



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 02:32 AM BST

PDB ID : 6OZH
Title : Crystal structure of Ciona intestinalis (Ci) Endonuclease V in complex with a 24mer DNA containing an inosine followed by a ribo-adenosine
Authors : Samara, N.L.; Yang, W.
Deposited on : 2019-05-15
Resolution : 3.03 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

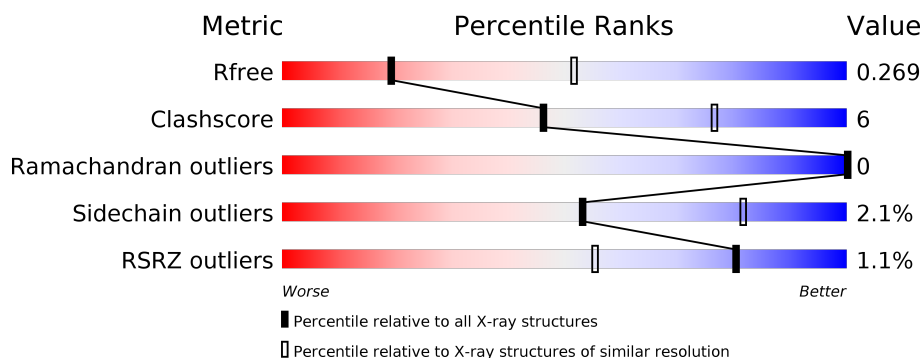
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	245	<div> <div>85%</div> <div>13%</div> <div>•</div> </div>
1	B	245	<div> <div>81%</div> <div>18%</div> <div>•</div> </div>
1	C	245	<div> <div>%</div> <div>79%</div> <div>18%</div> <div>•</div> </div>
1	D	245	<div> <div>84%</div> <div>13%</div> <div>•</div> </div>
2	E	24	<div> <div>46%</div> <div>33%</div> <div>21%</div> </div>
2	F	24	<div> <div>42%</div> <div>38%</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	24	<div><div></div><div>17%</div><div>54%</div><div>38%</div><div>8%</div></div>
2	H	24	<div><div></div><div>17%</div><div>54%</div><div>38%</div><div>8%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9267 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 endonuclease V isoform X2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	1	0
			1906	1218	325	354	9			
1	B	241	Total	C	N	O	S	0	0	0
			1904	1217	325	353	9			
1	C	239	Total	C	N	O	S	0	0	0
			1882	1200	321	352	9			
1	D	239	Total	C	N	O	S	0	1	0
			1883	1201	320	353	9			

- Molecule 2 is DNA/RNA hybrid called DNA/RNA (5'-D(P*CP*GP*GP*TP*AP*AP*CP*CP*GP*I)-R(P*A)-D(P*TP*AP*TP*GP*CP*AP*GP*CP*AP*TP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	19	Total	C	N	O	P	0	0	0
			390	186	71	114	19			
2	F	19	Total	C	N	O	P	0	0	0
			390	186	71	114	19			
2	G	22	Total	C	N	O	P	0	0	0
			452	215	81	134	22			
2	H	22	Total	C	N	O	P	0	0	0
			452	215	81	134	22			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	F	1	Total 1	Ca 1	0	0



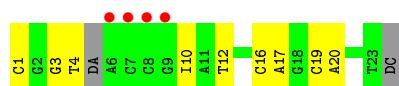
- Molecule 2: DNA/RNA (5'-D(P*CP*GP*GP*TP*AP*AP*CP*CP*GP*I)-R(P*A)-D(P*TP*A P*TP*GP*CP*AP*GP*CP*AP*TP*TP*TP*C)-3')



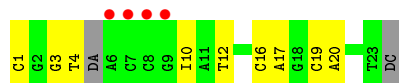
- Molecule 2: DNA/RNA (5'-D(P*CP*GP*GP*TP*AP*AP*CP*CP*GP*I)-R(P*A)-D(P*TP*A P*TP*GP*CP*AP*GP*CP*AP*TP*TP*TP*C)-3')



- Molecule 2: DNA/RNA (5'-D(P*CP*GP*GP*TP*AP*AP*CP*CP*GP*I)-R(P*A)-D(P*TP*A P*TP*GP*CP*AP*GP*CP*AP*TP*TP*TP*C)-3')



- Molecule 2: DNA/RNA (5'-D(P*CP*GP*GP*TP*AP*AP*CP*CP*GP*I)-R(P*A)-D(P*TP*A P*TP*GP*CP*AP*GP*CP*AP*TP*TP*TP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.25Å 121.97Å 79.92Å 90.00° 98.75° 90.00°	Depositor
Resolution (Å)	37.22 – 3.03 37.22 – 3.03	Depositor EDS
% Data completeness (in resolution range)	98.4 (37.22-3.03) 98.4 (37.22-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.233 , 0.269 0.233 , 0.269	Depositor DCC
R_{free} test set	1260 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 10.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9267	wwPDB-VP
Average B, all atoms (Å ²)	64.0	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 76.01 % 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 1.1315e-06. 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/1941	0.41	0/2607
1	B	0.25	0/1936	0.42	0/2600
1	C	0.25	0/1913	0.42	0/2570
1	D	0.25	0/1918	0.44	0/2579
2	E	0.53	0/412	0.96	0/631
2	F	0.52	0/412	0.96	0/631
2	G	0.59	0/480	0.99	0/734
2	H	0.60	0/480	0.97	0/734
All	All	0.33	0/9492	0.58	0/13086

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1906	0	1984	22	0
1	B	1904	0	1981	29	0
1	C	1882	0	1935	26	0
1	D	1883	0	1937	23	0
2	E	390	0	214	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	390	0	214	9	0
2	G	452	0	249	10	0
2	H	452	0	249	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
All	All	9267	0	8763	113	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 6.

The worst 5 of 113 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:C:17:GLN:HG3	1:C:127:CYS:HB3	1.68	0.76
1:A:129:ALA:H	2:E:10:DI:H1	1.39	0.70
1:B:129:ALA:H	2:F:10:DI:H1	1.40	0.69
1:B:177:ASP:OD1	1:B:189:LYS:NZ	2.27	0.66
1:A:177:ASP:OD1	1:A:189:LYS:NZ	2.28	0.66

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	240/245 (98%)	232 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	239/245 (98%)	229 (96%)	10 (4%)	0	100	100
1	C	235/245 (96%)	227 (97%)	8 (3%)	0	100	100
1	D	238/245 (97%)	228 (96%)	10 (4%)	0	100	100
All	All	952/980 (97%)	916 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	213/218 (98%)	211 (99%)	2 (1%)	78	92
1	B	212/218 (97%)	208 (98%)	4 (2%)	57	83
1	C	208/218 (95%)	199 (96%)	9 (4%)	29	64
1	D	209/218 (96%)	206 (99%)	3 (1%)	67	87
All	All	842/872 (97%)	824 (98%)	18 (2%)	53	81

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	LYS
1	C	73	THR
1	C	244	ILE
1	C	16	LYS
1	C	20	LEU

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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, 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	241/245 (98%)	-0.43	0 100 100	34, 50, 74, 90	0
1	B	241/245 (98%)	-0.44	0 100 100	37, 52, 72, 89	0
1	C	239/245 (97%)	-0.18	3 (1%) 77 51	40, 65, 98, 131	0
1	D	239/245 (97%)	-0.29	0 100 100	39, 56, 91, 102	0
2	E	18/24 (75%)	-0.14	0 100 100	43, 71, 152, 166	0
2	F	18/24 (75%)	-0.12	0 100 100	48, 68, 152, 158	0
2	G	21/24 (87%)	0.43	4 (19%) 1 0	52, 64, 159, 160	0
2	H	21/24 (87%)	0.36	4 (19%) 1 0	57, 63, 156, 157	0
All	All	1038/1076 (96%)	-0.30	11 (1%) 80 55	34, 56, 94, 166	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	7	DC	4.3
2	H	7	DC	3.9
2	G	8	DC	3.5
2	H	9	DG	3.2
2	G	9	DG	3.0

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

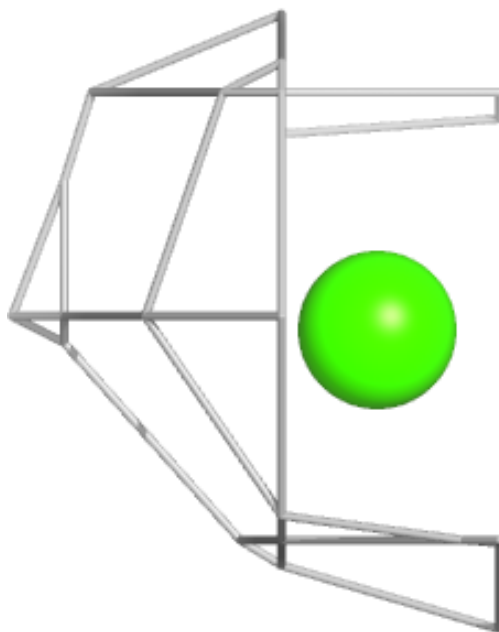
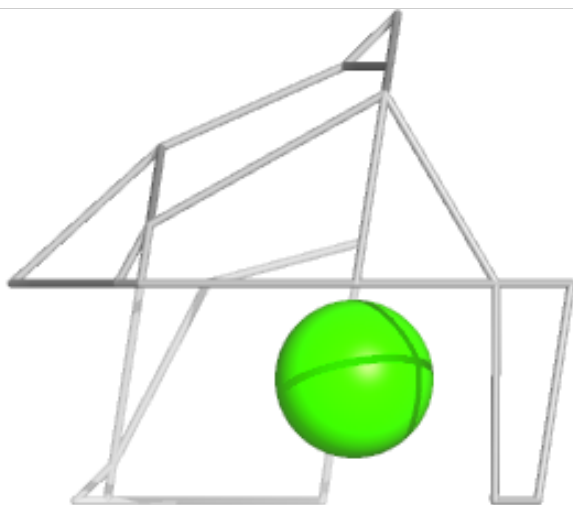
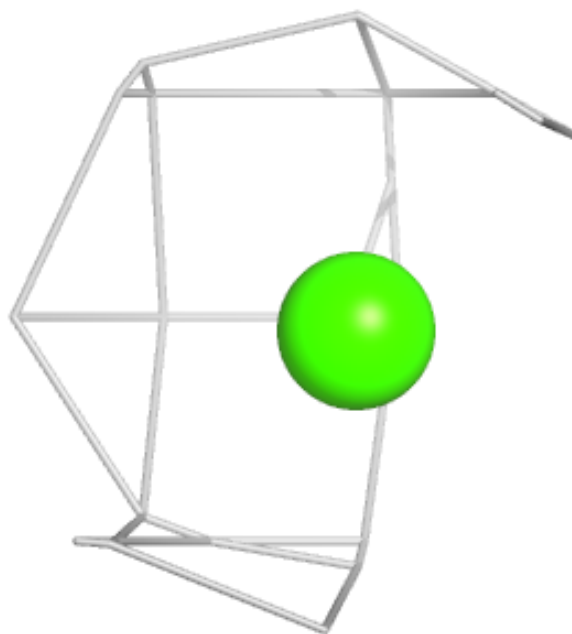
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CA	H	101	1/1	0.90	0.14	62,62,62,62	0
3	CA	E	101	1/1	0.90	0.17	52,52,52,52	0
3	CA	F	101	1/1	0.92	0.25	52,52,52,52	0
3	CA	A	301	1/1	0.94	0.18	46,46,46,46	0
3	CA	C	301	1/1	0.94	0.20	54,54,54,54	0
3	CA	G	101	1/1	0.95	0.20	59,59,59,59	0
3	CA	B	301	1/1	0.95	0.17	43,43,43,43	0
3	CA	D	301	1/1	0.95	0.20	48,48,48,48	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.

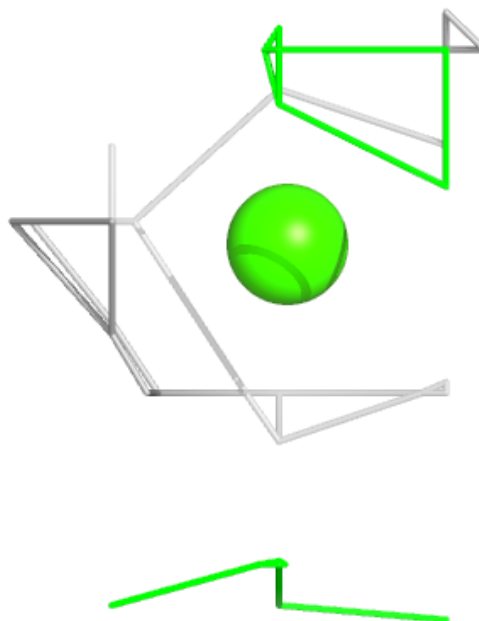
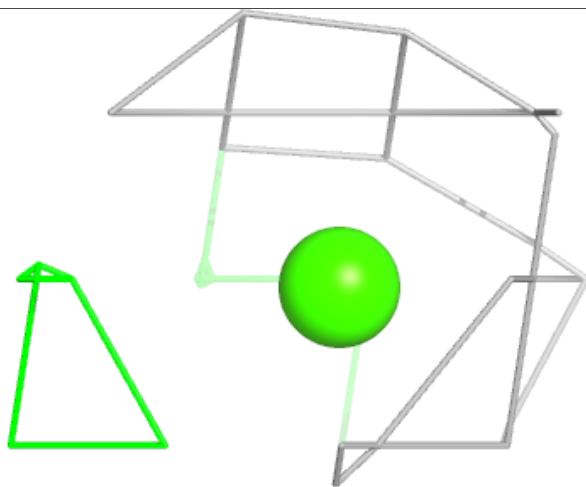
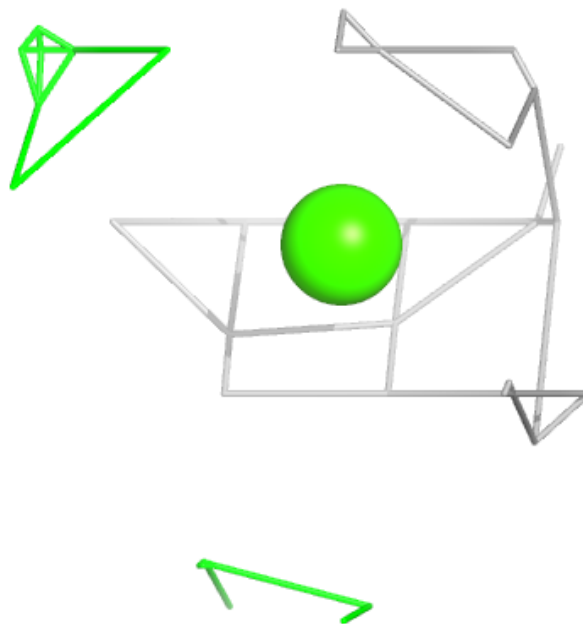
Electron density around CA H 101:

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



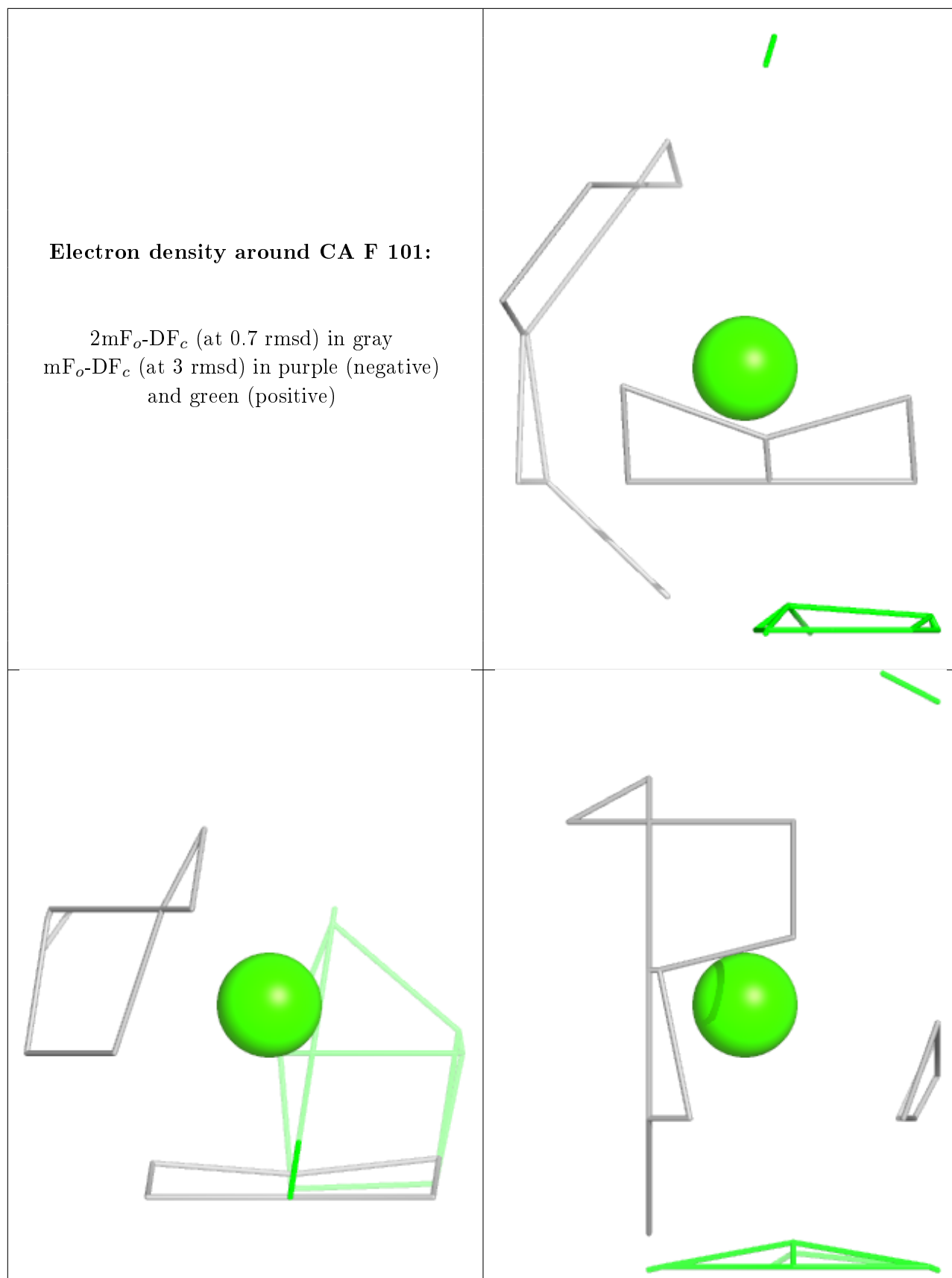
Electron density around CA E 101:

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



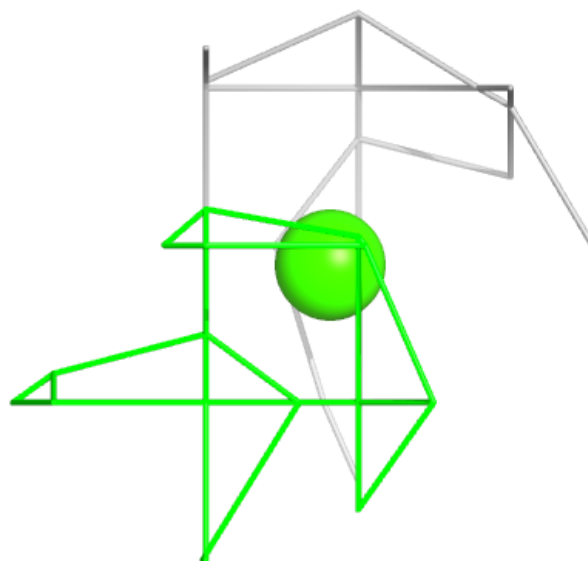
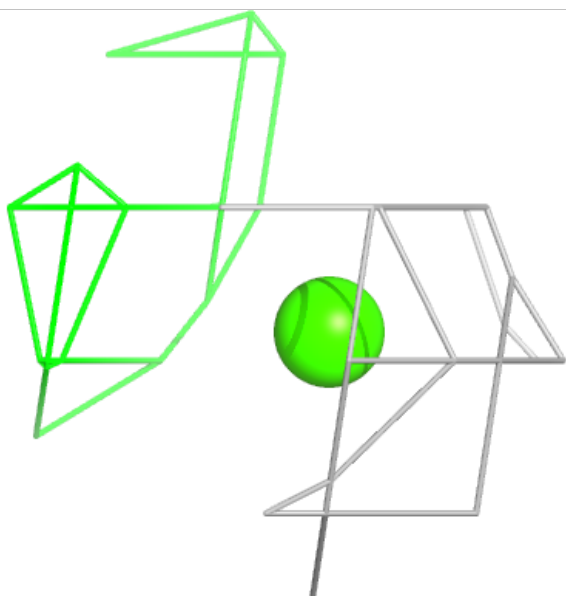
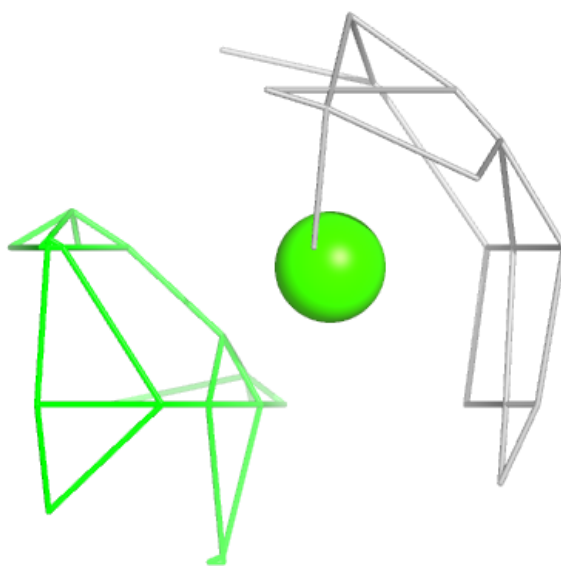
Electron density around CA F 101:

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



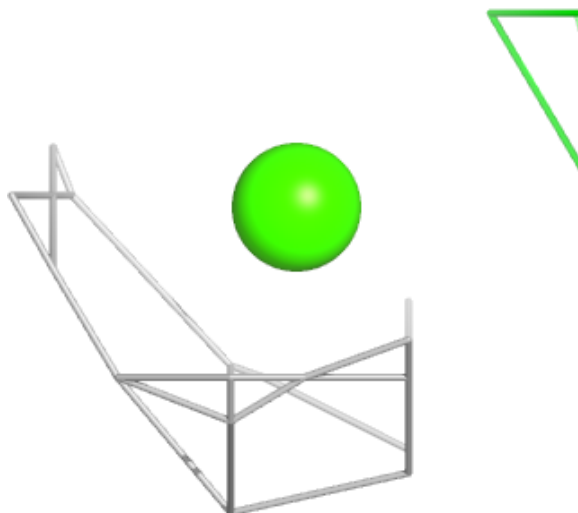
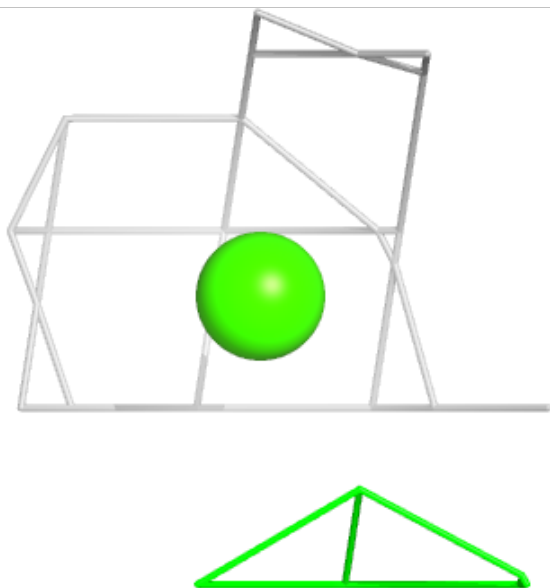
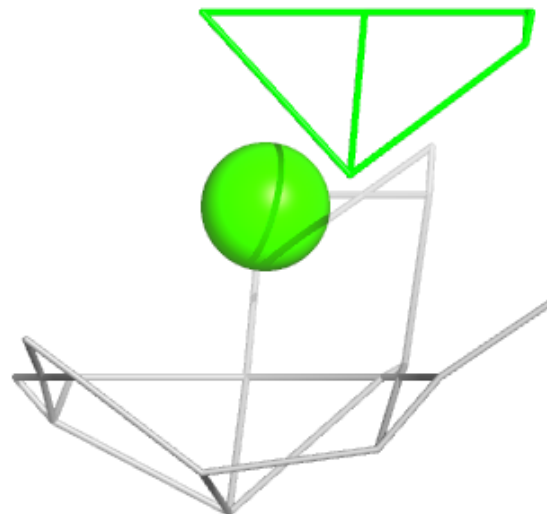
Electron density around CA A 301:

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



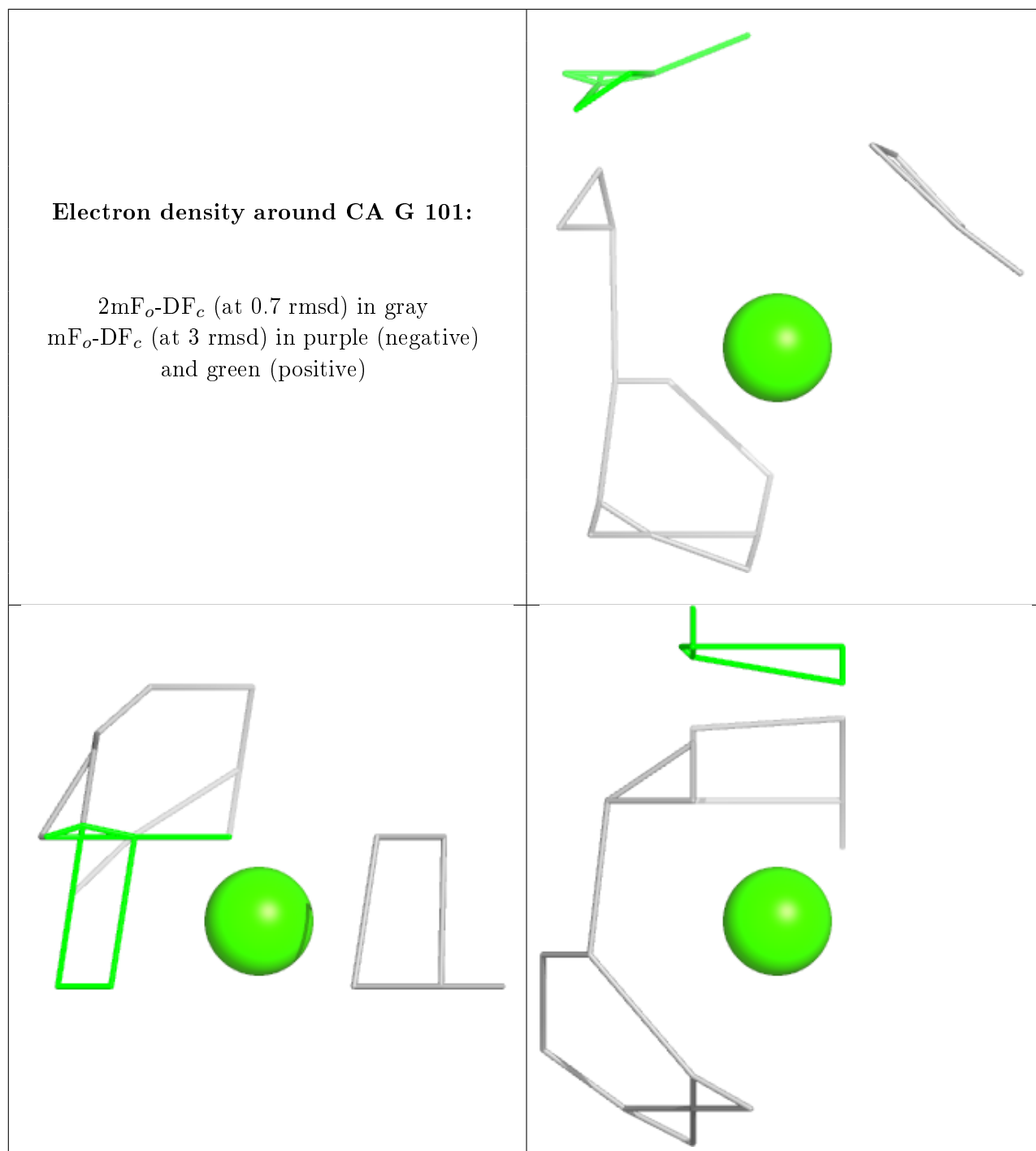
Electron density around CA C 301:

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



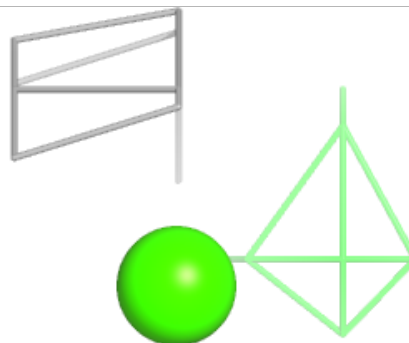
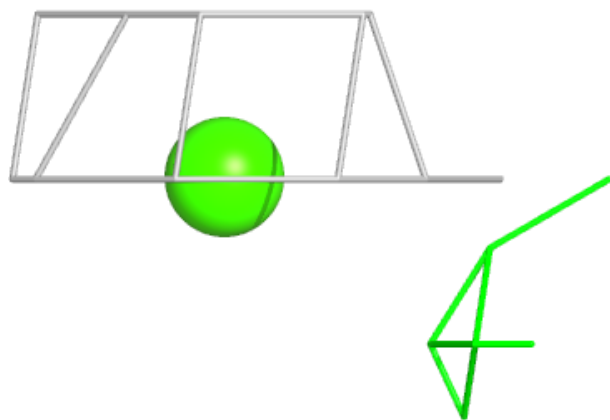
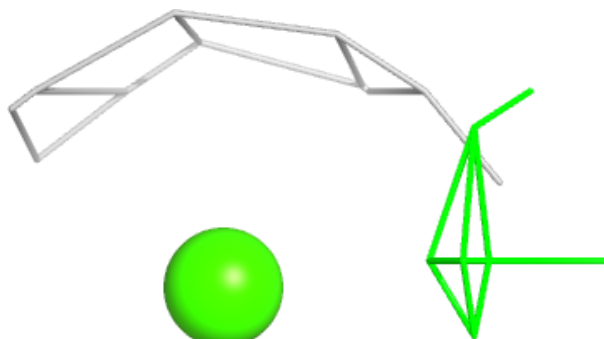
Electron density around CA G 101:

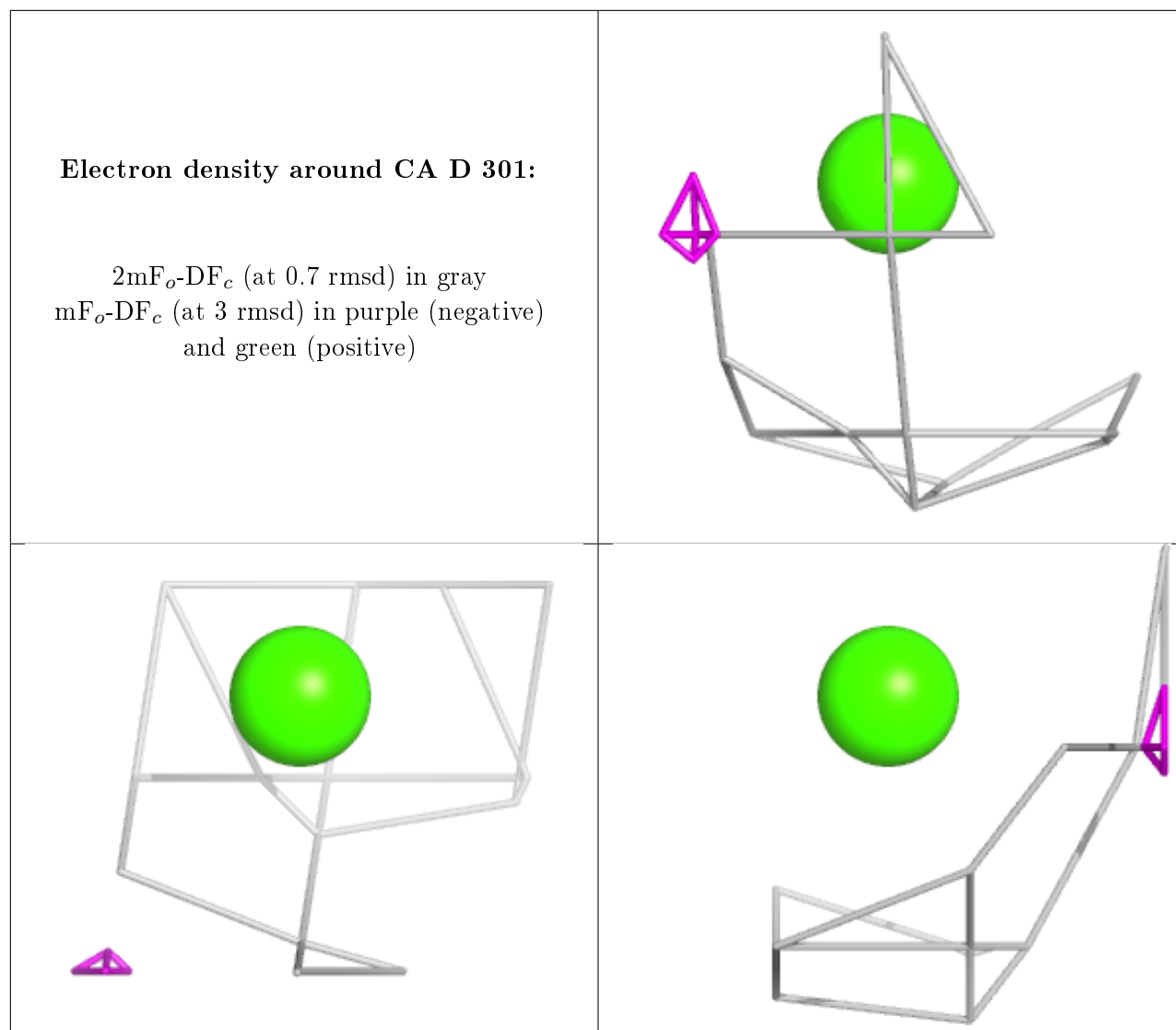
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 301:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.