



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2026 – 12:23 PM EDT

PDB ID : 9PH9 / pdb_00009ph9
Title : Crystal structure of SARS-CoV-2 nsp14 with SAH and GpppA bound
Authors : Caputo, A.T.; Dennis, M.L.; Blackman, L.D.
Deposited on : 2025-07-08
Resolution : 2.26 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

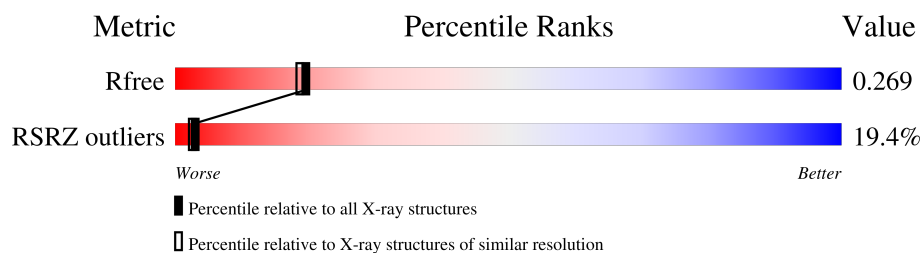
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12975 atoms, of which 6086 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 Guanine-N7 methyltransferase nsp14.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	427	Total	C	H	N	O	S	3042	1	0
			6500	2229	3042	584	613	32			
1	B	384	Total	C	H	N	O	S	2936	0	0
			6046	2005	2936	525	552	28			

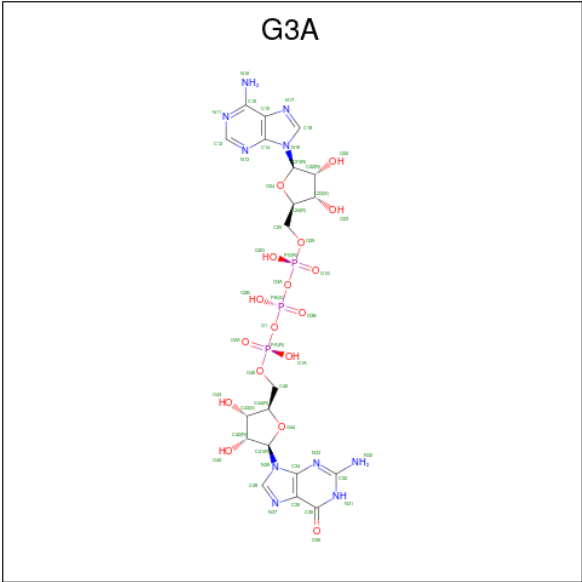
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	SER	-	expression tag	UNP P0DTD1
A	22	ASN	-	expression tag	UNP P0DTD1
A	23	GLY	-	expression tag	UNP P0DTD1
A	24	SER	-	expression tag	UNP P0DTD1
B	21	SER	-	expression tag	UNP P0DTD1
B	22	ASN	-	expression tag	UNP P0DTD1
B	23	GLY	-	expression tag	UNP P0DTD1
B	24	SER	-	expression tag	UNP P0DTD1

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

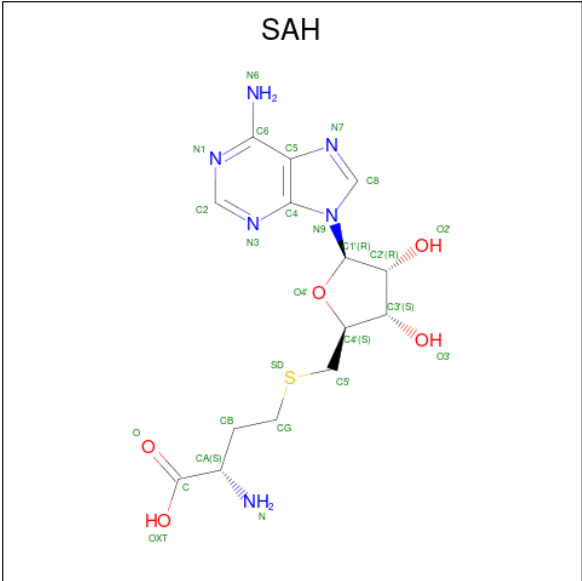
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Zn	0	0
			4	4		
2	B	4	Total	Zn	0	0
			4	4		

- Molecule 3 is GUANOSINE-P3-ADENOSINE-5',5'-TRIPHOSPHATE (CCD ID: G3A) (formula: C₂₀H₂₇N₁₀O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	27	0
			77	20	27	10	17	3		
3	B	1	Total	C	H	N	O	P	27	0
			77	20	27	10	17	3		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	20	0
			46	14	20	6	5	1		

Continued on next page...

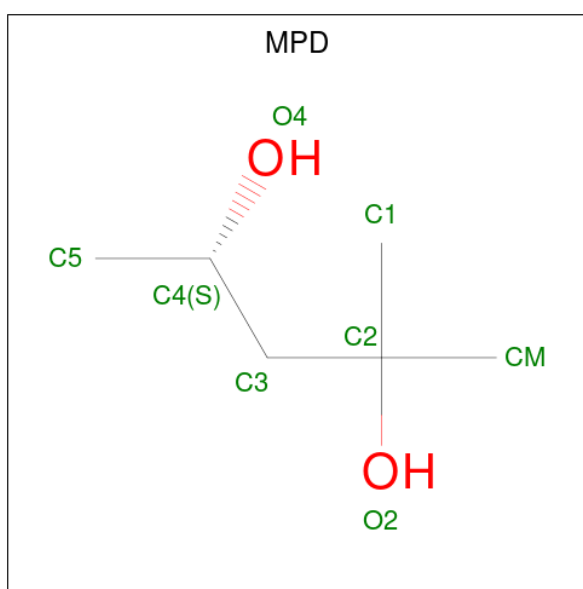
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	S	
			46	14	20	6	5	1	20
									0

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O		
			22	6	14	2	14	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	87	Total	O	0	0
			87	87		
7	B	65	Total	O	0	0
			65	65		

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.10Å 99.47Å 90.52Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	85.43 – 2.26 85.43 – 2.26	Depositor EDS
% Data completeness (in resolution range)	61.9 (85.43-2.26) 61.9 (85.43-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.25Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.234 , 0.266 0.228 , 0.269	Depositor DCC
R_{free} test set	1524 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12975	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 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	SAH	B	707	-	27,28,28	0.35	0	36,40,40	0.56	1 (2%)
4	SAH	A	706	-	27,28,28	0.34	0	36,40,40	0.49	0
3	G3A	A	705	-	55,55,55	0.25	0	81,86,86	0.38	0
6	MPD	B	705	-	7,7,7	0.19	0	9,10,10	0.34	0
3	G3A	B	706	-	55,55,55	0.34	0	81,86,86	0.46	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
4	SAH	B	707	-	-	2/15/31/31	0/3/3/3
4	SAH	A	706	-	-	2/15/31/31	0/3/3/3
3	G3A	A	705	-	-	8/32/64/64	0/6/6/6
6	MPD	B	705	-	-	0/5/5/5	-
3	G3A	B	706	-	-	8/32/64/64	0/6/6/6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	707	SAH	CB-CG-SD	-2.10	108.77	113.45

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	705	G3A	C25-O25-PG-O3A
3	A	705	G3A	C25-O25-PG-O2G
3	B	706	G3A	C25-O25-PG-O3A
3	B	706	G3A	C25-O25-PG-O2G
4	B	707	SAH	N-CA-CB-CG
4	A	706	SAH	C-CA-CB-CG
4	B	707	SAH	C-CA-CB-CG
3	A	705	G3A	PA-O1-PB-O2B

Continued on next page...

Continued from previous page...

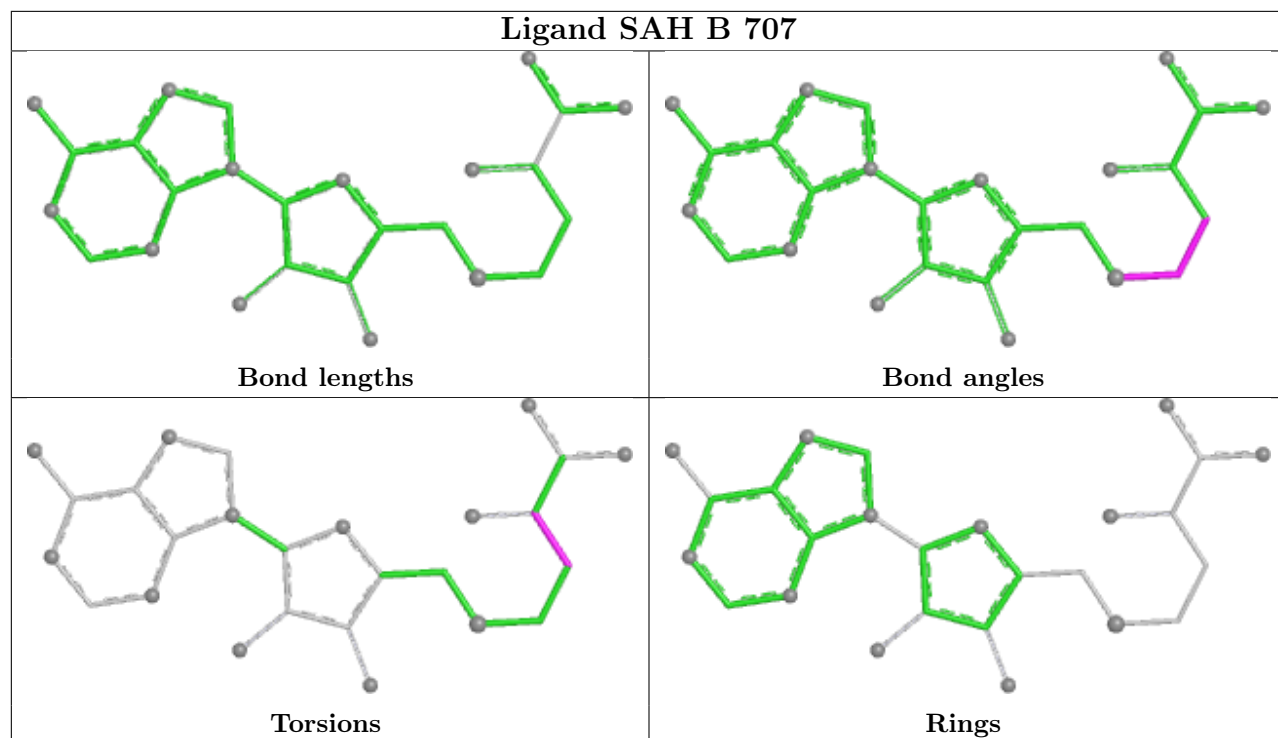
Mol	Chain	Res	Type	Atoms
3	B	706	G3A	PA-O1-PB-O2B
4	A	706	SAH	N-CA-CB-CG
3	A	705	G3A	PG-O3A-PB-O2B
3	B	706	G3A	PG-O3A-PB-O2B
3	B	706	G3A	PG-O3A-PB-O3B
3	A	705	G3A	PG-O3A-PB-O3B
3	A	705	G3A	C24-C25-O25-PG
3	A	705	G3A	O24-C24-C25-O25
3	B	706	G3A	O24-C24-C25-O25
3	B	706	G3A	C24-C25-O25-PG
3	A	705	G3A	PA-O1-PB-O3B
3	B	706	G3A	PA-O1-PB-O3B

There are no ring outliers.

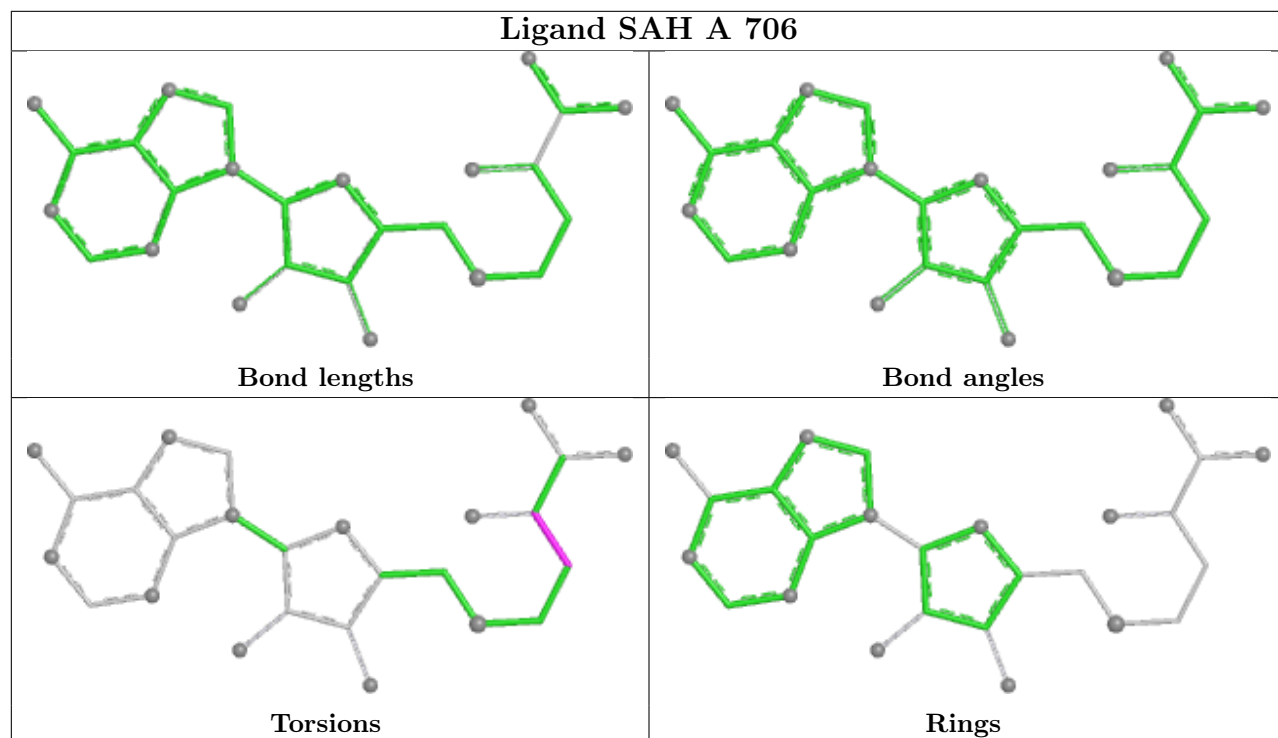
No monomer is involved in short contacts.

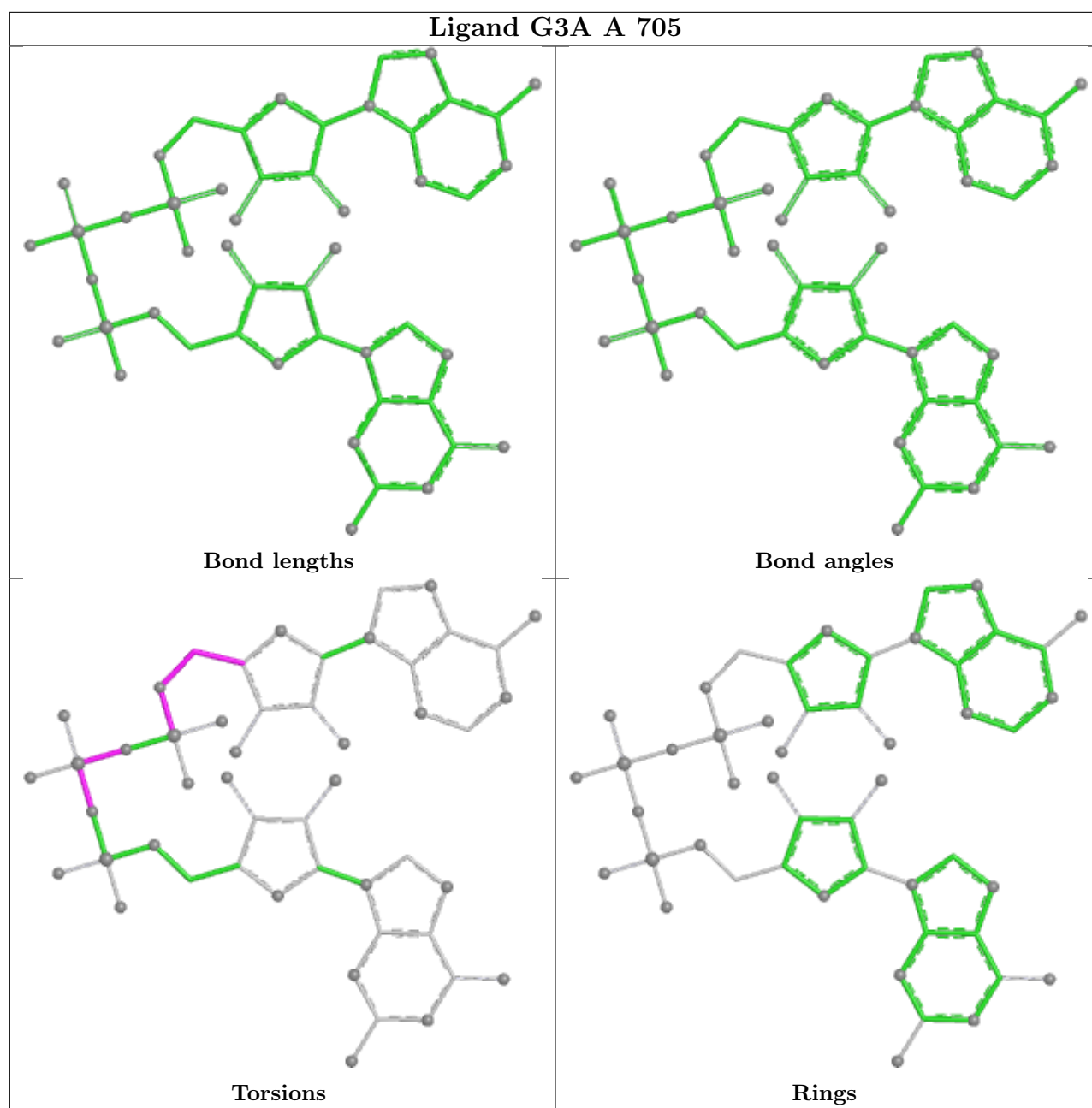
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

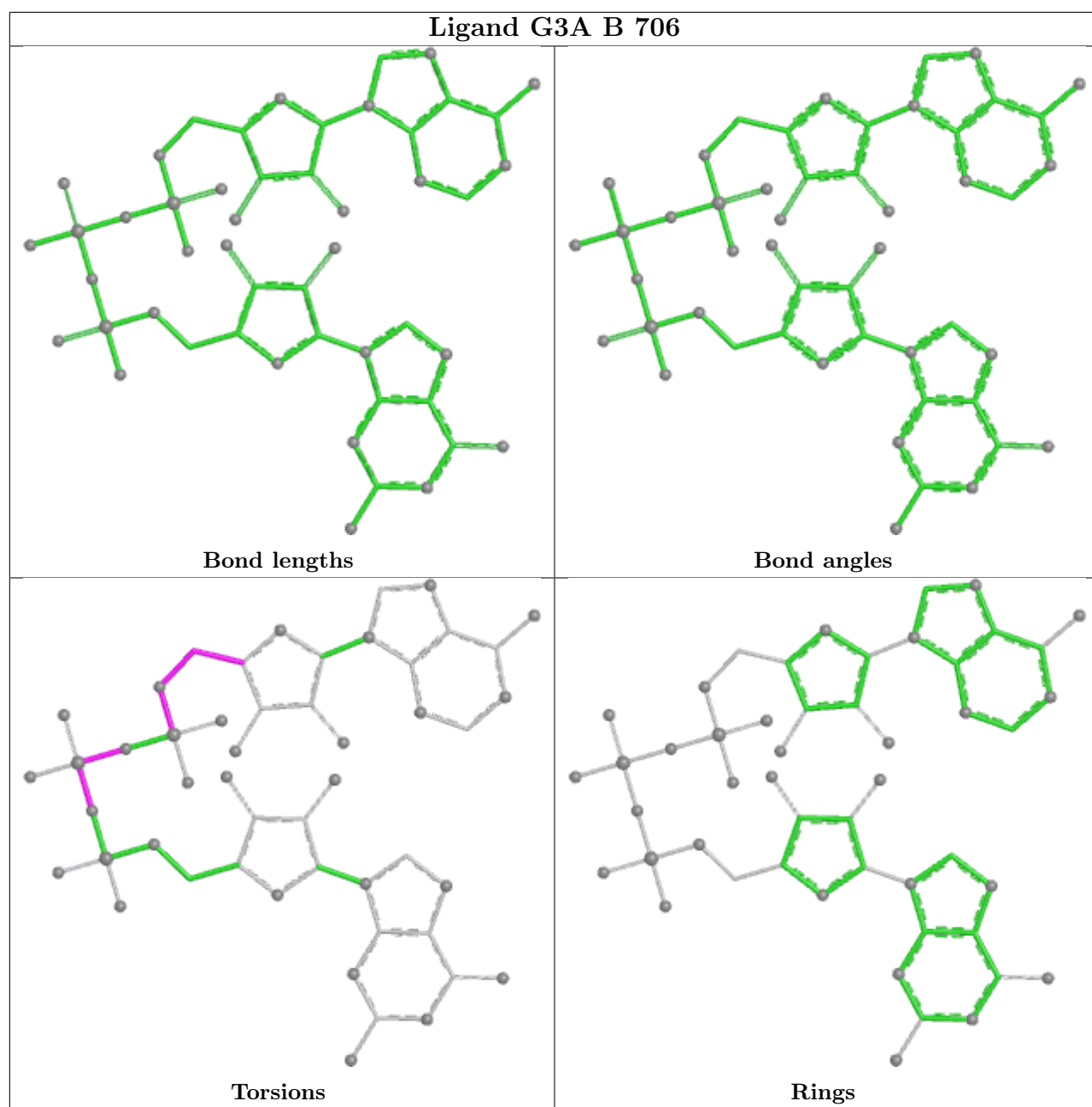
Ligand SAH B 707



Ligand SAH A 706







4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

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	427/531 (80%)	1.30	99 (23%) 2 1	17, 39, 138, 194	1 (0%)
1	B	384/531 (72%)	1.08	58 (15%) 5 5	23, 40, 61, 112	0
All	All	811/1062 (76%)	1.19	157 (19%) 3 2	17, 39, 72, 194	1 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	LEU	6.2
1	A	90	VAL	6.1
1	B	133	LEU	5.4
1	A	144	VAL	5.1
1	A	78	LEU	4.9
1	A	129	LEU	4.9
1	A	489	TYR	4.8
1	A	543	LEU	4.5
1	B	214	PHE	4.5
1	A	79	ILE	4.3
1	A	88	TYR	4.3
1	B	135	PHE	4.2
1	A	212	HIS	4.0
1	B	361	ALA	3.9
1	B	96	MET	3.9
1	B	190	ILE	3.9
1	B	225	ILE	3.8
1	A	292	HIS	3.8
1	A	490	VAL	3.8
1	A	545	ASN	3.7
1	B	401	PHE	3.7
1	B	94	PRO	3.6
1	A	93	TYR	3.6
1	B	132	GLN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	368	ALA	3.5
1	A	547	PHE	3.5
1	A	82	MET	3.5
1	B	474	SER	3.4
1	B	93	TYR	3.4
1	B	222	PHE	3.4
1	A	540	THR	3.4
1	A	469	PHE	3.3
1	A	91	ASN	3.3
1	A	233	LEU	3.3
1	A	312	LYS	3.3
1	A	289	GLY	3.3
1	A	216	LEU	3.3
1	A	92	GLY	3.2
1	A	478	SER	3.2
1	A	56	LYS	3.2
1	A	75	TYR	3.2
1	A	96	MET	3.2
1	A	97	PHE	3.1
1	B	244	ALA	3.1
1	B	475	PRO	3.1
1	A	57	PHE	3.1
1	A	83	GLY	3.1
1	A	213	GLY	3.1
1	B	221	TYR	3.0
1	B	490	VAL	3.0
1	B	288	HIS	3.0
1	B	207	PHE	3.0
1	B	186	VAL	3.0
1	A	266	ILE	3.0
1	B	255	ILE	3.0
1	B	183	TRP	3.0
1	B	504	GLY	2.9
1	A	538	PHE	2.9
1	B	113	PHE	2.9
1	A	542	ASN	2.9
1	A	55	THR	2.9
1	A	95	ASN	2.9
1	A	138	GLY	2.8
1	A	346	LEU	2.8
1	A	98	ILE	2.8
1	A	503	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	291	ALA	2.8
1	B	491	PRO	2.8
1	A	81	MET	2.8
1	A	60	GLU	2.8
1	A	360	LYS	2.8
1	B	138	GLY	2.7
1	A	101	GLU	2.7
1	B	382	ASP	2.7
1	A	209	LEU	2.7
1	B	503	LEU	2.7
1	B	343	ALA	2.7
1	A	271	TRP	2.7
1	A	313	ARG	2.7
1	A	383	LYS	2.7
1	A	349	LYS	2.6
1	A	270	GLN	2.6
1	A	84	PHE	2.6
1	A	137	THR	2.6
1	B	233	LEU	2.6
1	B	477	GLU	2.6
1	A	181	LEU	2.6
1	A	492	LEU	2.6
1	A	294	ALA	2.6
1	A	139	VAL	2.6
1	A	541	TYR	2.6
1	B	271	TRP	2.5
1	B	469	PHE	2.5
1	A	380	CYS	2.5
1	B	246	ASP	2.5
1	A	287	VAL	2.5
1	A	336	VAL	2.5
1	B	293	VAL	2.5
1	A	298	ALA	2.5
1	B	457	LYS	2.5
1	A	77	ARG	2.5
1	A	340	VAL	2.5
1	A	394	TYR	2.5
1	B	220	LYS	2.5
1	A	87	ASN	2.5
1	A	461	VAL	2.4
1	B	210	TRP	2.4
1	A	224[A]	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	58	LYS	2.4
1	B	227	PRO	2.4
1	A	333	CYS	2.4
1	A	362	ILE	2.4
1	A	352	VAL	2.4
1	A	345	LEU	2.4
1	A	504	GLY	2.3
1	A	505	GLY	2.3
1	A	255	ILE	2.3
1	B	181	LEU	2.3
1	A	385	TYR	2.3
1	A	544	TRP	2.3
1	B	229	ARG	2.3
1	A	290	ASN	2.3
1	B	465	GLN	2.3
1	A	105	ARG	2.2
1	A	284	TYR	2.2
1	B	277	LEU	2.2
1	A	214	PHE	2.2
1	A	369	ASP	2.2
1	A	211	ALA	2.2
1	A	366	PRO	2.2
1	A	495	ALA	2.2
1	B	274	THR	2.2
1	A	401	PHE	2.2
1	A	85	LYS	2.2
1	B	369	ASP	2.1
1	B	232	CYS	2.1
1	A	348	ASP	2.1
1	A	186	VAL	2.1
1	A	491	PRO	2.1
1	B	97	PHE	2.1
1	B	269	GLN	2.1
1	B	398	SER	2.1
1	A	390	LEU	2.1
1	B	394	TYR	2.1
1	B	313	ARG	2.1
1	B	387	ILE	2.1
1	B	513	ASN	2.1
1	B	507	VAL	2.1
1	B	509	ARG	2.1
1	B	137	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	73	MET	2.0
1	A	133	LEU	2.0
1	A	468	PHE	2.0
1	A	400	LYS	2.0
1	A	110	TRP	2.0
1	B	245	SER	2.0
1	B	209	LEU	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.

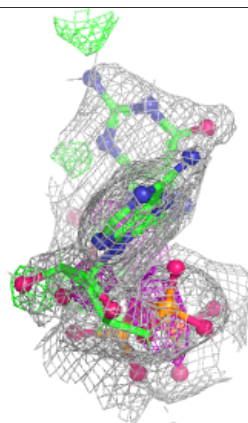
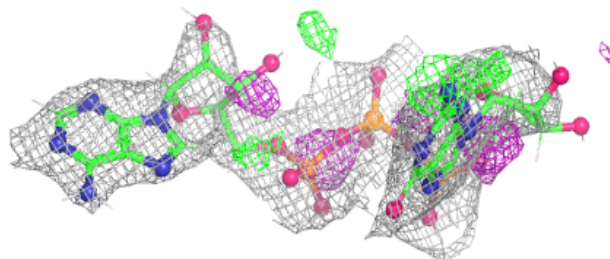
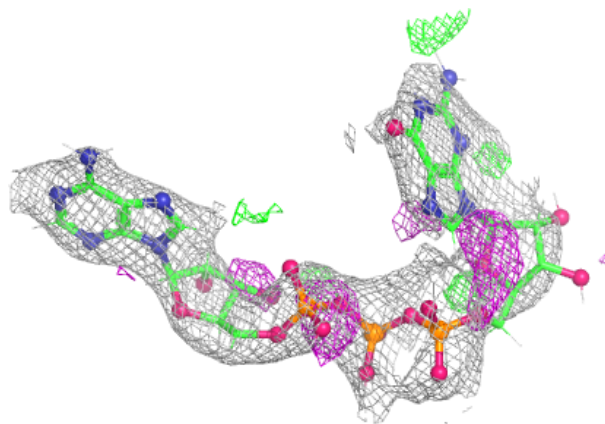
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	G3A	B	706	50/50	0.74	0.18	88,118,123,124	27
3	G3A	A	705	50/50	0.79	0.18	118,142,147,152	27
6	MPD	B	705	8/8	0.84	0.28	107,124,134,134	14
2	ZN	A	704	1/1	0.85	0.10	180,180,180,180	0
2	ZN	B	704	1/1	0.86	0.08	181,181,181,181	0
4	SAH	A	706	26/26	0.95	0.07	58,70,70,71	20
4	SAH	B	707	26/26	0.96	0.07	32,54,57,57	20
5	MN	A	707	1/1	0.97	0.09	60,60,60,60	0
2	ZN	B	701	1/1	0.99	0.05	80,80,80,80	0
2	ZN	B	702	1/1	0.99	0.04	77,77,77,77	0
2	ZN	B	703	1/1	0.99	0.06	102,102,102,102	0
2	ZN	A	703	1/1	0.99	0.06	105,105,105,105	0
2	ZN	A	702	1/1	0.99	0.07	66,66,66,66	0
2	ZN	A	701	1/1	1.00	0.07	66,66,66,66	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.

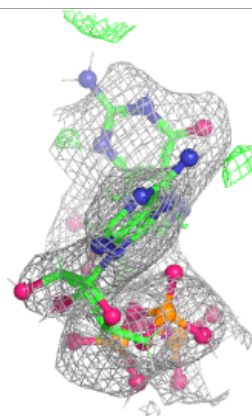
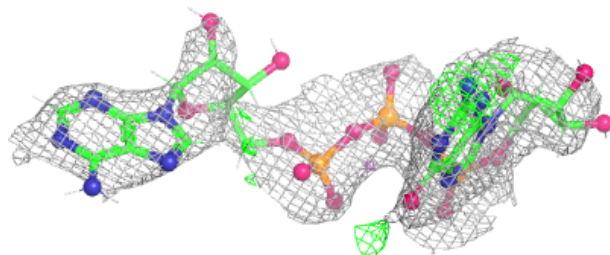
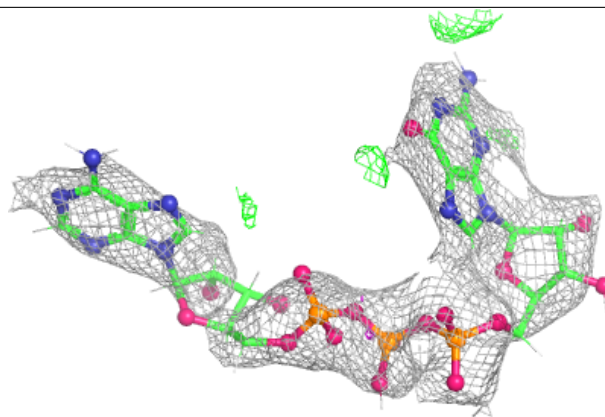
Electron density around G3A B 706:

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



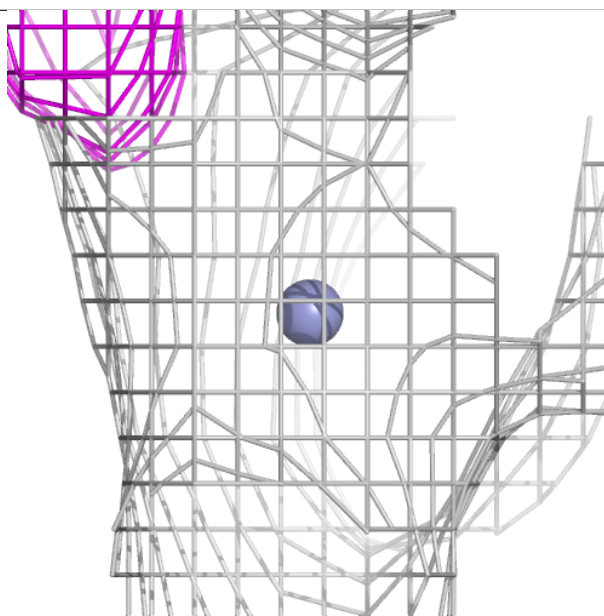
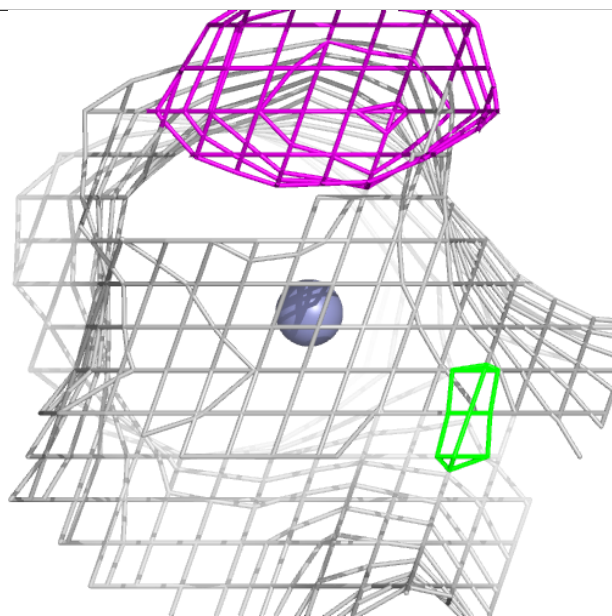
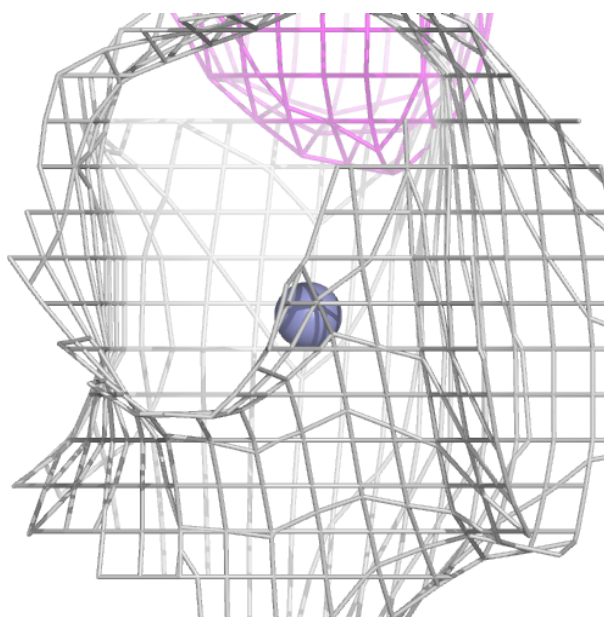
Electron density around G3A A 705:

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



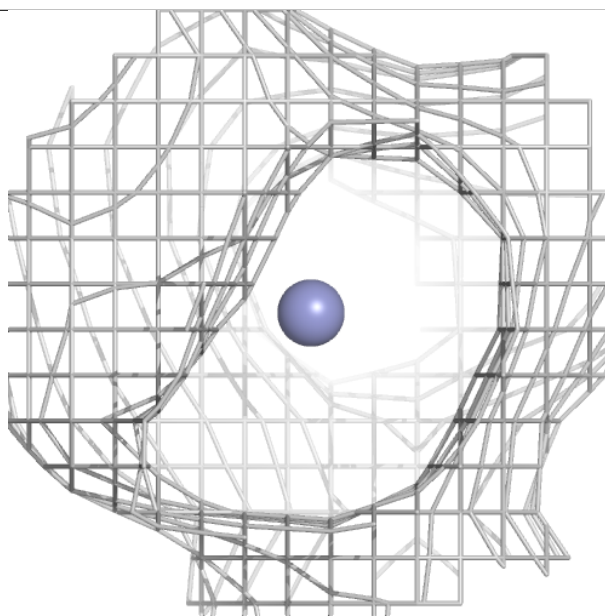
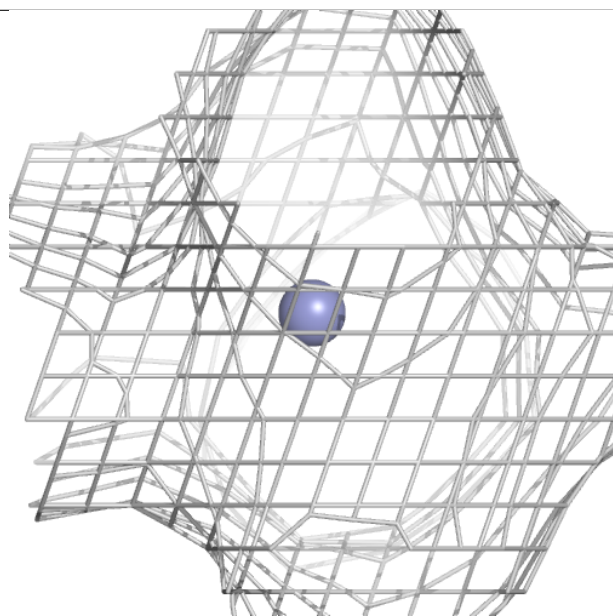
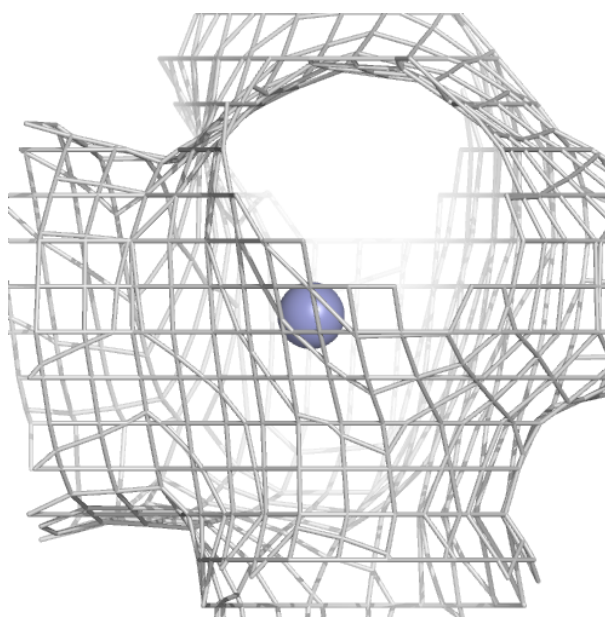
Electron density around ZN A 704:

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



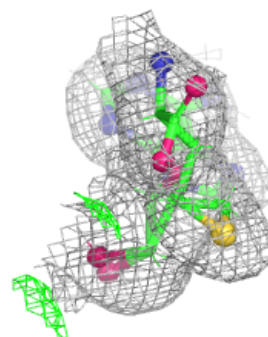
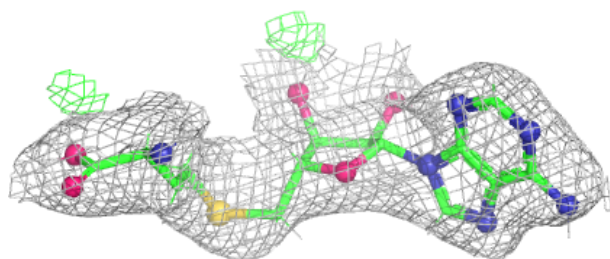
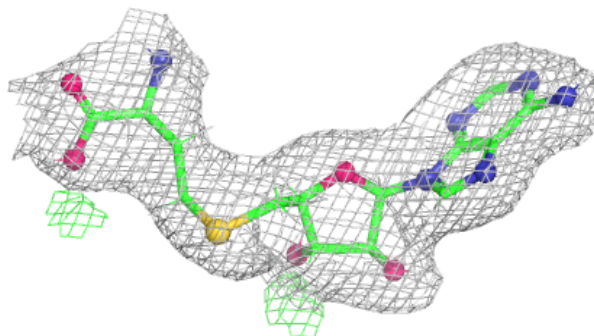
Electron density around ZN B 704:

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

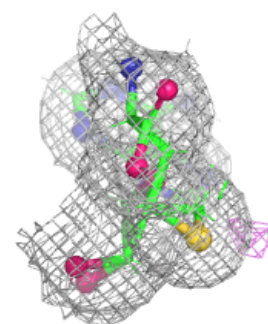
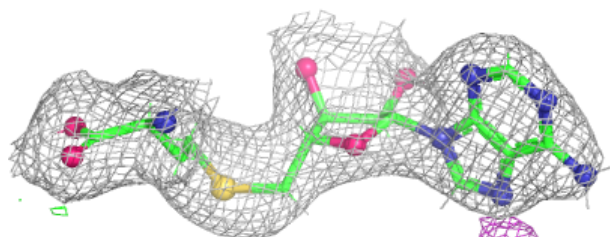
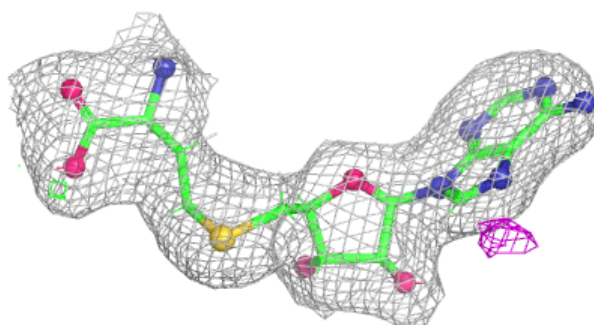


Electron density around SAH A 706:

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

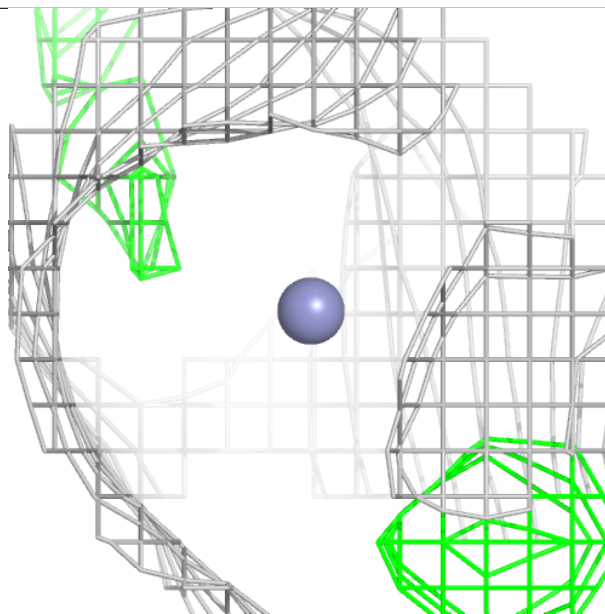
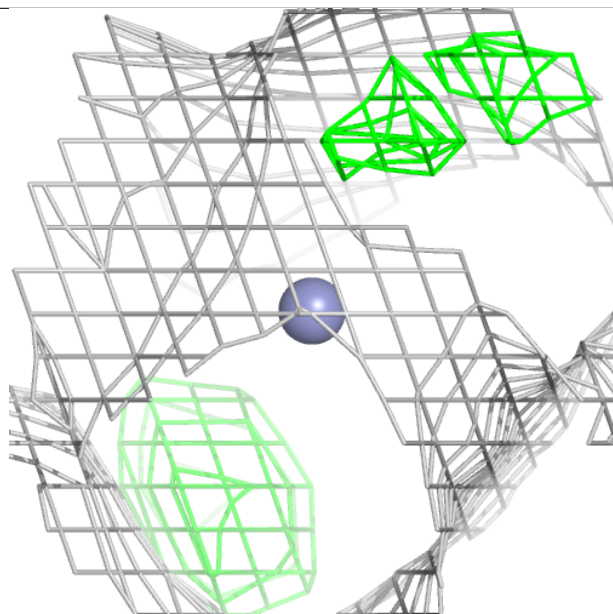
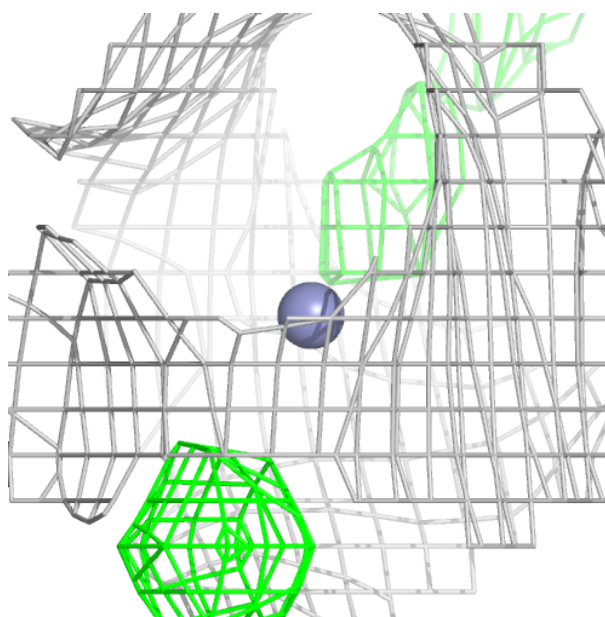
**Electron density around SAH B 707:**

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



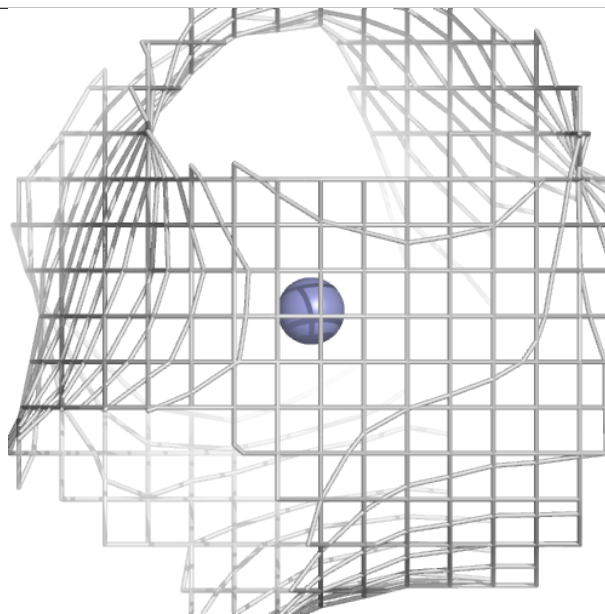
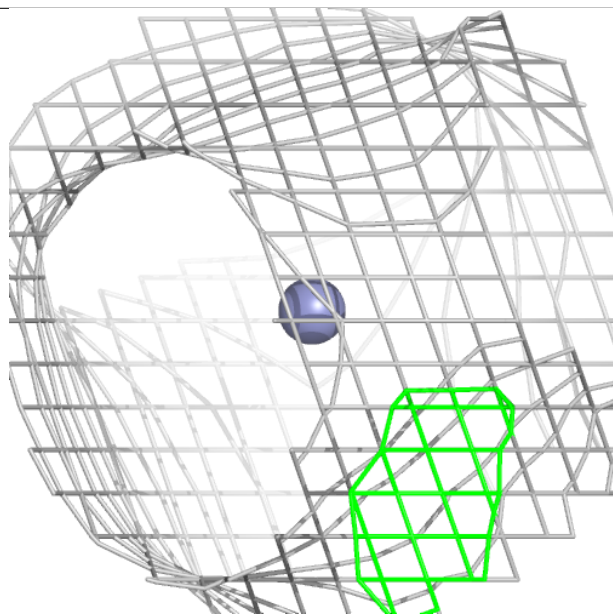
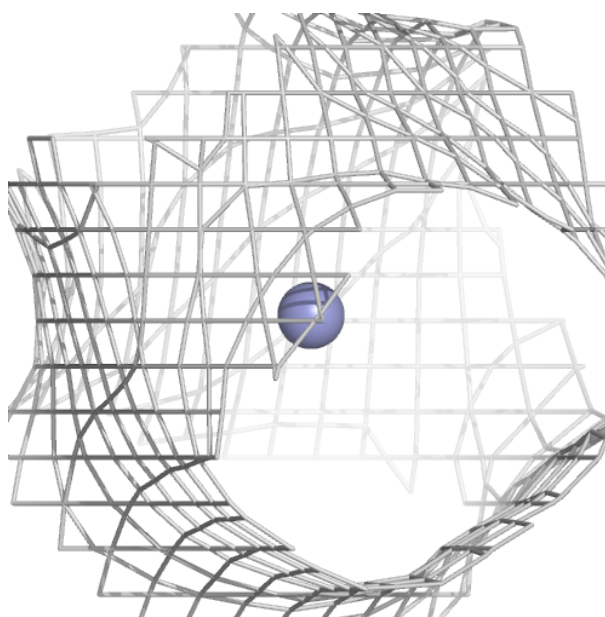
Electron density around ZN B 701:

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



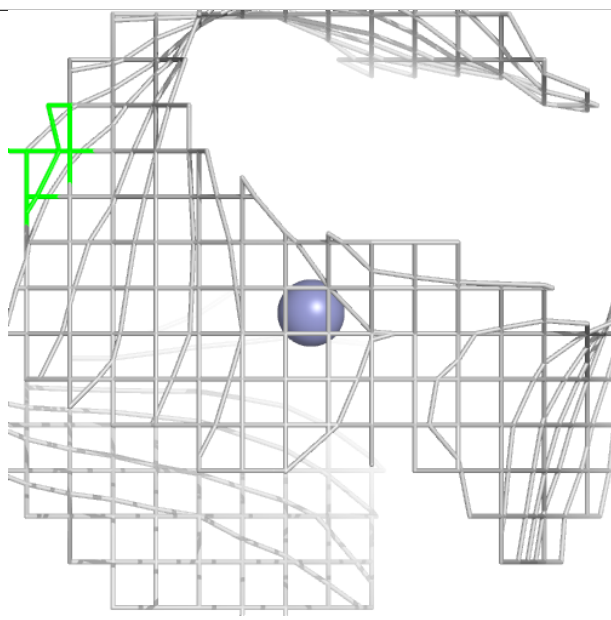
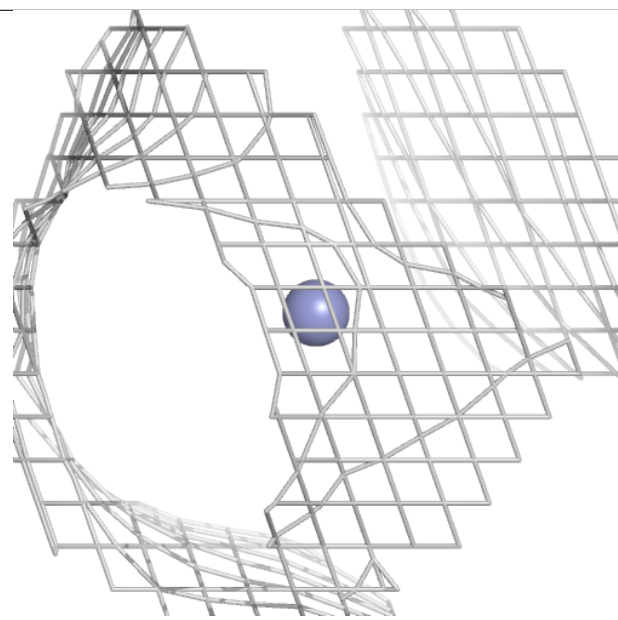
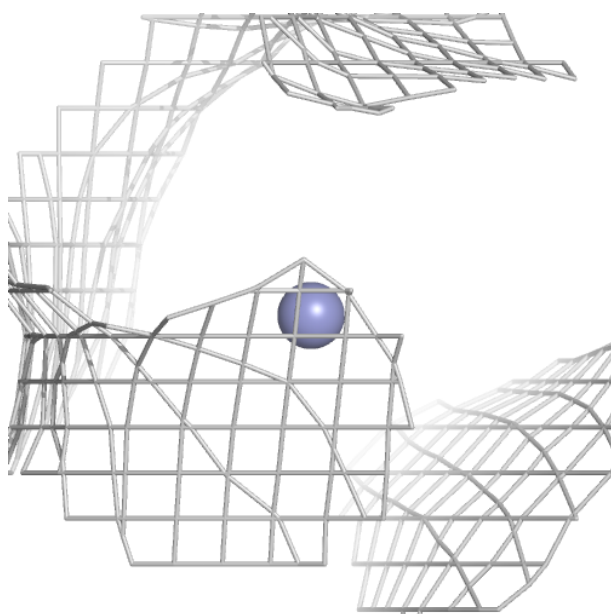
Electron density around ZN B 702:

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



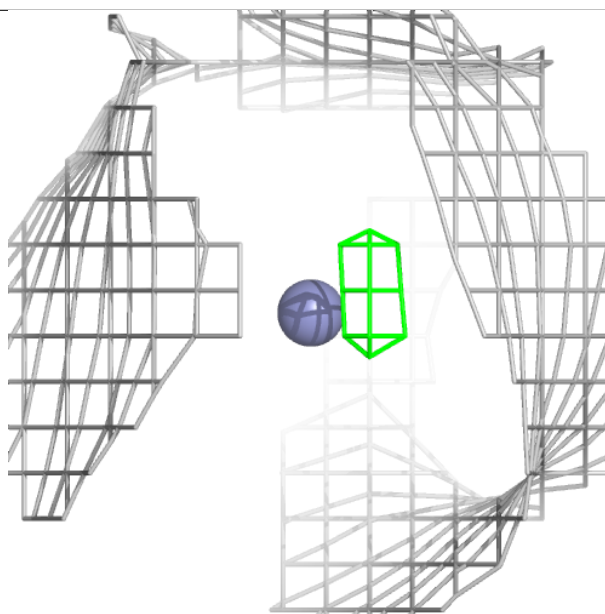
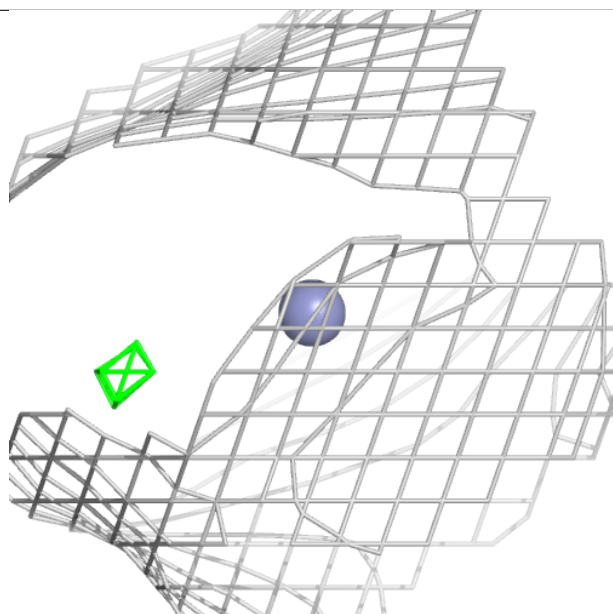
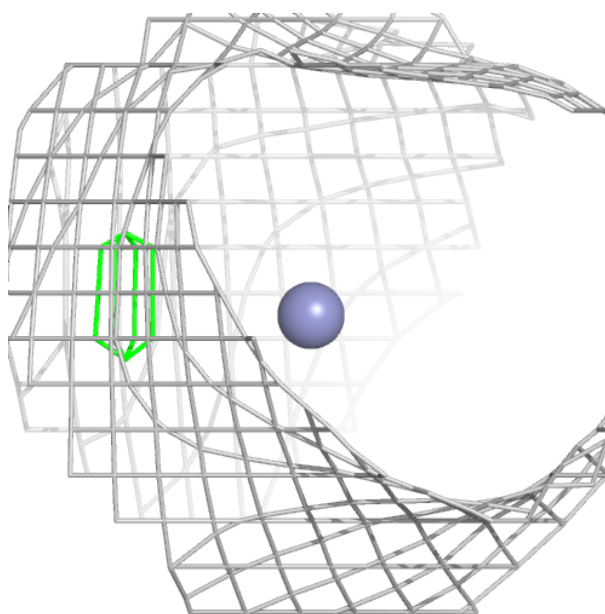
Electron density around ZN B 703:

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



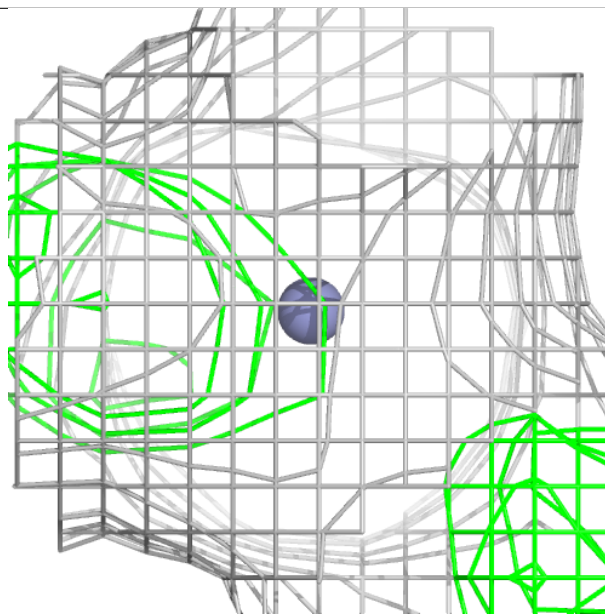
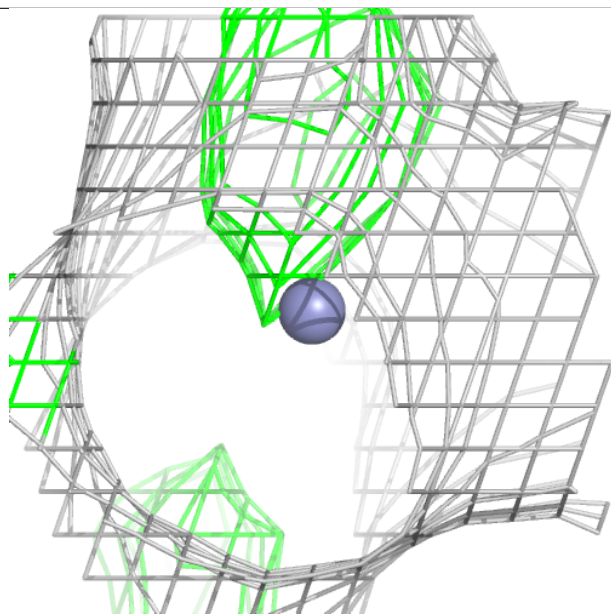
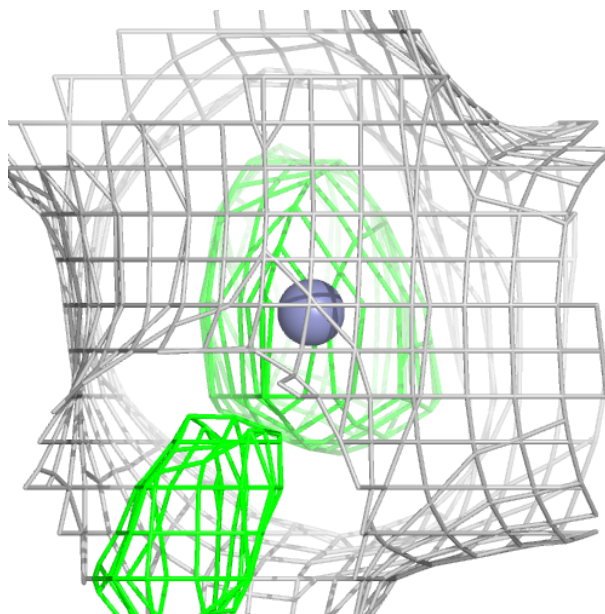
Electron density around ZN A 703:

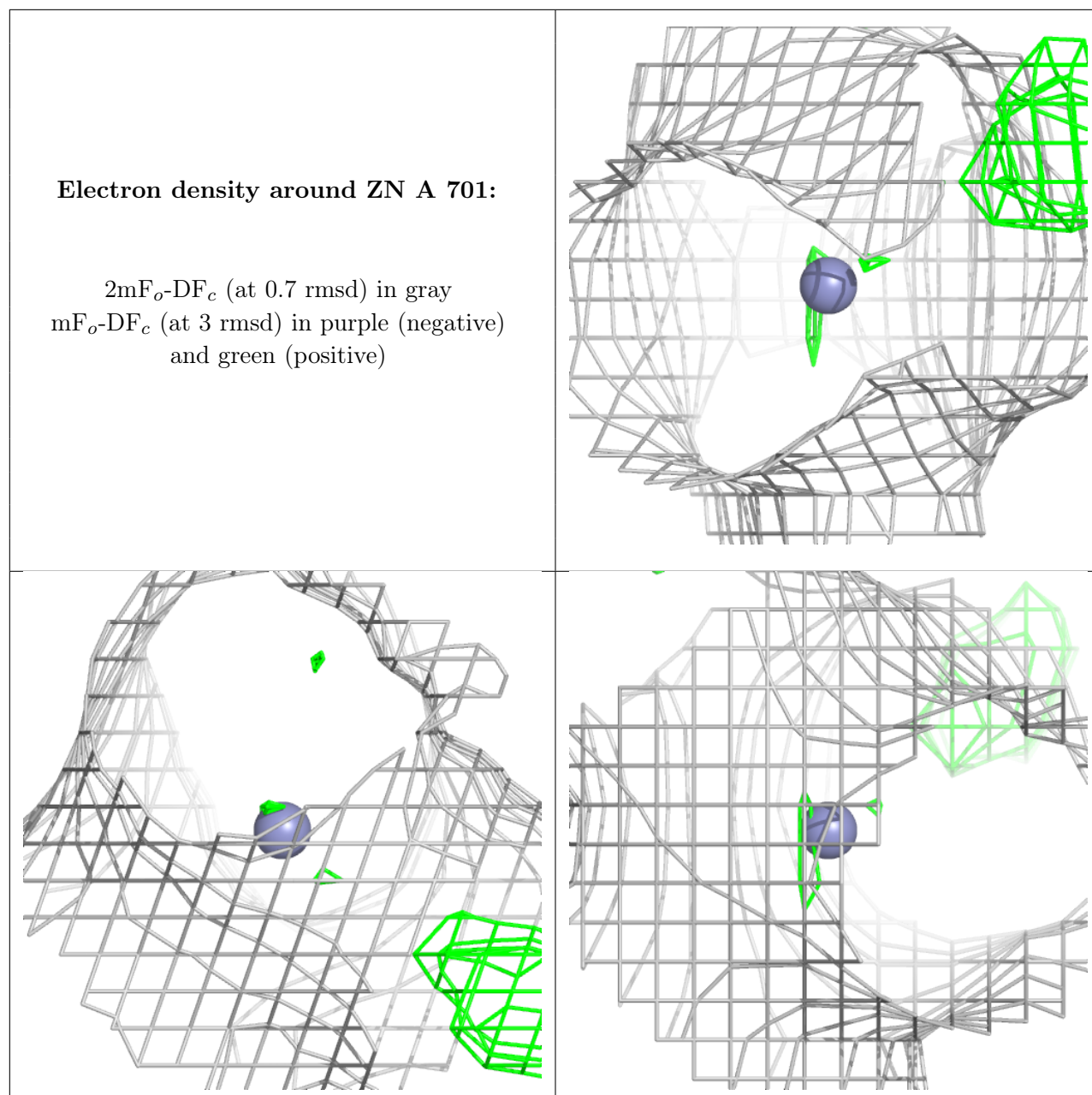
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 702:

$2mF_o-DF_c$ (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.