wwPDB X-ray Structure Validation Summary Report (i)

Sep 5, 2023 – 12:51 PM EDT

PDB ID	:	7RXY
Title	:	Hen egg-white lysozyme with ionic liquid ethylammonium nitrate 5 mol%
Authors	:	Han, Q.; Darmanin, C.; Smith, K.; Drummond, C.; Greaves, T.
Deposited on	:	2021-08-24
Resolution	:	1.60 Å(reported)

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

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

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

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

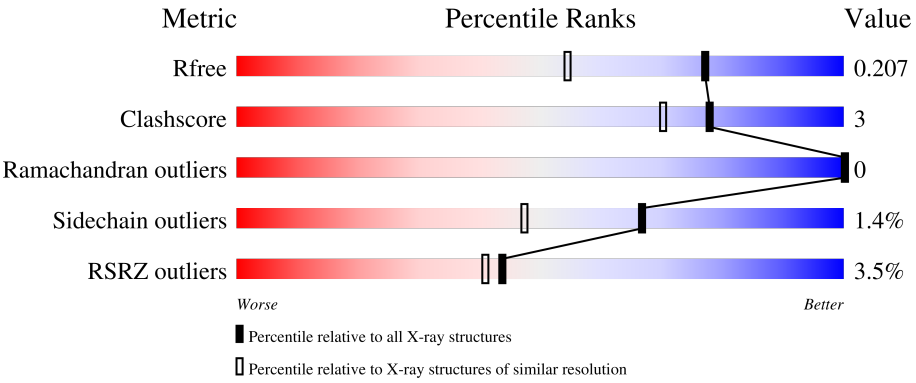
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	AAA	129	5% 91% 9%
1	BBB	129	2% 95% 5%

2 Entry composition (i)

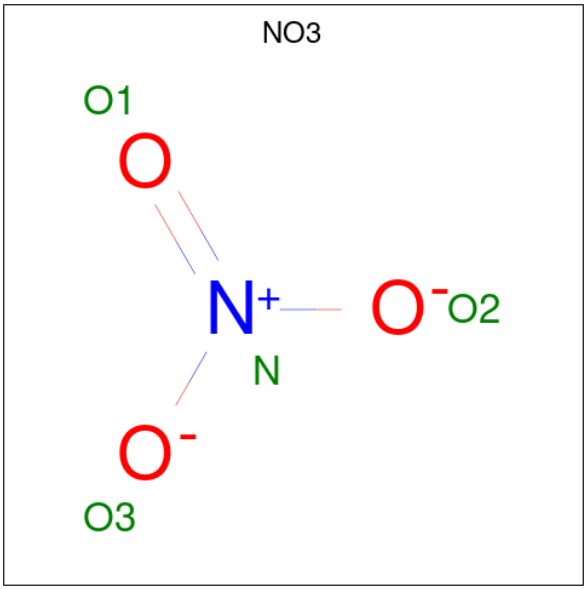
There are 3 unique types of molecules in this entry. The entry contains 2245 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysozyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	129	Total	C	N	O	S	0	2	0
			1022	625	201	186	10			
1	BBB	129	Total	C	N	O	S	0	4	0
			1027	629	201	187	10			

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	N	O		0	0
			4	1	3			
2	AAA	1	Total	N	O		0	0
			4	1	3			
2	AAA	1	Total	N	O		0	0
			4	1	3			
2	AAA	1	Total	N	O		0	0
			4	1	3			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total N O 4 1 3	0	0
2	AAA	1	Total N O 4 1 3	0	0
2	AAA	1	Total N O 4 1 3	0	0
2	BBB	1	Total N O 4 1 3	0	0
2	BBB	1	Total N O 4 1 3	0	0
2	BBB	1	Total N O 4 1 3	0	0
2	BBB	1	Total N O 4 1 3	0	0
2	BBB	1	Total N O 4 1 3	0	0
2	BBB	1	Total N O 4 1 3	0	0

- Molecule 3 is water.

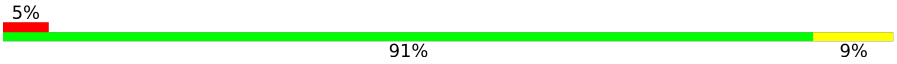
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	71	Total O 71 71	0	0
3	BBB	73	Total O 73 73	0	0

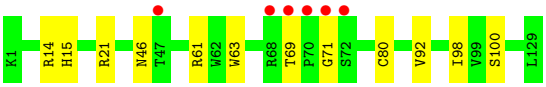
3 Residue-property plots (i)

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: Lysozyme C

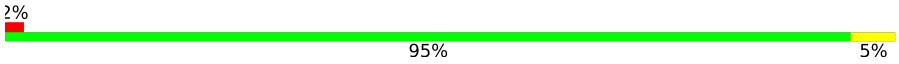
Chain AAA:

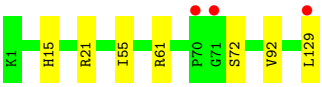




- Molecule 1: Lysozyme C

Chain BBB:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	27.53Å 62.48Å 59.65Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	29.84 – 1.60 29.82 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.84-1.60) 97.7 (29.82-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.30 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.140 , 0.207 0.139 , 0.207	Depositor DCC
R_{free} test set	1352 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h,-l,-k 0.000 for -h,l,k 0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2245	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7993e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NO3

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	AAA	0.63	0/1042	0.91	0/1407
1	BBB	0.62	0/1057	0.94	0/1427
All	All	0.62	0/2099	0.92	0/2834

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	AAA	1022	0	983	8	0
1	BBB	1027	0	993	4	0
2	AAA	28	0	0	2	0
2	BBB	24	0	0	0	0
3	AAA	71	0	0	0	0
3	BBB	73	0	0	0	0
All	All	2245	0	1976	12	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 3.

The worst 5 of 12 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:AAA:61:ARG:HA	1:AAA:69:THR:HG21	1.86	0.55
1:AAA:61:ARG:NH2	1:AAA:71:GLY:O	2.42	0.53
1:BBB:61:ARG:O	1:BBB:72:SER:HA	2.10	0.52
1:AAA:21[A]:ARG:HD2	1:AAA:100:SER:OG	2.13	0.49
1:BBB:15:HIS:HB3	1:BBB:92:VAL:HG11	1.94	0.49

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	AAA	129/129 (100%)	129 (100%)	0	0	100	100
1	BBB	131/129 (102%)	128 (98%)	3 (2%)	0	100	100
All	All	260/258 (101%)	257 (99%)	3 (1%)	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	AAA	107/105 (102%)	106 (99%)	1 (1%)	78	65
1	BBB	109/105 (104%)	107 (98%)	2 (2%)	59	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	216/210 (103%)	213 (99%)	3 (1%)	67 47

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

Mol	Chain	Res	Type
1	AAA	46	ASN
1	BBB	55	ILE
1	BBB	129	LEU

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NO3	BBB	202	-	1,3,3	0.37	0	0,3,3	-	-
2	NO3	AAA	204	-	1,3,3	0.42	0	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NO3	AAA	201	-	1,3,3	0.69	0	0,3,3	-	-
2	NO3	AAA	207	-	1,3,3	0.08	0	0,3,3	-	-
2	NO3	AAA	203	-	1,3,3	0.33	0	0,3,3	-	-
2	NO3	AAA	202	-	1,3,3	0.10	0	0,3,3	-	-
2	NO3	AAA	206	-	1,3,3	0.07	0	0,3,3	-	-
2	NO3	BBB	201	-	1,3,3	0.13	0	0,3,3	-	-
2	NO3	BBB	206	-	1,3,3	2.00	0	0,3,3	-	-
2	NO3	AAA	205	-	1,3,3	0.40	0	0,3,3	-	-
2	NO3	BBB	203	-	1,3,3	0.53	0	0,3,3	-	-
2	NO3	BBB	205	-	1,3,3	0.13	0	0,3,3	-	-
2	NO3	BBB	204	-	1,3,3	0.31	0	0,3,3	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

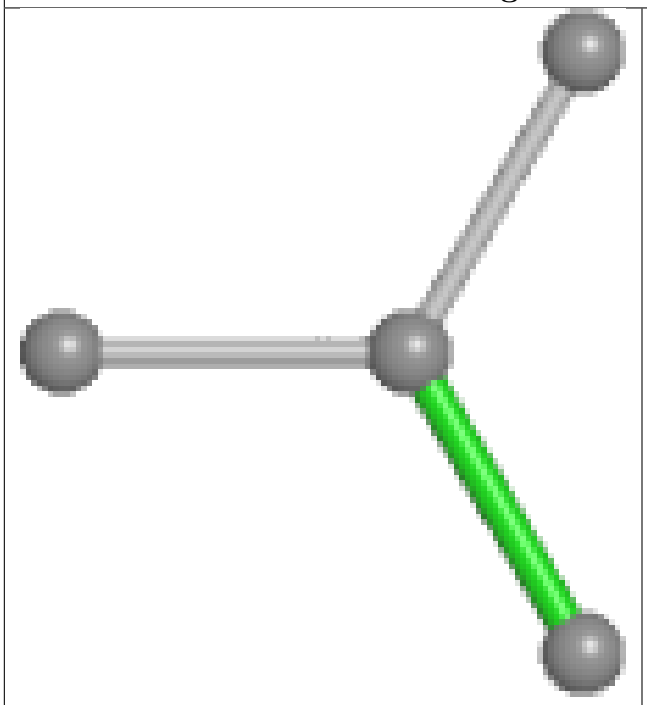
There are no ring outliers.

2 monomers are involved in 2 short contacts:

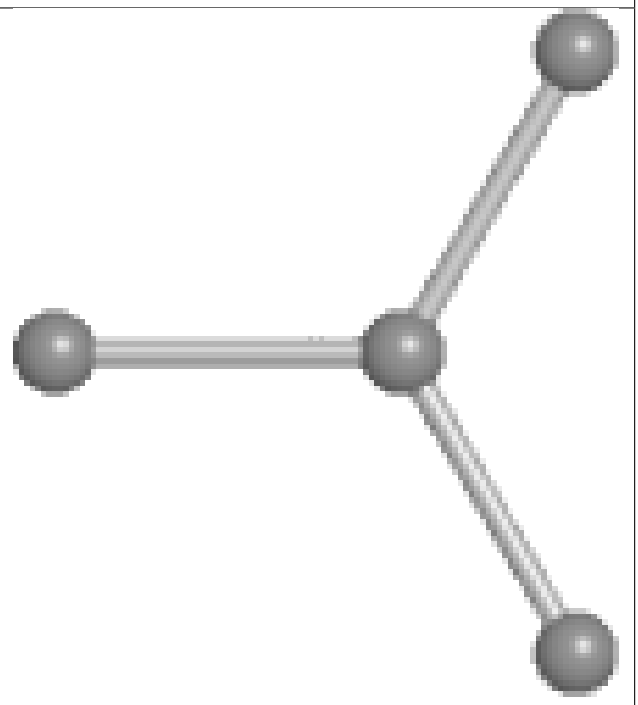
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	207	NO3	1	0
2	AAA	206	NO3	1	0

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.

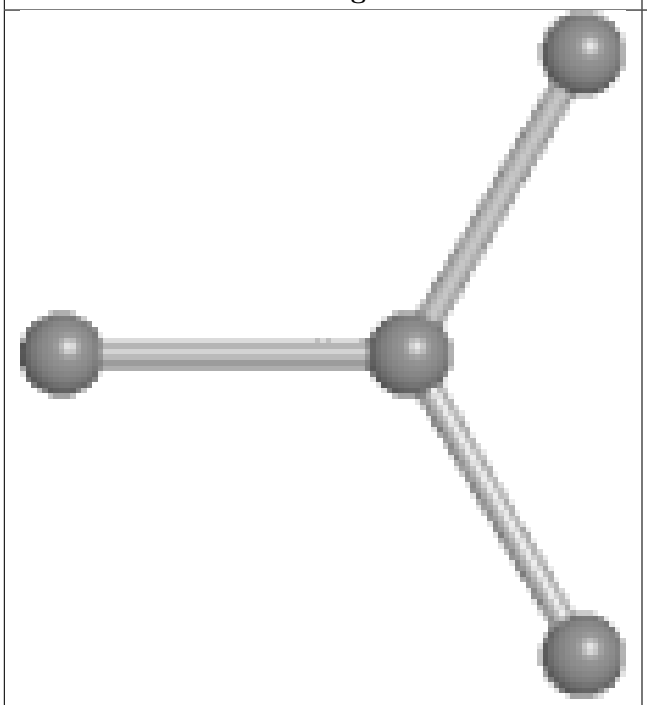
Ligand NO3 BBB 202



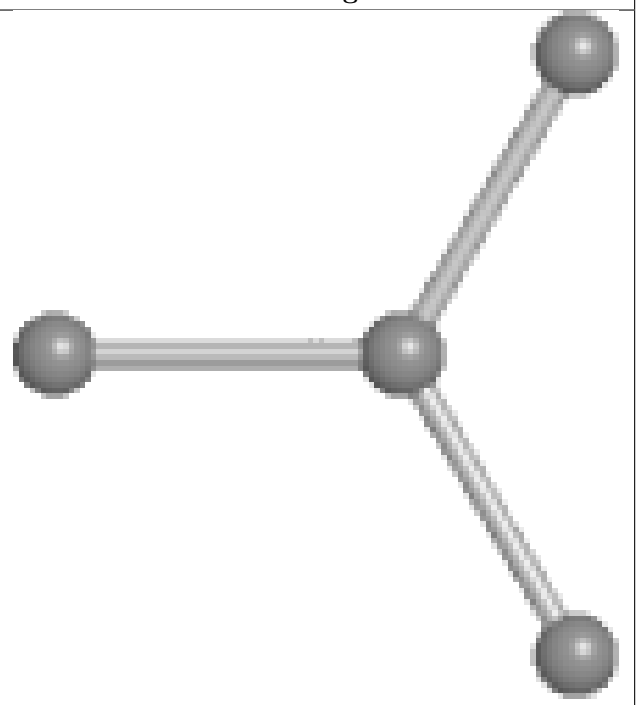
Bond lengths



Bond angles

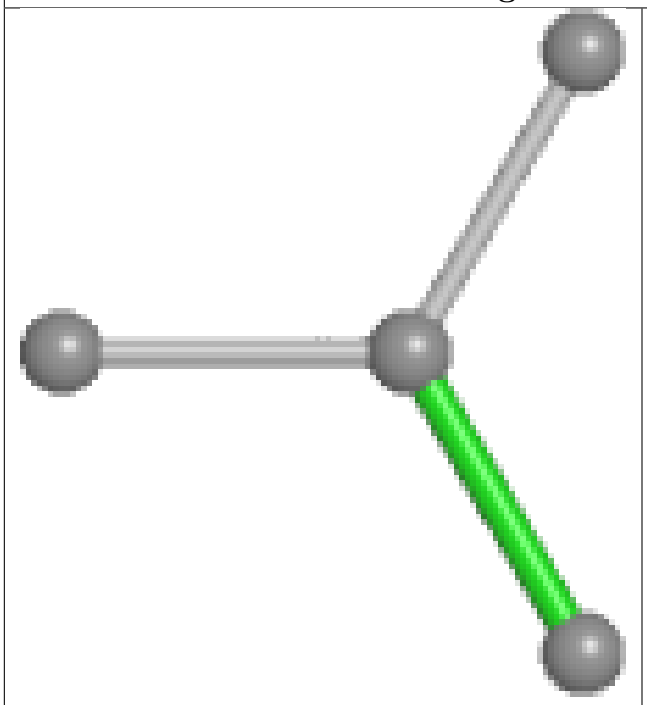


Torsions

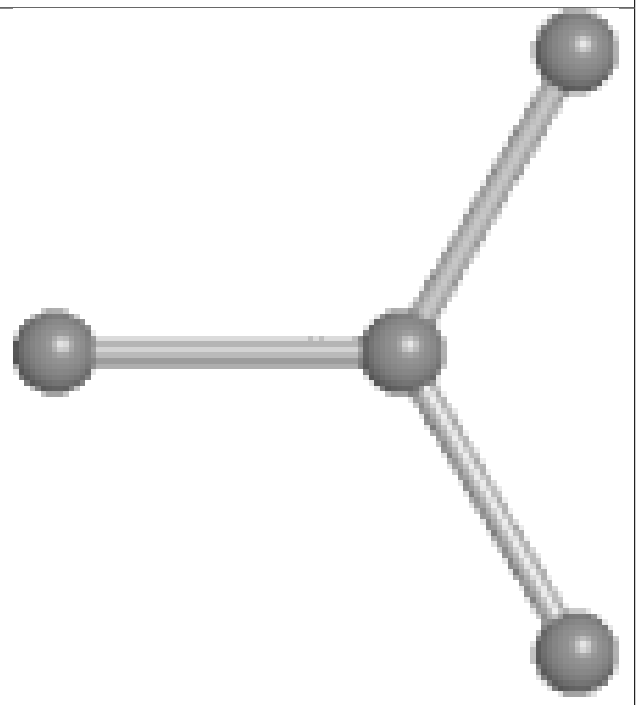


Rings

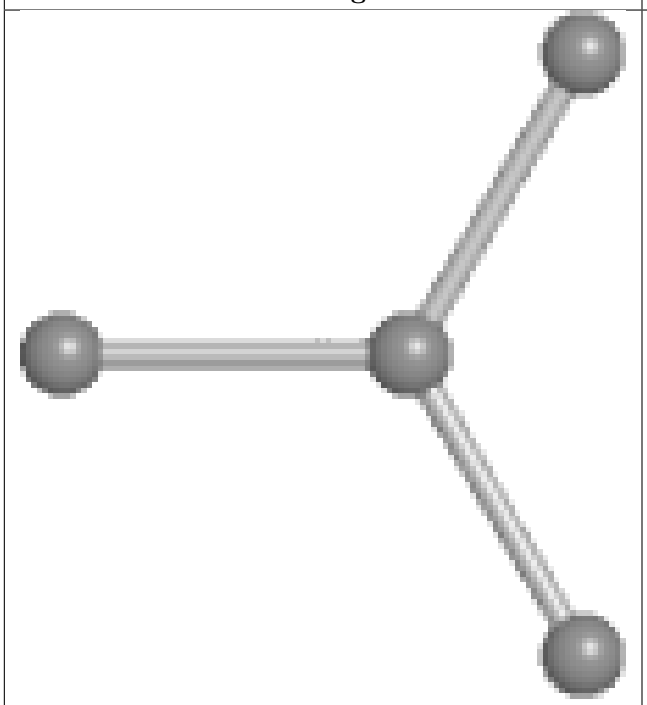
Ligand NO3 AAA 204



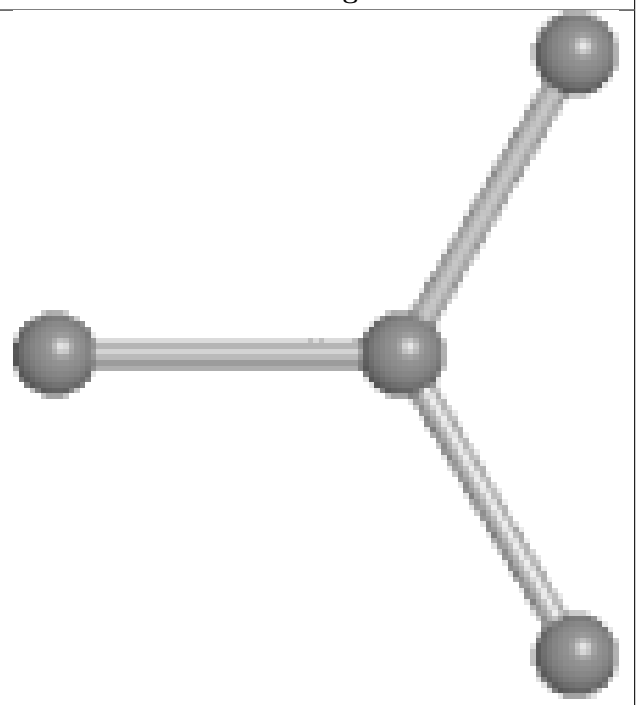
Bond lengths



Bond angles

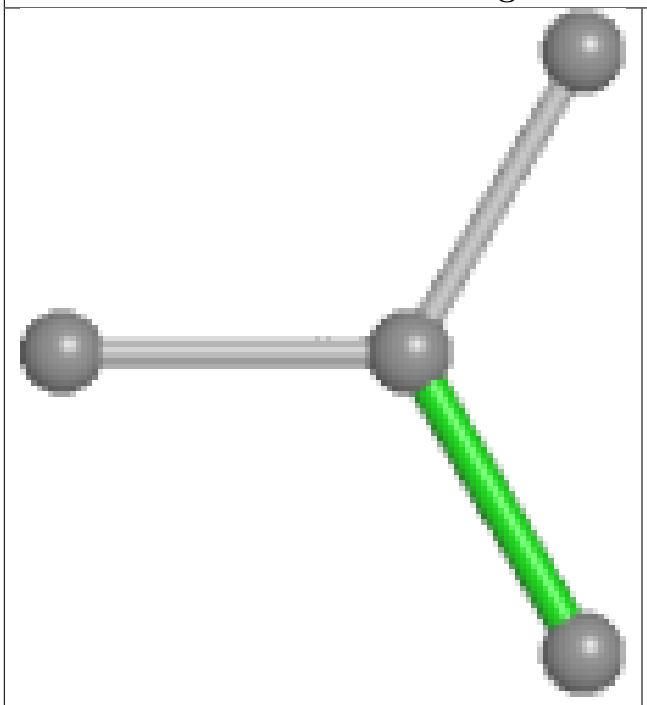


Torsions

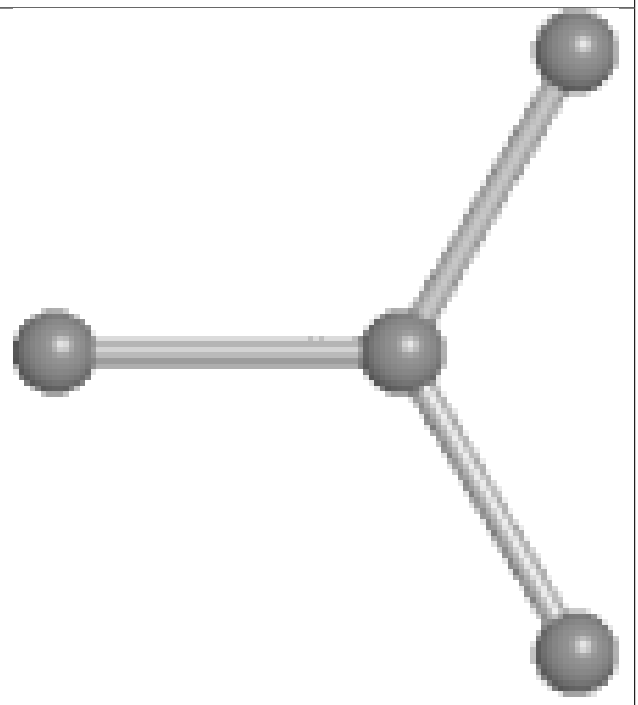


Rings

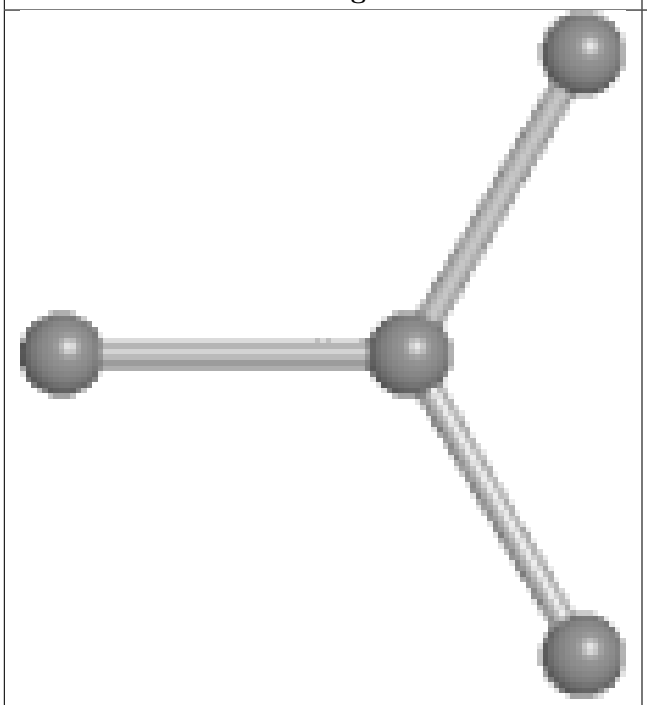
Ligand NO3 AAA 201



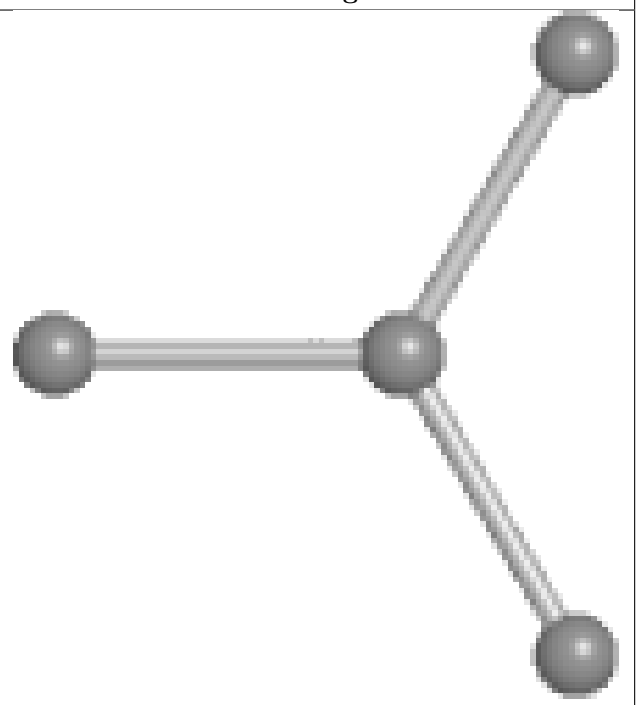
Bond lengths



Bond angles

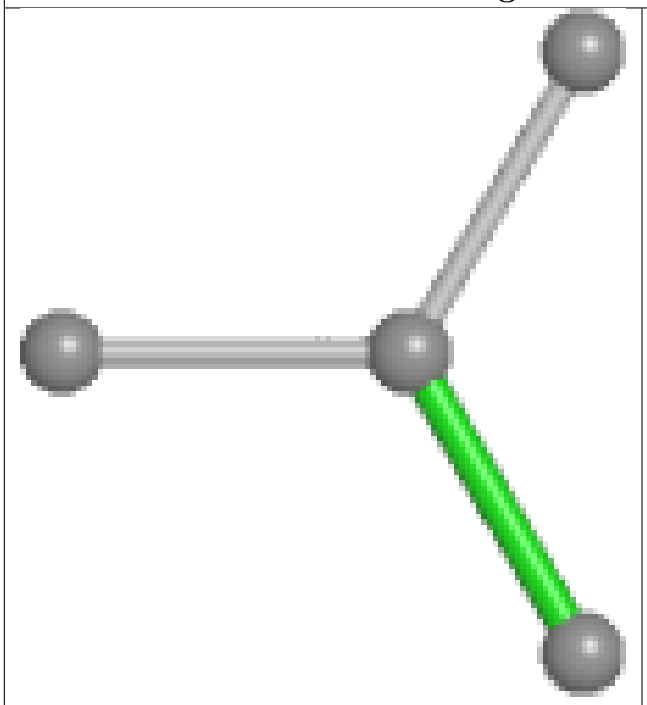


Torsions

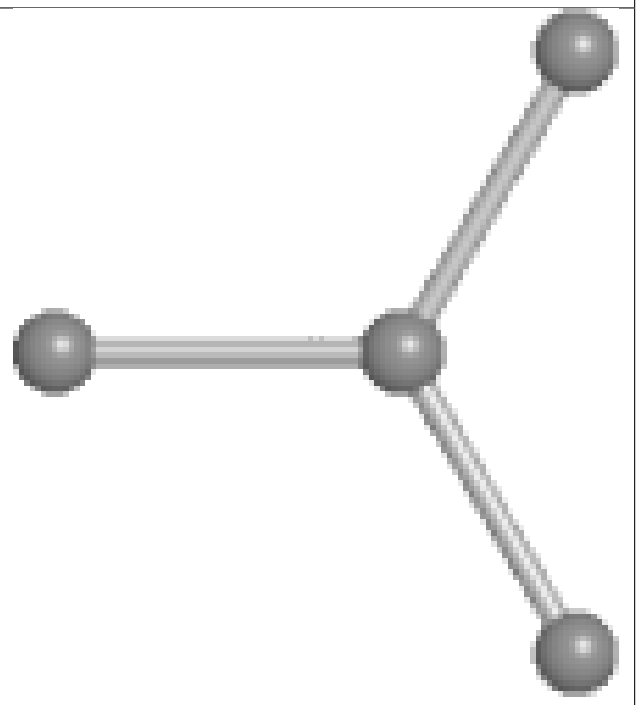


Rings

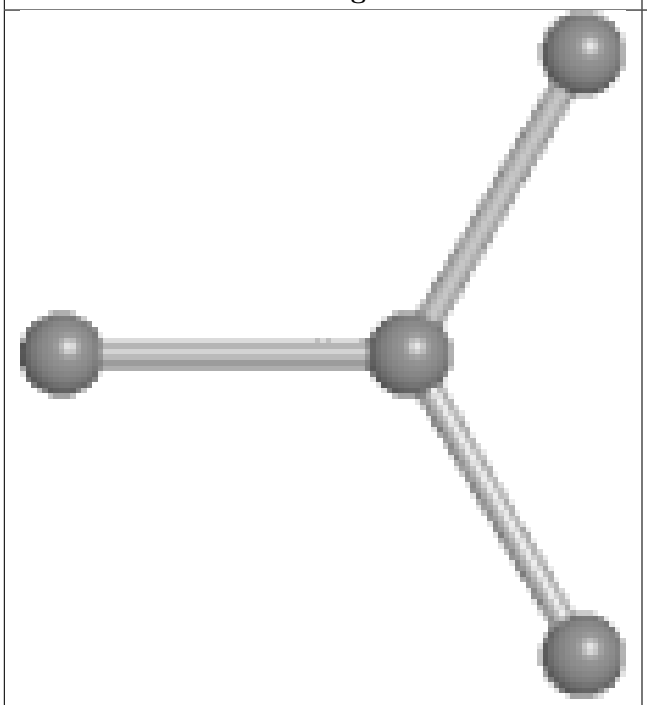
Ligand NO3 AAA 207



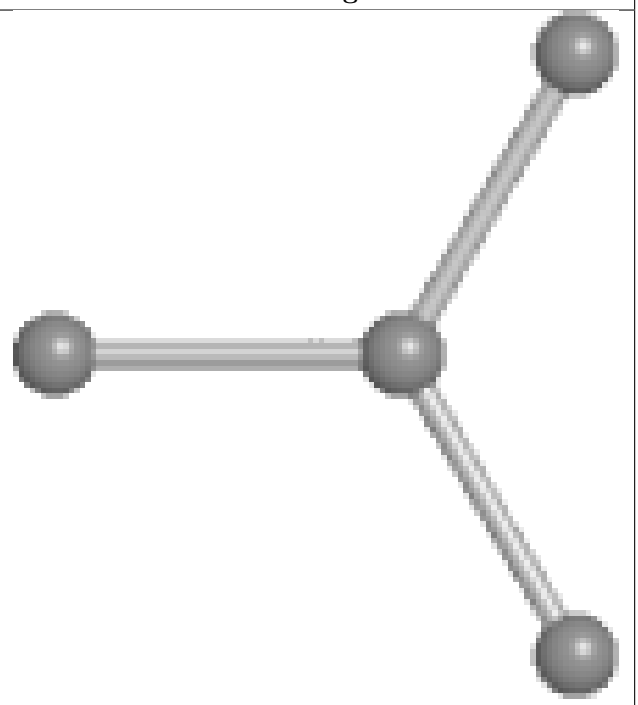
Bond lengths



Bond angles

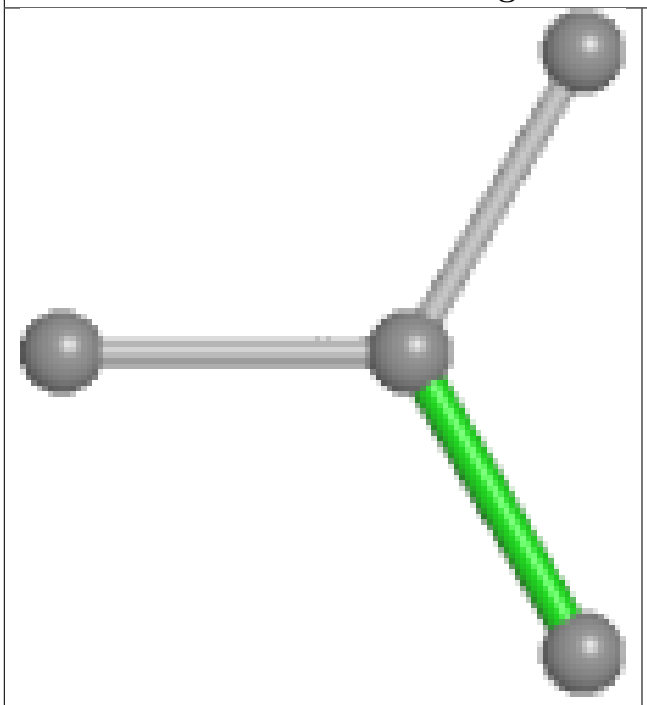


Torsions

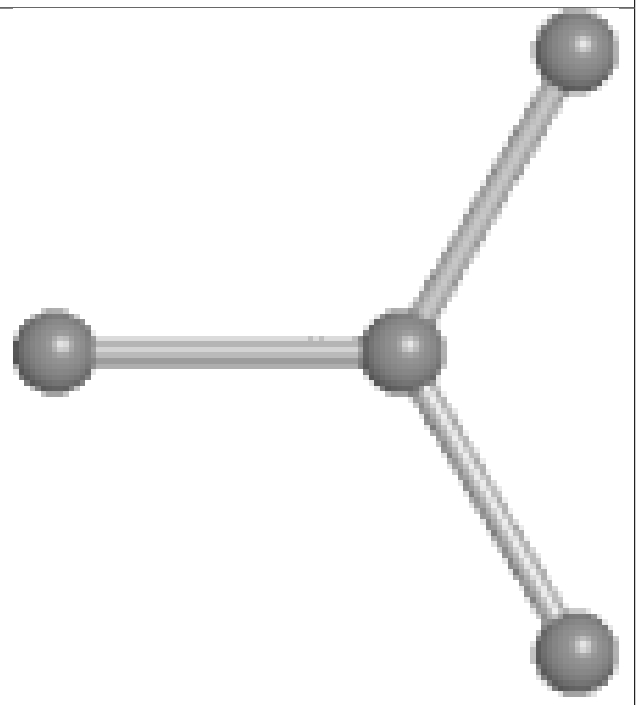


Rings

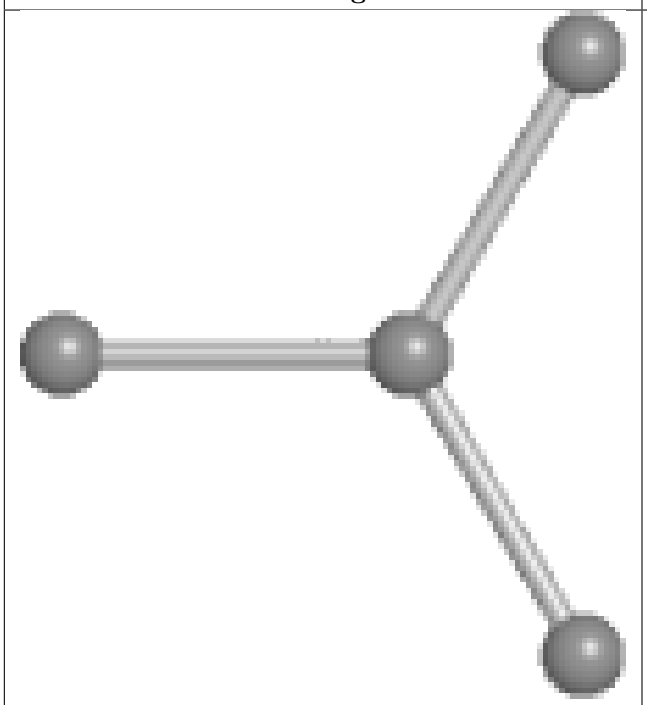
Ligand NO3 AAA 203



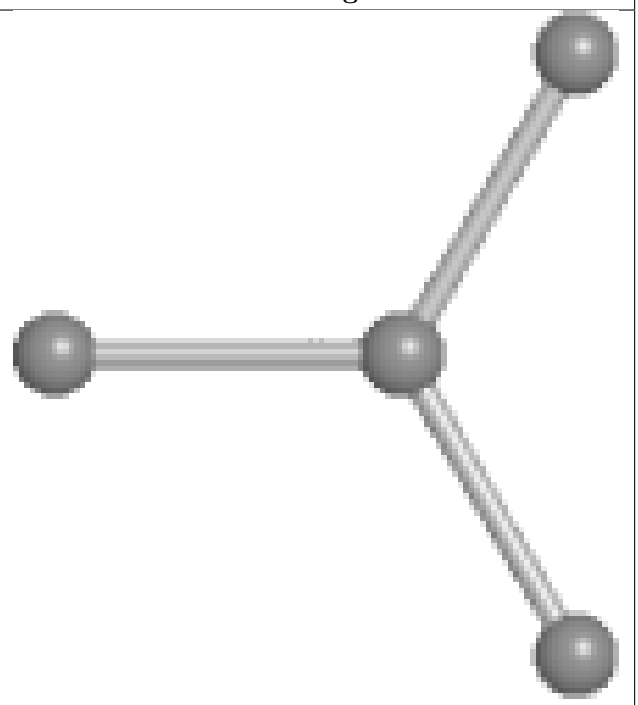
Bond lengths



Bond angles

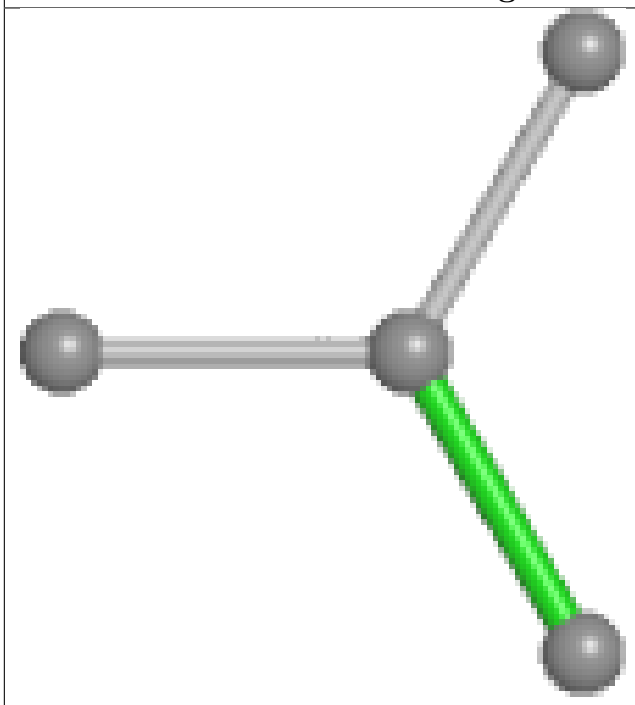


Torsions

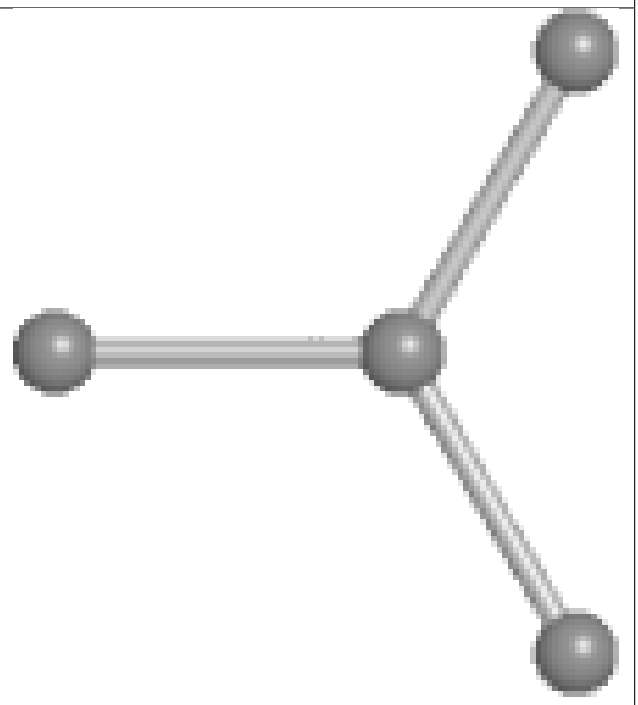


Rings

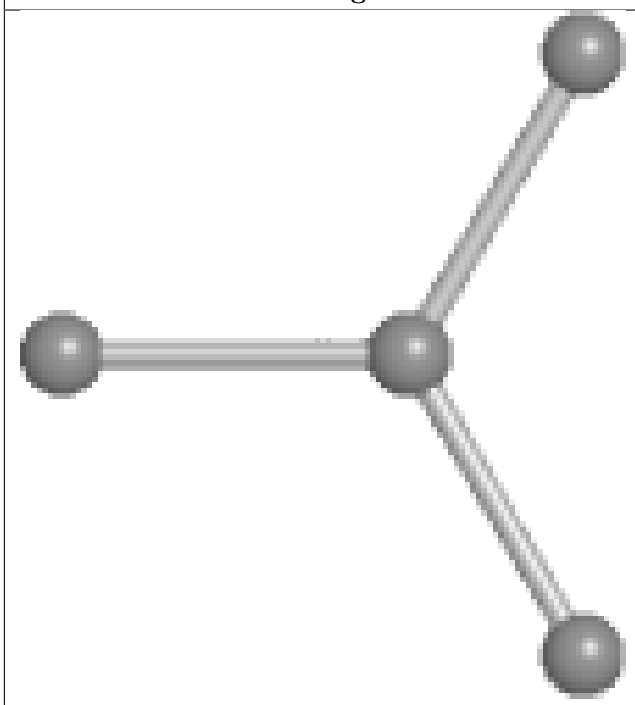
Ligand NO3 AAA 202



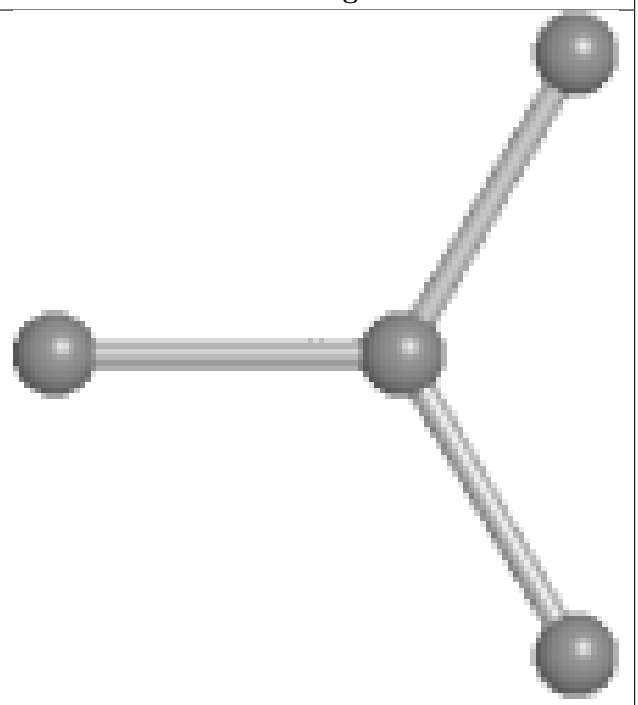
Bond lengths



Bond angles

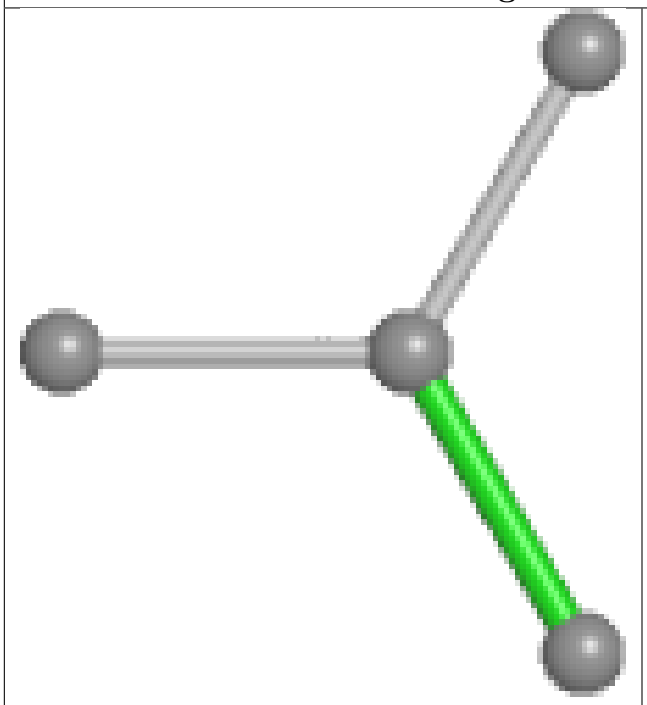


Torsions

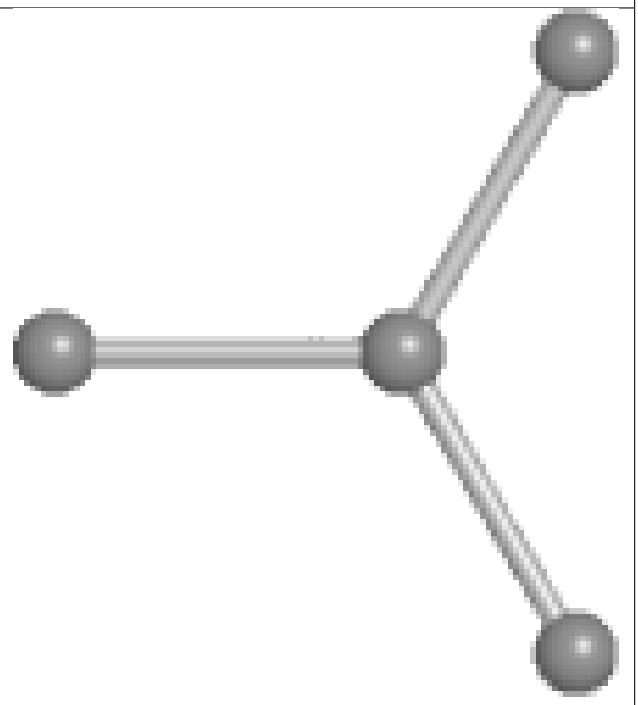


Rings

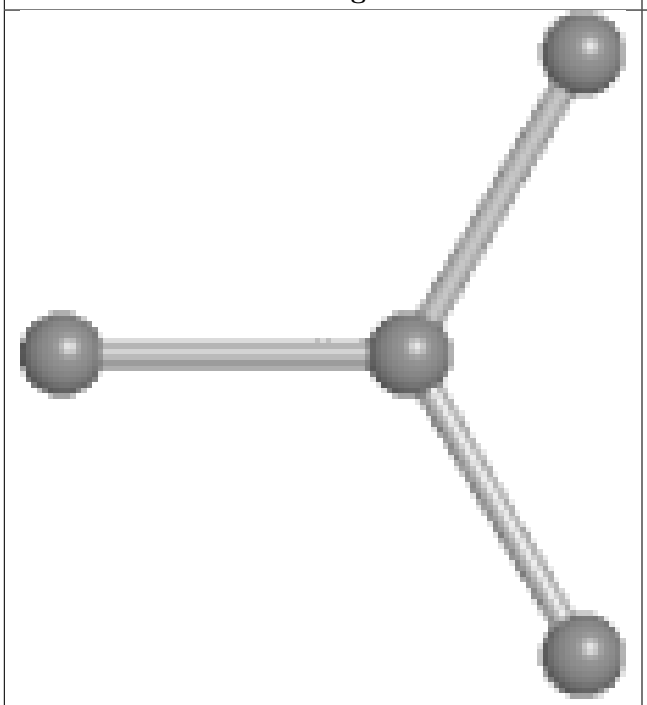
Ligand NO3 AAA 206



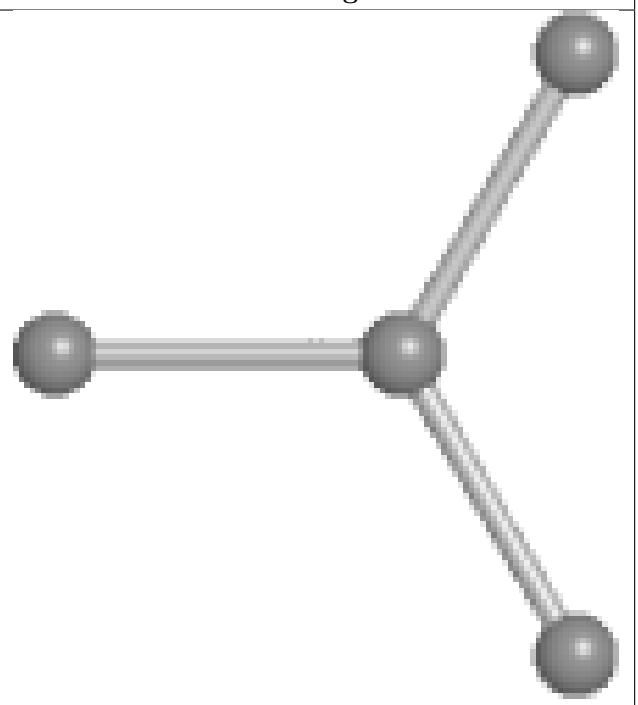
Bond lengths



Bond angles

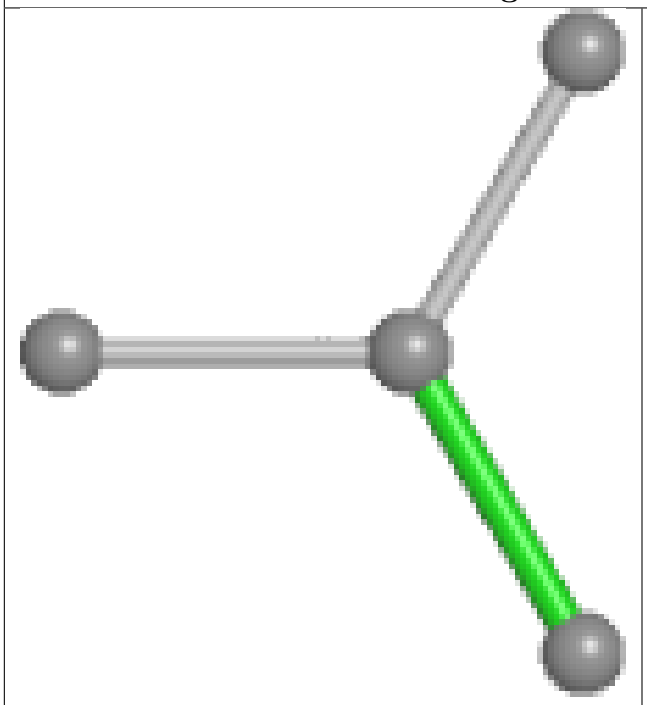


Torsions

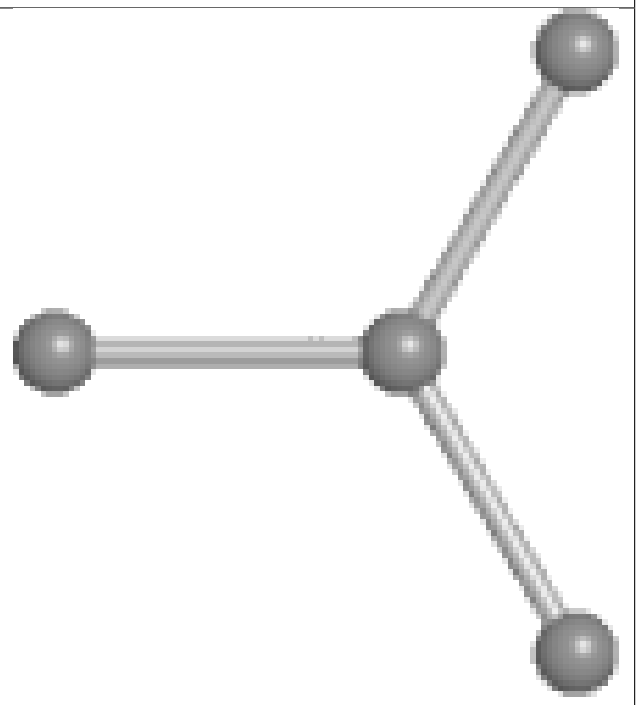


Rings

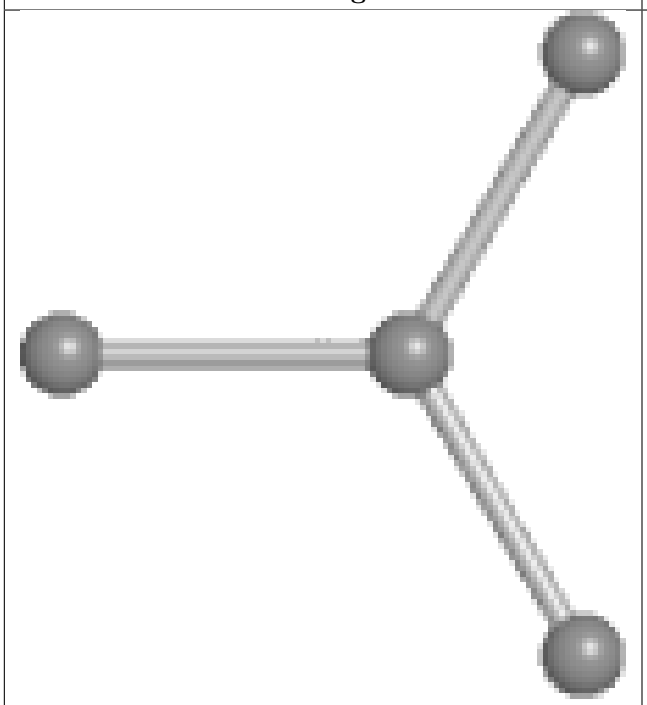
Ligand NO3 BBB 201



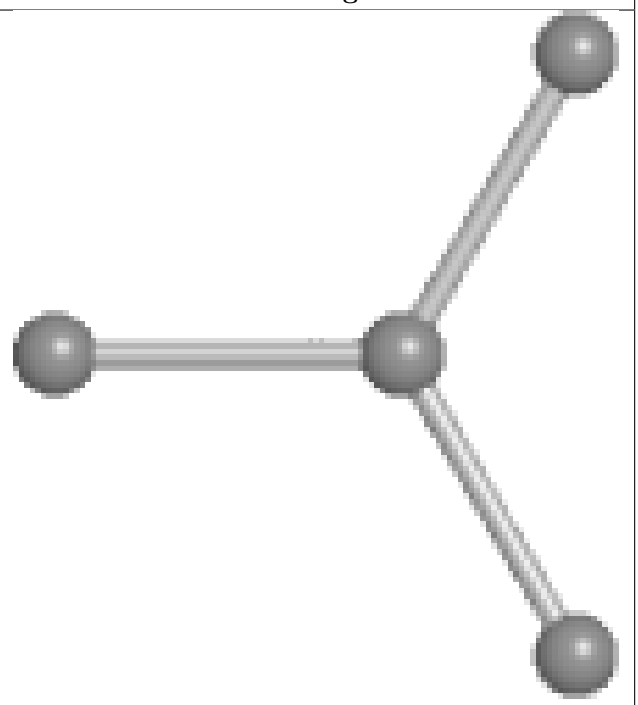
Bond lengths



Bond angles

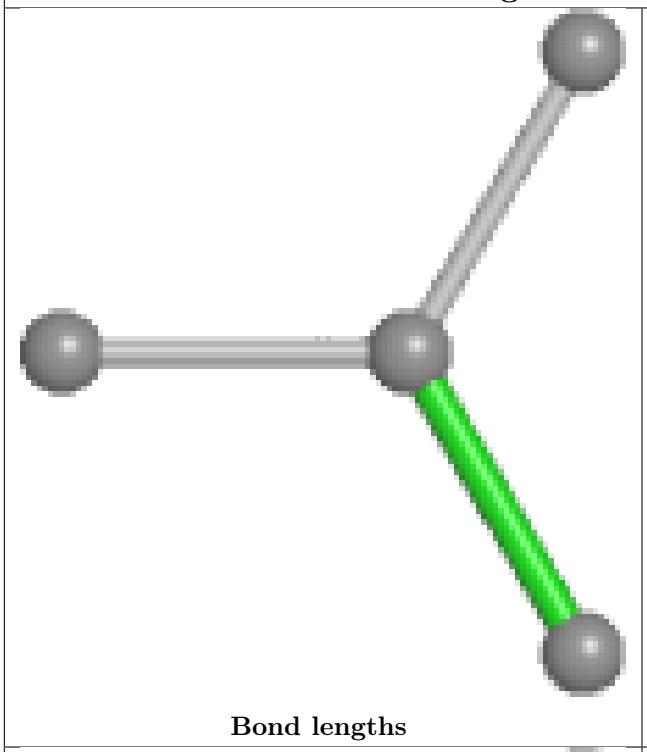


Torsions

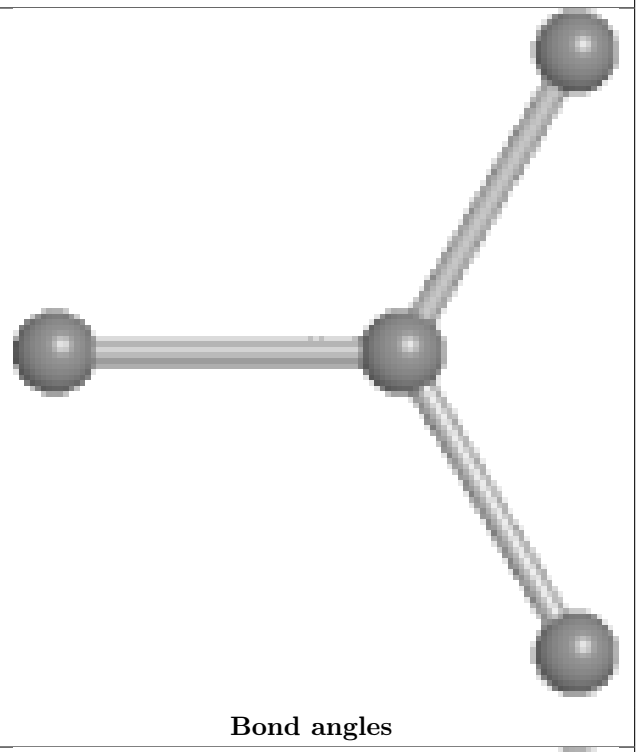


Rings

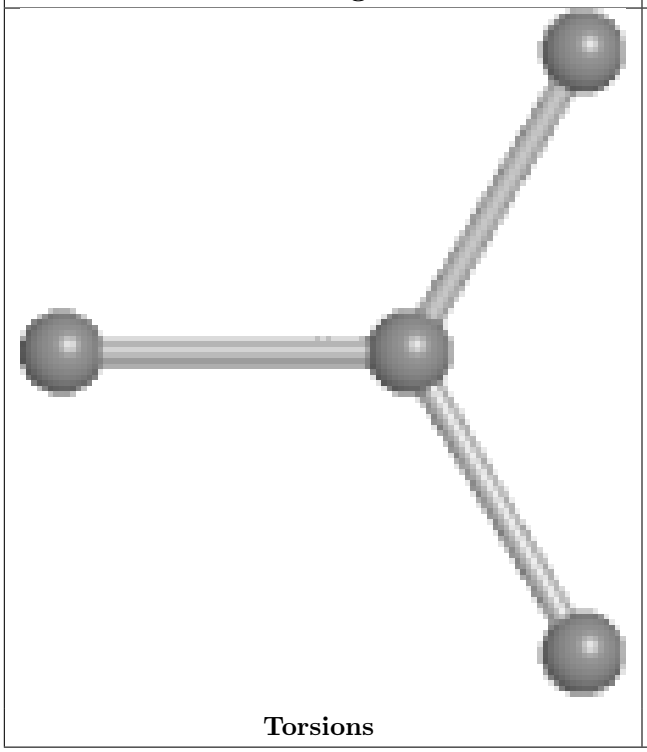
Ligand NO3 BBB 206



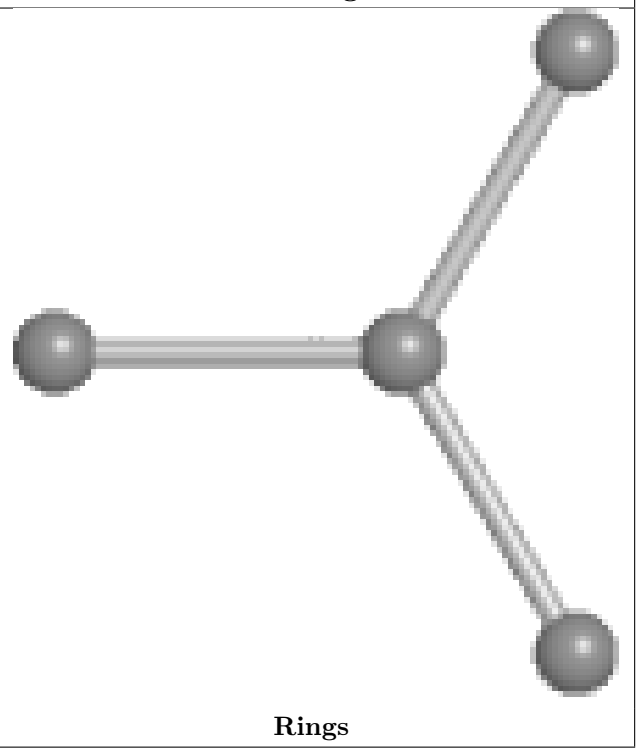
Bond lengths



Bond angles

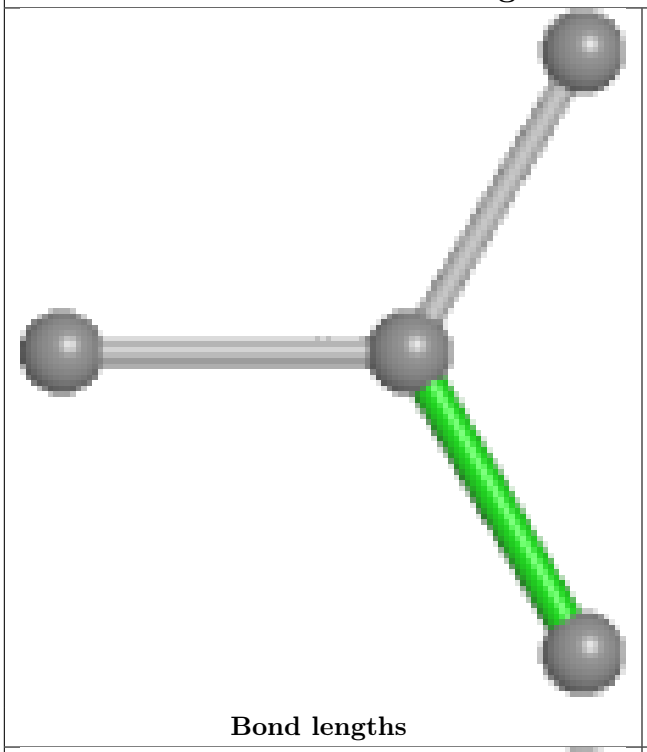


Torsions

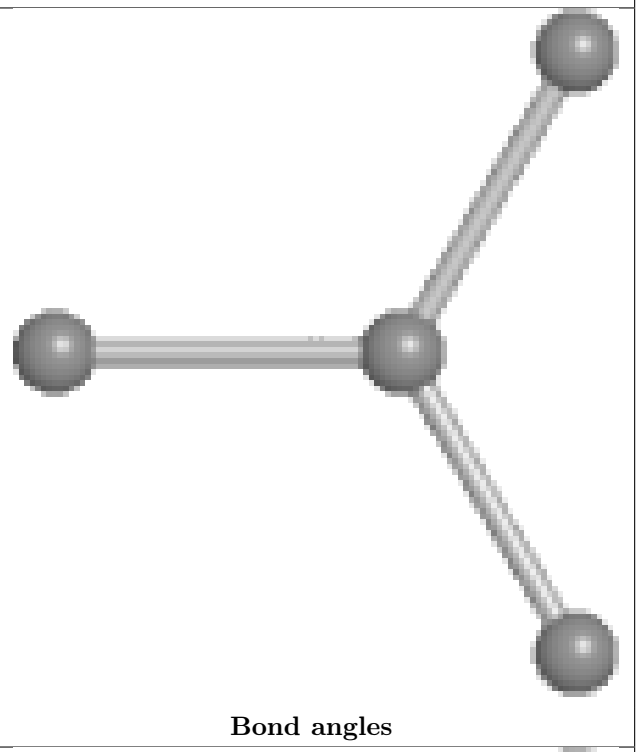


Rings

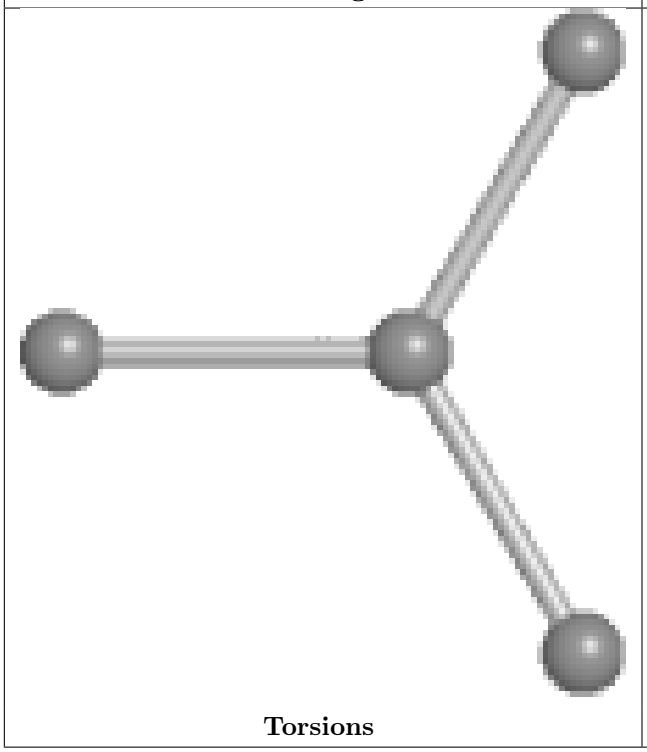
Ligand NO3 AAA 205



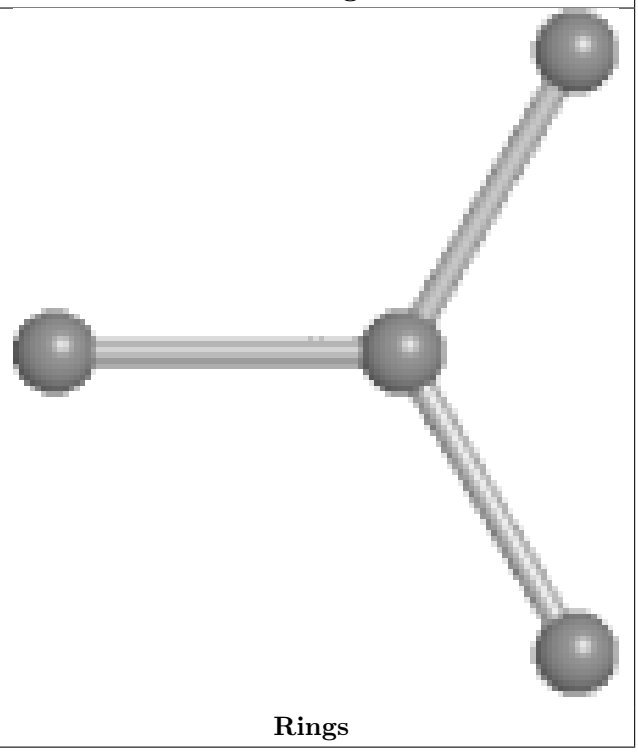
Bond lengths



Bond angles

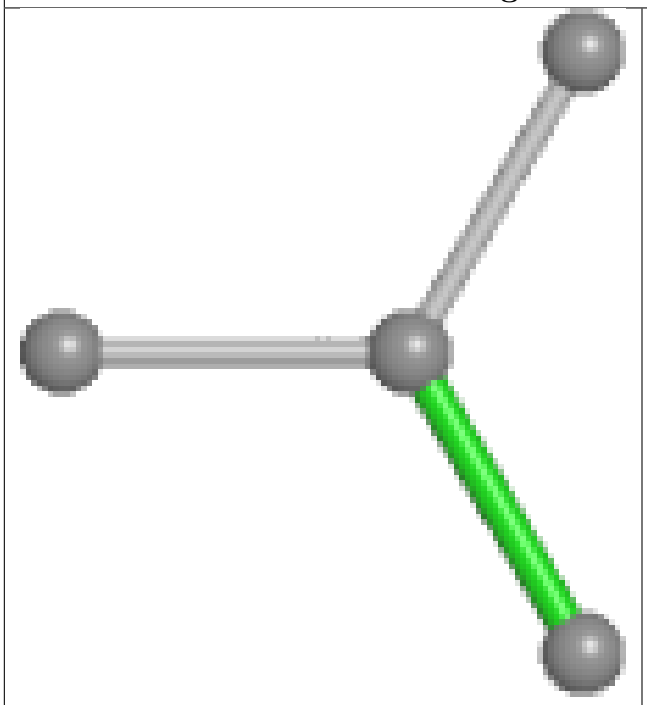


Torsions

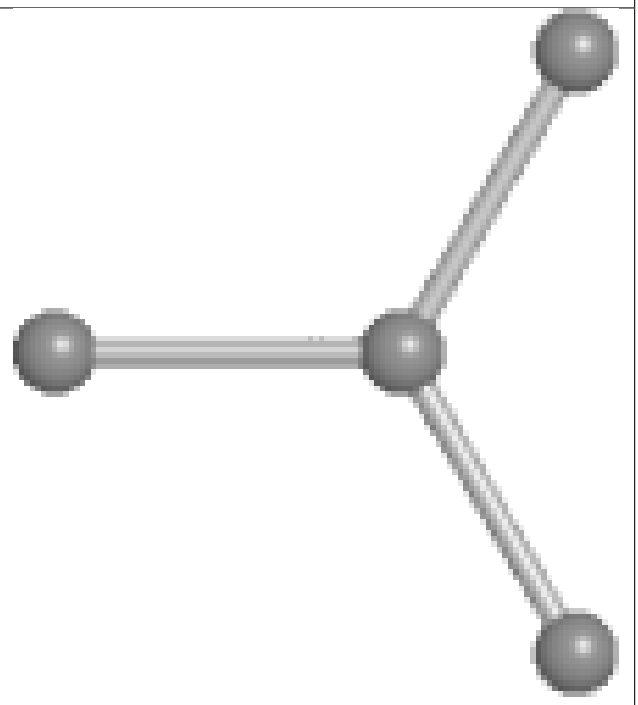


Rings

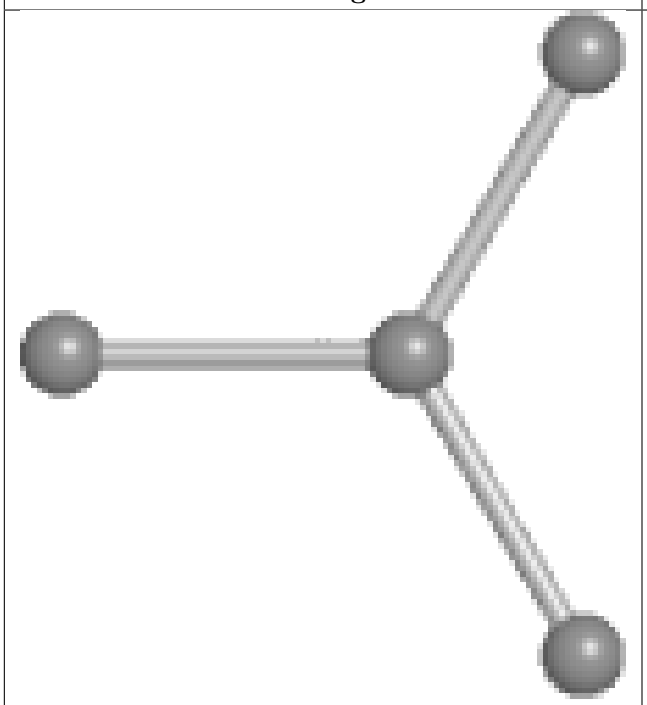
Ligand NO3 BBB 203



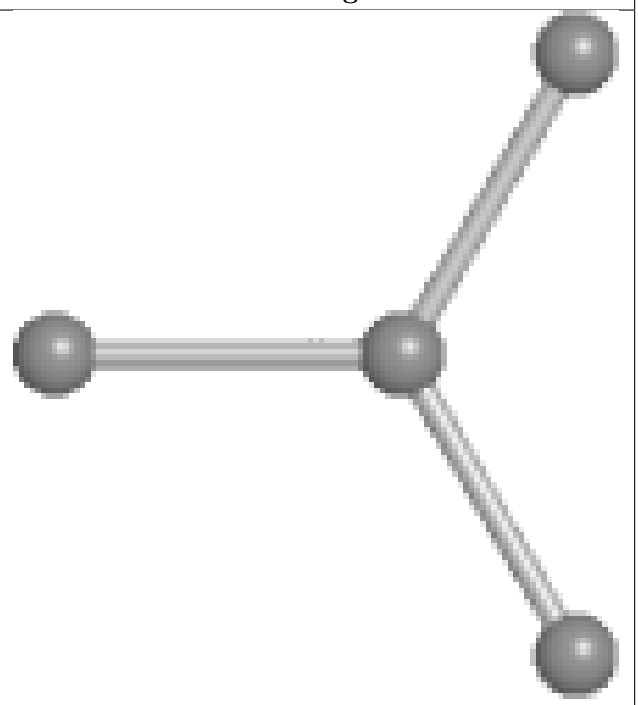
Bond lengths



Bond angles

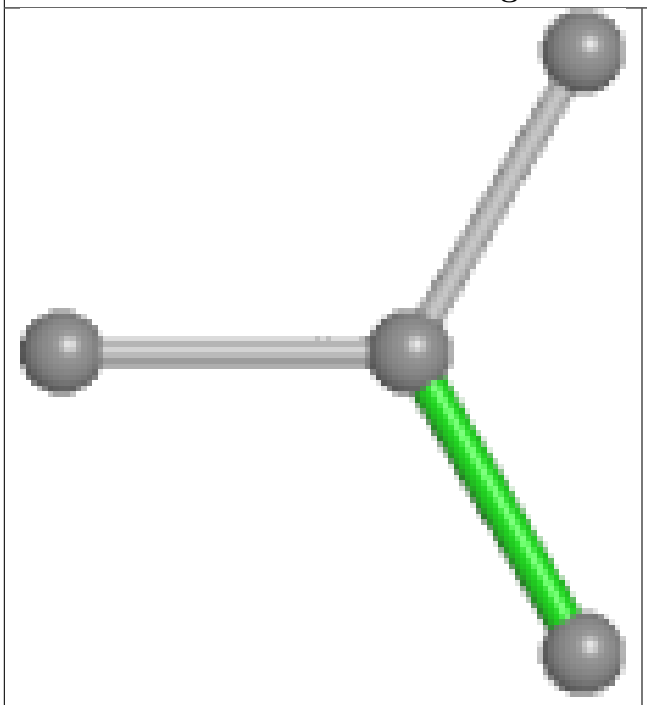


Torsions

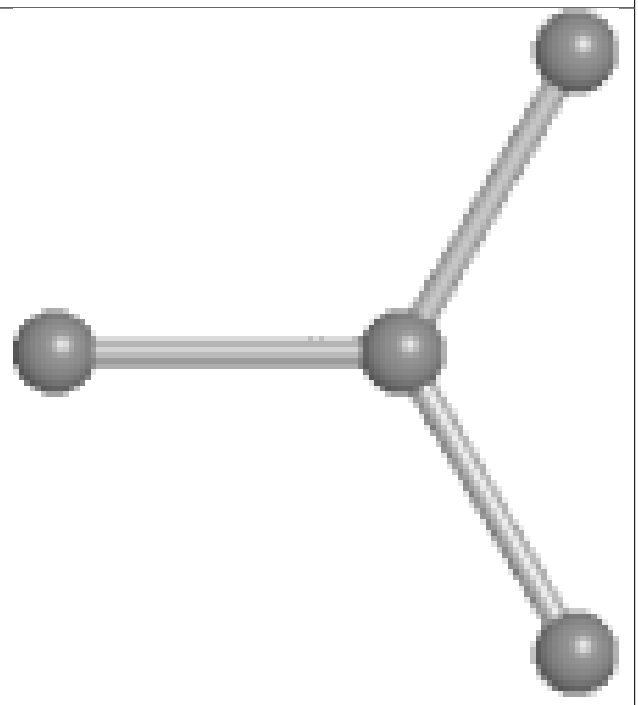


Rings

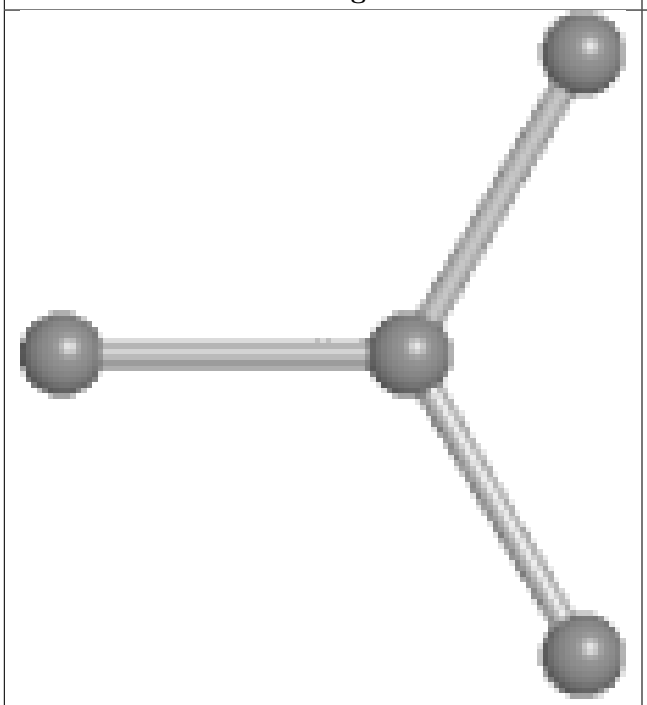
Ligand NO3 BBB 205



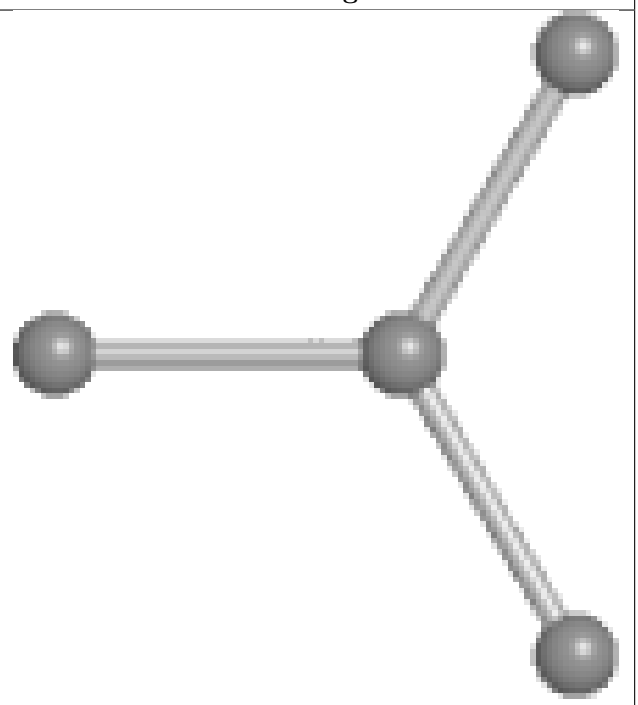
Bond lengths



Bond angles

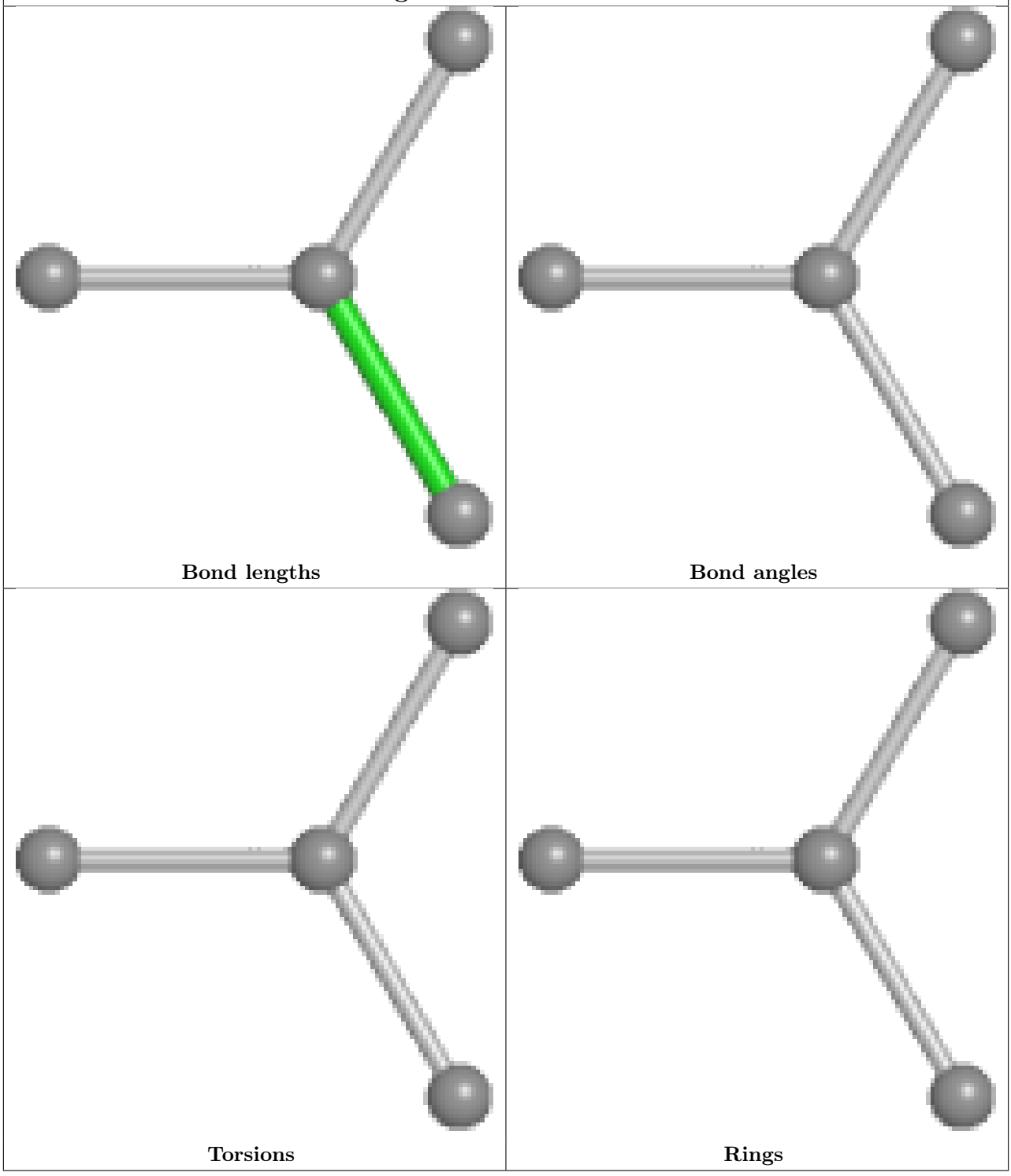


Torsions



Rings

Ligand NO3 BBB 204



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	AAA	129/129 (100%)	-0.37	6 (4%)	31	28	13, 22, 50, 73	0
1	BBB	129/129 (100%)	-0.52	3 (2%)	60	59	12, 21, 45, 54	0
All	All	258/258 (100%)	-0.44	9 (3%)	44	41	12, 21, 47, 73	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	69	THR	4.6
1	AAA	72	SER	4.1
1	AAA	70	PRO	3.9
1	AAA	47	THR	3.2
1	AAA	71	GLY	2.9

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

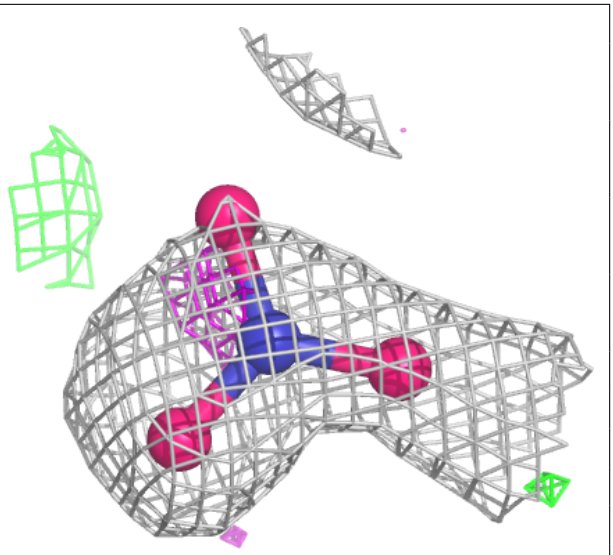
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

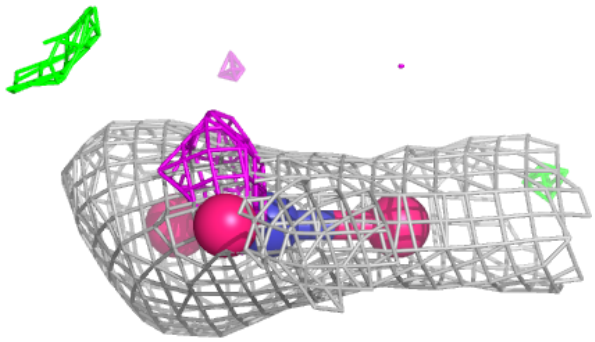
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NO3	AAA	207	4/4	0.82	0.21	33,59,63,73	0
2	NO3	BBB	206	4/4	0.86	0.18	37,51,58,71	0
2	NO3	BBB	205	4/4	0.91	0.24	44,50,67,71	0
2	NO3	AAA	203	4/4	0.93	0.14	36,38,44,49	0
2	NO3	AAA	202	4/4	0.93	0.17	39,42,44,49	0
2	NO3	AAA	206	4/4	0.94	0.11	43,46,50,51	0
2	NO3	BBB	203	4/4	0.97	0.07	30,31,33,34	0
2	NO3	BBB	204	4/4	0.97	0.07	34,34,37,40	0
2	NO3	AAA	204	4/4	0.97	0.10	32,33,36,41	0
2	NO3	AAA	205	4/4	0.97	0.13	34,39,40,44	0
2	NO3	BBB	201	4/4	0.98	0.14	27,31,46,56	0
2	NO3	BBB	202	4/4	0.98	0.08	32,33,37,39	0
2	NO3	AAA	201	4/4	0.99	0.07	23,26,30,33	0

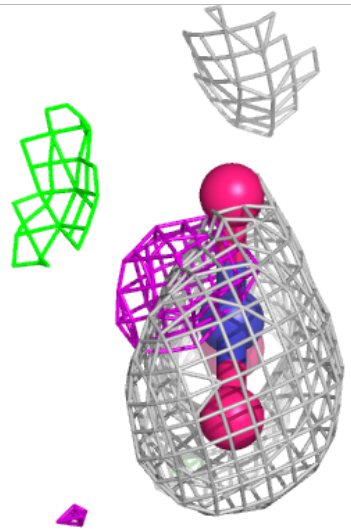
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NO3 AAA 207:

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

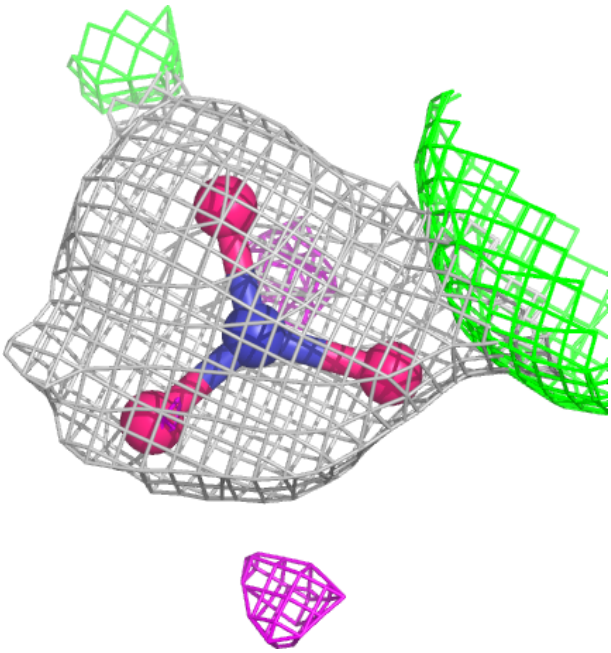


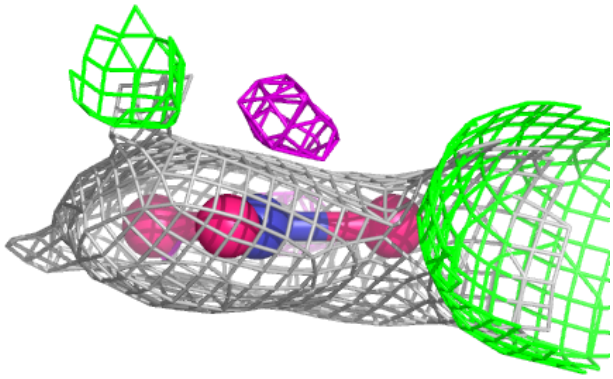


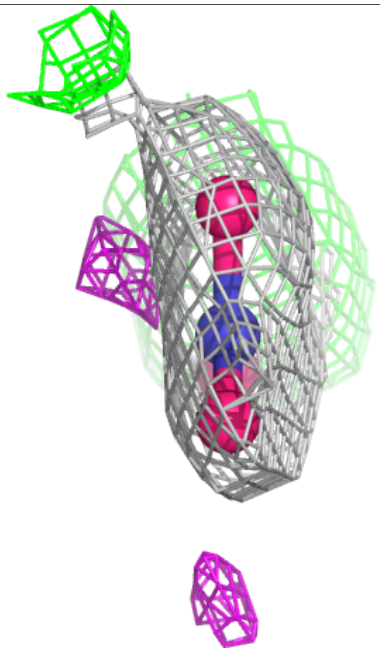


Electron density around NO3 BBB 206:

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

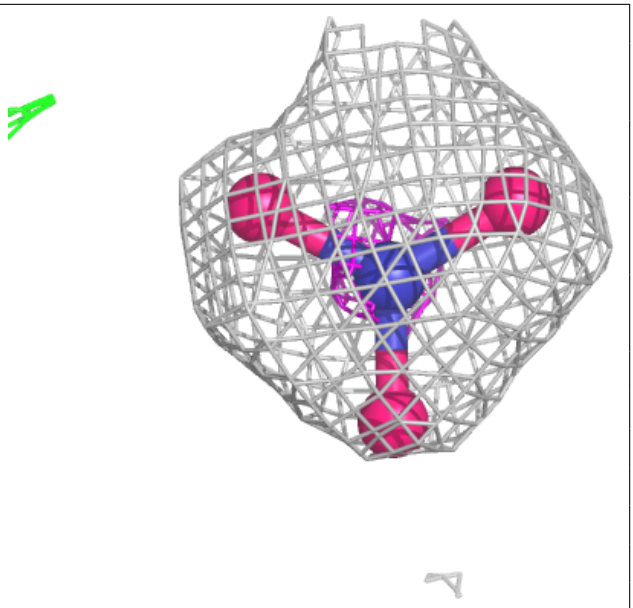


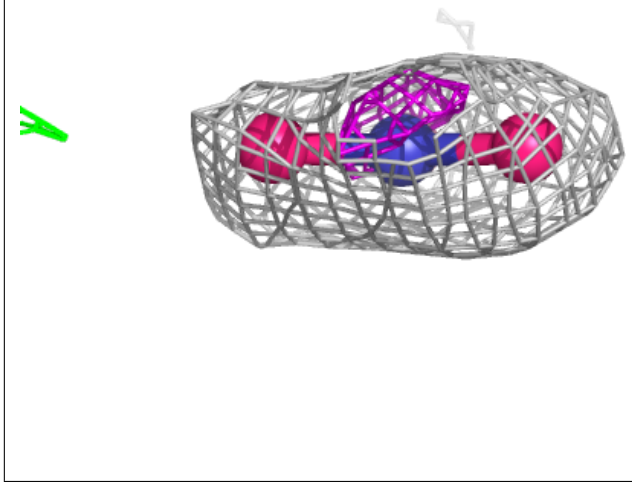


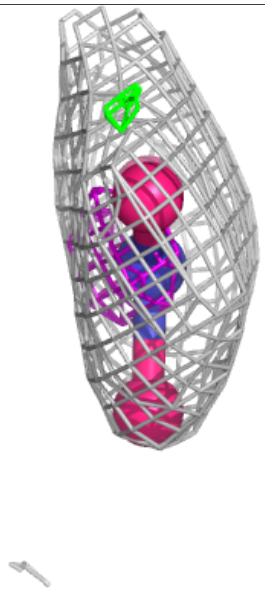


Electron density around NO3 BBB 205:

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

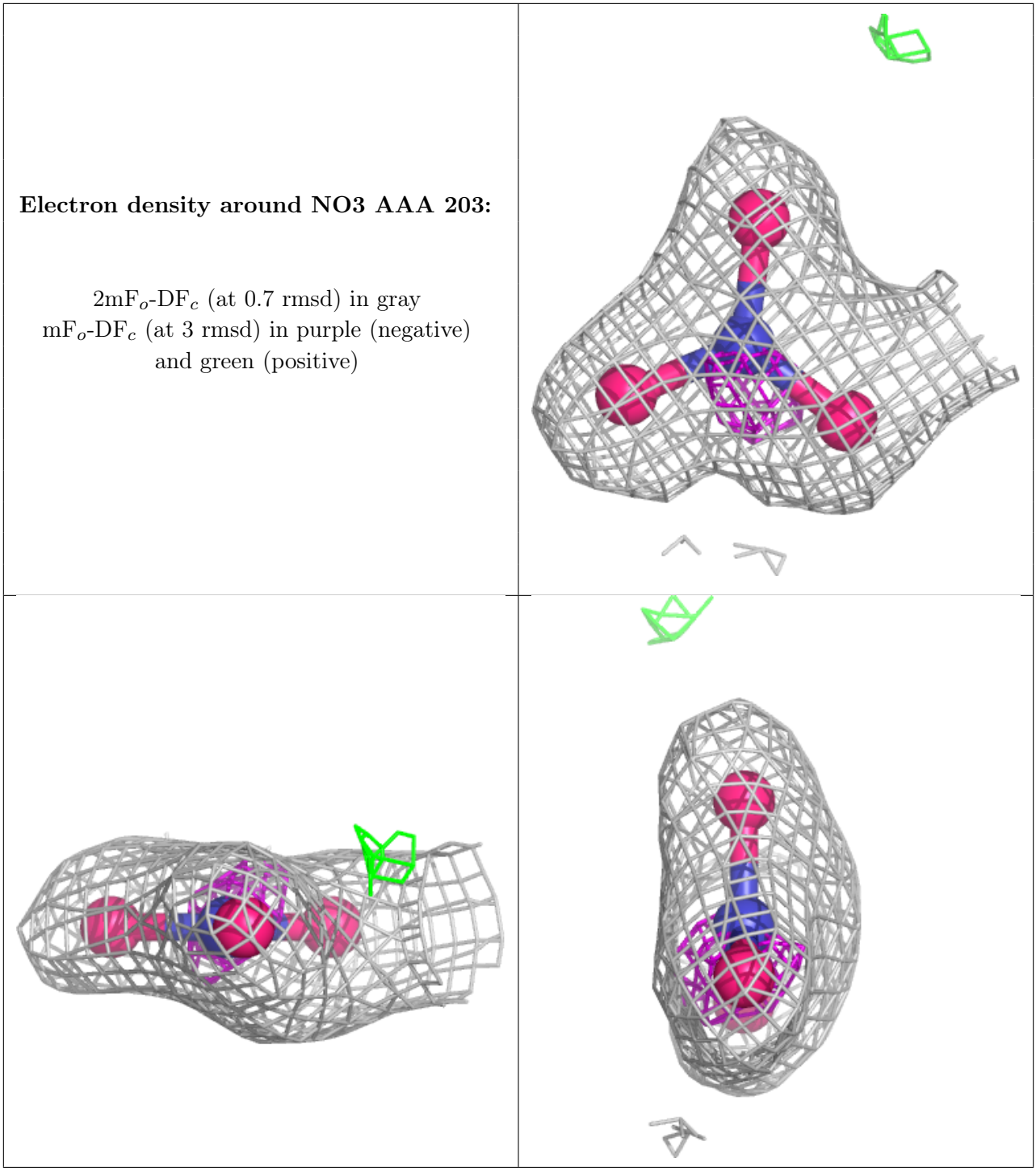






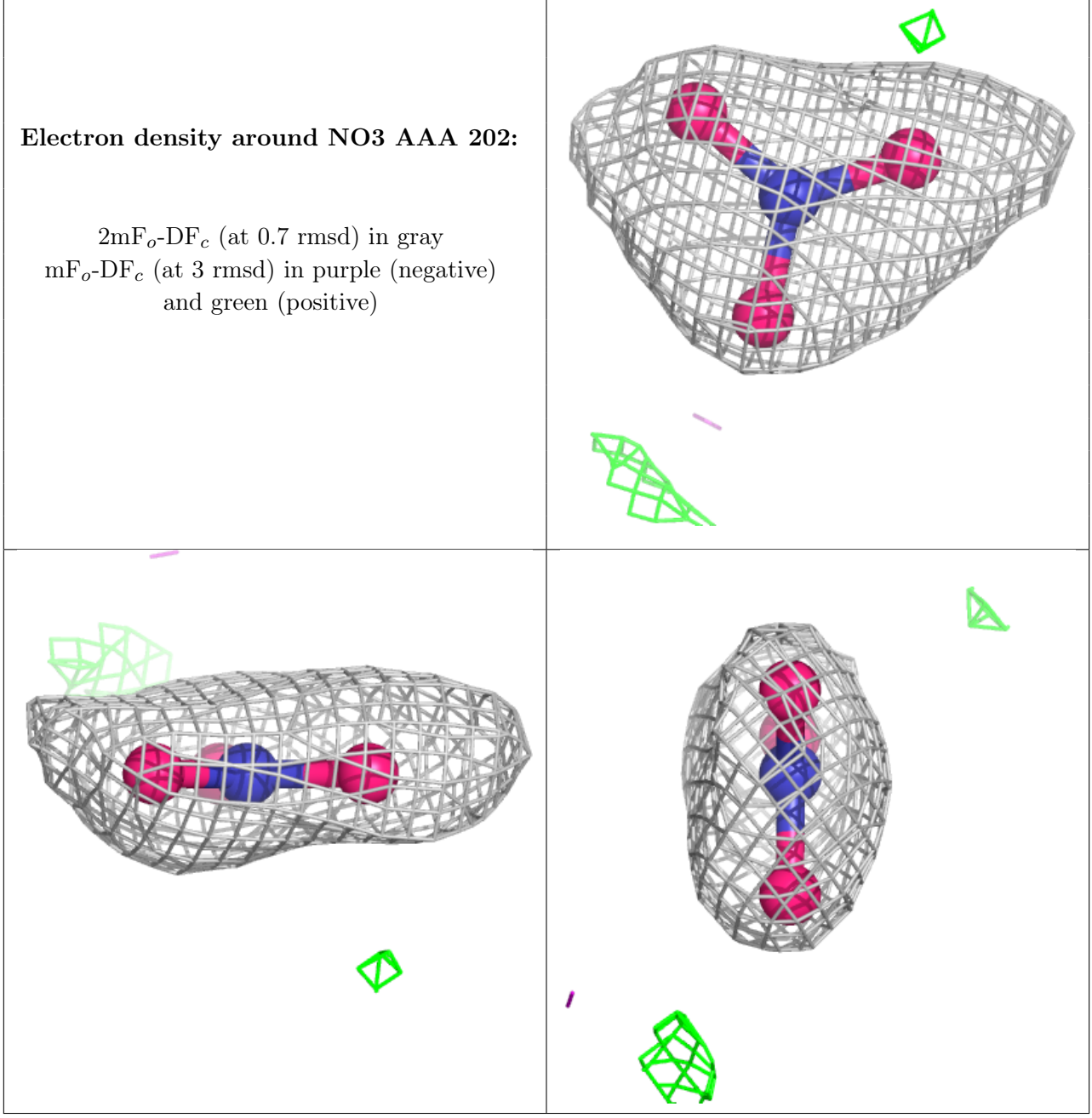
Electron density around NO3 AAA 203:

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



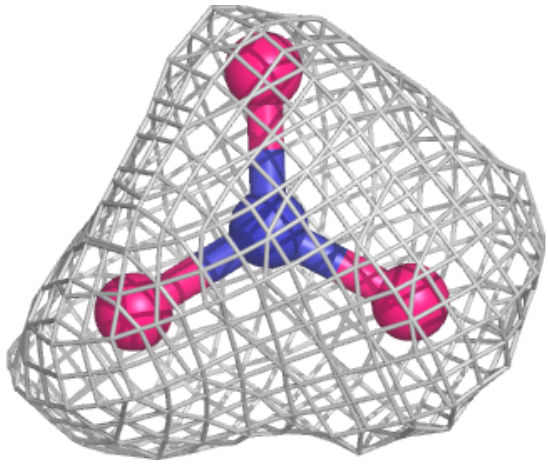
Electron density around NO3 AAA 202:

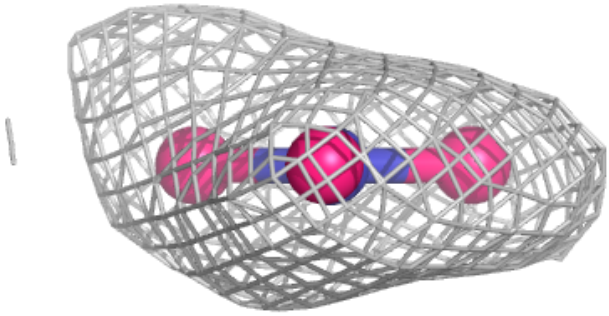
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

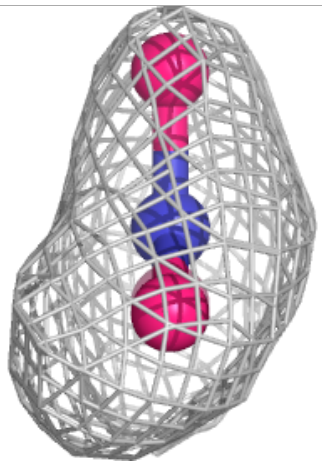


Electron density around NO3 AAA 206:

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

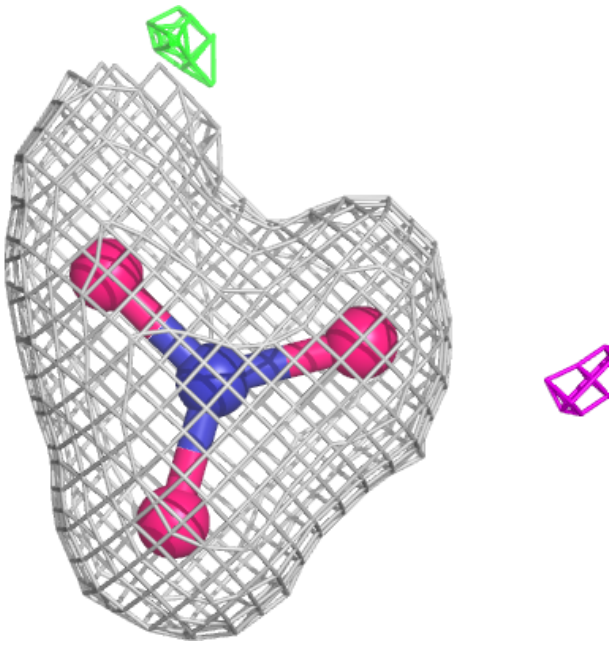


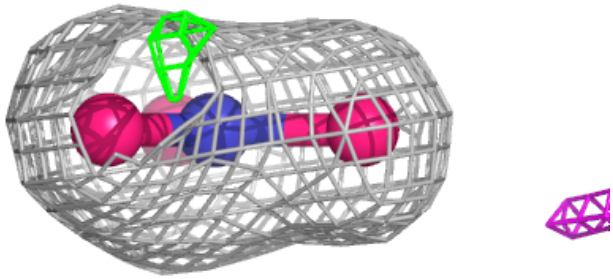


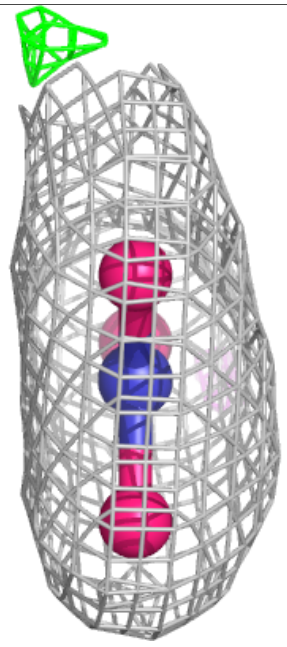


Electron density around NO3 BBB 203:

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

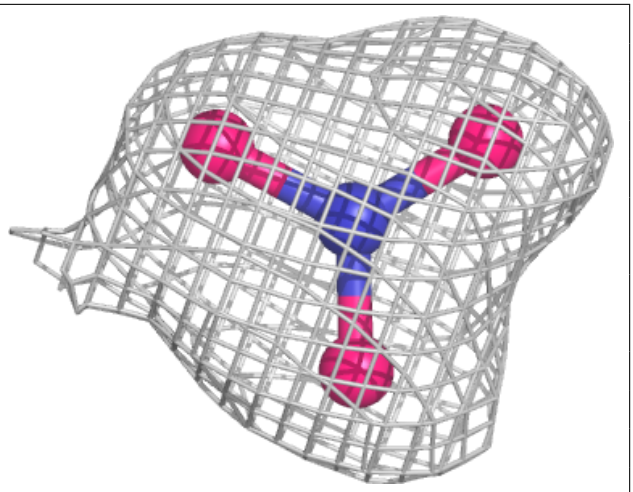


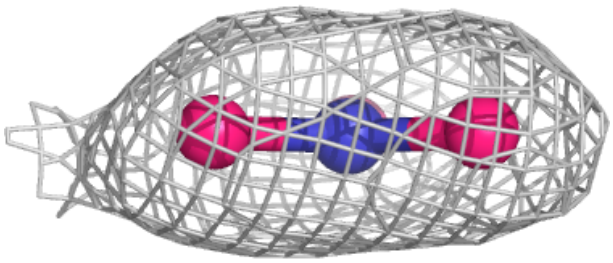


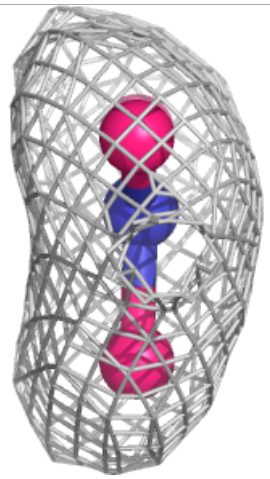


Electron density around NO3 BBB 204:

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

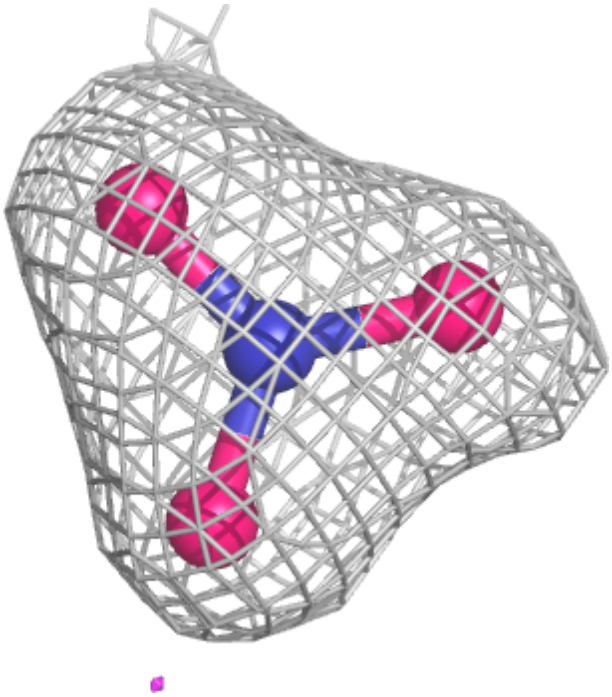


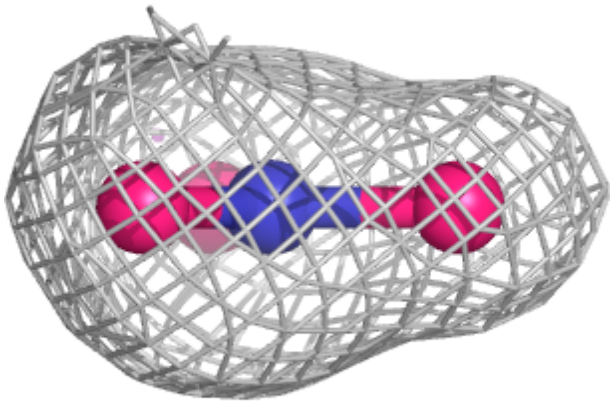


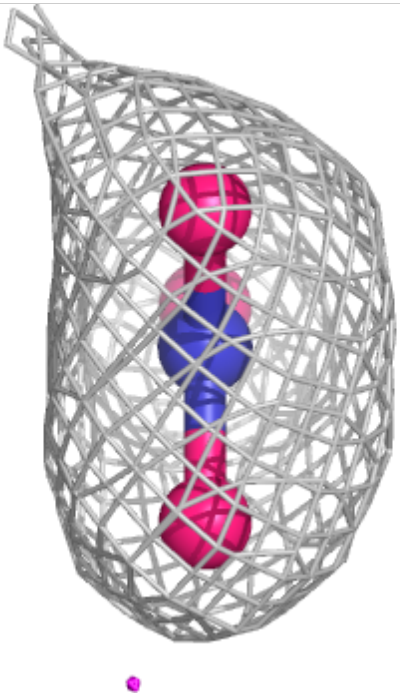


Electron density around NO3 AAA 204:

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

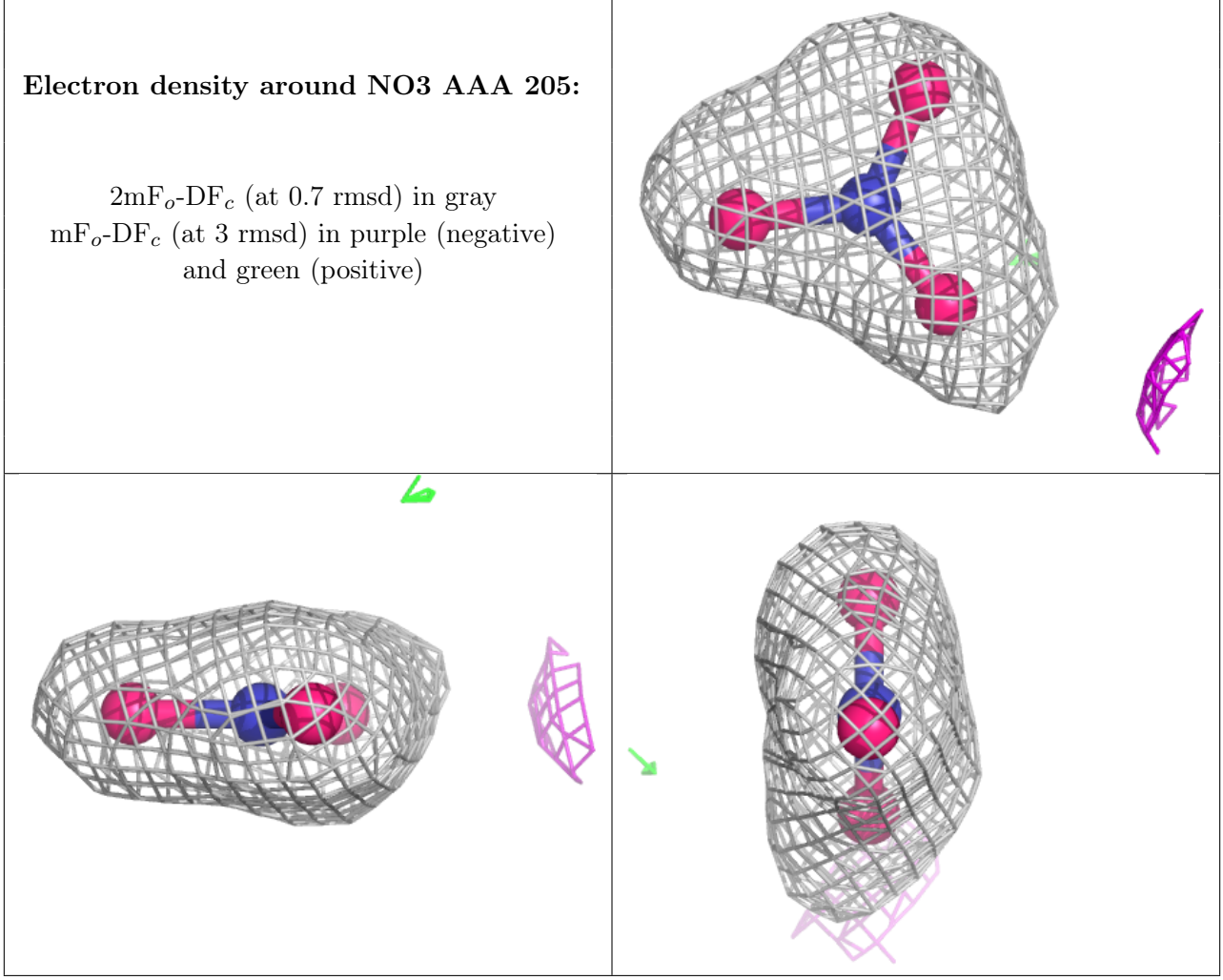






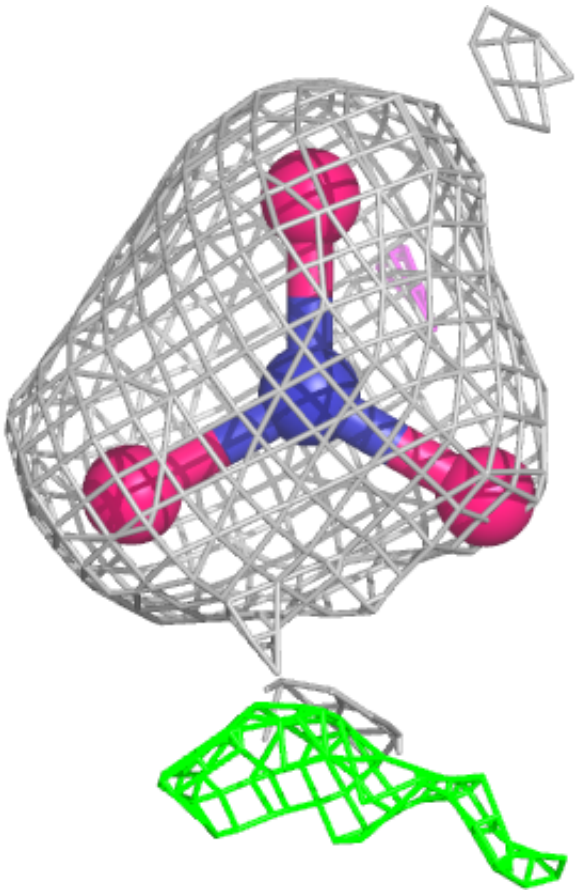
Electron density around NO3 AAA 205:

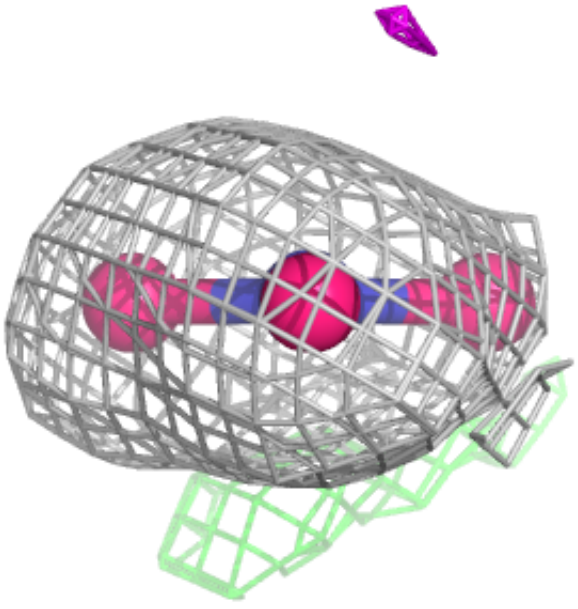
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

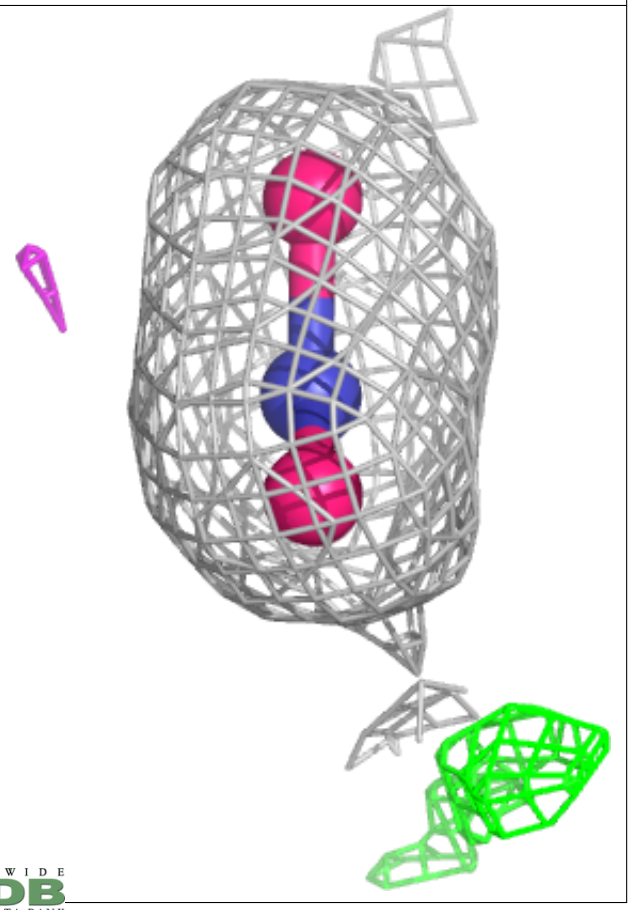


Electron density around NO3 BBB 201:

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

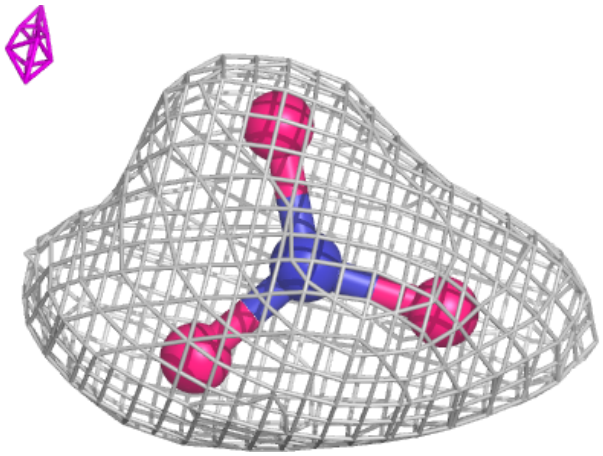


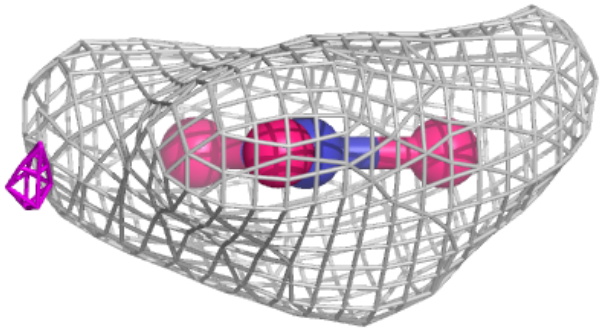


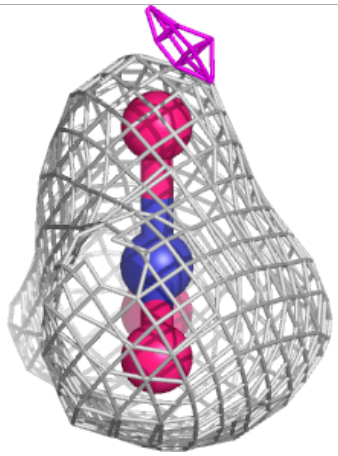


Electron density around NO3 BBB 202:

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

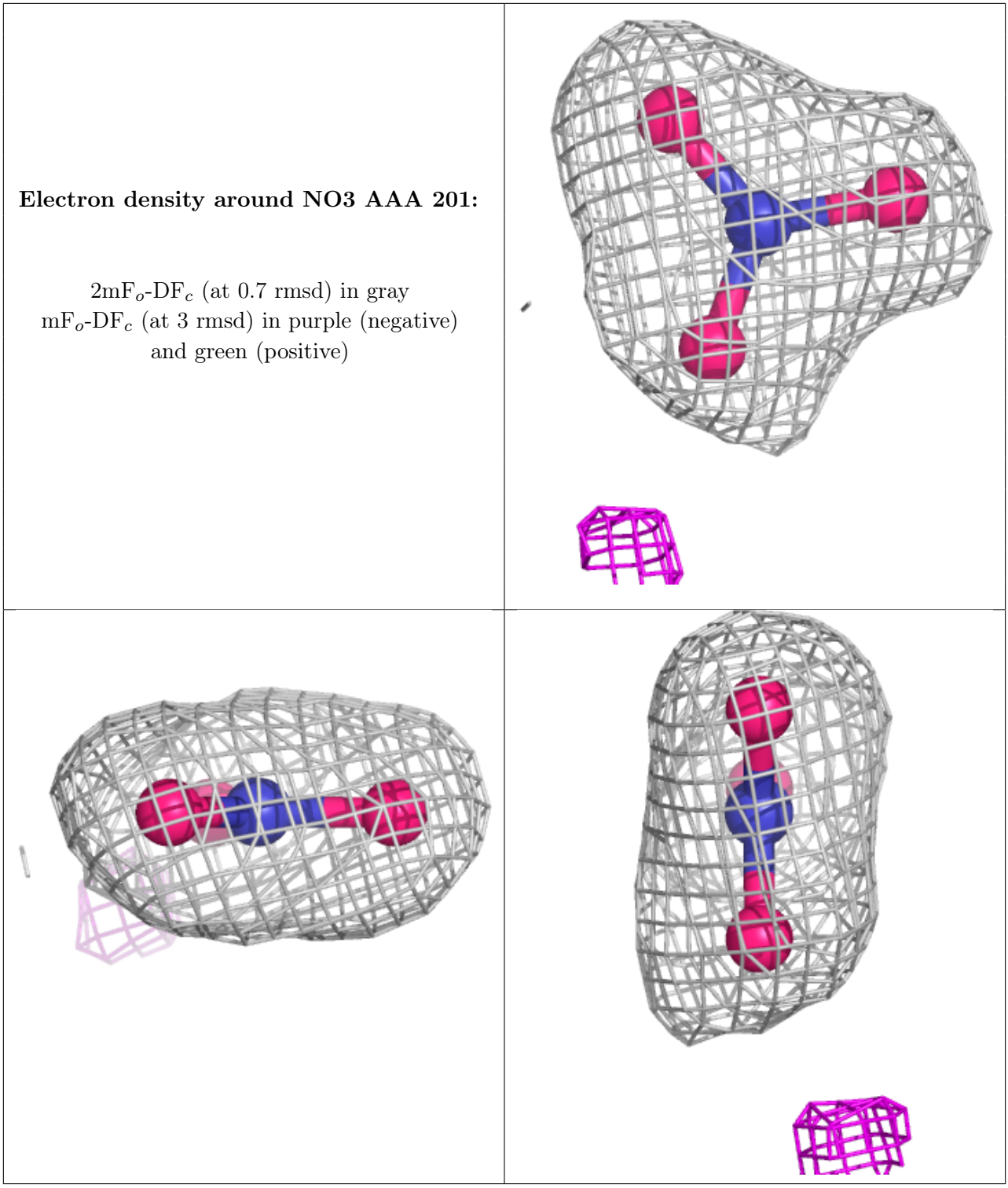






Electron density around NO3 AAA 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.