



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 08:55 AM UTC

PDB ID : 7PVK / pdb_00007pvk
Title : X-ray structure of dimeric PorX (T272A mutant), in complex with pGpG.
Authors : Schmitz, C.A.; Madej, M.; Potempa, J.; Sola, M.
Deposited on : 2021-10-04
Resolution : 2.40 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 : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

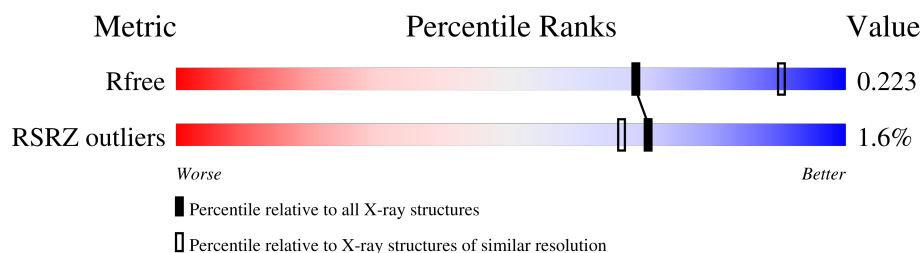
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 34841 atoms, of which 17042 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 Response regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	513	Total	C	H	N	O	Se	0	4	0
			8465	2730	4208	707	800	20			
1	B	513	Total	C	H	N	O	Se	0	4	0
			8463	2730	4206	707	800	20			
1	C	513	Total	C	H	N	O	Se	0	2	0
			8437	2722	4194	705	797	19			
1	D	513	Total	C	H	N	O	Se	0	2	0
			8437	2722	4194	705	797	19			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q7MVV4
A	-3	PRO	-	expression tag	UNP Q7MVV4
A	-2	LEU	-	expression tag	UNP Q7MVV4
A	-1	GLY	-	expression tag	UNP Q7MVV4
A	0	SER	-	expression tag	UNP Q7MVV4
A	272	ALA	THR	engineered mutation	UNP Q7MVV4
B	-4	GLY	-	expression tag	UNP Q7MVV4
B	-3	PRO	-	expression tag	UNP Q7MVV4
B	-2	LEU	-	expression tag	UNP Q7MVV4
B	-1	GLY	-	expression tag	UNP Q7MVV4
B	0	SER	-	expression tag	UNP Q7MVV4
B	272	ALA	THR	engineered mutation	UNP Q7MVV4
C	-4	GLY	-	expression tag	UNP Q7MVV4
C	-3	PRO	-	expression tag	UNP Q7MVV4
C	-2	LEU	-	expression tag	UNP Q7MVV4
C	-1	GLY	-	expression tag	UNP Q7MVV4
C	0	SER	-	expression tag	UNP Q7MVV4
C	272	ALA	THR	engineered mutation	UNP Q7MVV4
D	-4	GLY	-	expression tag	UNP Q7MVV4
D	-3	PRO	-	expression tag	UNP Q7MVV4
D	-2	LEU	-	expression tag	UNP Q7MVV4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP Q7MVV4
D	0	SER	-	expression tag	UNP Q7MVV4
D	272	ALA	THR	engineered mutation	UNP Q7MVV4

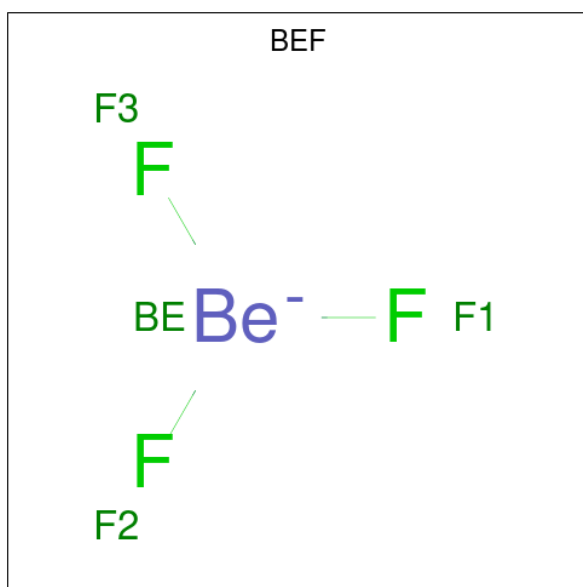
- Molecule 2 is a RNA chain called pGpG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	2	Total 68	C 20	H 22	N 10	O 14	P 2	0	0	0
2	F	2	Total 70	C 20	H 23	N 10	O 15	P 2	0	0	0
2	G	2	Total 70	C 20	H 23	N 10	O 15	P 2	0	0	0
2	H	2	Total 70	C 20	H 23	N 10	O 15	P 2	0	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Be	F	0	0
			4	1	3		
4	B	1	Total	Be	F	0	0
			4	1	3		
4	C	1	Total	Be	F	0	0
			4	1	3		
4	D	1	Total	Be	F	0	0
			4	1	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	B	2	Total	Zn	0	0
			2	2		
5	C	3	Total	Zn	0	1
			4	4		
5	D	2	Total	Zn	0	0
			2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



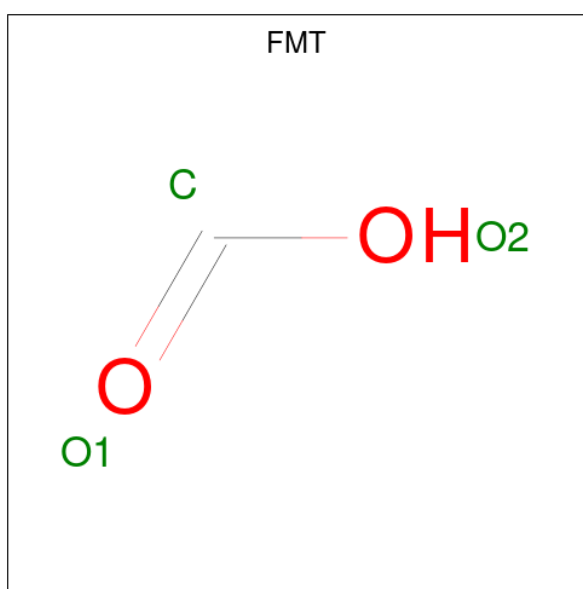
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			13	3	7	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		
6	C	1	Total	C	H	O	0	0
			14	3	8	3		
6	C	1	Total	C	H	O	0	0
			14	3	8	3		
6	C	1	Total	C	H	O	0	0
			14	3	8	3		
6	C	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	H	O	0	0
			14	3	8	3		
6	D	1	Total	C	H	O	0	0
			14	3	8	3		
6	D	1	Total	C	H	O	0	0
			14	3	8	3		
6	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 7 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			4	1	1	2		
7	A	1	Total	C	H	O	0	0
			4	1	1	2		
7	A	1	Total	C	H	O	0	0
			4	1	1	2		
7	B	1	Total	C	H	O	0	0
			4	1	1	2		
7	C	1	Total	C	H	O	0	0
			4	1	1	2		
7	D	1	Total	C	H	O	0	0
			4	1	1	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	72	Total 72	O 72	0	0
8	B	107	Total 107	O 107	0	0
8	C	138	Total 138	O 138	0	0
8	D	130	Total 130	O 130	0	0
8	E	2	Total 2	O 2	0	0
8	F	2	Total 2	O 2	0	0
8	G	3	Total 3	O 3	0	0
8	H	2	Total 2	O 2	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.63Å 103.77Å 132.21Å 90.00° 98.50° 90.00°	Depositor
Resolution (Å)	51.90 – 2.40 51.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (51.90-2.40) 99.5 (51.90-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.11.1	Depositor
R, R_{free}	0.194 , 0.223 0.196 , 0.223	Depositor DCC
R_{free} test set	1041 reflections (0.75%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34841	wwPDB-VP
Average B, all atoms (Å ²)	98.0	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 40.92 % 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 2.5493e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 14 are monoatomic - leaving 28 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	GOL	B	604	-	5,5,5	0.44	0	5,5,5	0.51	0
6	GOL	C	605	-	5,5,5	0.38	0	5,5,5	0.31	0
6	GOL	D	606	-	5,5,5	0.49	0	5,5,5	0.32	0
7	FMT	A	610	-	2,2,2	0.74	0	1,1,1	0.44	0
4	BEF	A	602	1	0,3,3	-	-	-		
7	FMT	D	607	-	2,2,2	0.74	0	1,1,1	0.42	0
7	FMT	A	611	-	2,2,2	0.73	0	1,1,1	0.38	0
6	GOL	D	604	-	5,5,5	0.39	0	5,5,5	0.26	0
6	GOL	B	606	-	5,5,5	0.34	0	5,5,5	0.33	0
7	FMT	C	609	-	2,2,2	0.74	0	1,1,1	0.42	0
4	BEF	B	602	1	0,3,3	-	-	-		
6	GOL	A	608	-	5,5,5	0.37	0	5,5,5	0.27	0
6	GOL	B	605	-	5,5,5	0.37	0	5,5,5	0.26	0
6	GOL	D	605	-	5,5,5	0.40	0	5,5,5	0.25	0
6	GOL	C	604	-	5,5,5	0.41	0	5,5,5	0.22	0
6	GOL	A	605	-	5,5,5	0.36	0	5,5,5	0.21	0
6	GOL	B	608	-	5,5,5	0.39	0	5,5,5	0.21	0
6	GOL	A	609	-	5,5,5	0.44	0	5,5,5	0.16	0
6	GOL	A	607	-	5,5,5	0.38	0	5,5,5	0.22	0
6	GOL	A	606	-	5,5,5	0.36	0	5,5,5	0.13	0
4	BEF	C	602	1	0,3,3	-	-	-		
7	FMT	A	612	-	2,2,2	0.75	0	1,1,1	0.41	0
6	GOL	B	607	-	5,5,5	0.36	0	5,5,5	0.35	0
4	BEF	D	602	1	0,3,3	-	-	-		
7	FMT	B	609	-	2,2,2	0.74	0	1,1,1	0.41	0
6	GOL	C	606	-	5,5,5	0.42	0	5,5,5	0.17	0
6	GOL	C	607	-	5,5,5	0.35	0	5,5,5	0.22	0
6	GOL	C	608	-	5,5,5	0.37	0	5,5,5	0.26	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
6	GOL	B	607	-	-	0/4/4/4	-
6	GOL	D	606	-	-	0/4/4/4	-
6	GOL	A	605	-	-	0/4/4/4	-
6	GOL	B	608	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	605	-	-	0/4/4/4	-
6	GOL	C	606	-	-	0/4/4/4	-
6	GOL	A	609	-	-	0/4/4/4	-
6	GOL	A	607	-	-	2/4/4/4	-
6	GOL	A	606	-	-	0/4/4/4	-
6	GOL	C	607	-	-	3/4/4/4	-
6	GOL	B	606	-	-	2/4/4/4	-
6	GOL	D	604	-	-	1/4/4/4	-
6	GOL	A	608	-	-	1/4/4/4	-
6	GOL	B	604	-	-	2/4/4/4	-
6	GOL	B	605	-	-	2/4/4/4	-
6	GOL	C	608	-	-	0/4/4/4	-
6	GOL	D	605	-	-	0/4/4/4	-
6	GOL	C	604	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

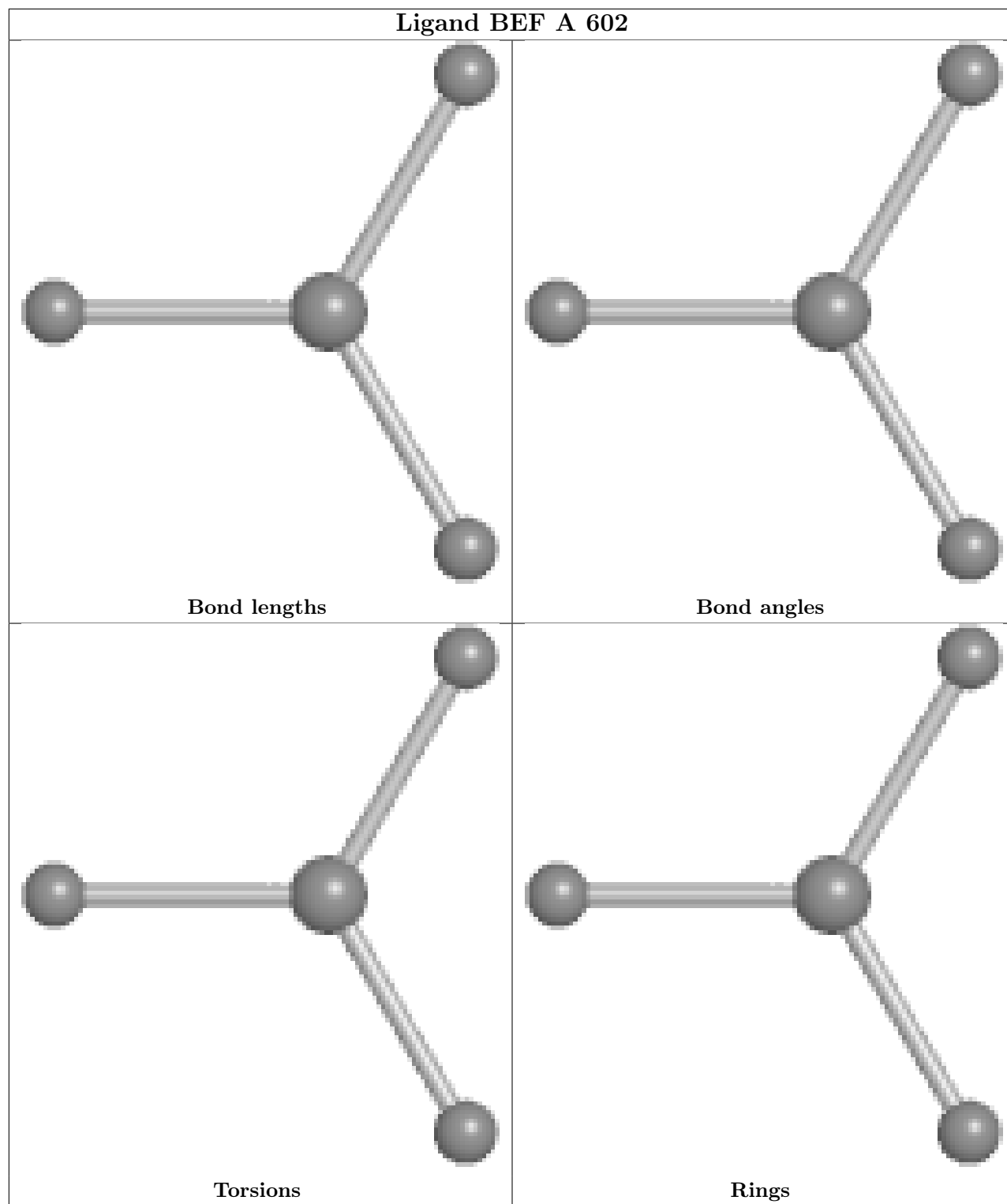
All (17) torsion outliers are listed below:

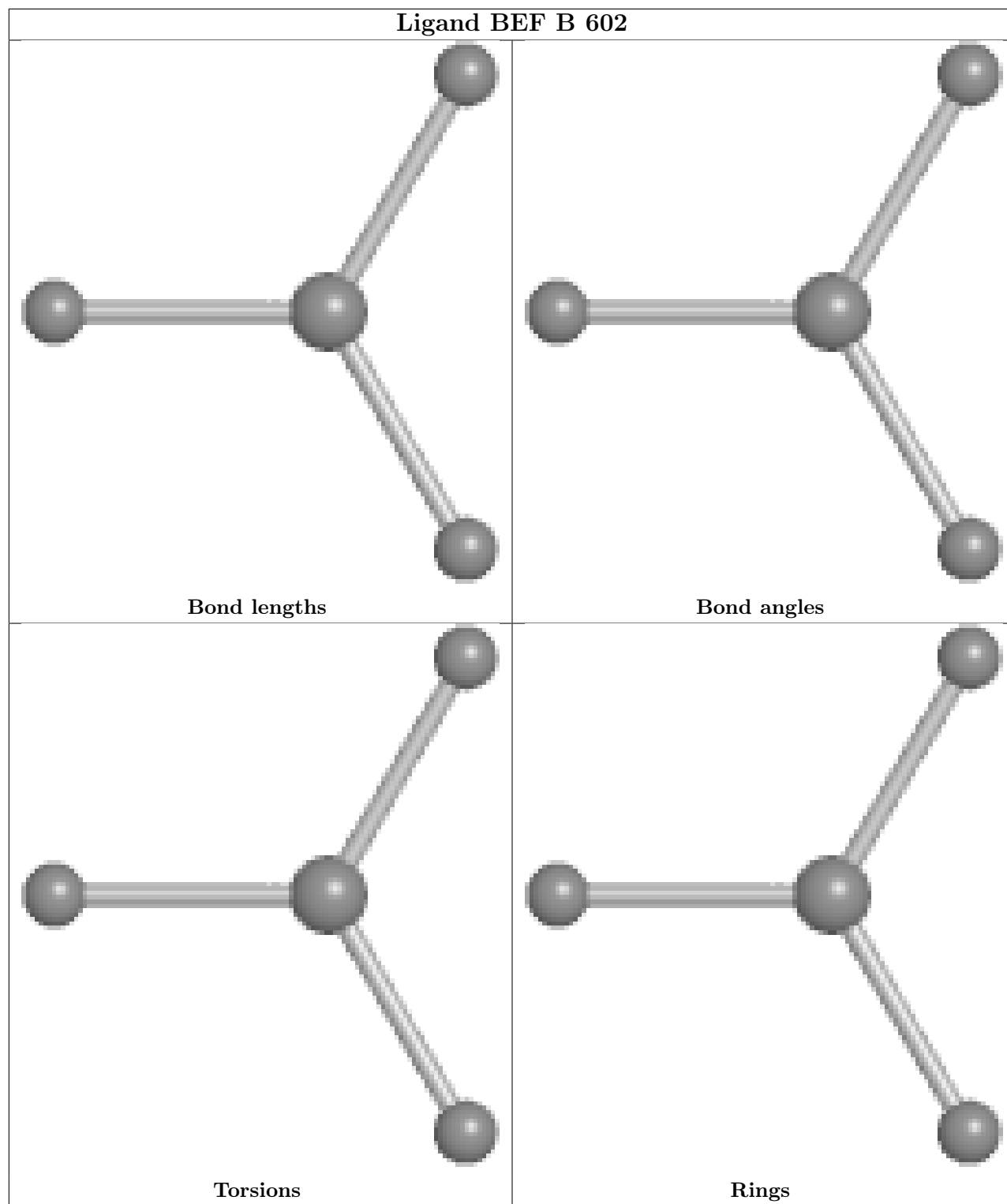
Mol	Chain	Res	Type	Atoms
6	B	604	GOL	C1-C2-C3-O3
6	B	605	GOL	O1-C1-C2-O2
6	B	605	GOL	O1-C1-C2-C3
6	B	606	GOL	O1-C1-C2-C3
6	B	608	GOL	O1-C1-C2-O2
6	B	608	GOL	O1-C1-C2-C3
6	C	607	GOL	C1-C2-C3-O3
6	C	607	GOL	O2-C2-C3-O3
6	A	607	GOL	O1-C1-C2-C3
6	C	604	GOL	O1-C1-C2-C3
6	A	607	GOL	O1-C1-C2-O2
6	B	604	GOL	O2-C2-C3-O3
6	B	606	GOL	O1-C1-C2-O2
6	C	604	GOL	O1-C1-C2-O2
6	D	604	GOL	O1-C1-C2-O2
6	C	607	GOL	O1-C1-C2-O2
6	A	608	GOL	O2-C2-C3-O3

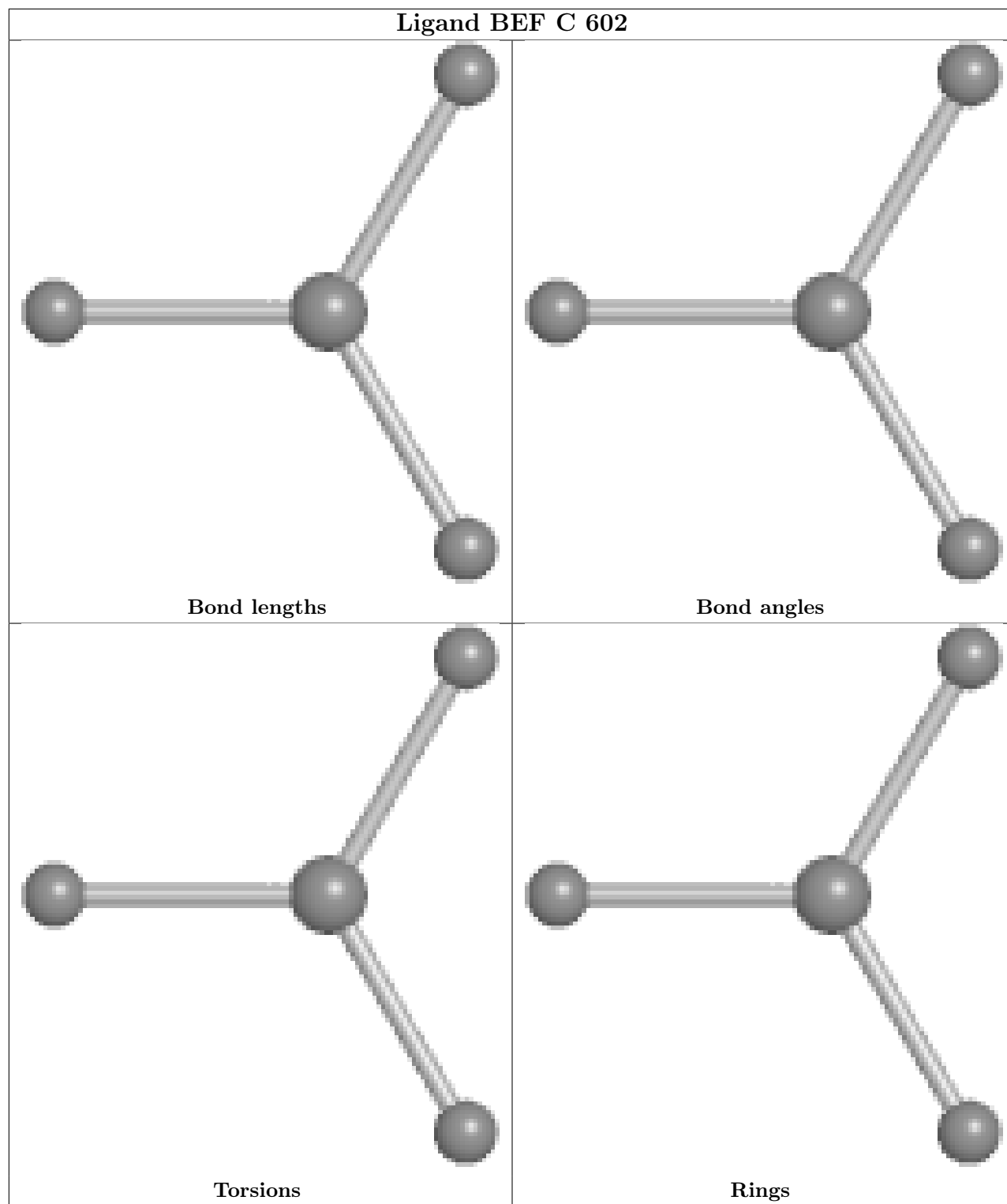
There are no ring outliers.

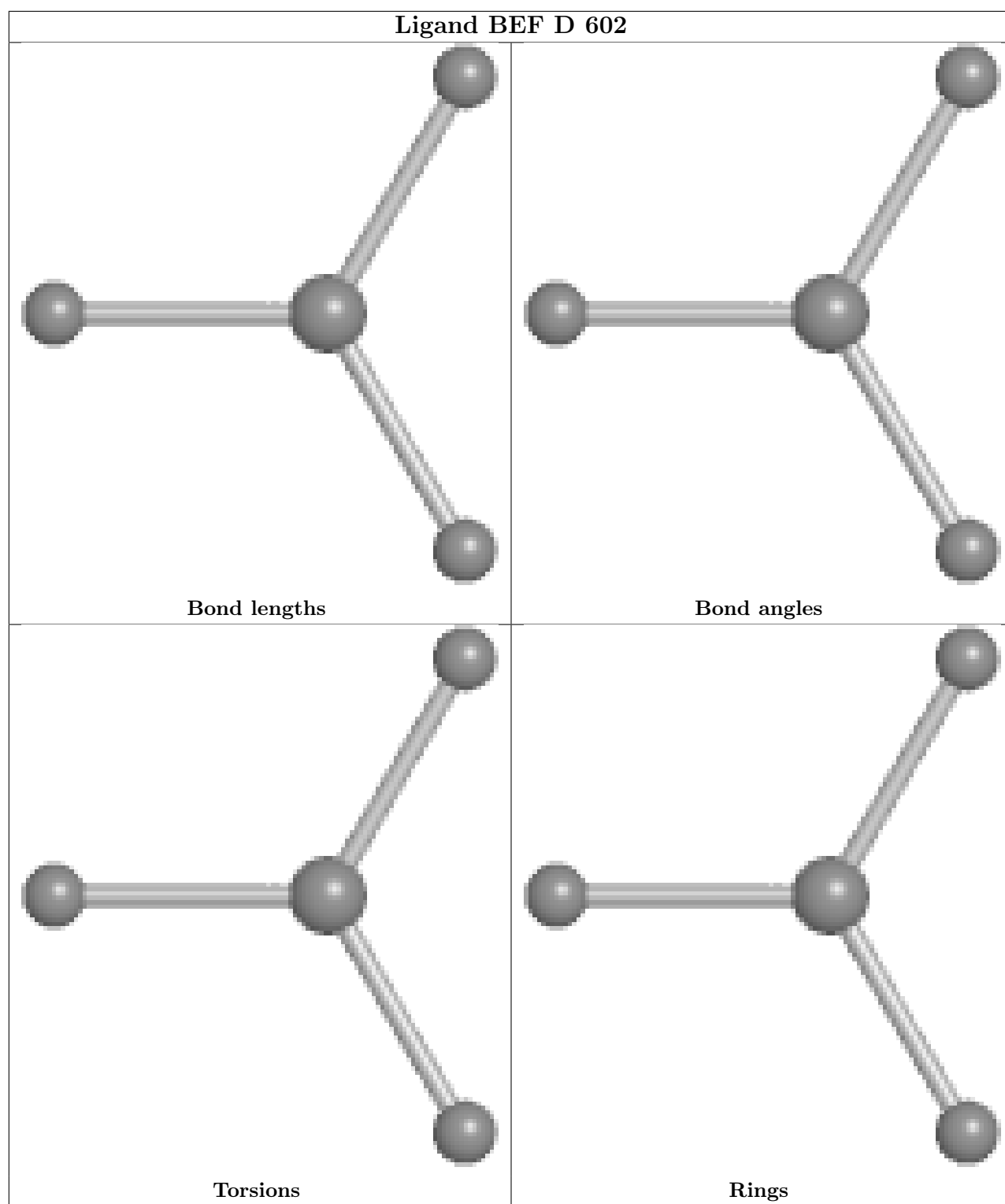
No monomer is involved in short contacts.

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









4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	495/523 (94%)	0.12	12 (2%) 59 55	41, 105, 162, 217	1 (0%)
1	B	495/523 (94%)	0.07	7 (1%) 73 69	37, 91, 158, 211	1 (0%)
1	C	495/523 (94%)	-0.03	7 (1%) 73 69	54, 85, 148, 213	0
1	D	495/523 (94%)	-0.06	6 (1%) 76 73	55, 85, 141, 203	0
2	E	2/2 (100%)	0.52	0 100 100	94, 94, 94, 150	0
2	F	2/2 (100%)	0.58	0 100 100	90, 90, 90, 215	0
2	G	2/2 (100%)	0.02	0 100 100	84, 84, 84, 176	0
2	H	2/2 (100%)	0.16	0 100 100	81, 81, 81, 155	0
All	All	1988/2100 (94%)	0.02	32 (1%) 70 66	37, 92, 155, 217	2 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	LEU	3.5
1	A	441	ILE	3.2
1	A	238	ILE	3.1
1	A	357	LEU	2.9
1	A	472	PHE	2.6
1	D	24	ILE	2.6
1	C	429	GLY	2.5
1	A	360	VAL	2.5
1	B	399	LEU	2.4
1	D	323	HIS	2.4
1	A	237	LEU	2.4
1	B	105	TYR	2.4
1	A	241	PHE	2.3
1	C	332	TYR	2.3
1	B	19	LEU	2.3
1	A	195	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	399	LEU	2.2
1	C	295	LEU	2.2
1	B	32	TYR	2.2
1	A	303	GLU	2.2
1	B	332	TYR	2.2
1	B	174	ALA	2.1
1	D	174	ALA	2.1
1	A	445	LEU	2.1
1	C	376	LEU	2.1
1	D	265	LEU	2.1
1	C	90	GLU	2.1
1	B	66	GLY	2.0
1	D	303	GLU	2.0
1	D	175	ASP	2.0
1	C	445	LEU	2.0
1	A	334	THR	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	D	605	6/6	0.54	0.13	129,155,159,160	0
6	GOL	B	608	6/6	0.55	0.24	126,152,153,154	0
6	GOL	A	606	6/6	0.64	0.11	121,145,152,154	0
6	GOL	B	604	6/6	0.67	0.14	138,150,180,180	0
7	FMT	A	611	3/3	0.67	0.21	125,126,128,151	0
6	GOL	C	607	6/6	0.70	0.15	128,154,156,156	0
6	GOL	A	609	6/6	0.73	0.08	136,164,166,166	0

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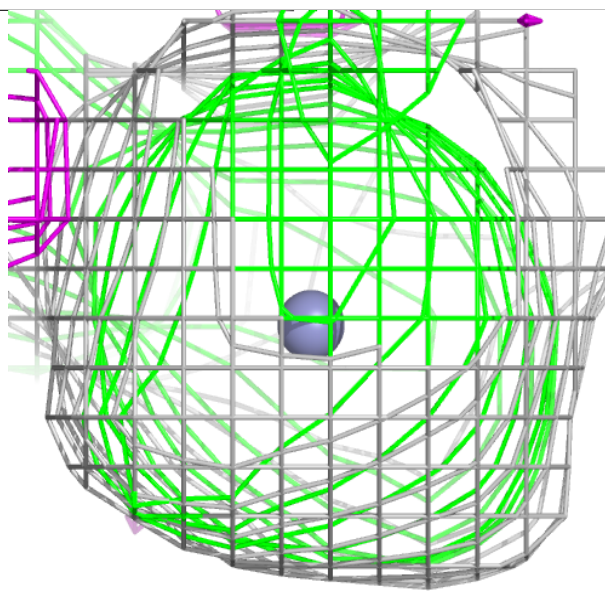
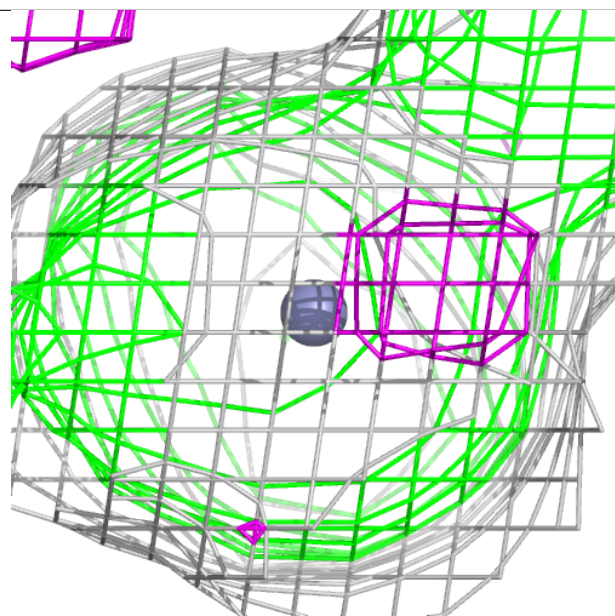
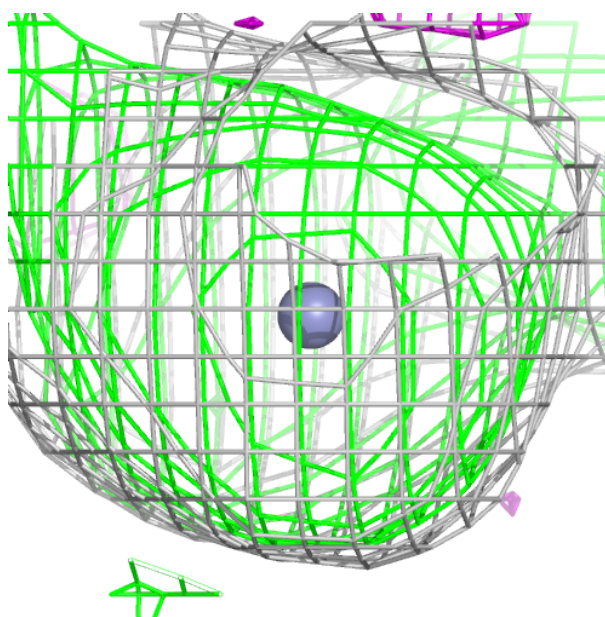
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	A	607	6/6	0.74	0.16	132,158,161,161	0
6	GOL	B	606	6/6	0.74	0.15	81,97,106,108	0
6	GOL	B	605	6/6	0.75	0.10	119,143,148,150	0
7	FMT	D	607	3/3	0.75	0.21	133,133,133,160	0
6	GOL	B	607	6/6	0.76	0.11	118,142,145,147	0
6	GOL	D	606	6/6	0.78	0.16	117,141,143,143	0
6	GOL	D	604	6/6	0.79	0.14	96,116,121,124	0
6	GOL	C	608	6/6	0.80	0.11	116,140,141,141	0
5	ZN	C	610[B]	1/1	0.81	0.26	166,166,166,166	1
7	FMT	B	609	3/3	0.81	0.20	124,125,126,151	0
7	FMT	C	609	3/3	0.81	0.10	128,128,128,153	0
5	ZN	C	610[A]	1/1	0.81	0.26	166,166,166,166	1
6	GOL	A	608	6/6	0.82	0.11	111,133,137,137	0
7	FMT	A	612	3/3	0.83	0.19	132,134,134,158	0
4	BEF	B	602	4/4	0.83	0.10	110,113,114,114	0
7	FMT	A	610	3/3	0.84	0.11	128,128,128,154	0
6	GOL	C	605	6/6	0.86	0.14	98,118,125,126	0
6	GOL	A	605	6/6	0.89	0.10	108,129,137,137	0
6	GOL	C	606	6/6	0.93	0.10	98,118,123,124	0
6	GOL	C	604	6/6	0.93	0.09	98,118,123,123	0
3	MG	B	601	1/1	0.93	0.09	114,114,114,114	0
4	BEF	D	602	4/4	0.94	0.07	73,74,77,79	0
4	BEF	C	602	4/4	0.96	0.07	51,53,53,57	0
5	ZN	A	603	1/1	0.97	0.08	72,72,72,72	0
4	BEF	A	602	4/4	0.97	0.07	68,71,75,80	0
3	MG	A	601	1/1	0.97	0.05	73,73,73,73	0
3	MG	D	601	1/1	0.98	0.04	81,81,81,81	0
5	ZN	B	610	1/1	0.99	0.03	60,60,60,60	0
3	MG	C	601	1/1	0.99	0.03	61,61,61,61	0
5	ZN	B	603	1/1	0.99	0.05	59,59,59,59	0
5	ZN	C	611	1/1	0.99	0.02	59,59,59,59	0
5	ZN	C	603	1/1	1.00	0.04	56,56,56,56	0
5	ZN	A	604	1/1	1.00	0.08	72,72,72,72	0
5	ZN	D	603	1/1	1.00	0.04	60,60,60,60	0
5	ZN	D	608	1/1	1.00	0.03	59,59,59,59	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.

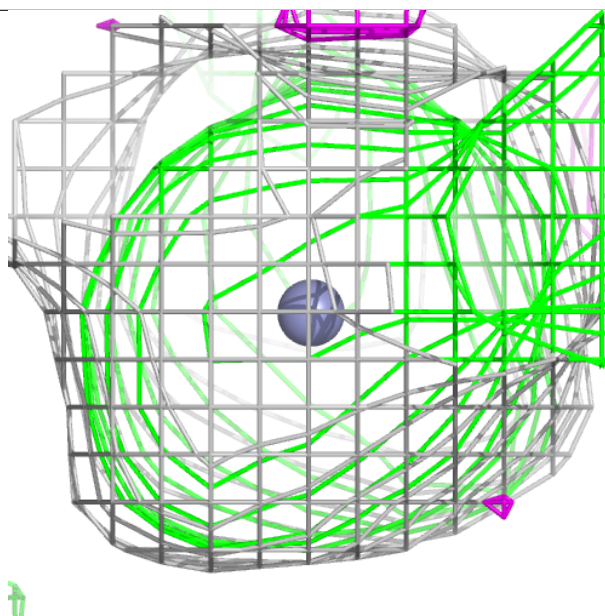
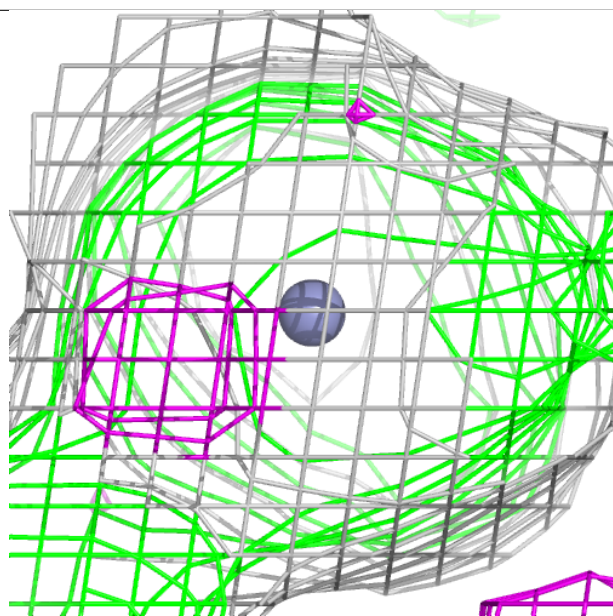
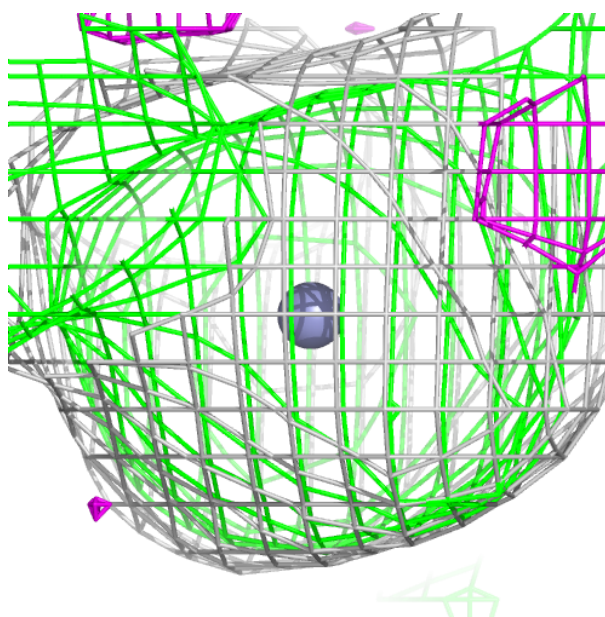
Electron density around ZN C 610 (B):

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



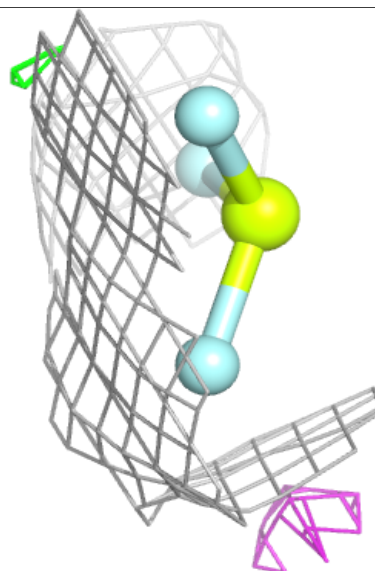
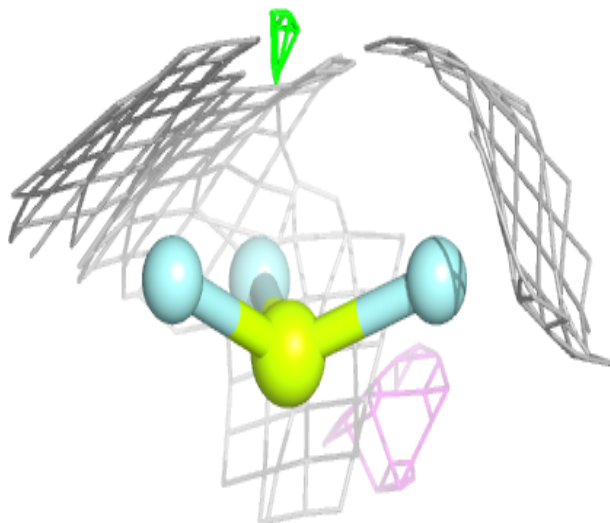
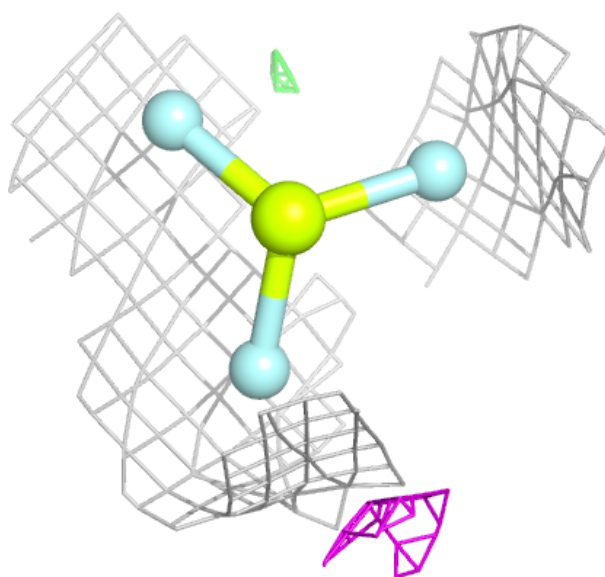
Electron density around ZN C 610 (A):

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



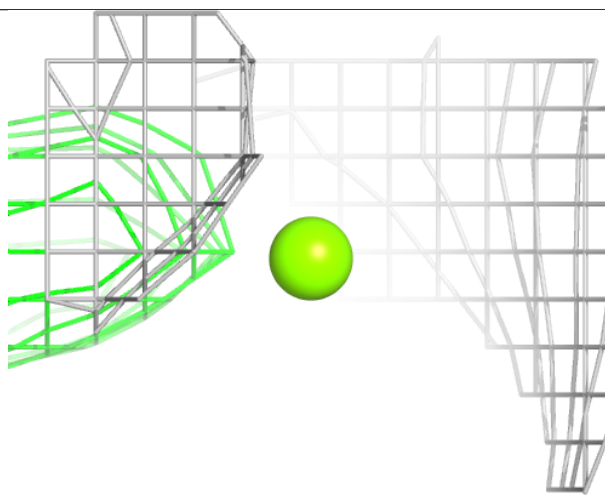
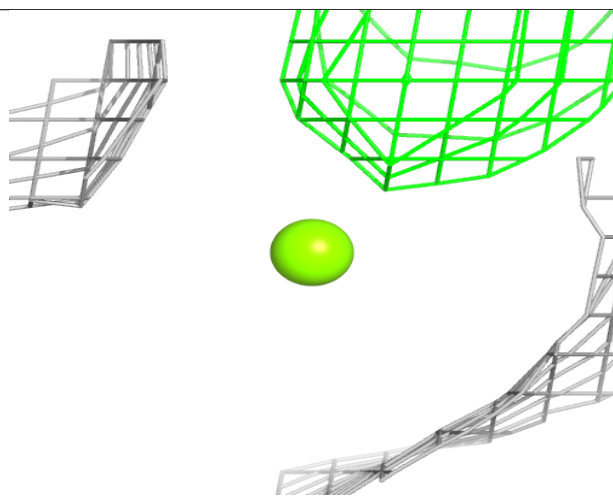
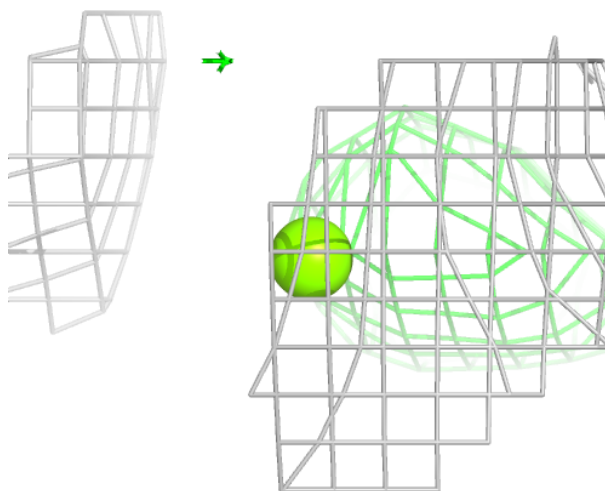
Electron density around BEF B 602:

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



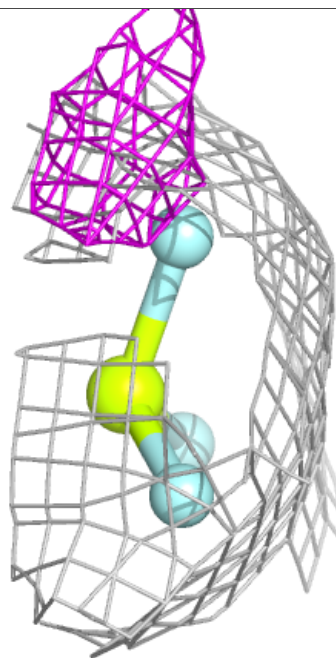
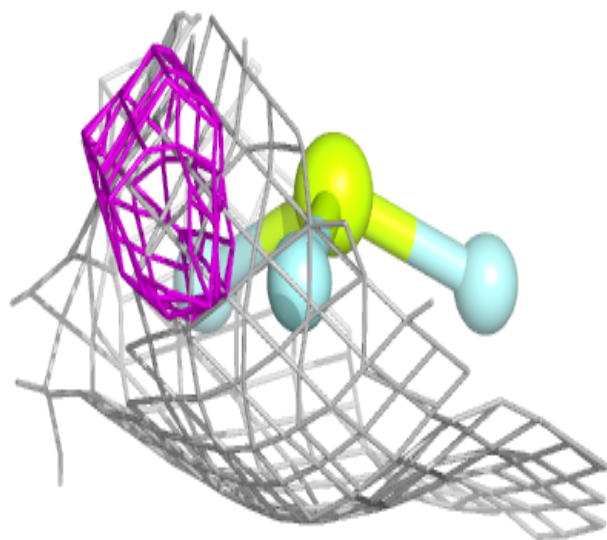
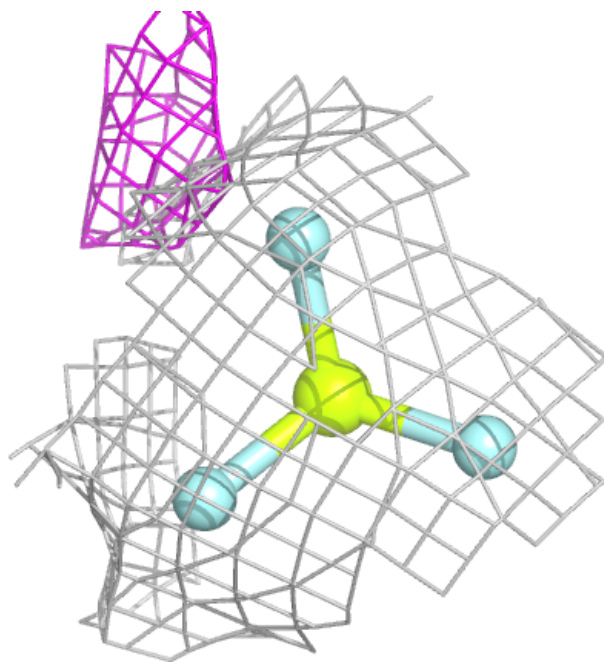
Electron density around MG B 601:

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



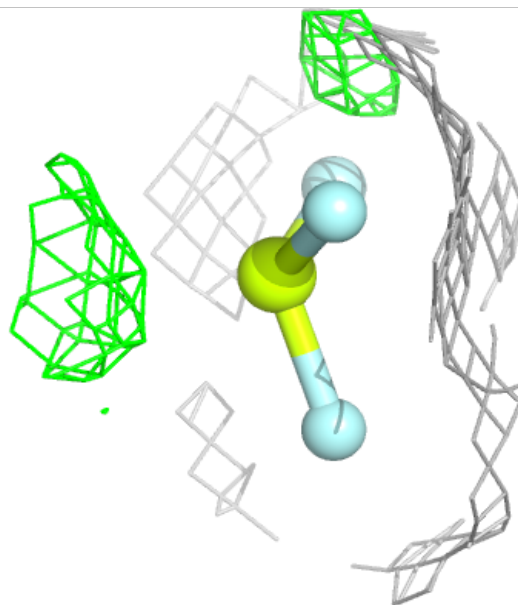
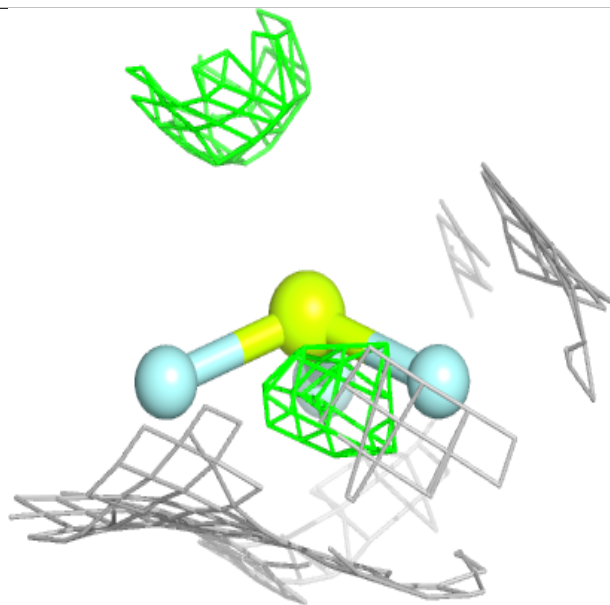
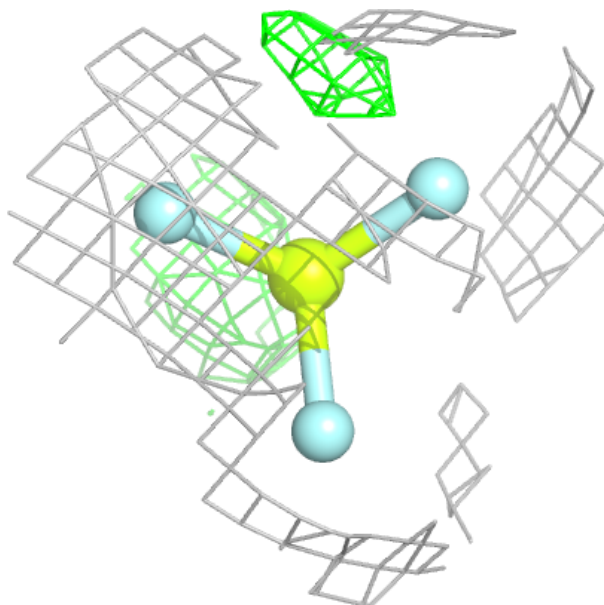
Electron density around BEF D 602:

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and green (positive)



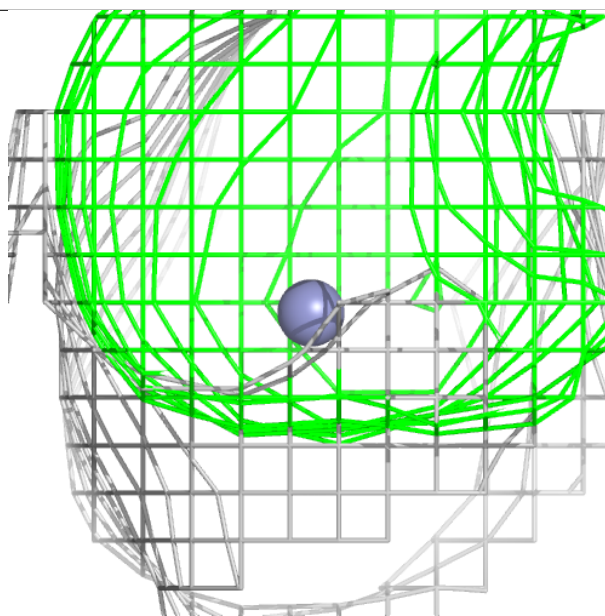
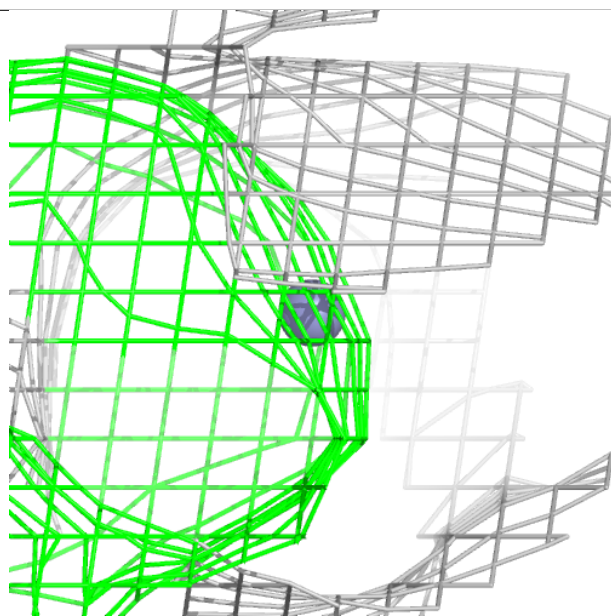
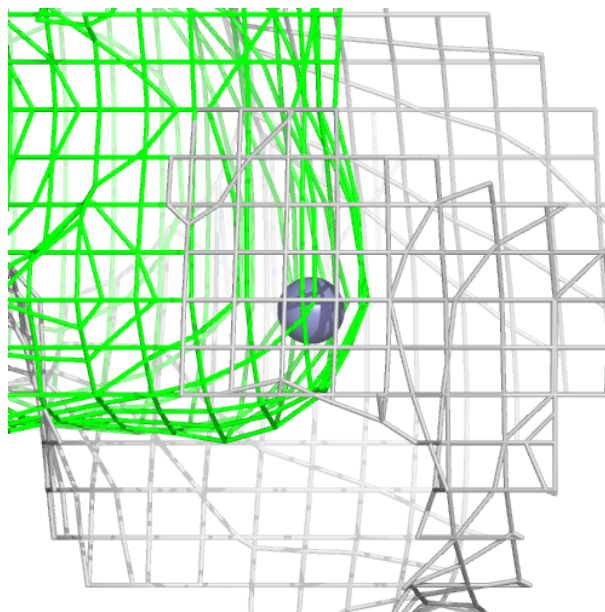
Electron density around BEF C 602:

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



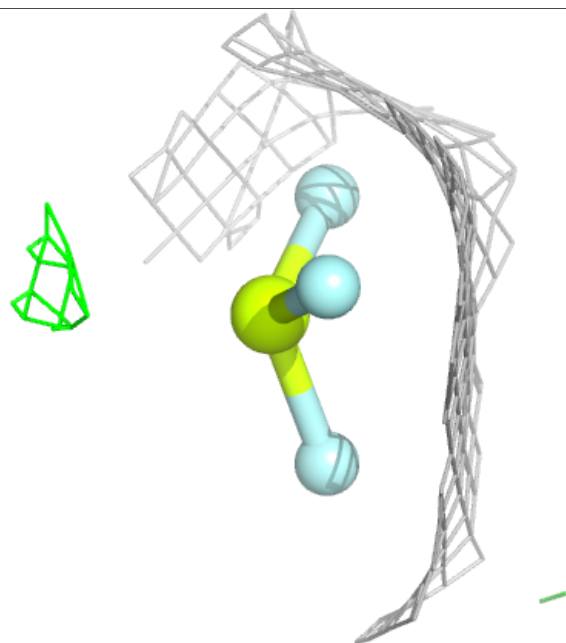
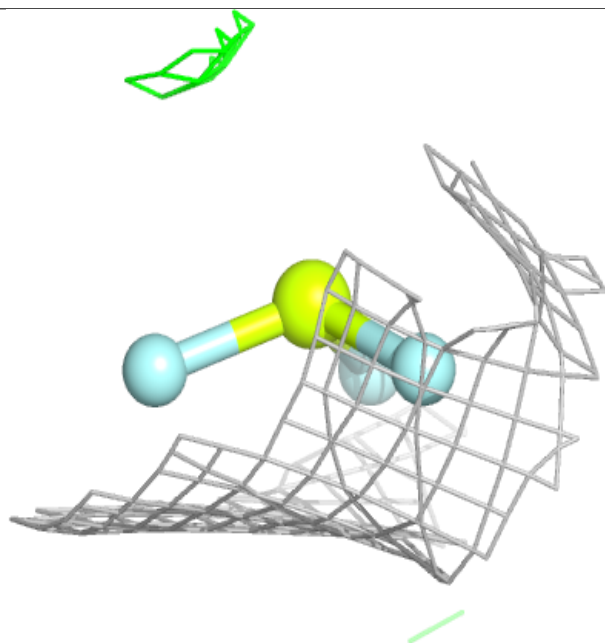
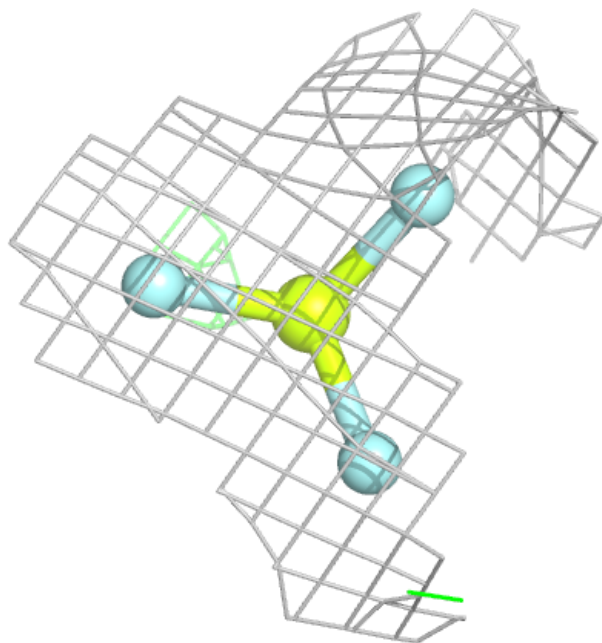
Electron density around ZN A 603:

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



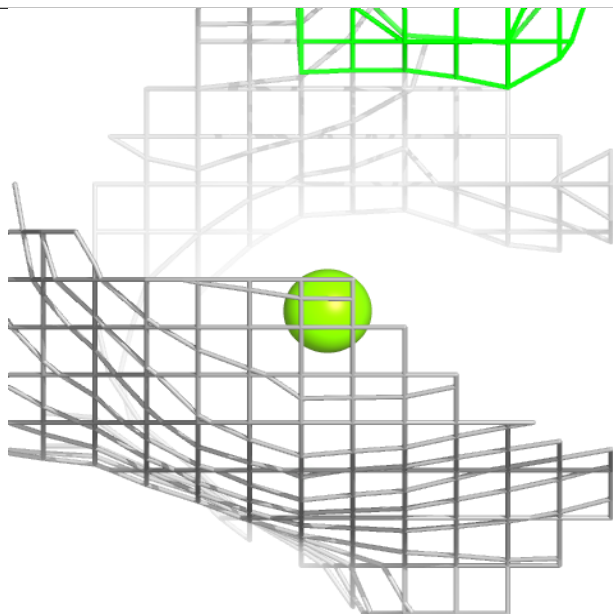
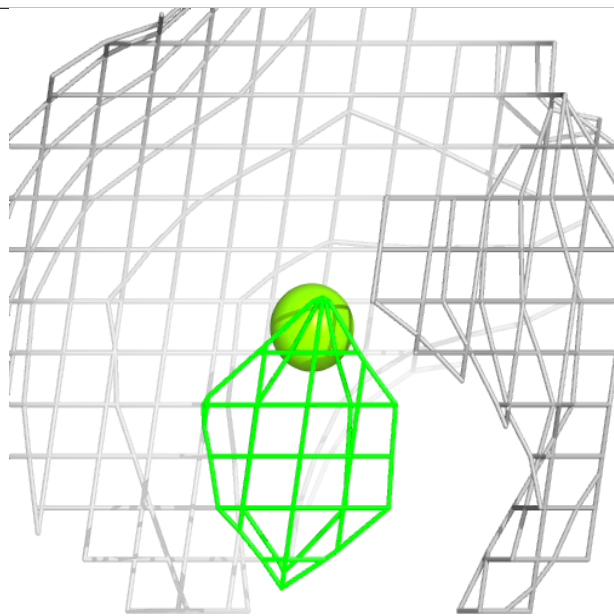
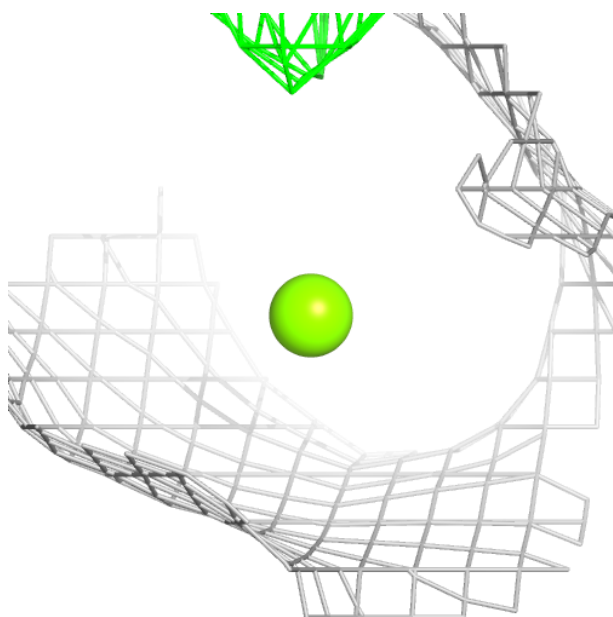
Electron density around BEF A 602:

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



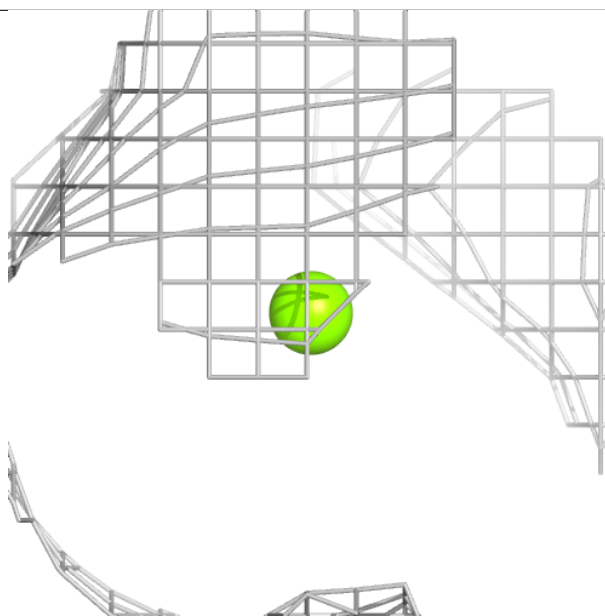
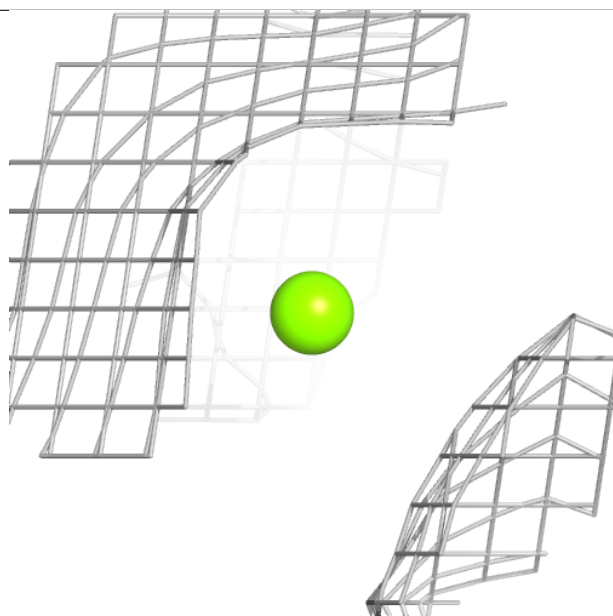
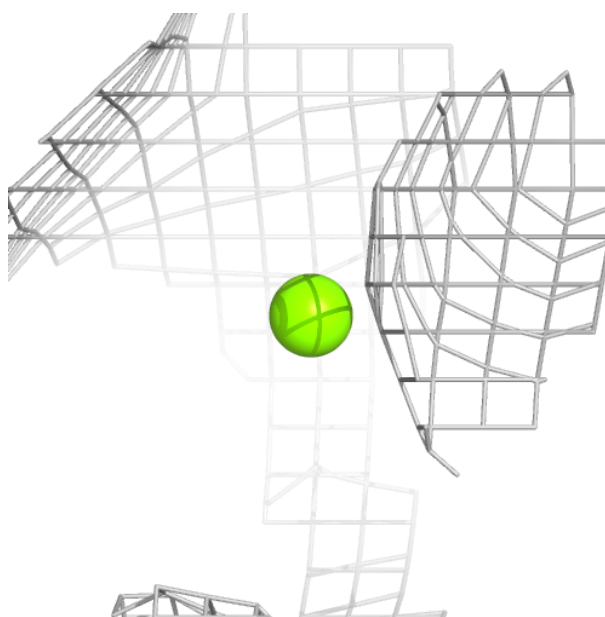
Electron density around MG A 601:

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and green (positive)



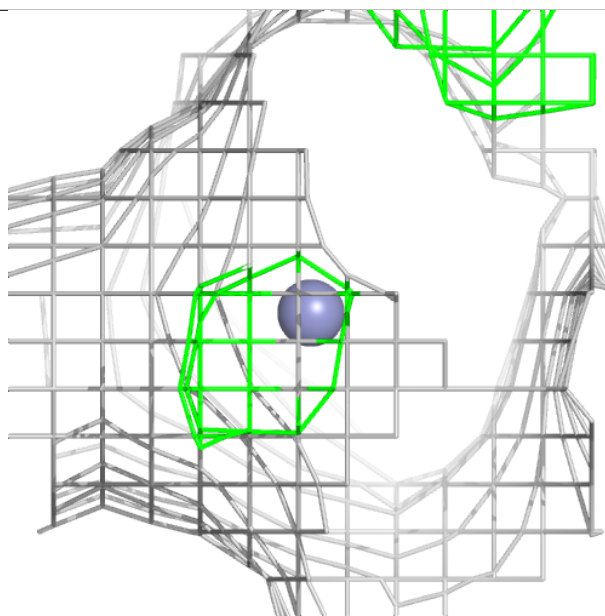
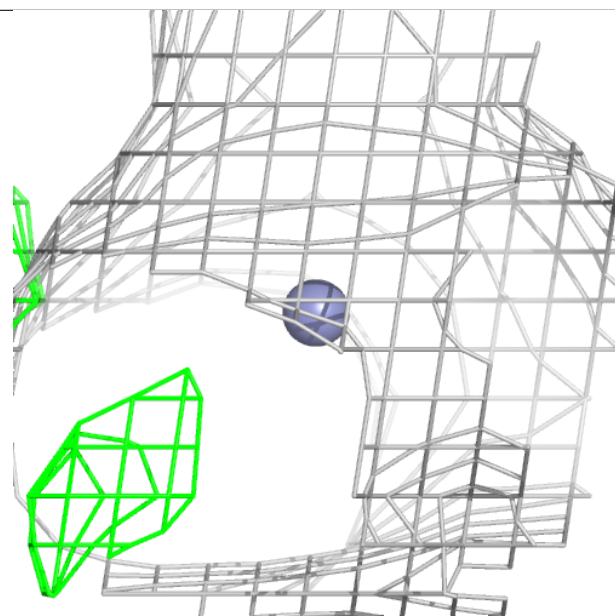
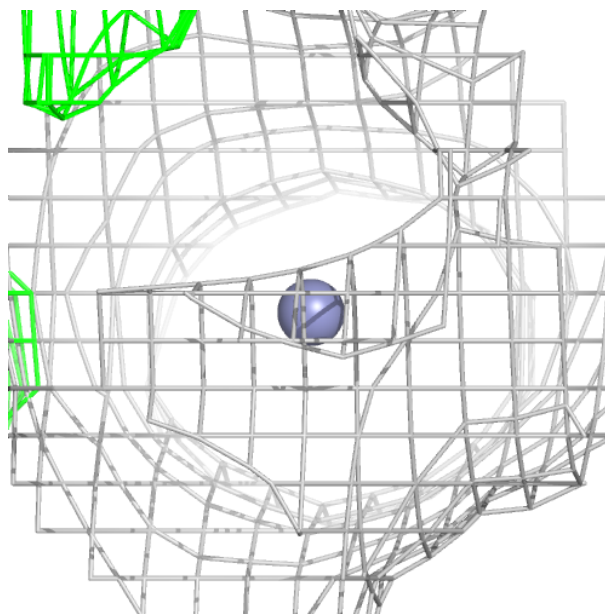
Electron density around MG D 601:

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



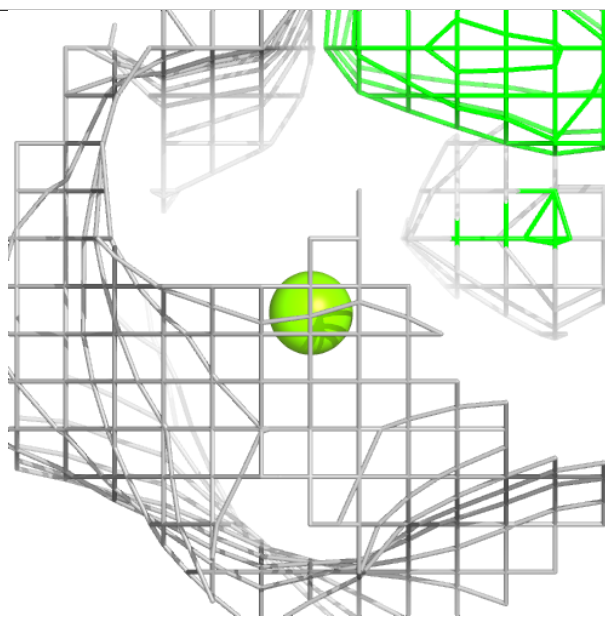
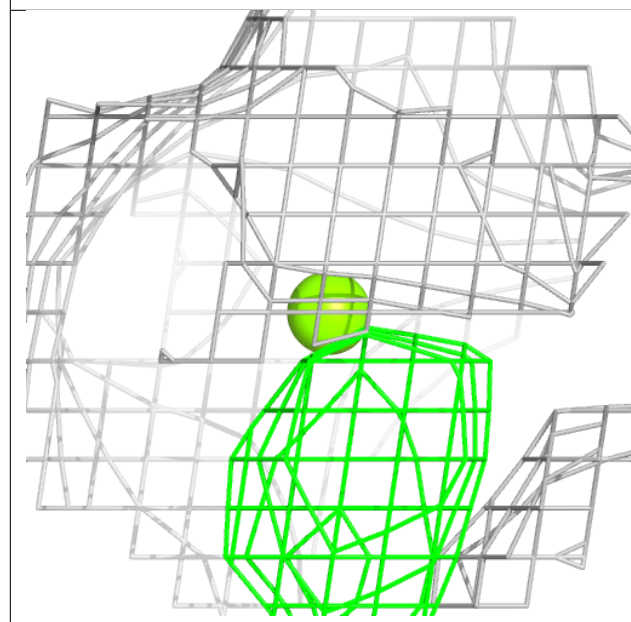
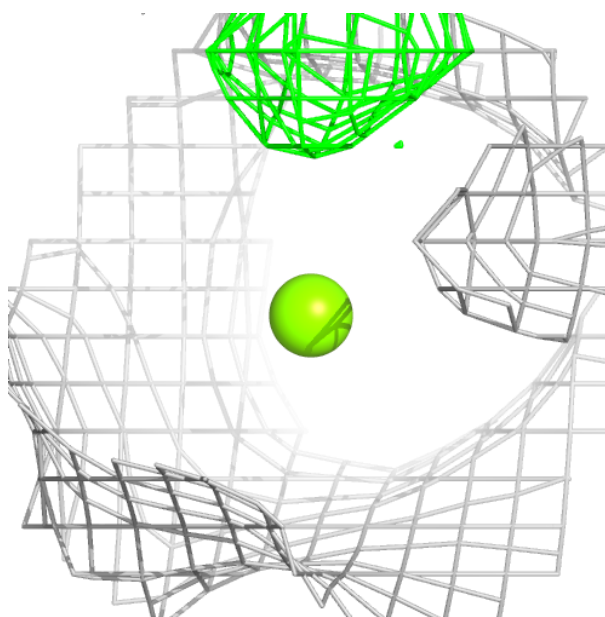
Electron density around ZN B 610:

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and green (positive)



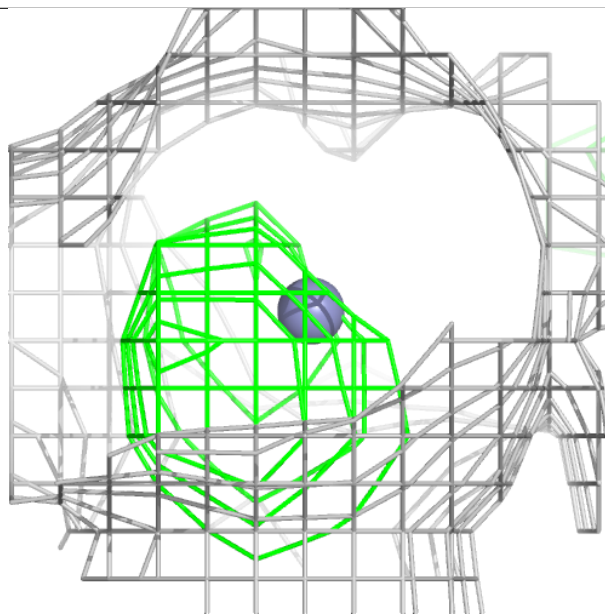
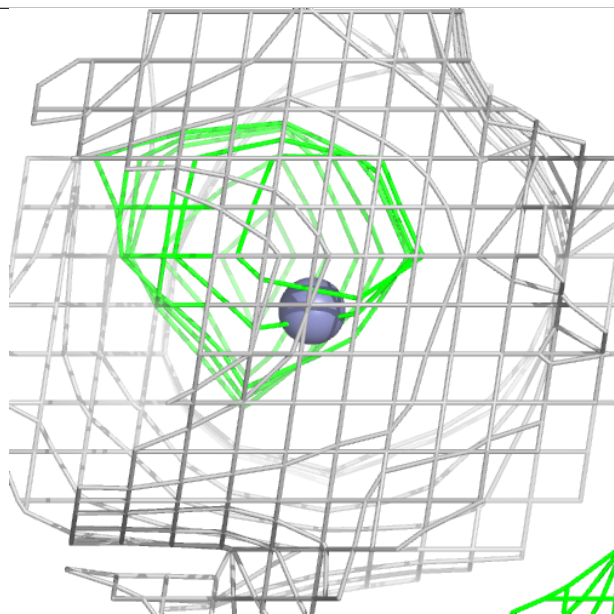
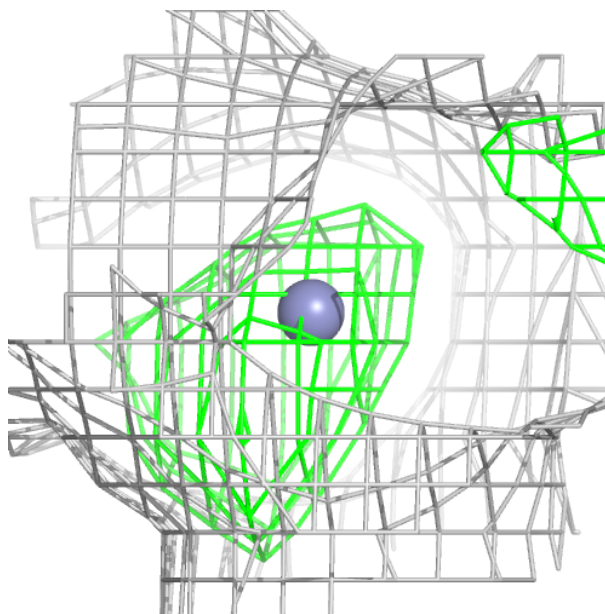
Electron density around MG C 601:

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and green (positive)



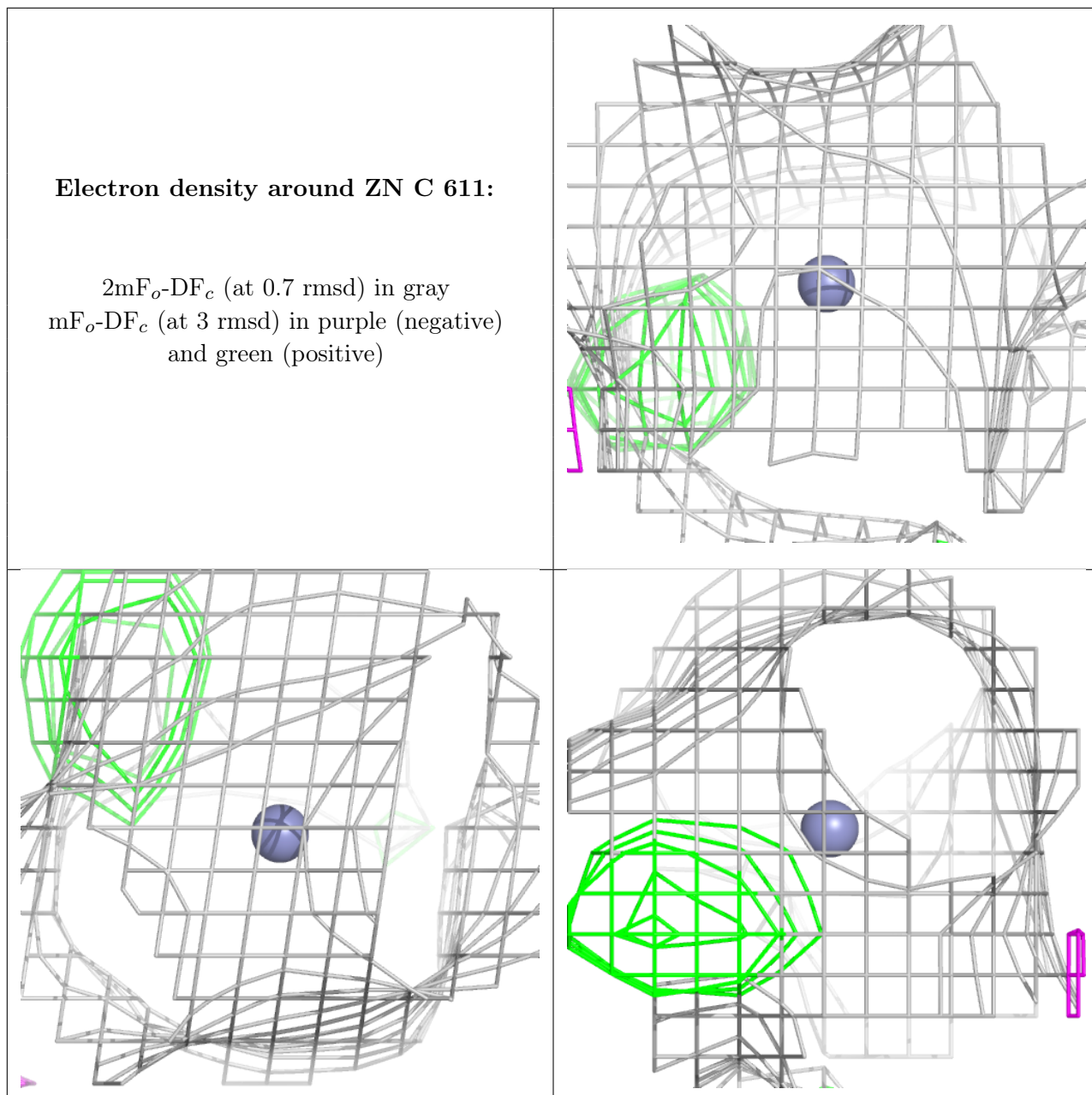
Electron density around ZN B 603:

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and green (positive)



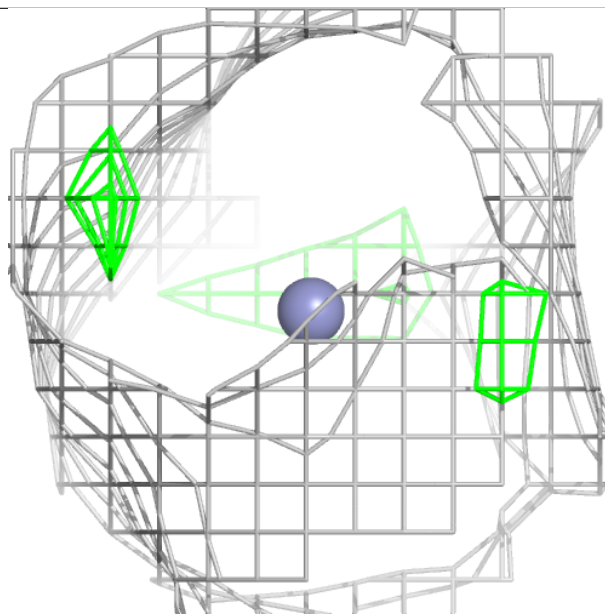
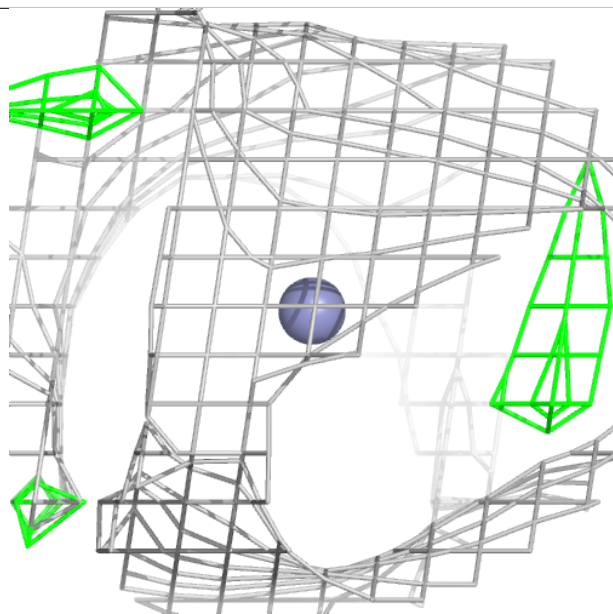
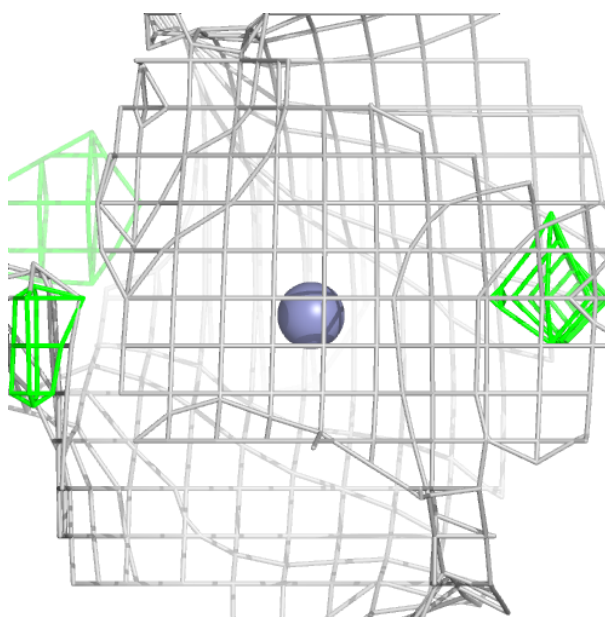
Electron density around ZN C 611:

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and green (positive)



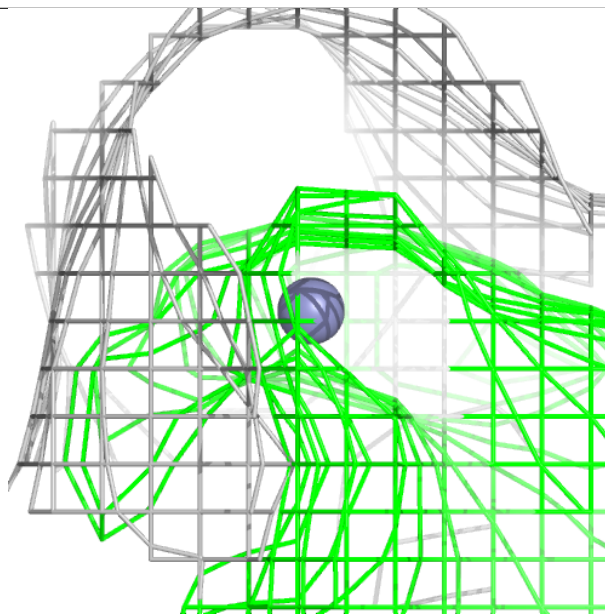
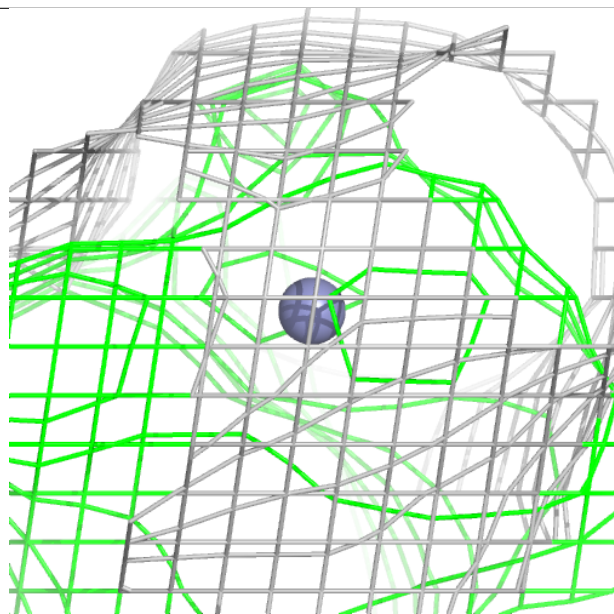
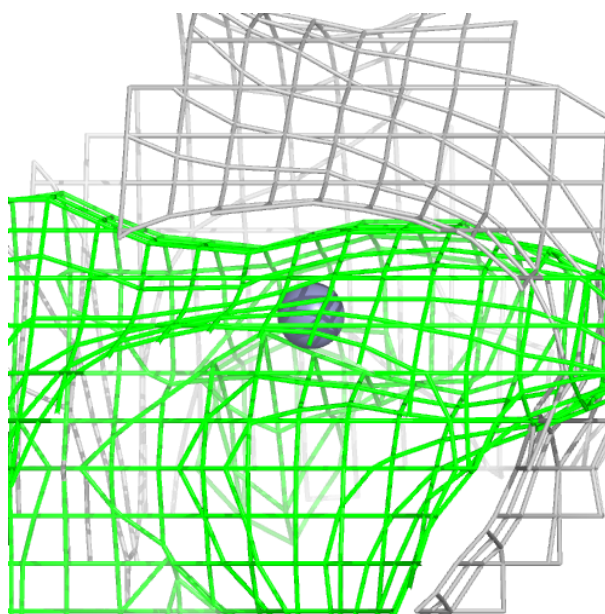
Electron density around ZN C 603:

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



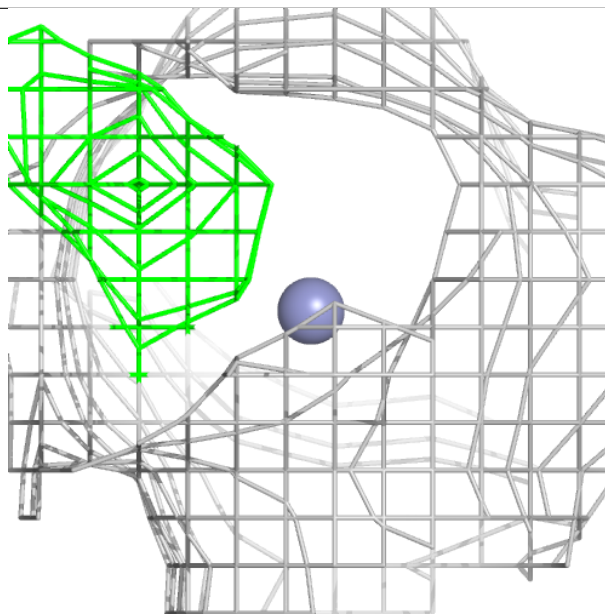
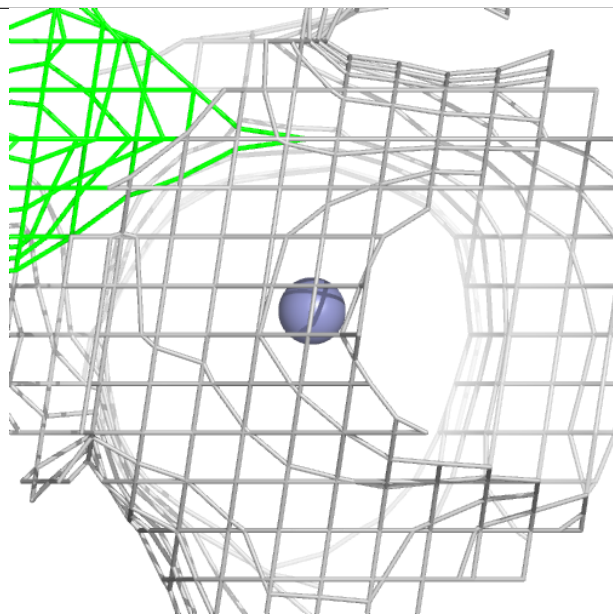
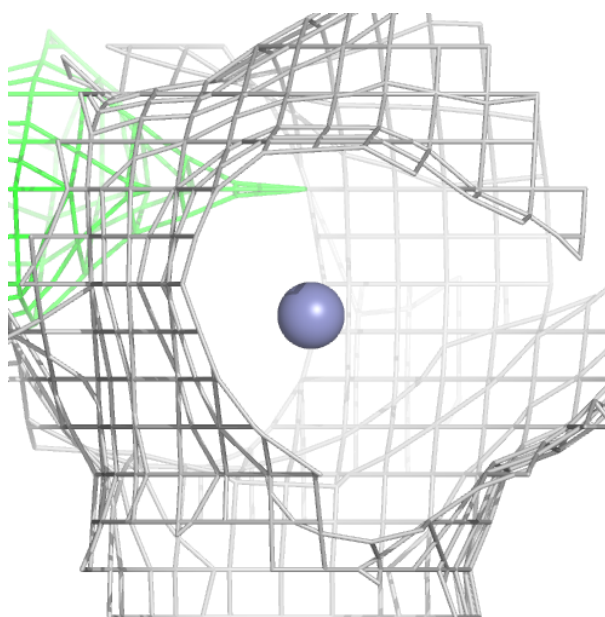
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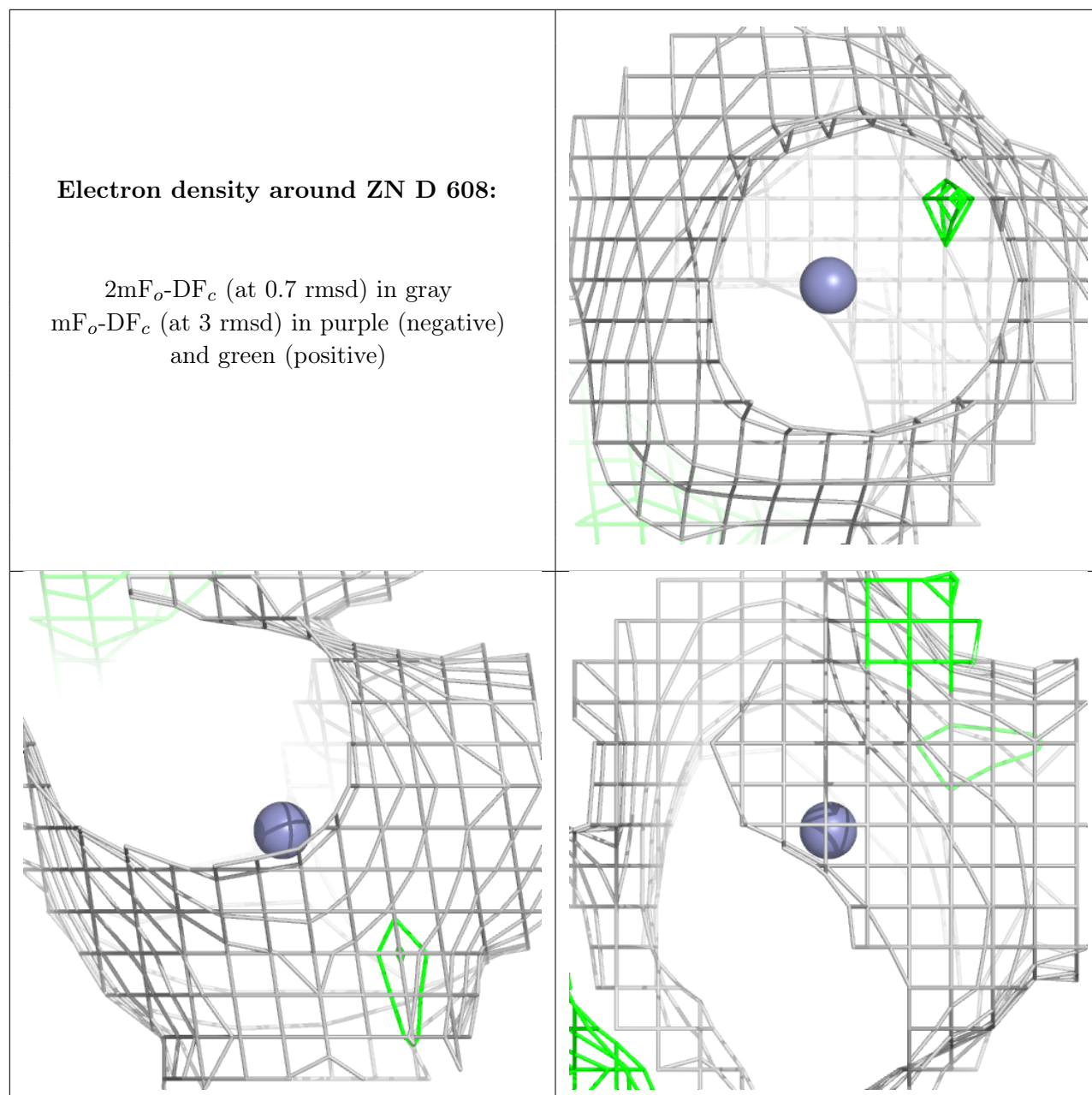
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN D 603:

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





5.5 Other polymers ⓘ

There are no such residues in this entry.