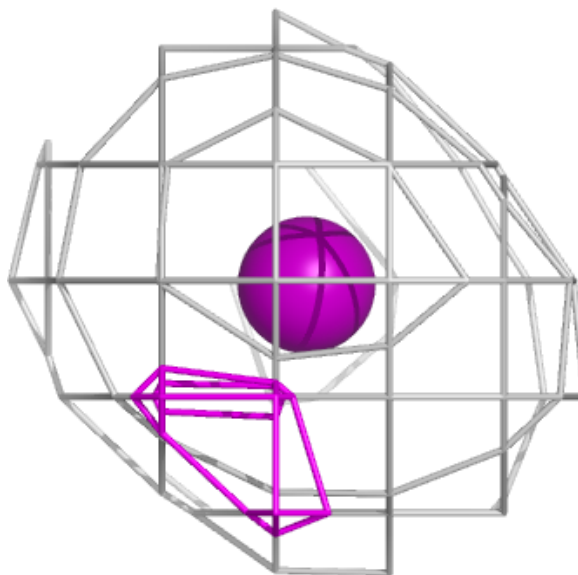
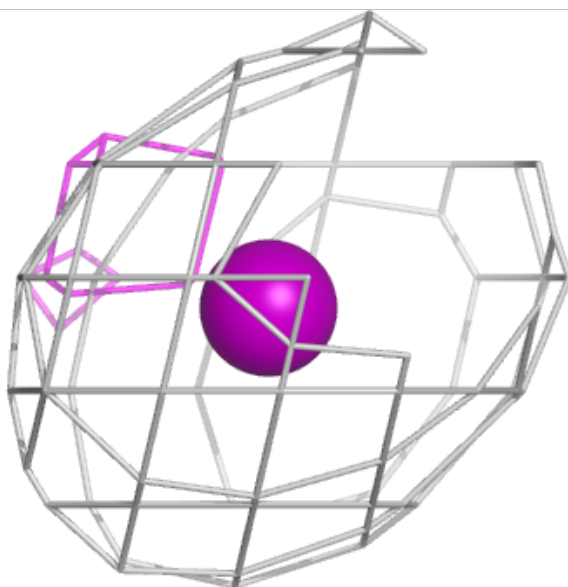
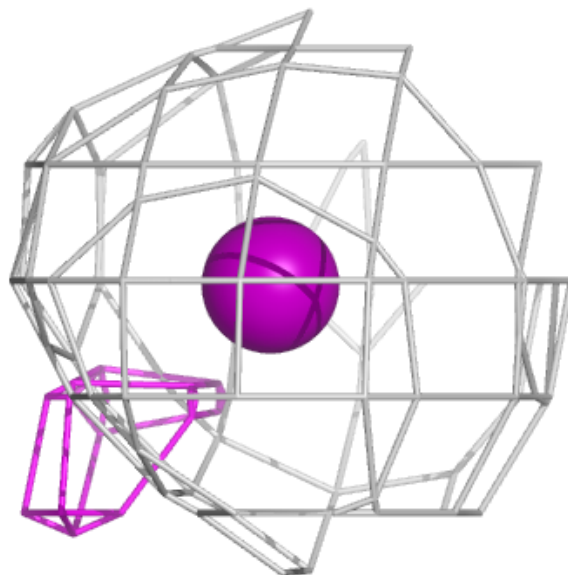
Electron density around NAG A 606:

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



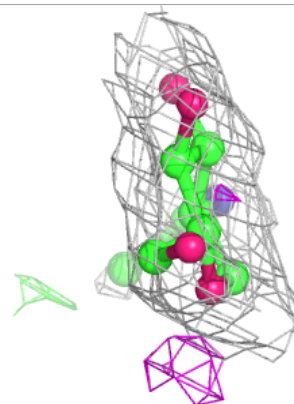
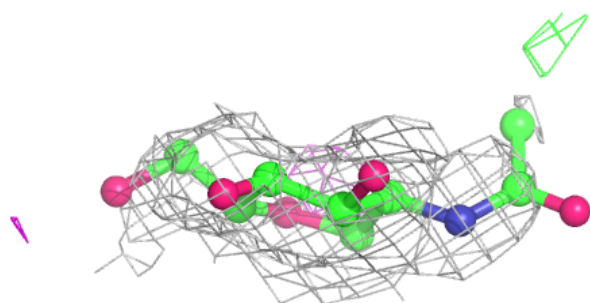
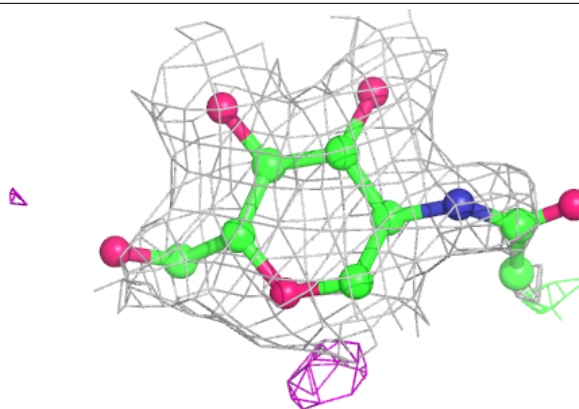
Electron density around IOD A 621:

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

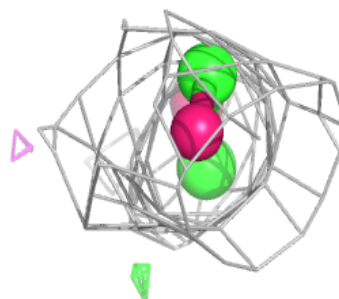
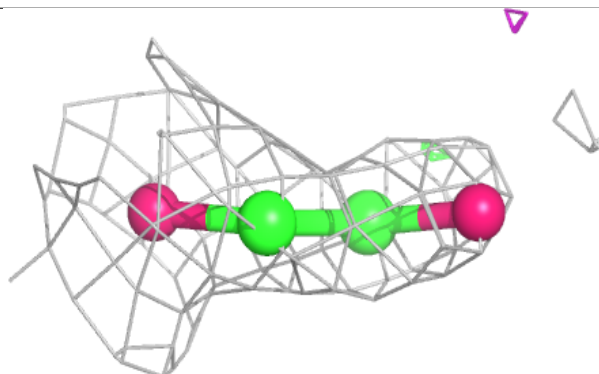
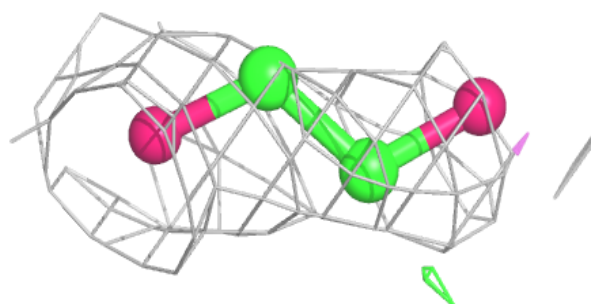


Electron density around NAG A 607:

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

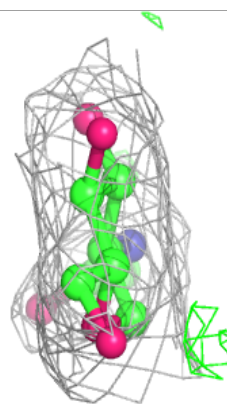
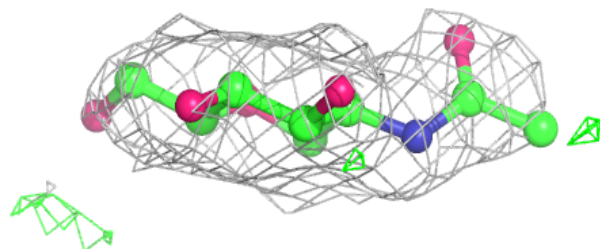
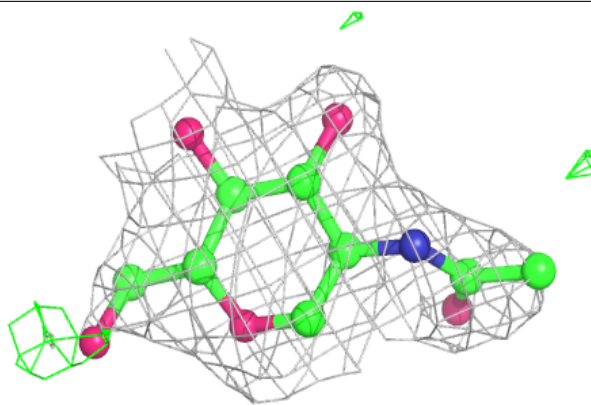
**Electron density around EDO A 623:**

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



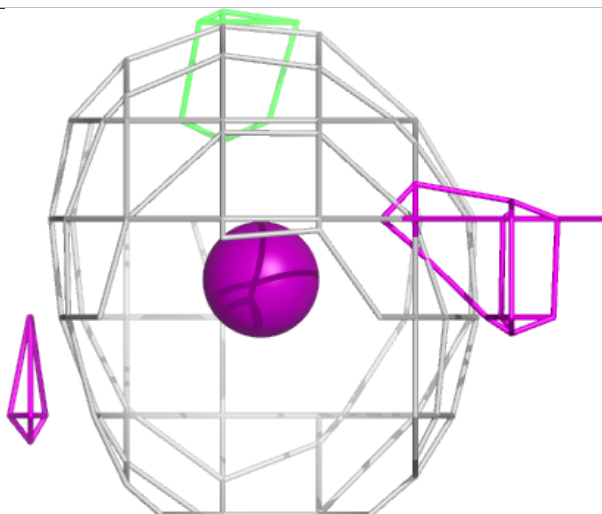
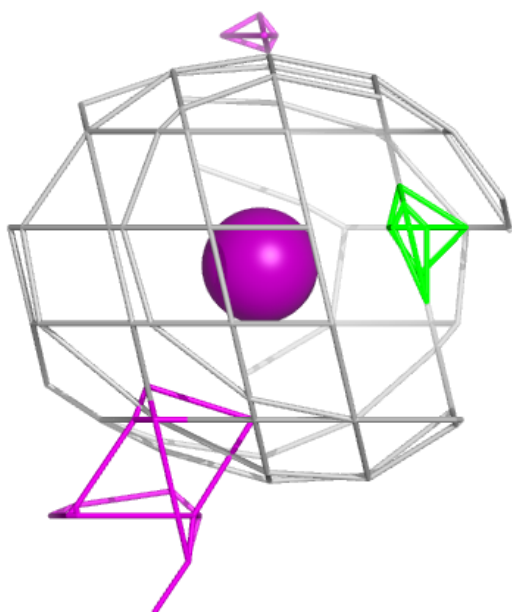
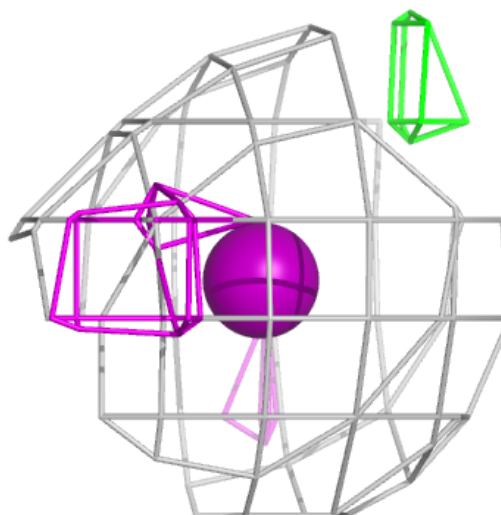
Electron density around NAG A 603:

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



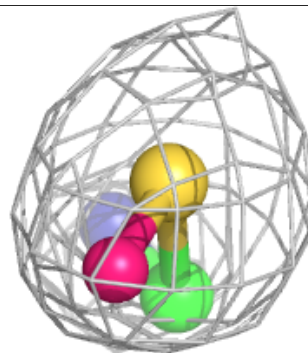
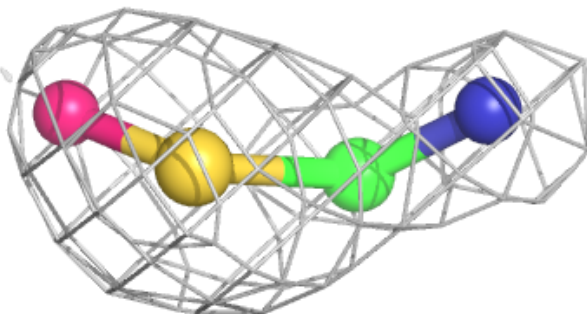
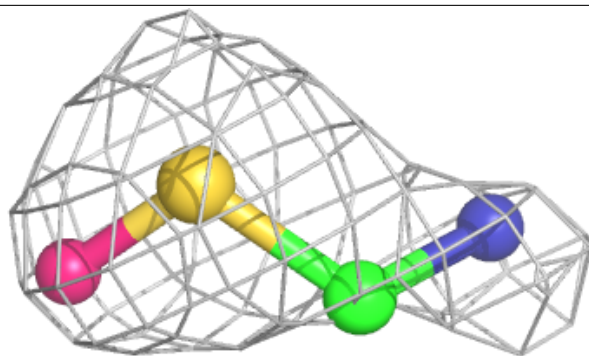
Electron density around IOD A 622:

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



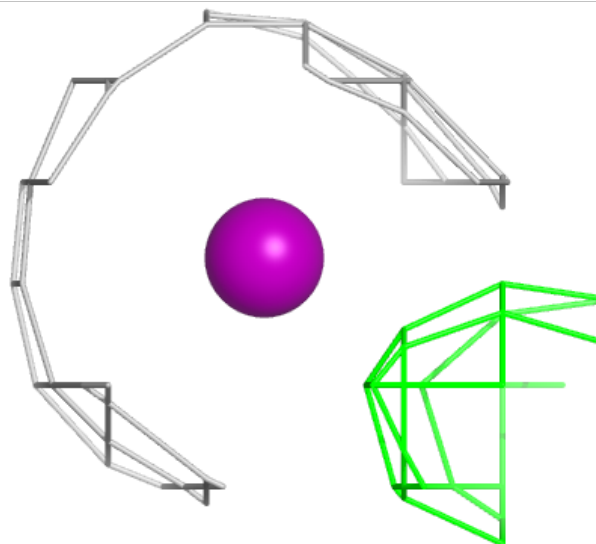
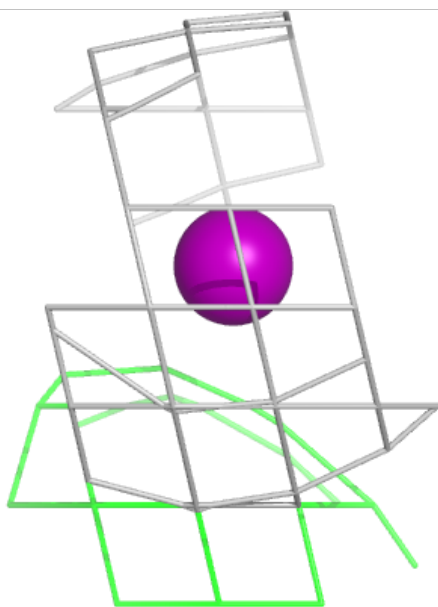
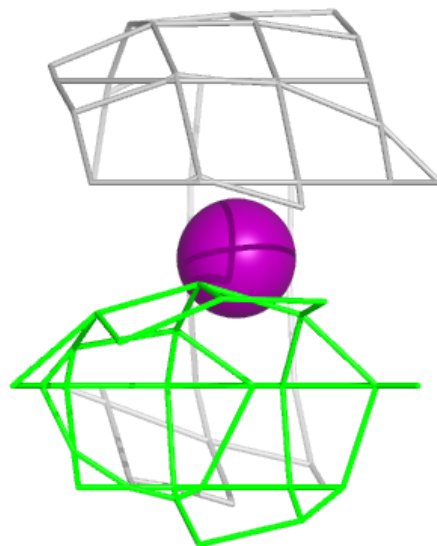
Electron density around OSM A 633:

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



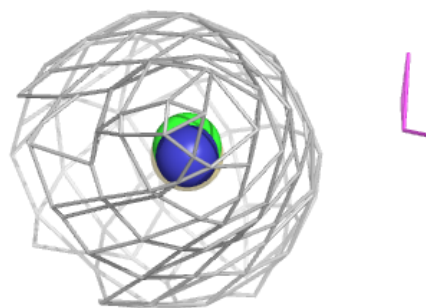
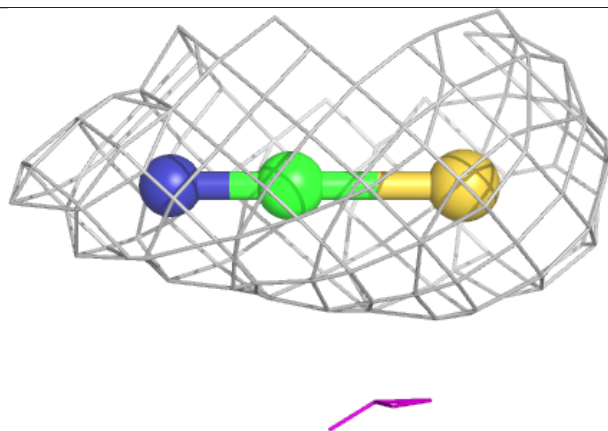
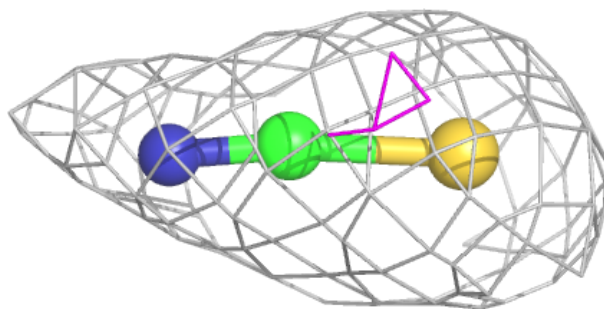
Electron density around IOD A 613:

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



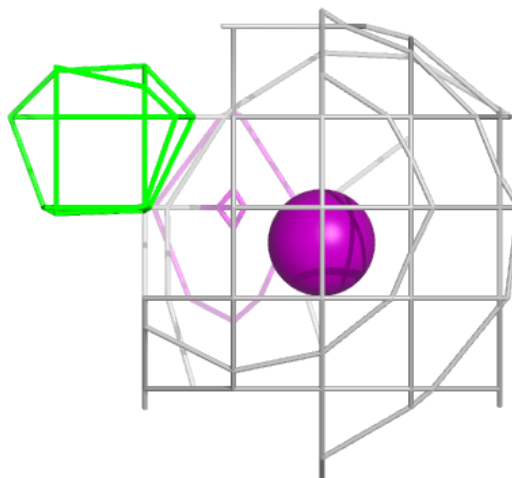
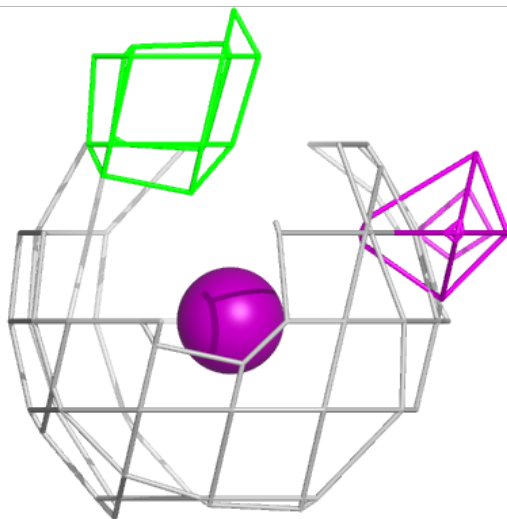
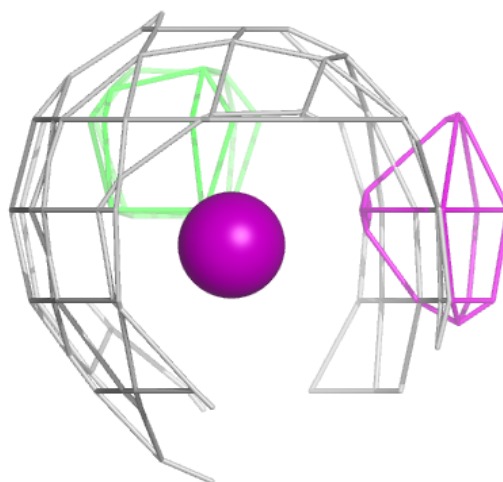
Electron density around SCN A 627:

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



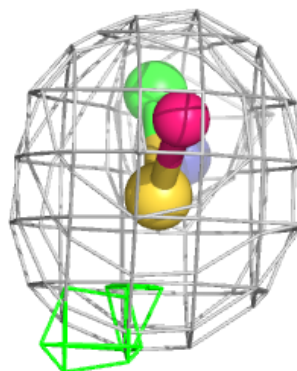
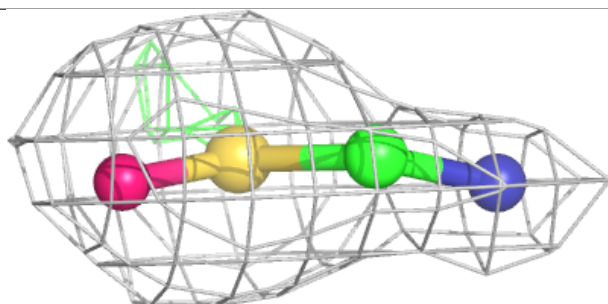
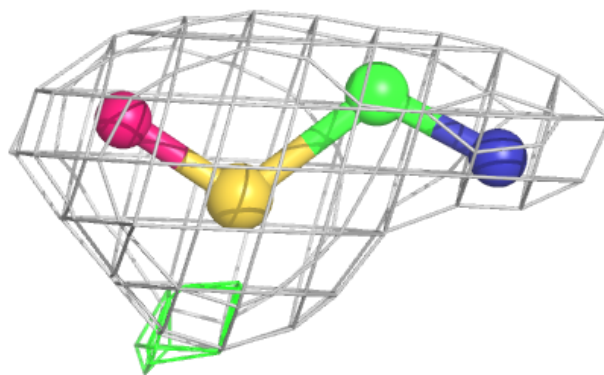
Electron density around IOD A 616:

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



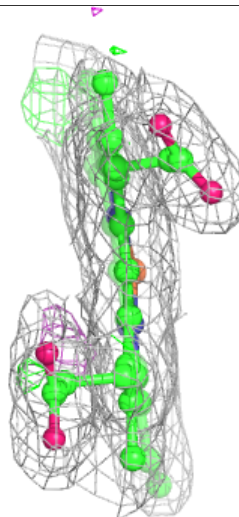
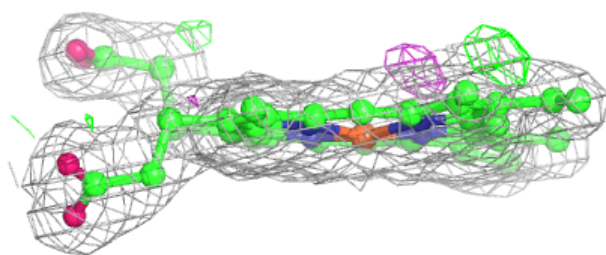
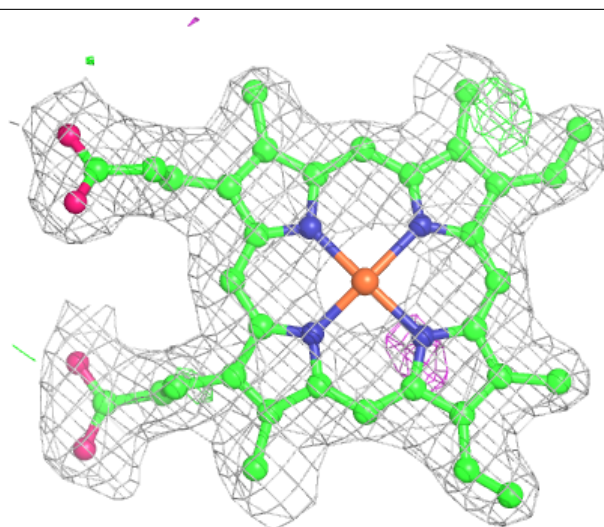
Electron density around OSM A 632:

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



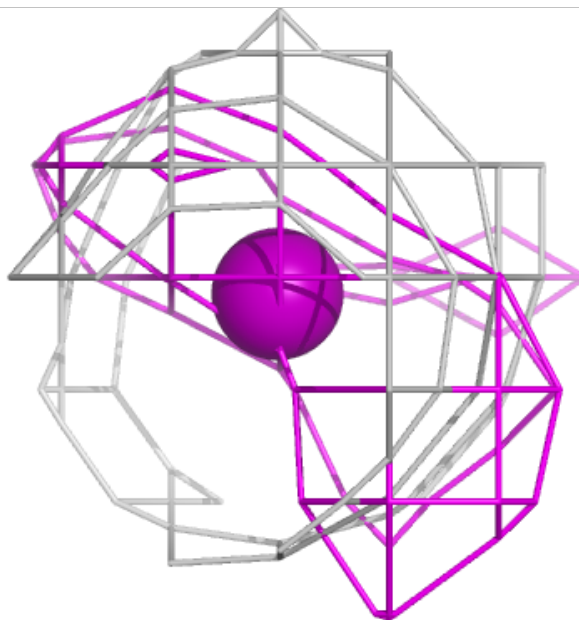
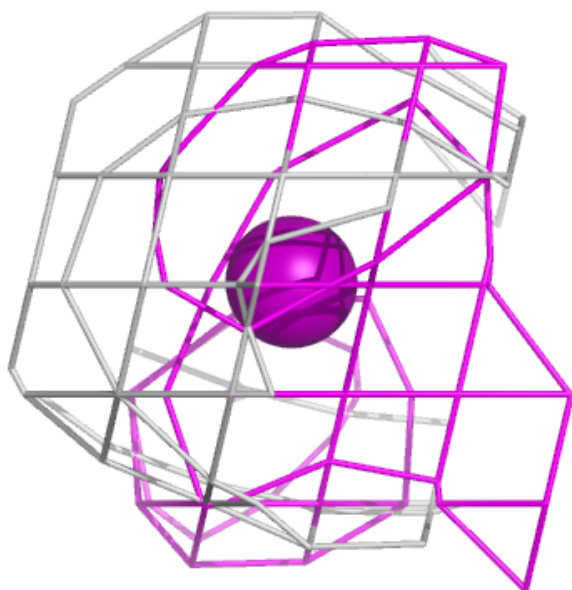
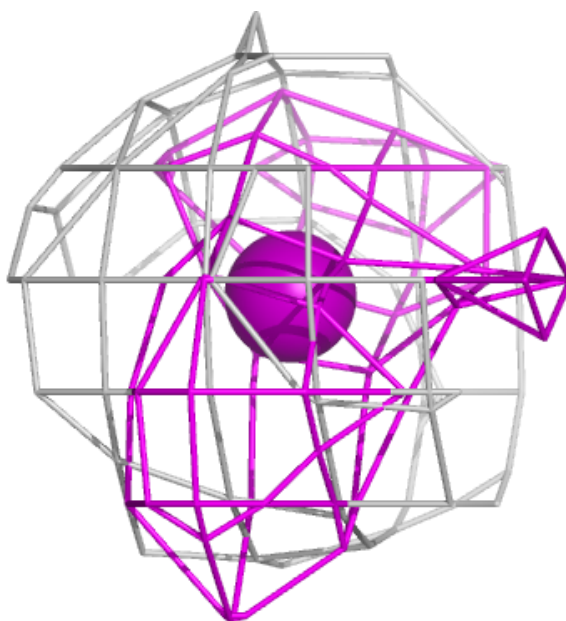
Electron density around HEM A 601:

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



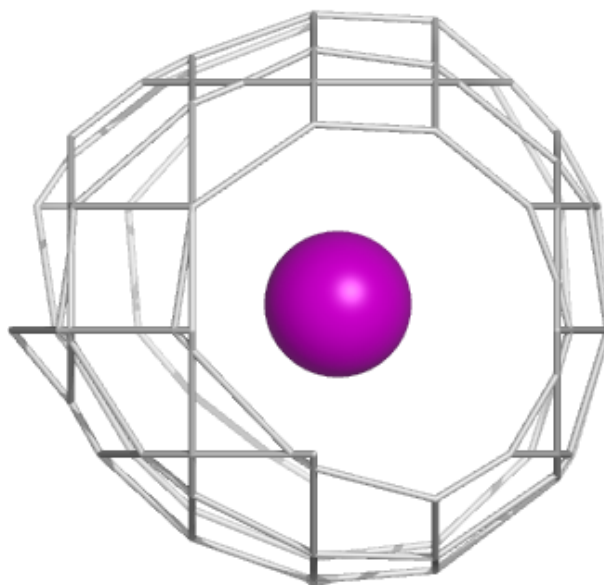
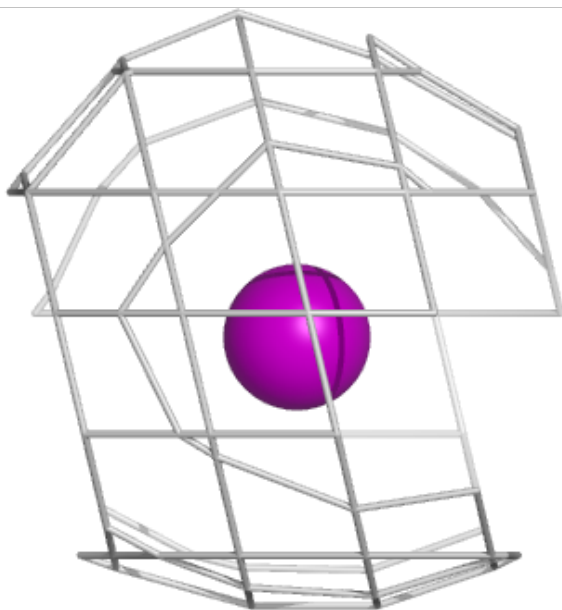
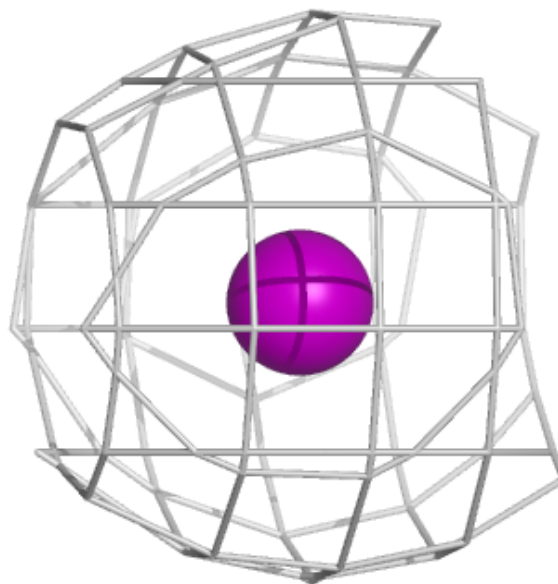
Electron density around IOD A 617:

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



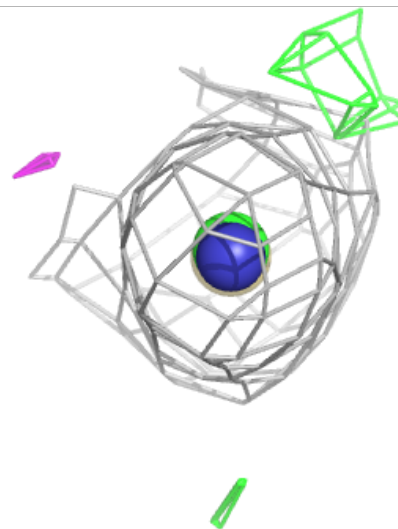
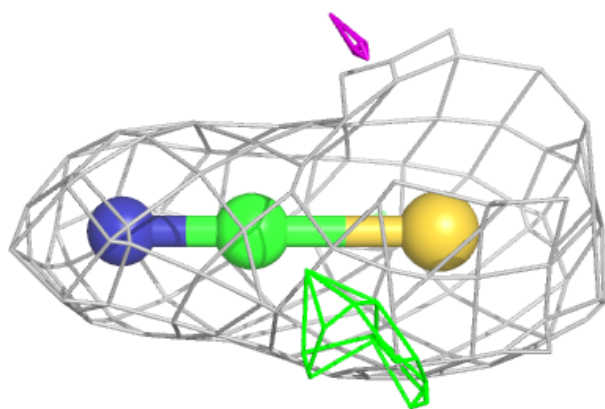
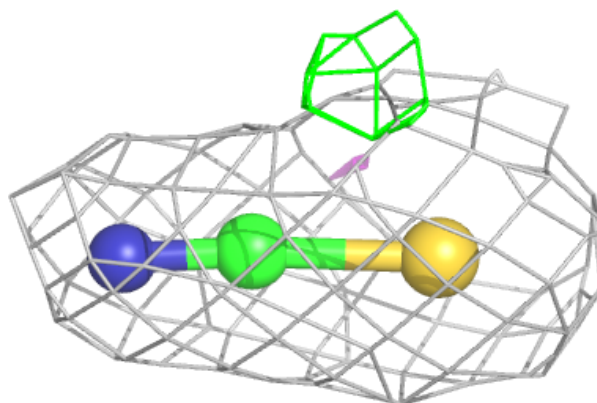
Electron density around IOD A 619:

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



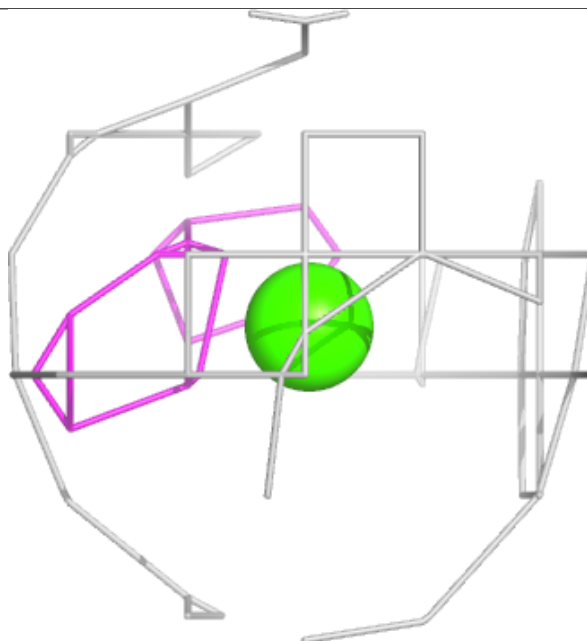
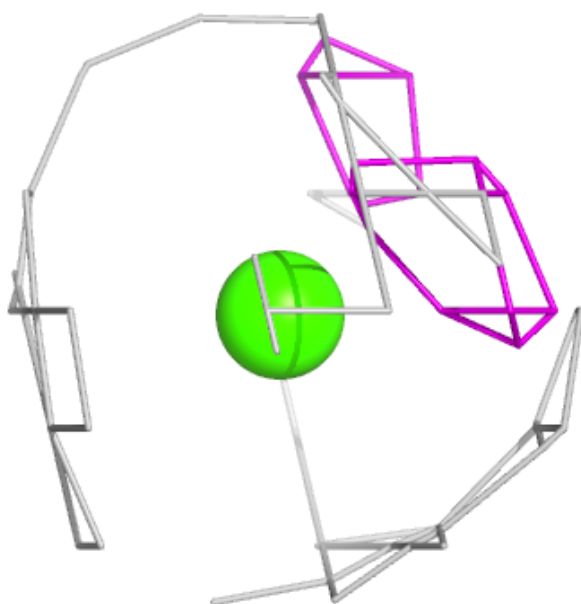
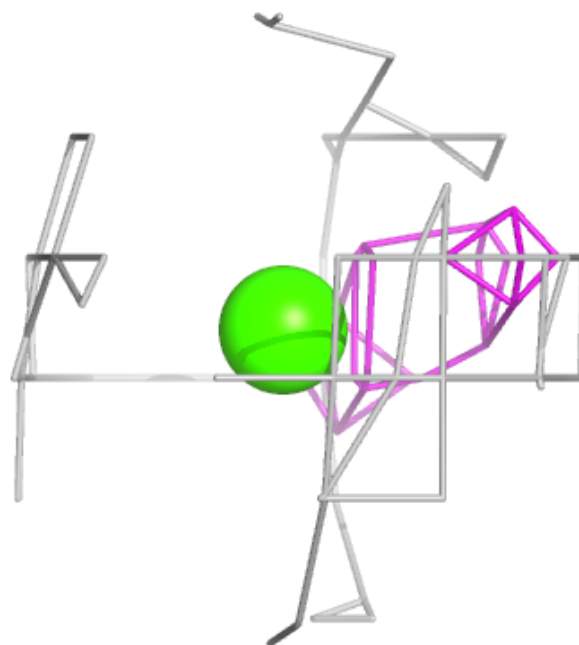
Electron density around SCN A 626:

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



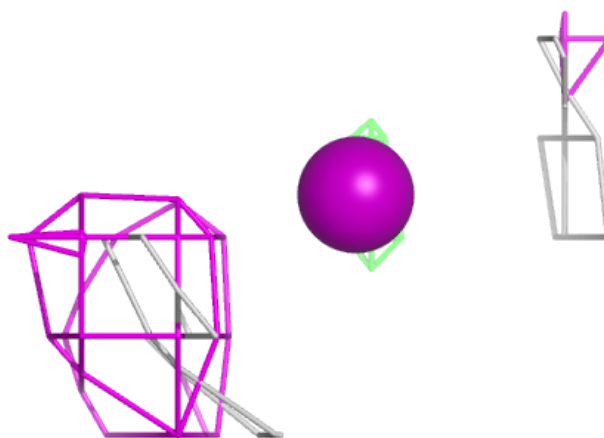
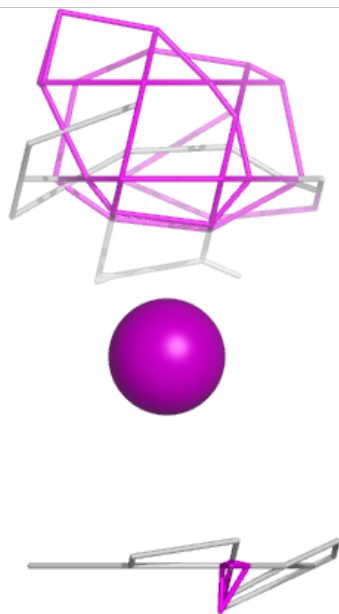
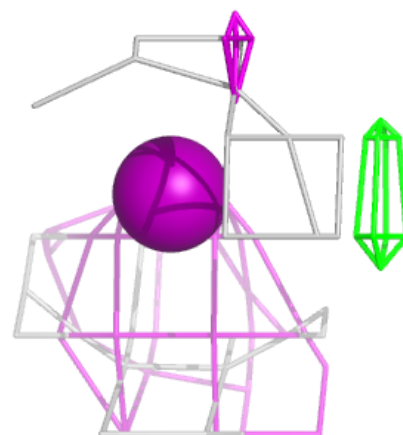
Electron density around CA A 602:

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



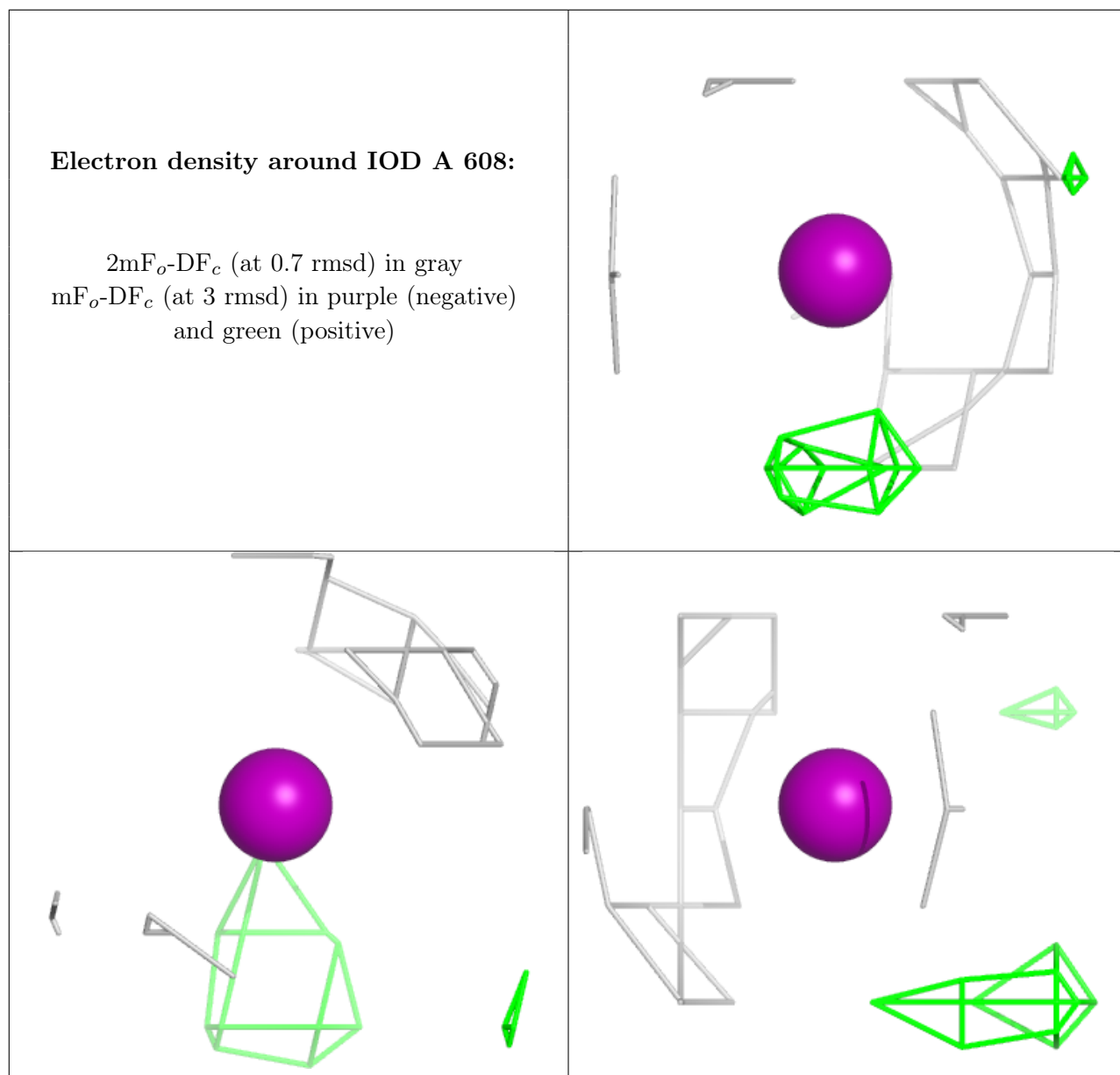
Electron density around IOD A 610:

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



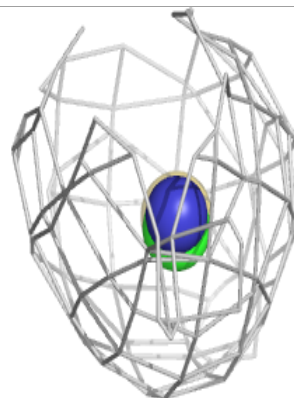
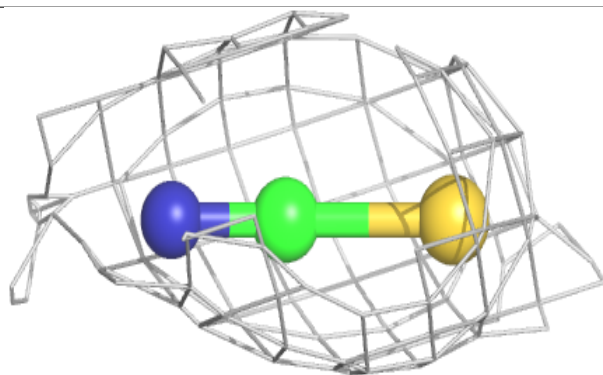
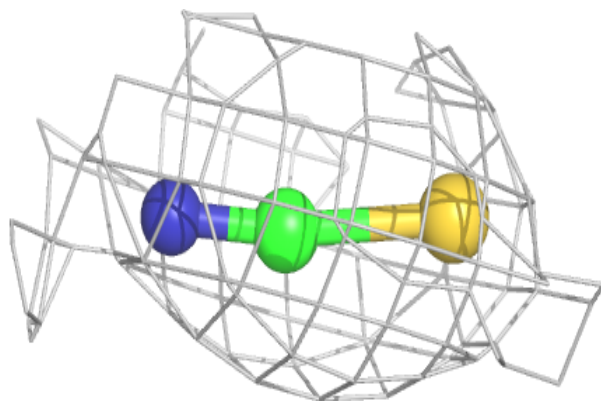
Electron density around IOD A 608:

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

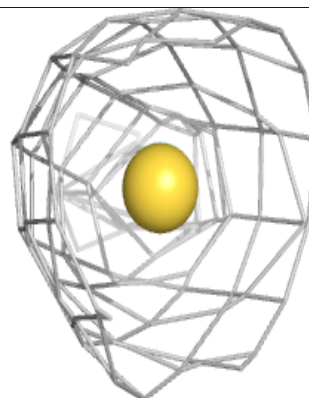
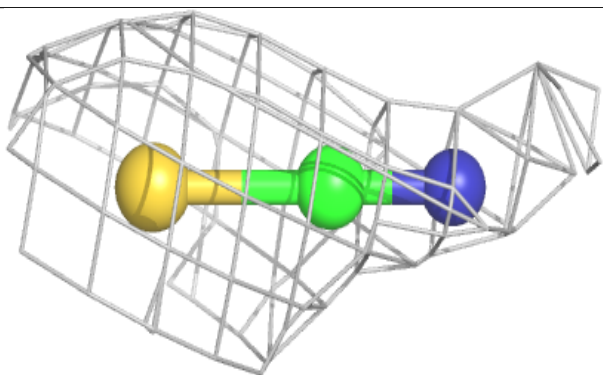
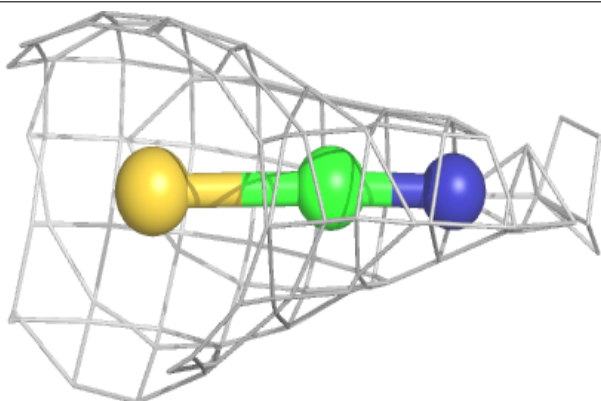


Electron density around SCN A 624:

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

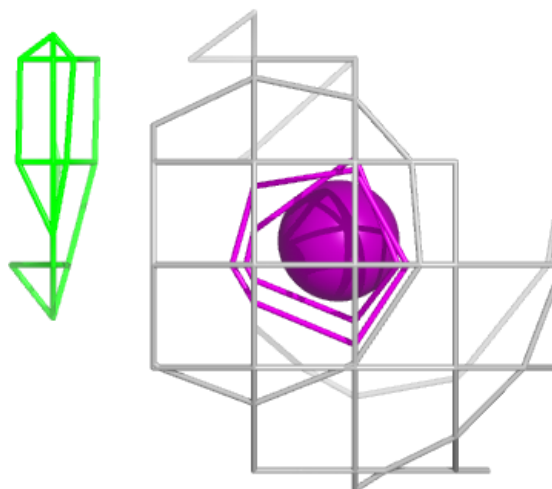
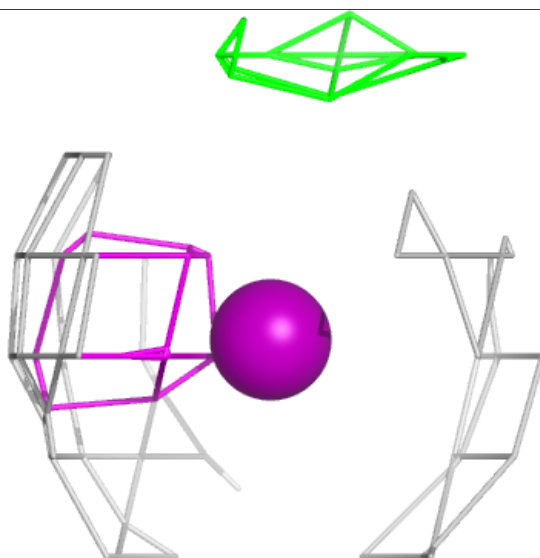
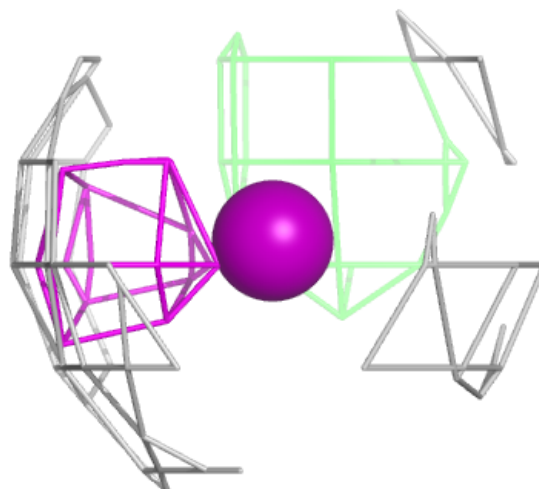
**Electron density around SCN A 625:**

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



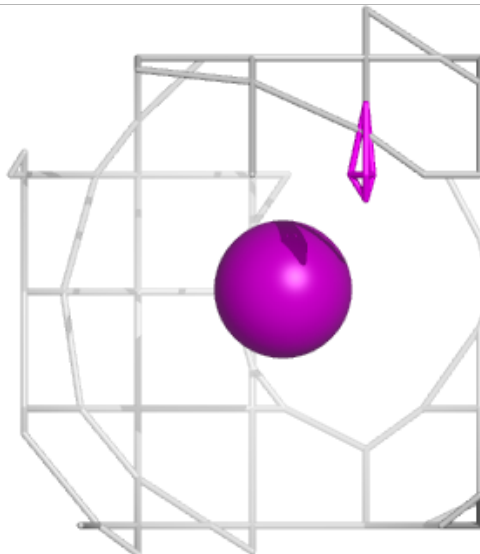
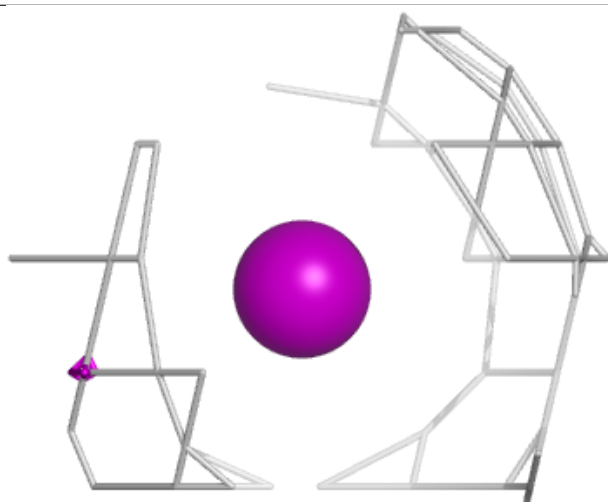
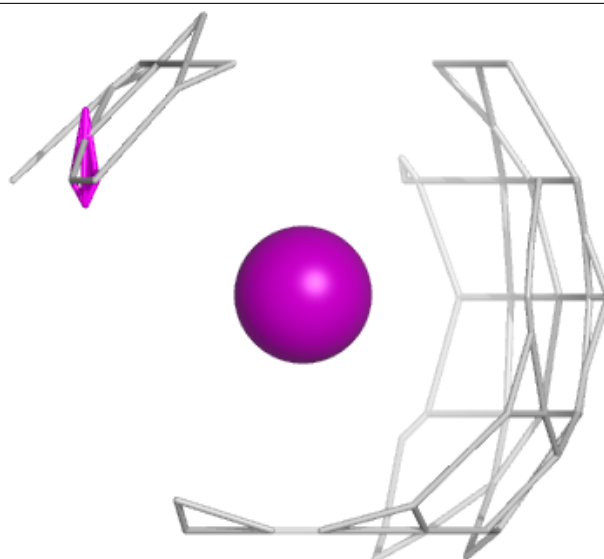
Electron density around IOD A 634:

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



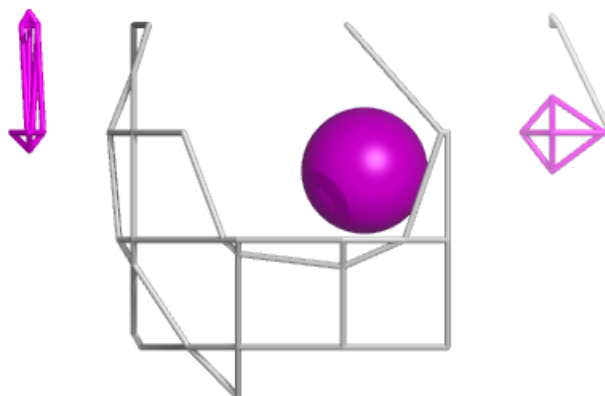
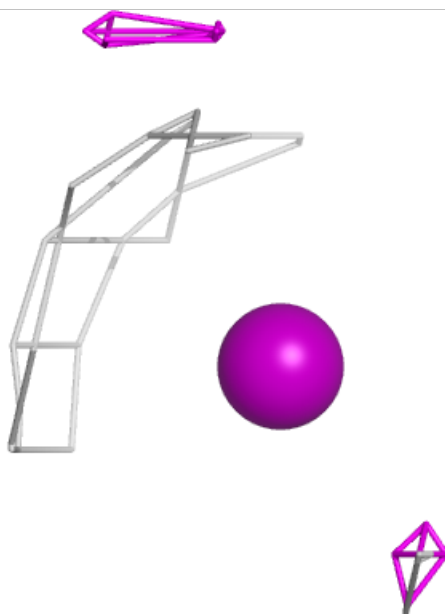
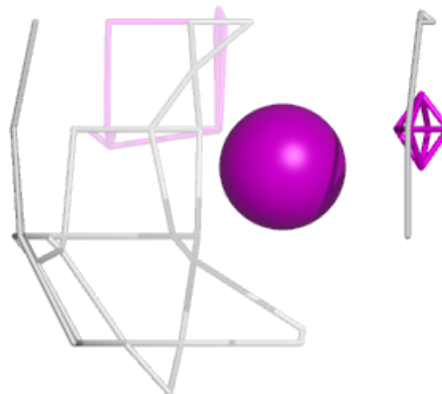
Electron density around IOD A 612:

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



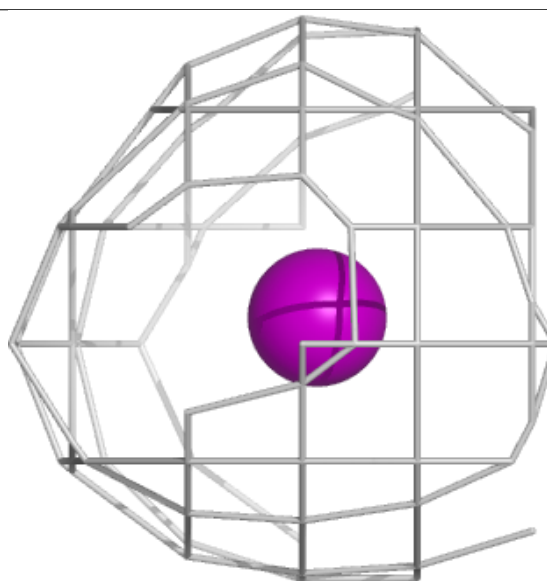
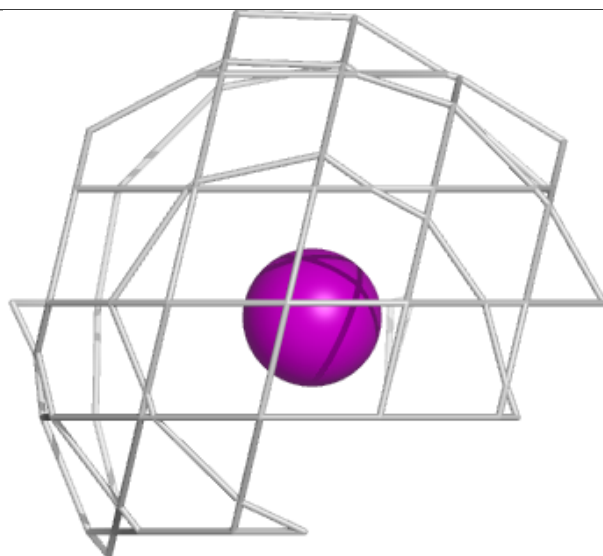
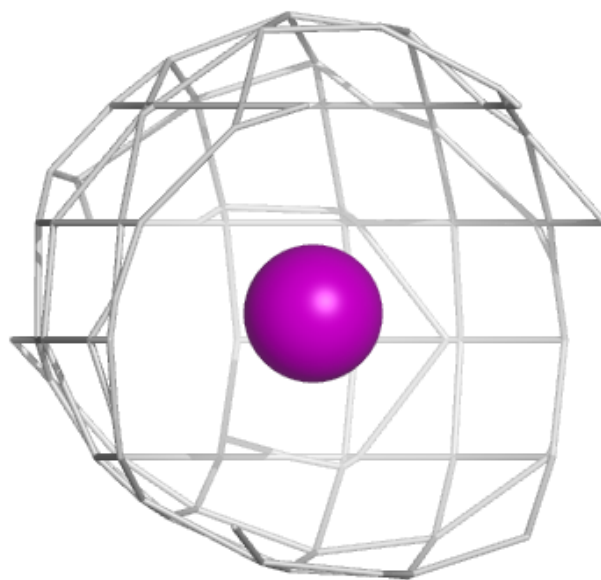
Electron density around IOD A 611:

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



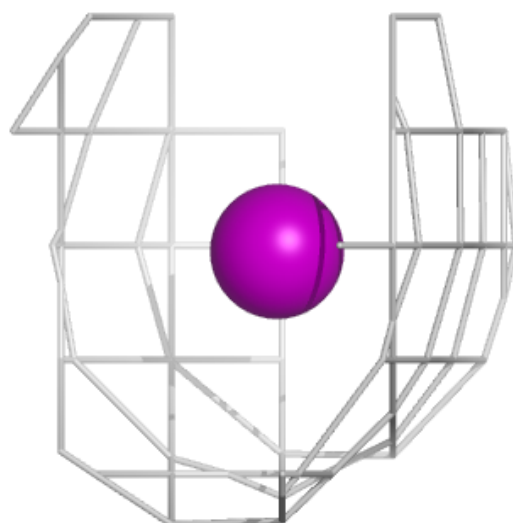
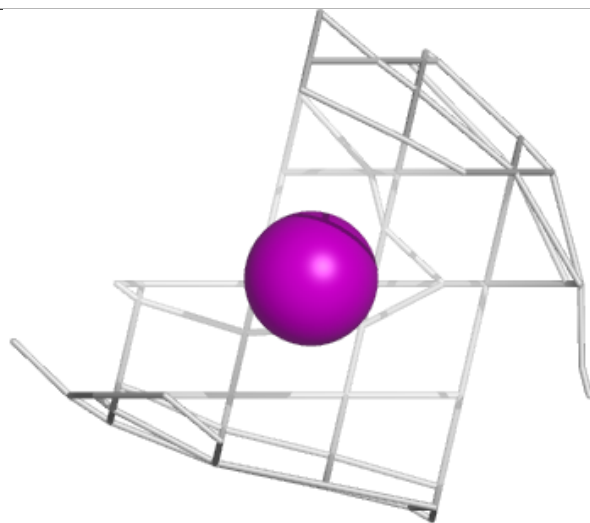
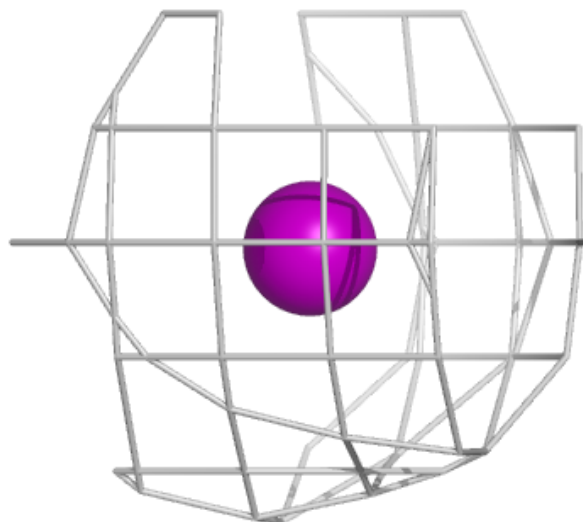
Electron density around IOD A 615:

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



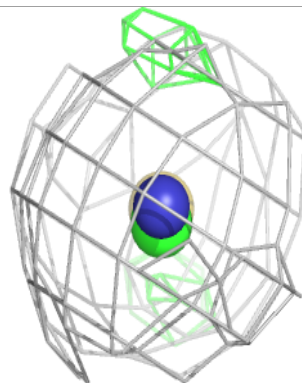
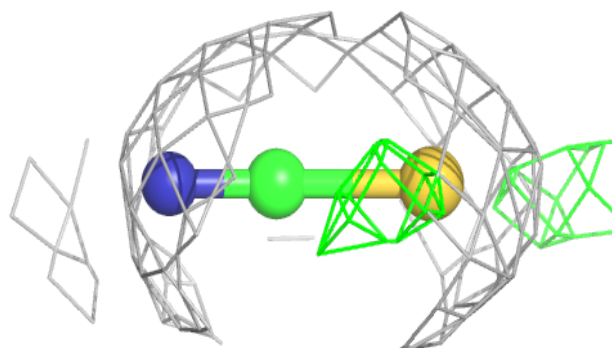
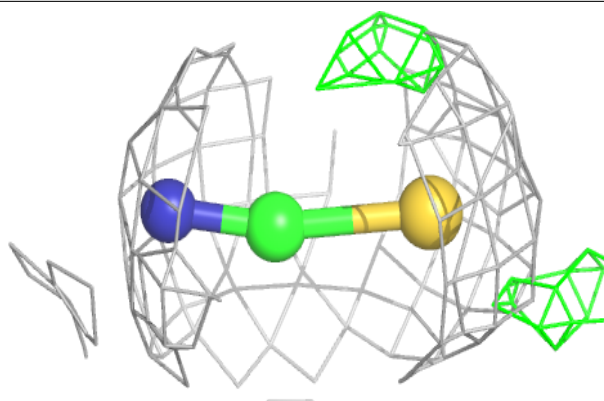
Electron density around IOD A 620:

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

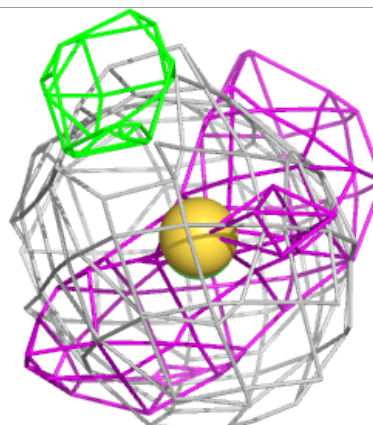
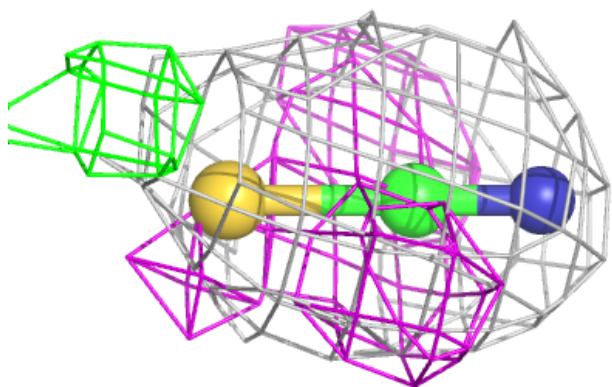
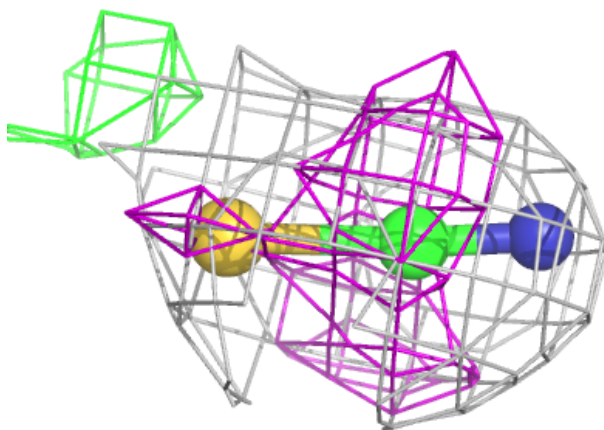


Electron density around SCN A 628:

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

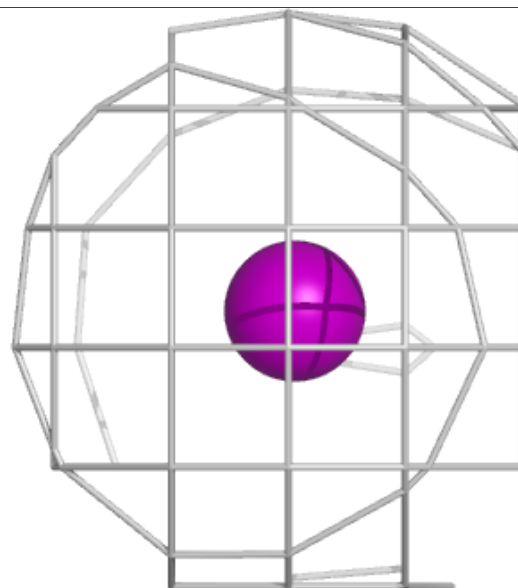
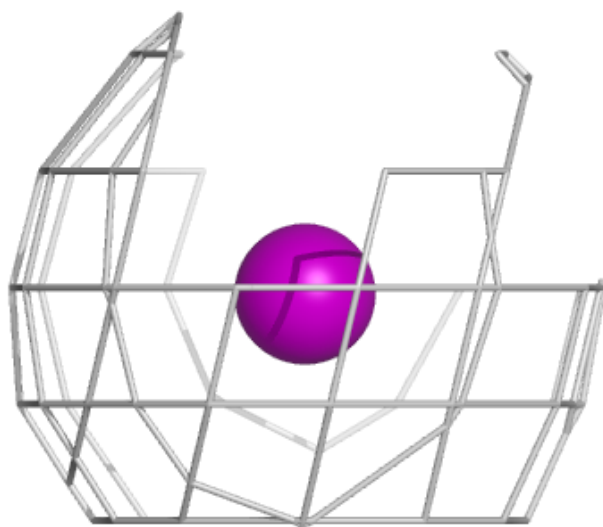
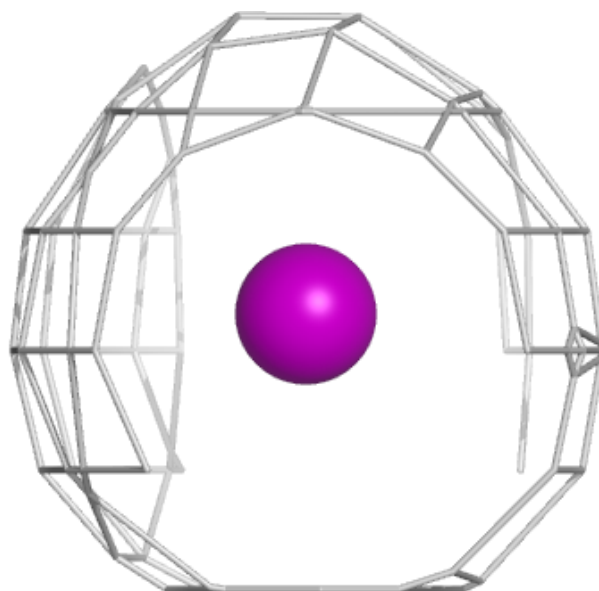
**Electron density around SCN A 629:**

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



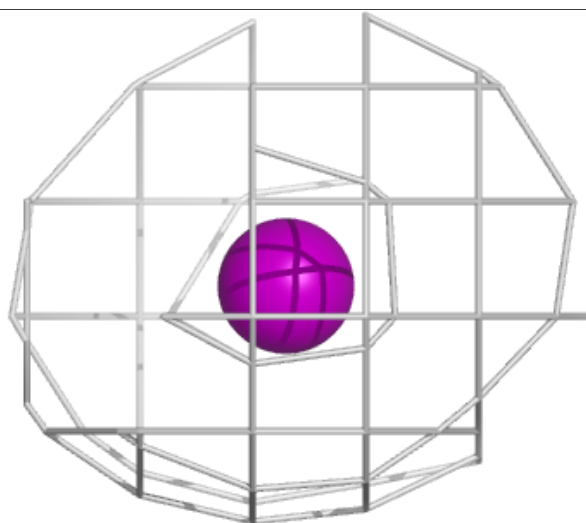
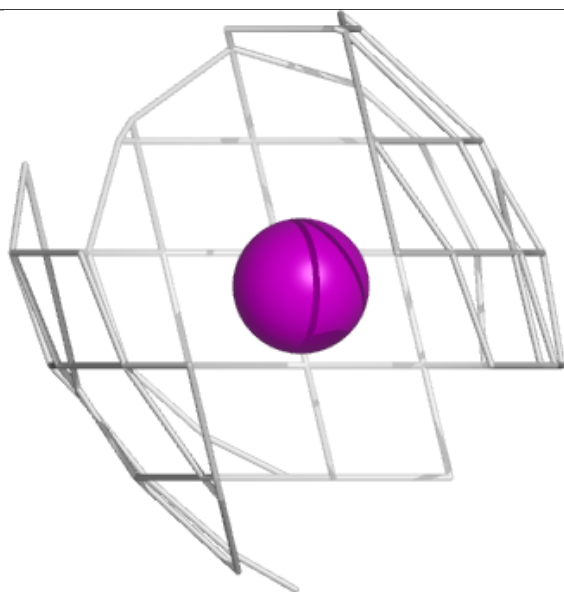
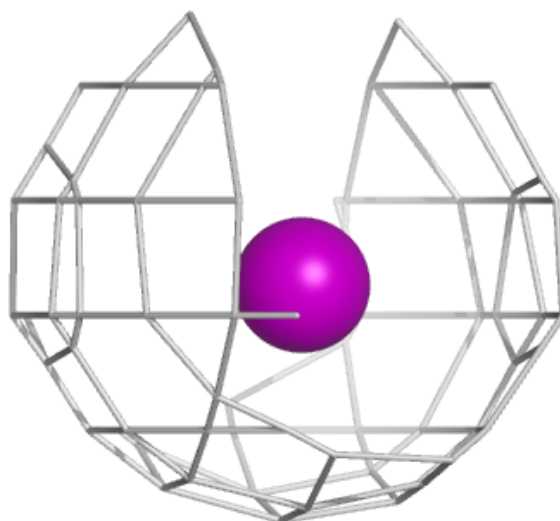
Electron density around IOD A 614:

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



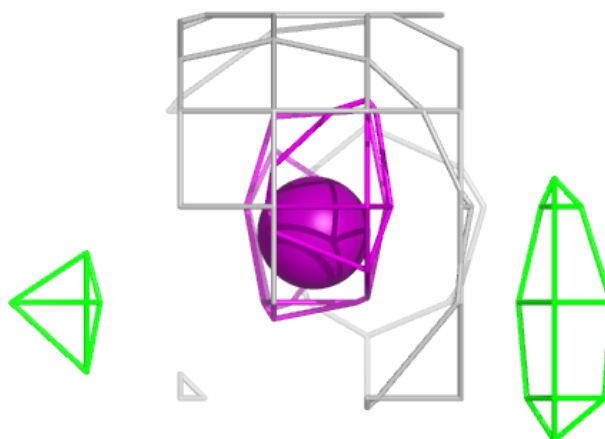
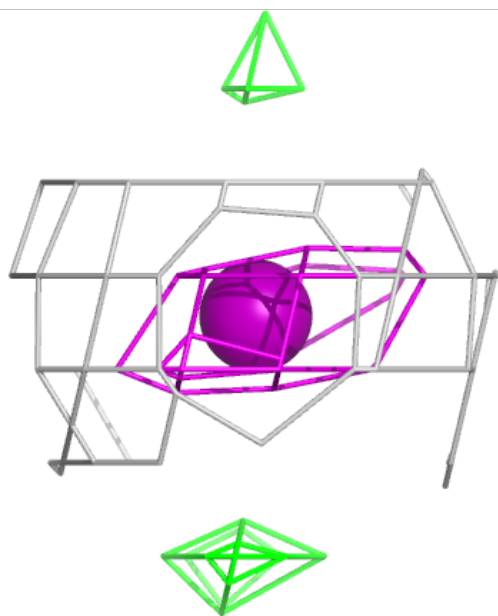
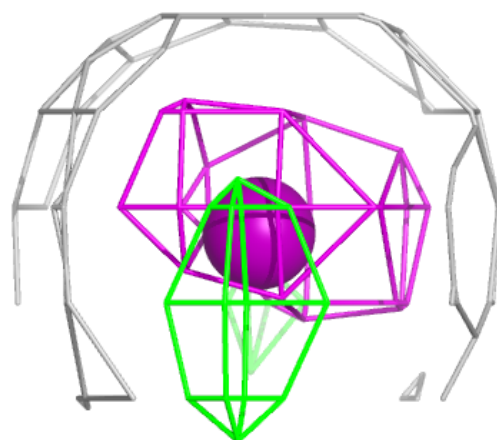
Electron density around IOD A 618:

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



Electron density around IOD A 609:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.