Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 09:00 PM JST

PDB ID	:	7F9A
Title	:	Homo sapiens Prolyl-tRNA Synthetase (HsPRS) in Complex with L-proline and compound L97
Authors	:	Manickam, Y.; Malhotra, N.; Sharma, A.
Deposited on	:	2021-07-04
Resolution	:	2.00 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:

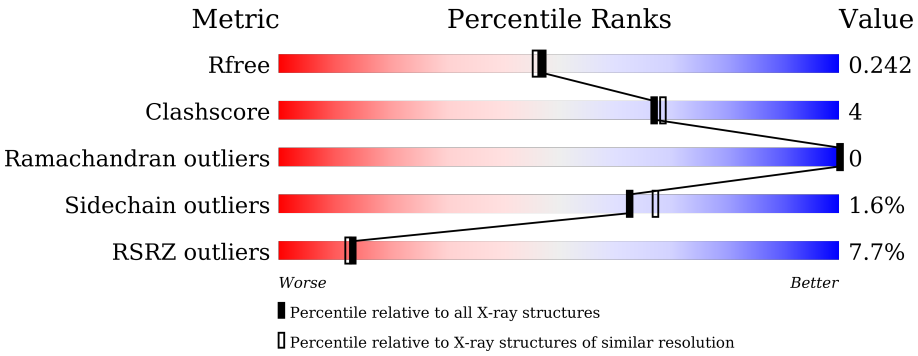
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	A	505	5% 90% 9% .
1	B	505	10% 84% 13% .

2 Entry composition

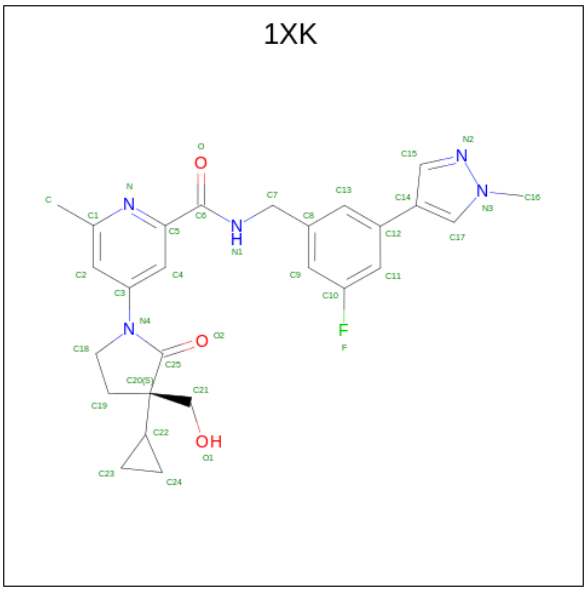
There are 7 unique types of molecules in this entry. The entry contains 8125 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional glutamate/proline--tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	2	0
			3941	2524	667	725	25			
1	B	488	Total	C	N	O	S	0	1	0
			3846	2466	645	710	25			

- Molecule 2 is 4-[(3S)-3-cyclopropyl-3-(hydroxymethyl)-2-oxidanylidene-pyrrolidin-1-yl]-N-[[3-fluoranyl-5-(1-methylpyrazol-4-yl)phenyl]methyl]-6-methyl-pyridine-2-carboxamide (three-letter code: 1XK) (formula: $C_{26}H_{28}FN_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			35	26	1	5	3		
2	B	1	Total	C	F	N	O	0	0
			35	26	1	5	3		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Inter-

est" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

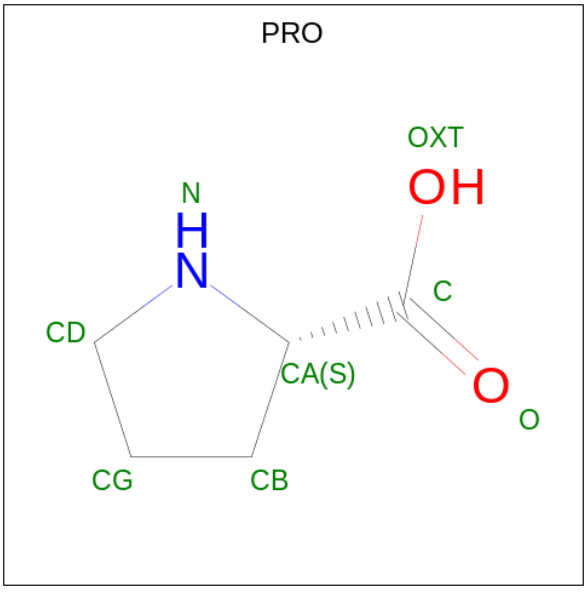
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total Ca 7 7	0	0
4	B	3	Total Ca 3 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Cl 3 3	0	0

- Molecule 6 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	5	1	2		
6	B	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 7 is water.

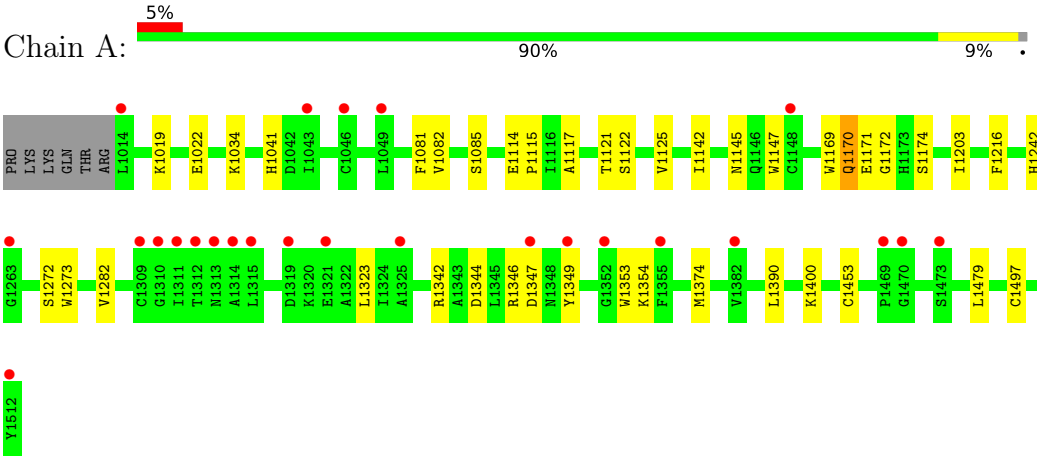
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	136	Total	O	0	1
			137	137		
7	B	100	Total	O	0	0
			100	100		

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.

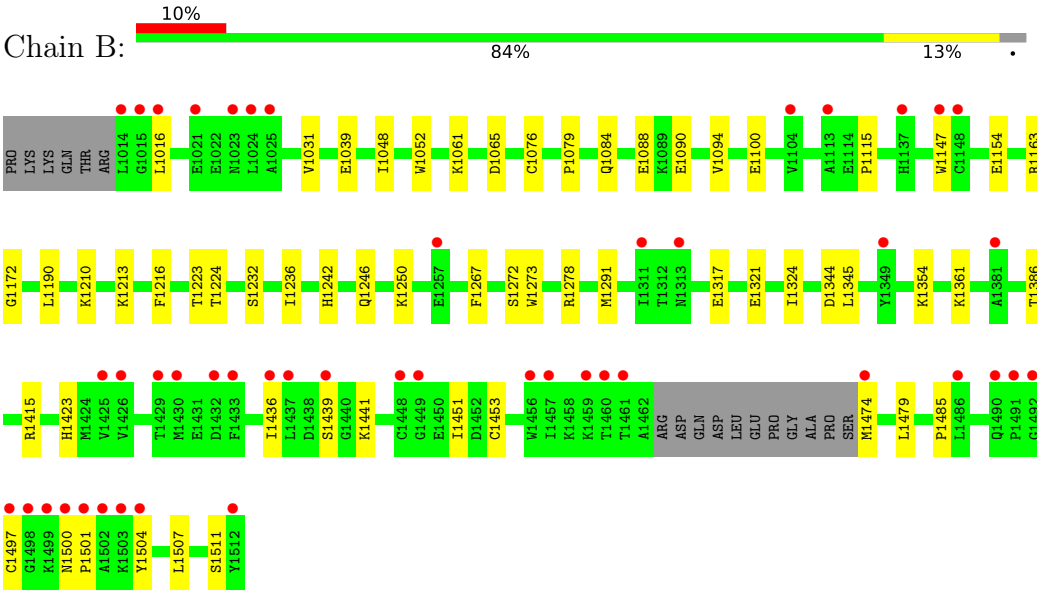
• Molecule 1: Bifunctional glutamate/proline--tRNA ligase

Chain A:



• Molecule 1: Bifunctional glutamate/proline--tRNA ligase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.74Å 105.92Å 145.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.93 – 2.00 59.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (59.93-2.00) 99.8 (59.93-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.15rc1_3423	Depositor
R, R_{free}	0.195 , 0.242 0.196 , 0.242	Depositor DCC
R_{free} test set	3728 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.3	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8125	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1XK, ZN, CA, CL

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	0.49	0/4044	0.60	0/5485
1	B	0.50	1/3943 (0.0%)	0.57	0/5352
All	All	0.49	1/7987 (0.0%)	0.59	0/10837

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1076	CYS	CB-SG	5.69	1.92	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3941	0	3846	25	0
1	B	3846	0	3739	37	0
2	A	35	0	0	0	0
2	B	35	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	7	0	0	0	0
4	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	3	0	0	1	0
6	A	8	0	7	1	0
6	B	8	0	7	0	0
7	A	137	0	0	0	0
7	B	100	0	0	1	0
All	All	8125	0	7599	60	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 4.

All (60) 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:B:1100:GLU:HG2	1:B:1154:GLU:HG2	1.58	0.84
1:B:1210:LYS:HE2	1:B:1224:THR:HG21	1.76	0.65
1:B:1423:HIS:HA	1:B:1441:LYS:HD3	1.80	0.63
1:A:1479:LEU:HD12	1:A:1507:LEU:HG	1.81	0.62
1:B:1500:ASN:HB3	1:B:1501:PRO:HD2	1.82	0.62
1:A:1344:ASP:O	1:A:1354:LYS:NZ	2.31	0.62
1:A:1082:VAL:HG22	1:A:1125:VAL:HG22	1.80	0.61
1:B:1163:ARG:NH2	7:B:2003:HOH:O	2.35	0.60
1:A:1216:PHE:HB2	1:A:1242:HIS:CE1	2.35	0.60
1:B:1436:ILE:O	1:B:1439:SER:HB3	2.05	0.57
1:B:1386:THR:HG22	1:B:1415:ARG:HH22	1.69	0.57
1:B:1494:LYS:HA	1:B:1501:PRO:HA	1.88	0.55
1:B:1479:LEU:HD12	1:B:1507:LEU:HG	1.89	0.55
1:A:1145:ASN:OD1	1:A:1170:GLN:HG2	2.08	0.54
1:A:1258:ASP:OD1	1:A:1259:PRO:HD2	2.07	0.54
1:A:1082:VAL:HG22	1:A:1125:VAL:CG2	2.38	0.53
1:A:1346:ARG:HH21	1:A:1353:TRP:HZ3	1.57	0.52
1:B:1016:LEU:HD11	1:B:1031:VAL:HG22	1.92	0.51
1:B:1216:PHE:HB2	1:B:1242:HIS:CE1	2.46	0.51
1:B:1147:TRP:CE3	1:B:1170:GLN:HB3	2.45	0.51
1:B:1061:LYS:O	1:B:1065:ASP:HB2	2.12	0.50
1:B:1236:ILE:HG12	1:B:1278:ARG:HD3	1.94	0.49
1:B:1324:ILE:HG23	1:B:1345:LEU:HD13	1.94	0.49
1:A:1019:LYS:HB2	1:A:1022:GLU:HG3	1.93	0.49
1:B:1317:GLU:O	1:B:1321:GLU:HG3	2.12	0.49
1:B:1088:GLU:HG3	1:B:1094:VAL:HG21	1.95	0.48
1:B:1213:LYS:HG3	1:B:1451:ILE:HG23	1.96	0.48
1:B:1495:CYS:SG	1:B:1496:VAL:N	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1052:TRP:CE2	1:B:1361:LYS:HB3	2.48	0.47
1:A:1034:LYS:HE3	5:A:1909:CL:CL	2.51	0.47
1:A:1147:TRP:CE3	1:A:1170:GLN:HB2	2.49	0.47
1:B:1190:LEU:HD22	1:B:1223:THR:HB	1.96	0.46
1:A:1172:GLY:O	1:A:1272:SER:HA	2.15	0.45
1:A:1114:GLU:HG2	1:A:1115:PRO:O	2.16	0.45
1:A:1453:CYS:SG	1:A:1497:CYS:HB3	2.55	0.45
1:B:1453:CYS:SG	1:B:1497:CYS:HB3	2.56	0.45
1:B:1423:HIS:O	1:B:1441:LYS:HB3	2.17	0.44
1:A:1323:LEU:HA	1:A:1374:MET:SD	2.58	0.43
1:B:1016:LEU:HD11	1:B:1031:VAL:CG2	2.48	0.43
1:A:1347:ASP:OD1	1:A:1347:ASP:N	2.50	0.43
1:B:1291:MET:HE3	1:B:1291:MET:HB3	1.93	0.43
1:B:1039:GLU:HB3	1:B:1048:ILE:HB	2.01	0.42
1:B:1246:GLN:O	1:B:1250:LYS:HG3	2.19	0.42
1:A:1041:HIS:CG	1:B:1079:PRO:HG2	2.54	0.42
1:B:1344:ASP:OD1	1:B:1354:LYS:HE2	2.19	0.42
1:B:1090:GLU:O	1:B:1094:VAL:HG12	2.19	0.42
1:B:1084:GLN:HE22	1:B:1115:PRO:HD2	1.84	0.42
1:B:1250:LYS:HA	1:B:1267:PHE:CE1	2.55	0.42
1:B:1172:GLY:O	1:B:1272:SER:HA	2.20	0.42
1:A:1122:SER:HB2	1:A:1171:GLU:OE1	2.20	0.41
1:B:1474:MET:HE1	1:B:1511:SER:O	2.20	0.41
1:A:1041:HIS:CD2	1:B:1079:PRO:HG2	2.55	0.41
1:B:1439:SER:OG	1:B:1441:LYS:HE2	2.19	0.41
1:A:1121:THR:HG1	6:A:1913:PRO:N	2.19	0.41
1:A:1203:ILE:HD13	1:A:1282:VAL:HG12	2.01	0.41
1:A:1390:LEU:HD13	1:A:1400:LYS:HE3	2.03	0.41
1:A:1081:PHE:HA	1:A:1117:ALA:O	2.21	0.41
1:A:1142:ILE:O	1:A:1174:SER:HA	2.21	0.41
1:A:1346:ARG:HG3	1:A:1349:TYR:HD2	1.86	0.41
1:B:1016:LEU:HA	1:B:1016:LEU:HD23	1.82	0.40

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	499/505 (99%)	491 (98%)	8 (2%)	0	100	100
1	B	485/505 (96%)	478 (99%)	7 (1%)	0	100	100
All	All	984/1010 (97%)	969 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/435 (95%)	406 (98%)	6 (2%)	65	69
1	B	403/435 (93%)	396 (98%)	7 (2%)	60	65
All	All	815/870 (94%)	802 (98%)	13 (2%)	62	67

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1085	SER
1	A	1169	TRP
1	A	1170	GLN
1	A	1273	TRP
1	A	1342	ARG
1	A	1504	TYR
1	B	1169	TRP
1	B	1170	GLN
1	B	1232	SER
1	B	1273	TRP
1	B	1400	LYS
1	B	1485	PRO
1	B	1504	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1093	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 15 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	1XK	A	1901	-	35,39,39	0.34	0	46,58,58	0.77	2 (4%)
2	1XK	B	1901	-	35,39,39	0.35	0	46,58,58	0.76	1 (2%)
6	PRO	A	1913	-	8,8,8	0.86	1 (12%)	10,10,10	1.36	2 (20%)
6	PRO	B	1906	-	8,8,8	0.80	0	10,10,10	1.34	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1XK	A	1901	-	-	0/24/44/44	0/5/5/5
2	1XK	B	1901	-	-	4/24/44/44	0/5/5/5
6	PRO	A	1913	-	-	2/4/11/11	0/1/1/1
6	PRO	B	1906	-	-	0/4/11/11	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1913	PRO	OXT-C	-2.06	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1901	1XK	C3-N4-C25	3.18	128.96	126.30
6	A	1913	PRO	OXT-C-CA	2.55	121.89	113.40
6	B	1906	PRO	OXT-C-O	-2.51	118.40	124.09
6	A	1913	PRO	OXT-C-O	-2.39	118.66	124.09
2	A	1901	1XK	C18-N4-C3	-2.24	117.54	120.76
6	B	1906	PRO	OXT-C-CA	2.18	120.64	113.40
2	A	1901	1XK	C2-C3-N4	2.09	122.84	119.85

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1901	1XK	C19-C20-C21-O1
2	B	1901	1XK	C22-C20-C21-O1
2	B	1901	1XK	C25-C20-C21-O1
2	B	1901	1XK	C25-C20-C22-C24
6	A	1913	PRO	O-C-CA-CB
6	A	1913	PRO	OXT-C-CA-CB

There are no ring outliers.

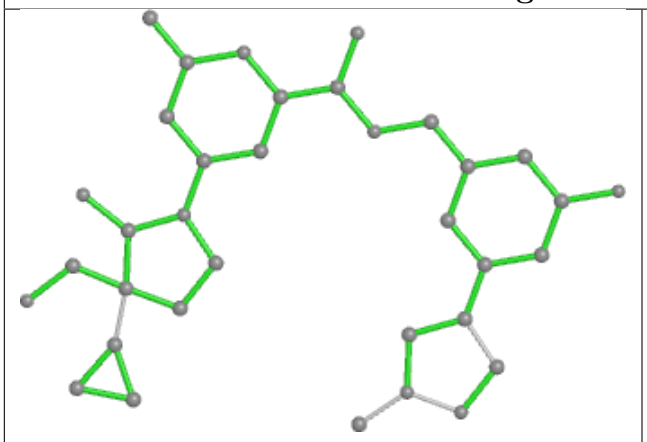
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1913	PRO	1	0

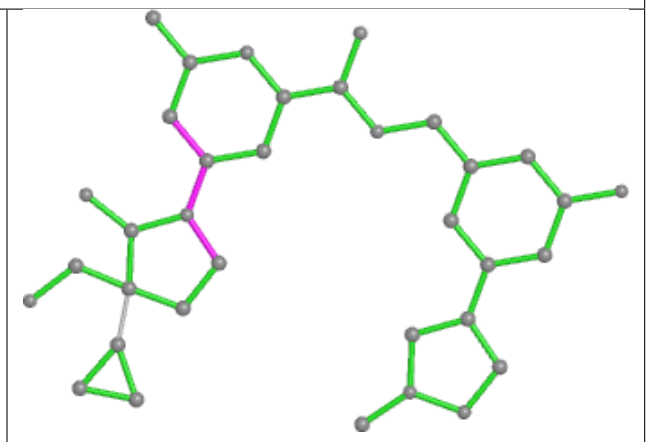
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

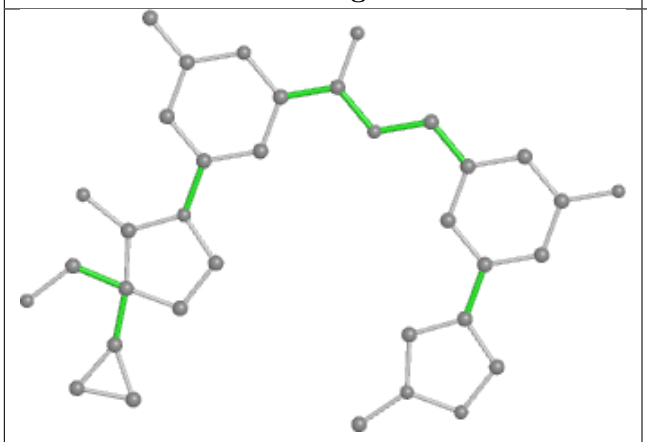
Ligand 1XK A 1901



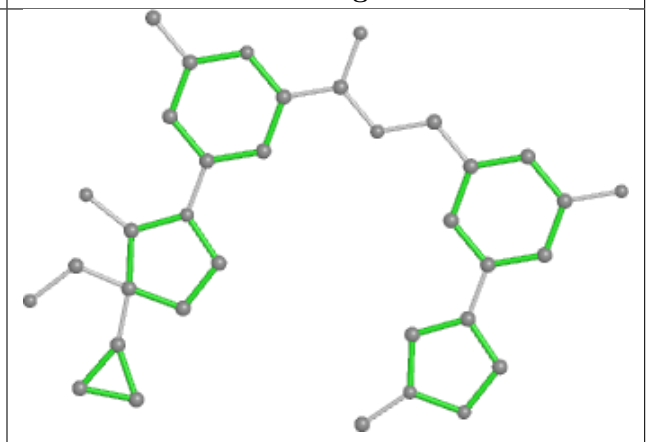
Bond lengths



Bond angles

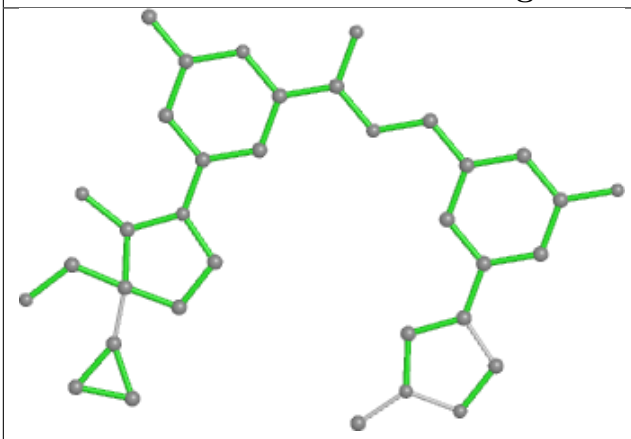


Torsions

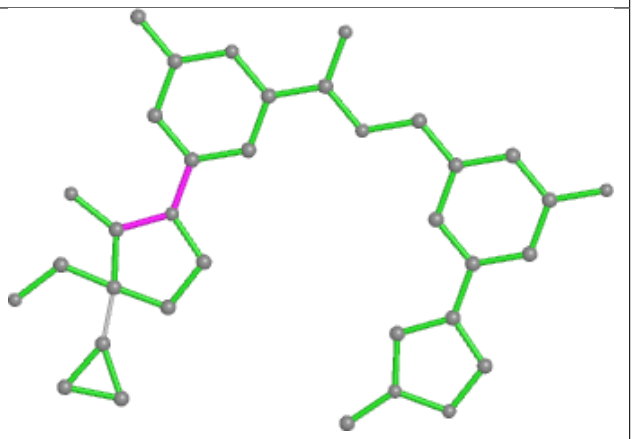


Rings

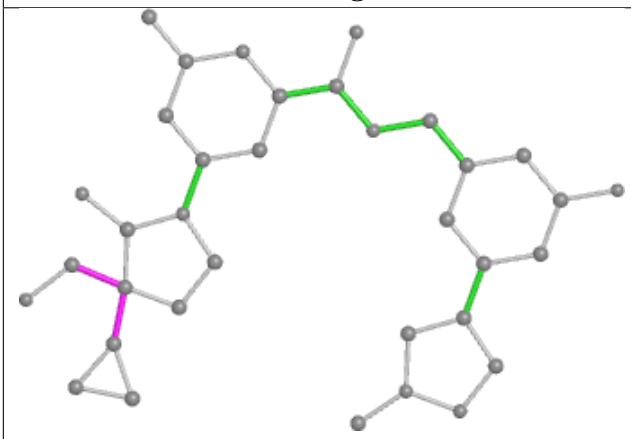
Ligand 1XK B 1901



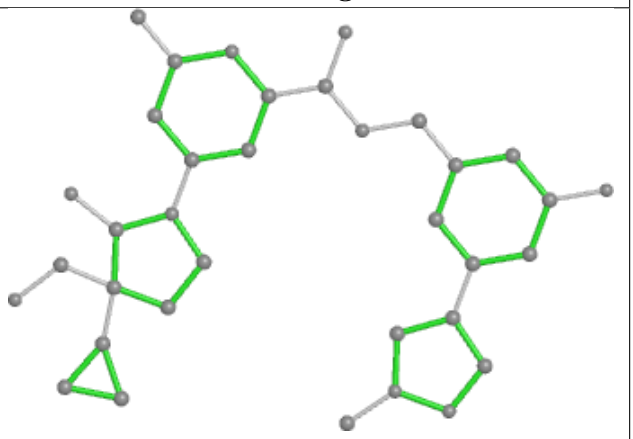
Bond lengths



Bond angles



Torsions



Rings

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	A	499/505 (98%)	0.56	27 (5%) 25 24	40, 56, 92, 126	0
1	B	488/505 (96%)	0.83	49 (10%) 7 6	42, 61, 96, 140	0
All	All	987/1010 (97%)	0.69	76 (7%) 13 12	40, 58, 95, 140	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1497	CYS	7.2
1	A	1315	LEU	6.6
1	A	1314	ALA	6.5
1	B	1498	GLY	6.3
1	B	1491	PRO	6.2
1	B	1504	TYR	5.6
1	B	1501	PRO	5.5
1	B	1461	THR	5.4
1	B	1460	THR	4.7
1	B	1432	ASP	4.7
1	B	1436	ILE	4.6
1	B	1512	TYR	4.3
1	B	1496	VAL	4.3
1	A	1313	ASN	4.2
1	B	1499	LYS	4.1
1	B	1500	ASN	4.1
1	B	1349	TYR	4.0
1	A	1259	PRO	4.0
1	B	1425	VAL	3.9
1	B	1492	GLY	3.9
1	A	1312	THR	3.7
1	B	1433	PHE	3.7
1	A	1311	ILE	3.7
1	B	1456	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	1490	GLN	3.4
1	B	1457	ILE	3.3
1	A	1263	GLY	3.2
1	B	1437	LEU	3.1
1	B	1448	CYS	3.1
1	B	1459	LYS	3.1
1	B	1429	THR	3.1
1	B	1023	ASN	3.0
1	A	1046	CYS	3.0
1	A	1148	CYS	3.0
1	B	1439	SER	2.9
1	B	1449	GLY	2.9
1	B	1502	ALA	2.9
1	A	1512	TYR	2.9
1	B	1147	TRP	2.9
1	A	1014	LEU	2.9
1	A	1347	ASP	2.8
1	B	1113	ALA	2.7
1	B	1474	MET	2.7
1	B	1313	ASN	2.6
1	A	1473	SER	2.6
1	A	1309	CYS	2.6
1	B	1381	ALA	2.6
1	B	1430	MET	2.6
1	B	1311	ILE	2.6
1	A	1319	ASP	2.6
1	A	1349	TYR	2.4
1	B	1015	GLY	2.4
1	A	1469	PRO	2.4
1	A	1325	ALA	2.3
1	A	1352	GLY	2.3
1	B	1016	LEU	2.3
1	A	1504	TYR	2.3
1	B	1137[A]	HIS	2.3
1	A	1382	VAL	2.2
1	A	1049	LEU	2.2
1	B	1148	CYS	2.2
1	B	1389	LYS	2.2
1	B	1014	LEU	2.2
1	A	1310	GLY	2.2
1	A	1043	ILE	2.1
1	B	1021	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1321	GLU	2.1
1	B	1503	LYS	2.1
1	A	1355	PHE	2.1
1	B	1024	LEU	2.1
1	B	1486	LEU	2.1
1	B	1025	ALA	2.1
1	B	1104	VAL	2.1
1	B	1257	GLU	2.0
1	B	1426	VAL	2.0
1	A	1470	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	A	1908	1/1	0.58	0.16	104,104,104,104	0
4	CA	B	1903	1/1	0.79	0.10	96,96,96,96	0
5	CL	A	1910	1/1	0.80	0.11	97,97,97,97	0
4	CA	A	1903	1/1	0.86	0.07	63,63,63,63	1
4	CA	B	1904	1/1	0.89	0.08	112,112,112,112	0
4	CA	A	1911	1/1	0.89	0.08	79,79,79,79	0
4	CA	A	1905	1/1	0.91	0.06	86,86,86,86	0
4	CA	A	1907	1/1	0.93	0.10	97,97,97,97	0
4	CA	A	1904	1/1	0.93	0.06	71,71,71,71	0
2	1XK	A	1901	35/35	0.93	0.13	39,48,72,75	0
4	CA	B	1905	1/1	0.94	0.04	110,110,110,110	0
2	1XK	B	1901	35/35	0.94	0.15	42,49,67,70	0
6	PRO	B	1906	8/8	0.94	0.20	33,47,52,54	0

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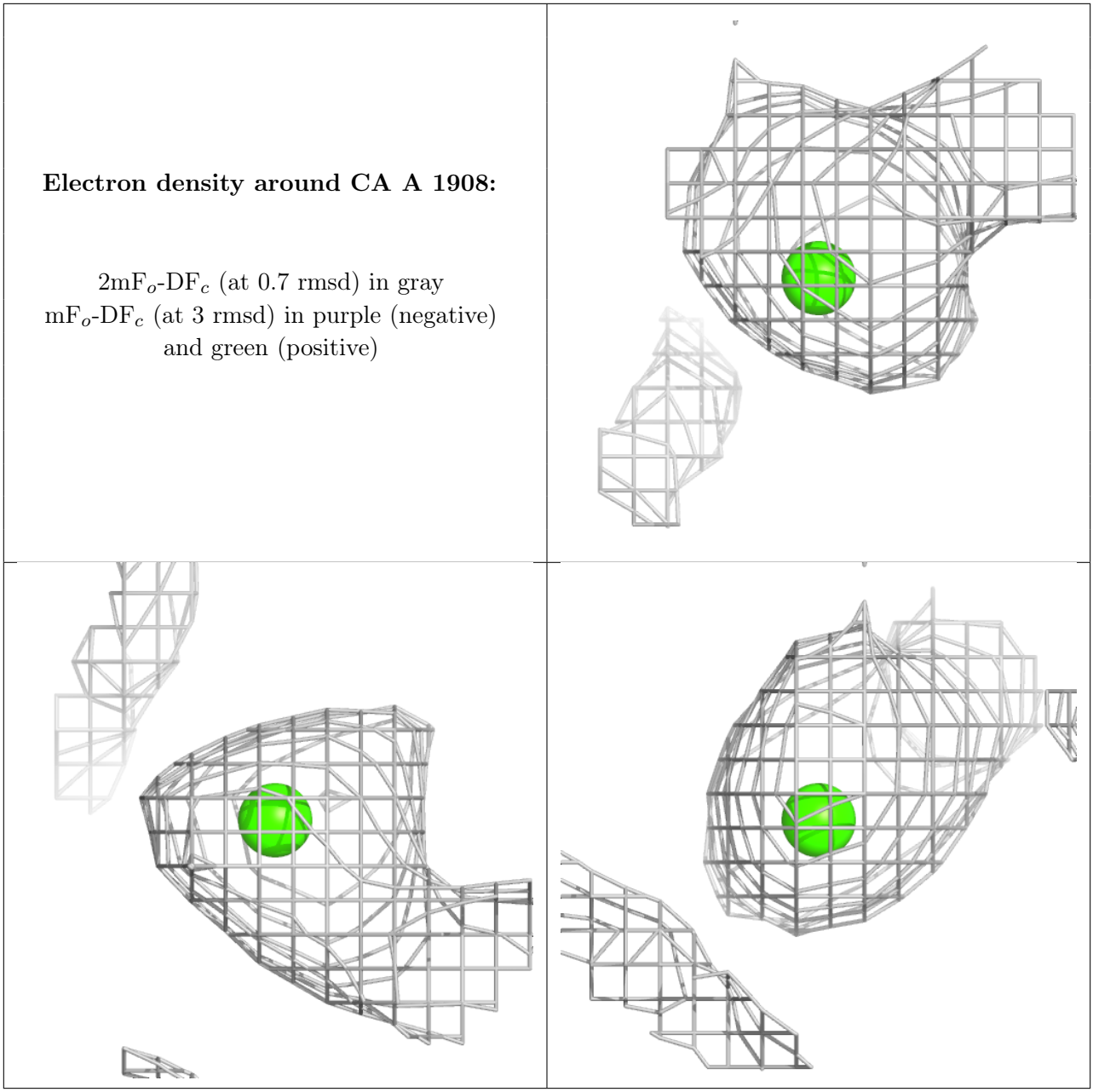
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	B	1902	1/1	0.96	0.06	79,79,79,79	1
5	CL	A	1909	1/1	0.96	0.13	57,57,57,57	1
4	CA	A	1906	1/1	0.97	0.19	82,82,82,82	1
6	PRO	A	1913	8/8	0.98	0.14	35,39,41,49	0
3	ZN	A	1902	1/1	0.99	0.11	48,48,48,48	1
5	CL	A	1912	1/1	0.99	0.15	58,58,58,58	1

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.

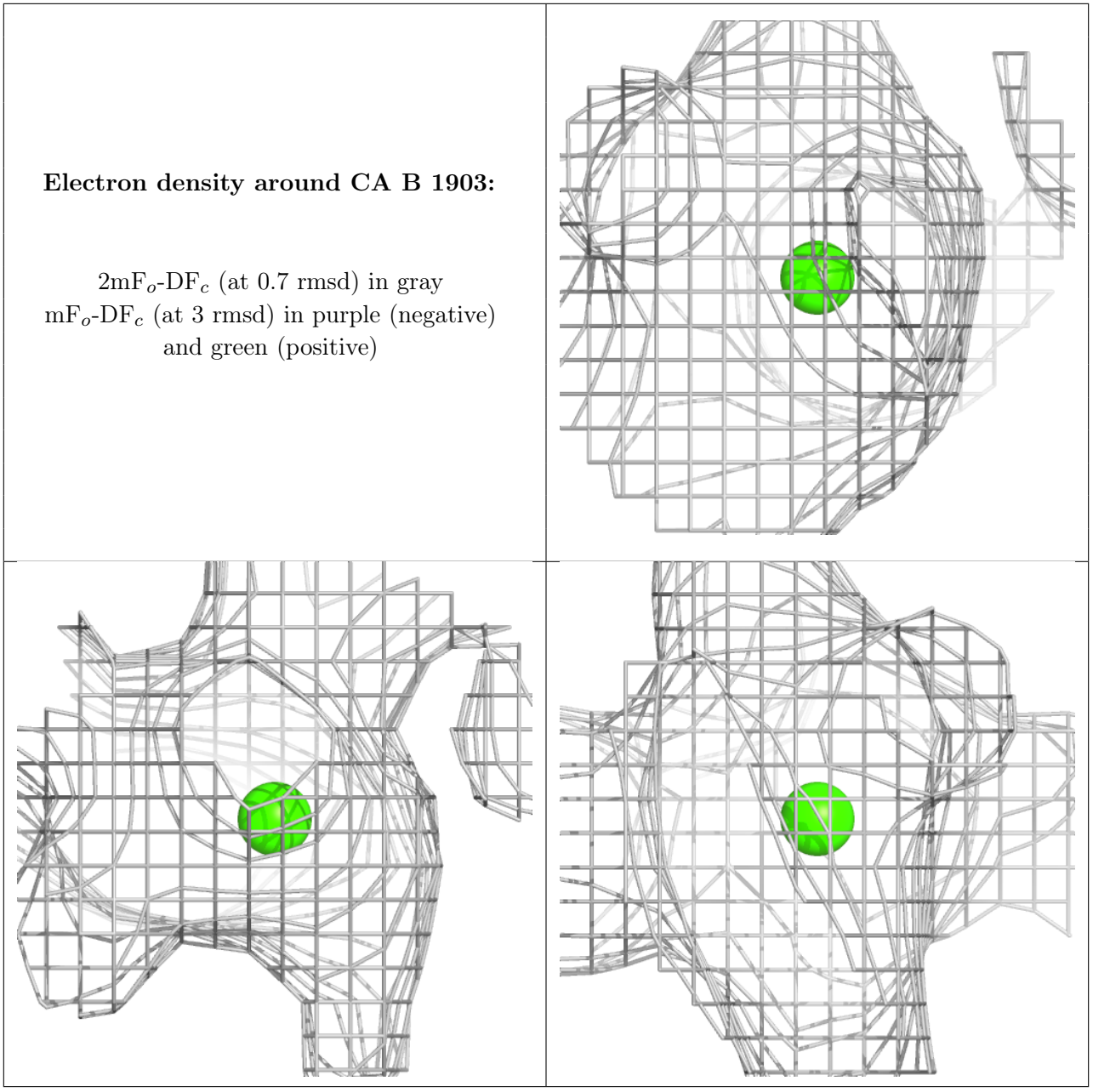
Electron density around CA A 1908:

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



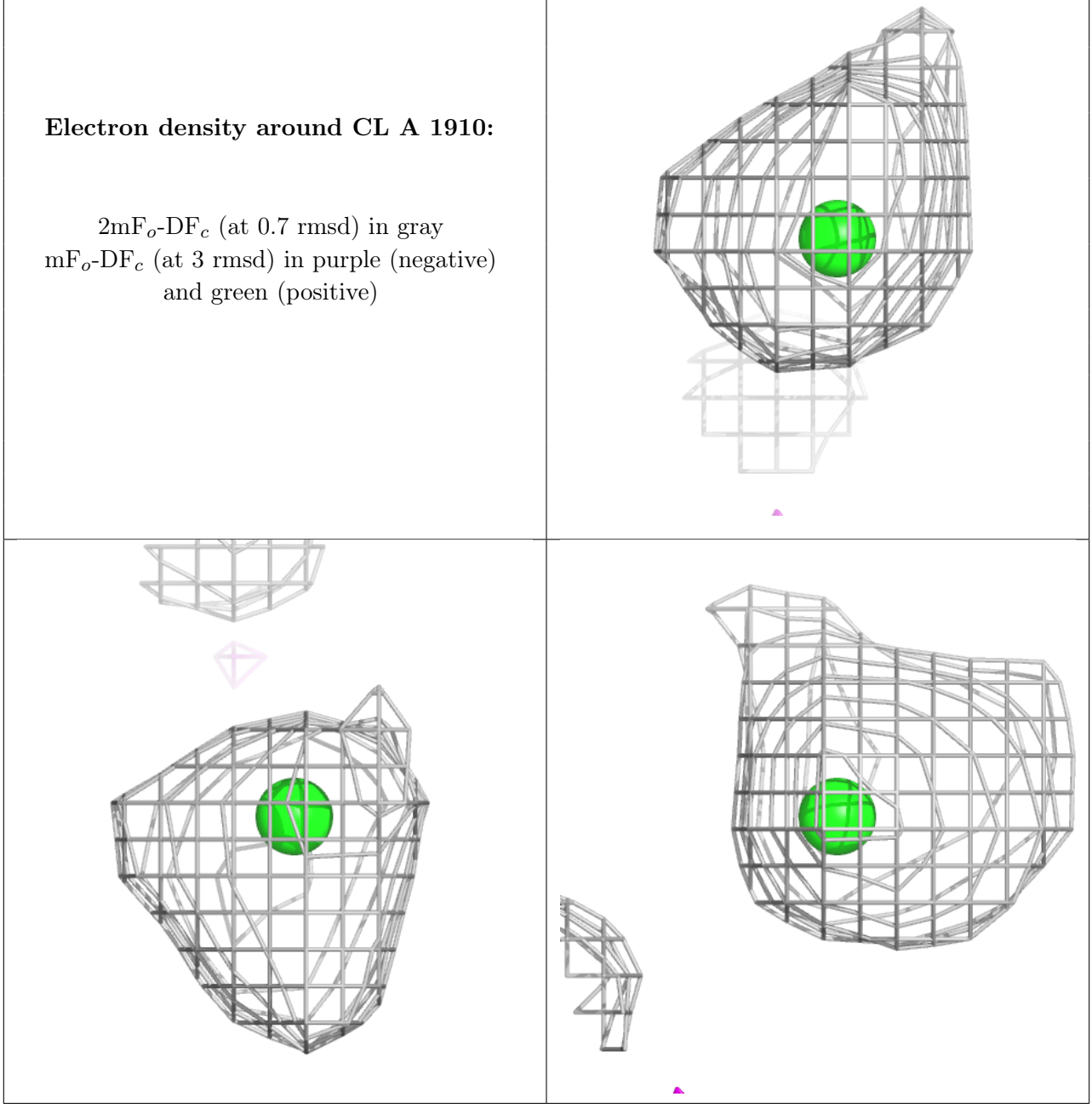
Electron density around CA B 1903:

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



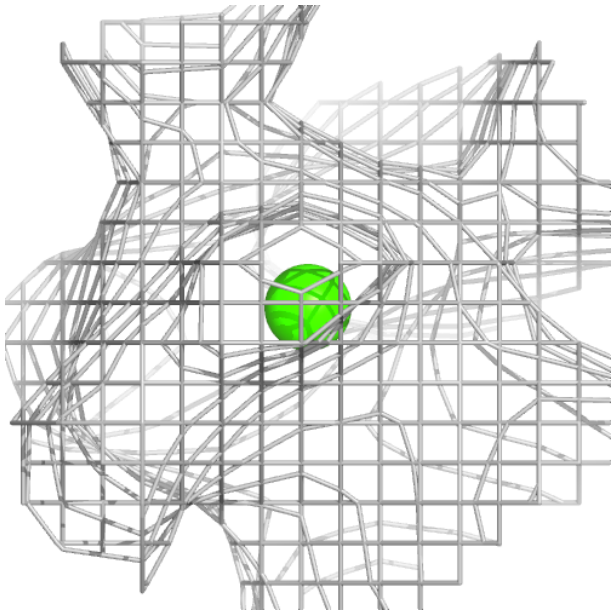
Electron density around CL A 1910:

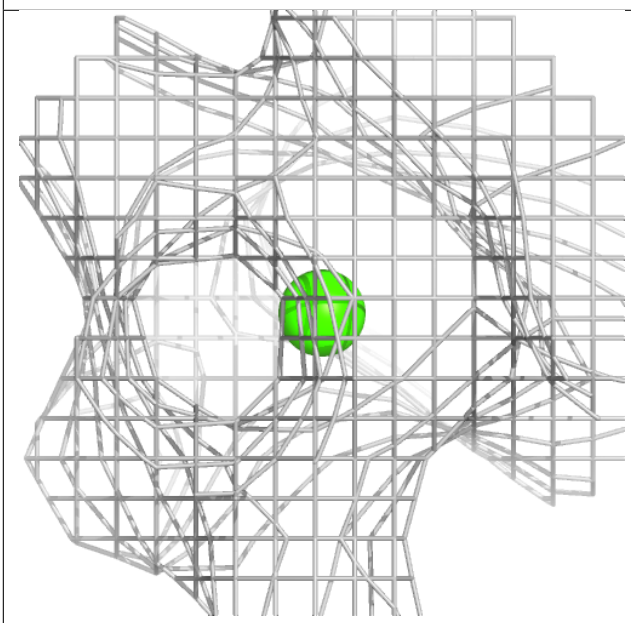
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

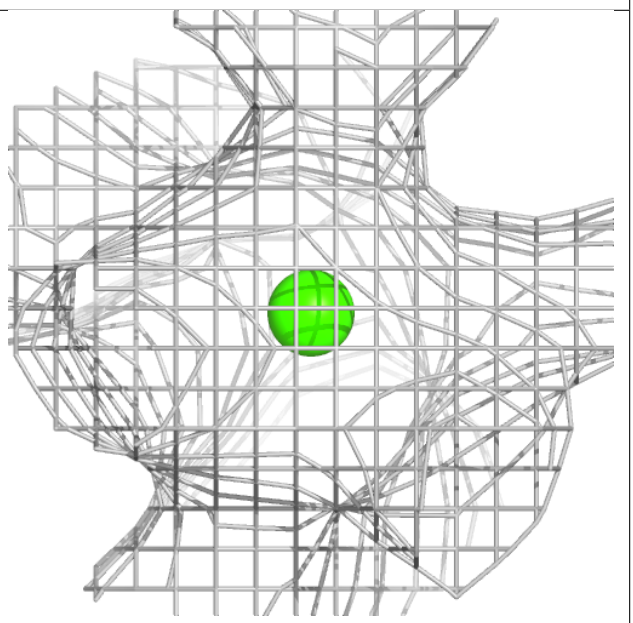


Electron density around CA A 1903:

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

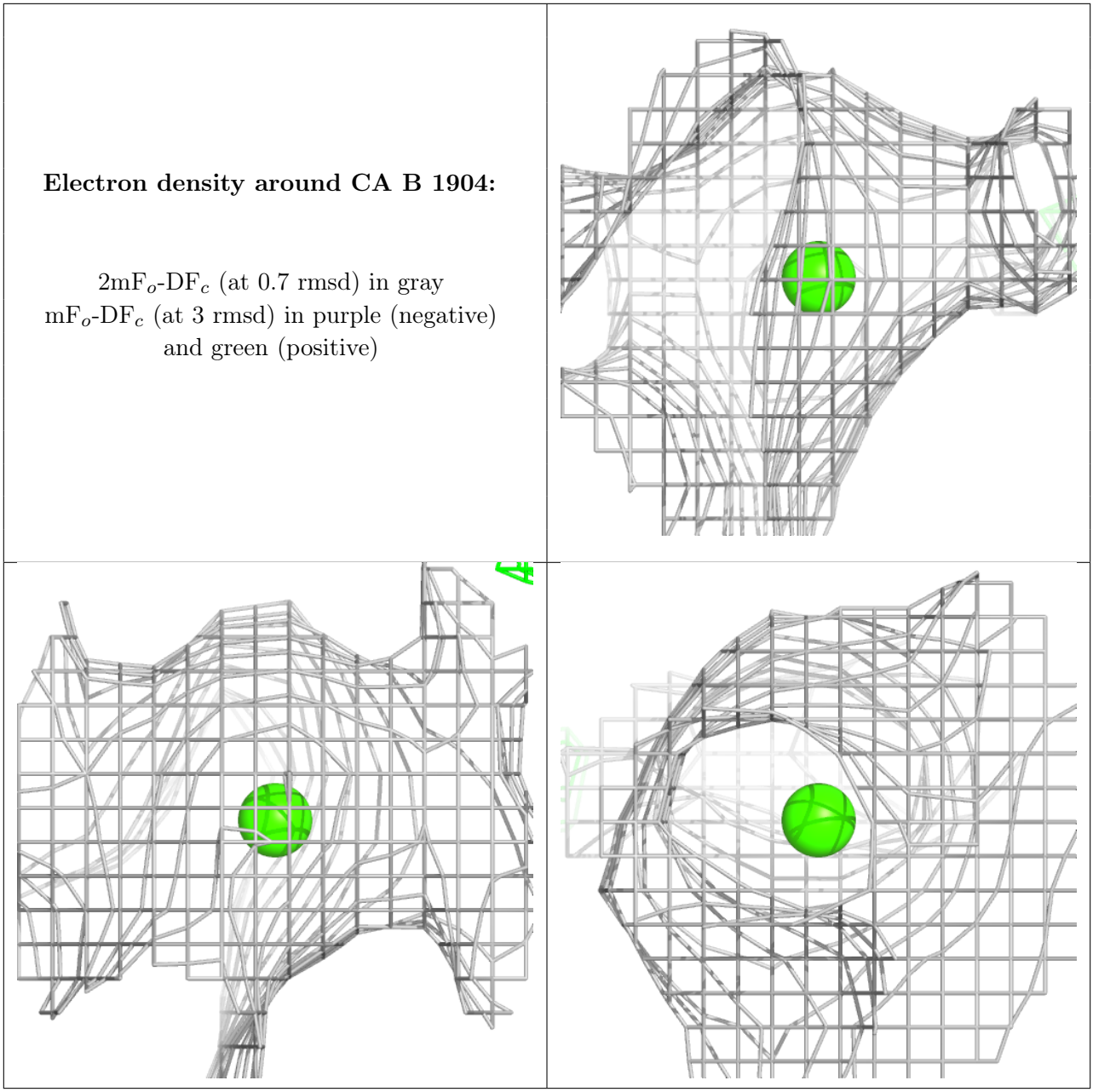






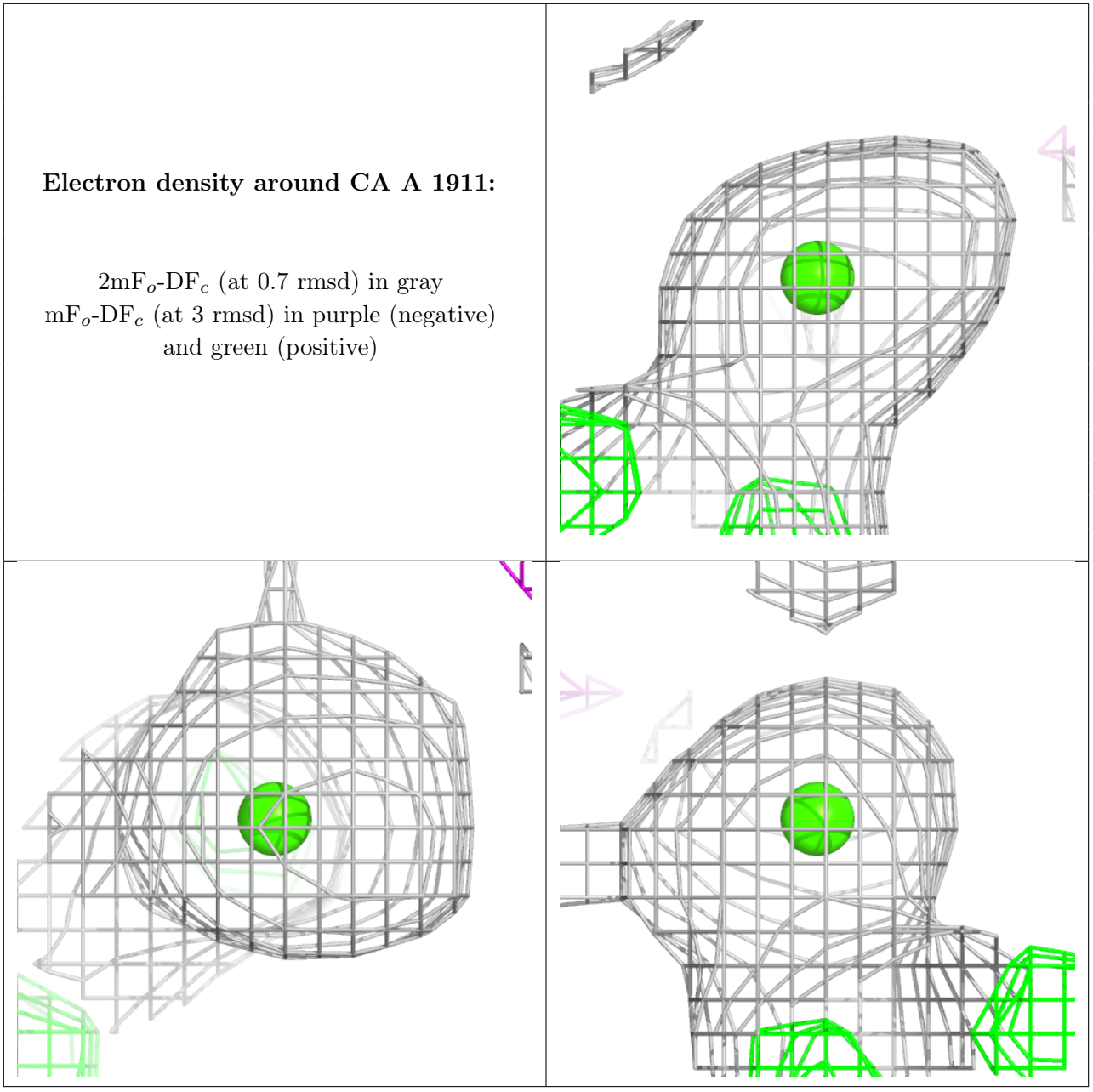
Electron density around CA B 1904:

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



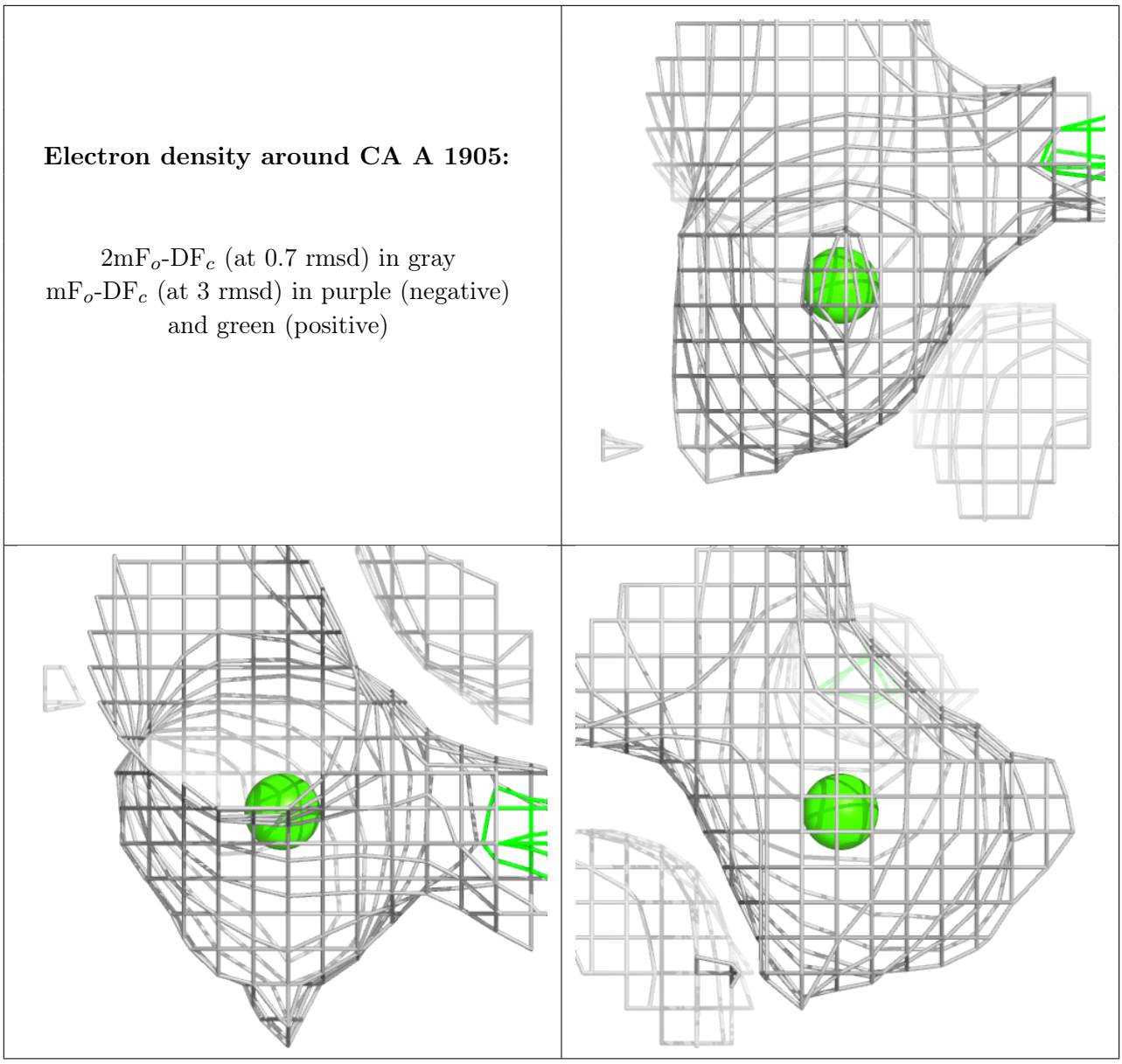
Electron density around CA A 1911:

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



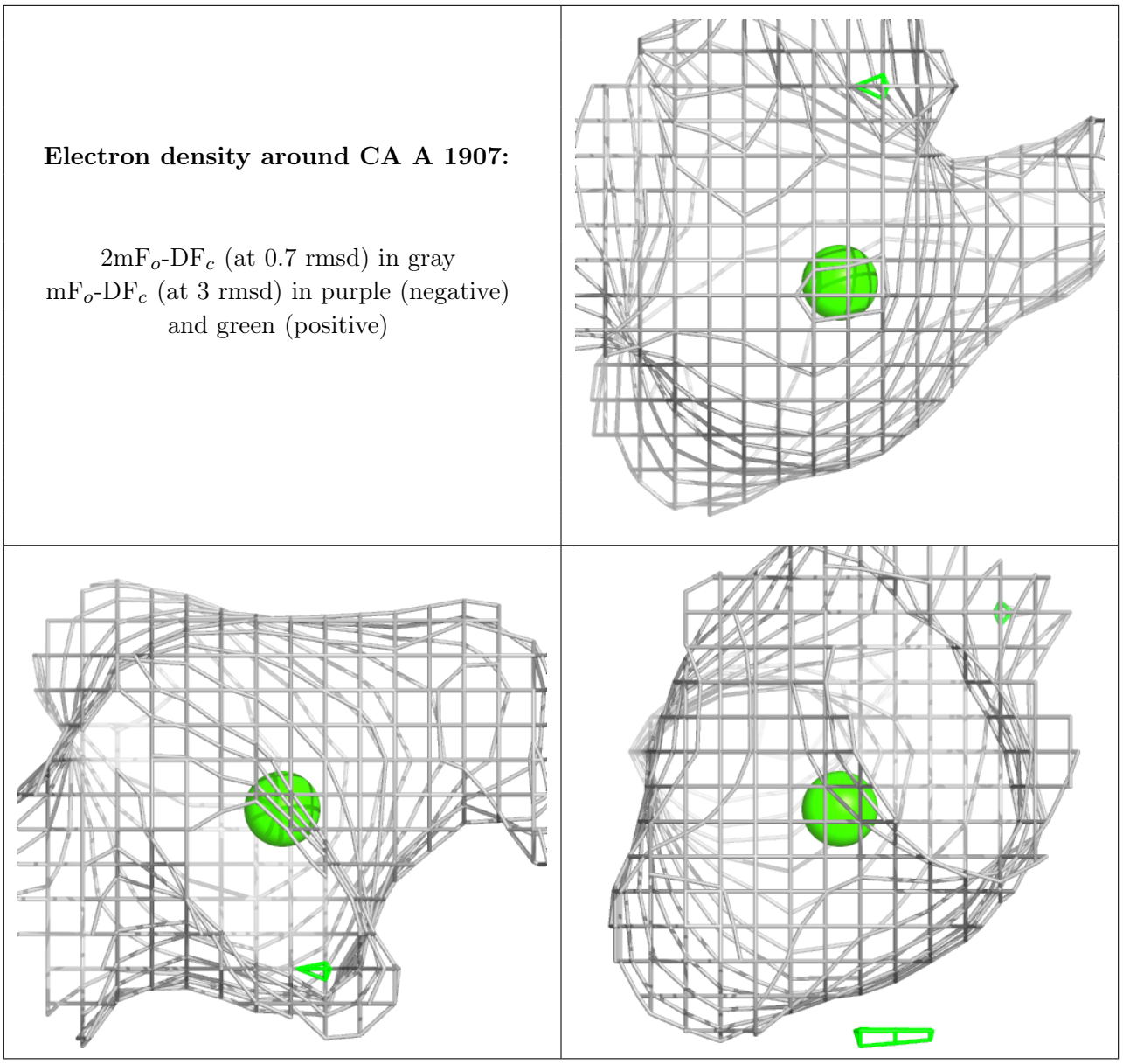
Electron density around CA A 1905:

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



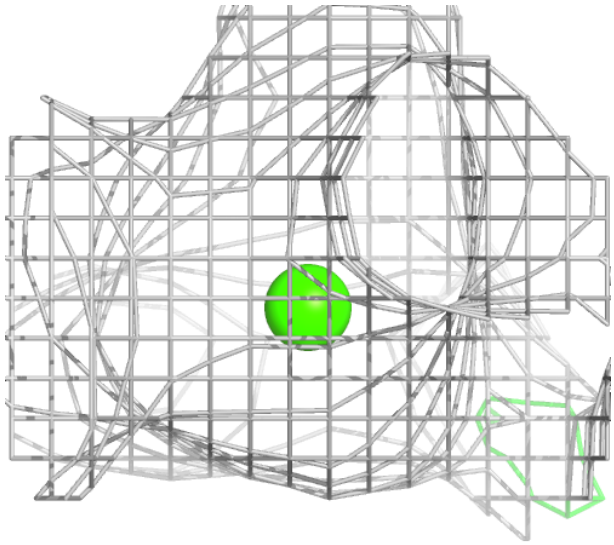
Electron density around CA A 1907:

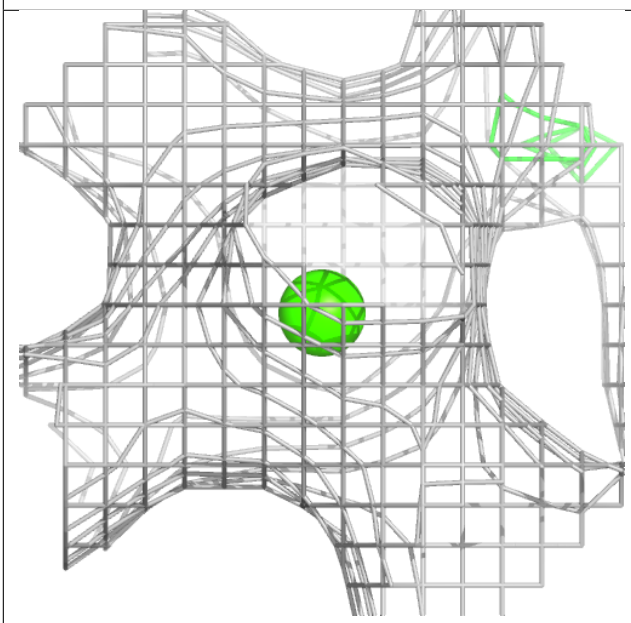
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

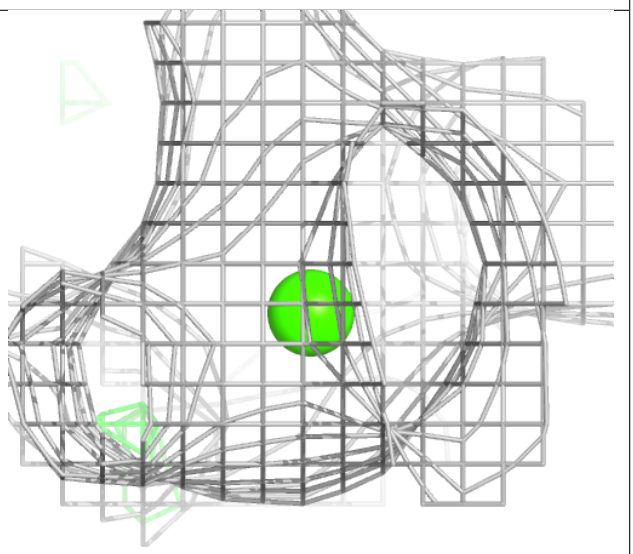


Electron density around CA A 1904:

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

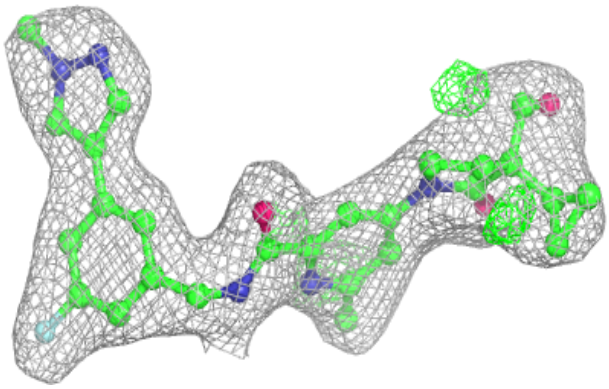


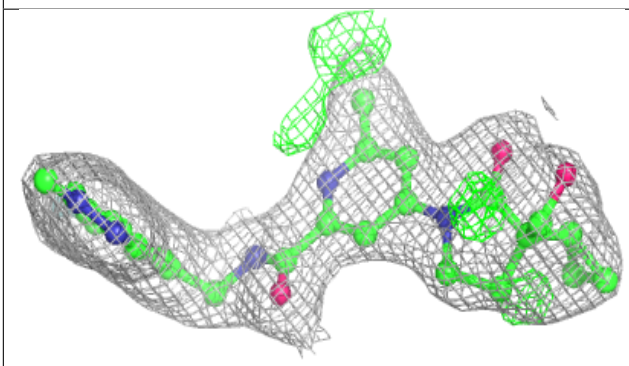


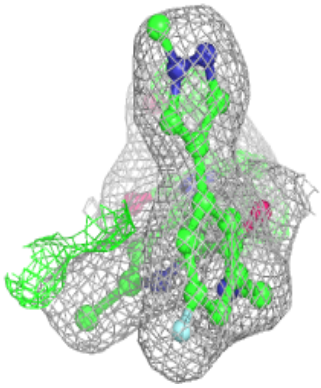


Electron density around 1XK A 1901:

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

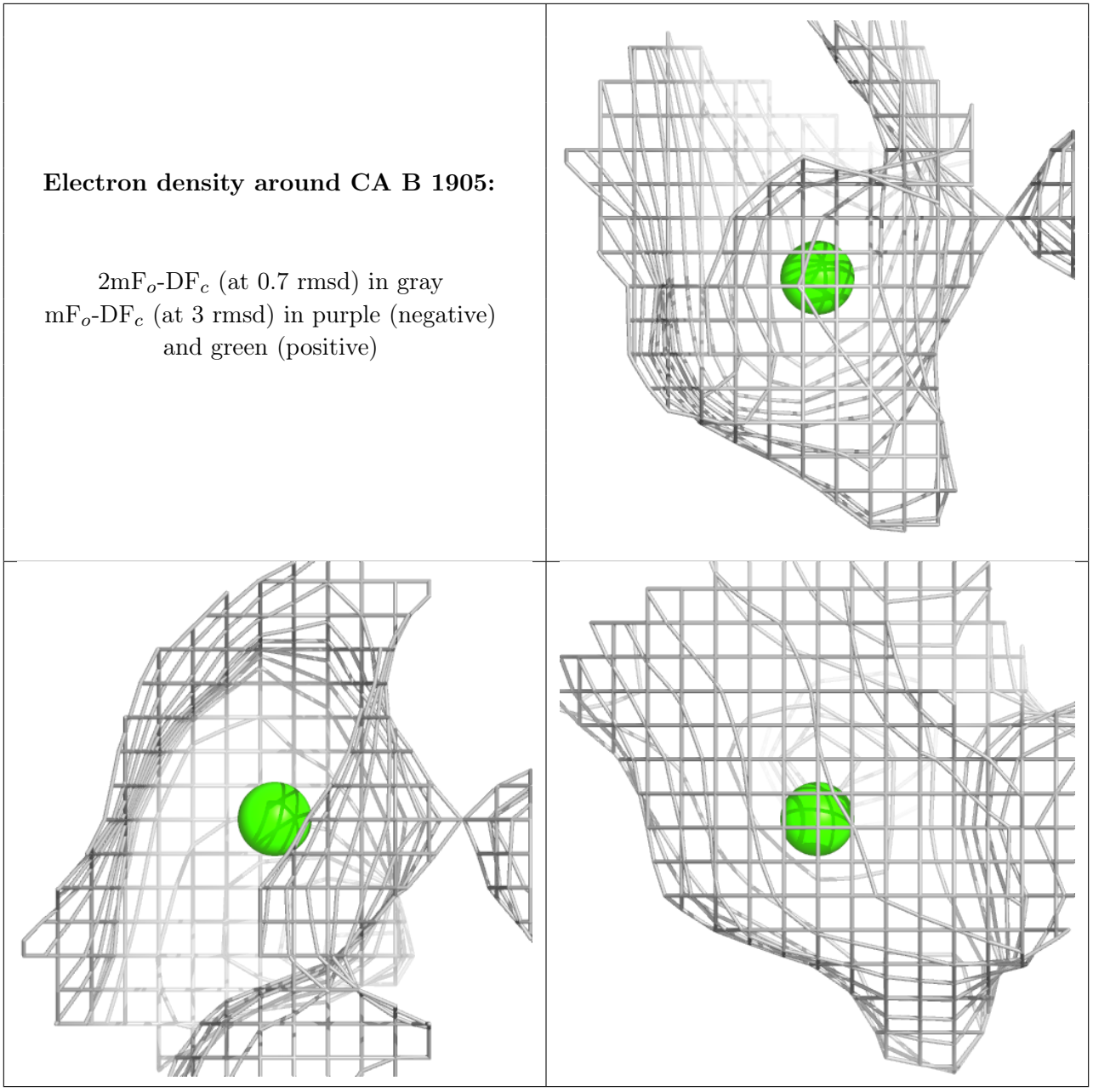






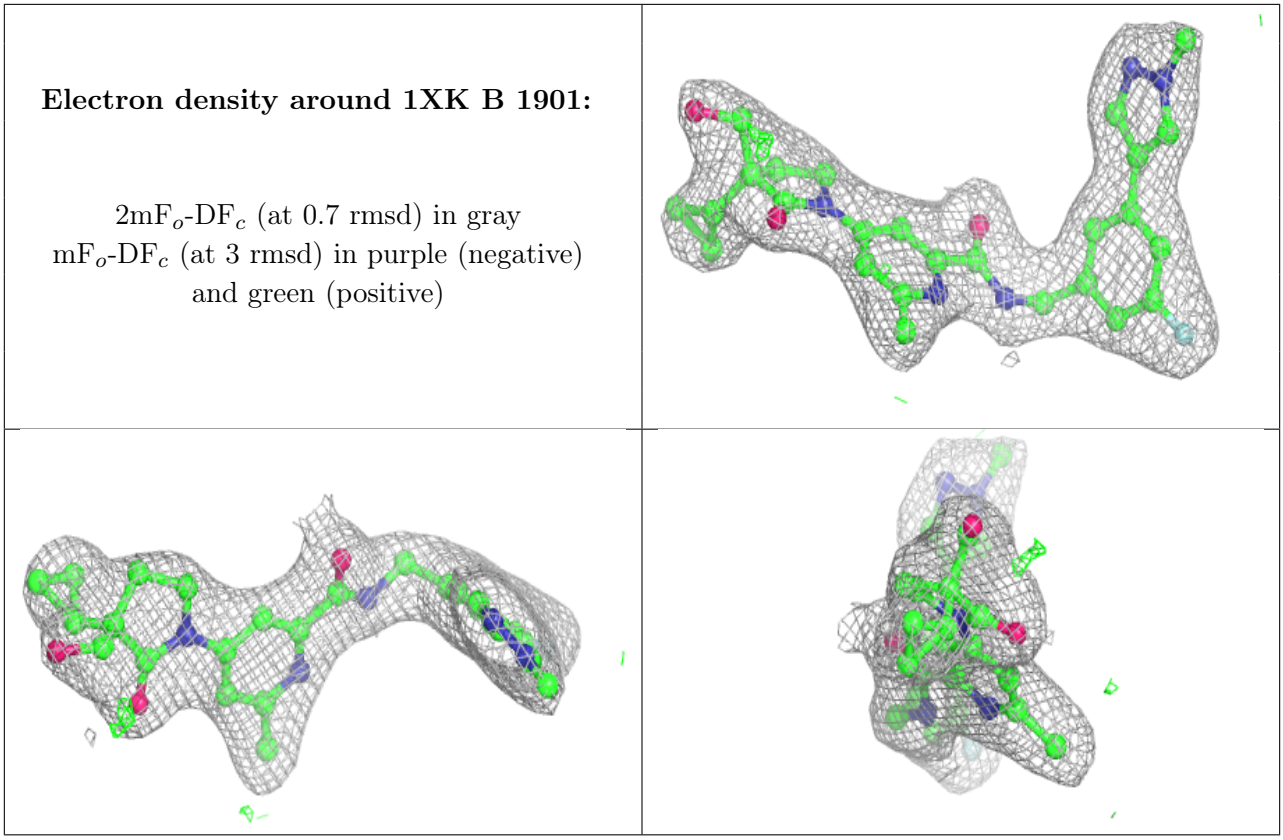
Electron density around CA B 1905:

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



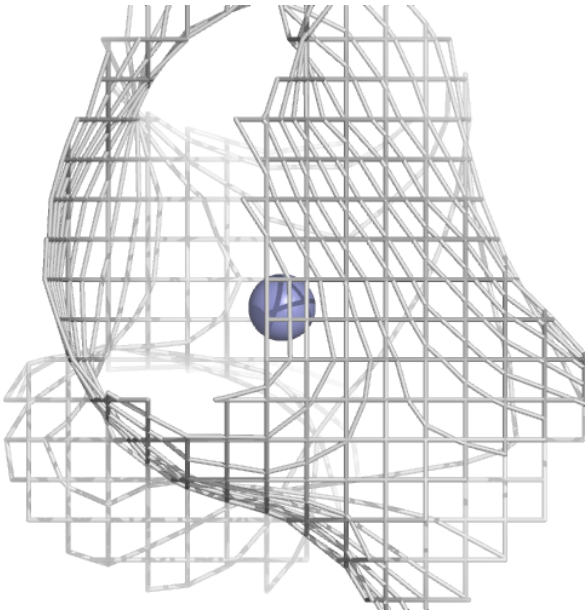
Electron density around 1XK B 1901:

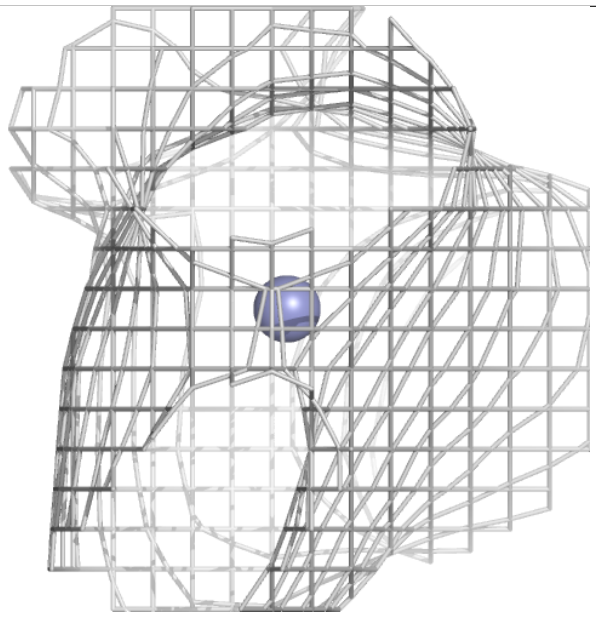
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

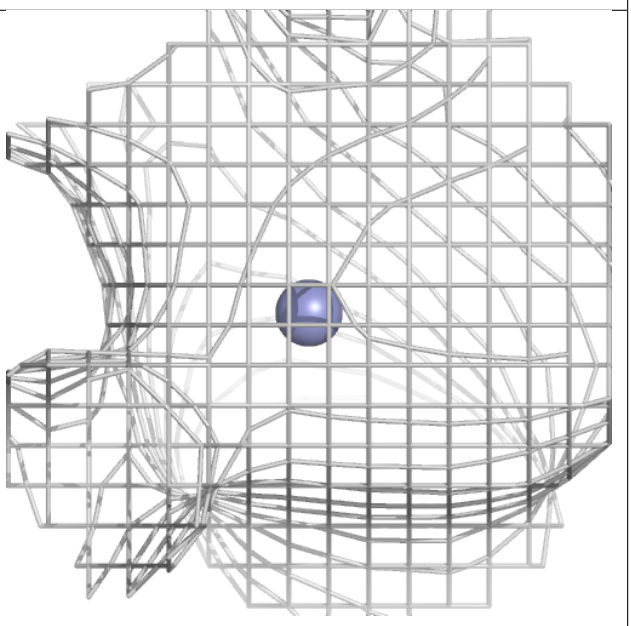


Electron density around ZN B 1902:

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

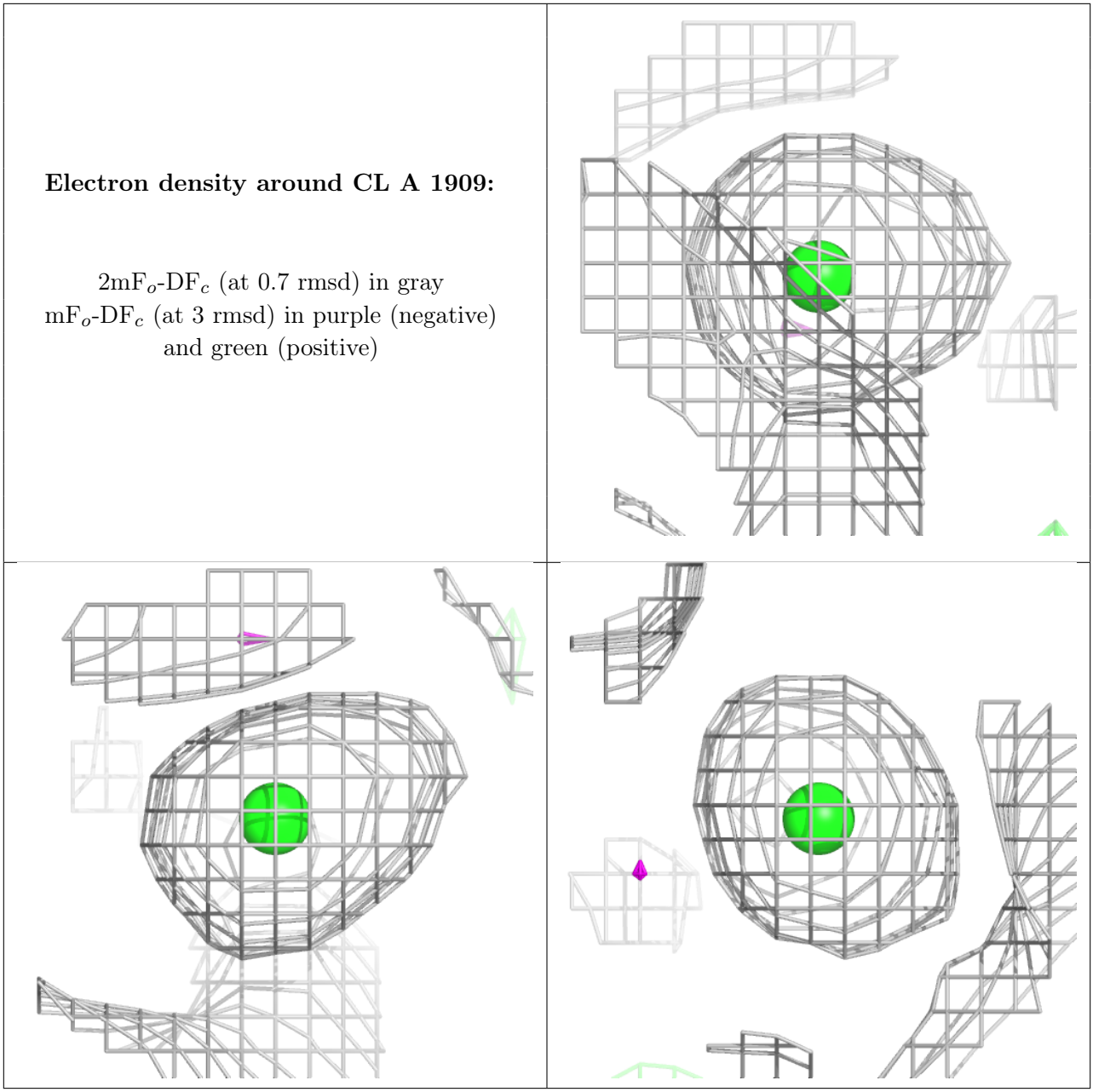






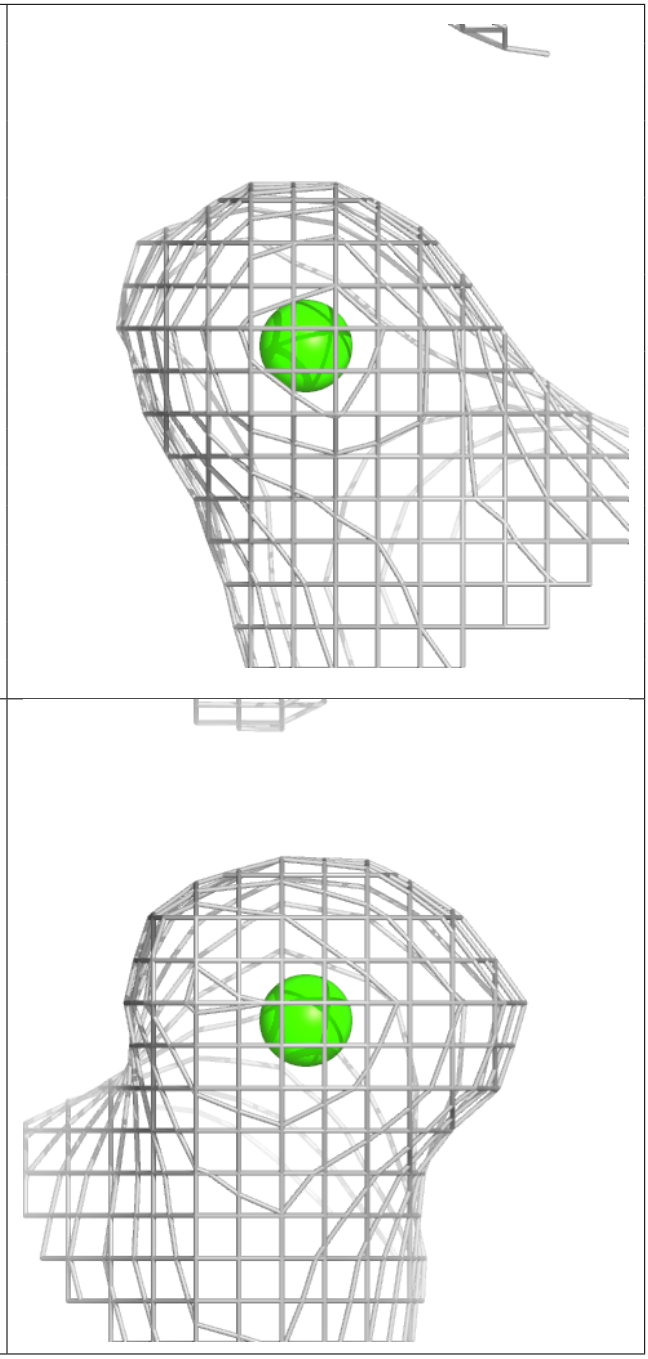
Electron density around CL A 1909:

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



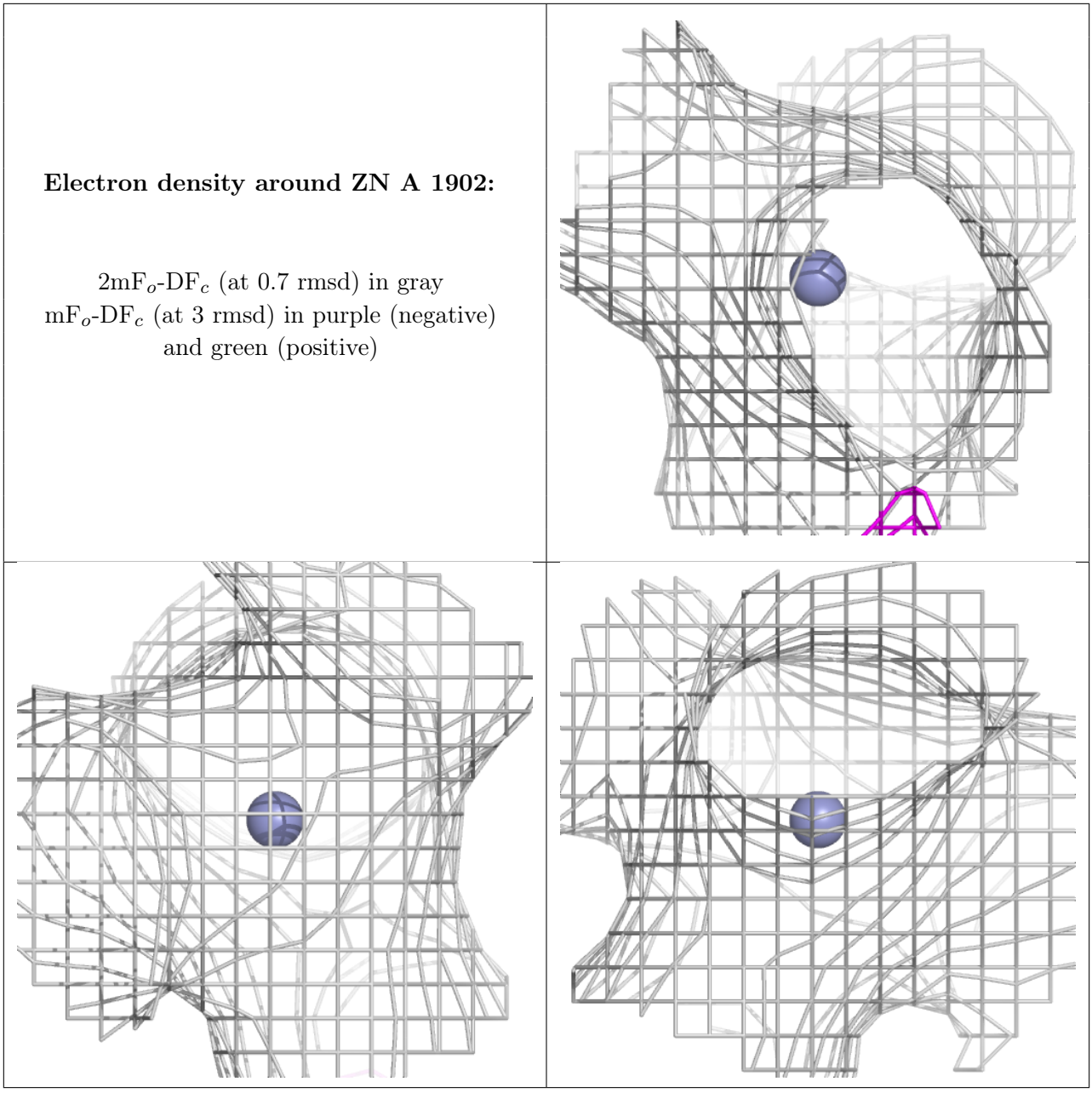
Electron density around CA A 1906:

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



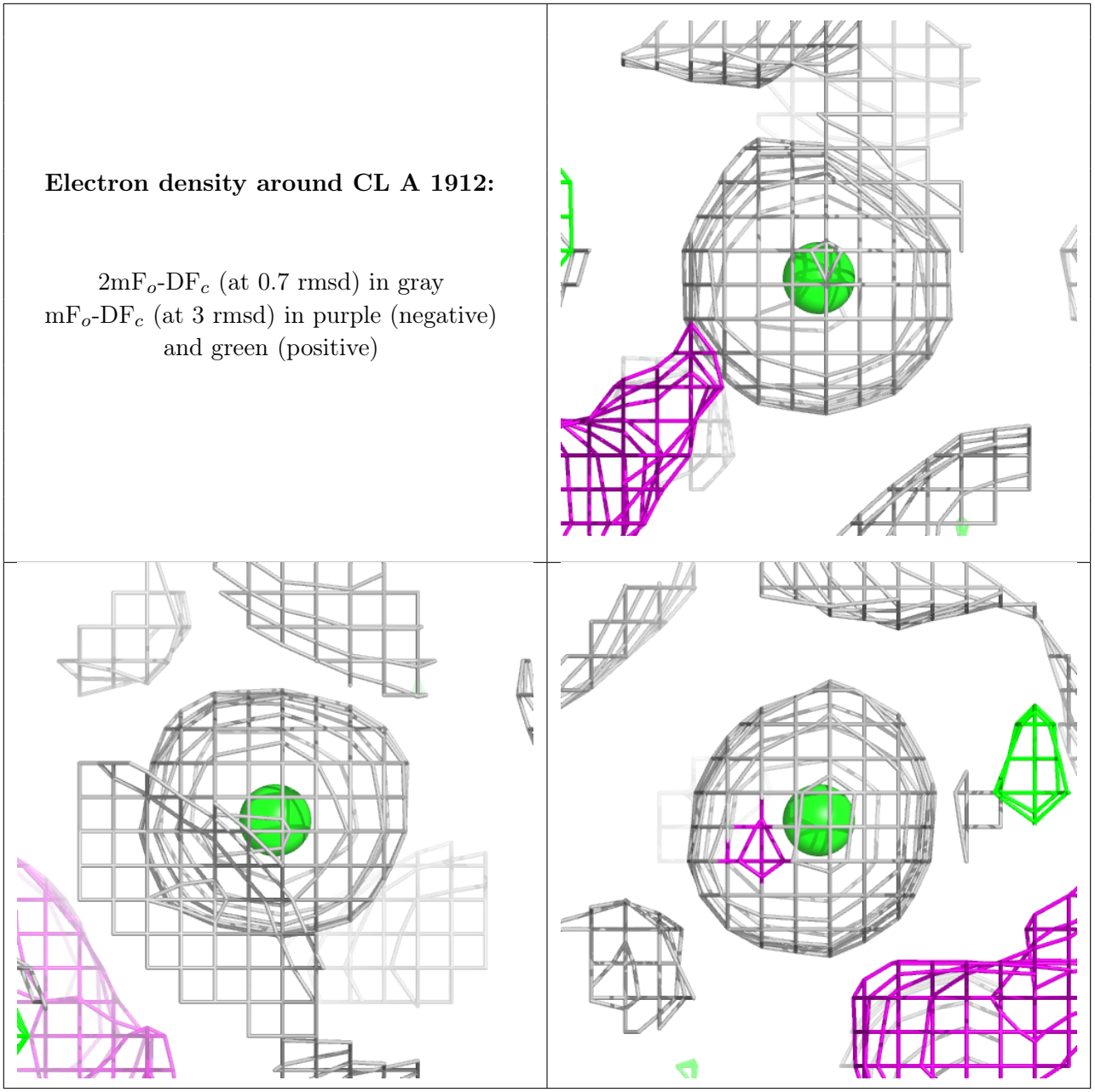
Electron density around ZN A 1902:

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



Electron density around CL A 1912:

$2mF_o$-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.