Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2020 – 09:11 AM GMT

PDB ID	:	7AHB
Title	:	Acyltransferase domain of the polyketide synthase PpsC of Mycobacterium tuberculosis
Authors	:	Faille, A.; Mourey, L.; Pedelacq, J.D.
Deposited on	:	2020-09-24
Resolution	:	1.90 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:

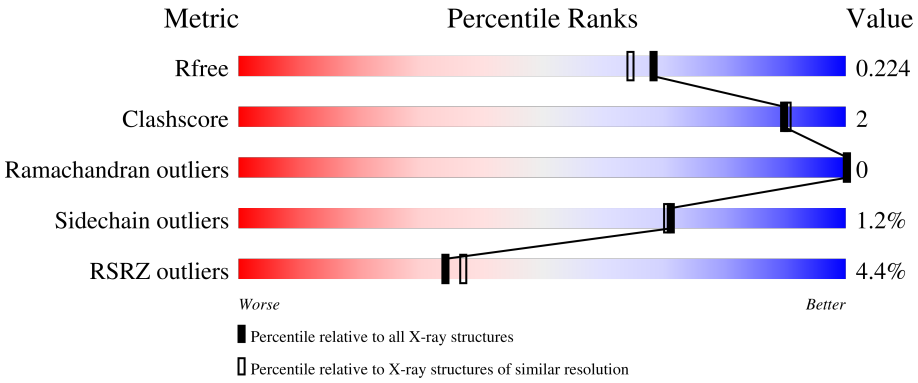
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	360	4% 88% . 9%
1	B	360	4% 86% 5% 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10377 atoms, of which 4868 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 Phthiocerol synthesis polyketide synthase type I PpsC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	329	Total	C	H	N	O	S	0	3	0
			4877	1538	2431	432	467	9			
1	B	329	Total	C	H	N	O	S	0	2	0
			4867	1536	2426	431	465	9			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	523	MET	-	initiating methionine	UNP P96202
A	524	GLY	-	expression tag	UNP P96202
A	525	SER	-	expression tag	UNP P96202
A	526	SER	-	expression tag	UNP P96202
A	527	HIS	-	expression tag	UNP P96202
A	528	HIS	-	expression tag	UNP P96202
A	529	HIS	-	expression tag	UNP P96202
A	530	HIS	-	expression tag	UNP P96202
A	531	HIS	-	expression tag	UNP P96202
A	532	HIS	-	expression tag	UNP P96202
A	533	SER	-	expression tag	UNP P96202
A	534	SER	-	expression tag	UNP P96202
A	535	GLY	-	expression tag	UNP P96202
A	536	LEU	-	expression tag	UNP P96202
A	537	VAL	-	expression tag	UNP P96202
A	538	PRO	-	expression tag	UNP P96202
A	539	ARG	-	expression tag	UNP P96202
A	540	GLY	-	expression tag	UNP P96202
A	541	SER	-	expression tag	UNP P96202
A	542	HIS	-	expression tag	UNP P96202
A	543	MET	-	expression tag	UNP P96202
A	544	SER	-	expression tag	UNP P96202
A	545	GLY	-	expression tag	UNP P96202
A	877	ALA	-	expression tag	UNP P96202
A	878	SER	-	expression tag	UNP P96202

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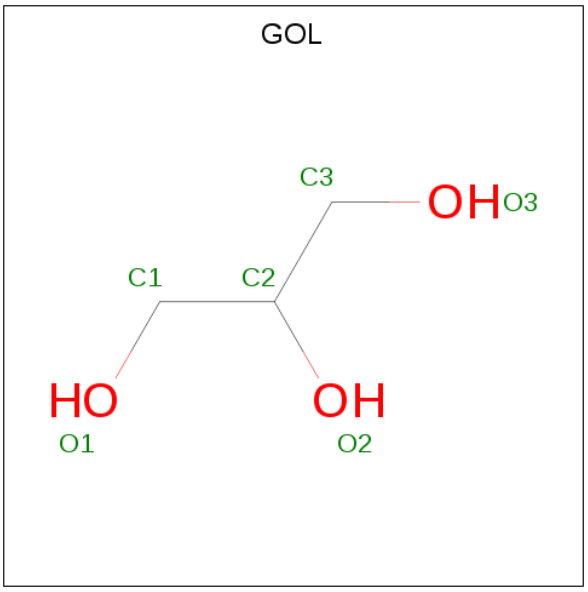
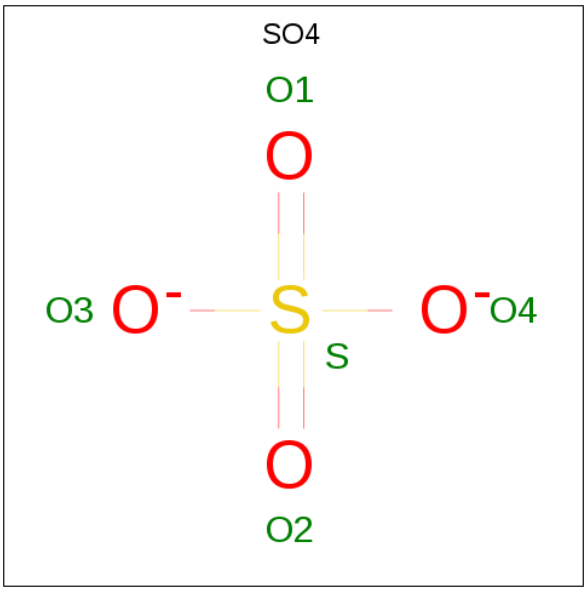
Chain	Residue	Modelled	Actual	Comment	Reference
A	879	THR	-	expression tag	UNP P96202
A	880	SER	-	expression tag	UNP P96202
A	881	GLY	-	expression tag	UNP P96202
A	882	SER	-	expression tag	UNP P96202
B	523	MET	-	initiating methionine	UNP P96202
B	524	GLY	-	expression tag	UNP P96202
B	525	SER	-	expression tag	UNP P96202
B	526	SER	-	expression tag	UNP P96202
B	527	HIS	-	expression tag	UNP P96202
B	528	HIS	-	expression tag	UNP P96202
B	529	HIS	-	expression tag	UNP P96202
B	530	HIS	-	expression tag	UNP P96202
B	531	HIS	-	expression tag	UNP P96202
B	532	HIS	-	expression tag	UNP P96202
B	533	SER	-	expression tag	UNP P96202
B	534	SER	-	expression tag	UNP P96202
B	535	GLY	-	expression tag	UNP P96202
B	536	LEU	-	expression tag	UNP P96202
B	537	VAL	-	expression tag	UNP P96202
B	538	PRO	-	expression tag	UNP P96202
B	539	ARG	-	expression tag	UNP P96202
B	540	GLY	-	expression tag	UNP P96202
B	541	SER	-	expression tag	UNP P96202
B	542	HIS	-	expression tag	UNP P96202
B	543	MET	-	expression tag	UNP P96202
B	544	SER	-	expression tag	UNP P96202
B	545	GLY	-	expression tag	UNP P96202
B	877	ALA	-	expression tag	UNP P96202
B	878	SER	-	expression tag	UNP P96202
B	879	THR	-	expression tag	UNP P96202
B	880	SER	-	expression tag	UNP P96202
B	881	GLY	-	expression tag	UNP P96202
B	882	SER	-	expression tag	UNP P96202

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by author).



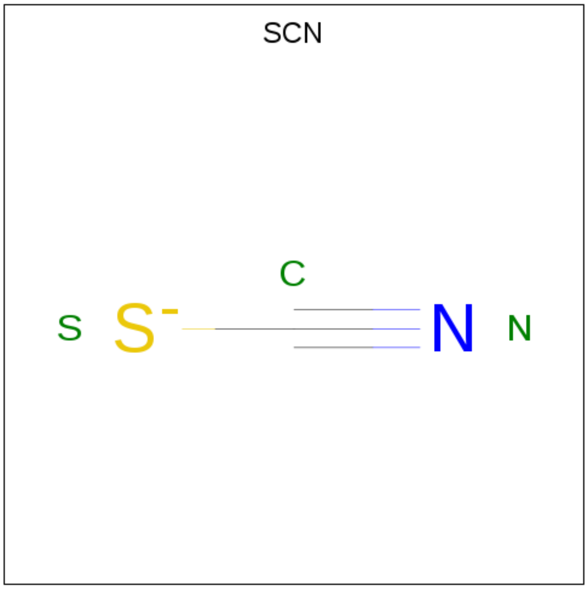
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 9 3 3 3	0	0
2	B	1	Total C H O 14 3 8 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS) (labeled as "Ligand of Interest" by author).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N S 3 1 1 1	0	0
4	B	1	Total C N S 3 1 1 1	0	0
4	B	1	Total C N S 3 1 1 1	0	0
4	B	1	Total C N S 3 1 1 1	0	0
4	B	1	Total C N S 3 1 1 1	0	0
4	B	1	Total C N S 3 1 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	4	Total Na 4 4	0	0
5	A	4	Total Na 4 4	0	0

- Molecule 6 is water.

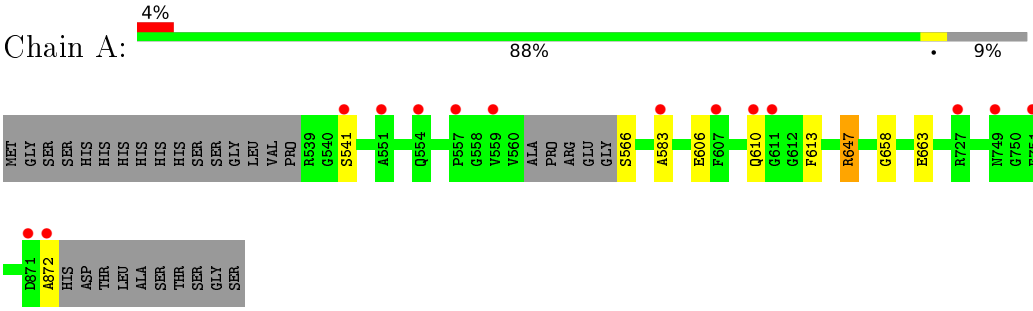
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	267	Total O 267 267	0	0
6	B	276	Total O 276 276	0	0

3 Residue-property plots (i)

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

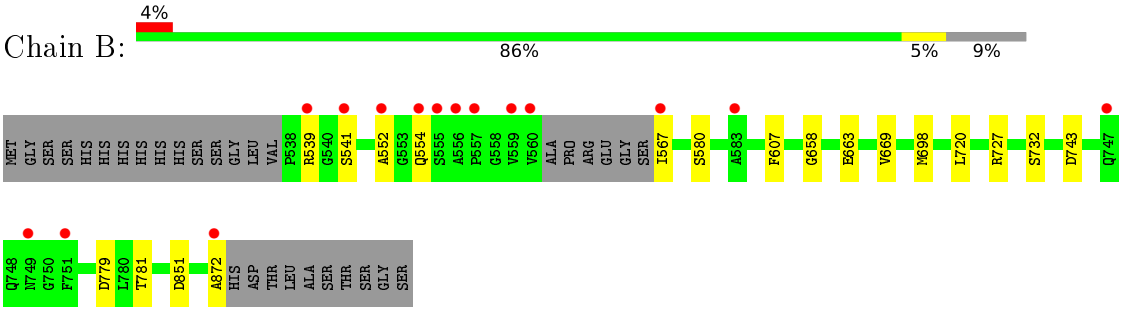
- Molecule 1: Phthiocerol synthesis polyketide synthase type I PpsC

Chain A:



- Molecule 1: Phthiocerol synthesis polyketide synthase type I PpsC

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.37Å 58.35Å 65.86Å 65.84° 73.28° 71.02°	Depositor
Resolution (Å)	48.12 – 1.90 48.12 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (48.12-1.90) 84.4 (48.12-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.37 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.188 , 0.224 0.188 , 0.224	Depositor DCC
R_{free} test set	1965 reflections (3.40%)	wwPDB-VP
Wilson B-factor (Å^2)	16.7	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10377	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.31% 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: GOL, SCN, SO4, NA

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	0.46	0/2502	0.57	0/3408
1	B	0.44	0/2496	0.54	0/3401
All	All	0.45	0/4998	0.56	0/6809

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	2446	2431	2427	8	1
1	B	2441	2426	2420	10	1
2	A	6	3	7	0	0
2	B	6	8	8	1	0
3	A	5	0	0	0	0
4	A	30	0	0	1	0
4	B	24	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	267	0	0	1	1
6	B	276	0	0	0	1
All	All	5509	4868	4862	18	2

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 2.

All (18) 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:647:ARG:HH11	1:A:647:ARG:HG3	1.57	0.68
1:B:779:ASP:O	1:B:781:THR:HG23	2.03	0.58
1:B:658:GLY:HA3	1:B:663:GLU:HA	1.89	0.55
1:A:658:GLY:HA3	1:A:663:GLU:HA	1.91	0.53
1:B:720:LEU:HD23	1:B:720:LEU:C	2.32	0.50
1:B:567:ILE:HD12	1:B:567:ILE:O	2.12	0.49
1:A:647:ARG:HH11	1:A:647:ARG:CG	2.26	0.48
1:A:790:ILE:HD11	4:A:1009:SCN:S	2.56	0.45
1:B:698:MET:CE	1:B:732:SER:HB2	2.47	0.45
1:B:698:MET:HE2	1:B:732:SER:HB2	2.00	0.44
1:A:606:GLU:O	1:A:610[A]:GLN:HB2	2.18	0.43
1:A:606:GLU:O	1:A:610[B]:GLN:HG3	2.19	0.43
1:B:552:ALA:HB3	1:B:554:GLN:HG3	2.01	0.43
1:B:669:VAL:HG22	2:B:902:GOL:O2	2.18	0.43
1:A:541:SER:HB2	1:A:872:ALA:HB1	2.01	0.42
1:B:541:SER:HB2	1:B:872:ALA:HB1	2.01	0.42
1:B:727:ARG:NH2	1:B:851:ASP:OD2	2.53	0.42
1:A:774:ARG:NH1	6:A:1102:HOH:O	2.32	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:ALA:H	1:B:743:ASP:OD1[1_546]	1.59	0.01
6:A:1303:HOH:O	6:B:1092:HOH:O[1_655]	2.19	0.01

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	328/360 (91%)	319 (97%)	9 (3%)	0	100	100
1	B	327/360 (91%)	319 (98%)	8 (2%)	0	100	100
All	All	655/720 (91%)	638 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	251/274 (92%)	248 (99%)	3 (1%)	71	70
1	B	250/274 (91%)	247 (99%)	3 (1%)	71	70
All	All	501/548 (91%)	495 (99%)	6 (1%)	71	70

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	566	SER
1	A	613	PHE
1	A	647	ARG
1	B	539	ARG
1	B	580	SER
1	B	607	PHE

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 8 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
4	SCN	A	1004	-	1,2,2	0.63	0	0,1,1	0.00	-
4	SCN	A	1003	-	1,2,2	0.41	0	0,1,1	0.00	-
4	SCN	B	904	-	1,2,2	0.49	0	0,1,1	0.00	-
4	SCN	B	908	-	1,2,2	1.00	0	0,1,1	0.00	-
4	SCN	A	1005	-	1,2,2	0.35	0	0,1,1	0.00	-
4	SCN	A	1007	-	1,2,2	0.48	0	0,1,1	0.00	-
4	SCN	A	1012	-	1,2,2	0.42	0	0,1,1	0.00	-
4	SCN	A	1008	-	1,2,2	0.60	0	0,1,1	0.00	-
4	SCN	B	901	-	1,2,2	0.87	0	0,1,1	0.00	-
4	SCN	A	1006	-	1,2,2	0.72	0	0,1,1	0.00	-
4	SCN	A	1010	-	1,2,2	0.52	0	0,1,1	0.00	-
3	SO4	A	1002	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SCN	B	905	-	1,2,2	1.07	0	0,1,1	0.00	-
4	SCN	A	1011	-	1,2,2	0.28	0	0,1,1	0.00	-
4	SCN	A	1009	-	1,2,2	0.95	0	0,1,1	0.00	-
4	SCN	B	906	-	1,2,2	0.73	0	0,1,1	0.00	-
4	SCN	B	909	-	1,2,2	0.39	0	0,1,1	0.00	-
4	SCN	B	903	-	1,2,2	0.87	0	0,1,1	0.00	-
4	SCN	B	907	-	1,2,2	0.70	0	0,1,1	0.00	-
2	GOL	A	1001	5	5,5,5	1.13	1 (20%)	5,5,5	0.34	0
2	GOL	B	902	-	5,5,5	0.90	0	5,5,5	0.31	0

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	GOL	A	1001	5	-	4/4/4/4	-
2	GOL	B	902	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GOL	O2-C2	-2.32	1.36	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	902	GOL	C1-C2-C3-O3
2	B	902	GOL	O2-C2-C3-O3
2	A	1001	GOL	O1-C1-C2-C3
2	A	1001	GOL	C1-C2-C3-O3
2	A	1001	GOL	O2-C2-C3-O3
2	B	902	GOL	O1-C1-C2-C3
2	B	902	GOL	O1-C1-C2-O2
2	A	1001	GOL	O1-C1-C2-O2

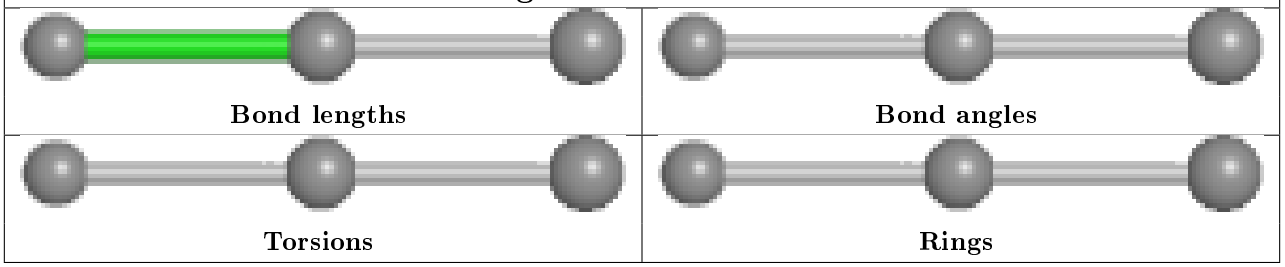
There are no ring outliers.

2 monomers are involved in 2 short contacts:

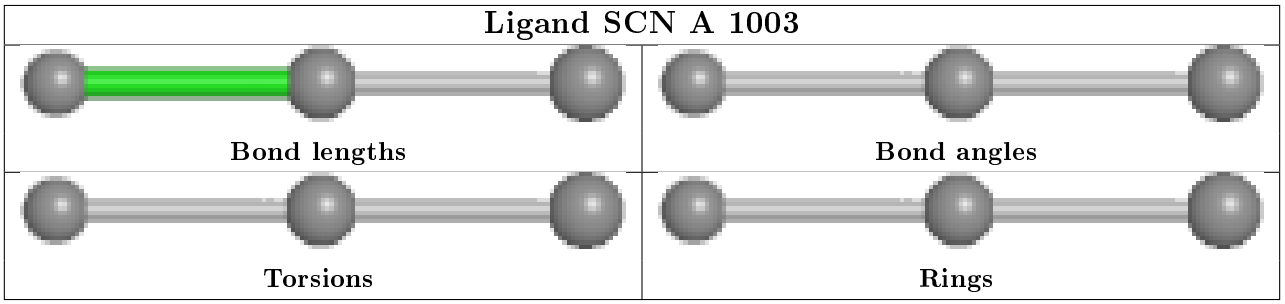
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1009	SCN	1	0
2	B	902	GOL	1	0

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

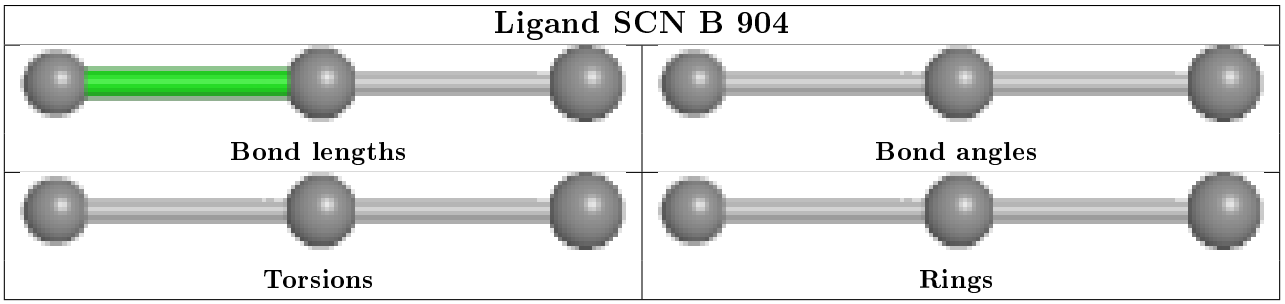
Ligand SCN A 1004



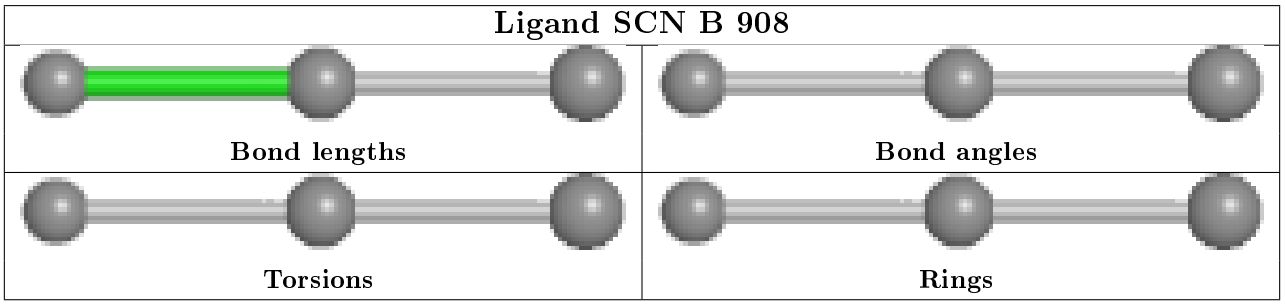
Ligand SCN A 1003



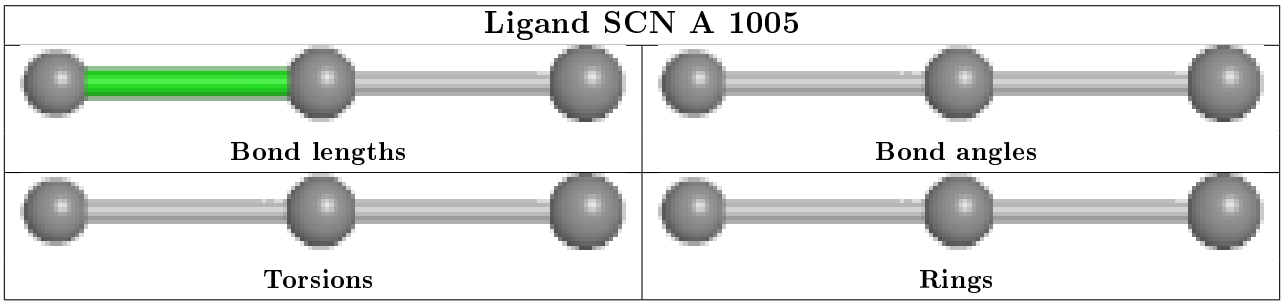
Ligand SCN B 904

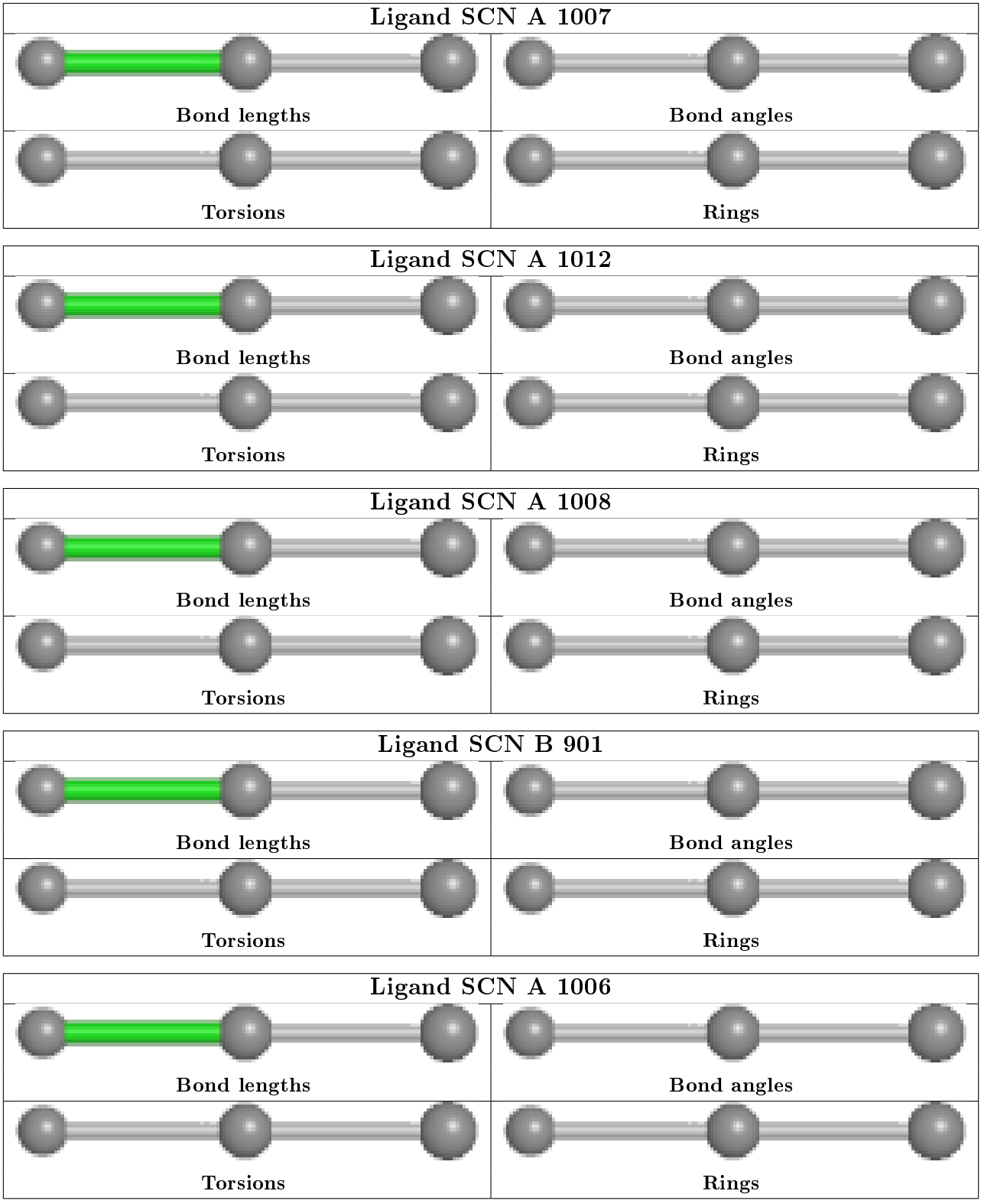


Ligand SCN B 908

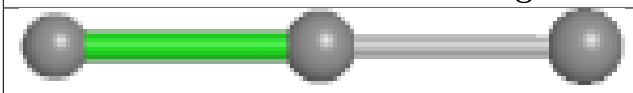


Ligand SCN A 1005

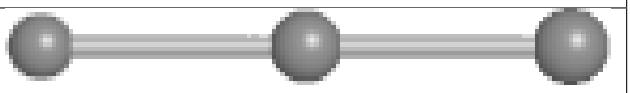



Ligand SCN A 1007
Bond lengths
Bond angles
Torsions
Rings
Ligand SCN A 1012
Bond lengths
Bond angles
Torsions
Rings
Ligand SCN A 1008
Bond lengths
Bond angles
Torsions
Rings
Ligand SCN B 901
Bond lengths
Bond angles
Torsions
Rings
Ligand SCN A 1006
Bond lengths
Bond angles
Torsions
Rings

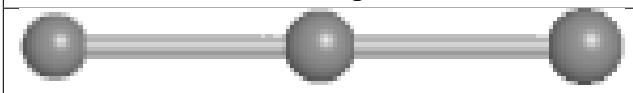
Ligand SCN A 1010



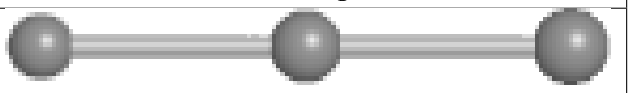
Bond lengths



Bond angles

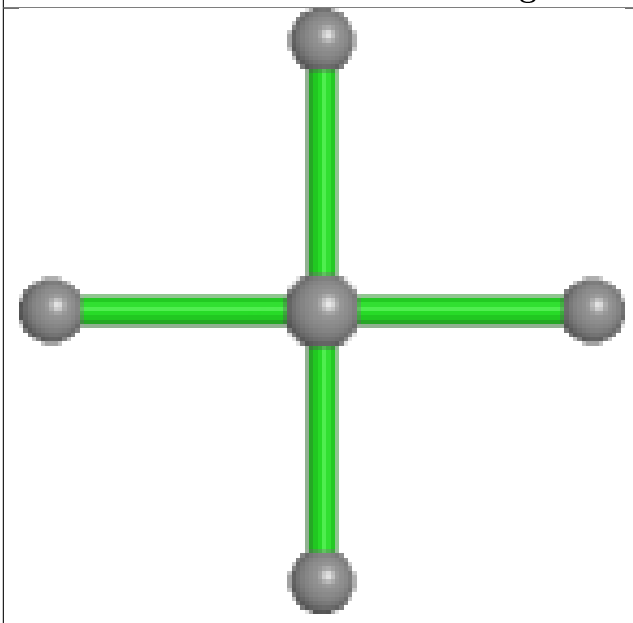


Torsions

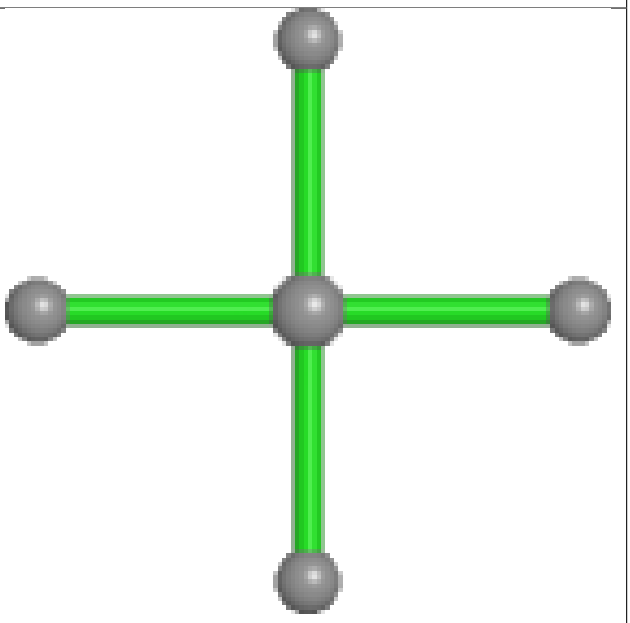


Rings

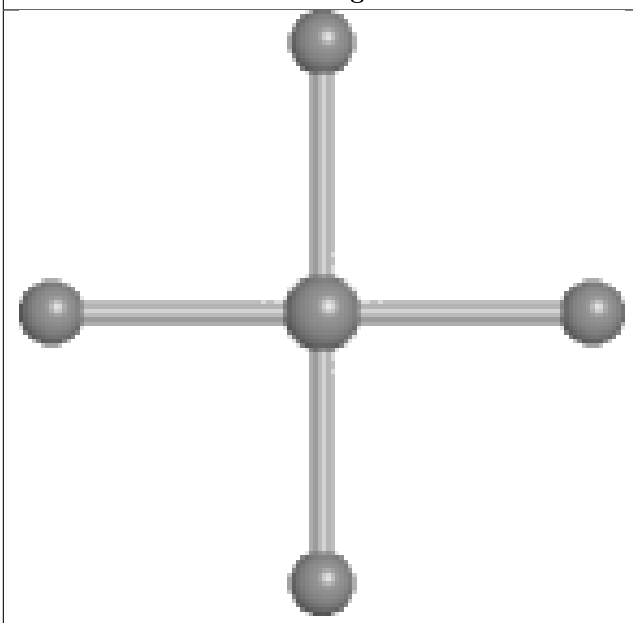
Ligand SO4 A 1002



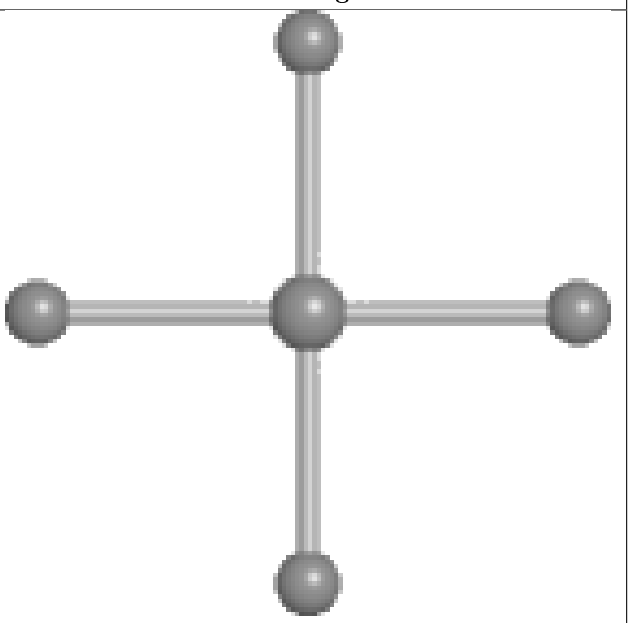
Bond lengths



Bond angles

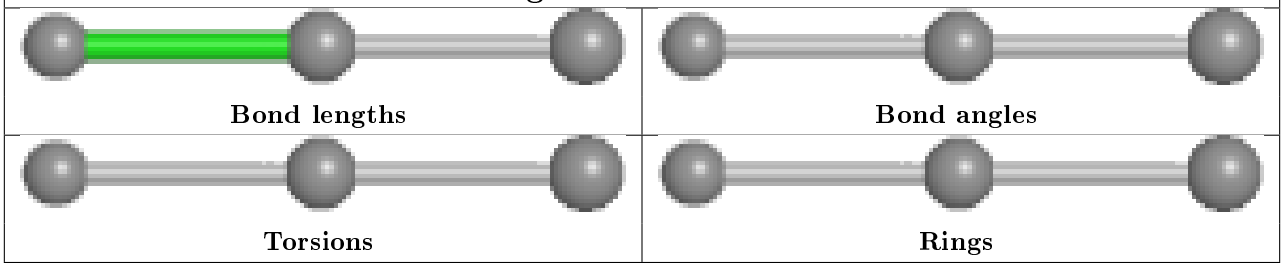


Torsions

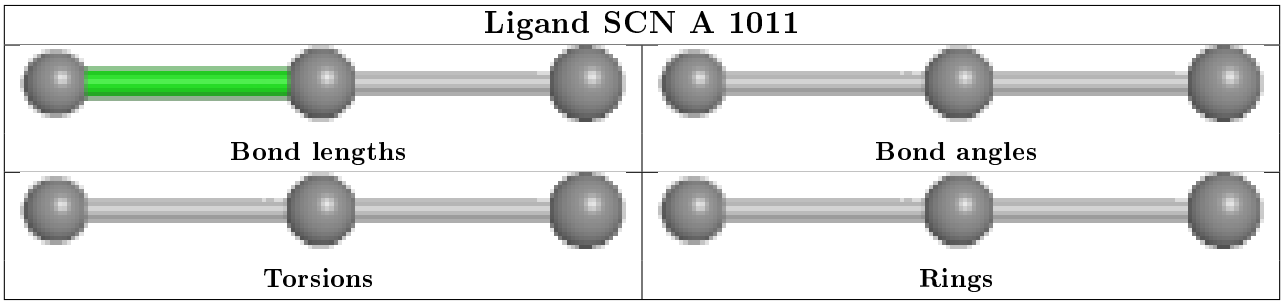


Rings

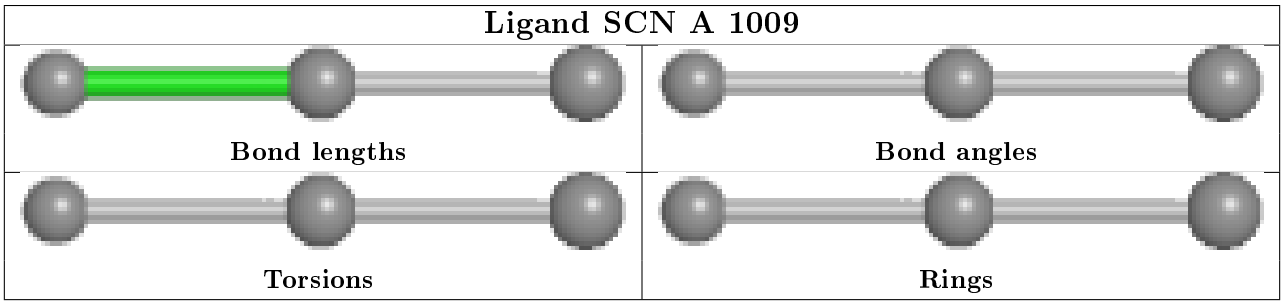
Ligand SCN B 905



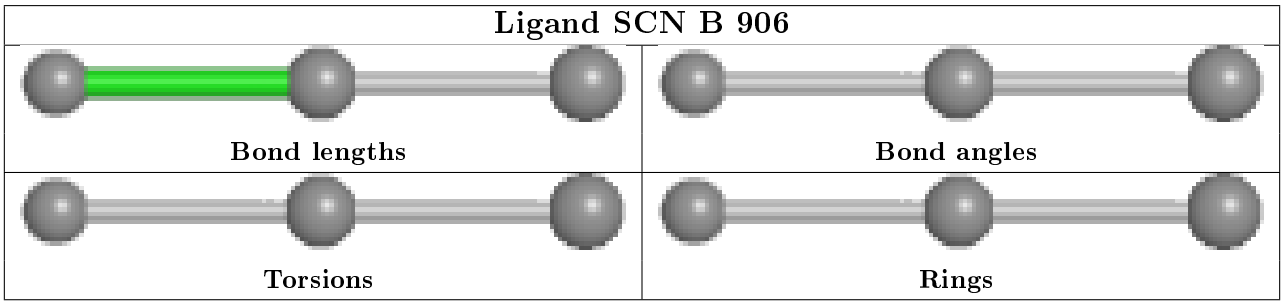
Ligand SCN A 1011



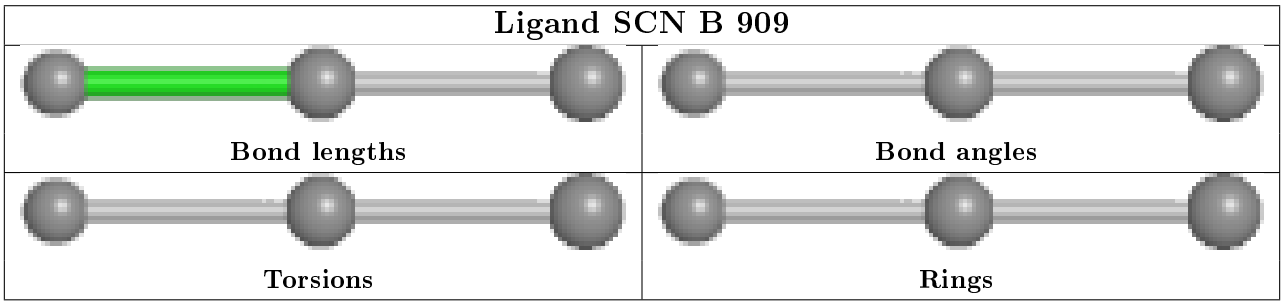
Ligand SCN A 1009



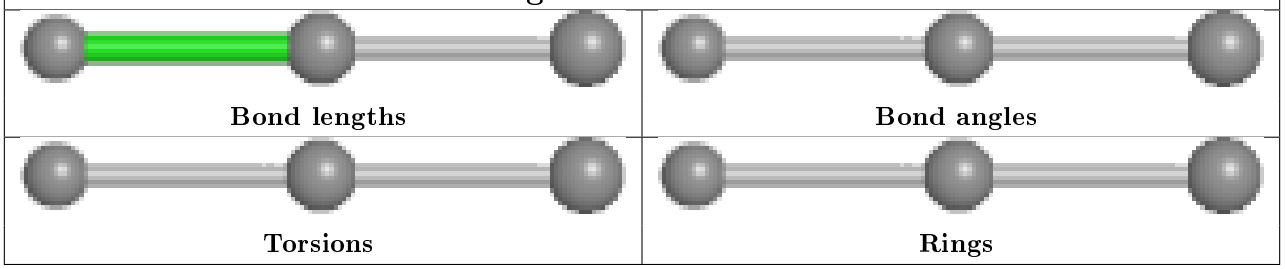
Ligand SCN B 906



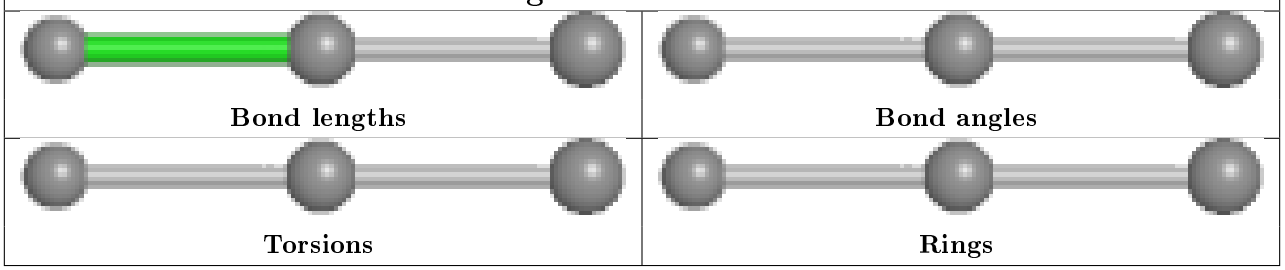
Ligand SCN B 909



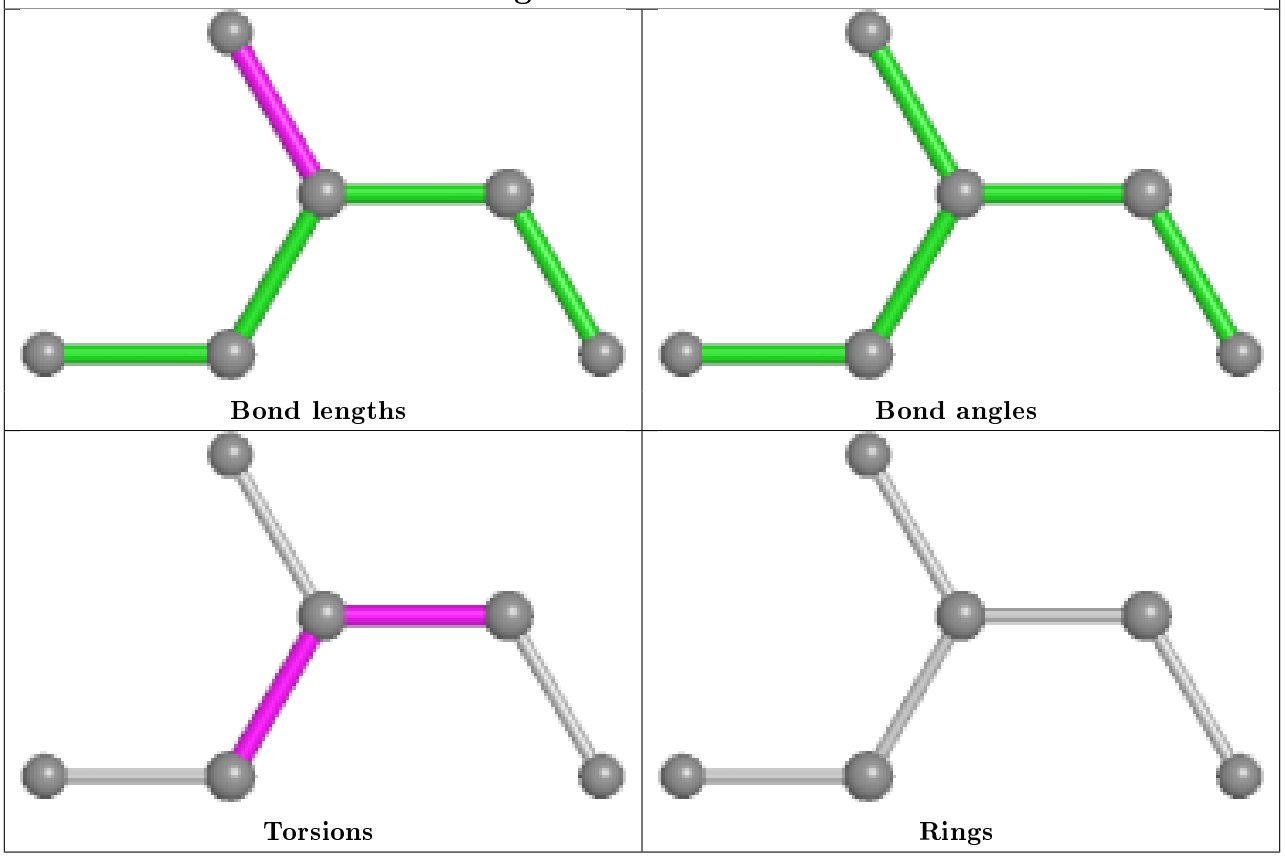
Ligand SCN B 903

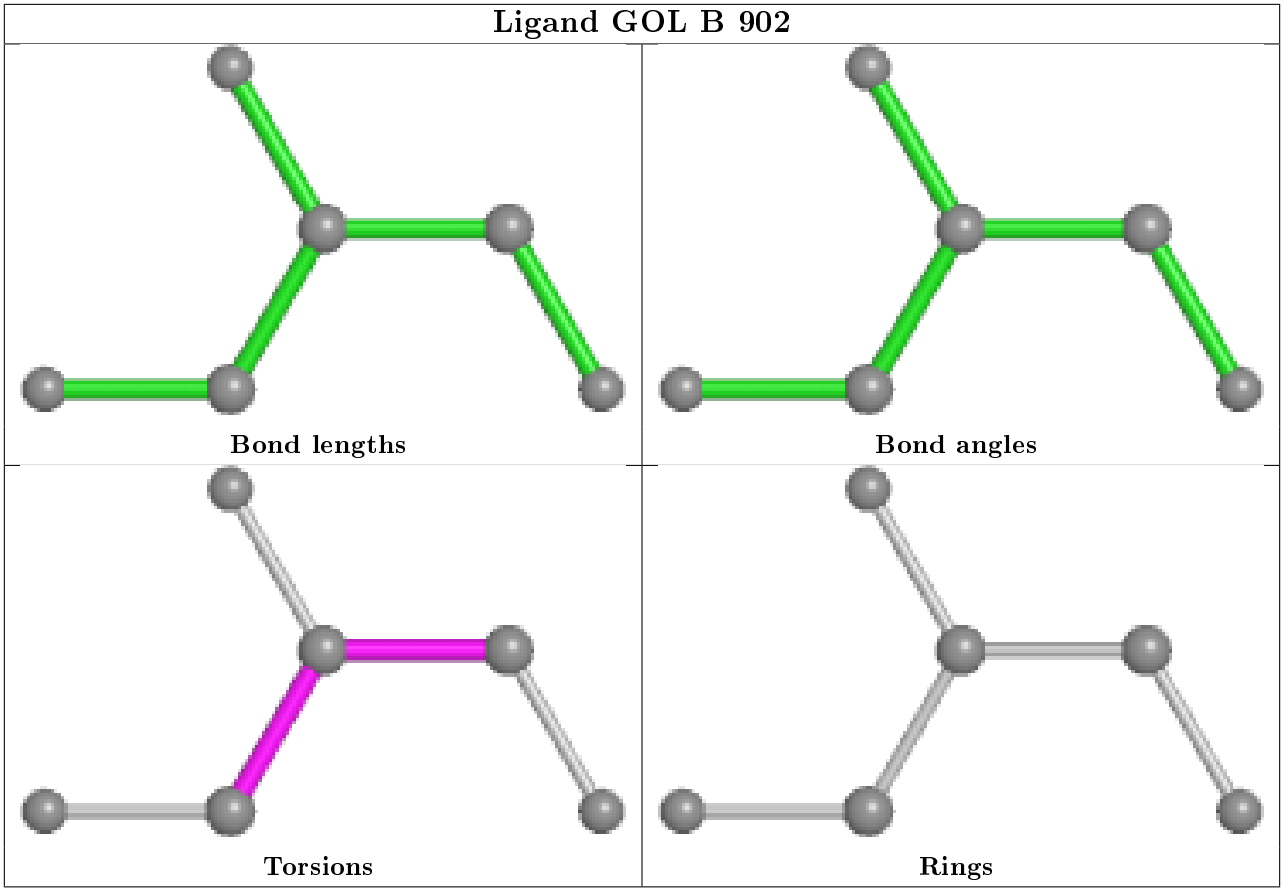


Ligand SCN B 907



Ligand GOL A 1001





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	329/360 (91%)	0.03	14 (4%)	35	38	15, 24, 54, 84	0
1	B	329/360 (91%)	0.01	15 (4%)	32	35	14, 25, 53, 85	0
All	All	658/720 (91%)	0.02	29 (4%)	34	37	14, 25, 55, 85	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	567	ILE	3.8
1	A	751	PHE	3.8
1	B	554	GLN	3.7
1	B	557	PRO	3.6
1	A	559	VAL	3.5
1	A	557	PRO	3.3
1	B	539	ARG	3.3
1	B	556	ALA	3.0
1	B	751	PHE	3.0
1	B	749	ASN	2.8
1	A	871	ASP	2.8
1	A	554	GLN	2.7
1	A	749	ASN	2.7
1	B	559	VAL	2.7
1	A	541	SER	2.5
1	A	611[A]	GLY	2.5
1	B	872	ALA	2.3
1	A	607	PHE	2.3
1	A	727	ARG	2.2
1	A	551	ALA	2.2
1	B	560	VAL	2.2
1	A	610[A]	GLN	2.2
1	B	583	ALA	2.2
1	B	541	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	552	ALA	2.1
1	A	583	ALA	2.1
1	A	872	ALA	2.1
1	B	747	GLN	2.0
1	B	555	SER	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 monosaccharides 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
4	SCN	A	1011	3/3	0.87	0.12	31,31,31,47	0
4	SCN	A	1009	3/3	0.90	0.12	26,26,27,55	0
4	SCN	A	1004	3/3	0.91	0.09	42,42,45,50	0
4	SCN	B	907	3/3	0.91	0.14	50,50,55,71	0
2	GOL	B	902	6/6	0.92	0.14	21,30,40,48	0
4	SCN	B	901	3/3	0.92	0.13	40,40,41,62	0
3	SO4	A	1002	5/5	0.92	0.17	67,78,83,90	0
4	SCN	A	1003	3/3	0.92	0.11	35,35,45,53	0
4	SCN	A	1006	3/3	0.92	0.11	48,48,52,57	0
4	SCN	B	909	3/3	0.92	0.14	30,30,30,35	0
4	SCN	A	1012	3/3	0.93	0.11	30,30,30,38	0
5	NA	B	912	1/1	0.93	0.15	35,35,35,35	0
4	SCN	A	1010	3/3	0.94	0.08	25,25,29,47	0
4	SCN	A	1007	3/3	0.94	0.16	37,37,44,59	0
4	SCN	B	906	3/3	0.94	0.14	44,44,48,64	0
2	GOL	A	1001	6/6	0.94	0.25	24,34,43,45	0
5	NA	B	913	1/1	0.95	0.11	33,33,33,33	0
4	SCN	B	905	3/3	0.95	0.20	17,17,31,69	0

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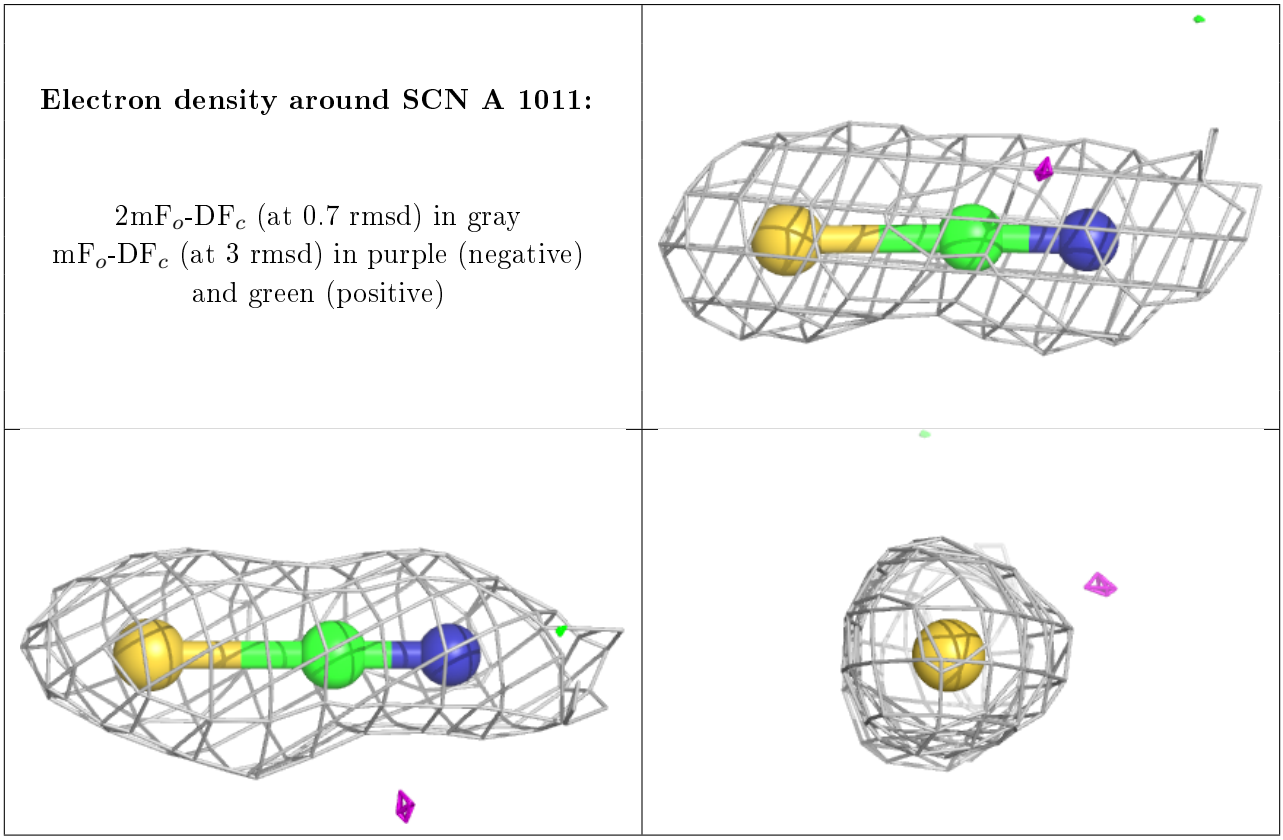
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	B	911	1/1	0.95	0.08	34,34,34,34	0
4	SCN	B	908	3/3	0.96	0.09	26,26,28,35	0
5	NA	A	1015	1/1	0.96	0.11	47,47,47,47	0
5	NA	A	1016	1/1	0.96	0.10	27,27,27,27	0
4	SCN	A	1008	3/3	0.96	0.09	37,37,40,59	0
4	SCN	B	904	3/3	0.98	0.07	37,37,40,60	0
5	NA	A	1014	1/1	0.98	0.07	25,25,25,25	0
5	NA	B	910	1/1	0.99	0.13	26,26,26,26	0
4	SCN	B	903	3/3	0.99	0.13	24,24,34,38	0
4	SCN	A	1005	3/3	0.99	0.11	23,23,31,48	0
5	NA	A	1013	1/1	0.99	0.08	31,31,31,31	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.

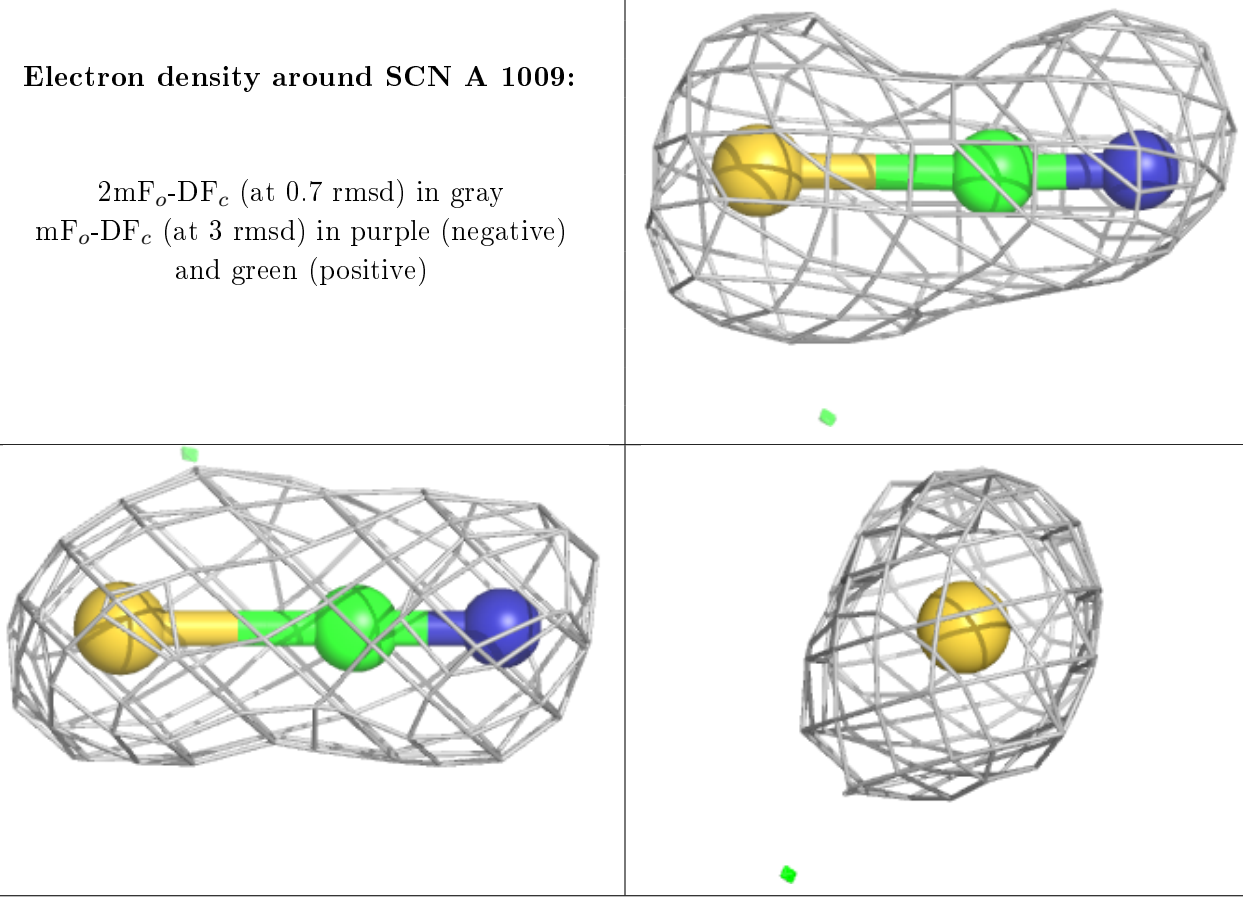
Electron density around SCN A 1011:

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



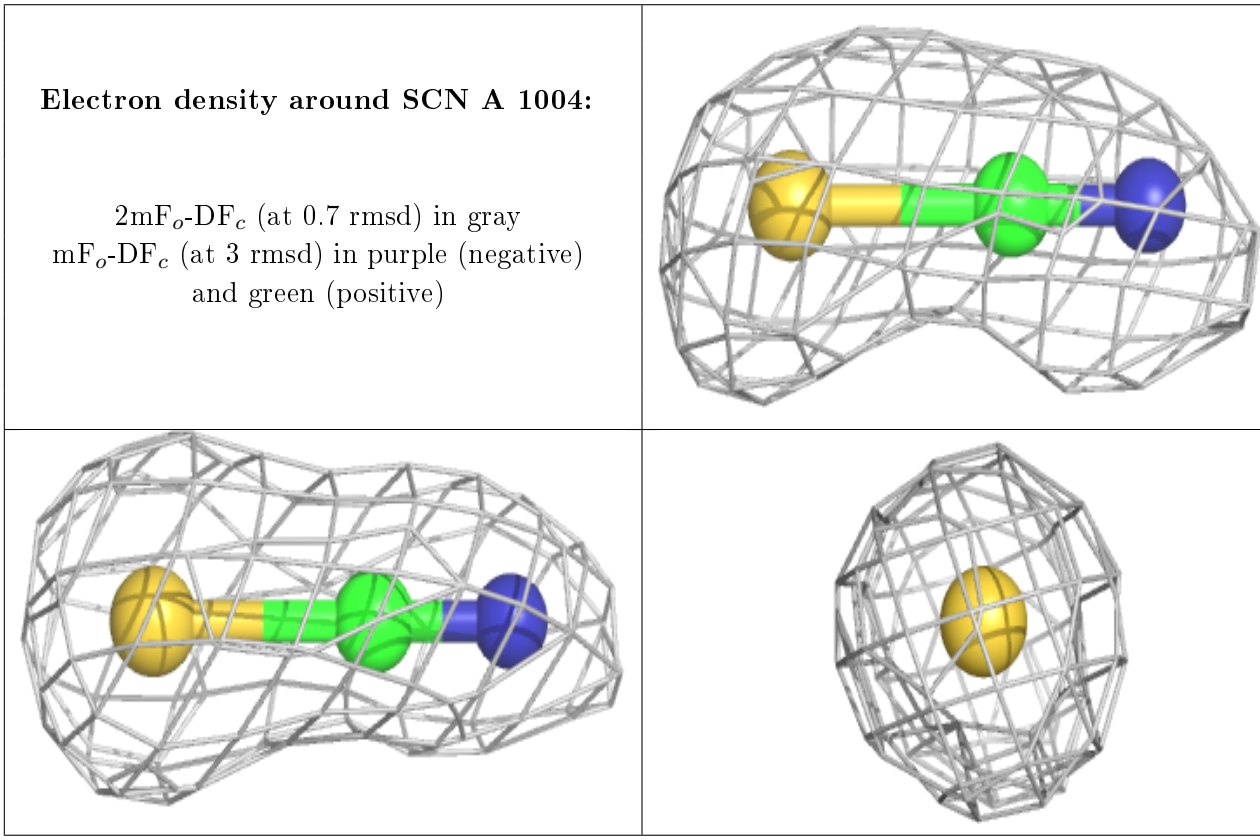
Electron density around SCN A 1009:

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



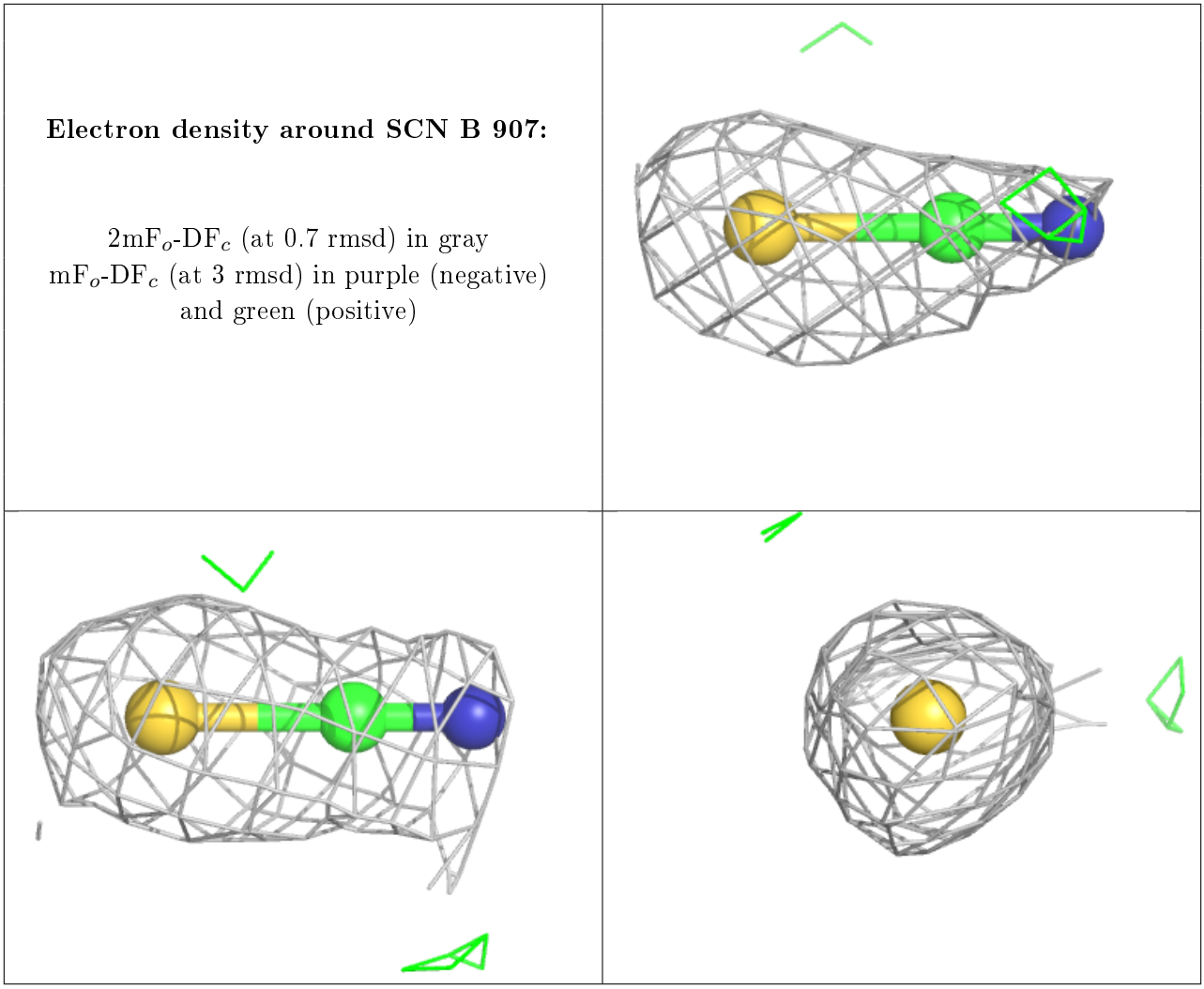
Electron density around SCN A 1004:

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



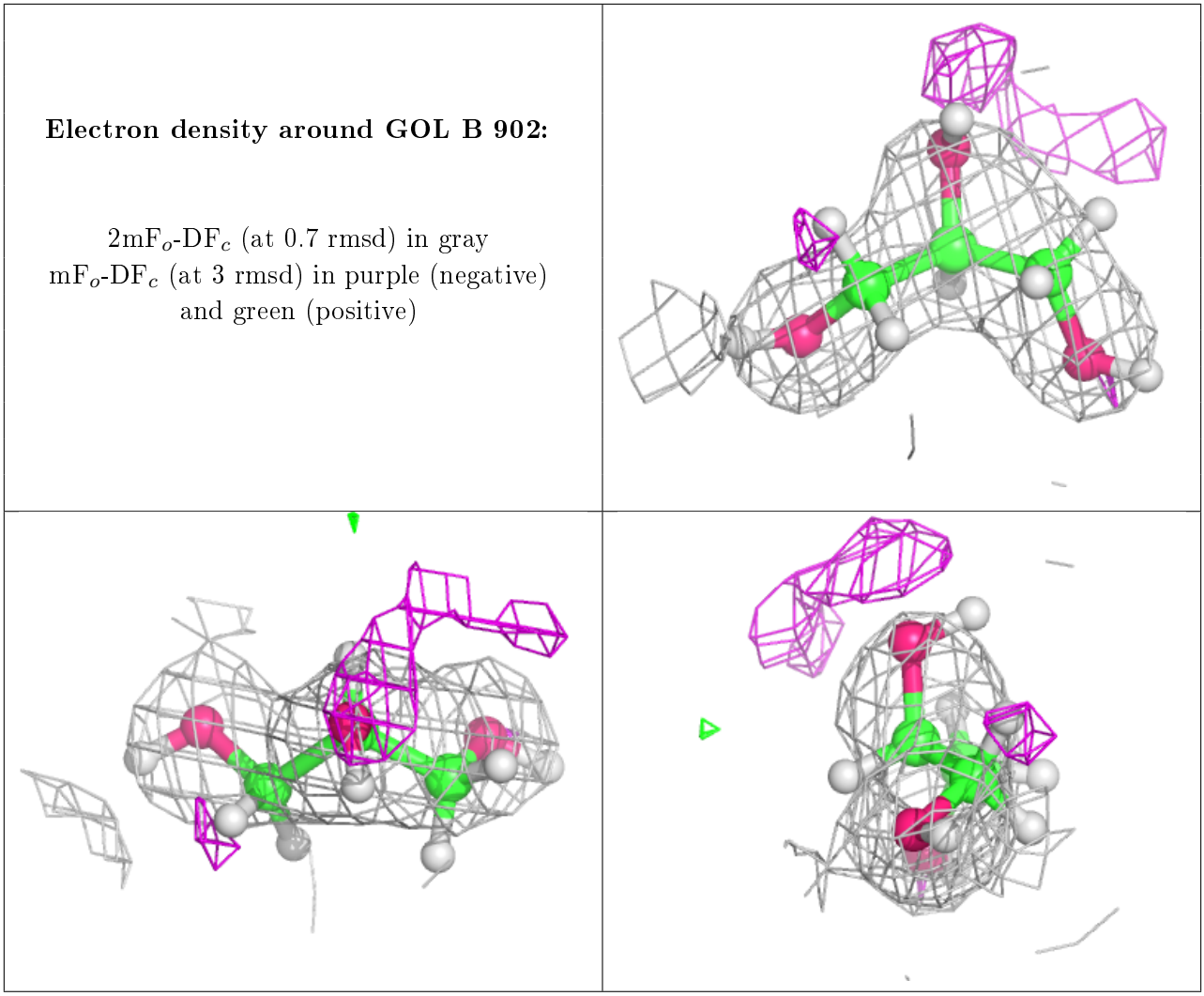
Electron density around SCN B 907:

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



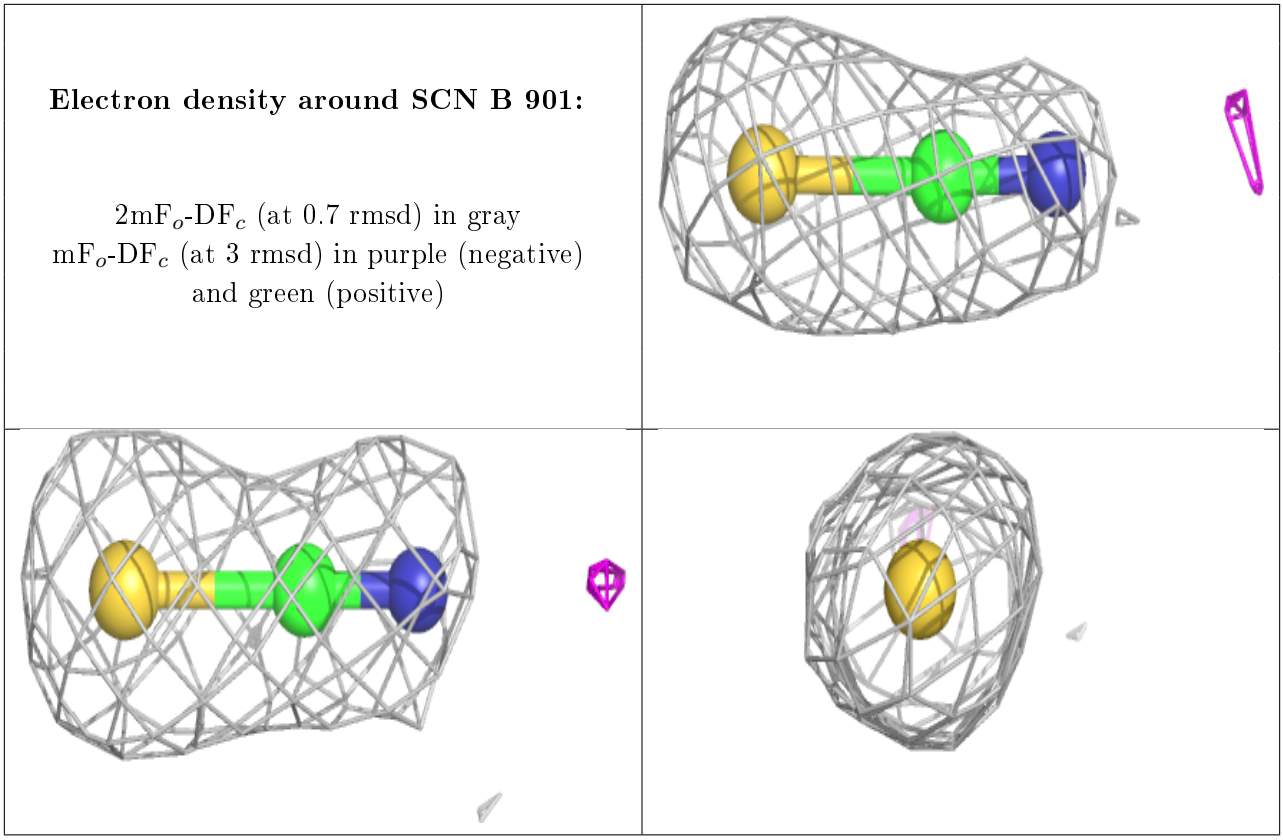
Electron density around GOL B 902:

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



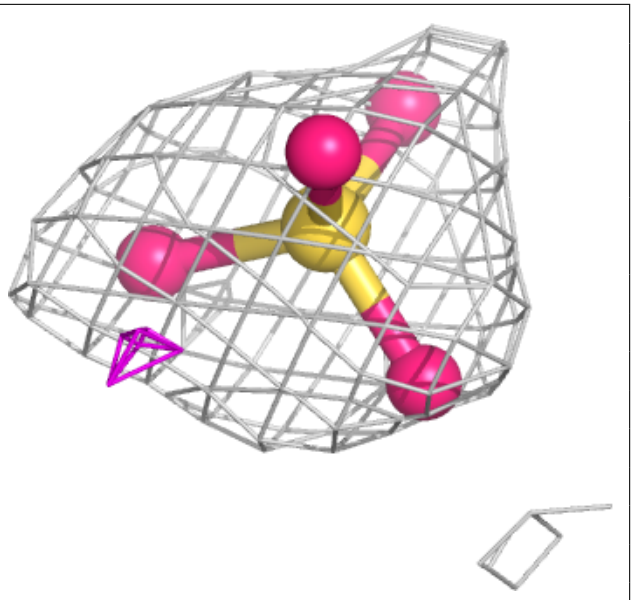
Electron density around SCN B 901:

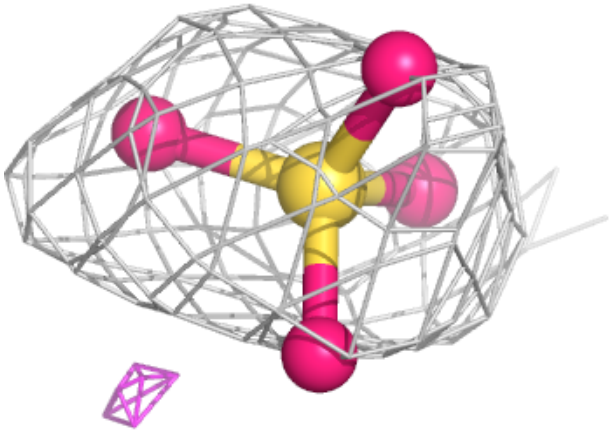
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

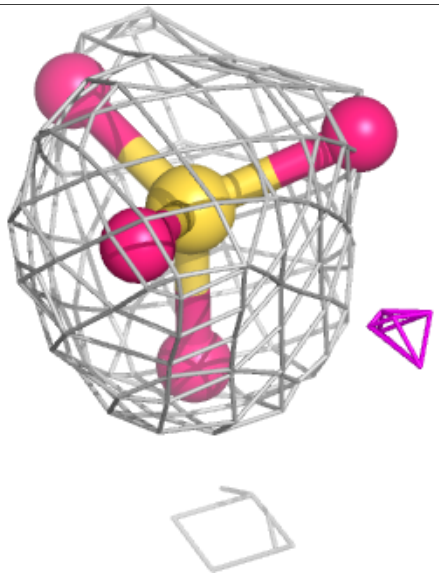


Electron density around SO4 A 1002:

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

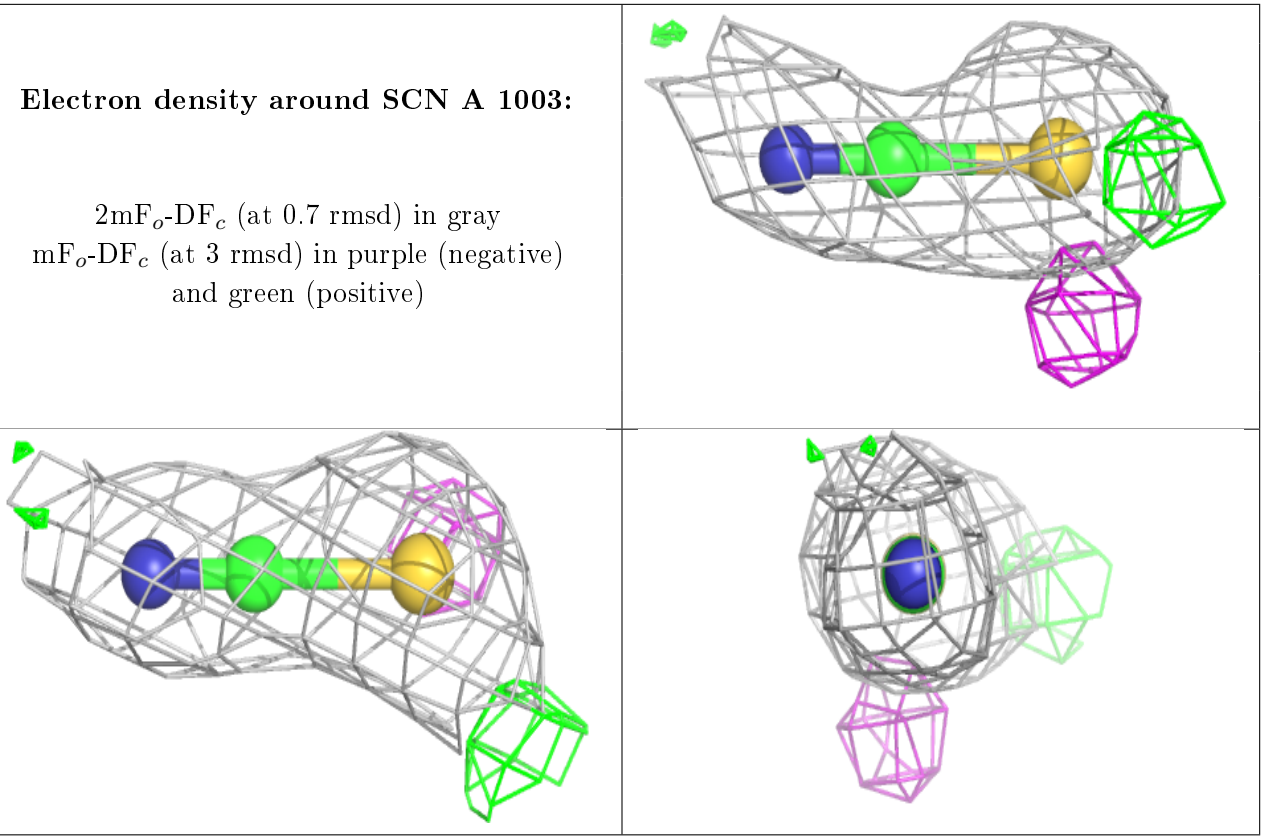






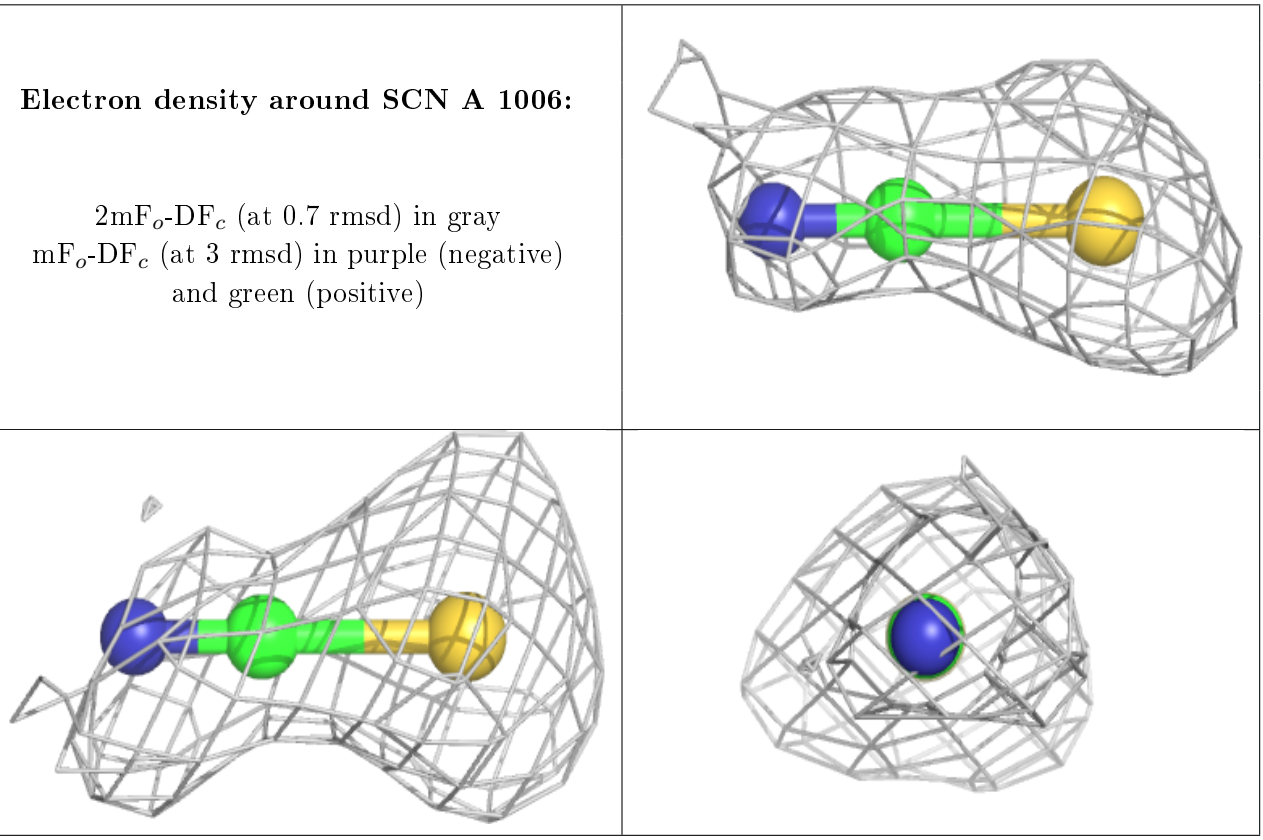
Electron density around SCN A 1003:

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



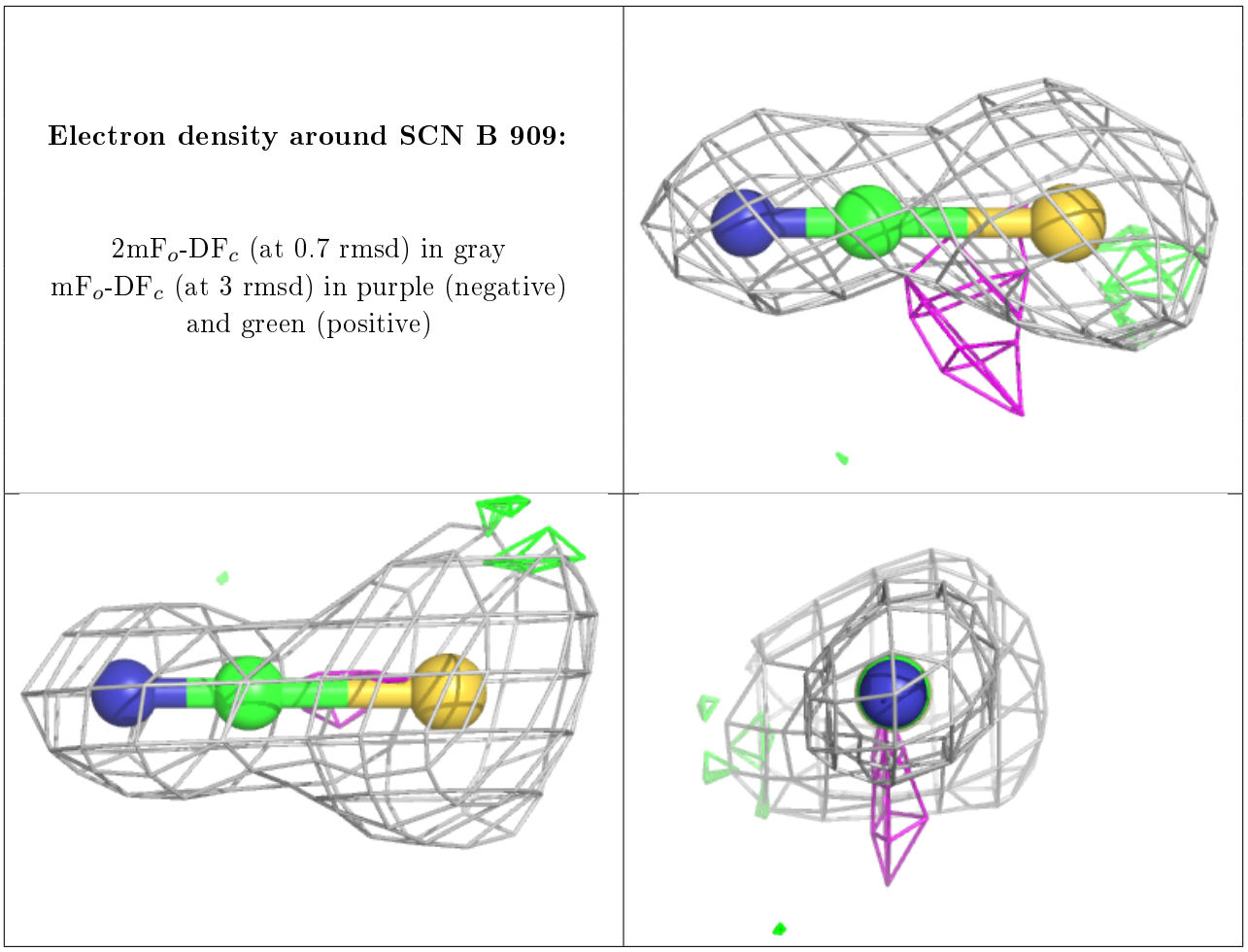
Electron density around SCN A 1006:

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



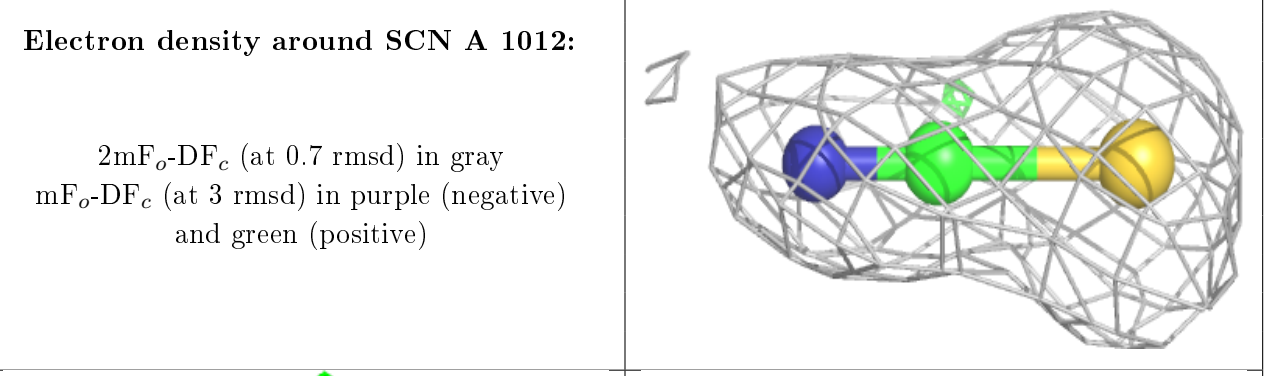
Electron density around SCN B 909:

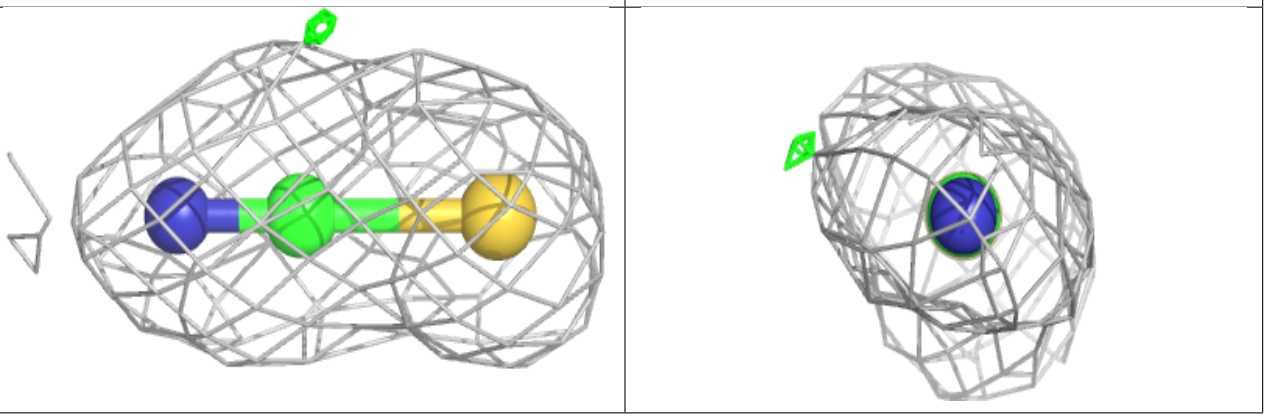
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SCN A 1012:

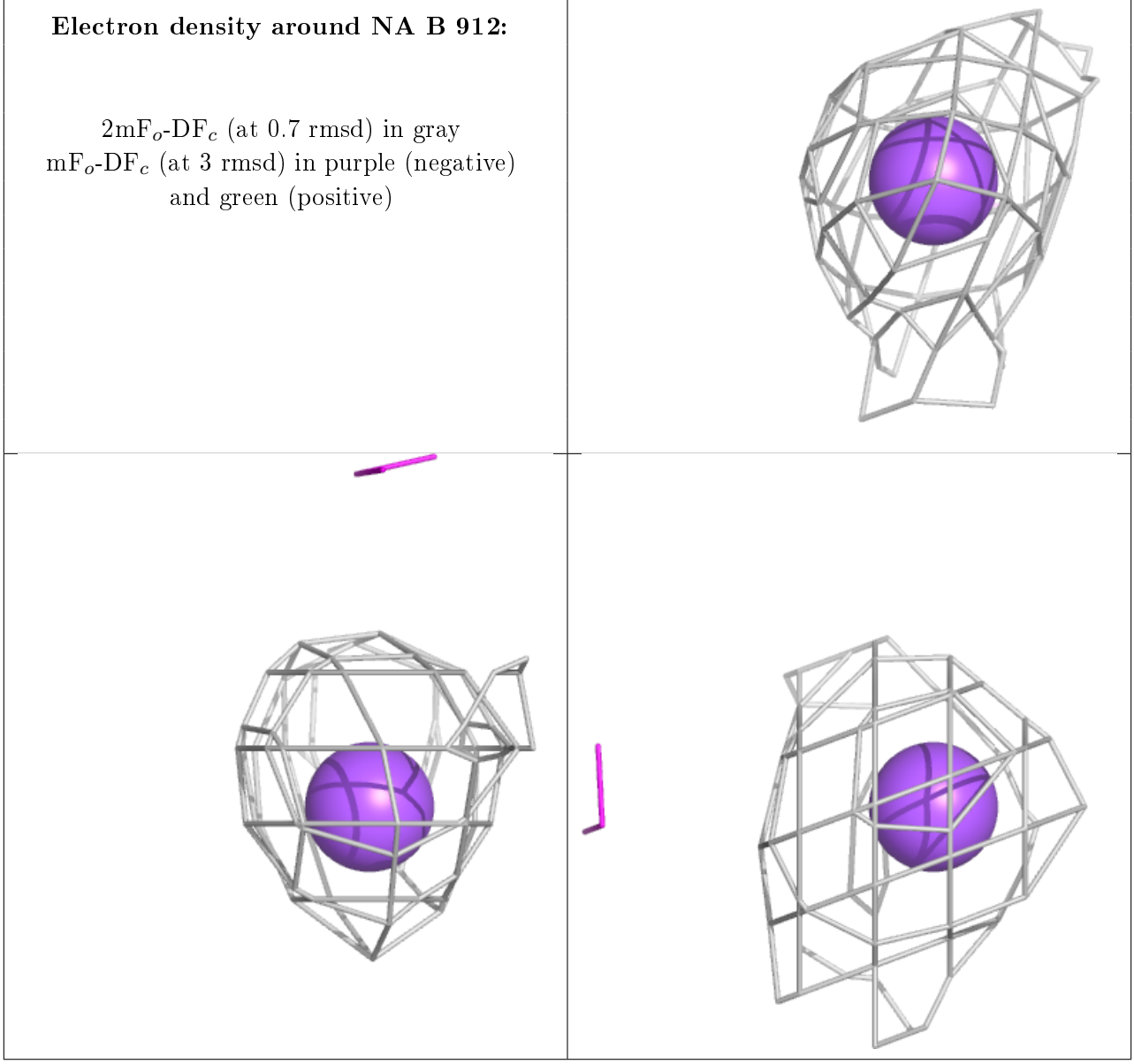
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





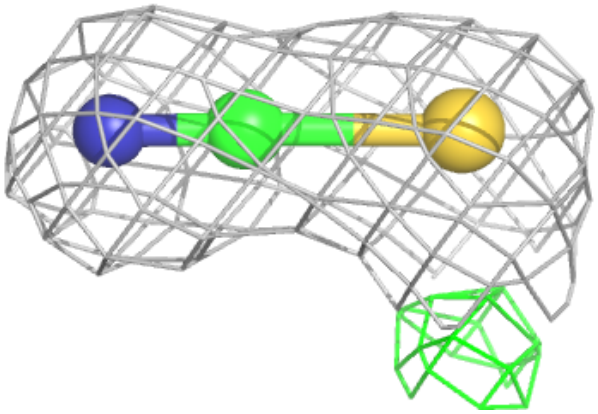
Electron density around NA B 912:

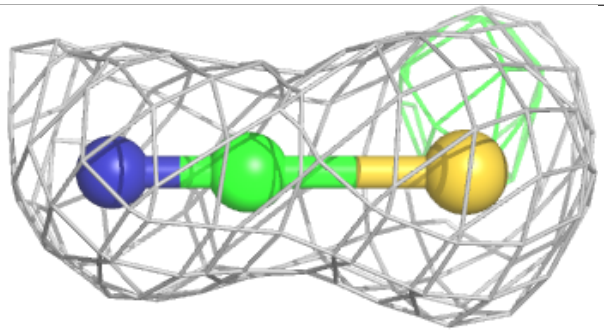
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

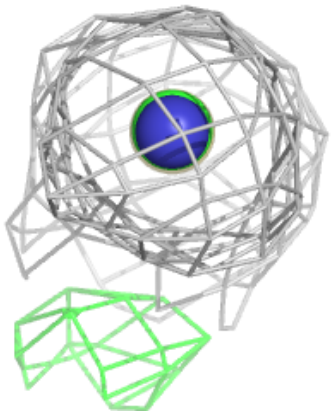


Electron density around SCN A 1010:

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

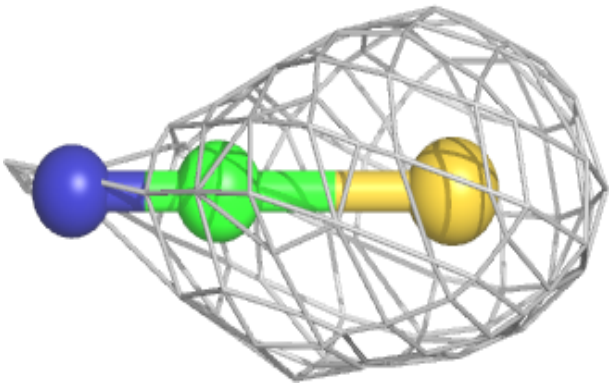


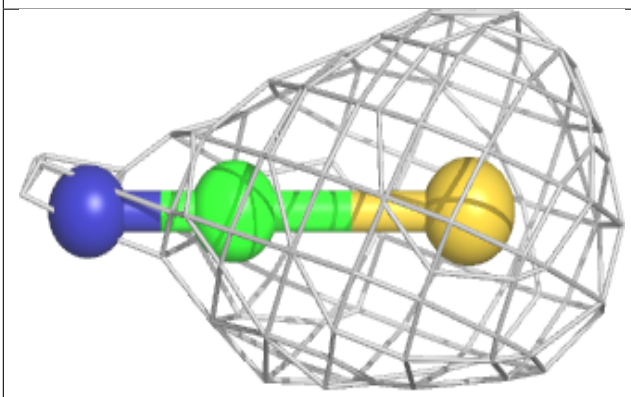


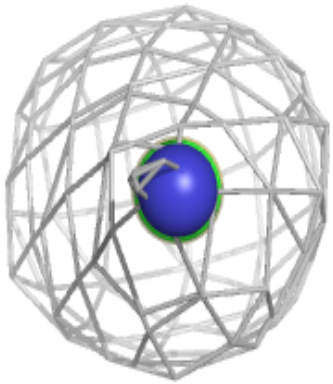


Electron density around SCN A 1007:

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

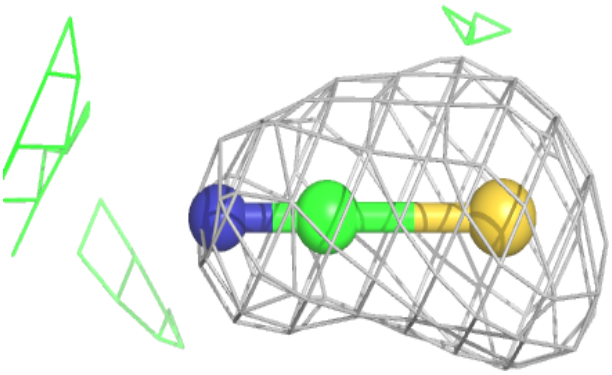


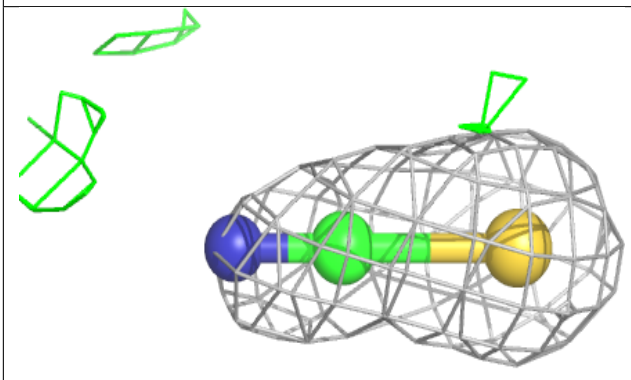


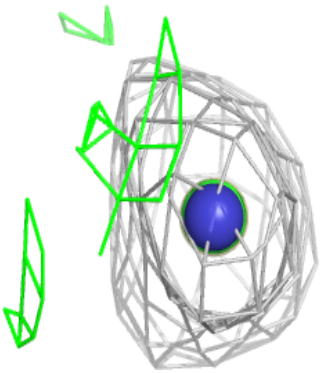


Electron density around SCN B 906:

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

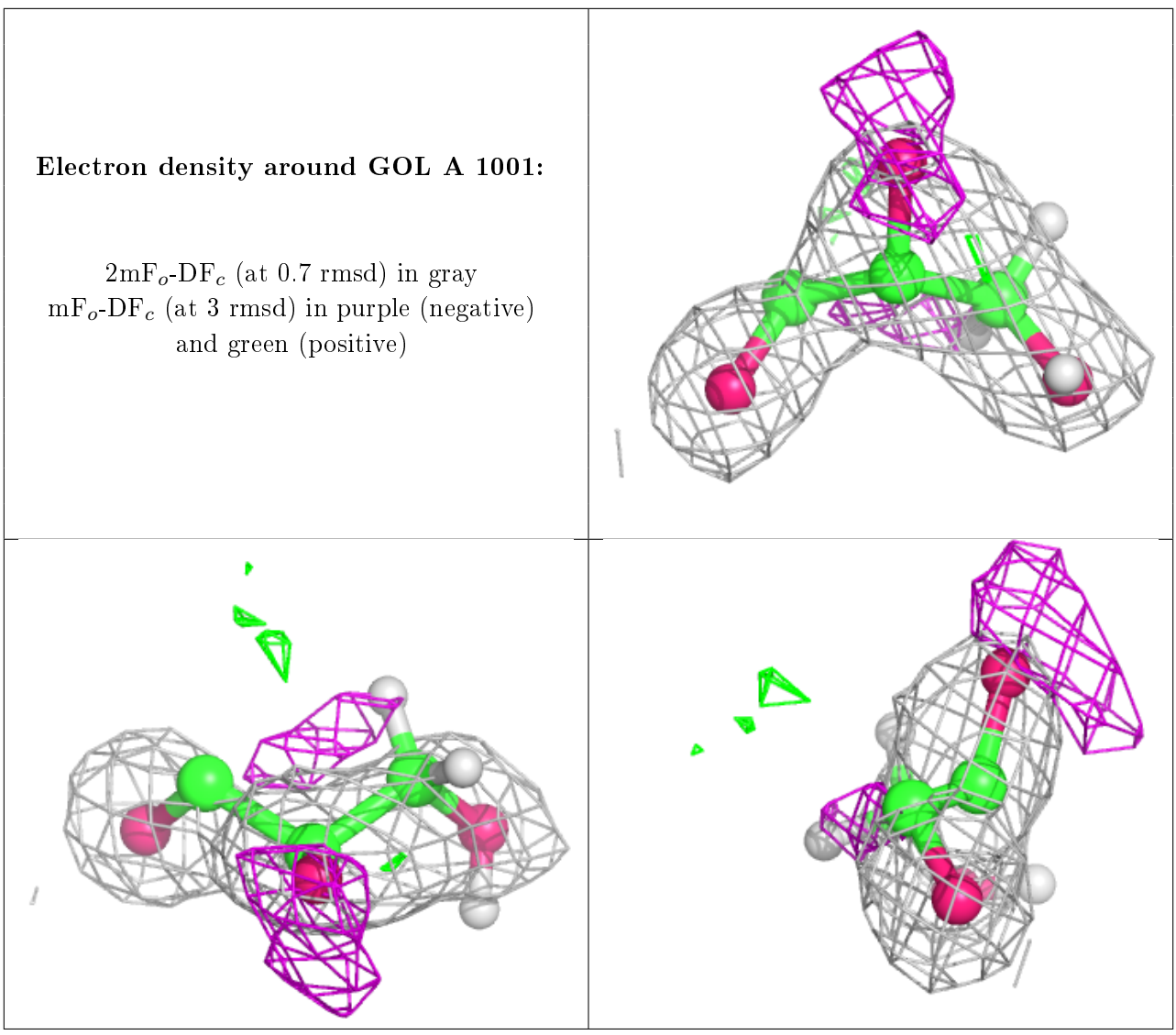






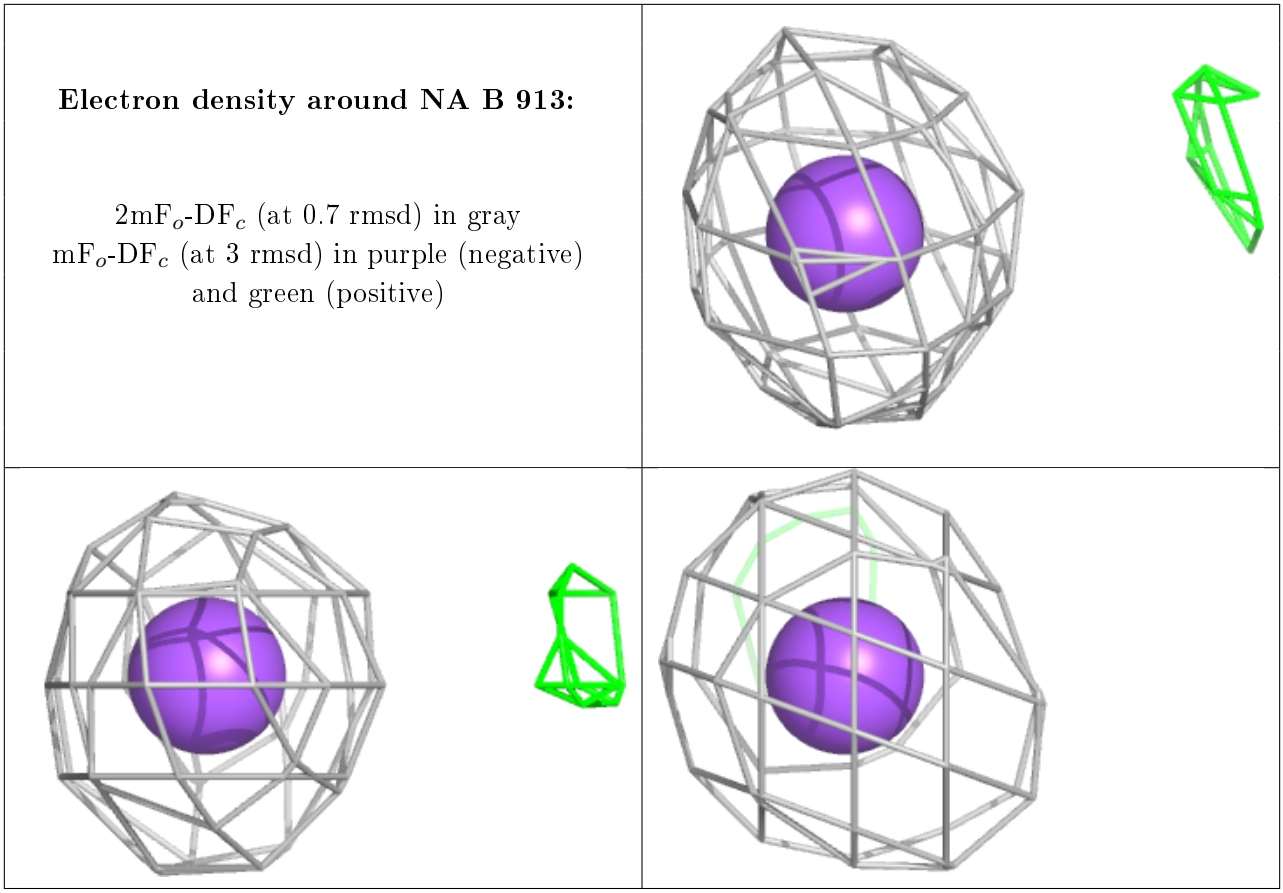
Electron density around GOL A 1001:

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



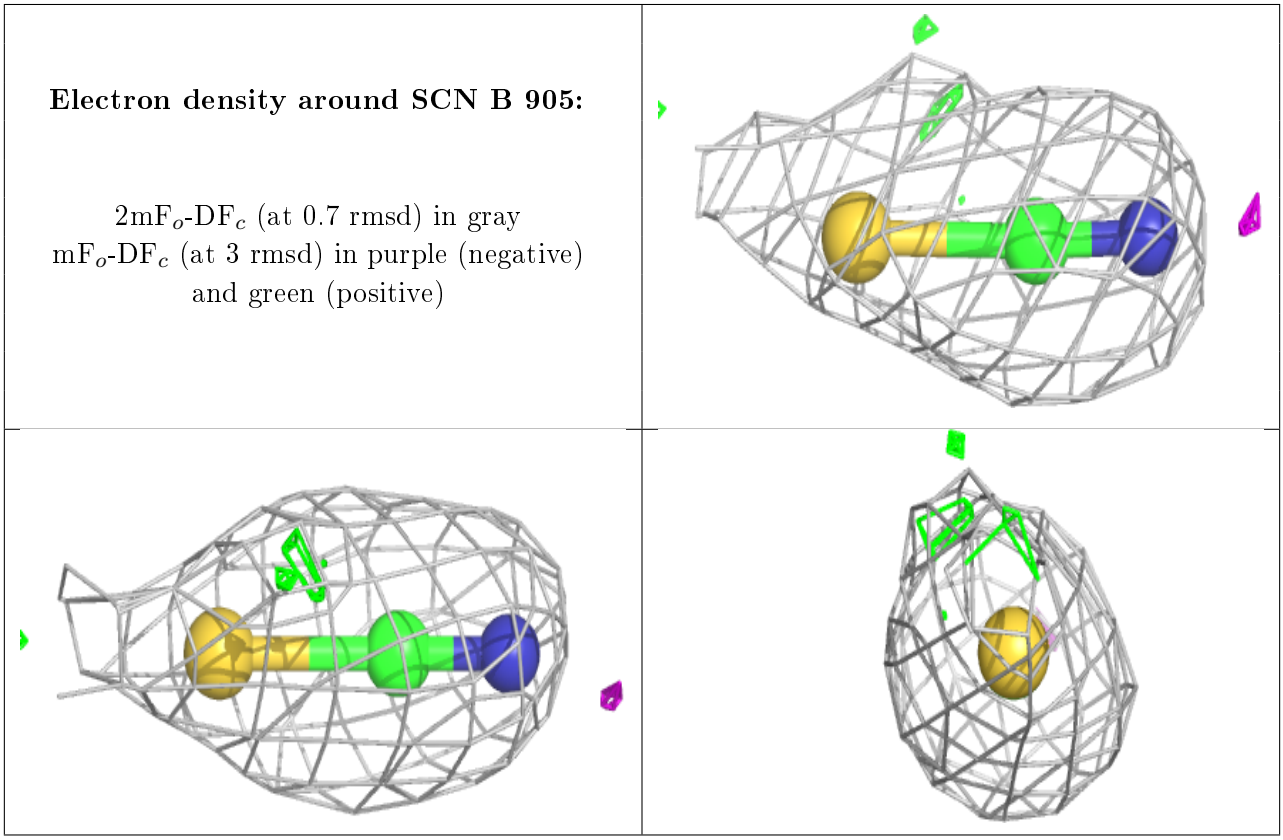
Electron density around NA B 913:

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



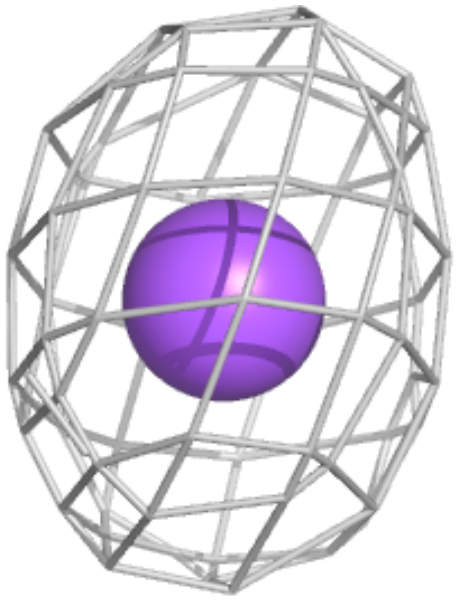
Electron density around SCN B 905:

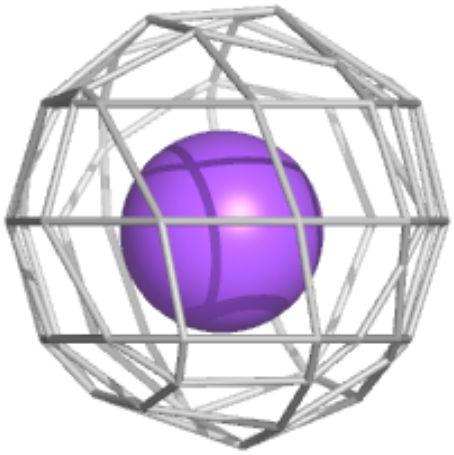
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

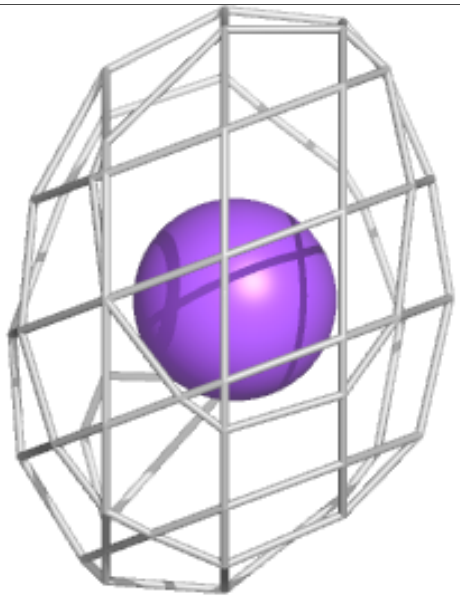


Electron density around NA B 911:

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

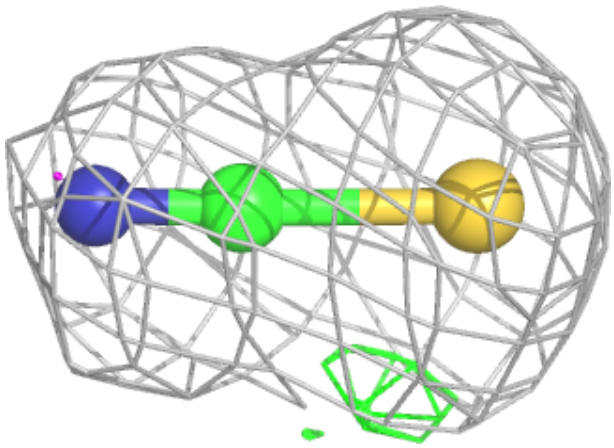


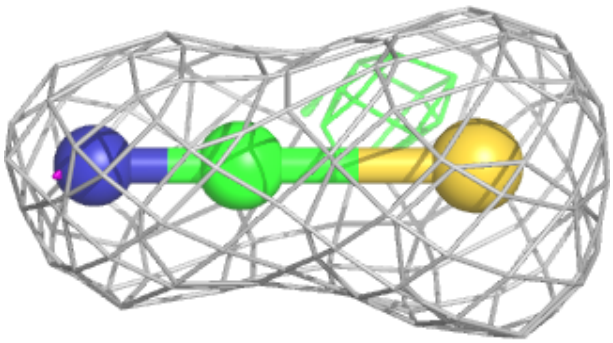


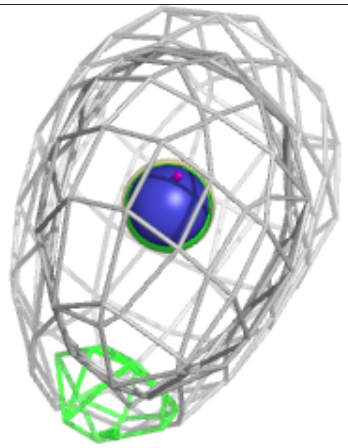


Electron density around SCN B 908:

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

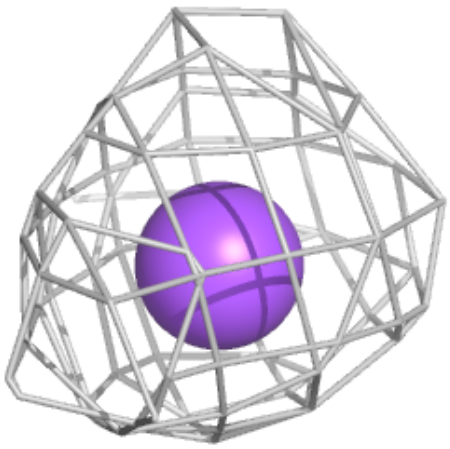


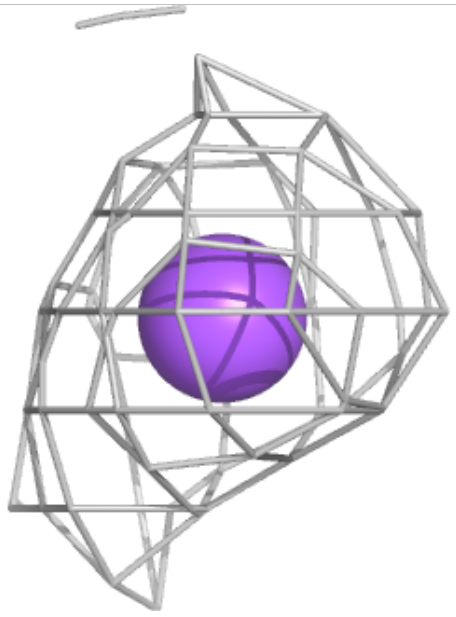


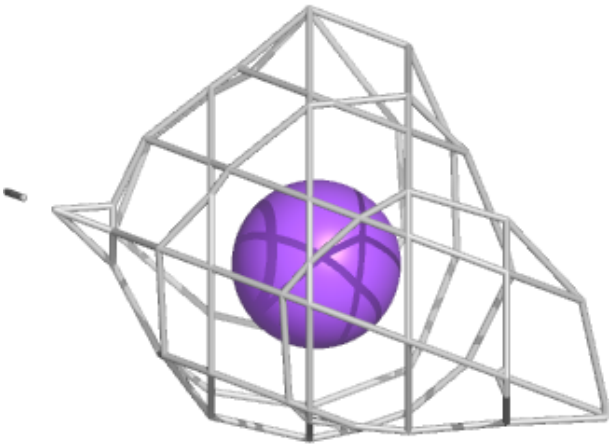


Electron density around NA A 1015:

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

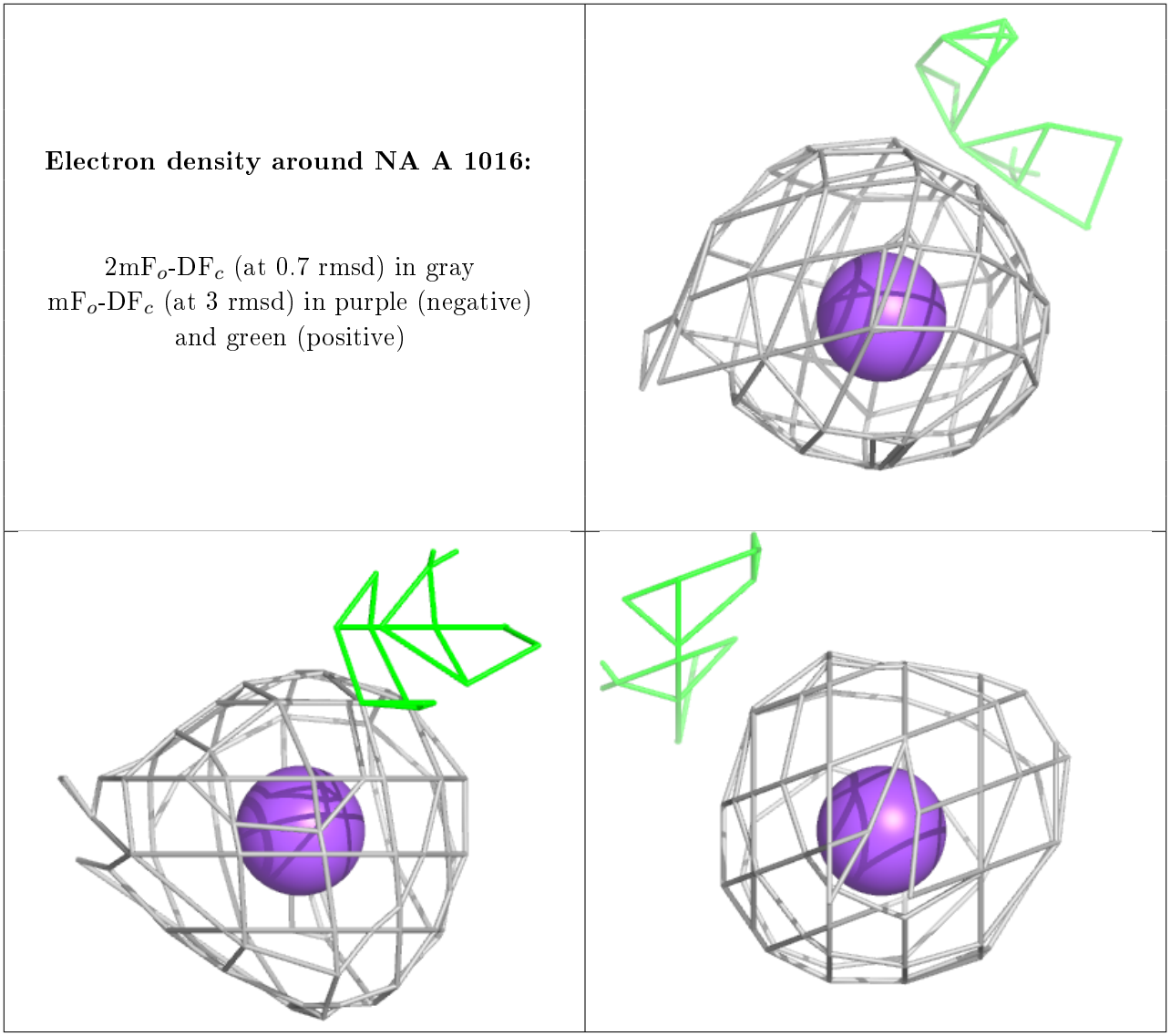






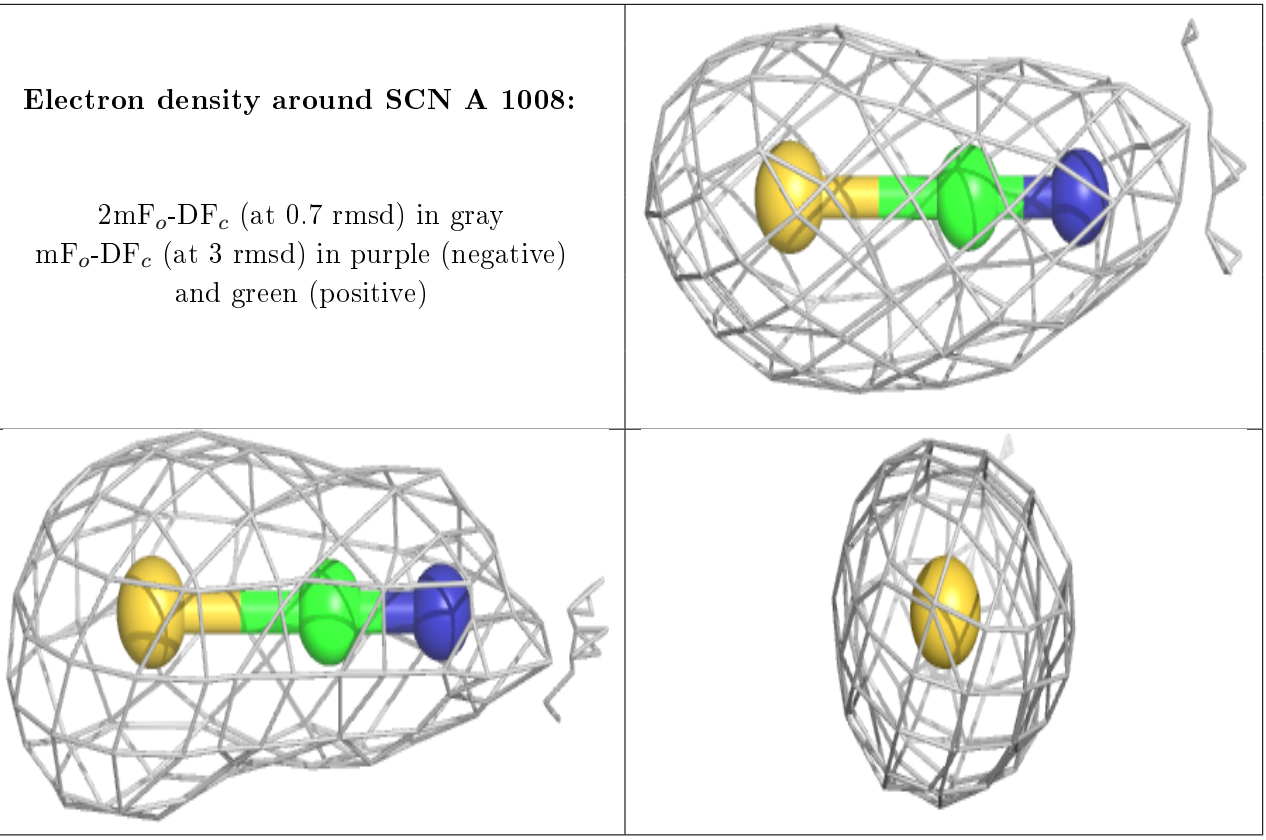
Electron density around NA A 1016:

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



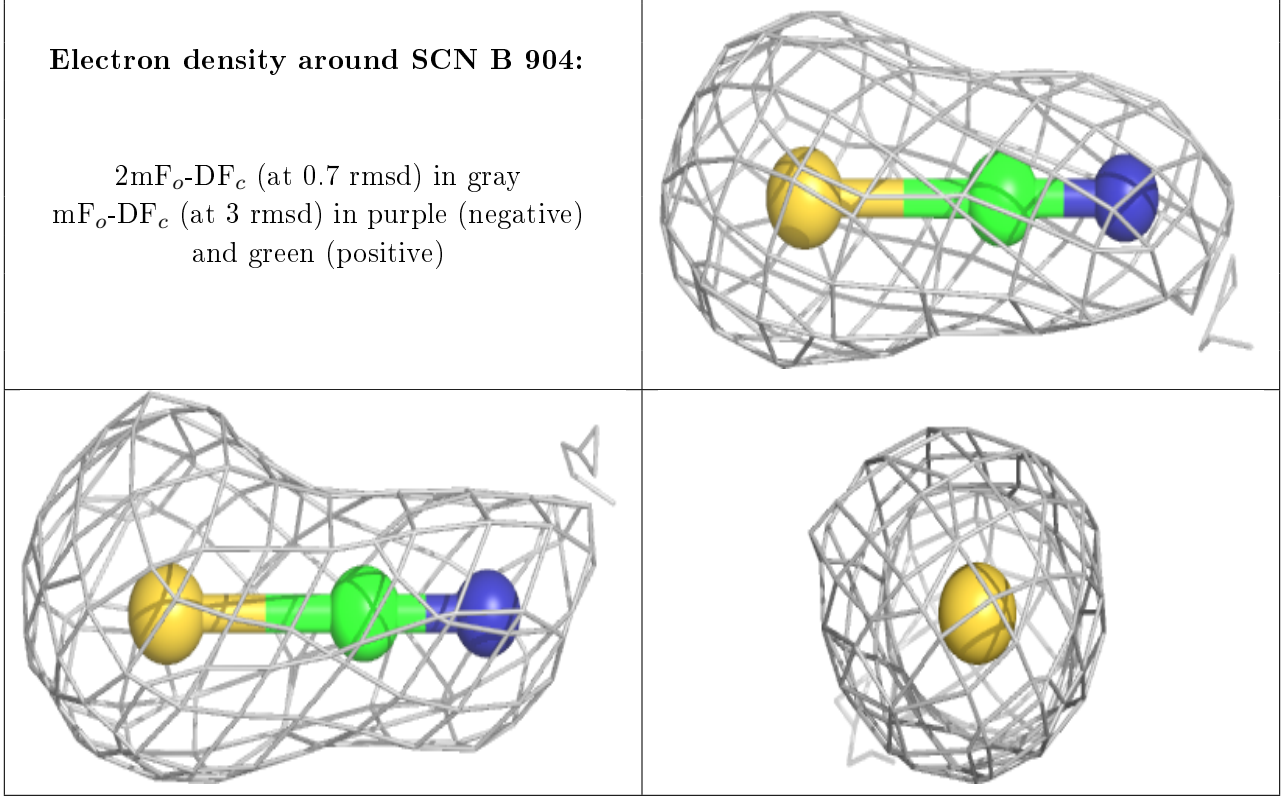
Electron density around SCN A 1008:

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



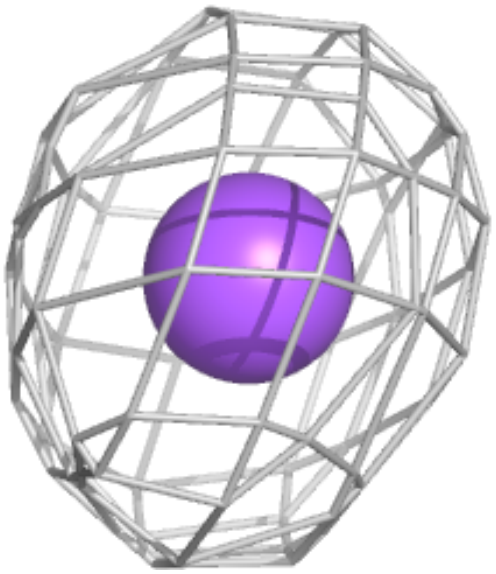
Electron density around SCN B 904:

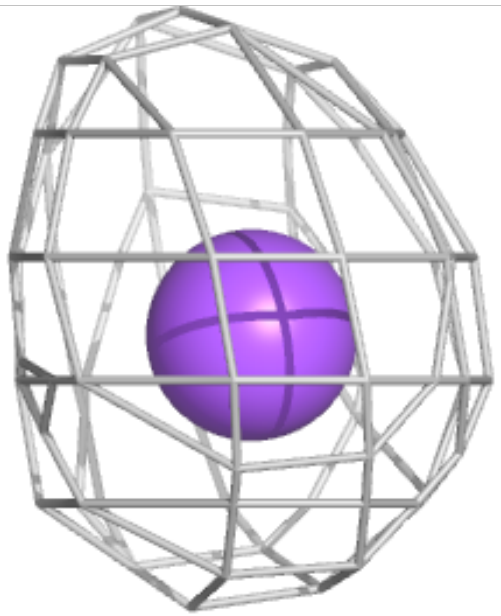
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

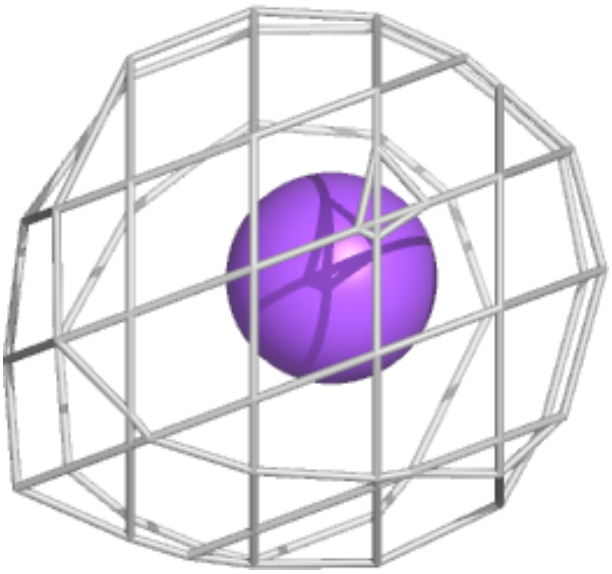


Electron density around NA A 1014:

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

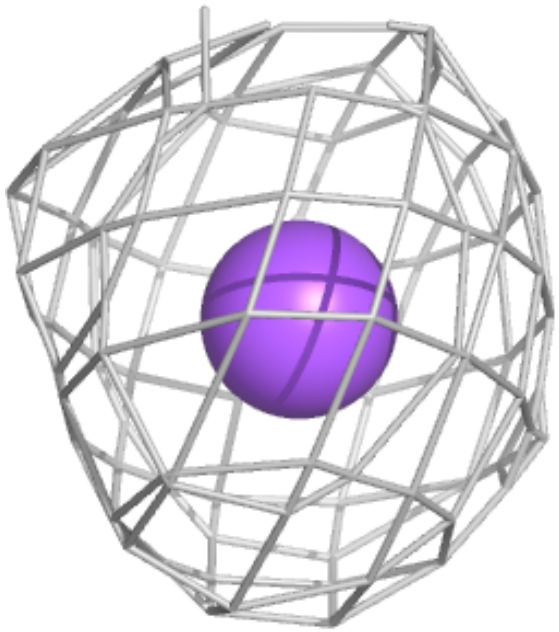


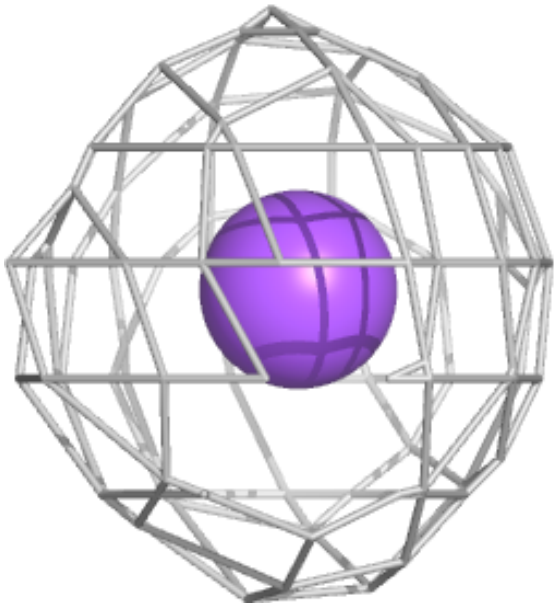


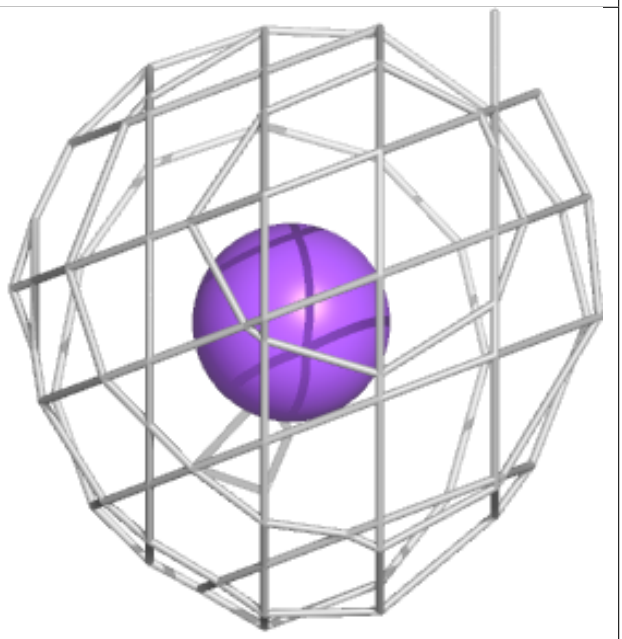


Electron density around NA B 910:

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

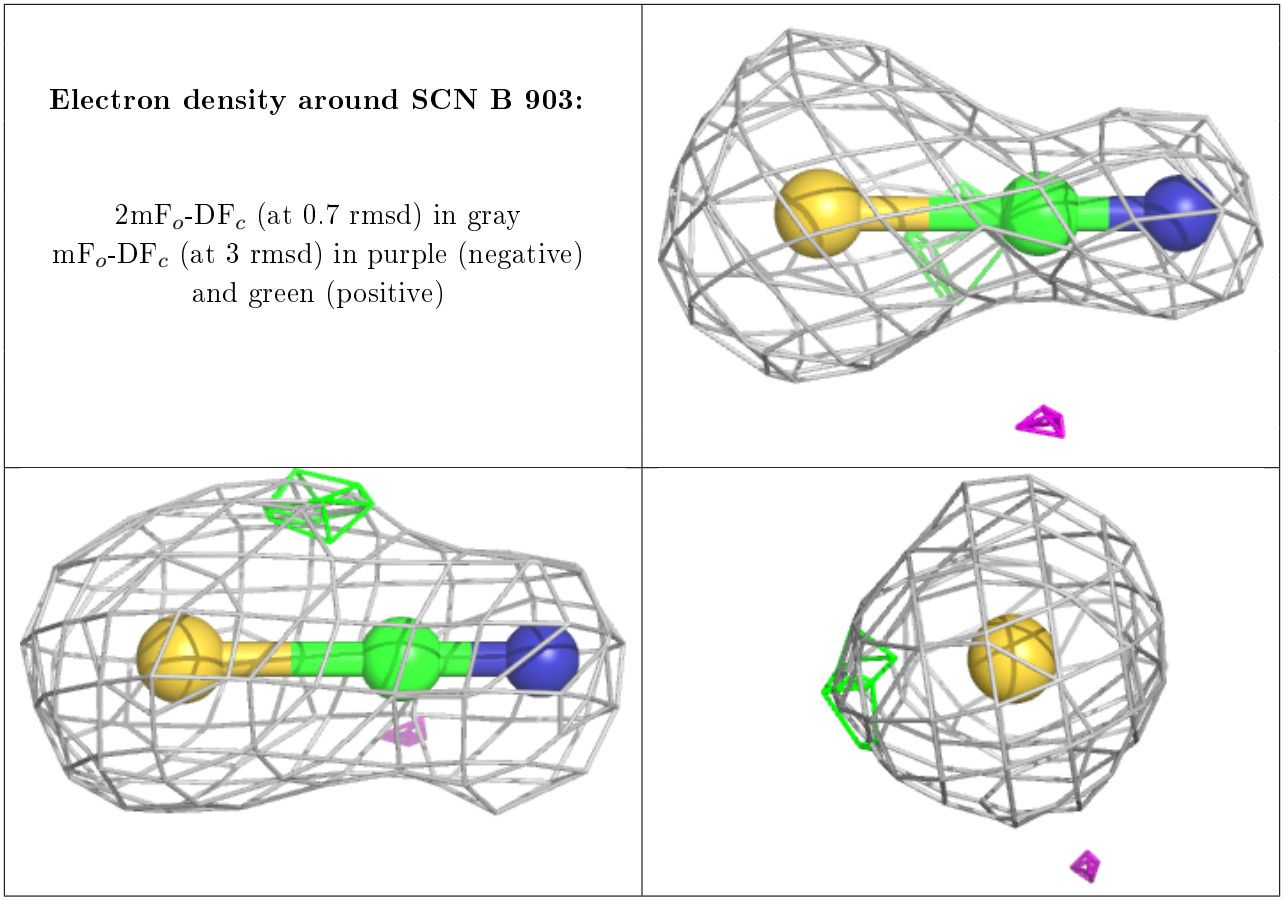






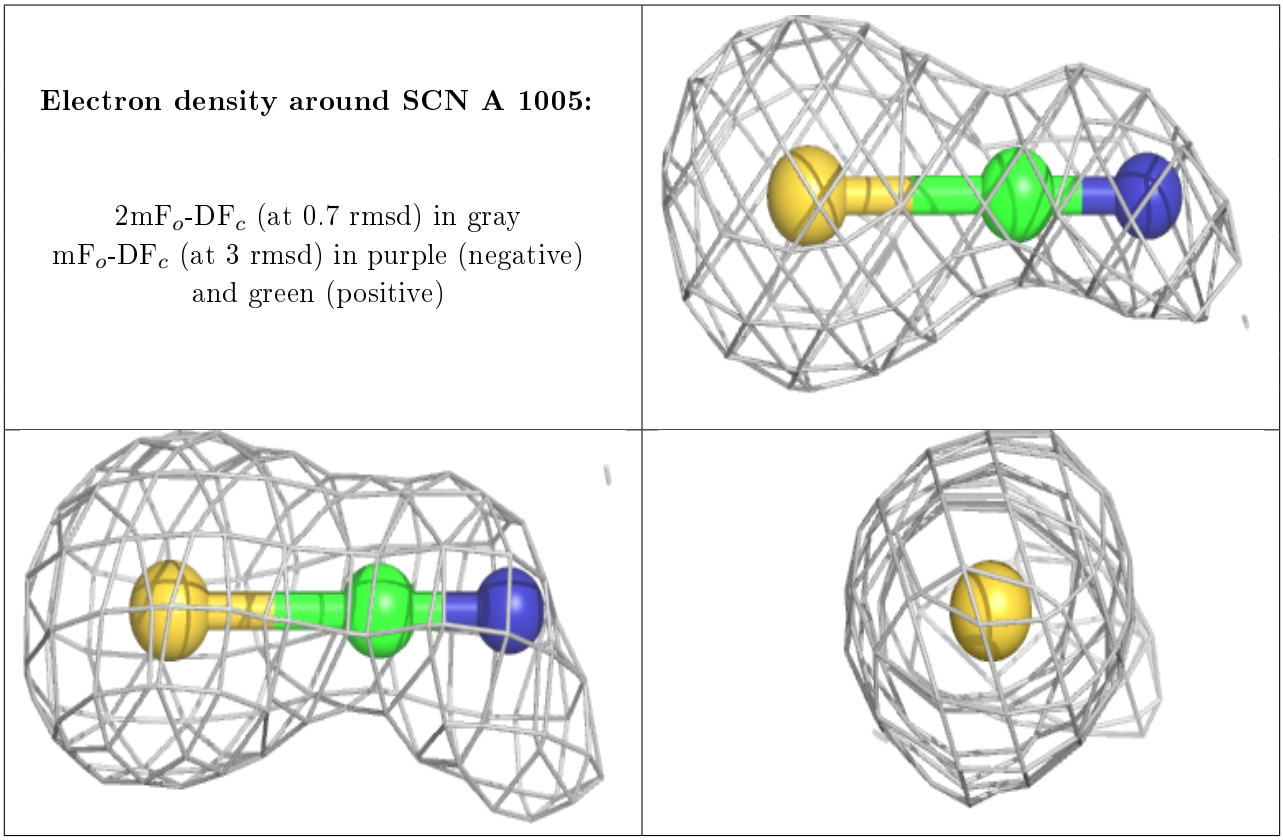
Electron density around SCN B 903:

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



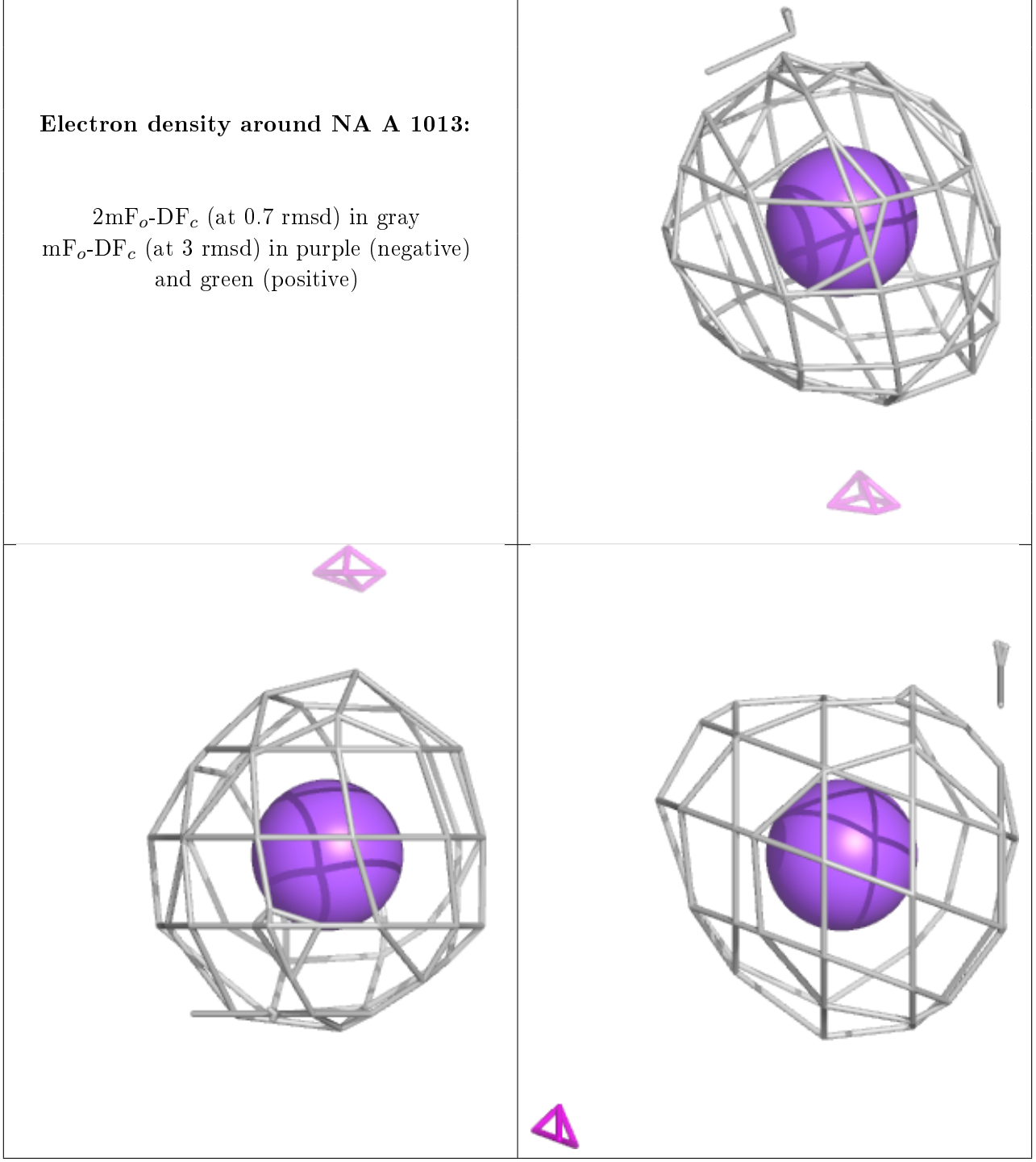
Electron density around SCN A 1005:

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



Electron density around NA A 1013:

$2mF_o$-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.