Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:34 PM JST

PDB ID	:	6LF7 / pdb_00006lf7
Title	:	Crystal structure of the complex of goat lactoperoxidase with hypothiocyanite and hydrogen peroxide at 1.79 A resolution.
Authors	:	Viswanathan, V.; Tyagi, T.K.; Singh, R.P.; Singh, A.K.; Singh, A.; Bhushan, A.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2019-11-30
Resolution	:	1.79 Å(reported)

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

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

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

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

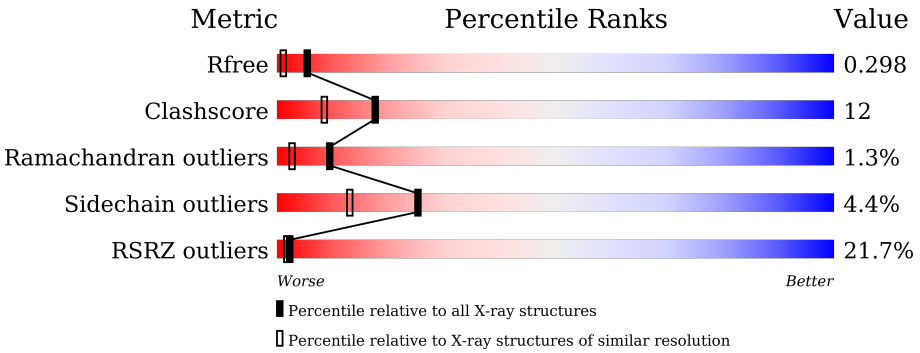
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.79 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	595	22% 80% 17%

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
10	GOL	A	638	-	-	X	-
7	PEO	A	618	-	-	X	-
8	OSM	A	622[A]	-	-	X	-
8	OSM	A	622[B]	-	-	X	-
8	OSM	A	625	-	-	X	-
8	OSM	A	626	-	-	X	-
8	OSM	A	628	-	-	X	-
9	SCN	A	631	-	-	X	-
9	SCN	A	632	-	-	X	-
9	SCN	A	633	-	-	X	-

2 Entry composition

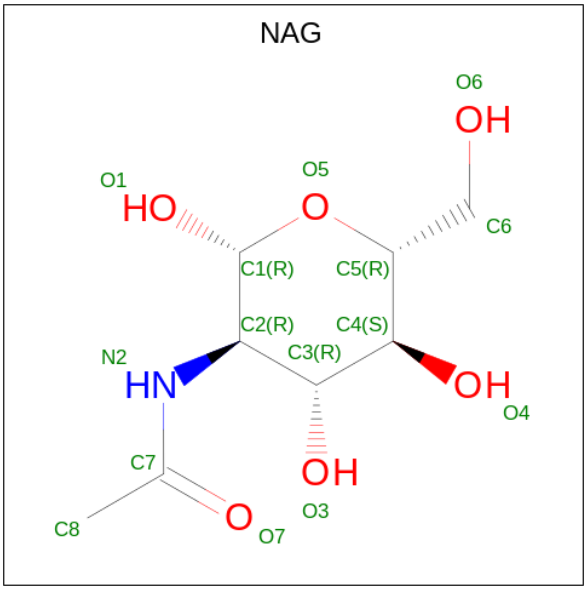
There are 11 unique types of molecules in this entry. The entry contains 5467 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

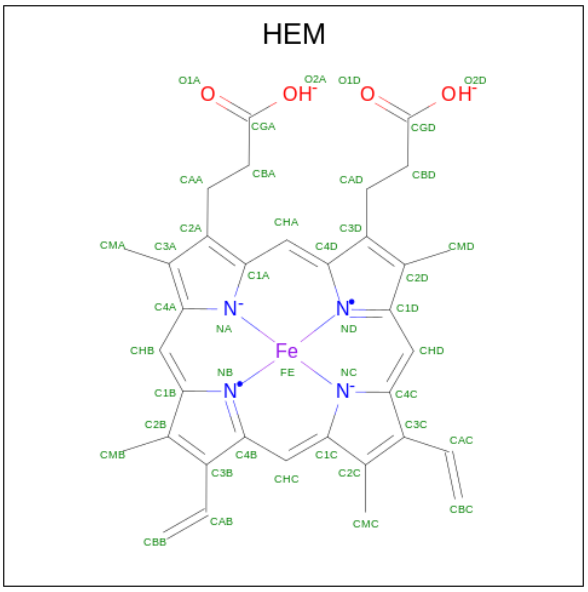
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	595	4800	3057	852	862	29	0	8	0

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



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

- Molecule 3 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
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

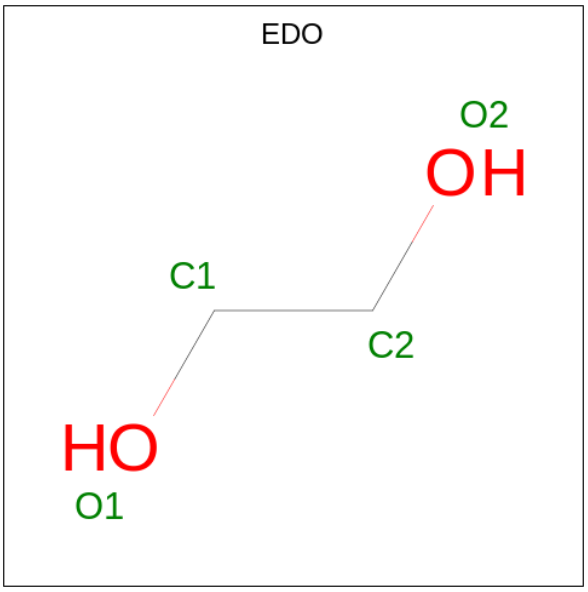
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

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

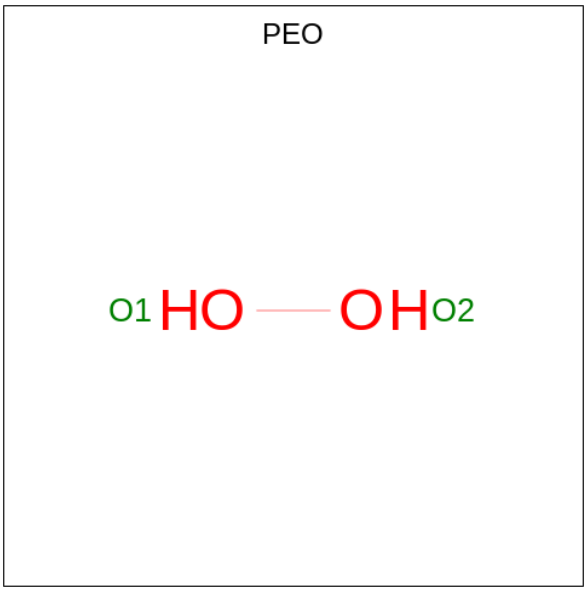
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	I	0	0
			12	12		

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



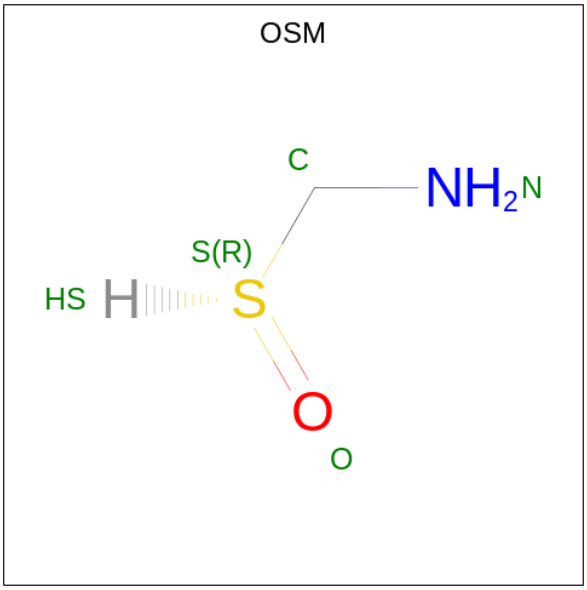
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0

- Molecule 7 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H_2O_2) (labeled as "Ligand of Interest" by depositor).



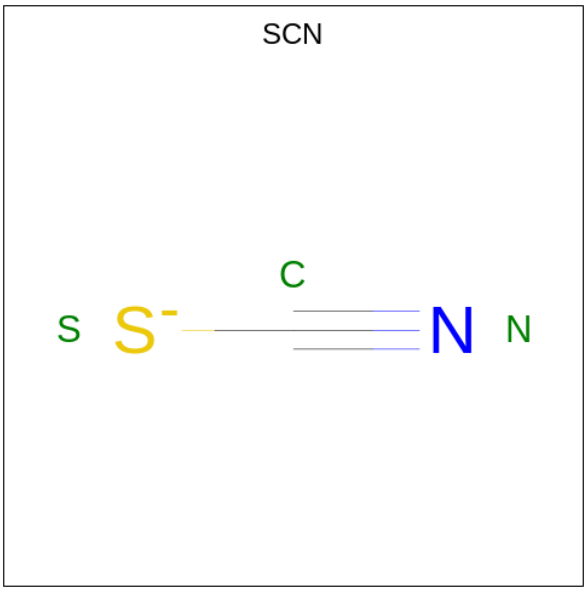
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 2 2	0	0

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



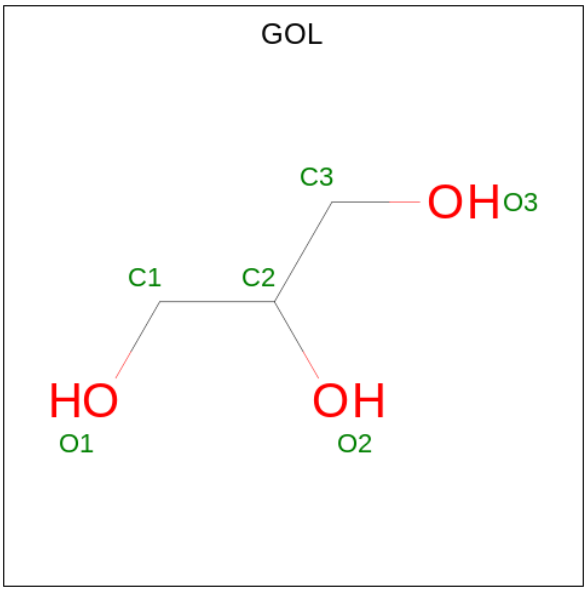
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O S 8 2 2 2 2	0	1
8	A	1	Total C N O S 4 1 1 1 1	0	0
8	A	1	Total C N O S 4 1 1 1 1	0	0
8	A	1	Total C N O S 4 1 1 1 1	0	0
8	A	1	Total C N O S 4 1 1 1 1	0	0
8	A	1	Total C N O S 4 1 1 1 1	0	0
8	A	1	Total C N O S 4 1 1 1 1	0	0
8	A	1	Total C N O S 4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

- Molecule 9 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is water.

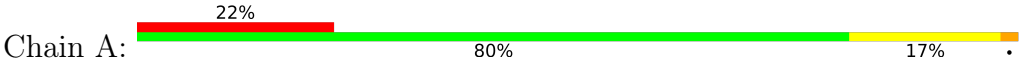
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	488	Total	O	0	0
			488	488		

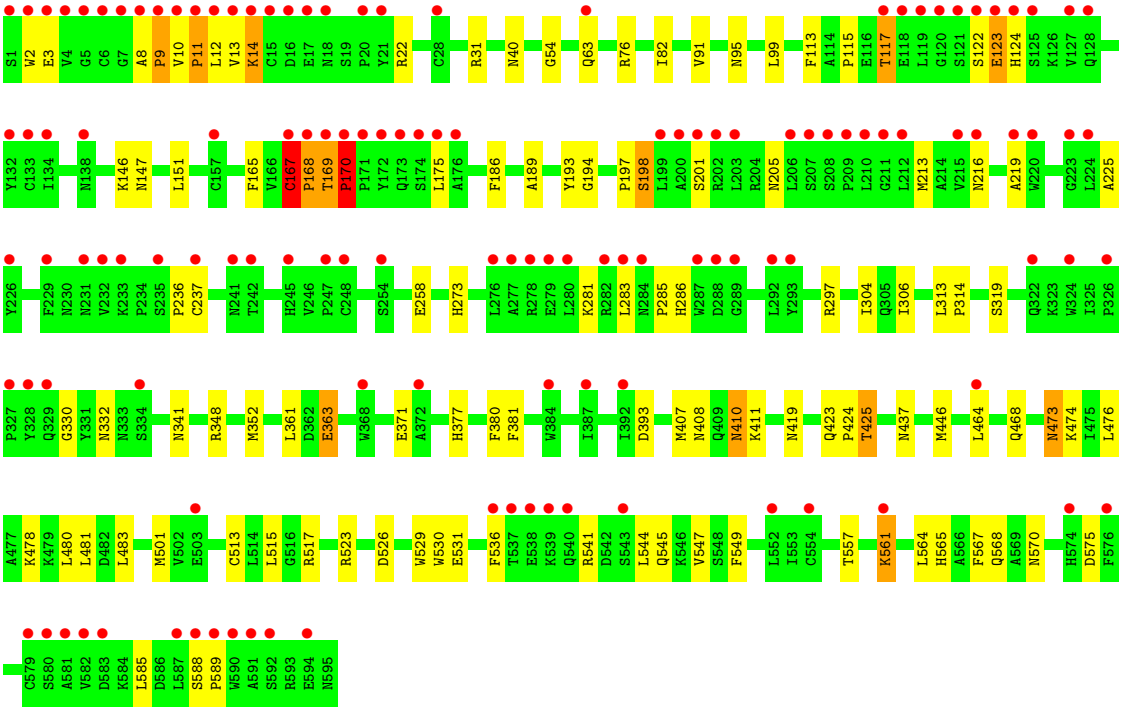
3 Residue-property plots (i)

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

- Molecule 1: Lactoperoxidase

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.88Å 80.73Å 75.14Å 90.00° 101.53° 90.00°	Depositor
Resolution (Å)	27.21 – 1.79 27.21 – 1.79	Depositor EDS
% Data completeness (in resolution range)	96.4 (27.21-1.79) 96.4 (27.21-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.23 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.231 , 0.297 0.237 , 0.298	Depositor DCC
R_{free} test set	2871 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5467	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.03	1/4953 (0.0%)	1.33	4/6721 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	PHE	C-O	6.51	1.32	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	330	GLY	CA-C-O	-5.35	118.54	122.23
1	A	170	PRO	N-CA-CB	-5.32	97.92	103.08
1	A	515	LEU	N-CA-C	-5.17	105.73	111.36
1	A	194	GLY	CA-C-O	-5.14	118.68	122.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	CYS	Peptide
1	A	169	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4800	0	4733	109	0
2	A	42	0	39	3	0
3	A	43	0	30	7	0
4	A	1	0	0	0	0
5	A	12	0	0	5	0
6	A	16	0	23	5	0
7	A	2	0	0	2	0
8	A	36	0	45	16	0
9	A	21	0	0	10	0
10	A	6	0	8	4	0
11	A	488	0	0	36	0
All	All	5467	0	4878	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (122) 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:258:GLU:OE2	3:A:604:HEM:CMB	1.66	1.44
1:A:446:MET:HE1	9:A:631:SCN:N	1.59	1.17
1:A:258:GLU:OE2	3:A:604:HEM:HMB1	0.86	1.04
1:A:198:SER:HB2	10:A:638:GOL:O2	1.70	0.89
6:A:637:EDO:H11	11:A:832:HOH:O	1.77	0.83
1:A:529:TRP:HE3	11:A:708:HOH:O	1.62	0.83
1:A:446:MET:CE	9:A:631:SCN:N	2.41	0.82
1:A:11:PRO:HA	11:A:748:HOH:O	1.78	0.81
1:A:526:ASP:HB3	11:A:708:HOH:O	1.82	0.80
1:A:258:GLU:HG3	8:A:622[A]:OSM:H2	1.67	0.75
8:A:629:OSM:N	11:A:707:HOH:O	2.19	0.75
7:A:618:PEO:O1	8:A:622[B]:OSM:O	2.05	0.75
5:A:614:IOD:I	11:A:1012:HOH:O	2.74	0.74
1:A:407:MET:HB3	1:A:501:MET:HE2	1.71	0.72
1:A:258:GLU:CD	3:A:604:HEM:CMB	2.61	0.72
1:A:258:GLU:CD	3:A:604:HEM:HMB1	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:HIS:HB3	8:A:626:OSM:H1	1.72	0.71
1:A:22:ARG:HD2	11:A:999:HOH:O	1.90	0.71
1:A:541:ARG:HH22	8:A:625:OSM:HS	1.38	0.71
1:A:219:ALA:HB2	8:A:628:OSM:N	2.06	0.71
1:A:567:PHE:H	8:A:626:OSM:HS	1.37	0.70
8:A:622[B]:OSM:H1	11:A:1083:HOH:O	1.90	0.70
1:A:423:GLN:NE2	11:A:710:HOH:O	2.24	0.70
1:A:410:ASN:OD1	11:A:703:HOH:O	2.11	0.68
7:A:618:PEO:O1	8:A:622[A]:OSM:O	2.10	0.68
2:A:602:NAG:O7	11:A:702:HOH:O	2.10	0.68
1:A:258:GLU:OE2	3:A:604:HEM:HMB2	1.88	0.67
8:A:622[A]:OSM:N	11:A:709:HOH:O	2.22	0.67
1:A:197:PRO:HD2	9:A:632:SCN:N	2.10	0.65
1:A:168:PRO:HB3	11:A:1090:HOH:O	1.95	0.65
1:A:198:SER:C	10:A:638:GOL:O2	2.39	0.65
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.33	0.63
1:A:408:ASN:OD1	1:A:410:ASN:ND2	2.32	0.62
1:A:410:ASN:HB3	11:A:1029:HOH:O	2.00	0.61
1:A:531:GLU:OE1	11:A:704:HOH:O	2.15	0.61
1:A:117:THR:HB	11:A:894:HOH:O	2.02	0.60
1:A:348:ARG:HH11	1:A:437:ASN:ND2	1.99	0.60
1:A:82[A]:ILE:HD13	1:A:480:LEU:HD23	1.86	0.58
1:A:219:ALA:HB2	8:A:628:OSM:HN1	1.69	0.58
1:A:570:ASN:ND2	11:A:717:HOH:O	2.36	0.58
1:A:536:PHE:O	1:A:541:ARG:NH1	2.37	0.57
1:A:197:PRO:CD	9:A:632:SCN:N	2.67	0.57
1:A:332:ASN:ND2	11:A:716:HOH:O	2.34	0.56
1:A:8:ALA:N	1:A:9:PRO:HD3	2.20	0.56
1:A:258:GLU:HG3	8:A:622[A]:OSM:C	2.36	0.55
1:A:341:ASN:HB3	9:A:631:SCN:C	2.37	0.55
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.53	0.55
1:A:363:GLU:H	1:A:363:GLU:CD	2.15	0.55
1:A:237:CYS:HA	1:A:381:PHE:O	2.07	0.54
1:A:169:THR:HG22	11:A:1020:HOH:O	2.08	0.54
1:A:236:PRO:HA	5:A:609:IOD:I	2.78	0.54
1:A:352[B]:MET:HB3	1:A:407:MET:HG2	1.90	0.53
1:A:197:PRO:CG	9:A:632:SCN:N	2.72	0.52
1:A:407:MET:HE3	1:A:407:MET:C	2.34	0.52
8:A:623:OSM:N	11:A:712:HOH:O	2.28	0.52
1:A:529:TRP:CE3	11:A:708:HOH:O	2.46	0.51
5:A:615:IOD:I	11:A:892:HOH:O	2.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:O	1:A:547:VAL:HG22	2.11	0.51
1:A:319:SER:OG	11:A:705:HOH:O	2.19	0.50
1:A:167:CYS:N	1:A:168:PRO:HA	2.26	0.50
1:A:526:ASP:CB	11:A:708:HOH:O	2.49	0.50
1:A:393:ASP:OD1	1:A:557:THR:HB	2.11	0.50
1:A:205:ASN:HA	11:A:1010:HOH:O	2.11	0.50
1:A:529:TRP:HB2	11:A:708:HOH:O	2.10	0.50
1:A:113:PHE:O	1:A:115:PRO:HD3	2.11	0.50
6:A:612:EDO:H22	11:A:1043:HOH:O	2.11	0.50
1:A:352[A]:MET:SD	1:A:407:MET:SD	3.10	0.49
1:A:410:ASN:HB3	5:A:621:IOD:I	2.82	0.49
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.94	0.49
1:A:473:ASN:C	1:A:473:ASN:HD22	2.21	0.49
1:A:258:GLU:OE2	3:A:604:HEM:C2B	2.58	0.48
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.49	0.48
1:A:567:PHE:HD1	8:A:626:OSM:S	2.36	0.48
1:A:408:ASN:HB2	11:A:884:HOH:O	2.12	0.48
1:A:473:ASN:ND2	1:A:476:LEU:H	2.11	0.48
1:A:568:GLN:NE2	11:A:717:HOH:O	2.46	0.47
1:A:361:LEU:HD21	6:A:613:EDO:H21	1.95	0.47
1:A:352[B]:MET:CB	1:A:407:MET:HG2	2.44	0.47
1:A:306:ILE:HA	9:A:633:SCN:N	2.29	0.47
1:A:146:LYS:O	1:A:147:ASN:HB2	2.15	0.46
1:A:570:ASN:HD22	1:A:575:ASP:HB3	1.80	0.46
1:A:526:ASP:OD2	11:A:708:HOH:O	2.21	0.46
1:A:198:SER:CB	10:A:638:GOL:O2	2.53	0.46
1:A:513:CYS:O	1:A:517[A]:ARG:HG3	2.15	0.46
1:A:95:ASN:ND2	2:A:601:NAG:C7	2.79	0.45
1:A:410:ASN:H	1:A:410:ASN:HD22	1.63	0.45
1:A:8:ALA:N	1:A:9:PRO:CD	2.80	0.45
2:A:602:NAG:O4	11:A:706:HOH:O	2.19	0.45
1:A:10:VAL:HG23	11:A:947:HOH:O	2.16	0.45
1:A:588:SER:N	1:A:589:PRO:CD	2.80	0.44
1:A:541:ARG:NH2	8:A:625:OSM:HS	2.09	0.44
3:A:604:HEM:HMB2	3:A:604:HEM:HBB2	1.98	0.44
1:A:313:LEU:N	1:A:314:PRO:CD	2.82	0.43
1:A:258:GLU:HB2	8:A:622[A]:OSM:H1	2.00	0.43
1:A:14:LYS:HD2	11:A:1187:HOH:O	2.19	0.43
1:A:165:PHE:CE2	1:A:168:PRO:O	2.72	0.43
1:A:76:ARG:HH12	1:A:419:ASN:ND2	2.17	0.43
1:A:54:GLY:HA2	11:A:1047:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:CB	1:A:170:PRO:HD2	2.49	0.43
1:A:193:TYR:CZ	1:A:297:ARG:HA	2.54	0.43
1:A:31:ARG:NH1	11:A:757:HOH:O	2.52	0.43
1:A:197:PRO:HA	6:A:612:EDO:H12	2.01	0.43
1:A:561:LYS:N	9:A:634:SCN:N	2.66	0.43
1:A:198:SER:HB2	10:A:638:GOL:C2	2.45	0.42
1:A:281:LYS:HE3	1:A:285:PRO:O	2.20	0.42
1:A:530:TRP:NE1	9:A:633:SCN:N	2.67	0.42
1:A:332:ASN:OD1	1:A:332:ASN:C	2.62	0.42
1:A:91:VAL:HG12	1:A:411:LYS:HD3	2.01	0.42
1:A:216:ASN:HA	5:A:607:IOD:I	2.90	0.41
1:A:99:LEU:HD21	1:A:549:PHE:CD1	2.56	0.41
1:A:169:THR:O	1:A:170:PRO:C	2.63	0.41
1:A:197:PRO:HG2	9:A:632:SCN:N	2.34	0.41
1:A:225:ALA:N	6:A:637:EDO:O2	2.46	0.41
1:A:169:THR:CB	1:A:170:PRO:CD	2.99	0.41
1:A:63[A]:GLN:HG2	11:A:978:HOH:O	2.20	0.40
1:A:189:ALA:HB2	1:A:304:ILE:HD12	2.03	0.40
1:A:464:LEU:HA	1:A:481:LEU:HD12	2.03	0.40
1:A:169:THR:HB	1:A:170:PRO:CD	2.50	0.40
1:A:424:PRO:O	1:A:425:THR:HB	2.22	0.40
1:A:122:SER:O	1:A:123:GLU:C	2.64	0.40
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.56	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	601/595 (101%)	561 (93%)	32 (5%)	8 (1%)	9 3

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	167	CYS
1	A	168	PRO
1	A	170	PRO
1	A	117	THR
1	A	123	GLU
1	A	11	PRO
1	A	425	THR

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	525/517 (102%)	502 (96%)	23 (4%)	25 13

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	3	GLU
1	A	12	LEU
1	A	13	VAL
1	A	14	LYS
1	A	124	HIS
1	A	151	LEU
1	A	170	PRO
1	A	175	LEU
1	A	198	SER
1	A	201	SER
1	A	283	LEU
1	A	286	HIS
1	A	363	GLU
1	A	371	GLU
1	A	410	ASN
1	A	473	ASN
1	A	478	LYS
1	A	483	LEU

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Mol	Chain	Res	Type
1	A	545	GLN
1	A	561	LYS
1	A	564	LEU
1	A	585	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	250	GLN
1	A	329	GLN
1	A	410	ASN
1	A	419	ASN
1	A	423	GLN
1	A	437	ASN
1	A	468	GLN
1	A	473	ASN
1	A	497	ASN
1	A	545	GLN
1	A	556	ASN
1	A	558	HIS
1	A	565	HIS
1	A	568	GLN
1	A	570	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 13 are monoatomic - leaving 26 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	EDO	A	611	-	3,3,3	0.24	0	2,2,2	0.35	0
7	PEO	A	618	3	1,1,1	0.30	0	-		
9	SCN	A	634	-	1,2,2	0.36	0	0,1,1	-	-
8	OSM	A	624	-	1,3,3	0.01	0	0,2,2	-	-
6	EDO	A	612	-	3,3,3	0.36	0	2,2,2	0.35	0
3	HEM	A	604	1,7	50,50,50	1.80	10 (20%)	66,82,82	1.51	12 (18%)
9	SCN	A	633	-	1,2,2	1.32	0	0,1,1	-	-
8	OSM	A	626	-	1,3,3	0.05	0	0,2,2	-	-
9	SCN	A	636	-	1,2,2	0.71	0	0,1,1	-	-
2	NAG	A	603	1	14,14,15	0.76	0	17,19,21	1.72	3 (17%)
8	OSM	A	625	-	1,3,3	0.02	0	0,2,2	-	-
9	SCN	A	632	-	1,2,2	0.69	0	0,1,1	-	-
9	SCN	A	631	-	1,2,2	0.11	0	0,1,1	-	-
8	OSM	A	622[B]	-	1,3,3	0.09	0	0,2,2	-	-
9	SCN	A	630	-	1,2,2	0.89	0	0,1,1	-	-
2	NAG	A	602	1	14,14,15	1.13	2 (14%)	17,19,21	1.47	2 (11%)
6	EDO	A	613	-	3,3,3	0.69	0	2,2,2	0.19	0
8	OSM	A	627	-	1,3,3	0.01	0	0,2,2	-	-
8	OSM	A	622[A]	-	1,3,3	0.01	0	0,2,2	-	-
6	EDO	A	637	-	3,3,3	0.22	0	2,2,2	0.65	0
2	NAG	A	601	1	14,14,15	0.77	0	17,19,21	2.03	2 (11%)
8	OSM	A	628	-	1,3,3	0.05	0	0,2,2	-	-
8	OSM	A	629	-	1,3,3	0.05	0	0,2,2	-	-
9	SCN	A	635	-	1,2,2	0.58	0	0,1,1	-	-
10	GOL	A	638	-	5,5,5	0.61	0	5,5,5	0.61	0
8	OSM	A	623	-	1,3,3	0.09	0	0,2,2	-	-

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
6	EDO	A	611	-	-	1/1/1/1	-
6	EDO	A	612	-	-	0/1/1/1	-
10	GOL	A	638	-	-	4/4/4/4	-
3	HEM	A	604	1,7	-	4/14/54/54	-
8	OSM	A	626	-	-	0/0/1/1	-
2	NAG	A	603	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
6	EDO	A	613	-	-	0/1/1/1	-
8	OSM	A	628	-	-	0/0/1/1	-
8	OSM	A	627	-	-	0/0/1/1	-
8	OSM	A	622[A]	-	-	0/0/1/1	-
8	OSM	A	629	-	-	0/0/1/1	-
6	EDO	A	637	-	-	1/1/1/1	-
8	OSM	A	625	-	-	0/0/1/1	-
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1
8	OSM	A	624	-	-	0/0/1/1	-
8	OSM	A	622[B]	-	-	0/0/1/1	-
8	OSM	A	623	-	-	0/0/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	HEM	FE-NC	4.96	2.12	1.95
3	A	604	HEM	FE-NB	4.84	2.09	1.94
3	A	604	HEM	C4C-NC	-3.75	1.32	1.39
3	A	604	HEM	C4D-C3D	3.38	1.50	1.45
3	A	604	HEM	C1B-NB	-3.15	1.34	1.40
3	A	604	HEM	FE-NA	2.90	2.04	1.95
3	A	604	HEM	C1C-C2C	-2.80	1.39	1.45
2	A	602	NAG	C2-N2	-2.29	1.42	1.46
3	A	604	HEM	C4D-ND	-2.17	1.36	1.40
3	A	604	HEM	C3D-C2D	-2.13	1.32	1.36
3	A	604	HEM	C1C-NC	-2.09	1.35	1.39
2	A	602	NAG	O5-C1	-2.00	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	NAG	C2-N2-C7	-6.71	113.34	122.90
3	A	604	HEM	C1B-NB-C4B	4.60	109.83	105.07
2	A	603	NAG	C1-O5-C5	-4.34	106.31	112.19
3	A	604	HEM	C4C-NC-C1C	3.57	108.84	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	604	HEM	C3B-C2B-C1B	3.45	109.05	106.49
2	A	602	NAG	C1-O5-C5	3.34	116.72	112.19
2	A	603	NAG	C3-C4-C5	-3.31	104.33	110.24
2	A	601	NAG	C4-C3-C2	-3.15	106.41	111.02
2	A	602	NAG	C6-C5-C4	-3.03	105.90	113.00
3	A	604	HEM	CHC-C4B-NB	2.99	127.67	124.42
3	A	604	HEM	CHD-C1D-C2D	-2.76	120.67	124.98
3	A	604	HEM	C4B-C3B-C2B	-2.74	104.94	107.11
3	A	604	HEM	CHB-C1B-NB	2.65	127.64	124.37
3	A	604	HEM	C2D-C1D-ND	2.49	112.86	109.88
3	A	604	HEM	CHA-C4D-C3D	-2.43	120.77	125.33
2	A	603	NAG	C4-C3-C2	-2.19	107.81	111.02
3	A	604	HEM	C1A-CHA-C4D	-2.17	121.18	126.34
3	A	604	HEM	O2A-CGA-CBA	2.10	120.79	114.03
3	A	604	HEM	CHA-C4D-ND	2.08	126.94	124.37

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	611	EDO	O1-C1-C2-O2
2	A	601	NAG	C8-C7-N2-C2
2	A	601	NAG	O7-C7-N2-C2
10	A	638	GOL	O1-C1-C2-O2
10	A	638	GOL	O1-C1-C2-C3
10	A	638	GOL	C1-C2-C3-O3
10	A	638	GOL	O2-C2-C3-O3
6	A	637	EDO	O1-C1-C2-O2
3	A	604	HEM	CAD-CBD-CGD-O2D
3	A	604	HEM	CAA-CBA-CGA-O2A
3	A	604	HEM	CAD-CBD-CGD-O1D
3	A	604	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

19 monomers are involved in 45 short contacts:

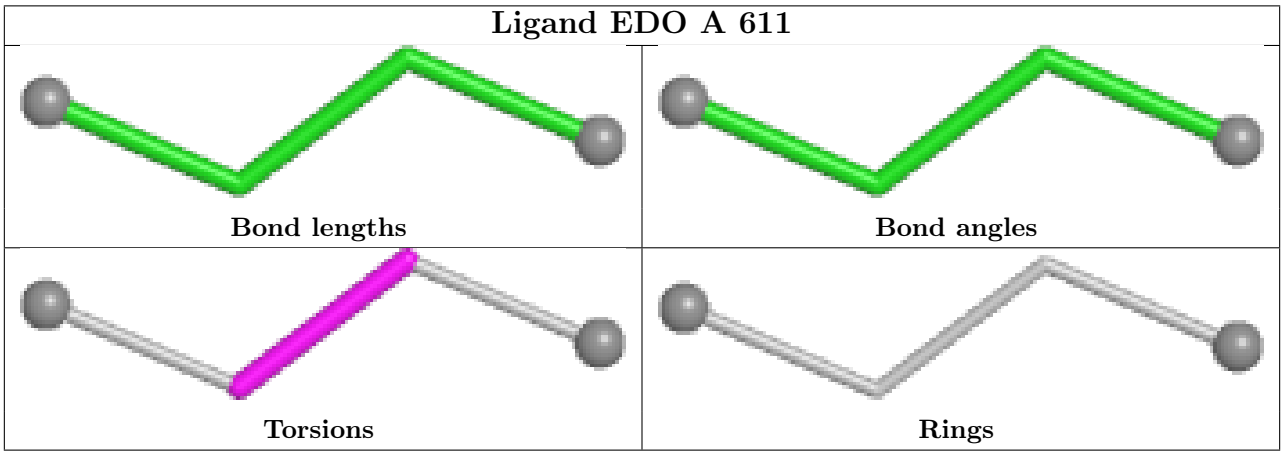
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	618	PEO	2	0
9	A	634	SCN	1	0
6	A	612	EDO	2	0
3	A	604	HEM	7	0

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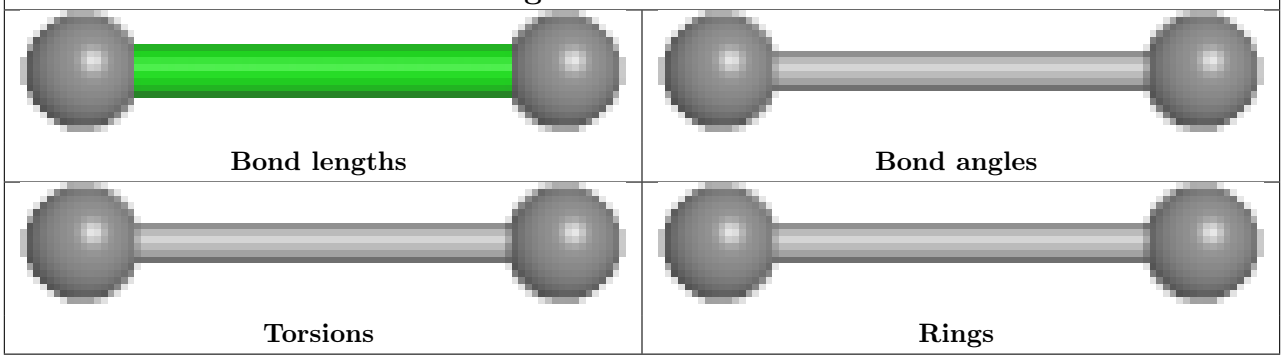
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	633	SCN	2	0
8	A	626	OSM	3	0
8	A	625	OSM	2	0
9	A	632	SCN	4	0
9	A	631	SCN	3	0
8	A	622[B]	OSM	2	0
2	A	602	NAG	2	0
6	A	613	EDO	1	0
8	A	622[A]	OSM	5	0
6	A	637	EDO	2	0
2	A	601	NAG	1	0
8	A	628	OSM	2	0
8	A	629	OSM	1	0
10	A	638	GOL	4	0
8	A	623	OSM	1	0

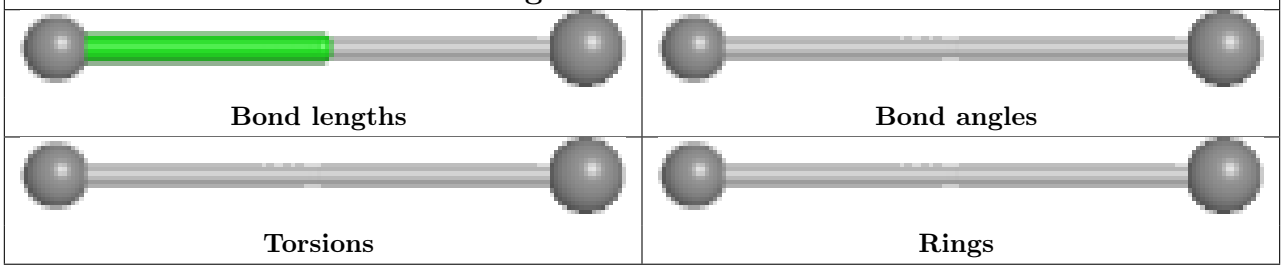
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



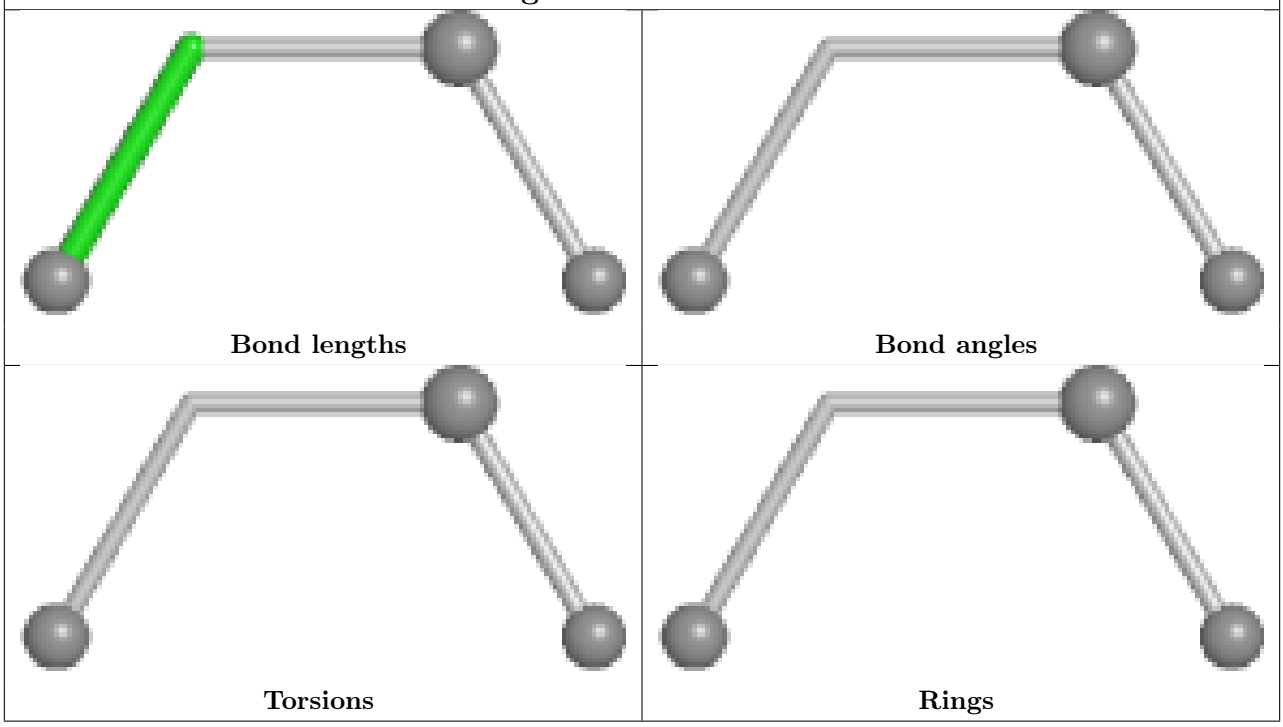
Ligand PEO A 618



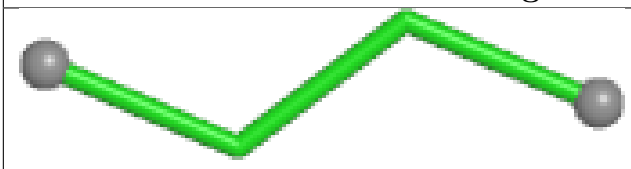
Ligand SCN A 634



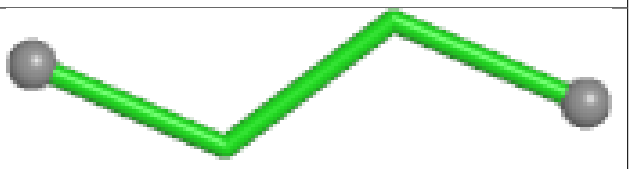
Ligand OSM A 624



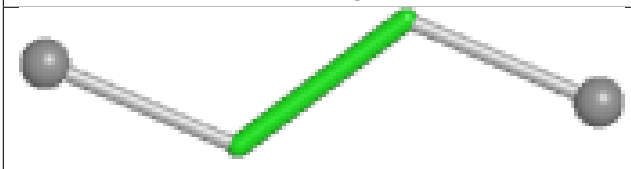
Ligand EDO A 612



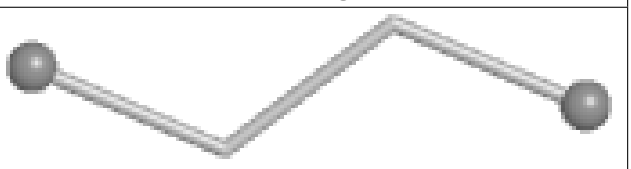
Bond lengths



Bond angles

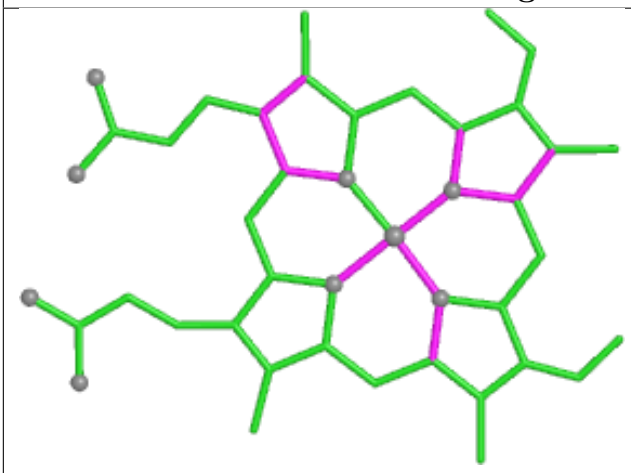


Torsions

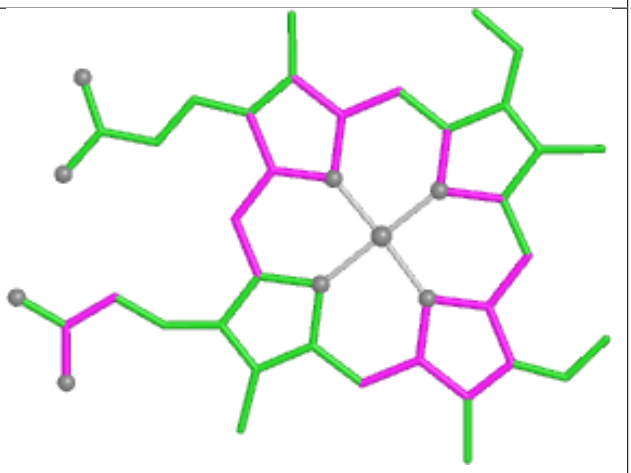


Rings

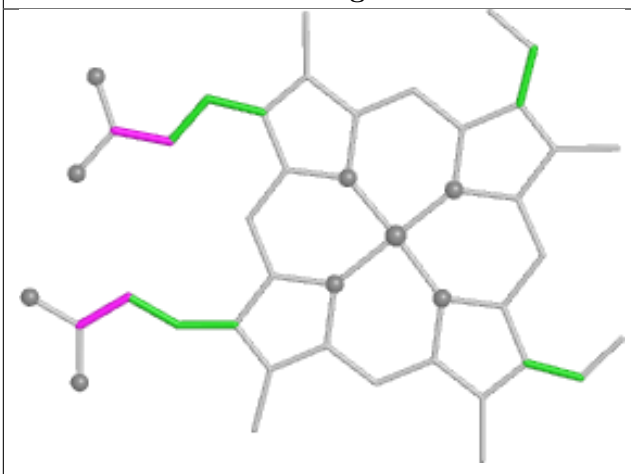
Ligand HEM A 604



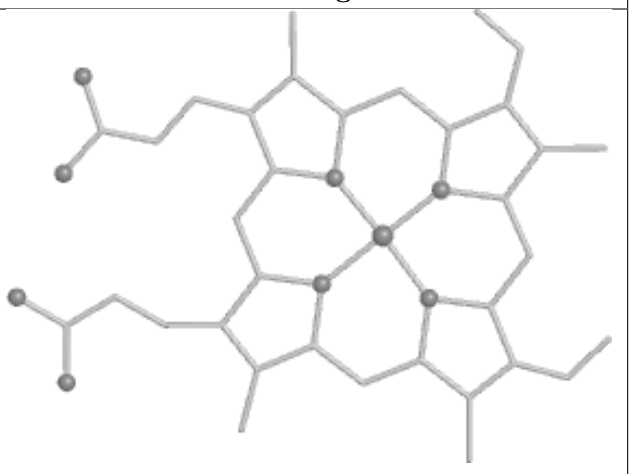
Bond lengths



Bond angles

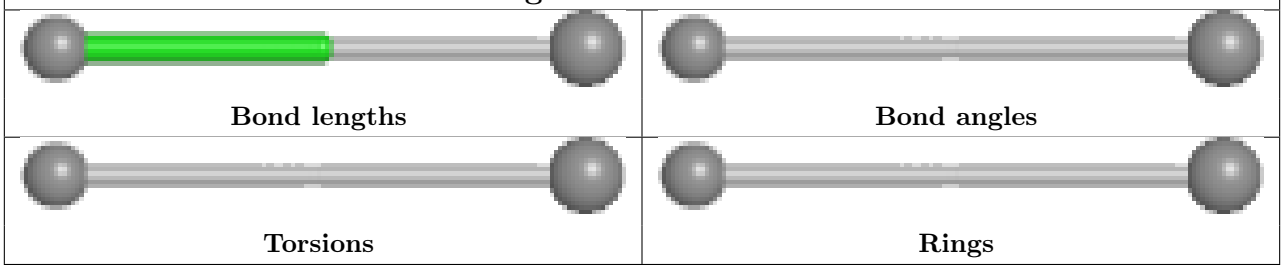


Torsions

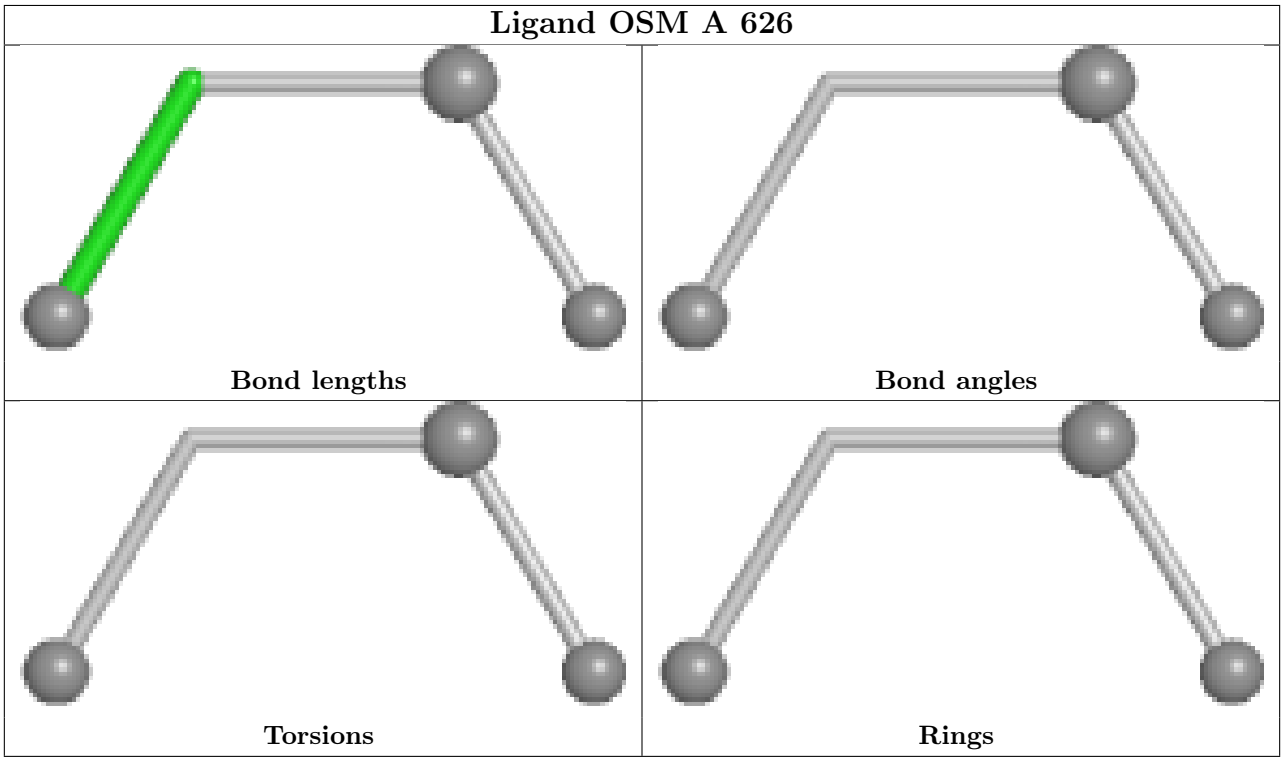


Rings

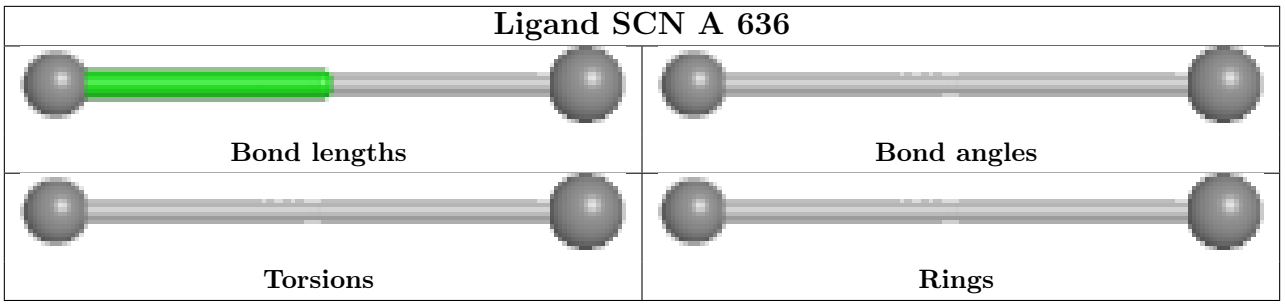
Ligand SCN A 633



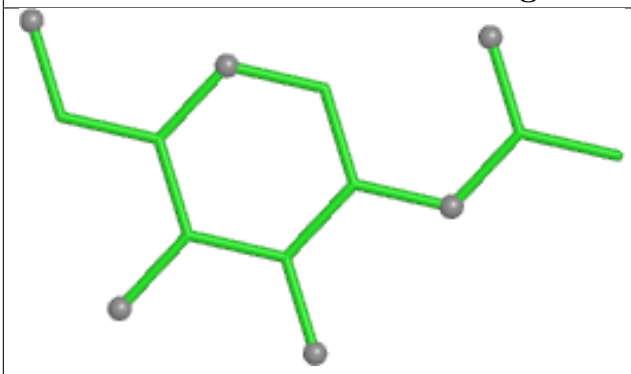
Ligand OSM A 626



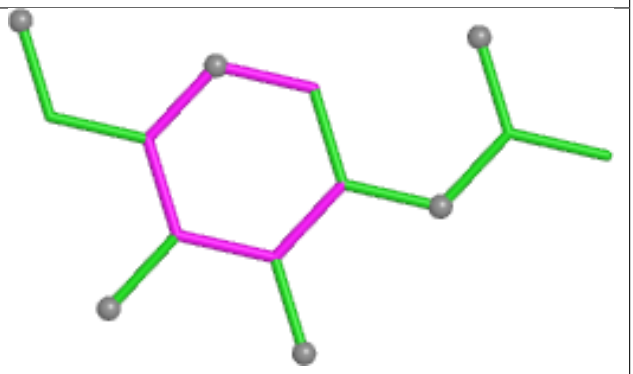
Ligand SCN A 636



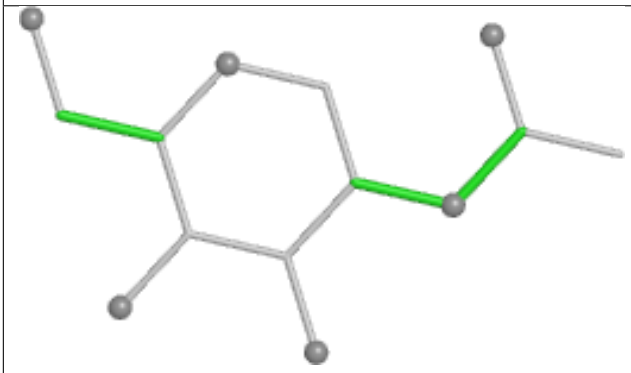
Ligand NAG A 603



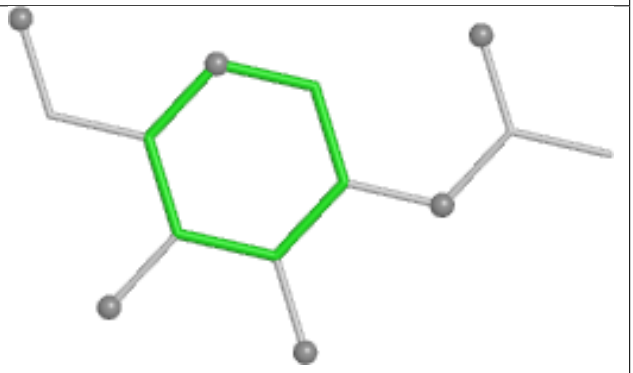
Bond lengths



Bond angles

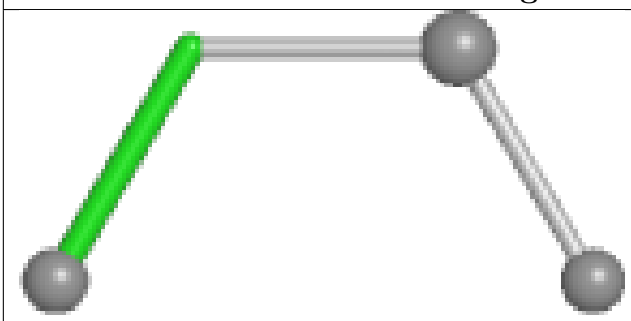


Torsions

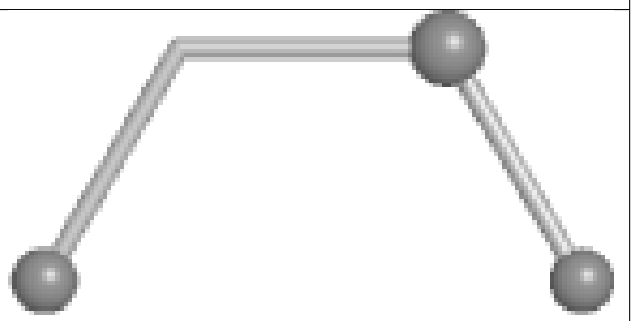


Rings

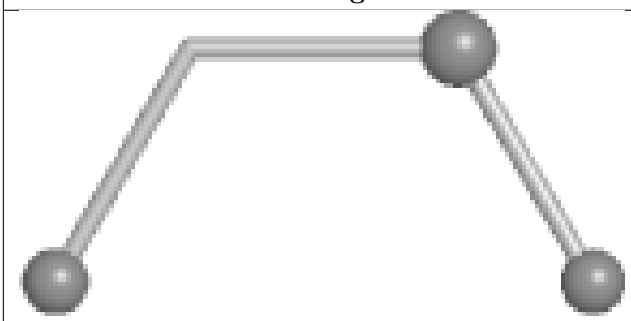
Ligand OSM A 625



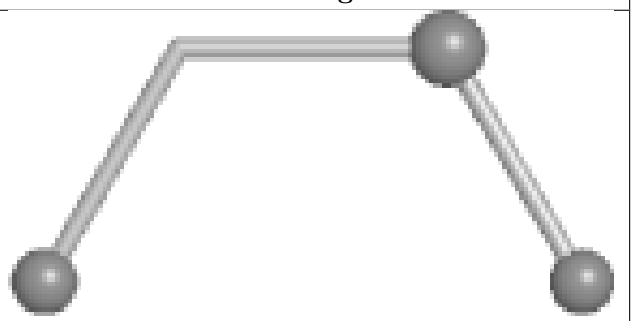
Bond lengths



Bond angles

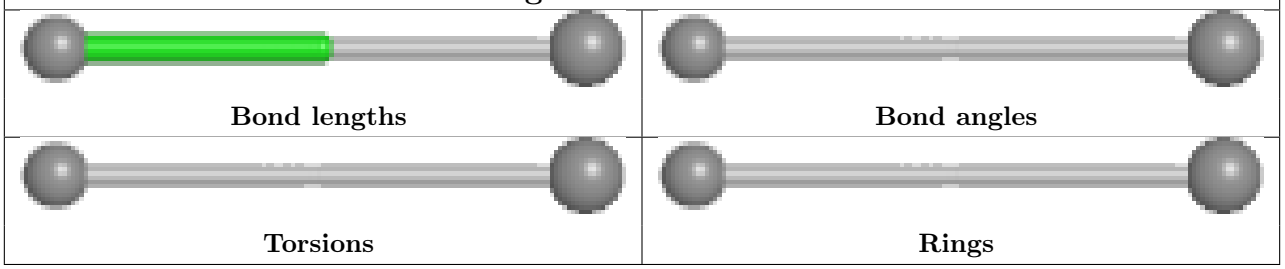


Torsions

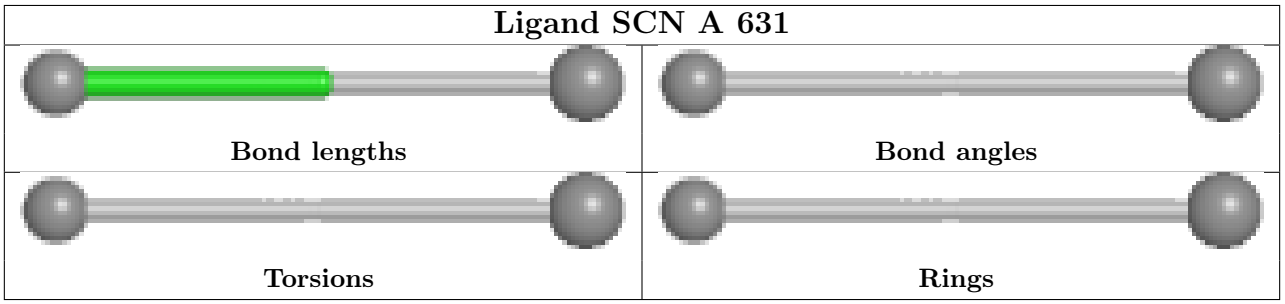


Rings

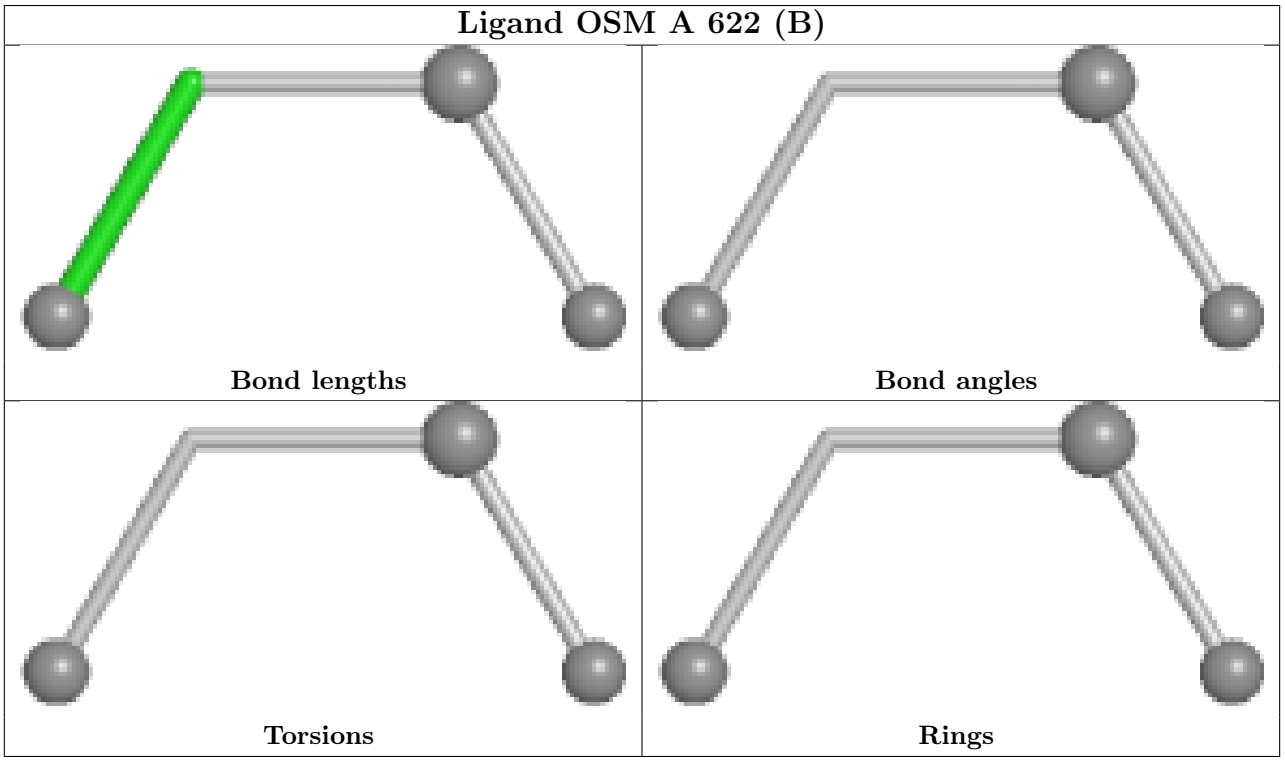
Ligand SCN A 632



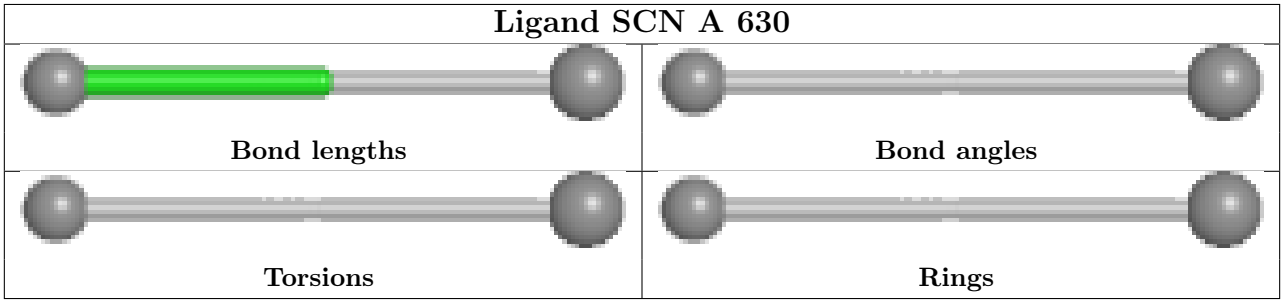
Ligand SCN A 631



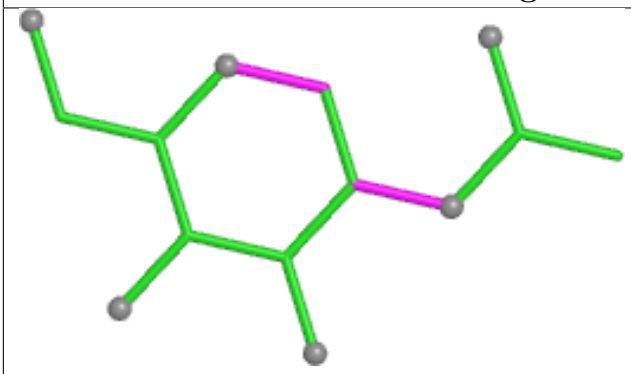
Ligand OSM A 622 (B)



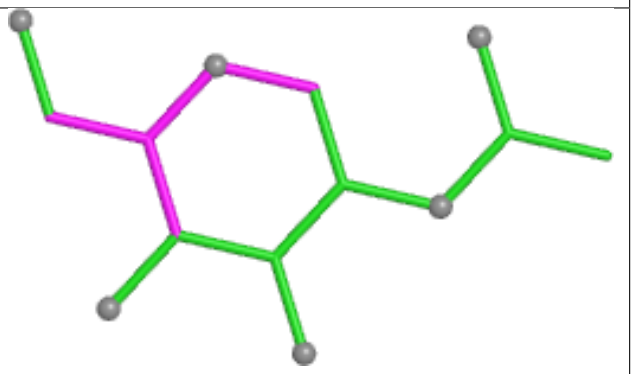
Ligand SCN A 630



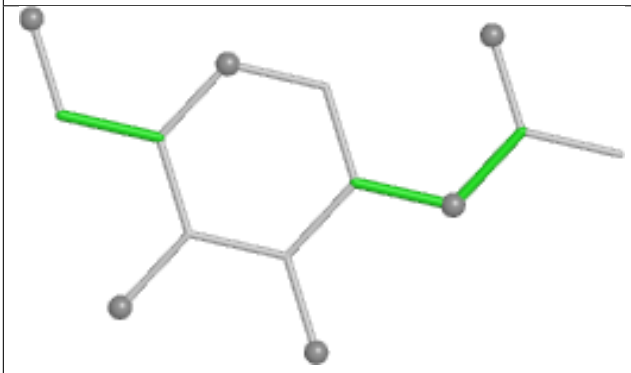
Ligand NAG A 602



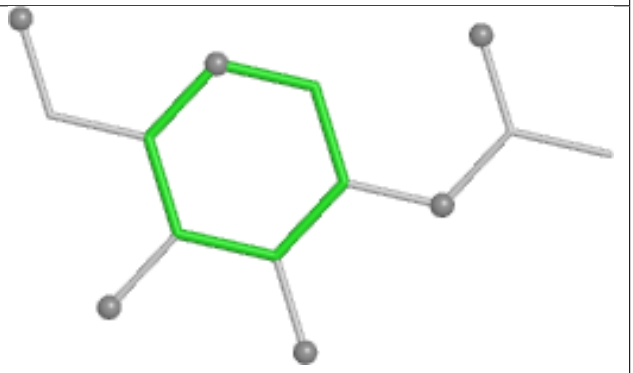
Bond lengths



Bond angles

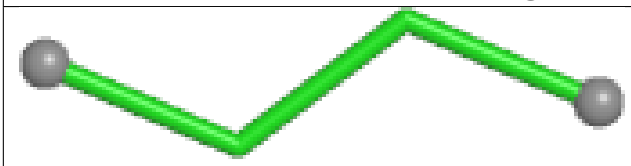


Torsions

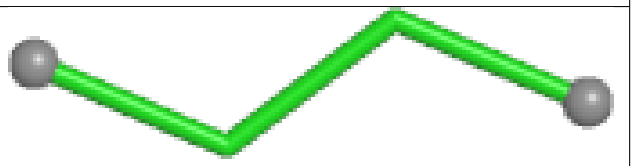


Rings

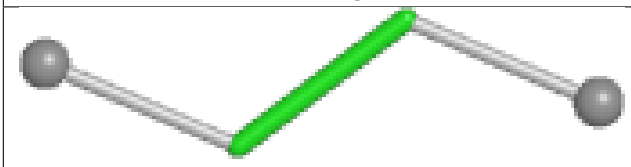
Ligand EDO A 613



Bond lengths



Bond angles

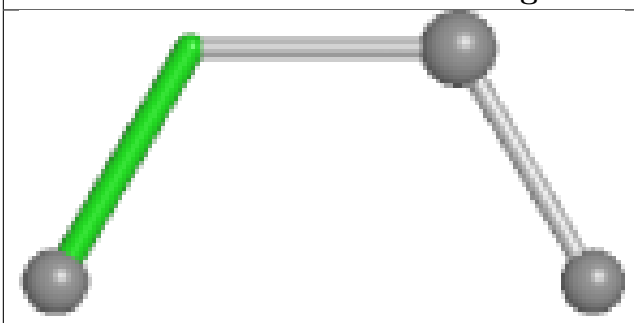


Torsions

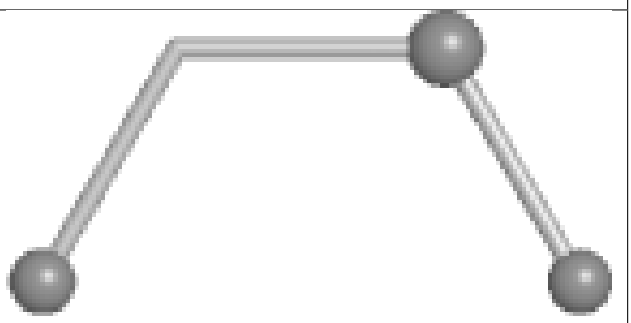


Rings

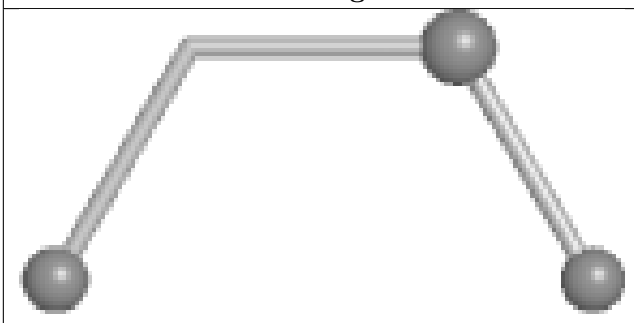
Ligand OSM A 627



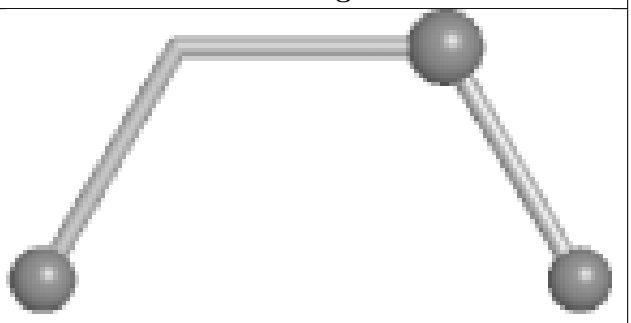
Bond lengths



Bond angles

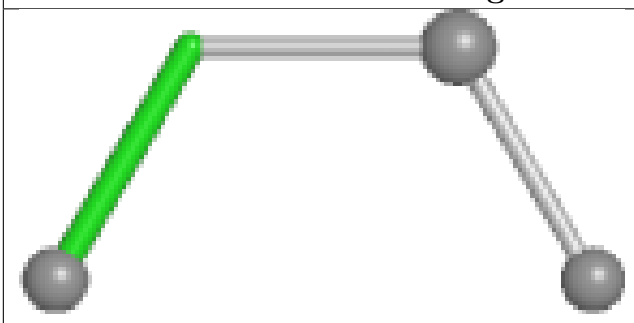


Torsions

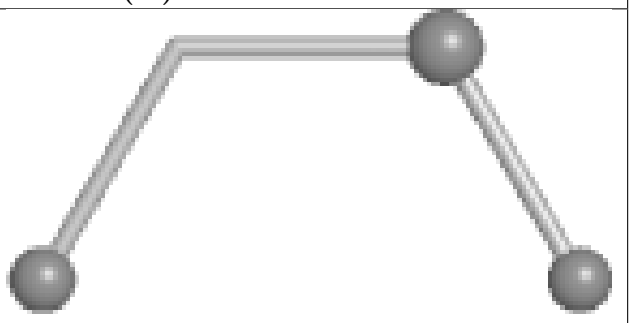


Rings

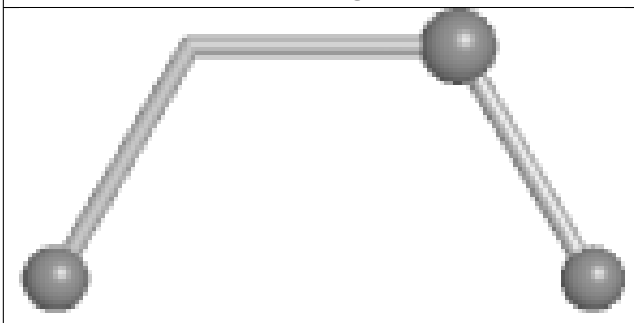
Ligand OSM A 622 (A)



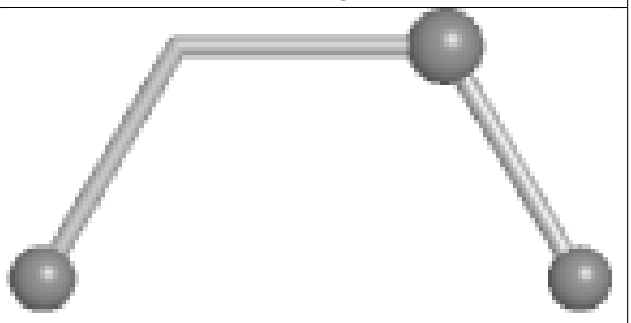
Bond lengths



Bond angles

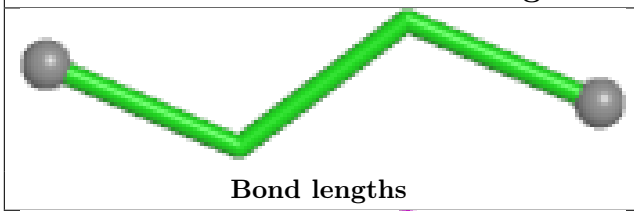


Torsions

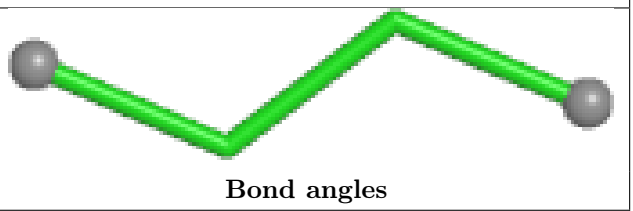


Rings

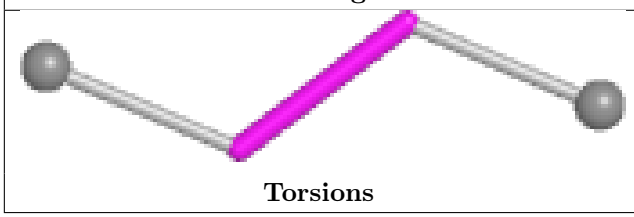
Ligand EDO A 637



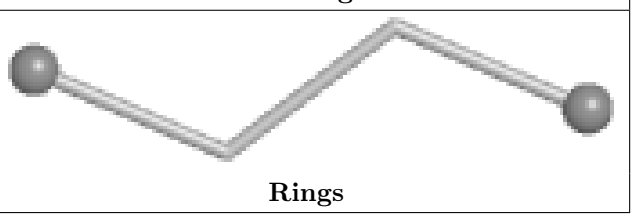
Bond lengths



Bond angles

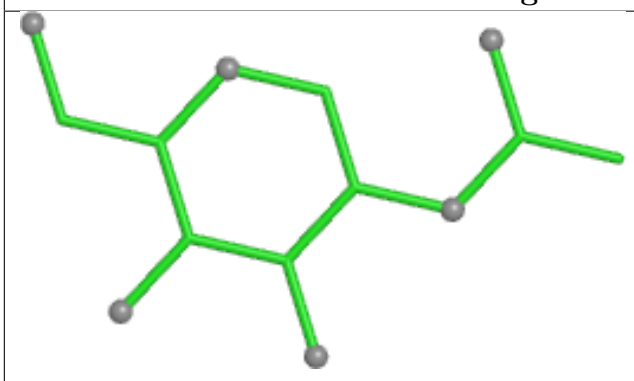


Torsions

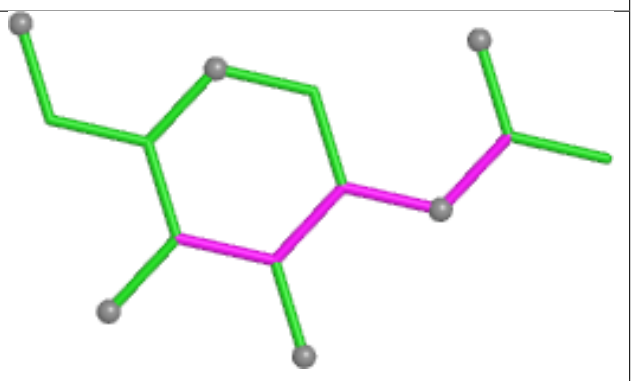


Rings

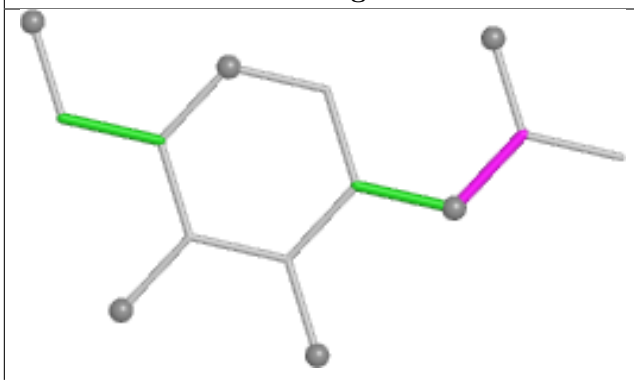
Ligand NAG A 601



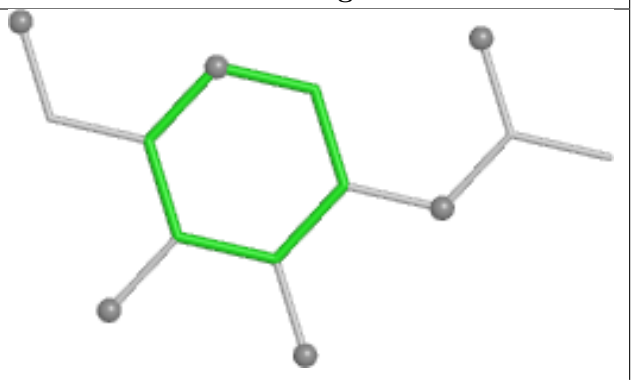
Bond lengths



Bond angles

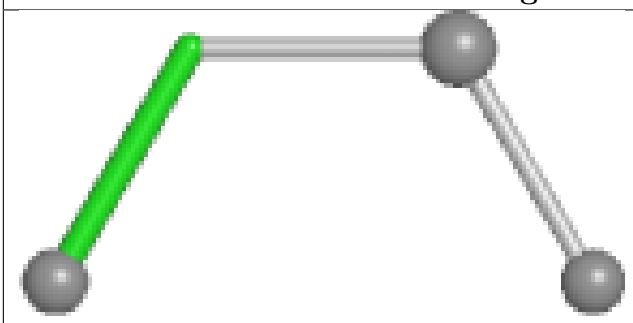


Torsions

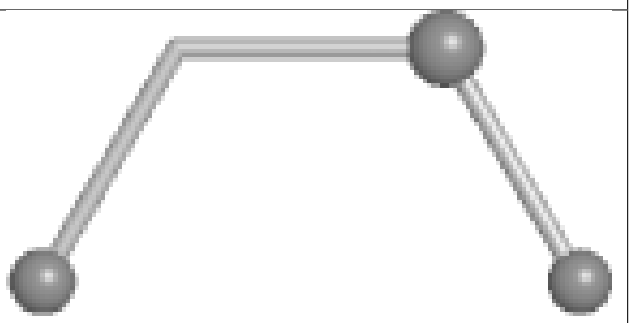


Rings

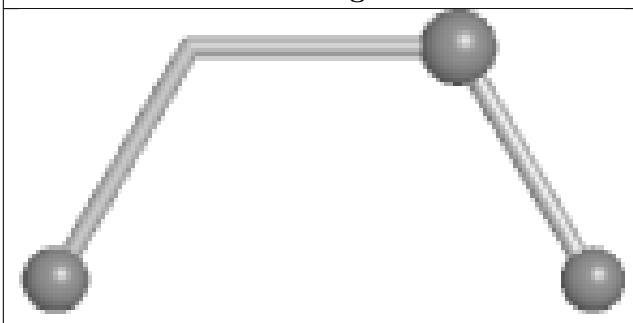
Ligand OSM A 628



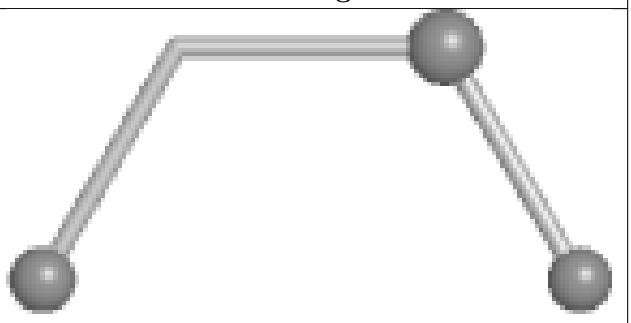
Bond lengths



Bond angles

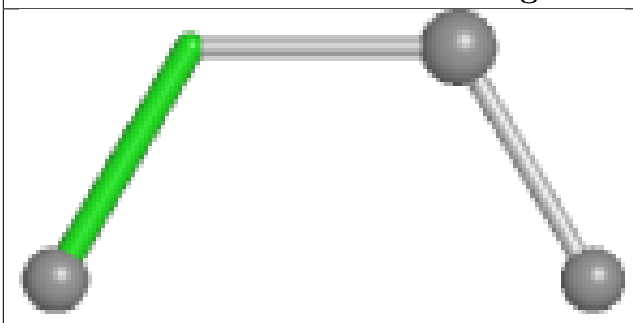


Torsions

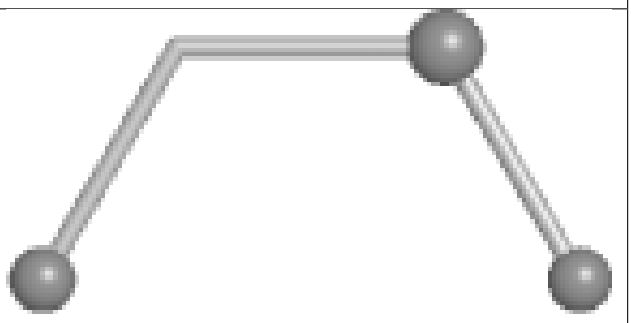


Rings

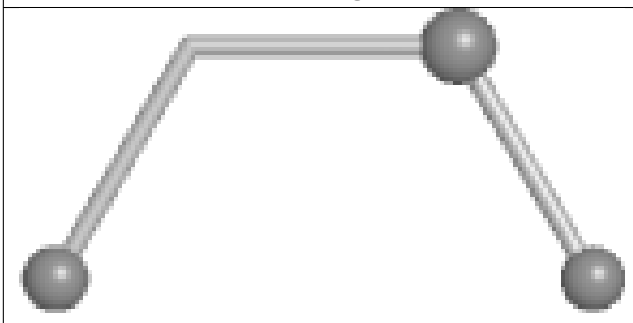
Ligand OSM A 629



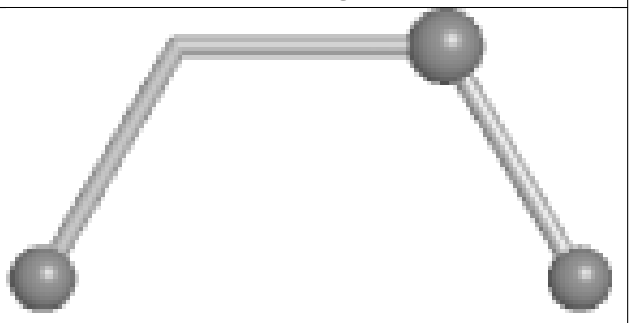
Bond lengths



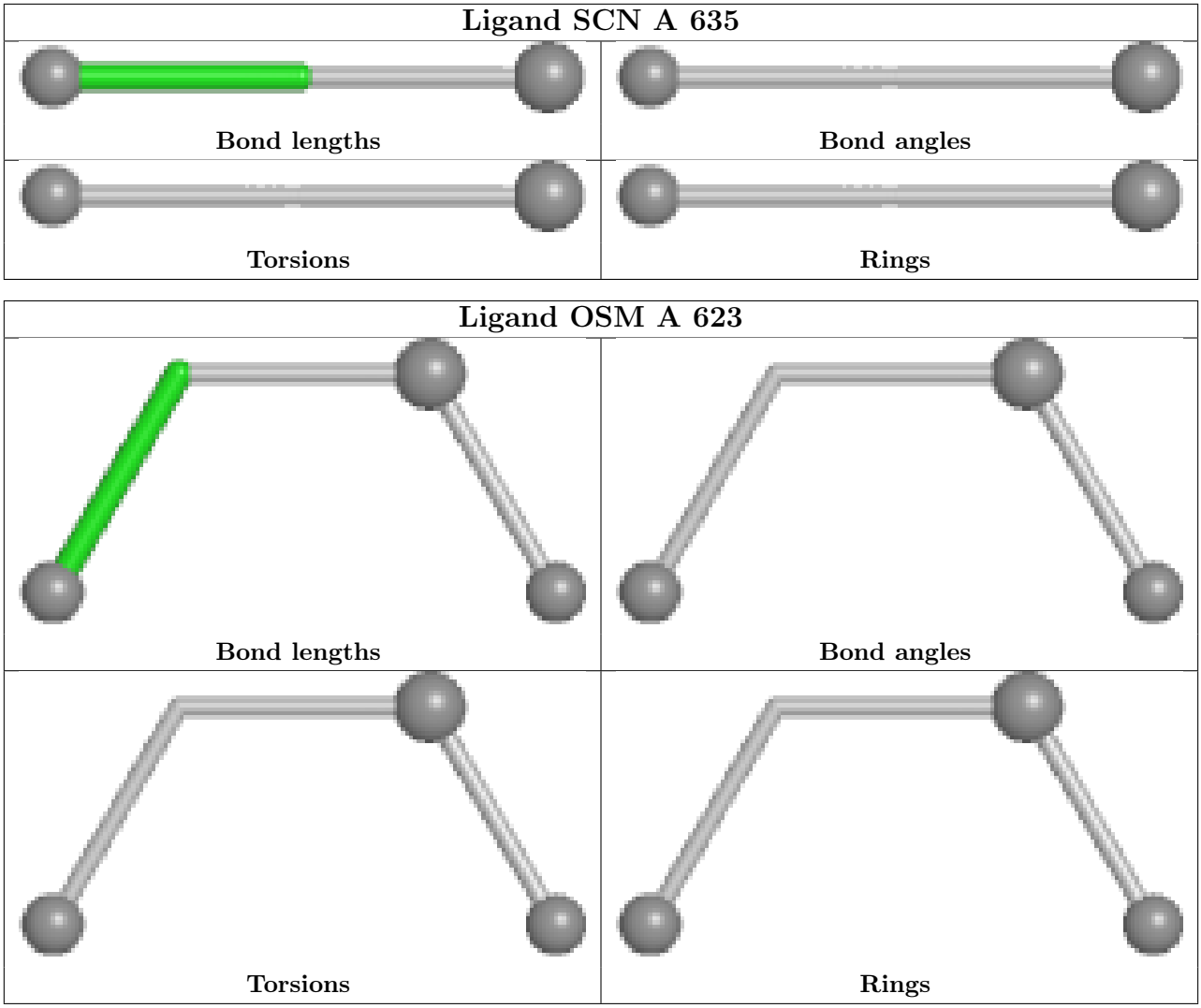
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	595/595 (100%)	1.24	129 (21%)	2 2	12, 31, 81, 159	8 (1%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	10.1
1	A	168	PRO	8.1
1	A	172	TYR	7.6
1	A	10	VAL	7.4
1	A	12	LEU	6.5
1	A	13	VAL	6.5
1	A	127	VAL	6.3
1	A	9	PRO	6.3
1	A	4	VAL	5.8
1	A	169	THR	5.6
1	A	117	THR	5.3
1	A	8	ALA	5.2
1	A	283	LEU	5.2
1	A	292	LEU	5.2
1	A	119	LEU	5.2
1	A	171	PRO	5.2
1	A	170	PRO	5.1
1	A	120	GLY	4.9
1	A	167	CYS	4.8
1	A	124	HIS	4.7
1	A	324	TRP	4.6
1	A	11	PRO	4.5
1	A	175	LEU	4.5
1	A	208	SER	4.4
1	A	173	GLN	4.4
1	A	122	SER	4.3
1	A	289	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	537	THR	4.1
1	A	174	SER	4.1
1	A	212	LEU	3.9
1	A	219	ALA	3.9
1	A	242	THR	3.9
1	A	229	PHE	3.8
1	A	277	ALA	3.7
1	A	20	PRO	3.6
1	A	287	TRP	3.6
1	A	579	CYS	3.6
1	A	284	ASN	3.5
1	A	224	LEU	3.4
1	A	276	LEU	3.4
1	A	5	GLY	3.4
1	A	3	GLU	3.4
1	A	543	SER	3.4
1	A	210	LEU	3.4
1	A	132	TYR	3.2
1	A	206	LEU	3.2
1	A	133	CYS	3.2
1	A	121	SER	3.1
1	A	591	ALA	3.1
1	A	232	VAL	3.1
1	A	211	GLY	3.1
1	A	6	CYS	3.1
1	A	138	ASN	3.0
1	A	209	PRO	3.0
1	A	220	TRP	3.0
1	A	201	SER	3.0
1	A	245	HIS	3.0
1	A	539	LYS	3.0
1	A	1	SER	2.9
1	A	279	GLU	2.9
1	A	288	ASP	2.9
1	A	322	GLN	2.9
1	A	223	GLY	2.9
1	A	125	SER	2.9
1	A	574	HIS	2.9
1	A	207	SER	2.9
1	A	282	ARG	2.8
1	A	293	TYR	2.8
1	A	134	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	202	ARG	2.8
1	A	280	LEU	2.8
1	A	7	GLY	2.8
1	A	247	PRO	2.7
1	A	226	TYR	2.7
1	A	580	SER	2.7
1	A	248	CYS	2.7
1	A	200	ALA	2.7
1	A	387	ILE	2.6
1	A	589	PRO	2.6
1	A	18	ASN	2.6
1	A	63[A]	GLN	2.6
1	A	334	SER	2.5
1	A	15	CYS	2.5
1	A	28	CYS	2.5
1	A	118	GLU	2.5
1	A	384	TRP	2.5
1	A	368	TRP	2.4
1	A	590	TRP	2.4
1	A	216	ASN	2.4
1	A	326	PRO	2.4
1	A	329	GLN	2.4
1	A	215	VAL	2.4
1	A	16	ASP	2.4
1	A	241	ASN	2.4
1	A	554	CYS	2.4
1	A	203	LEU	2.4
1	A	536	PHE	2.4
1	A	392	ILE	2.4
1	A	592	SER	2.3
1	A	503	GLU	2.3
1	A	176	ALA	2.3
1	A	372	ALA	2.3
1	A	123	GLU	2.3
1	A	582	VAL	2.3
1	A	581	ALA	2.3
1	A	538	GLU	2.3
1	A	254	SER	2.3
1	A	128	GLN	2.2
1	A	328	TYR	2.2
1	A	14	LYS	2.2
1	A	233	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	231	ASN	2.2
1	A	540	GLN	2.2
1	A	235	SER	2.2
1	A	587	LEU	2.1
1	A	588	SER	2.1
1	A	17	GLU	2.1
1	A	561	LYS	2.1
1	A	199	LEU	2.1
1	A	464	LEU	2.1
1	A	278	ARG	2.1
1	A	327	PRO	2.1
1	A	576	PHE	2.1
1	A	157	CYS	2.1
1	A	583	ASP	2.1
1	A	21	TYR	2.1
1	A	552	LEU	2.0
1	A	594	GLU	2.0
1	A	237	CYS	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	601	14/15	0.75	0.14	51,56,62,64	0
2	NAG	A	602	14/15	0.80	0.13	38,45,48,50	0
6	EDO	A	612	4/4	0.83	0.12	39,39,42,42	0
10	GOL	A	638	6/6	0.83	0.14	21,26,28,32	0
8	OSM	A	625	4/4	0.86	0.17	49,49,50,54	0

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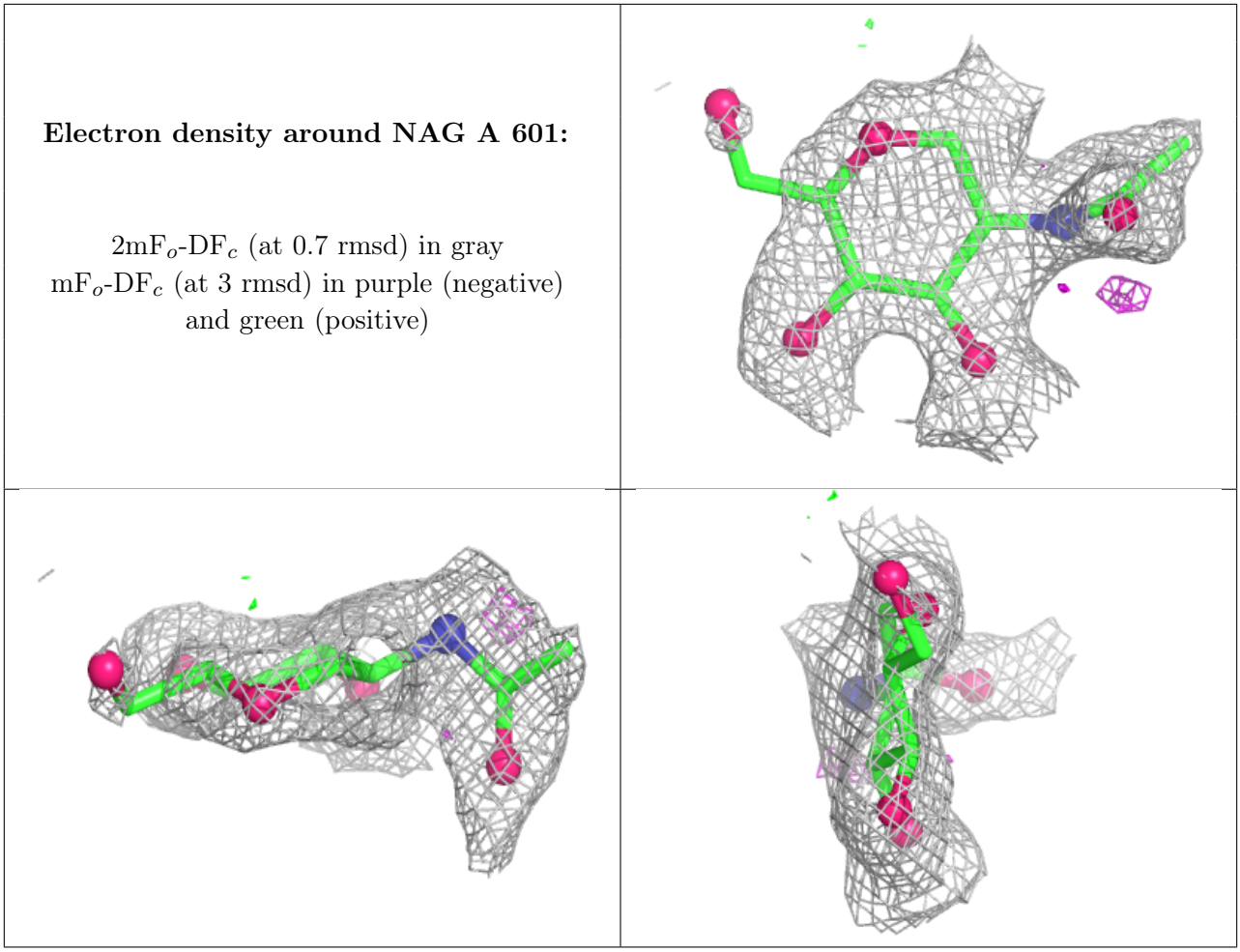
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	IOD	A	614	1/1	0.86	0.18	70,70,70,70	1
6	EDO	A	611	4/4	0.87	0.10	30,44,45,45	0
2	NAG	A	603	14/15	0.89	0.12	31,41,47,49	0
8	OSM	A	628	4/4	0.89	0.14	39,47,50,51	0
6	EDO	A	637	4/4	0.89	0.14	37,37,37,39	0
8	OSM	A	627	4/4	0.90	0.12	41,43,43,51	0
8	OSM	A	626	4/4	0.91	0.15	32,35,36,39	0
6	EDO	A	613	4/4	0.91	0.11	21,28,32,36	0
8	OSM	A	629	4/4	0.92	0.11	46,48,49,50	0
8	OSM	A	624	4/4	0.92	0.11	44,44,47,52	0
7	PEO	A	618	2/2	0.93	0.13	32,32,32,34	0
5	IOD	A	610	1/1	0.93	0.12	66,66,66,66	1
8	OSM	A	622[B]	4/4	0.94	0.10	11,13,15,17	4
8	OSM	A	622[A]	4/4	0.94	0.10	13,19,19,20	4
8	OSM	A	623	4/4	0.96	0.09	22,29,35,35	0
9	SCN	A	634	3/3	0.96	0.08	12,12,13,13	3
9	SCN	A	636	3/3	0.96	0.07	18,18,20,20	3
5	IOD	A	615	1/1	0.96	0.16	61,61,61,61	1
5	IOD	A	621	1/1	0.97	0.06	45,45,45,45	1
3	HEM	A	604	43/43	0.97	0.06	14,17,22,24	0
5	IOD	A	619	1/1	0.97	0.08	43,43,43,43	1
9	SCN	A	630	3/3	0.98	0.05	10,10,11,11	3
9	SCN	A	632	3/3	0.98	0.06	15,15,15,17	3
4	CA	A	605	1/1	0.98	0.04	21,21,21,21	0
9	SCN	A	635	3/3	0.98	0.05	10,10,10,11	3
5	IOD	A	607	1/1	0.98	0.09	55,55,55,55	1
5	IOD	A	620	1/1	0.98	0.03	31,31,31,31	1
5	IOD	A	616	1/1	0.99	0.04	27,27,27,27	1
9	SCN	A	633	3/3	0.99	0.06	9,9,10,11	3
5	IOD	A	617	1/1	0.99	0.03	27,27,27,27	1
5	IOD	A	609	1/1	0.99	0.03	35,35,35,35	1
5	IOD	A	608	1/1	0.99	0.02	33,33,33,33	1
9	SCN	A	631	3/3	0.99	0.09	13,13,15,16	3
5	IOD	A	606	1/1	1.00	0.01	18,18,18,18	0

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

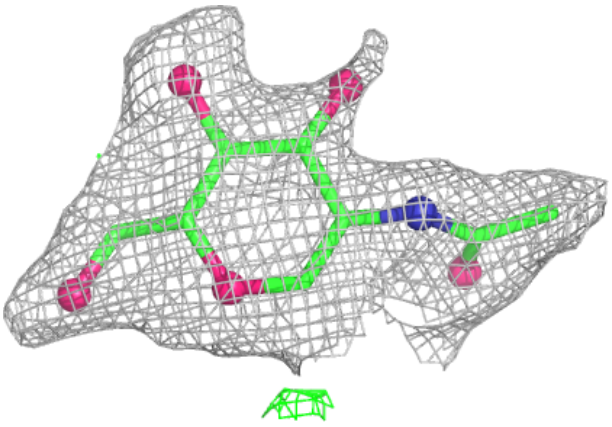
Electron density around NAG A 601:

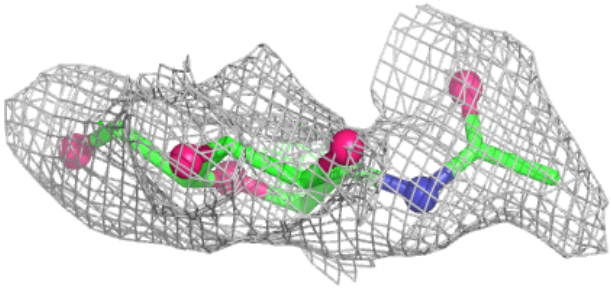
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

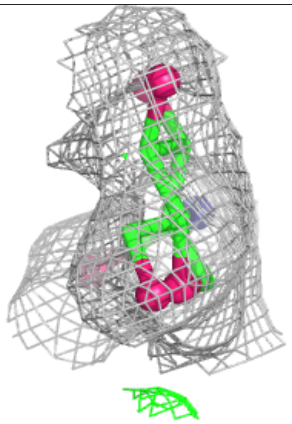


Electron density around NAG A 602:

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

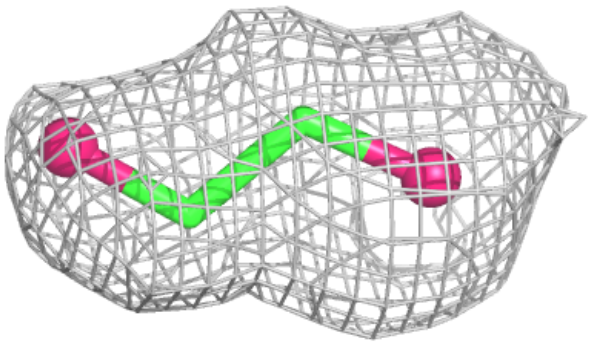


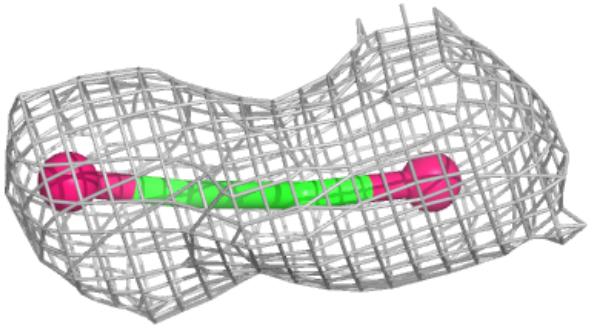


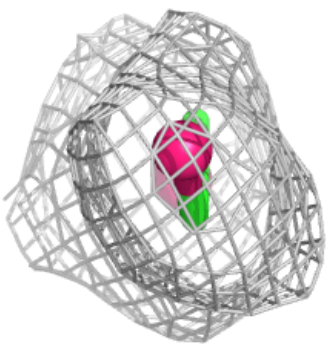


Electron density around EDO A 612:

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

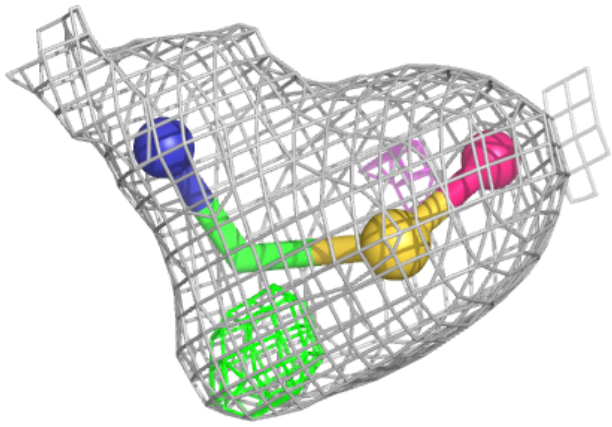


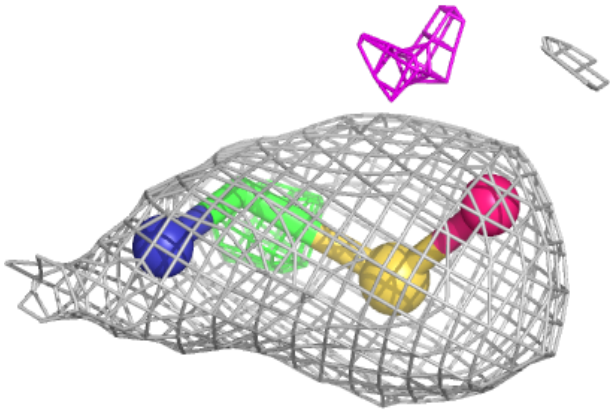


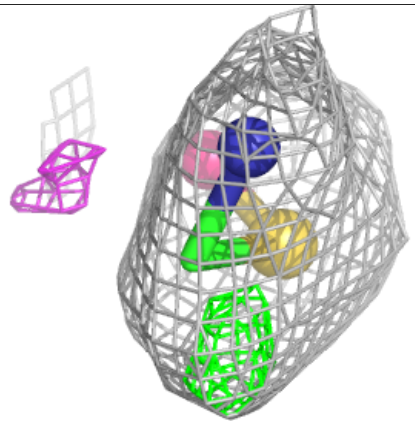


Electron density around OSM A 625:

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

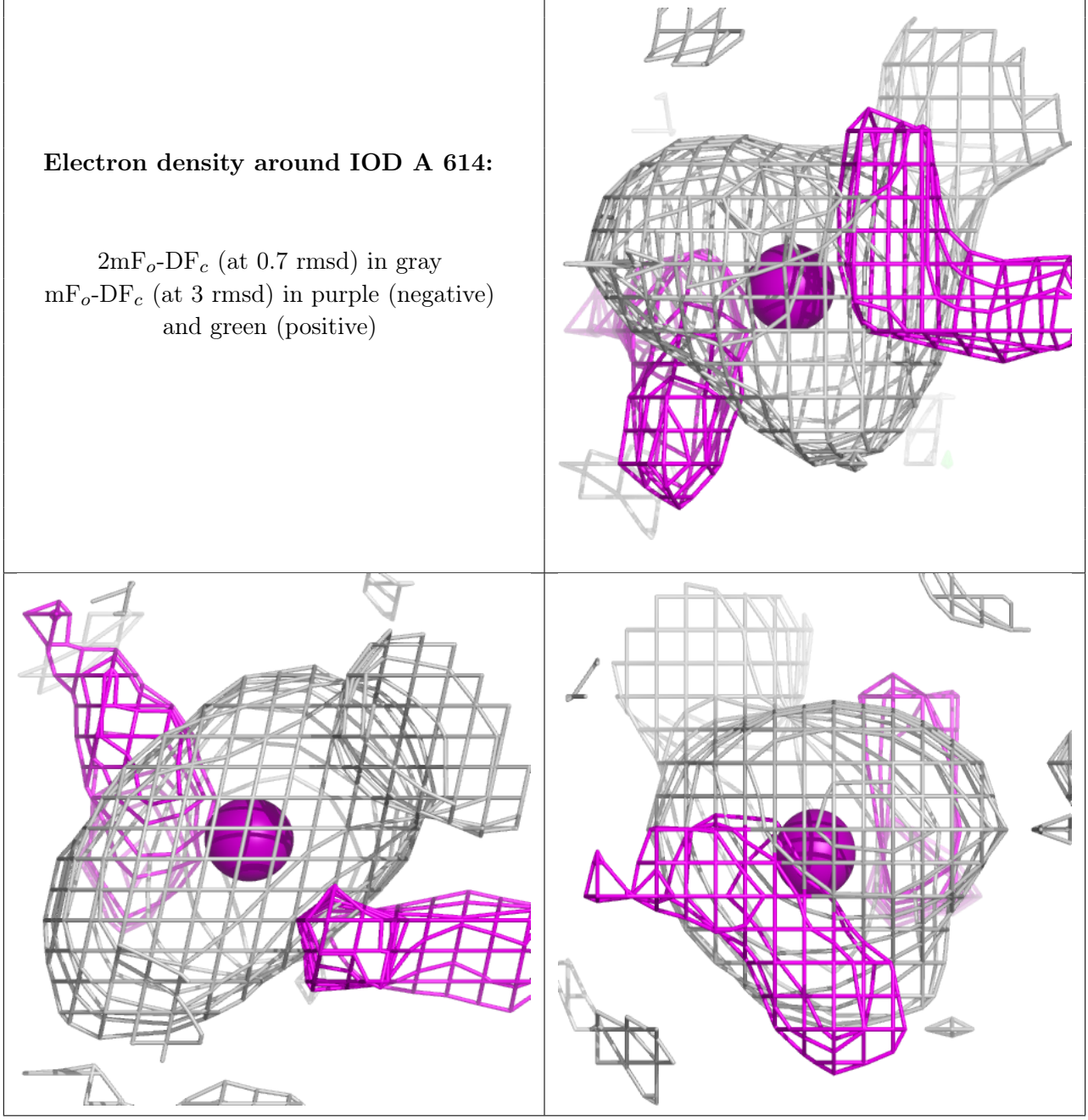






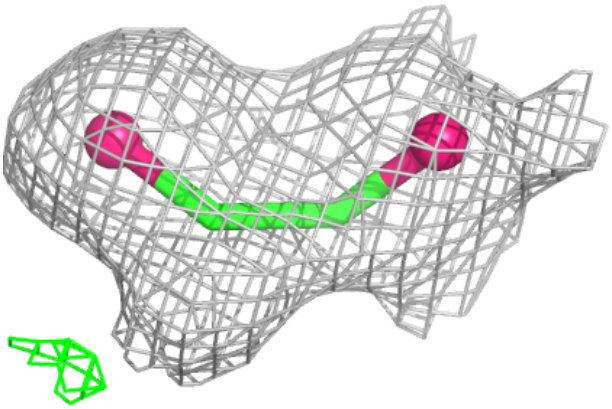
Electron density around IOD A 614:

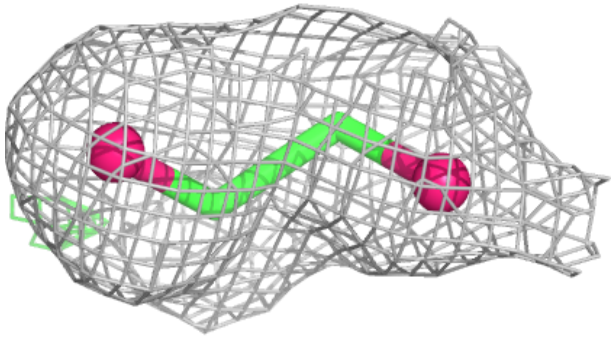
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

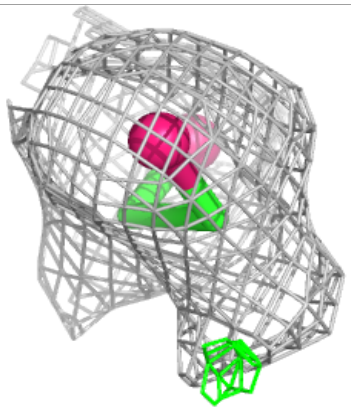


Electron density around EDO A 611:

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

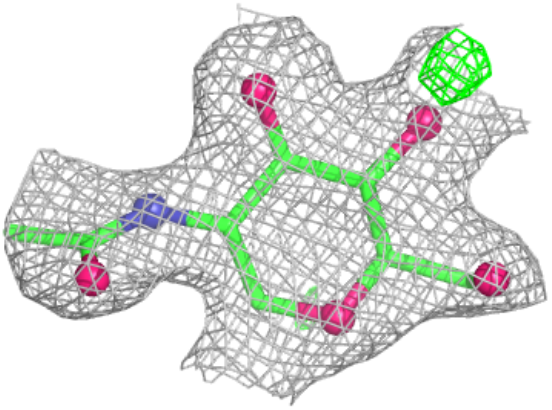


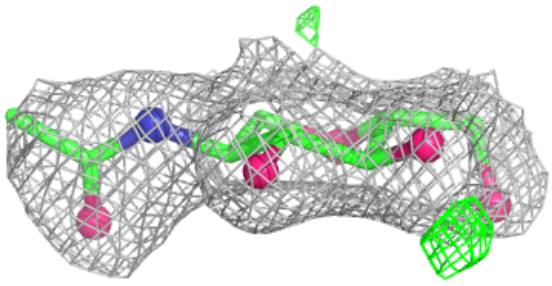


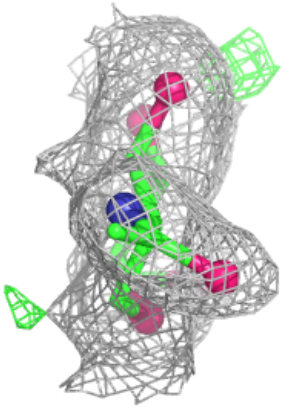


Electron density around NAG A 603:

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

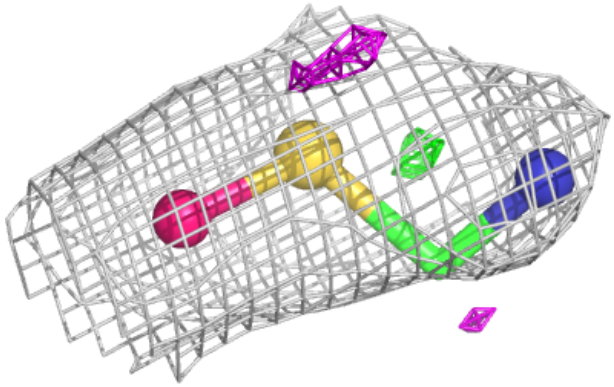


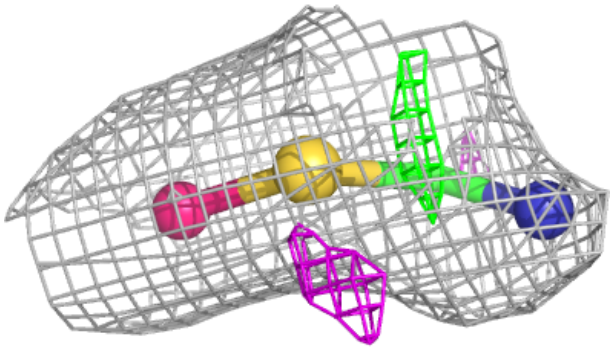


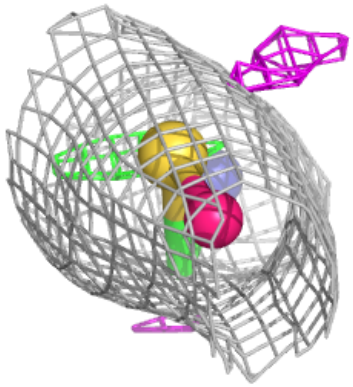


Electron density around OSM A 628:

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

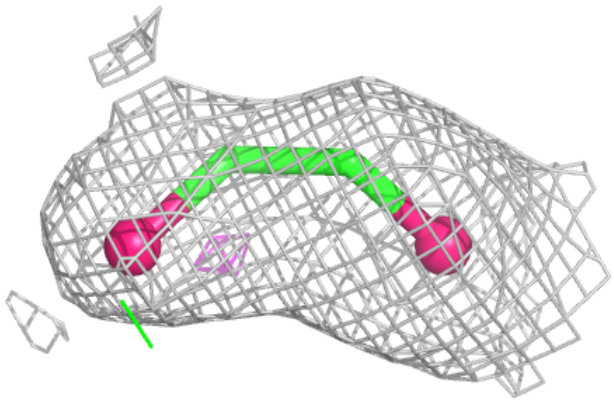


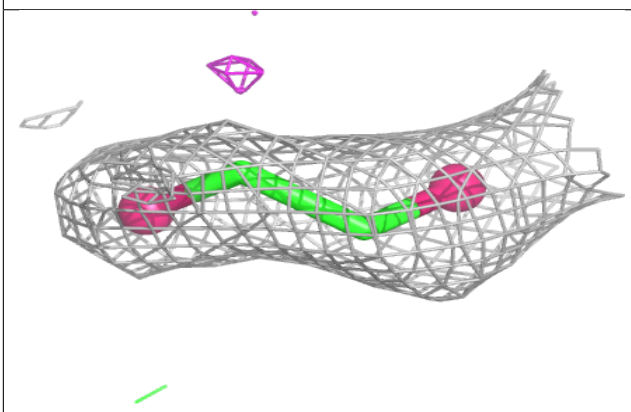


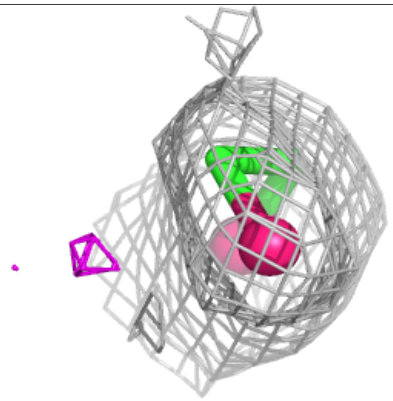


Electron density around EDO A 637:

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

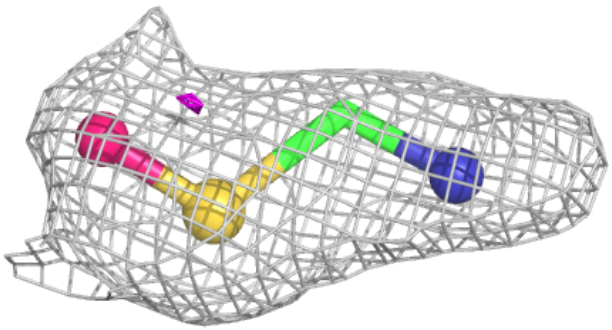


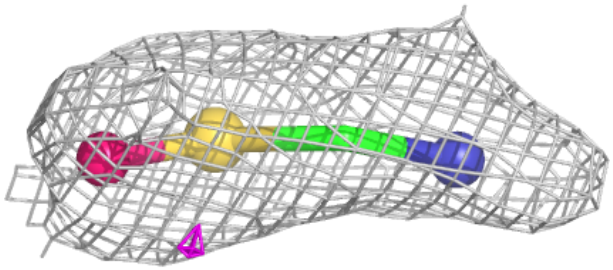


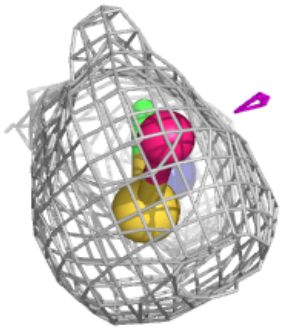


Electron density around OSM A 627:

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

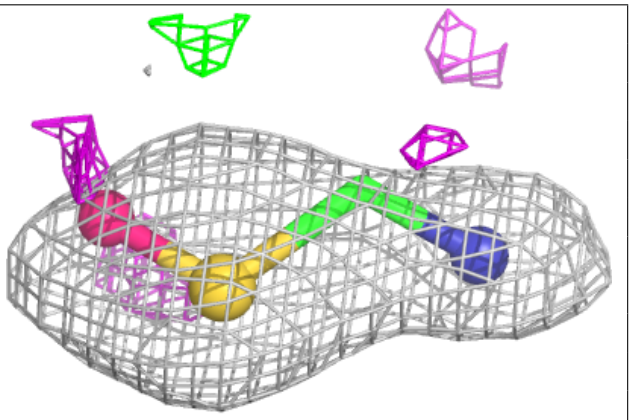


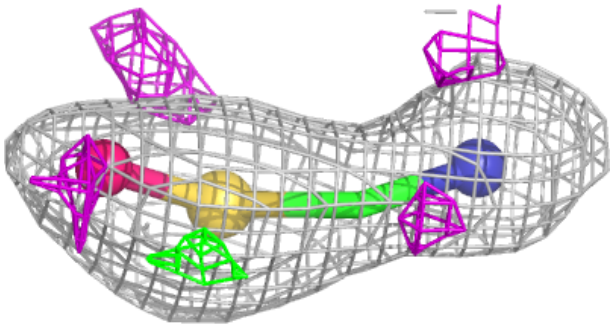


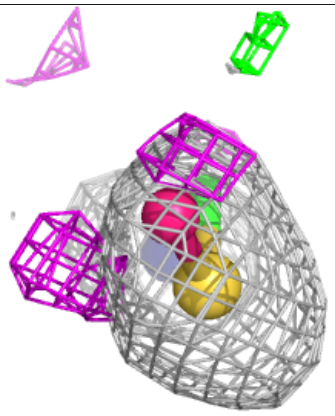


Electron density around OSM A 626:

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

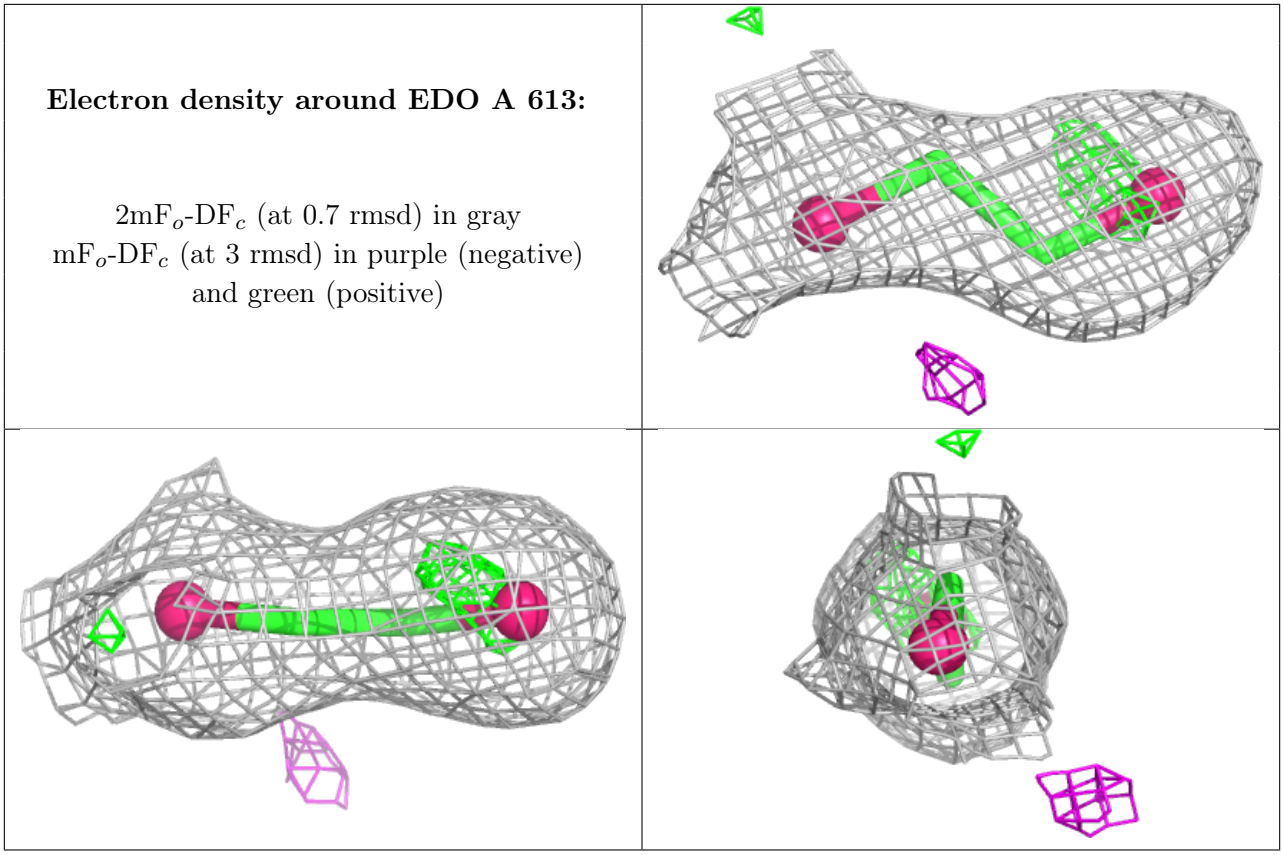






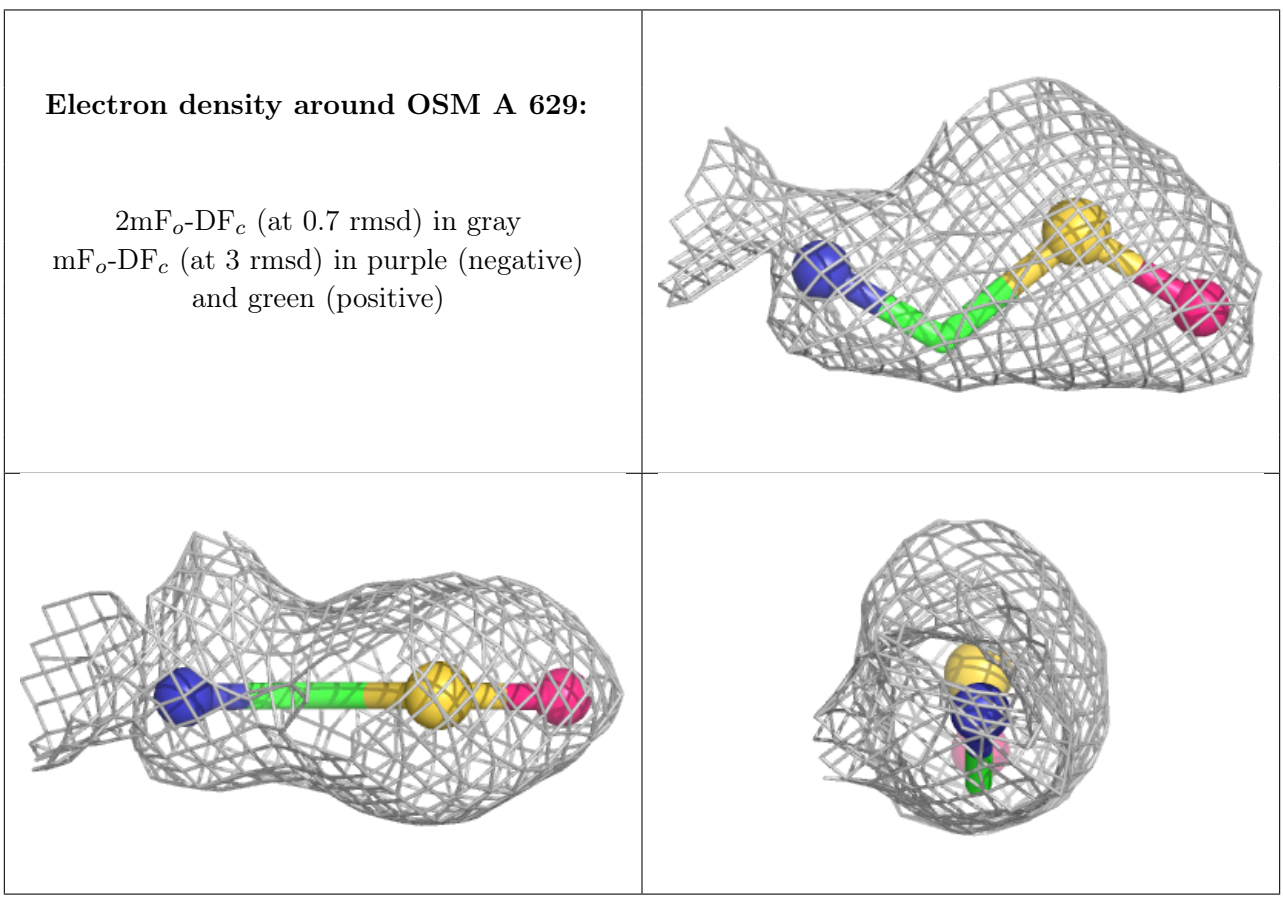
Electron density around EDO A 613:

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



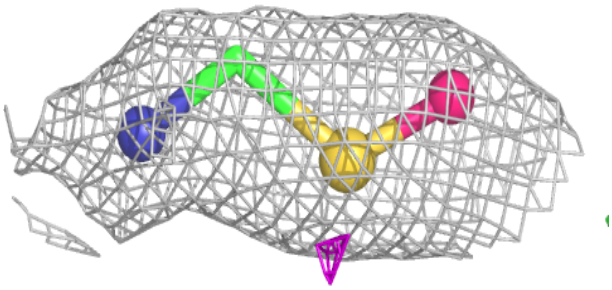
Electron density around OSM A 629:

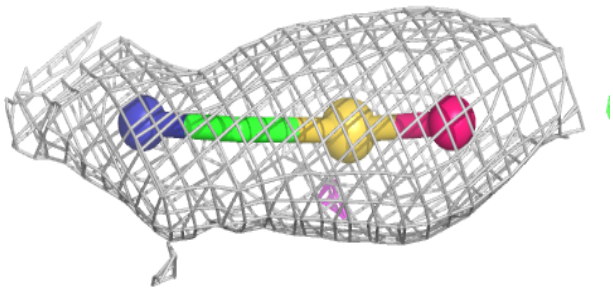
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

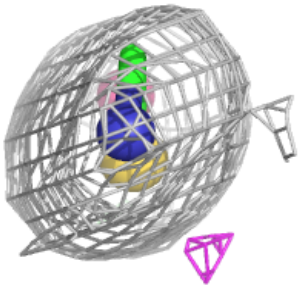


Electron density around OSM A 624:

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

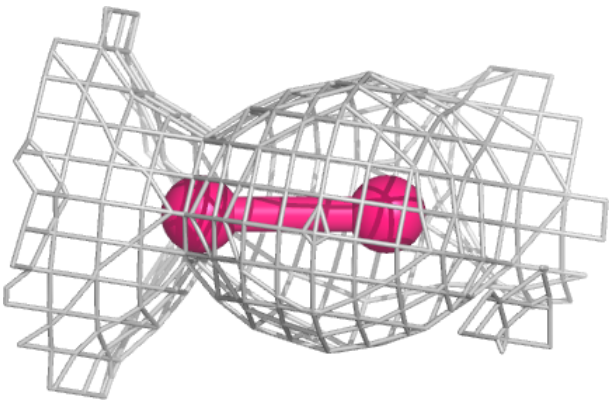


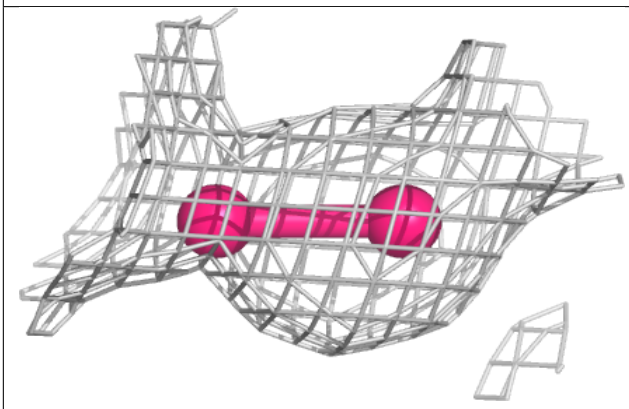


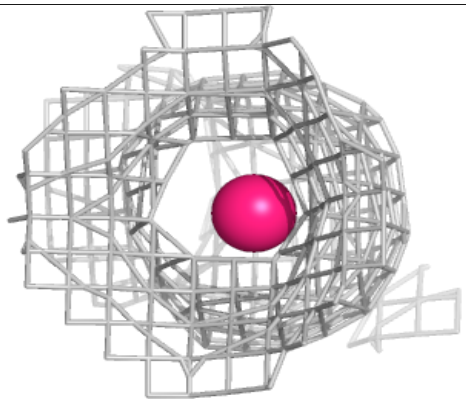


Electron density around PEO A 618:

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

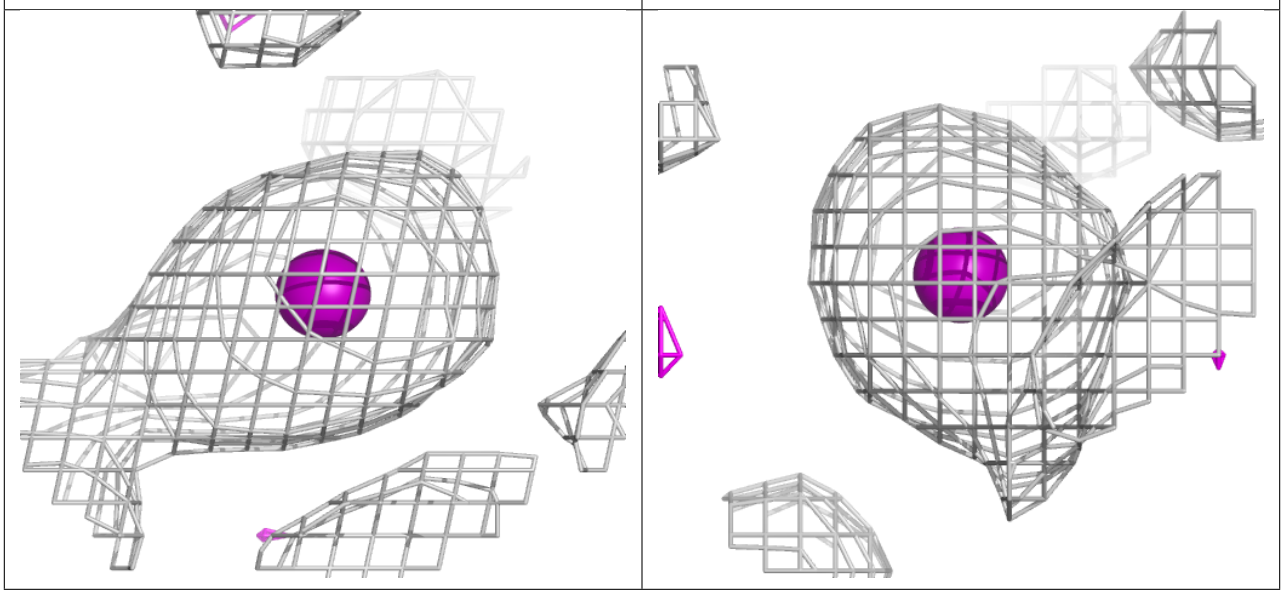






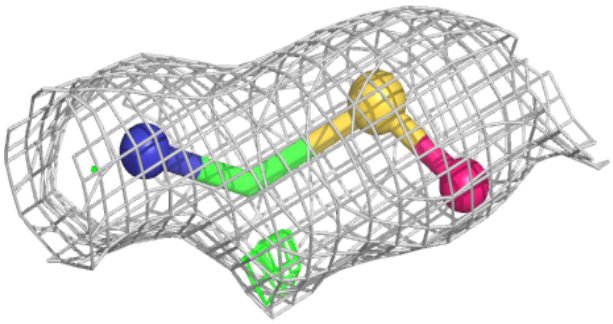
Electron density around IOD A 610:

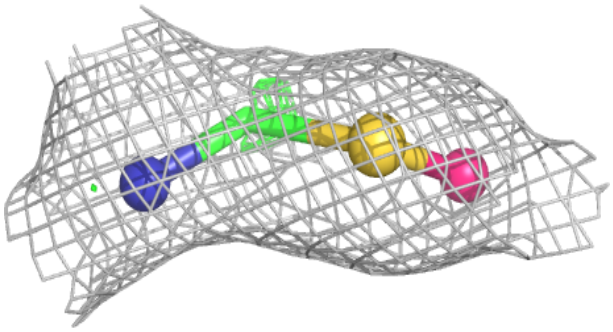
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

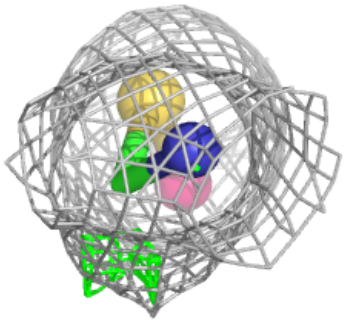


Electron density around OSM A 622 (B):

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

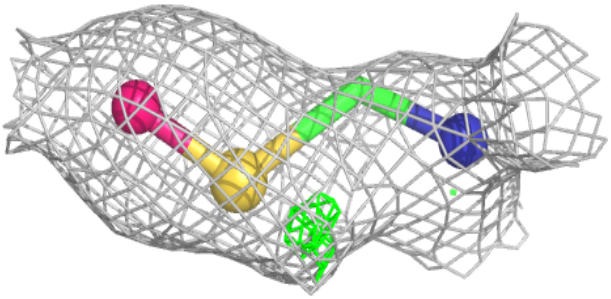


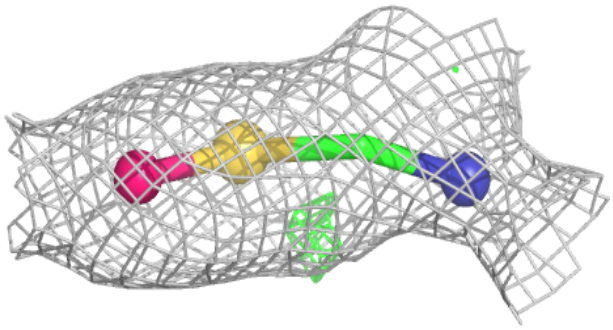


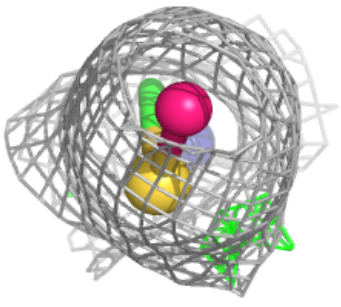


Electron density around OSM A 622 (A):

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

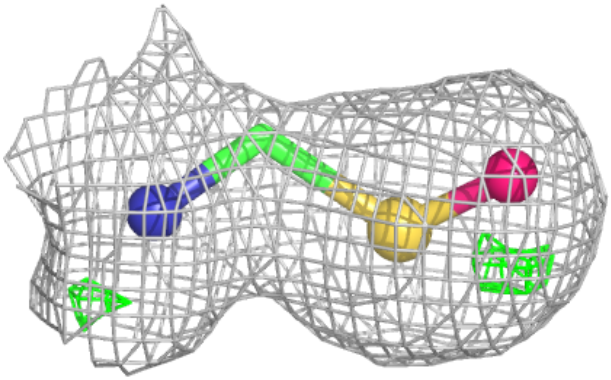


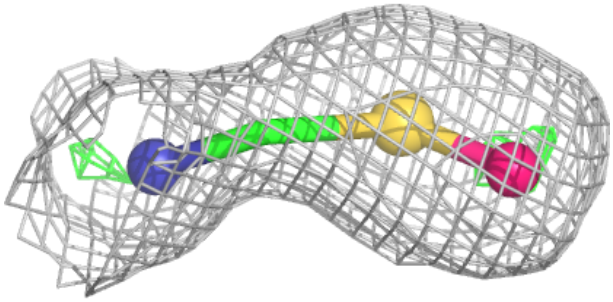


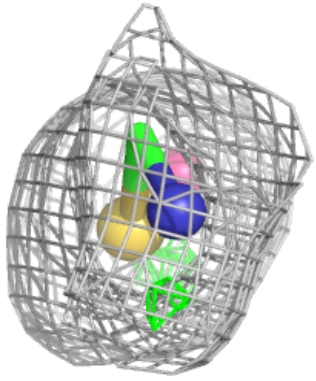


Electron density around OSM A 623:

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

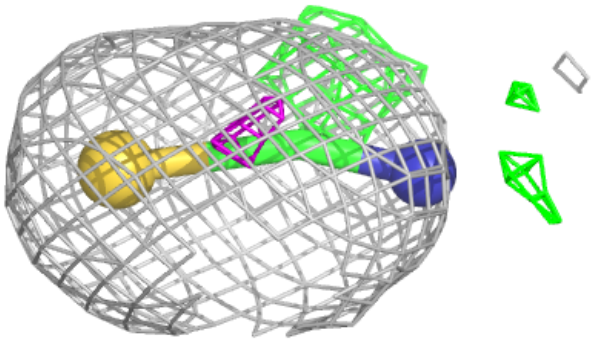


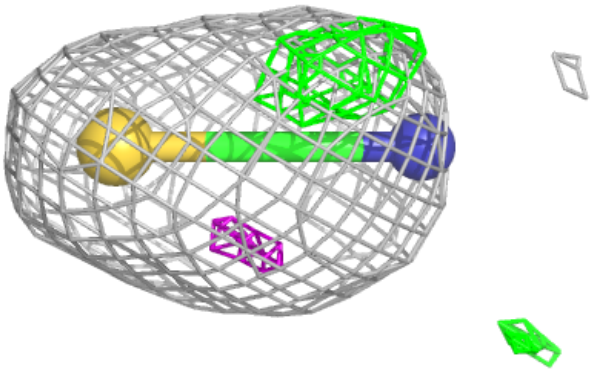


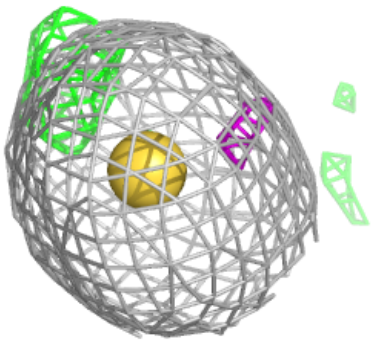


Electron density around SCN A 634:

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

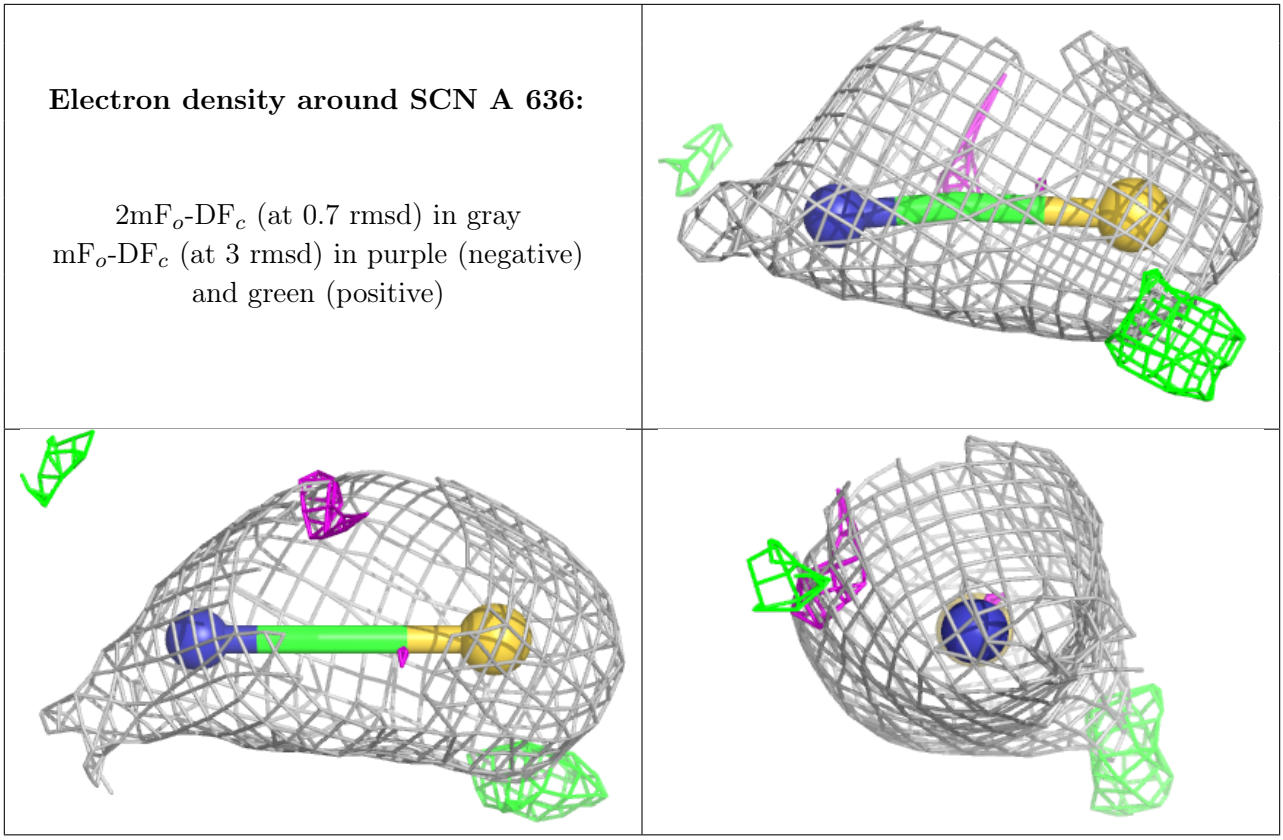






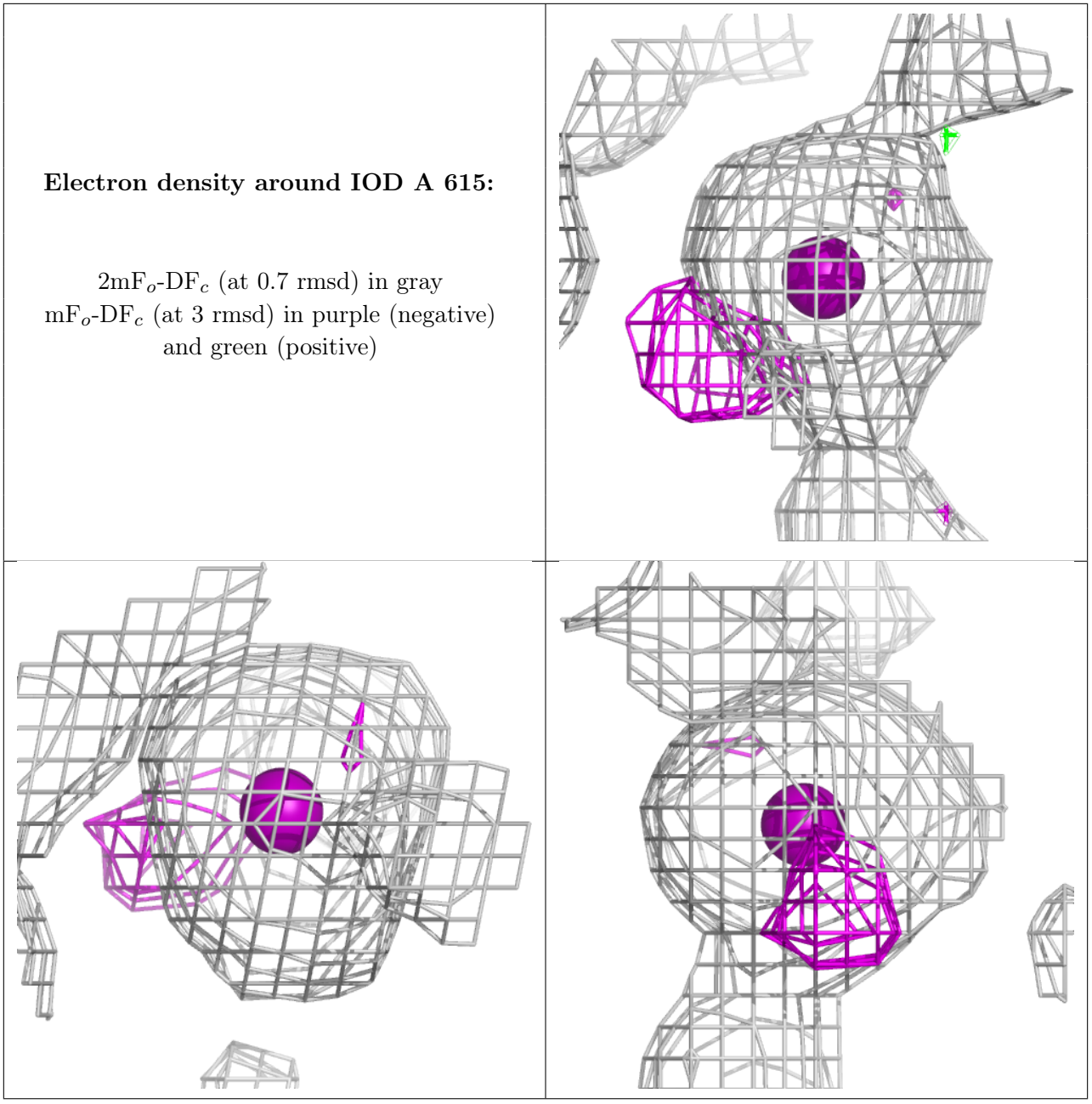
Electron density around SCN A 636:

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



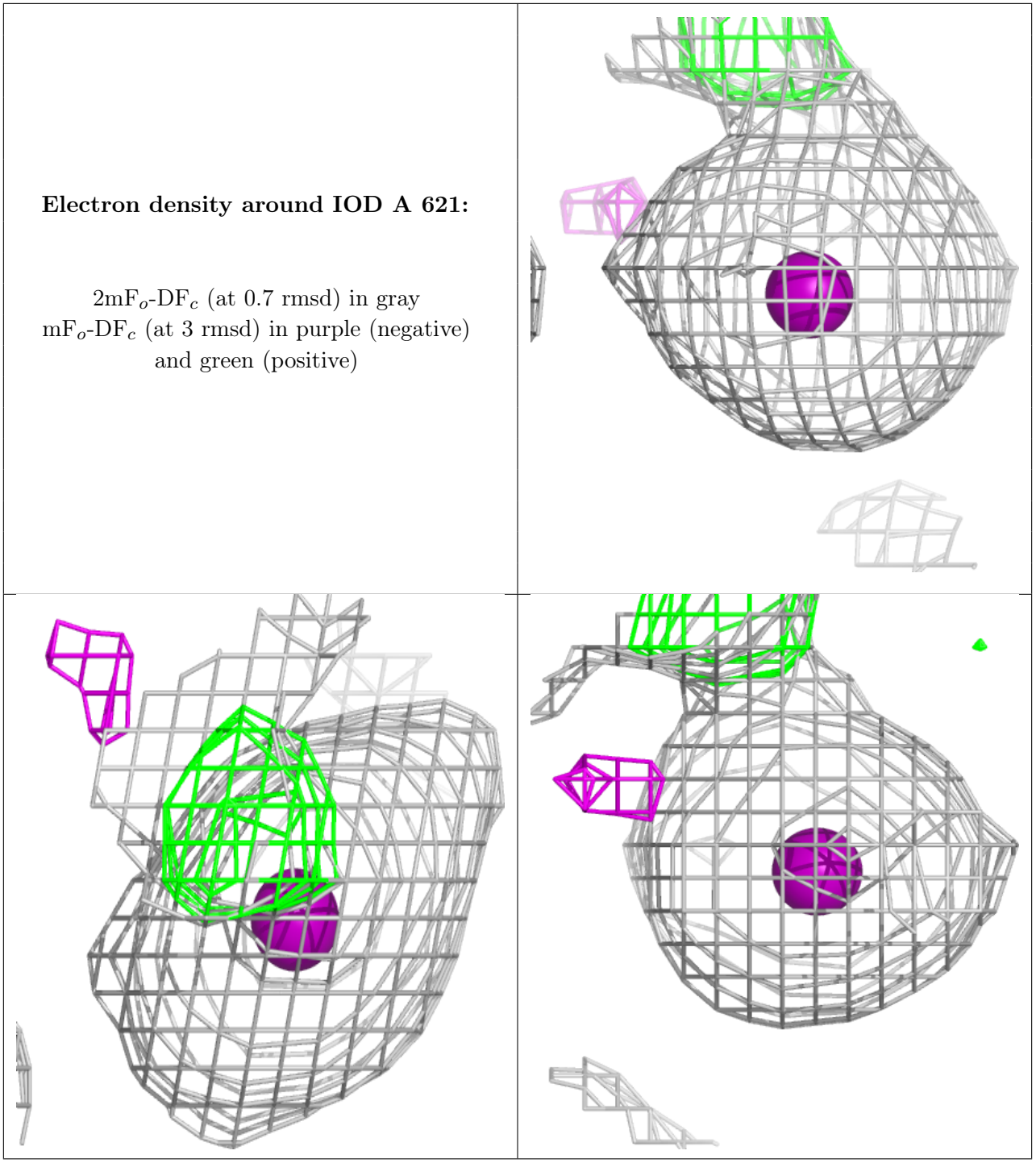
Electron density around IOD A 615:

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



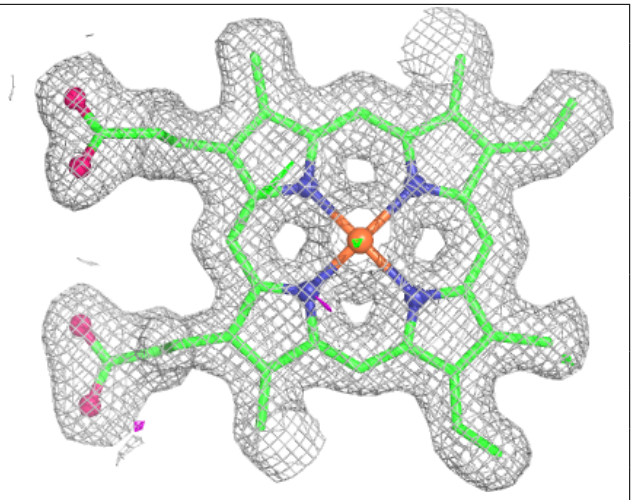
Electron density around IOD A 621:

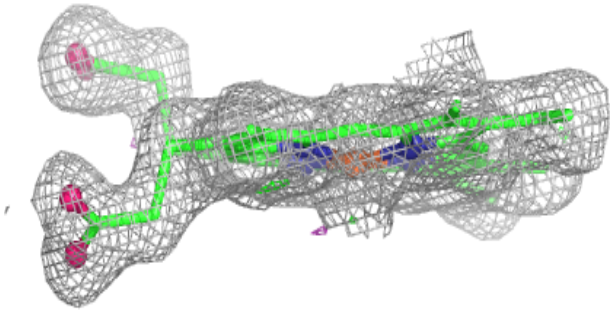
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

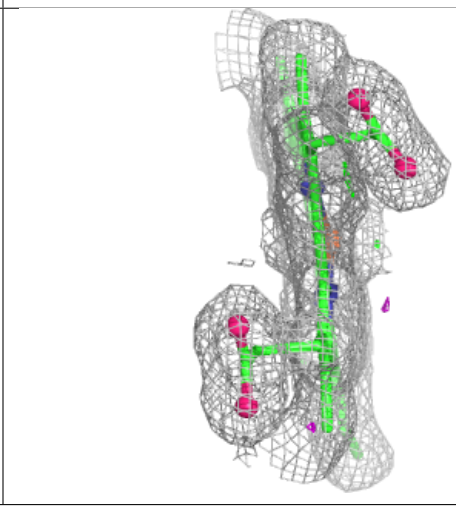


Electron density around HEM A 604:

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

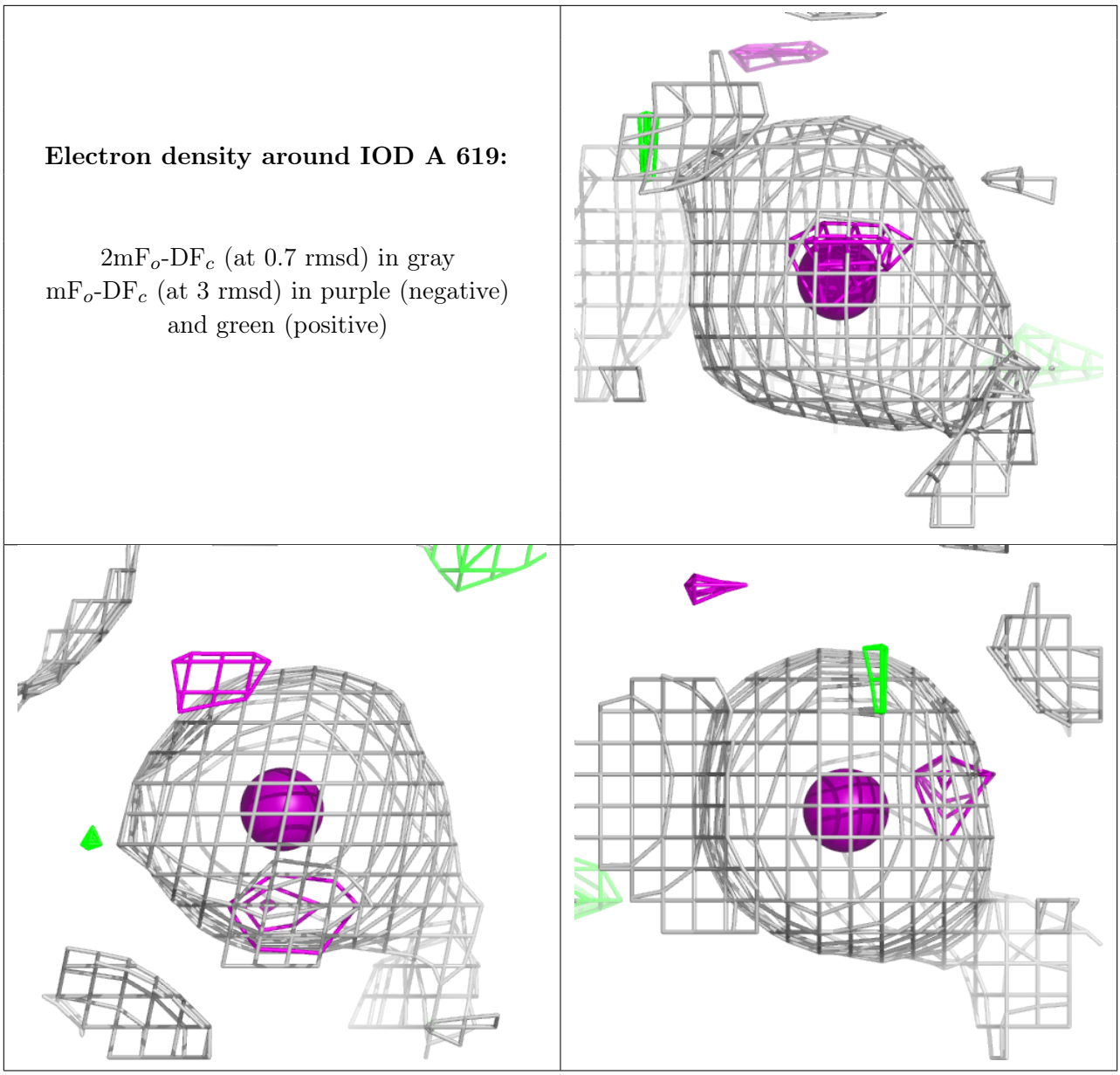






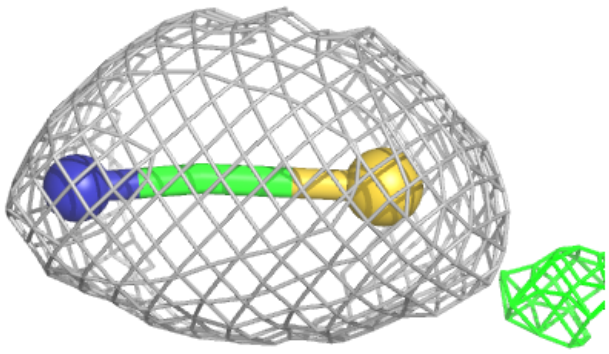
Electron density around IOD A 619:

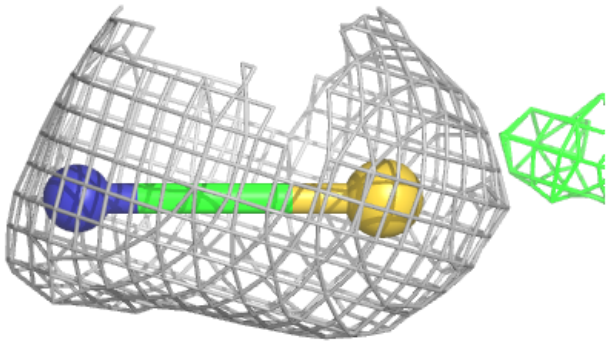
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

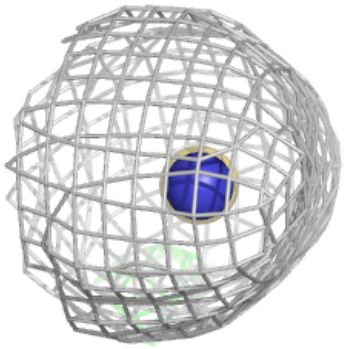


Electron density around SCN A 630:

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

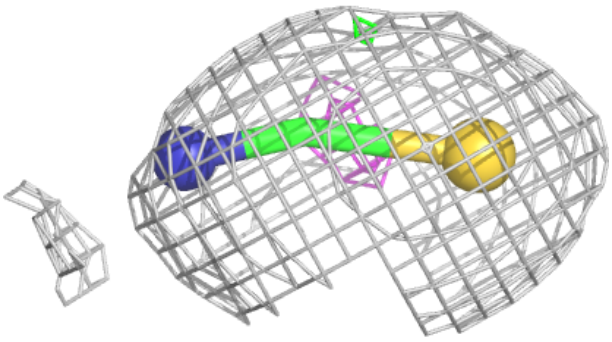


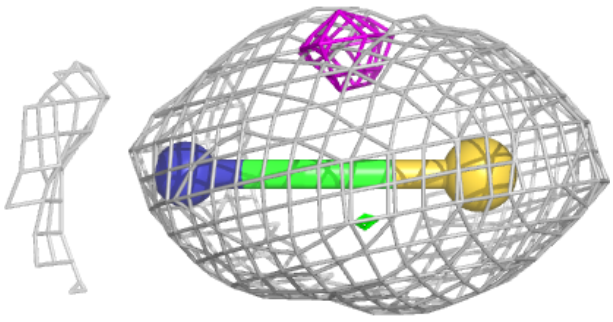


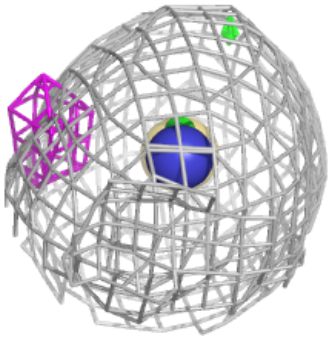


Electron density around SCN A 632:

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

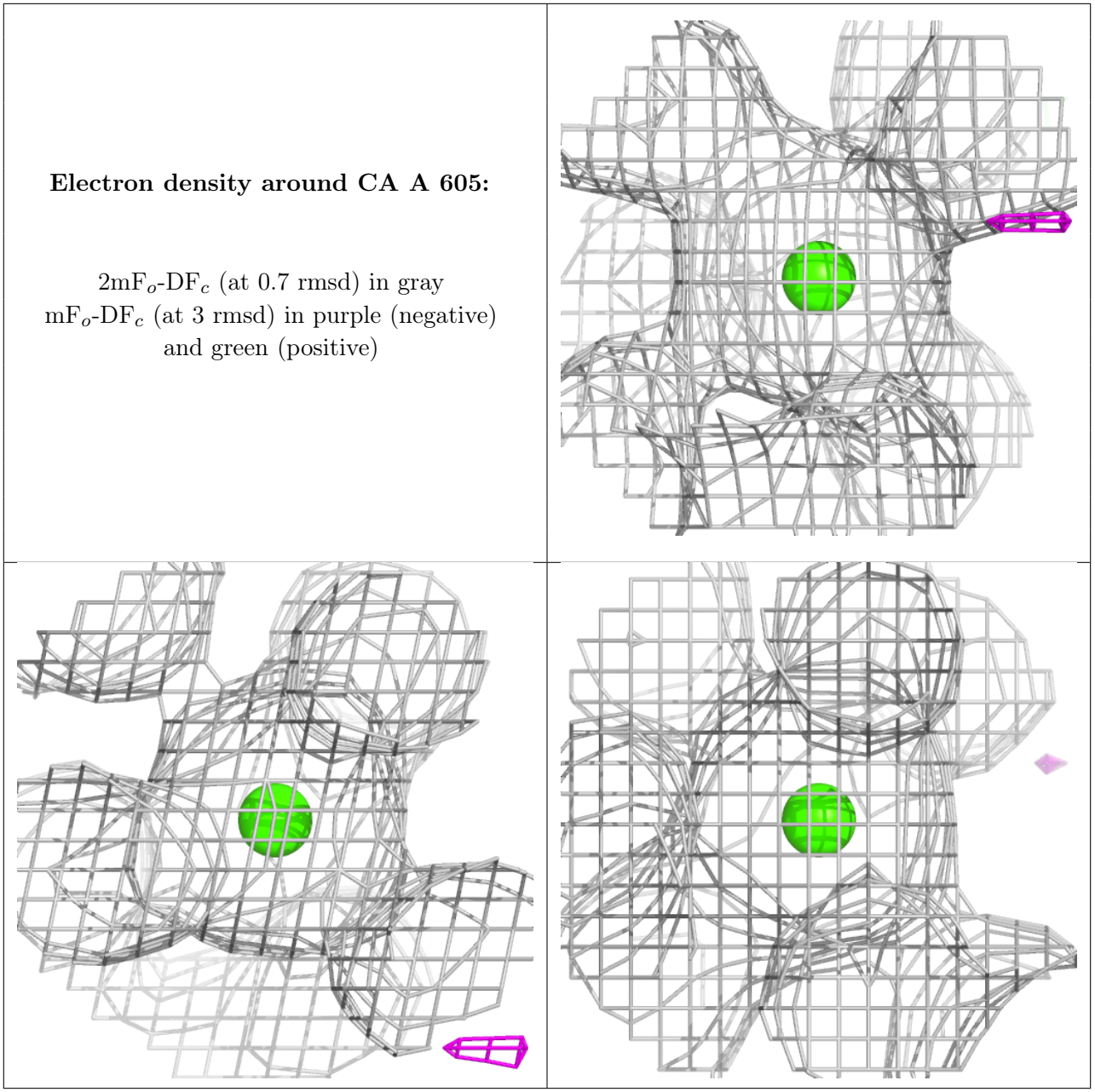






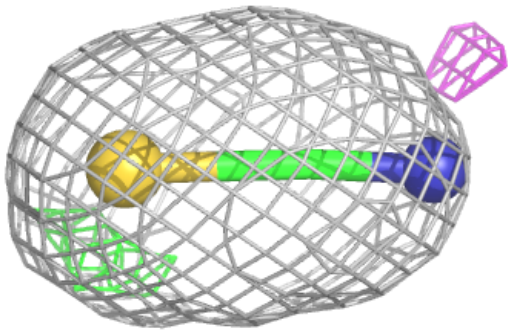
Electron density around CA A 605:

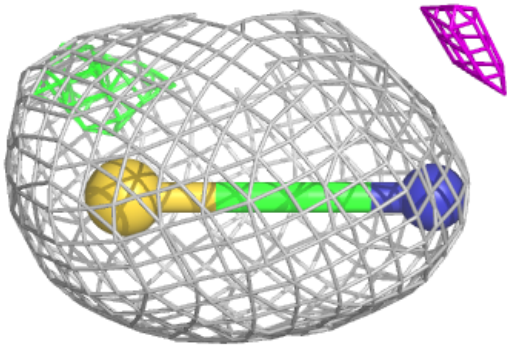
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

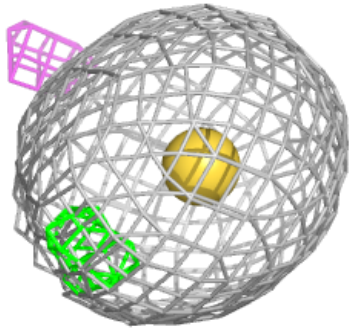


Electron density around SCN A 635:

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

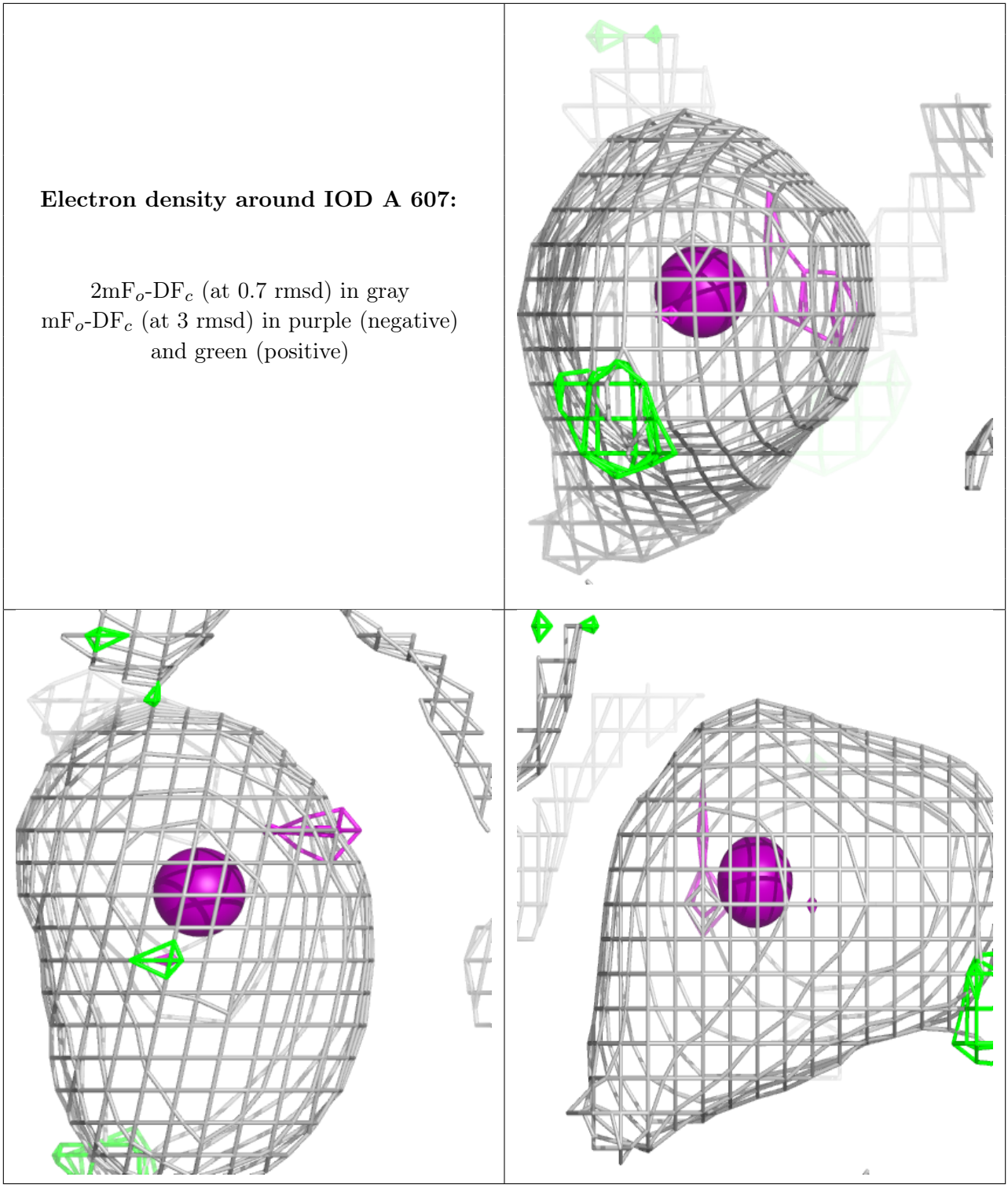






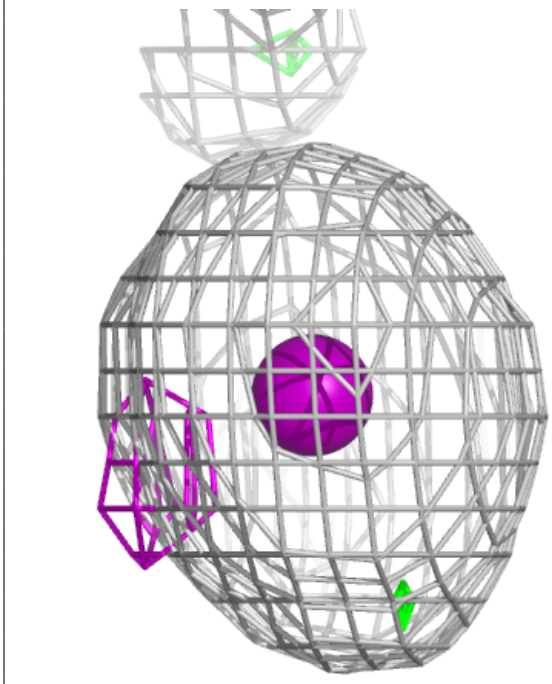
Electron density around IOD A 607:

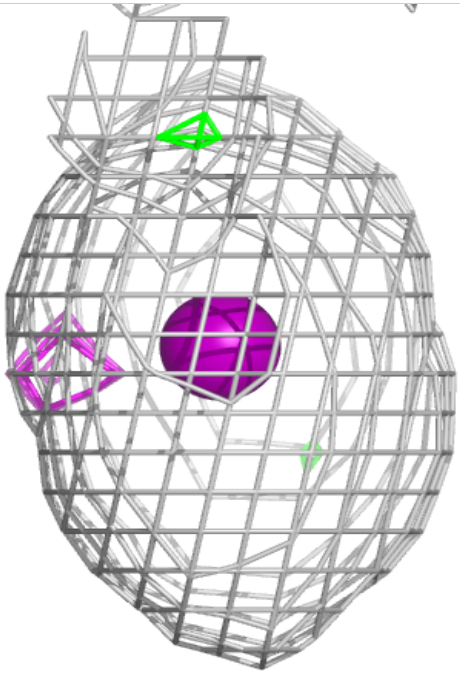
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

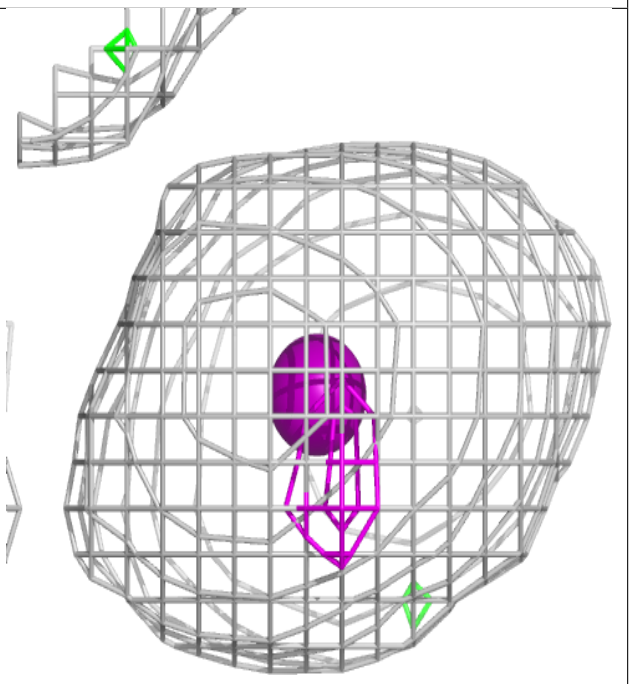


Electron density around IOD A 620:

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

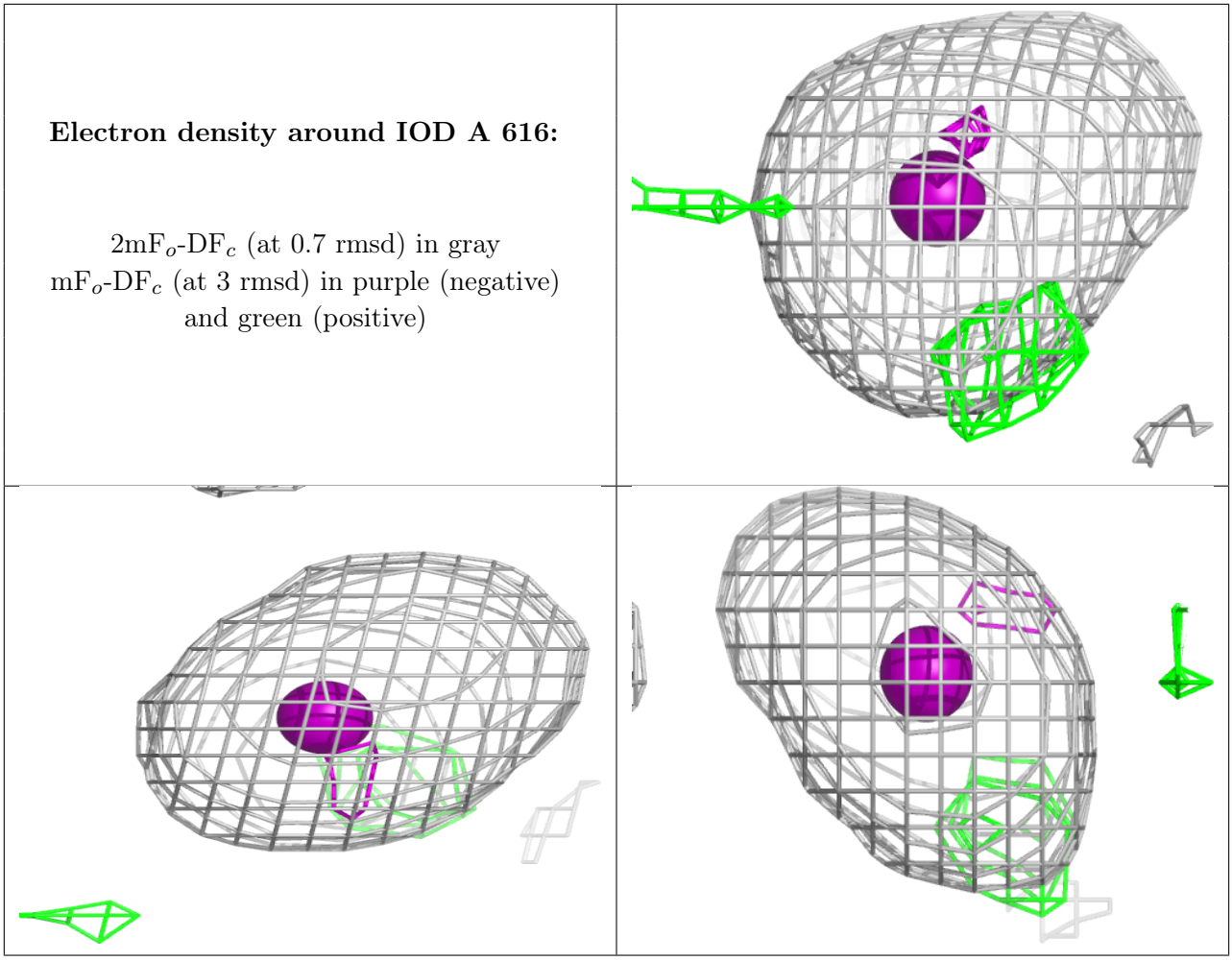






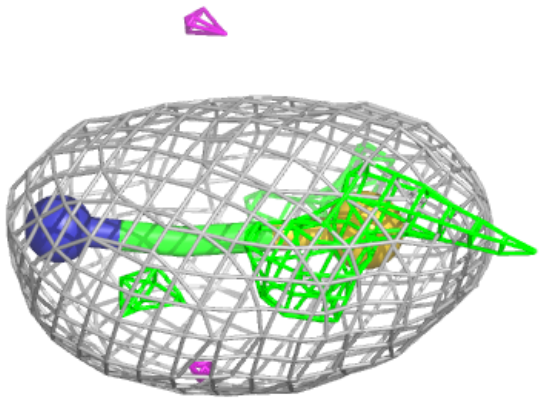
Electron density around IOD A 616:

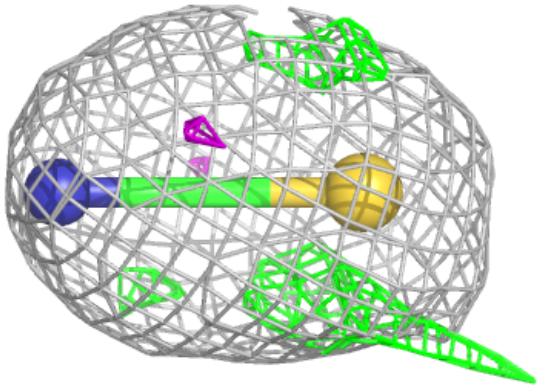
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

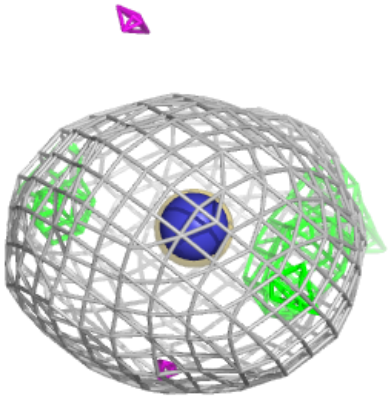


Electron density around SCN A 633:

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

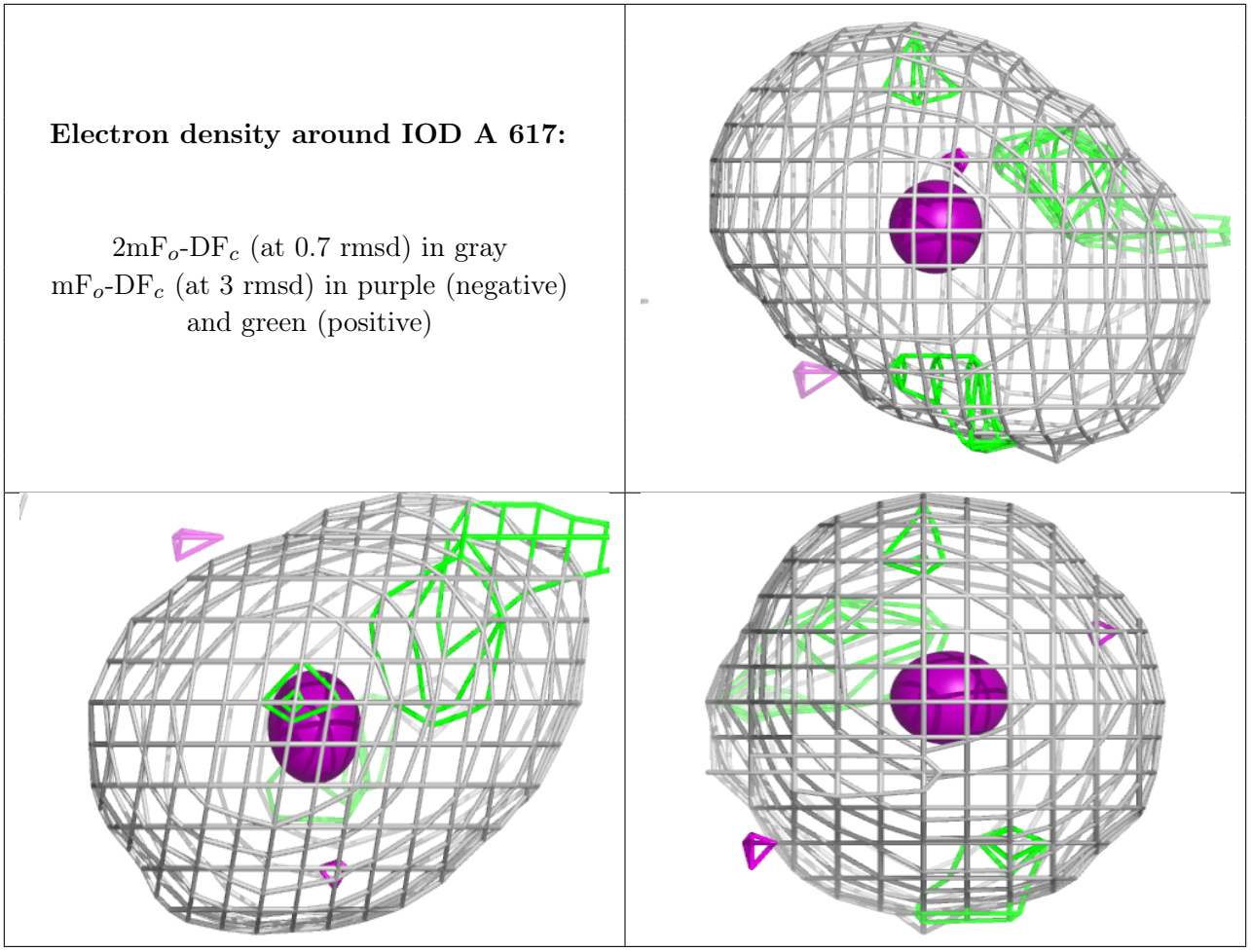






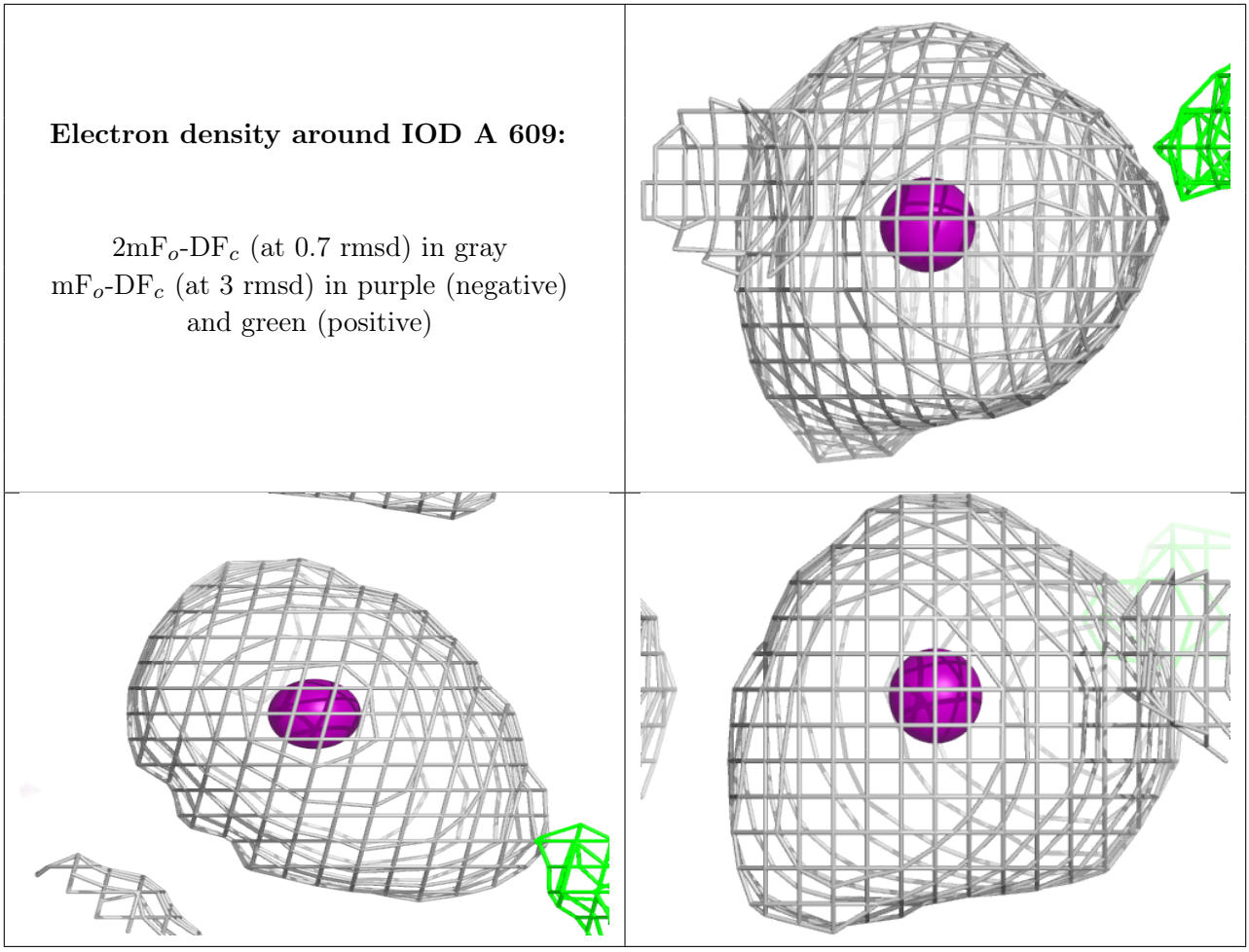
Electron density around IOD A 617:

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



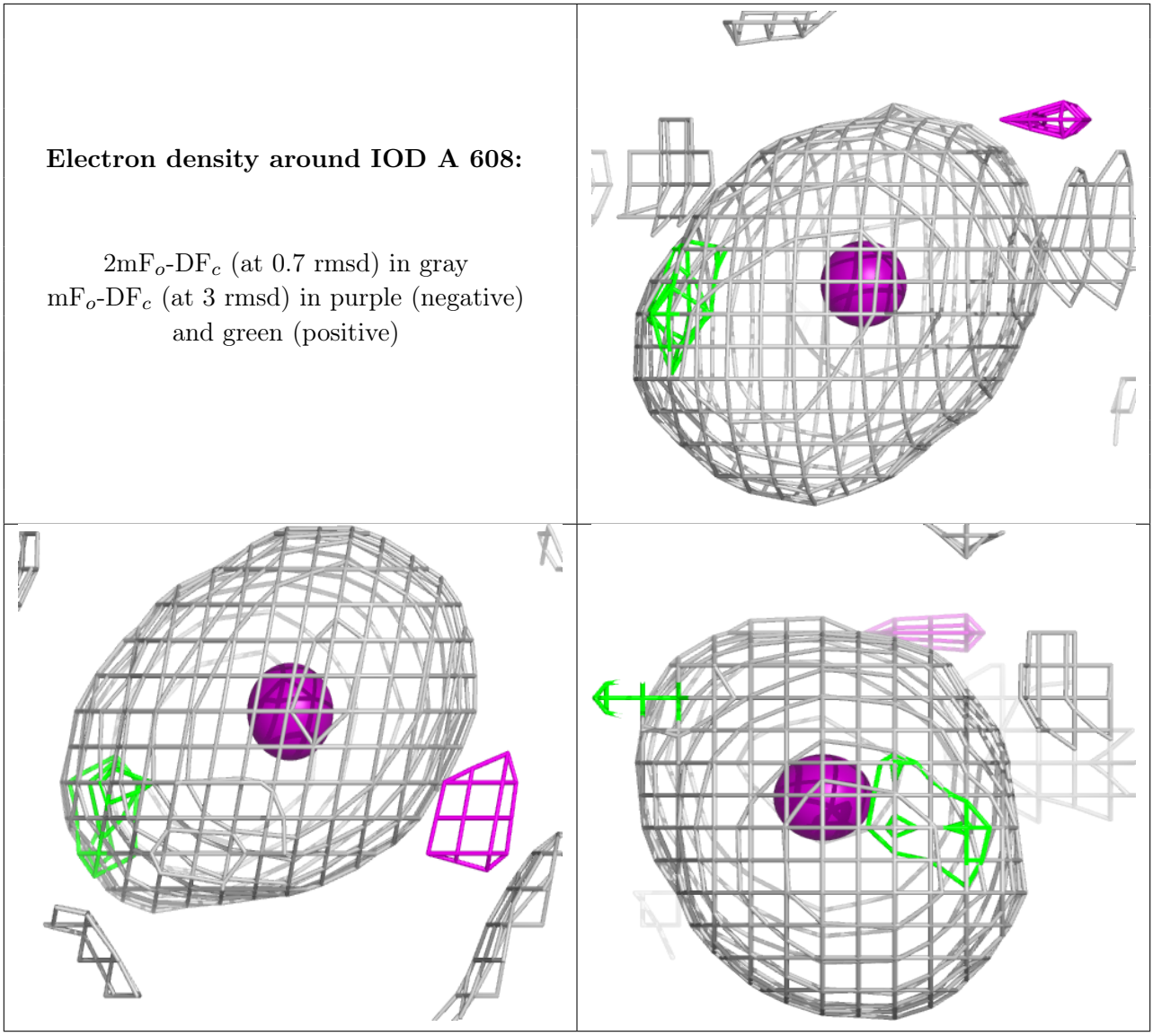
Electron density around IOD A 609:

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



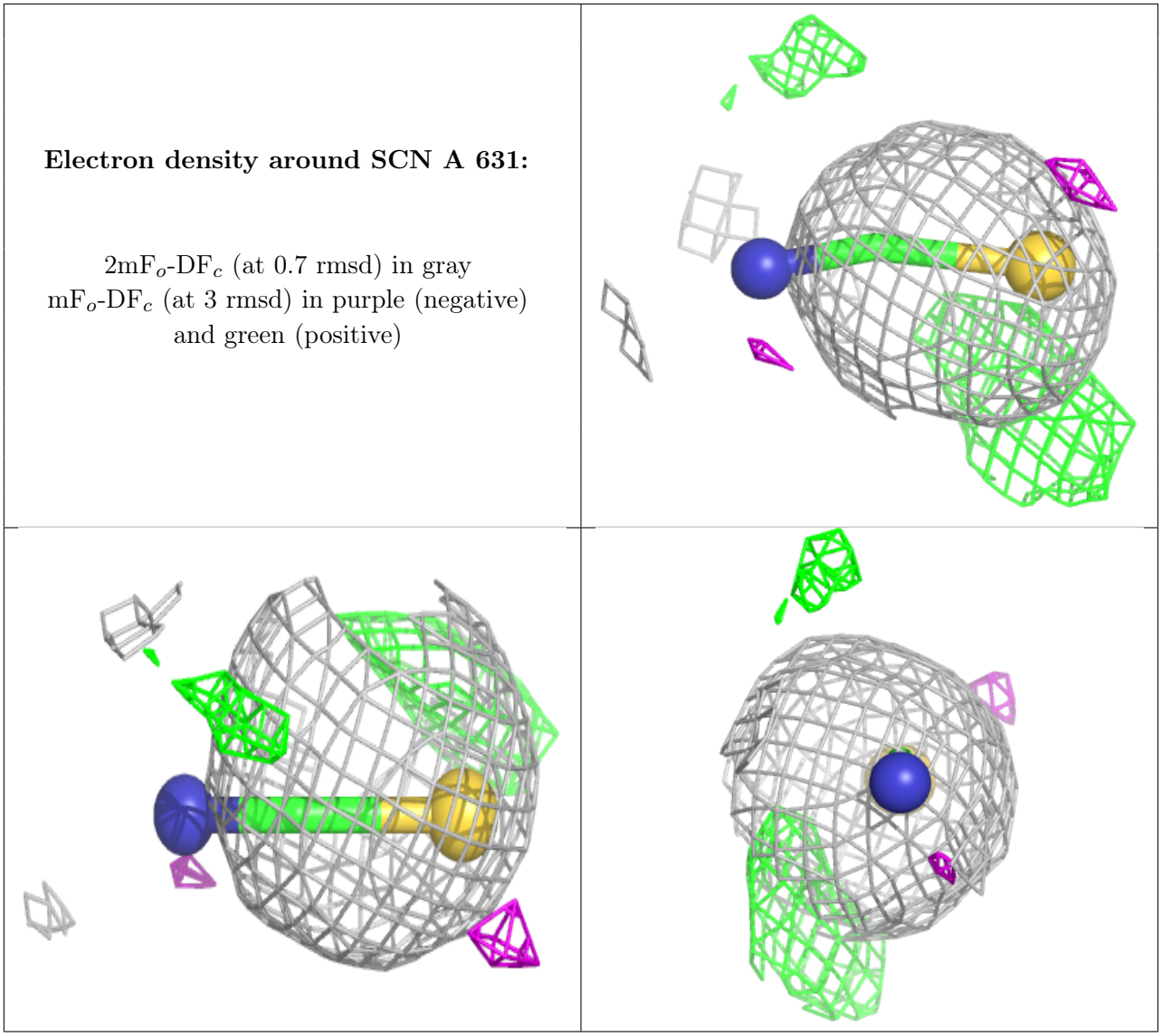
Electron density around IOD A 608:

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



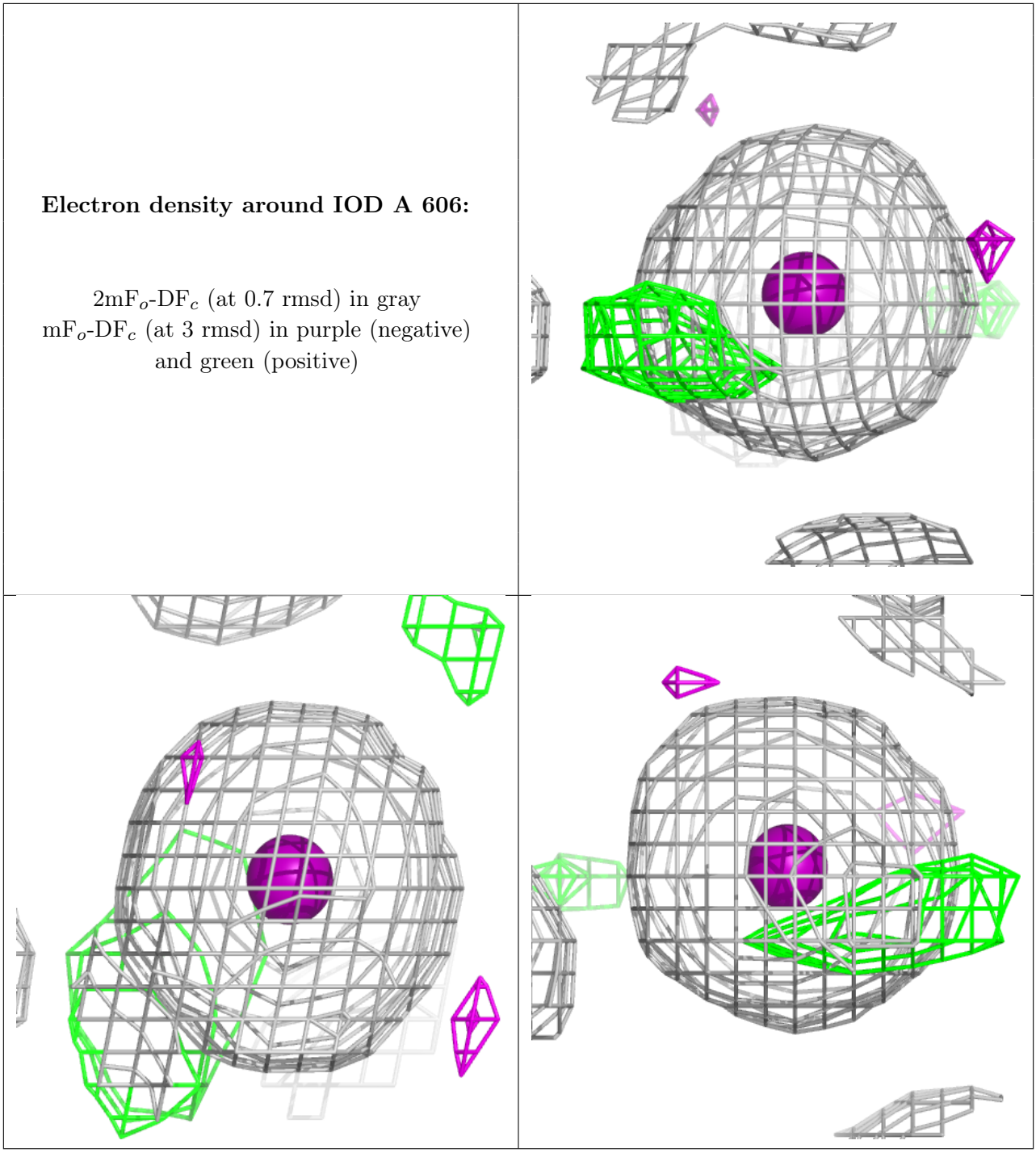
Electron density around SCN A 631:

$2mF_o$-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 606:

$2mF_o$-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.