Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2023 – 02:54 pm BST

PDB ID	:	7ZD0
Title	:	Crystal structure of Pseudomonas aeruginosa S-adenosyl-L-homocysteine hydrolase inhibited by Cd2+ ions
Authors	:	Malecki, P.H.; Gawel, M.; Brzezinski, K.
Deposited on	:	2022-03-29
Resolution	:	1.87 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:

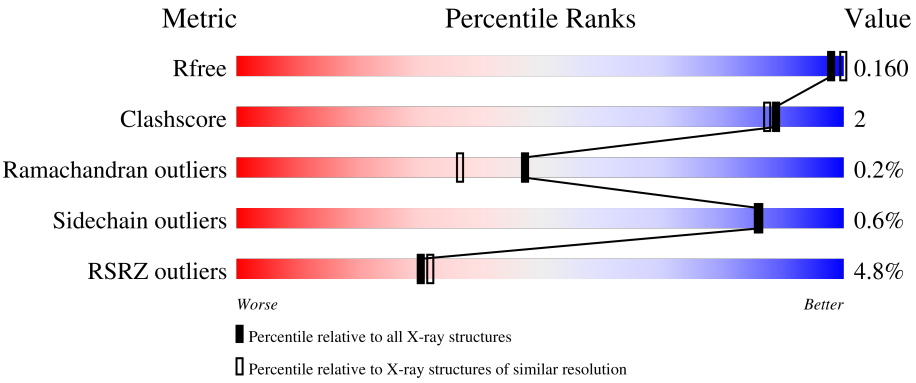
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	472	2% 93%
1	B	472	6% 93%
1	C	472	3% 93%
1	D	472	8% 92% 5%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 16326 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.

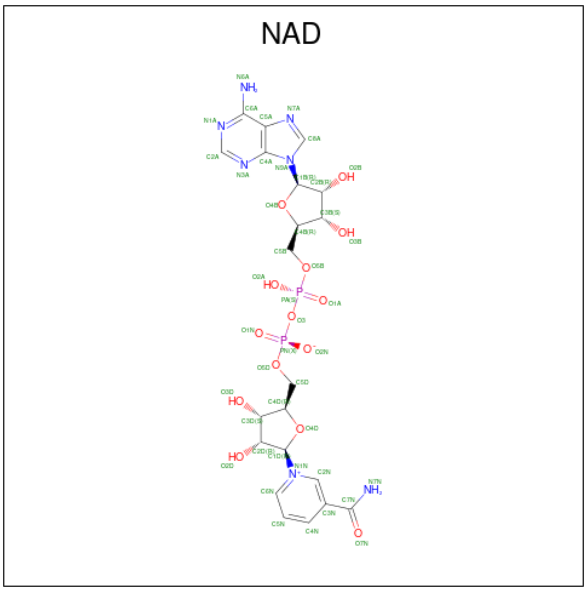
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	4	0
			3579	2256	618	682	23			
1	B	460	Total	C	N	O	S	0	3	0
			3567	2249	617	679	22			
1	C	461	Total	C	N	O	S	0	6	0
			3592	2265	622	681	24			
1	D	461	Total	C	N	O	S	0	6	0
			3591	2262	621	685	23			

There are 12 discrepancies between the modelled and reference sequences:

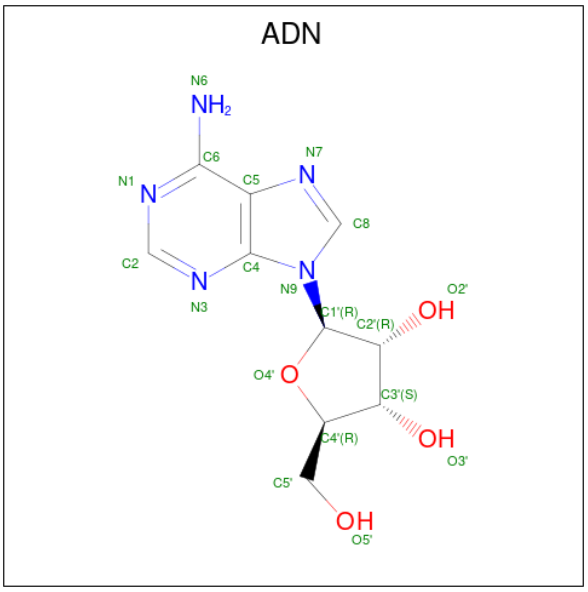
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9I685
A	-1	ASN	-	expression tag	UNP Q9I685
A	0	ALA	-	expression tag	UNP Q9I685
B	-2	SER	-	expression tag	UNP Q9I685
B	-1	ASN	-	expression tag	UNP Q9I685
B	0	ALA	-	expression tag	UNP Q9I685
C	-2	SER	-	expression tag	UNP Q9I685
C	-1	ASN	-	expression tag	UNP Q9I685
C	0	ALA	-	expression tag	UNP Q9I685
D	-2	SER	-	expression tag	UNP Q9I685
D	-1	ASN	-	expression tag	UNP Q9I685
D	0	ALA	-	expression tag	UNP Q9I685

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



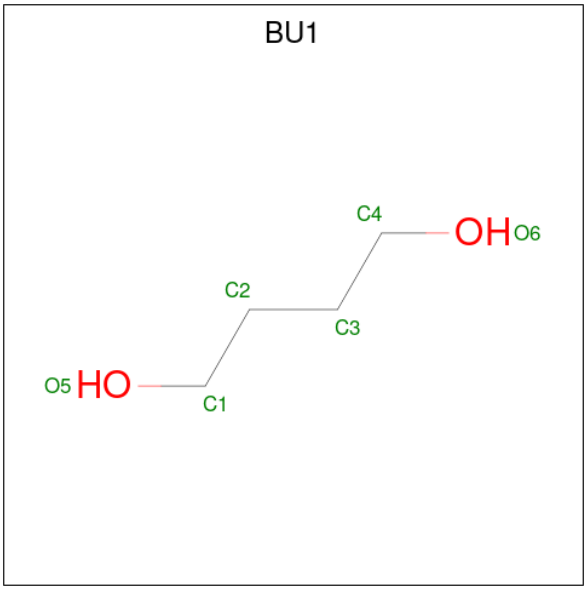
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$) (labeled as "Ligand of Interest" by depositor).



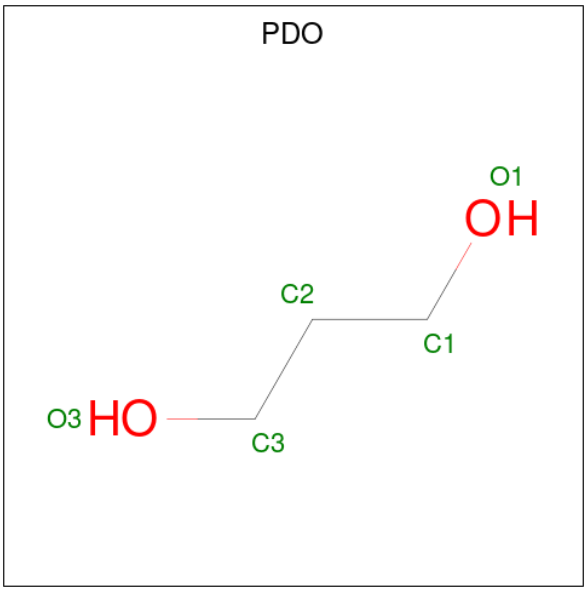
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	5	4		
3	B	1	Total	C	N	O	0	0
			19	10	5	4		
3	C	1	Total	C	N	O	0	0
			19	10	5	4		
3	D	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 4 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		
4	A	1	Total	C	O	0	0
			6	4	2		
4	C	1	Total	C	O	0	0
			6	4	2		
4	C	1	Total	C	O	0	0
			6	4	2		
4	C	1	Total	C	O	0	0
			6	4	2		
4	D	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is 1,3-PROPANDIOL (three-letter code: PDO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 5 3 2	0	0
5	A	1	Total C O 5 3 2	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K 1 1	0	0
6	B	1	Total K 1 1	0	0
6	C	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0

- Molecule 7 is CADMIUM ION (three-letter code: CD) (formula: Cd) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	5	Total Cd 5 5	0	0
7	B	5	Total Cd 6 6	0	1

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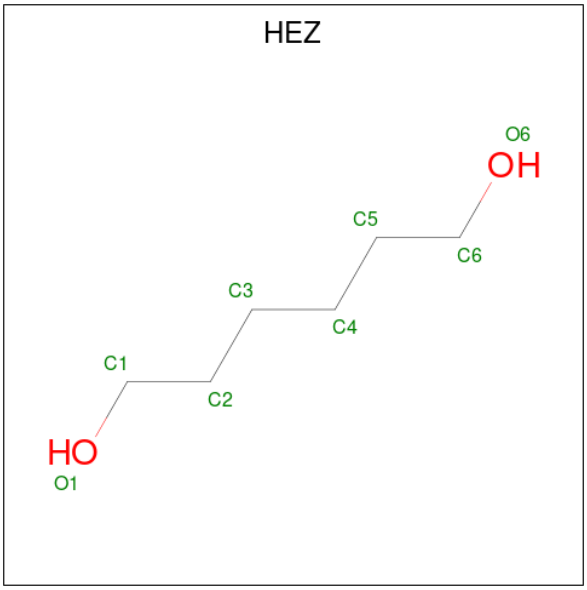
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	4	Total Cd 5 5	0	1
7	D	5	Total Cd 5 5	0	0

- Molecule 8 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total Cl 1 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	488	Total O 497 497	0	9
10	B	365	Total O 374 374	0	11
10	C	407	Total O 414 414	0	10

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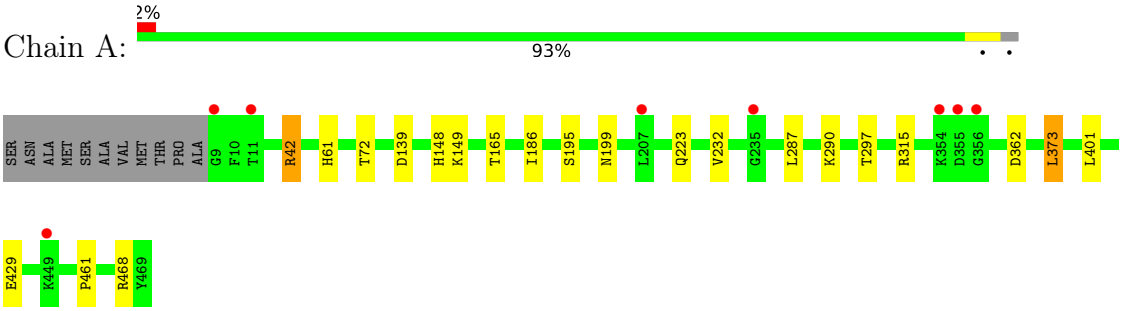
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	376	Total 380	O 380	0	5

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.

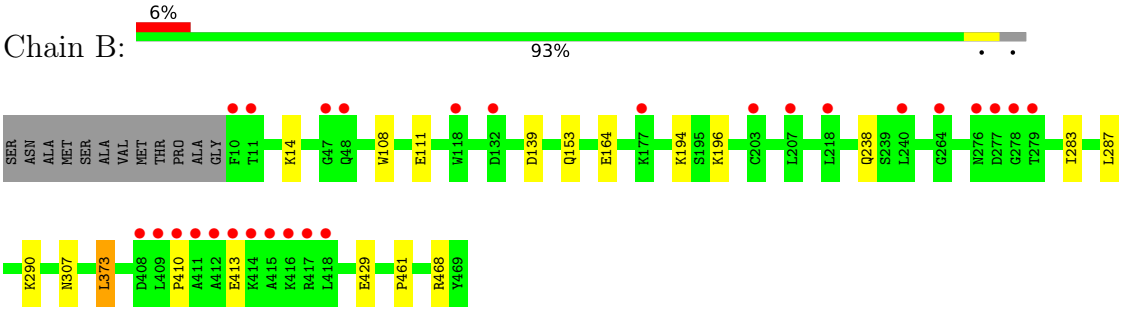
- Molecule 1: Adenosylhomocysteinase

Chain A:



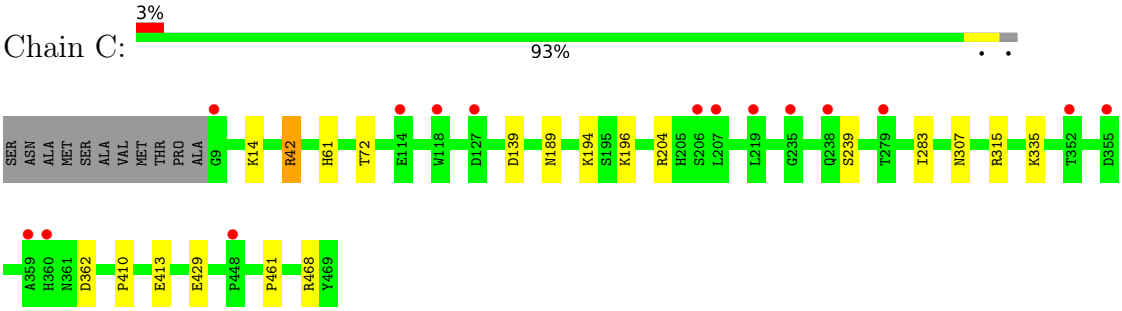
- Molecule 1: Adenosylhomocysteinase

Chain B:



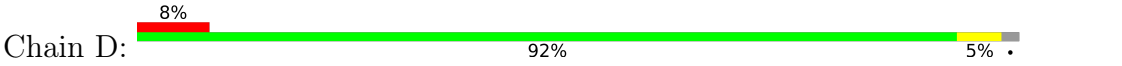
- Molecule 1: Adenosylhomocysteinase

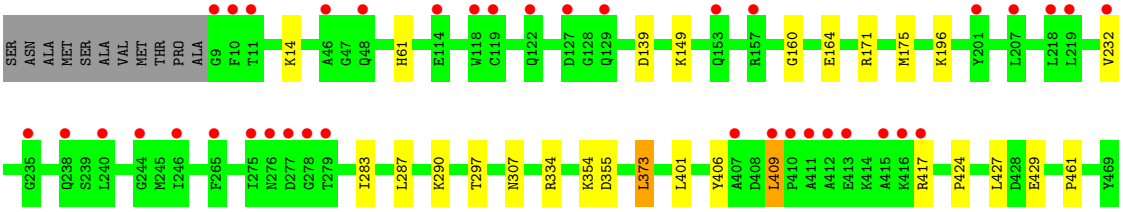
Chain C:



- Molecule 1: Adenosylhomocysteinase

Chain D:




SER
ASN
ALA
MET
SER
ALA
VAL
MET
THR
PRO
ALA
G9
F10
T11
K14
A46
G47
Q48
H61
E114
W118
C119
Q122
D127
G128
Q129
D139
K149
Q153
R157
G160
E164
R171
M175
K196
Y201
L207
L218
L219
V232
G235
Q238
S239
L240
G244
M245
I246
F265
I275
N276
D277
G278
T279
I283
L287
K290
T297
N307
R334
K354
D355
L373
L401
Y406
A407
D408
L409
P410
A411
A412
E413
K414
A415
K416
R417
P424
L427
D428
E429
P461
Y469

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	176.97Å 134.16Å 108.88Å 90.00° 106.06° 90.00°	Depositor
Resolution (Å)	44.10 – 1.87 44.10 – 1.87	Depositor EDS
% Data completeness (in resolution range)	92.5 (44.10-1.87) 93.3 (44.10-1.87)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.147 , 0.162 0.147 , 0.160	Depositor DCC
R_{free} test set	1029 reflections (0.55%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.000 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	16326	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: CL, NAD, BU1, K, PDO, HEZ, ADN, CD

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	0.40	0/3648	0.59	1/4931 (0.0%)
1	B	0.36	0/3636	0.58	1/4916 (0.0%)
1	C	0.37	0/3667	0.59	0/4955
1	D	0.36	0/3660	0.57	1/4947 (0.0%)
All	All	0.37	0/14611	0.58	3/19749 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	373	LEU	CA-CB-CG	5.71	128.43	115.30
1	D	373	LEU	CA-CB-CG	5.12	127.06	115.30
1	A	373	LEU	CA-CB-CG	5.03	126.86	115.30

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	3579	0	3584	12	0
1	B	3567	0	3575	14	0
1	C	3592	0	3608	11	0
1	D	3591	0	3592	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
3	A	19	0	13	2	0
3	B	19	0	13	2	0
3	C	19	0	13	2	0
3	D	19	0	13	2	0
4	A	12	0	20	2	0
4	C	18	0	30	1	0
4	D	6	0	10	1	0
5	A	10	0	16	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	5	0	0	0	0
7	B	6	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
8	B	8	0	14	1	0
9	D	1	0	0	0	0
10	A	497	0	0	2	0
10	B	374	0	0	3	0
10	C	414	0	0	0	0
10	D	380	0	0	2	0
All	All	16326	0	14605	55	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 2.

All (55) 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:14:LYS:HE2	4:C:503:BU1:H21	1.70	0.72
1:D:14:LYS:HE3	4:D:503:BU1:H32	1.76	0.67
1:B:287:LEU:HD12	10:B:781:HOH:O	1.96	0.65
1:A:148:HIS:HB3	4:A:504:BU1:H41	1.84	0.58
2:A:501:NAD:C4N	3:A:502:ADN:H3'	2.35	0.56
1:B:196:LYS:HE3	1:C:468:ARG:HB2	1.88	0.56
1:B:14:LYS:HE3	8:B:503:HEZ:H22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:501:NAD:C4N	3:D:502:ADN:H3'	2.36	0.55
1:C:189:ASN:HA	1:C:194:LYS:HD2	1.88	0.55
1:D:149:LYS:NZ	10:D:605:HOH:O	2.40	0.54
1:A:429:GLU:OE1	1:A:461:PRO:HA	2.08	0.54
1:A:315:ARG:NH1	1:A:362:ASP:HB2	2.23	0.53
1:D:287:LEU:HD12	10:D:852:HOH:O	2.08	0.53
2:C:501:NAD:C4N	3:C:502:ADN:H3'	2.38	0.53
1:B:139:ASP:OD2	1:B:164:GLU:HG2	2.09	0.52
1:C:204:ARG:HA	1:C:239:SER:HB2	1.92	0.52
1:C:42:ARG:HG3	1:C:72:THR:HG23	1.91	0.52
1:D:429:GLU:OE1	1:D:461:PRO:HA	2.11	0.51
1:A:186:ILE:HG12	1:A:401:LEU:HD11	1.92	0.51
1:D:283:ILE:HG13	1:D:307:ASN:HB3	1.93	0.50
1:D:409:LEU:HD21	1:D:417:ARG:HE	1.76	0.50
1:B:283:ILE:HG13	1:B:307:ASN:HB3	1.94	0.50
1:B:410:PRO:HD2	1:B:413:GLU:HG3	1.95	0.48
1:A:139:ASP:OD2	3:A:502:ADN:H4'	2.14	0.48
1:C:283:ILE:HG13	1:C:307:ASN:HB3	1.96	0.48
1:C:139:ASP:OD2	3:C:502:ADN:H4'	2.13	0.47
1:D:406:TYR:HA	1:D:409:LEU:HD22	1.96	0.47
1:D:139:ASP:OD2	1:D:164:GLU:HG2	2.14	0.47
1:D:139:ASP:OD2	3:D:502:ADN:H4'	2.15	0.47
1:A:42:ARG:HG3	1:A:72:THR:HG23	1.96	0.47
1:A:195:SER:O	1:A:199:ASN:HB2	2.15	0.46
1:A:149:LYS:HE2	4:A:504:BU1:H22	1.98	0.46
1:B:429:GLU:OE1	1:B:461:PRO:HA	2.16	0.45
1:D:232:VAL:HG12	1:D:297:THR:HB	1.98	0.45
2:B:501:NAD:C4N	3:B:502:ADN:H3'	2.47	0.45
1:C:315:ARG:NH1	1:C:362:ASP:HB2	2.32	0.45
1:B:238:GLN:HG2	10:B:877:HOH:O	2.16	0.44
1:C:429:GLU:OE1	1:C:461:PRO:HA	2.18	0.44
1:D:160:GLY:HA3	1:D:401:LEU:HD13	2.00	0.43
1:D:290:LYS:HB2	1:D:290:LYS:HE3	1.86	0.43
1:D:171:ARG:O	1:D:175:MET:HG3	2.19	0.43
1:A:232:VAL:HG12	1:A:297:THR:HB	2.01	0.43
1:B:468:ARG:HB2	1:C:196:LYS:HE3	2.01	0.43
1:C:410:PRO:HD2	1:C:413:GLU:HB2	2.01	0.43
1:D:354:LYS:HG3	1:D:355[B]:ASP:H	1.83	0.43
5:A:506:PDO:H21	10:A:913:HOH:O	2.19	0.42
1:B:153:GLN:HB2	10:B:845:HOH:O	2.19	0.42
1:B:290:LYS:HB3	1:B:290:LYS:HE3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:PRO:HD2	1:D:427:LEU:HD12	2.02	0.42
1:B:139:ASP:OD2	3:B:502:ADN:H4'	2.20	0.41
1:A:223:GLN:NE2	1:A:290:LYS:HE2	2.36	0.41
1:A:287:LEU:HD12	10:A:740:HOH:O	2.21	0.41
1:A:468:ARG:HB2	1:D:196:LYS:HE3	2.02	0.41
1:B:164:GLU:O	1:B:194:LYS:HE3	2.21	0.41
1:B:108:TRP:O	1:B:111:GLU:HG3	2.22	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	463/472 (98%)	452 (98%)	10 (2%)	1 (0%)	47	37
1	B	461/472 (98%)	453 (98%)	8 (2%)	0	100	100
1	C	465/472 (98%)	455 (98%)	9 (2%)	1 (0%)	47	37
1	D	465/472 (98%)	455 (98%)	9 (2%)	1 (0%)	47	37
All	All	1854/1888 (98%)	1815 (98%)	36 (2%)	3 (0%)	47	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	C	61	HIS
1	D	61	HIS

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	381/385 (99%)	378 (99%)	3 (1%)	81	80
1	B	380/385 (99%)	379 (100%)	1 (0%)	92	92
1	C	383/385 (100%)	381 (100%)	2 (0%)	88	88
1	D	382/385 (99%)	379 (99%)	3 (1%)	81	80
All	All	1526/1540 (99%)	1517 (99%)	9 (1%)	86	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	165	THR
1	A	373	LEU
1	B	373	LEU
1	C	42	ARG
1	C	335	LYS
1	D	334	ARG
1	D	373	LEU
1	D	409	LEU

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

Mol	Chain	Res	Type
1	C	129	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 43 ligands modelled in this entry, 26 are monoatomic - leaving 17 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	BU1	D	503	-	5,5,5	0.39	0	4,4,4	0.40	0
3	ADN	C	502	-	18,21,21	0.66	0	18,31,31	0.84	1 (5%)
4	BU1	A	503	-	5,5,5	0.34	0	4,4,4	0.52	0
5	PDO	A	505	-	4,4,4	0.36	0	3,3,3	0.36	0
3	ADN	A	502	-	18,21,21	0.64	0	18,31,31	0.93	1 (5%)
3	ADN	D	502	-	18,21,21	0.67	0	18,31,31	0.87	1 (5%)
5	PDO	A	506	-	4,4,4	0.33	0	3,3,3	0.38	0
2	NAD	C	501	-	42,48,48	0.57	0	50,73,73	0.71	1 (2%)
4	BU1	A	504	-	5,5,5	0.33	0	4,4,4	0.60	0
4	BU1	C	504	-	5,5,5	0.38	0	4,4,4	0.47	0
2	NAD	A	501	-	42,48,48	0.55	0	50,73,73	0.78	1 (2%)
4	BU1	C	503	-	5,5,5	0.32	0	4,4,4	0.44	0
4	BU1	C	505	-	5,5,5	0.33	0	4,4,4	0.38	0
8	HEZ	B	503	-	7,7,7	0.12	0	6,6,6	0.42	0
2	NAD	D	501	-	42,48,48	0.55	0	50,73,73	0.72	1 (2%)
3	ADN	B	502	-	18,21,21	0.64	0	18,31,31	0.89	1 (5%)
2	NAD	B	501	-	42,48,48	0.54	0	50,73,73	0.74	1 (2%)

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	BU1	D	503	-	-	2/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADN	C	502	-	-	0/2/22/22	0/3/3/3
4	BU1	A	503	-	-	1/3/3/3	-
5	PDO	A	505	-	-	2/2/2/2	-
3	ADN	A	502	-	-	0/2/22/22	0/3/3/3
3	ADN	D	502	-	-	0/2/22/22	0/3/3/3
5	PDO	A	506	-	-	1/2/2/2	-
2	NAD	C	501	-	-	5/26/62/62	0/5/5/5
4	BU1	A	504	-	-	2/3/3/3	-
4	BU1	C	504	-	-	2/3/3/3	-
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5
4	BU1	C	503	-	-	2/3/3/3	-
4	BU1	C	505	-	-	0/3/3/3	-
8	HEZ	B	503	-	-	3/5/5/5	-
2	NAD	D	501	-	-	5/26/62/62	0/5/5/5
3	ADN	B	502	-	-	0/2/22/22	0/3/3/3
2	NAD	B	501	-	-	5/26/62/62	0/5/5/5

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	ADN	C5-C6-N6	2.33	123.90	120.35
2	C	501	NAD	C5A-C6A-N6A	2.29	123.83	120.35
3	B	502	ADN	C5-C6-N6	2.27	123.81	120.35
2	B	501	NAD	C5A-C6A-N6A	2.27	123.80	120.35
2	A	501	NAD	C5A-C6A-N6A	2.26	123.79	120.35
3	D	502	ADN	C5-C6-N6	2.24	123.75	120.35
2	D	501	NAD	C5A-C6A-N6A	2.23	123.75	120.35
3	C	502	ADN	C5-C6-N6	2.09	123.53	120.35

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	B	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	O4D-C1D-N1N-C2N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	C	501	NAD	C2D-C1D-N1N-C2N
2	C	501	NAD	C2D-C1D-N1N-C6N
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C2N
2	D	501	NAD	C2D-C1D-N1N-C6N
5	A	505	PDO	O1-C1-C2-C3
5	A	505	PDO	C1-C2-C3-O3
5	A	506	PDO	C1-C2-C3-O3
8	B	503	HEZ	C3-C4-C5-C6
8	B	503	HEZ	C1-C2-C3-C4
4	D	503	BU1	C2-C3-C4-O6
4	C	503	BU1	O5-C1-C2-C3
4	C	504	BU1	O5-C1-C2-C3
4	A	503	BU1	O5-C1-C2-C3
4	A	504	BU1	O5-C1-C2-C3
4	C	503	BU1	C2-C3-C4-O6
4	A	504	BU1	C1-C2-C3-C4
8	B	503	HEZ	C4-C5-C6-O6
4	D	503	BU1	O5-C1-C2-C3
2	B	501	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	O4B-C4B-C5B-O5B
2	D	501	NAD	O4B-C4B-C5B-O5B
4	C	504	BU1	C1-C2-C3-C4

There are no ring outliers.

13 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	503	BU1	1	0
3	C	502	ADN	2	0
3	A	502	ADN	2	0
3	D	502	ADN	2	0
5	A	506	PDO	1	0
2	C	501	NAD	1	0
4	A	504	BU1	2	0

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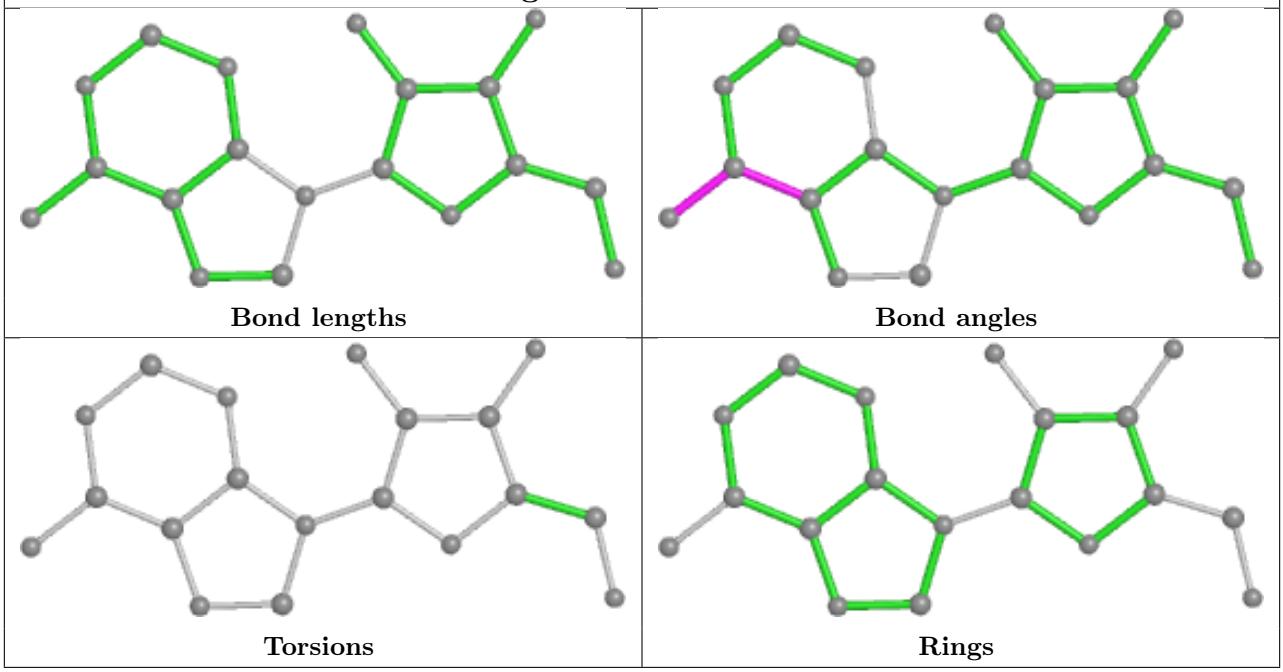
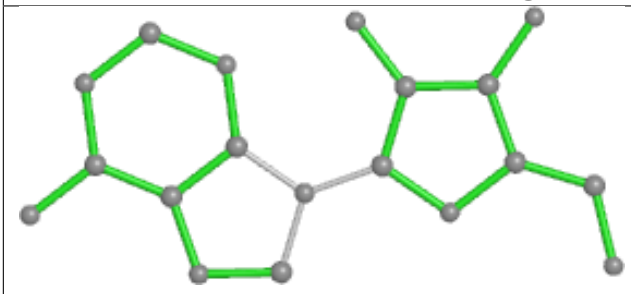
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAD	1	0
4	C	503	BU1	1	0
8	B	503	HEZ	1	0
2	D	501	NAD	1	0
3	B	502	ADN	2	0
2	B	501	NAD	1	0

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.

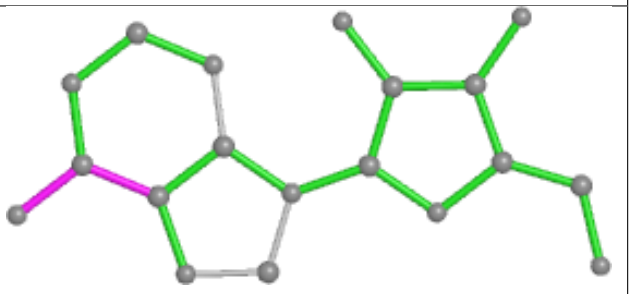
Ligand ADN C 502



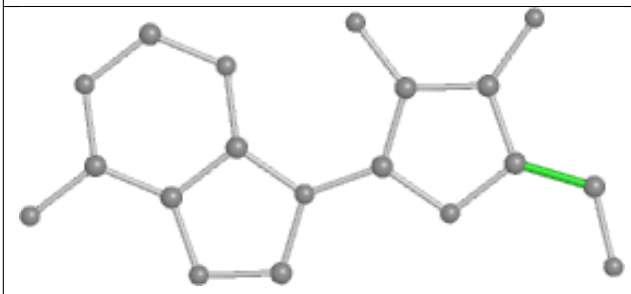
Ligand ADN A 502



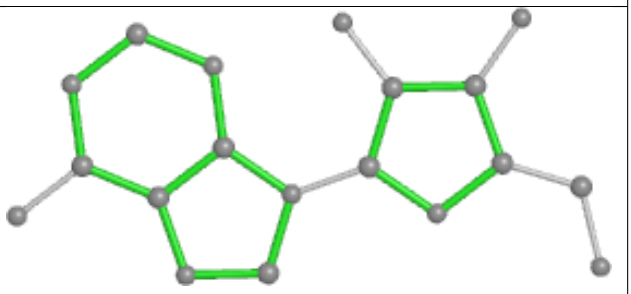
Bond lengths



Bond angles

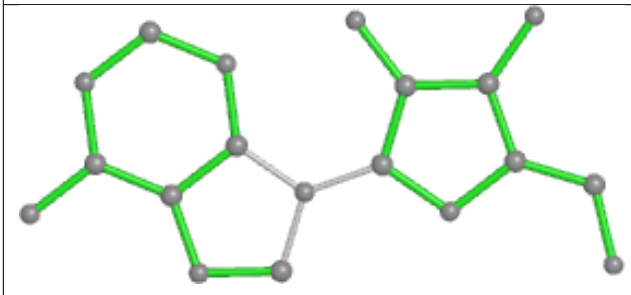


Torsions



Rings

Ligand ADN D 502



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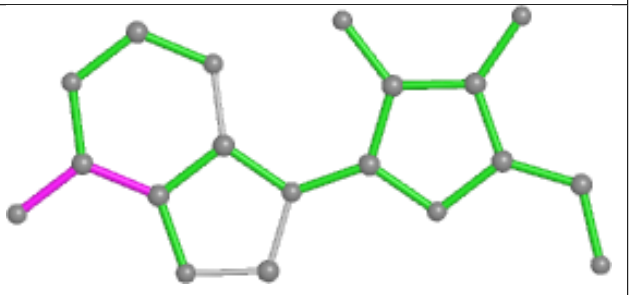

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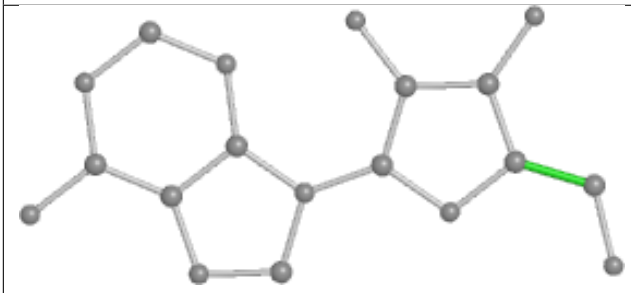

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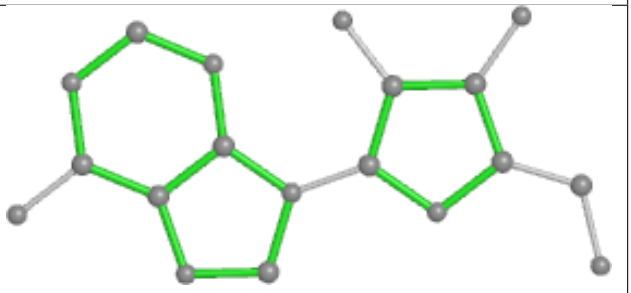
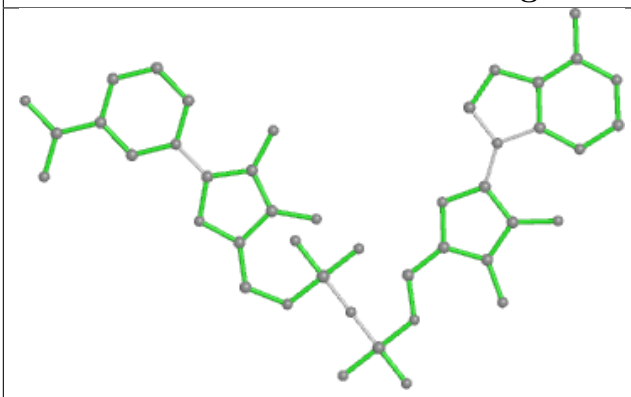


Rings

Ligand NAD C 501



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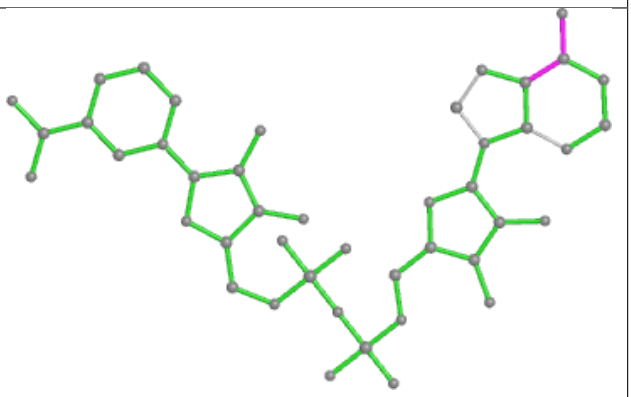

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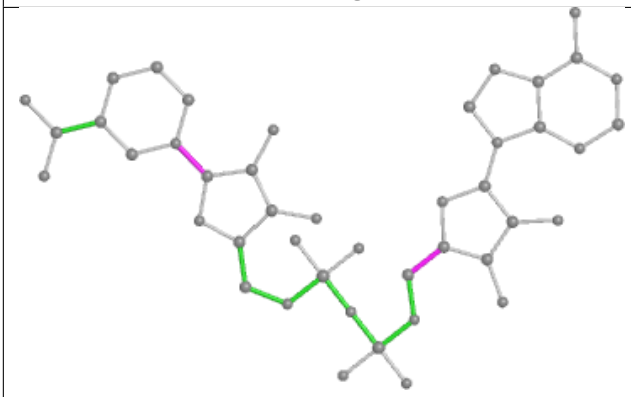

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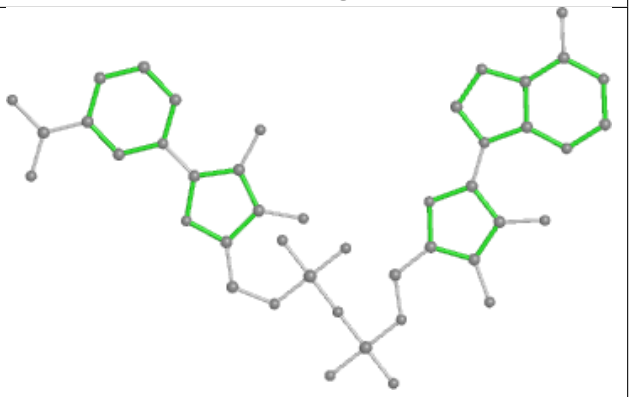
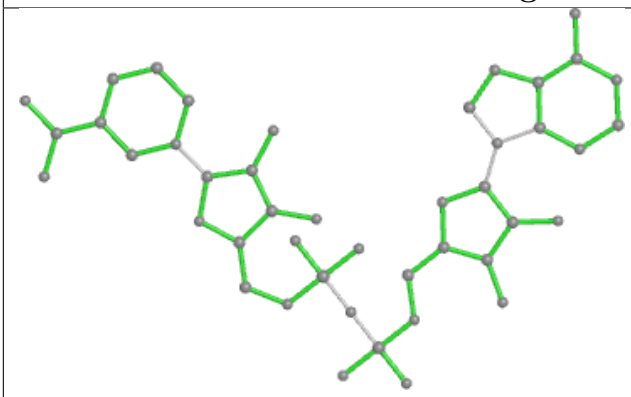


Rings

Ligand NAD A 501



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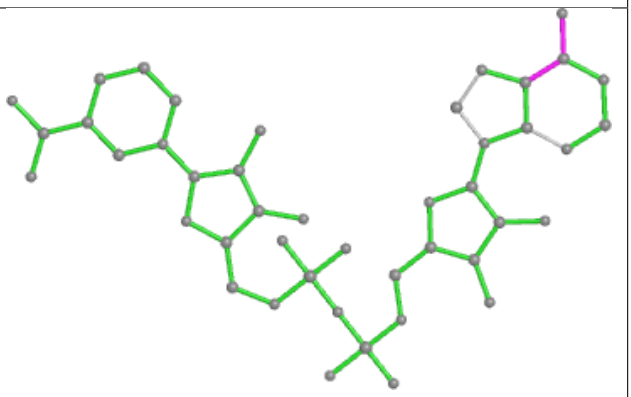
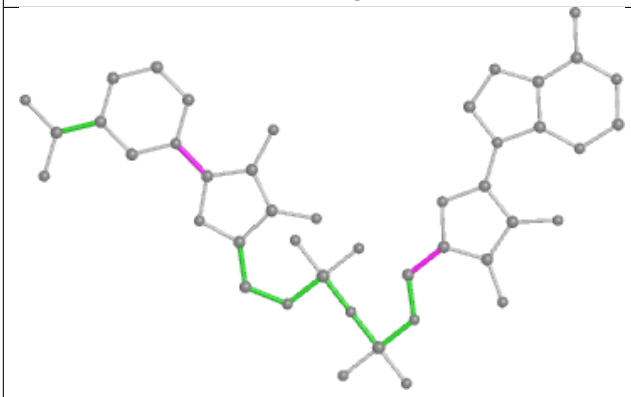


Bond angles



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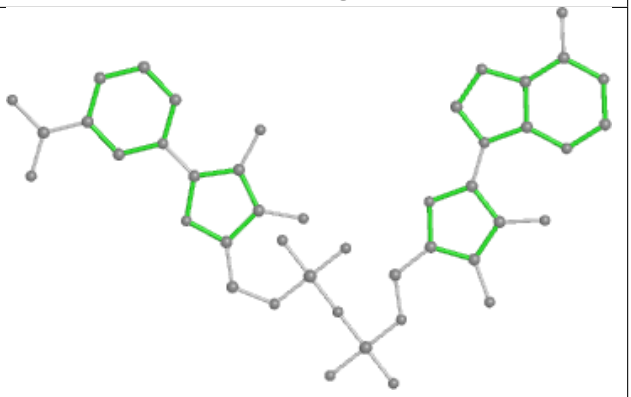
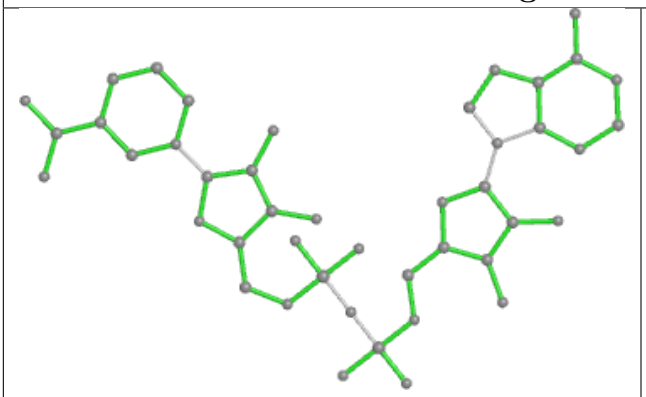


Rings

Ligand NAD D 501



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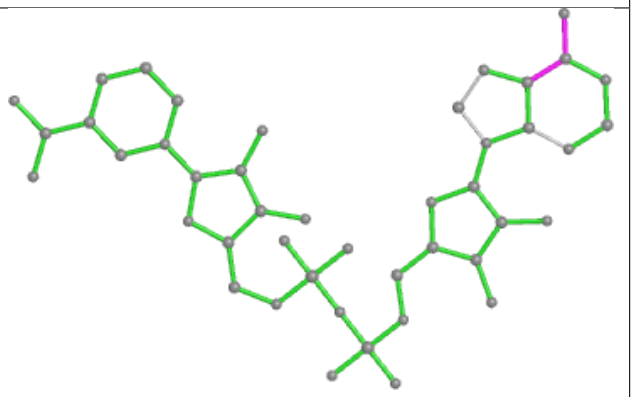

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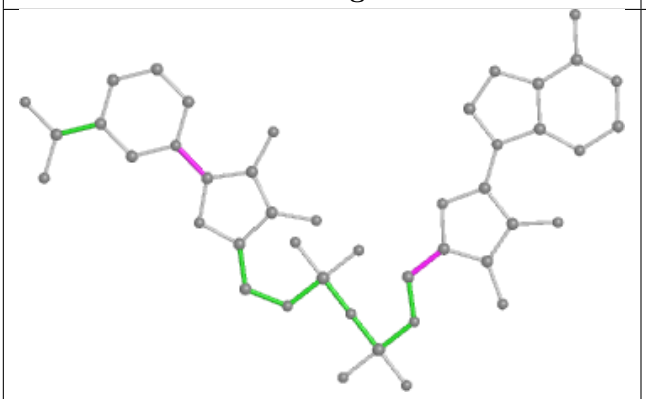

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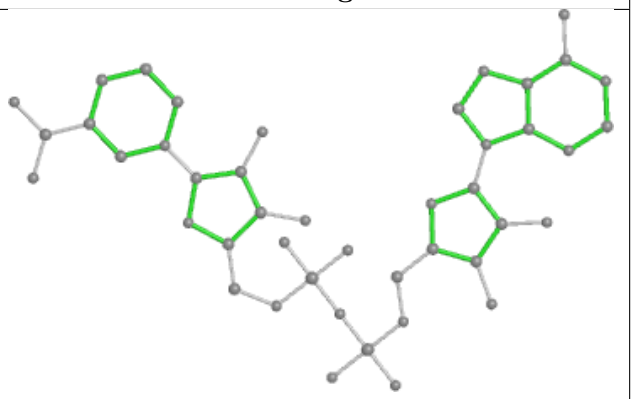
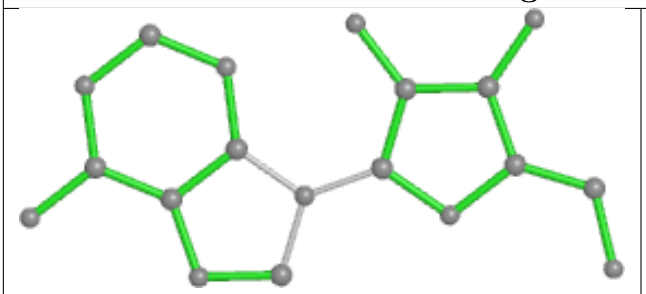
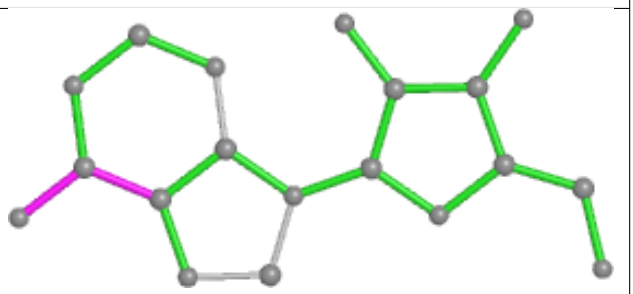


Rings

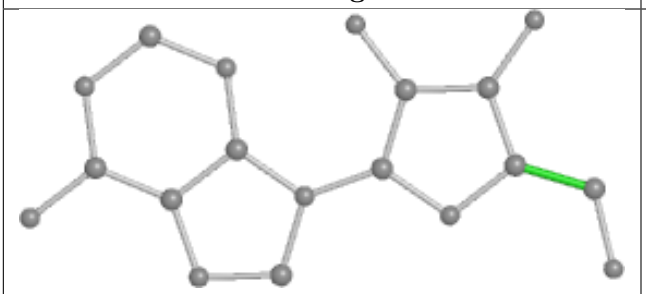
Ligand ADN B 502



Bond lengths



Bond angles



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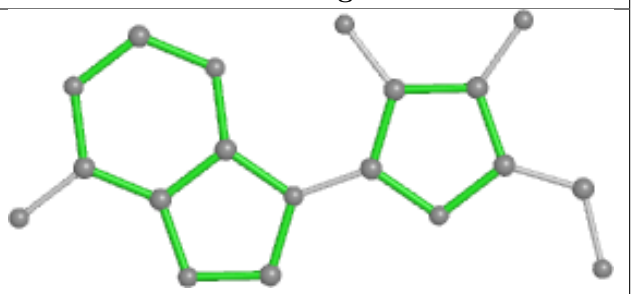
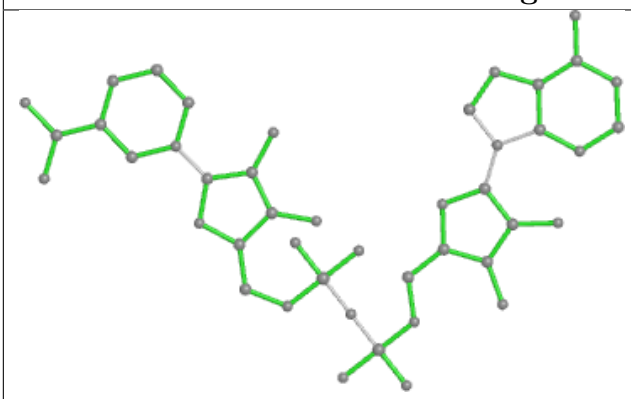
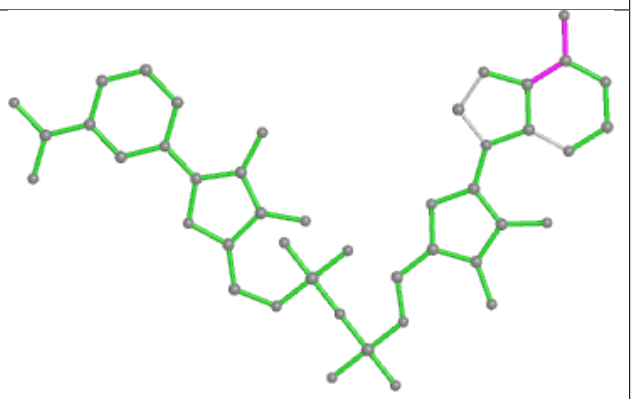


Rings

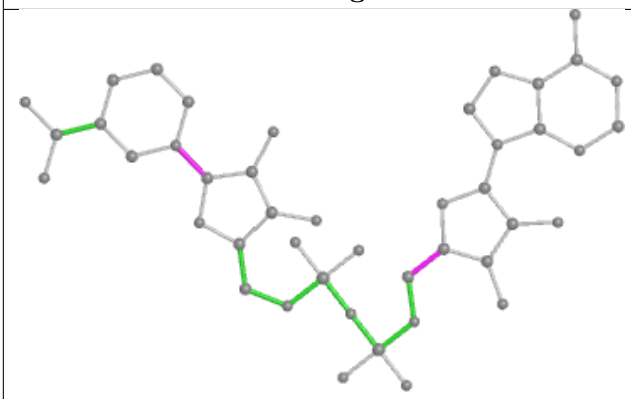
Ligand NAD B 501



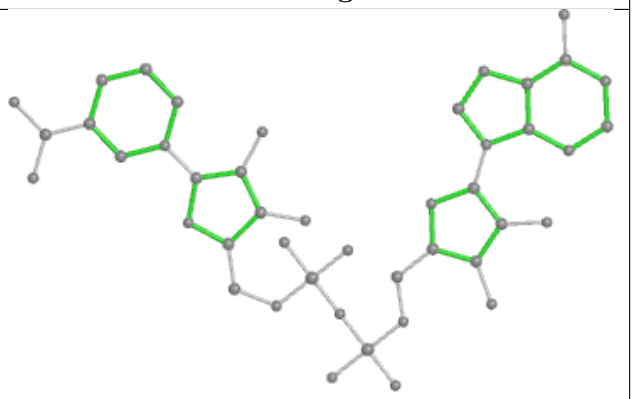
Bond lengths



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	461/472 (97%)	-0.06	8 (1%)	70	72	22, 32, 50, 73	0
1	B	460/472 (97%)	0.15	27 (5%)	22	24	23, 38, 64, 79	0
1	C	461/472 (97%)	-0.01	15 (3%)	46	47	25, 35, 54, 72	0
1	D	461/472 (97%)	0.27	38 (8%)	11	12	23, 37, 62, 76	0
All	All	1843/1888 (97%)	0.09	88 (4%)	30	32	22, 35, 59, 79	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	PHE	7.5
1	B	409	LEU	5.8
1	D	412	ALA	5.6
1	A	355	ASP	5.4
1	D	411	ALA	5.3
1	D	413	GLU	4.9
1	D	9	GLY	4.9
1	A	9	GLY	4.7
1	B	414	LYS	4.6
1	D	415	ALA	4.4
1	B	413	GLU	4.2
1	C	355	ASP	4.1
1	B	411	ALA	4.0
1	B	410	PRO	3.9
1	B	412	ALA	3.7
1	C	9	GLY	3.6
1	D	118	TRP	3.6
1	D	238[A]	GLN	3.5
1	B	10	PHE	3.5
1	D	240	LEU	3.5
1	D	410	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	360	HIS	3.4
1	D	11	THR	3.4
1	B	415	ALA	3.3
1	D	48	GLN	3.3
1	D	409	LEU	3.2
1	C	238[A]	GLN	3.2
1	D	207	LEU	3.1
1	D	46	ALA	3.1
1	B	279	THR	3.0
1	D	218	LEU	2.9
1	B	277	ASP	2.9
1	D	278	GLY	2.9
1	D	416	LYS	2.9
1	D	407	ALA	2.7
1	B	417	ARG	2.7
1	C	207	LEU	2.7
1	B	47	GLY	2.7
1	B	278	GLY	2.7
1	B	276	ASN	2.7
1	C	219	LEU	2.6
1	D	265	PHE	2.6
1	B	416	LYS	2.6
1	D	279	THR	2.5
1	D	129	GLN	2.5
1	D	275	ILE	2.4
1	B	11	THR	2.4
1	B	118	TRP	2.4
1	B	48	GLN	2.4
1	D	244	GLY	2.4
1	D	201	TYR	2.4
1	A	11	THR	2.4
1	D	276	ASN	2.4
1	B	132	ASP	2.3
1	D	417	ARG	2.3
1	B	207	LEU	2.3
1	C	359	ALA	2.3
1	D	219	LEU	2.3
1	D	157	ARG	2.3
1	D	127	ASP	2.3
1	B	218	LEU	2.3
1	D	235	GLY	2.3
1	C	279	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	354	LYS	2.3
1	B	408	ASP	2.2
1	A	235	GLY	2.2
1	B	264	GLY	2.2
1	C	114	GLU	2.2
1	B	240	LEU	2.2
1	A	356	GLY	2.2
1	B	177	LYS	2.2
1	D	246	ILE	2.2
1	D	277	ASP	2.2
1	A	449	LYS	2.1
1	C	235	GLY	2.1
1	C	127	ASP	2.1
1	D	119	CYS	2.1
1	C	206	SER	2.1
1	C	448	PRO	2.1
1	A	207	LEU	2.1
1	C	352	THR	2.0
1	D	232	VAL	2.0
1	C	118	TRP	2.0
1	D	122	GLN	2.0
1	D	153	GLN	2.0
1	B	418	LEU	2.0
1	B	203	CYS	2.0
1	D	114	GLU	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)

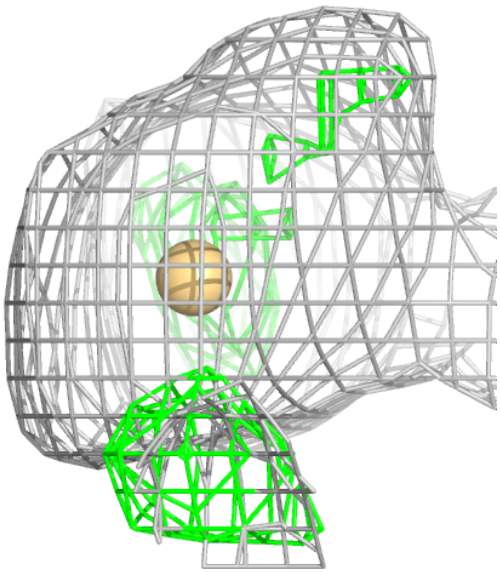
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

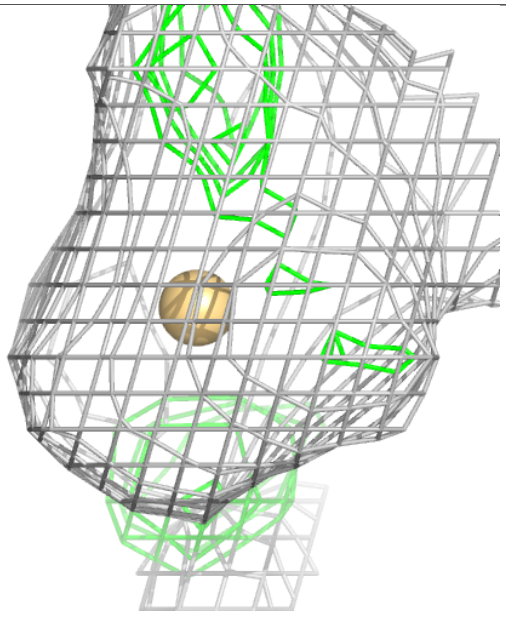
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BU1	C	505	6/6	0.59	0.19	54,62,66,71	0
4	BU1	C	504	6/6	0.70	0.21	54,60,70,76	0
4	BU1	D	503	6/6	0.75	0.17	55,61,68,81	0
4	BU1	A	503	6/6	0.76	0.09	49,57,60,64	0
5	PDO	A	506	5/5	0.84	0.22	52,55,68,69	0
8	HEZ	B	503	8/8	0.85	0.11	52,58,69,71	0
7	CD	C	510	1/1	0.88	0.11	98,98,98,98	1
5	PDO	A	505	5/5	0.89	0.08	49,52,61,61	0
4	BU1	A	504	6/6	0.90	0.12	50,58,69,73	0
7	CD	A	511	1/1	0.90	0.09	100,100,100,100	1
4	BU1	C	503	6/6	0.91	0.09	51,54,64,71	0
7	CD	D	509	1/1	0.92	0.06	69,69,69,69	1
7	CD	B	506	1/1	0.92	0.05	92,92,92,92	1
7	CD	C	508	1/1	0.93	0.09	99,99,99,99	1
3	ADN	D	502	19/19	0.95	0.09	28,31,37,38	0
2	NAD	C	501	44/44	0.95	0.09	25,29,33,38	0
3	ADN	C	502	19/19	0.95	0.11	25,28,36,39	0
2	NAD	B	501	44/44	0.96	0.08	26,29,31,33	0
7	CD	A	512	1/1	0.96	0.04	91,91,91,91	1
2	NAD	A	501	44/44	0.96	0.10	24,27,29,30	0
2	NAD	D	501	44/44	0.96	0.08	24,28,31,37	0
3	ADN	A	502	19/19	0.96	0.10	21,25,30,31	0
3	ADN	B	502	19/19	0.96	0.11	27,30,34,39	0
7	CD	A	510	1/1	0.96	0.07	73,73,73,73	1
6	K	D	504	1/1	0.97	0.09	38,38,38,38	1
7	CD	D	507	1/1	0.97	0.12	81,81,81,81	1
7	CD	C	509[A]	1/1	0.98	0.05	55,55,55,55	1
7	CD	C	509[B]	1/1	0.98	0.05	81,81,81,81	1
7	CD	B	507[A]	1/1	0.98	0.07	58,58,58,58	1
7	CD	B	507[B]	1/1	0.98	0.07	74,74,74,74	1
7	CD	D	508	1/1	0.98	0.07	66,66,66,66	1
7	CD	B	509	1/1	0.98	0.04	54,54,54,54	1
6	K	B	504	1/1	0.98	0.10	41,41,41,41	1
7	CD	B	508	1/1	0.99	0.03	96,96,96,96	1
6	K	C	506	1/1	0.99	0.10	37,37,37,37	1
7	CD	A	509	1/1	0.99	0.05	49,49,49,49	1
7	CD	D	505	1/1	0.99	0.04	44,44,44,44	1
7	CD	D	506	1/1	1.00	0.05	36,36,36,36	1
6	K	A	507	1/1	1.00	0.07	39,39,39,39	1
7	CD	A	508	1/1	1.00	0.05	31,31,31,31	0
7	CD	C	507	1/1	1.00	0.07	37,37,37,37	1
7	CD	B	505	1/1	1.00	0.06	39,39,39,39	1
9	CL	D	510	1/1	1.00	0.10	32,32,32,32	1

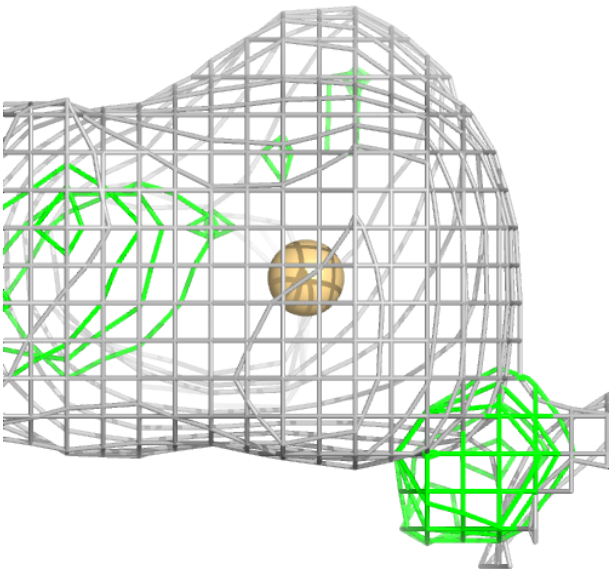
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CD C 510:

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

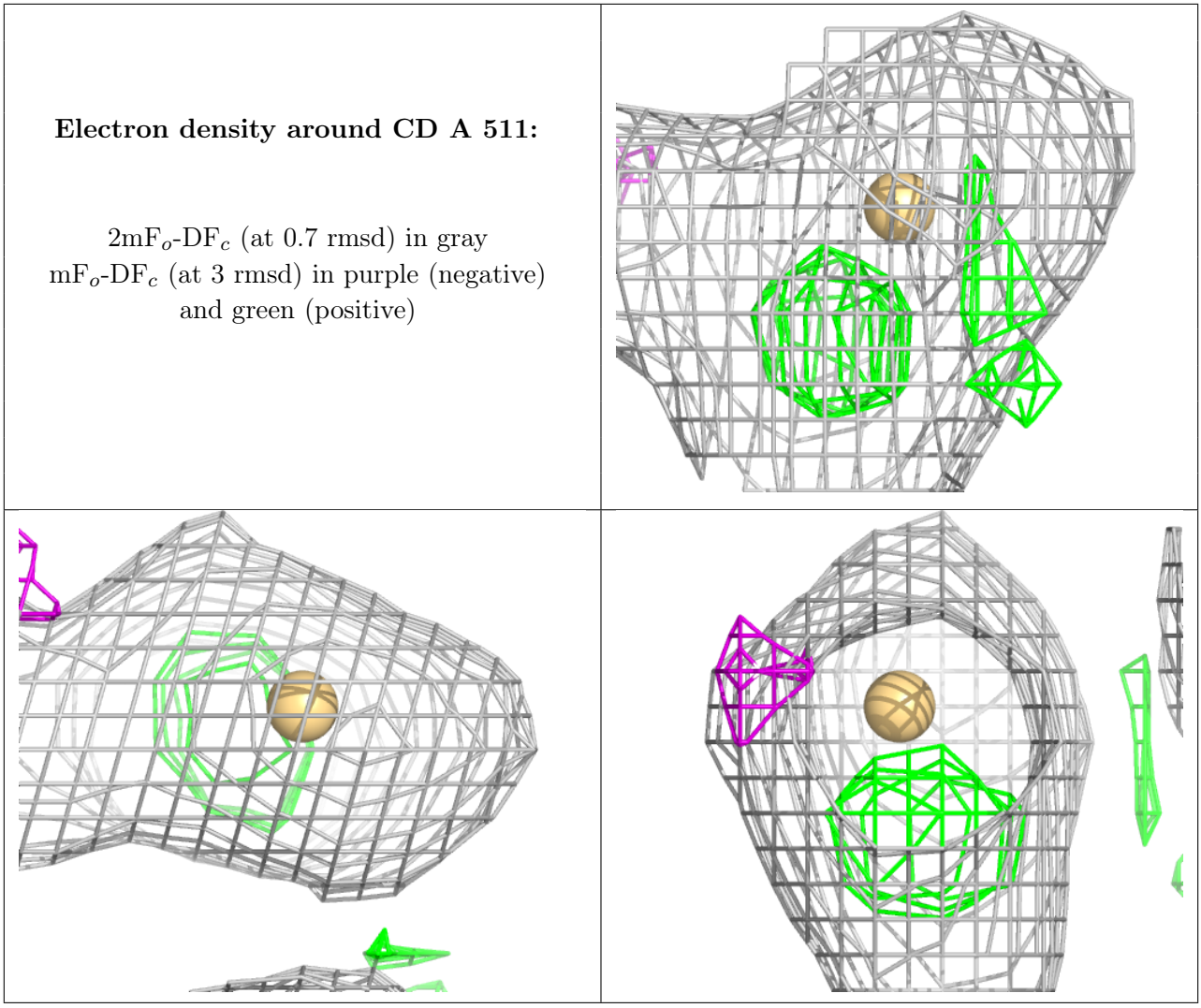






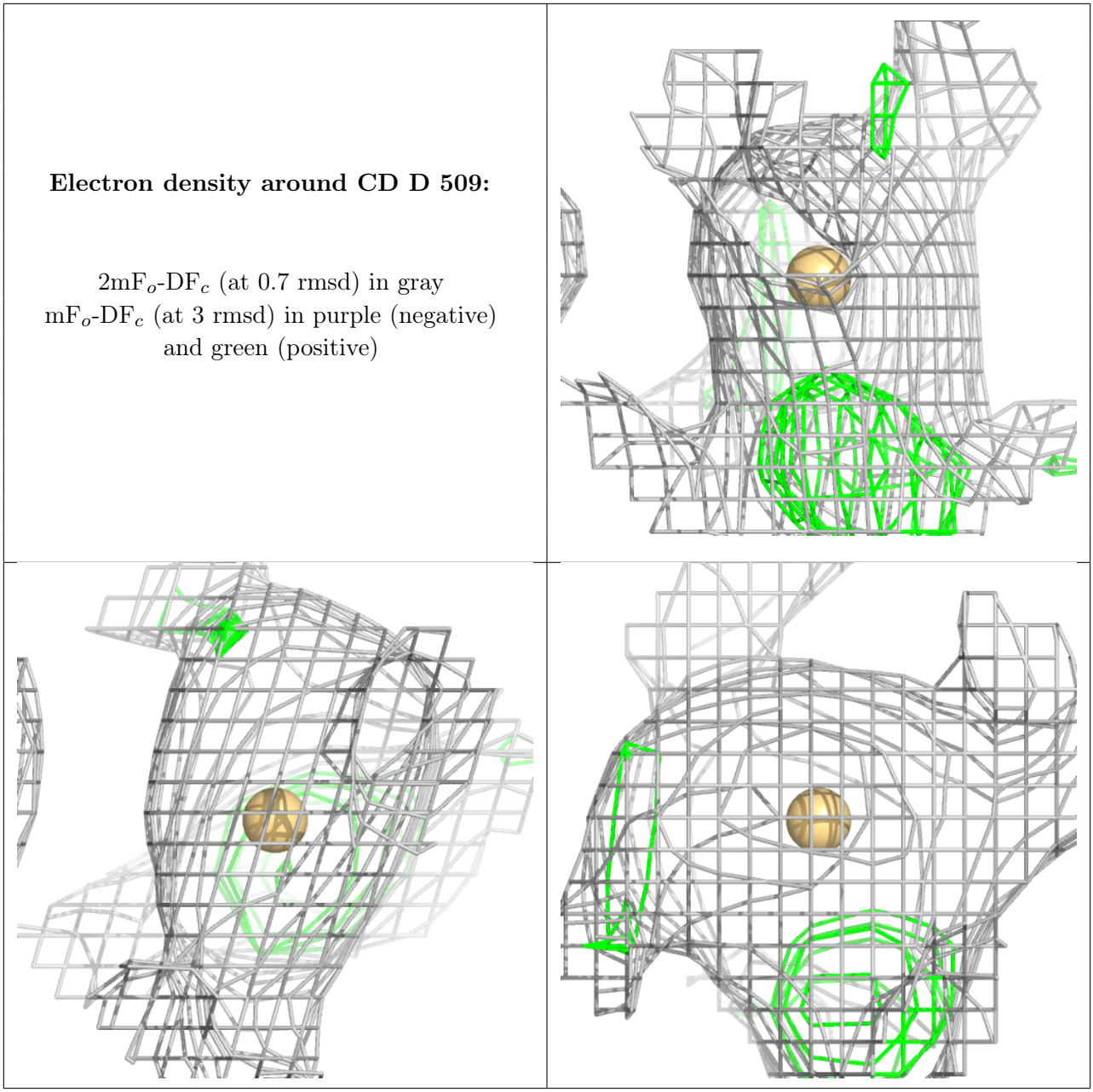
Electron density around CD A 511:

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



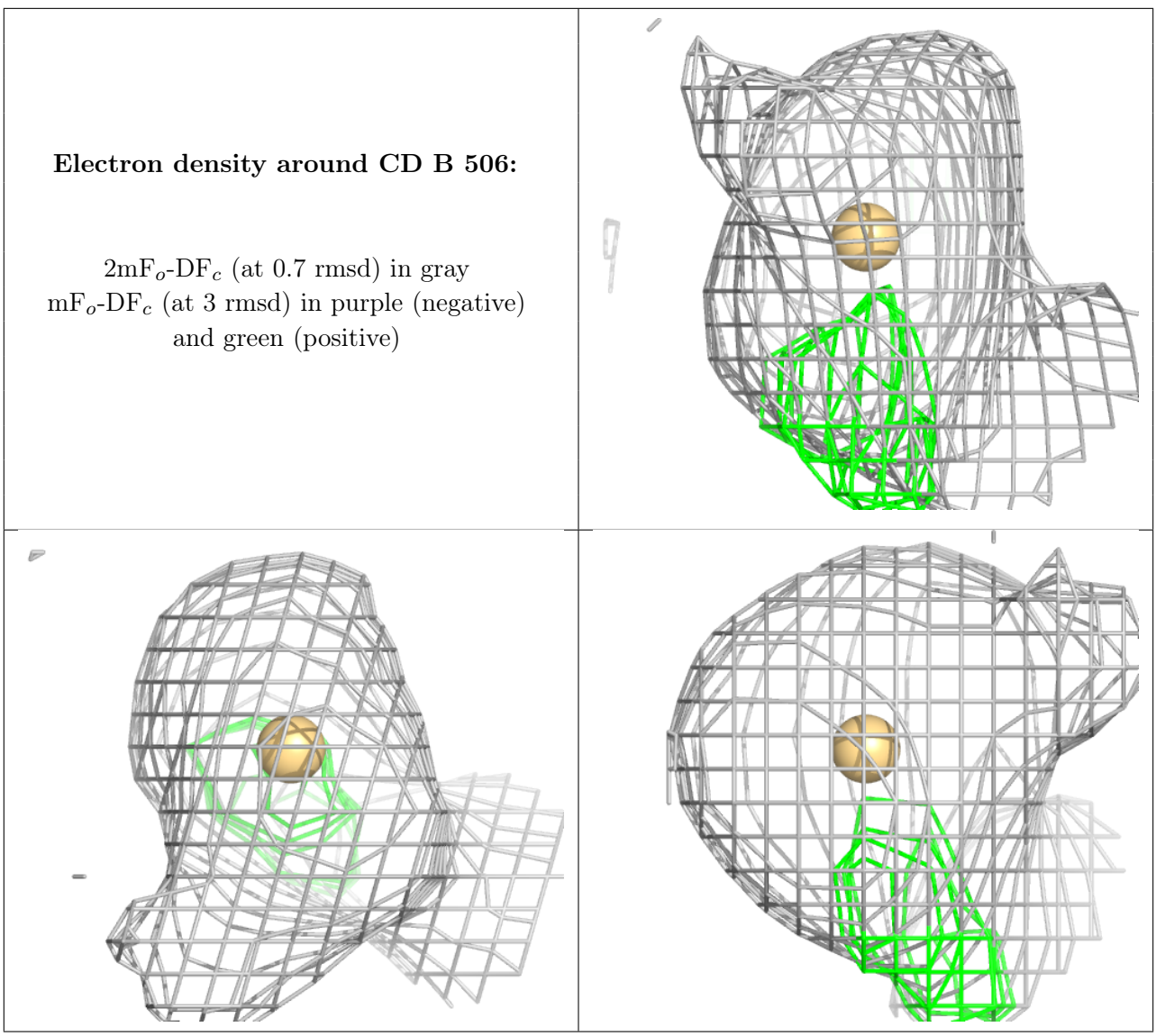
Electron density around CD D 509:

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



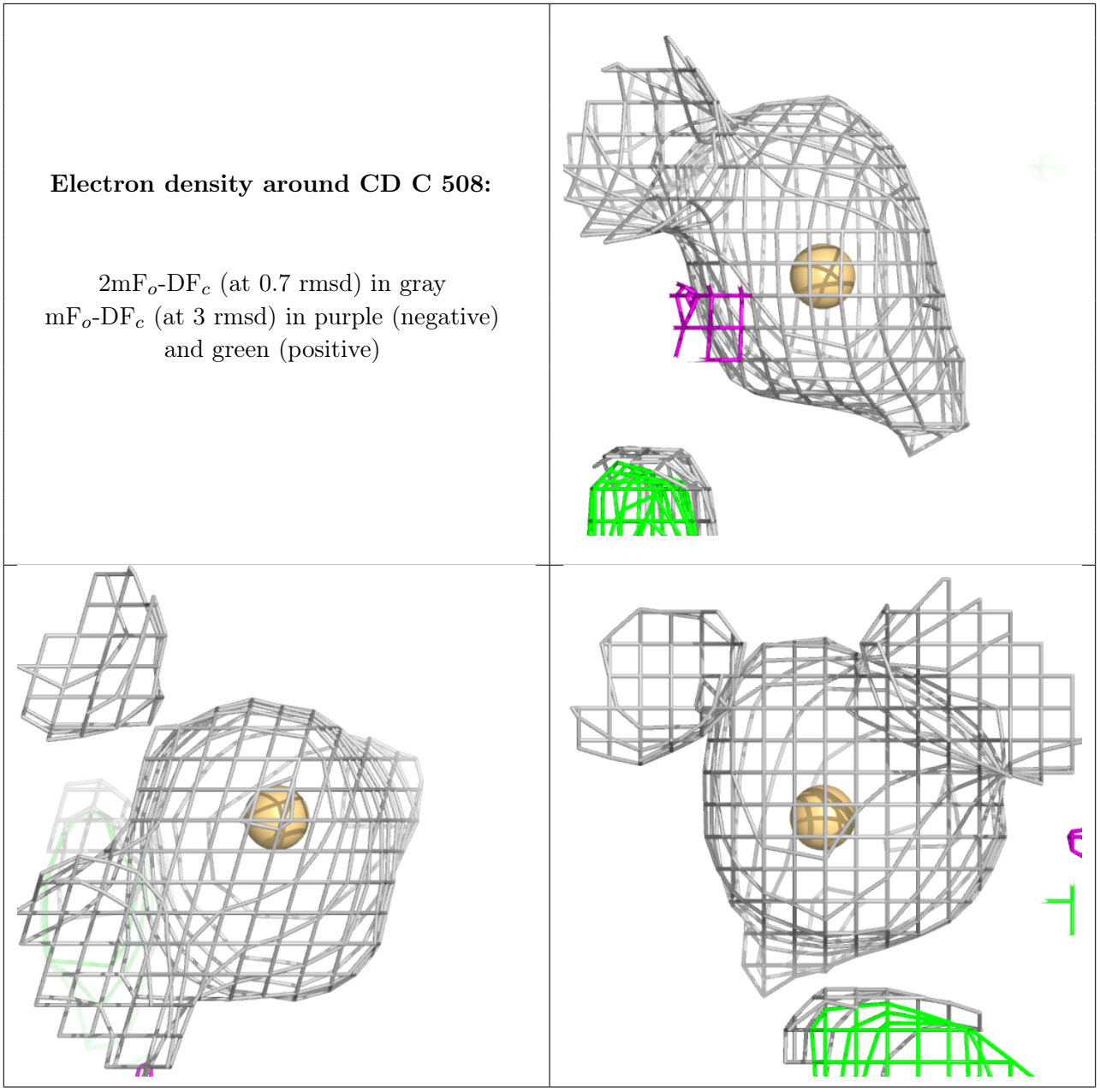
Electron density around CD B 506:

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



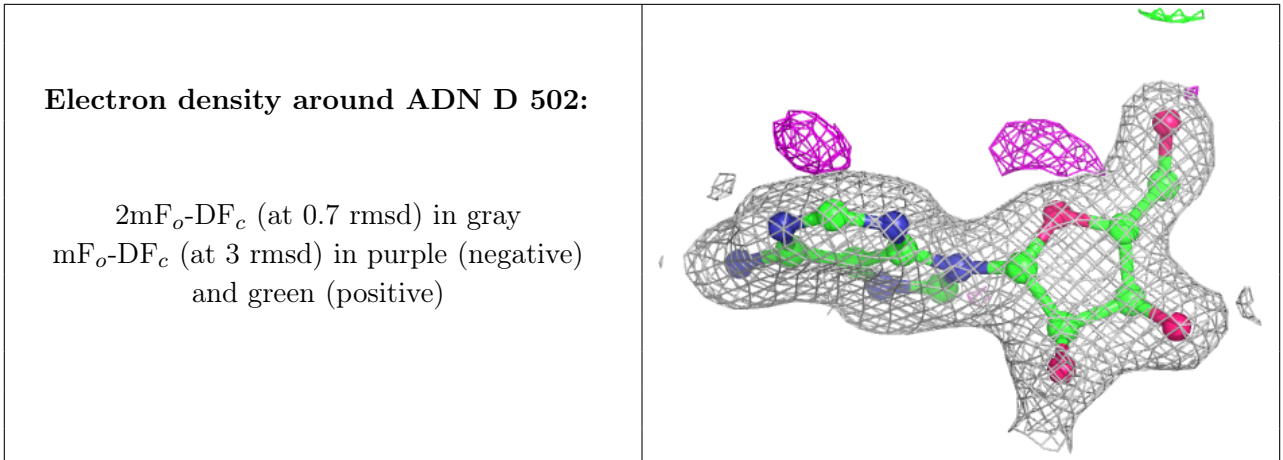
Electron density around CD C 508:

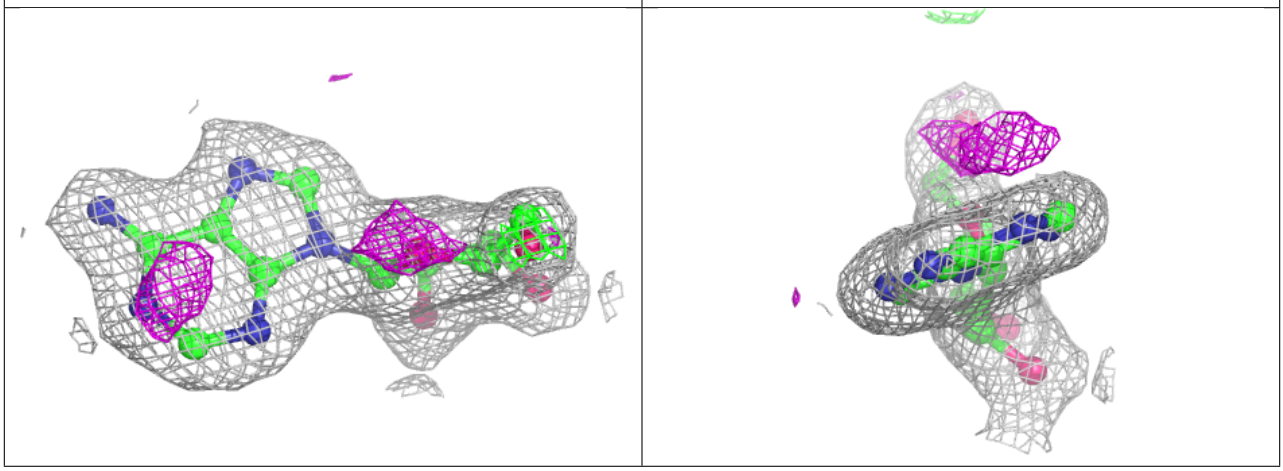
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ADN D 502:

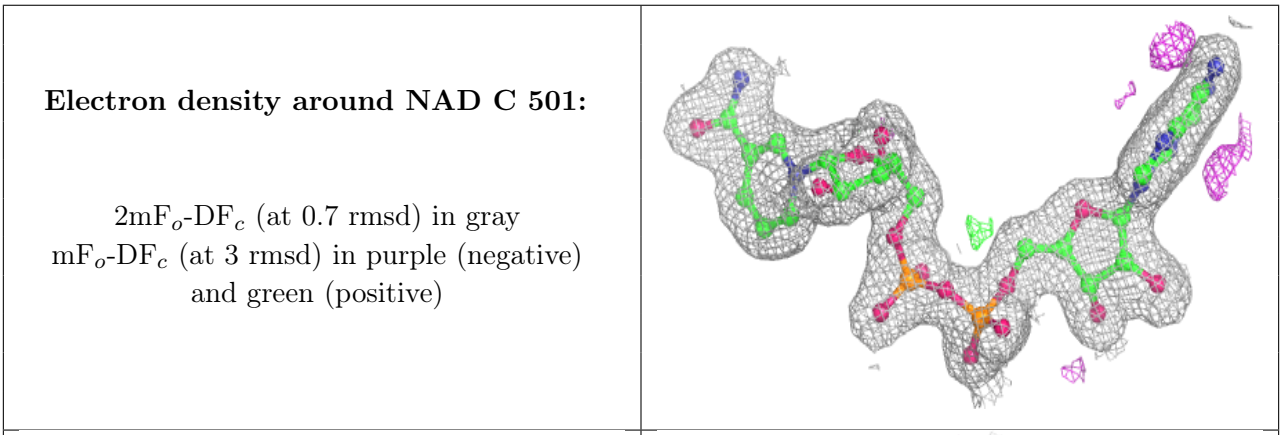
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

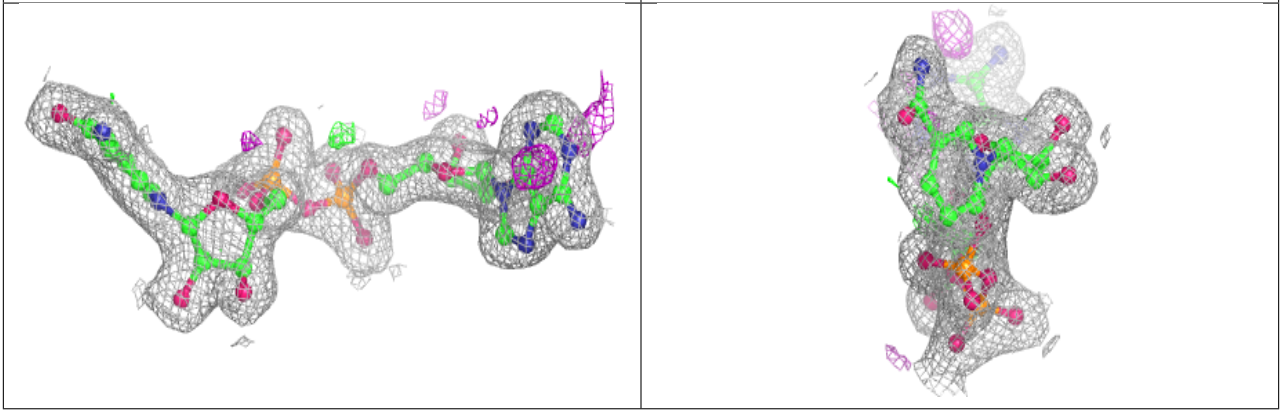




Electron density around NAD C 501:

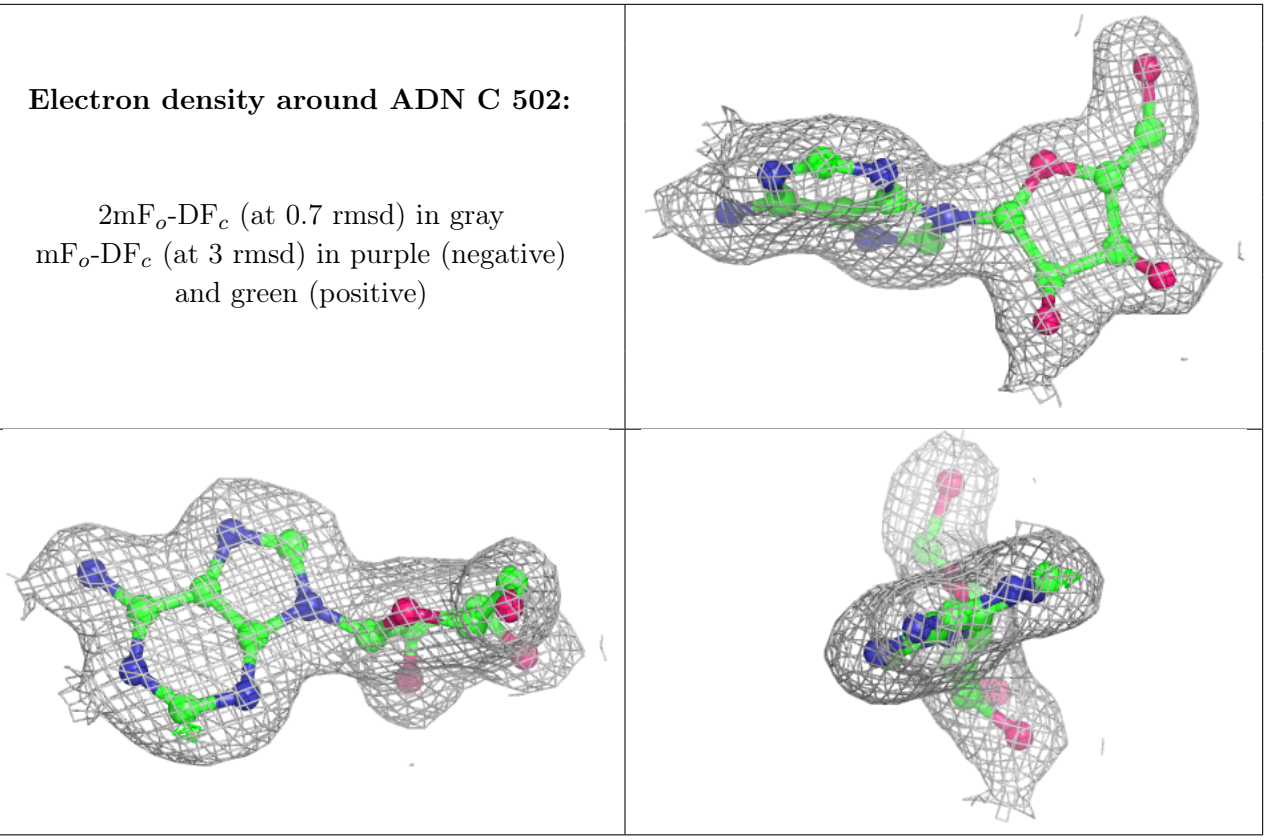
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





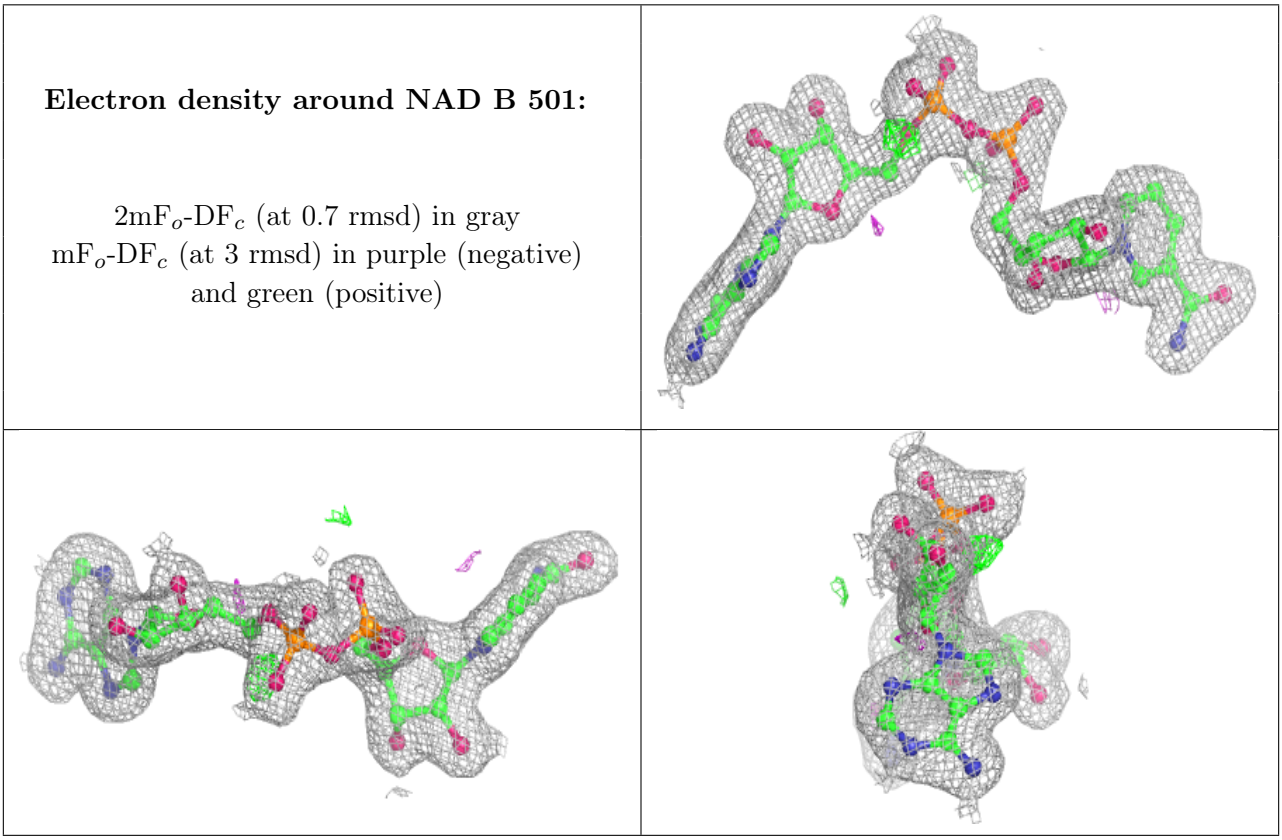
Electron density around ADN C 502:

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



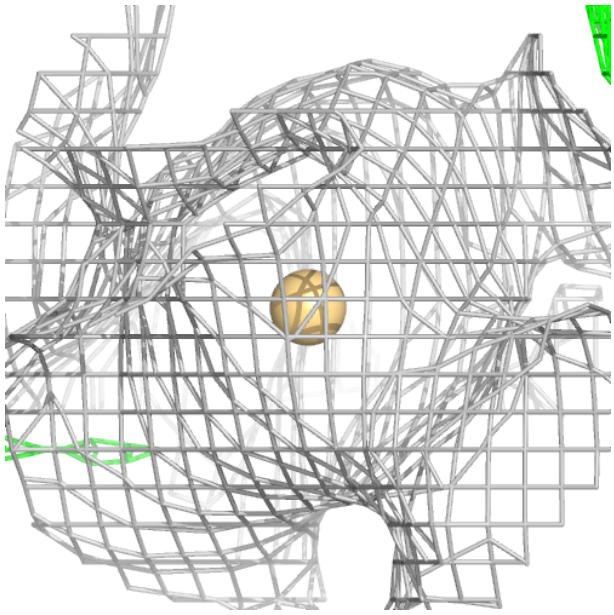
Electron density around NAD B 501:

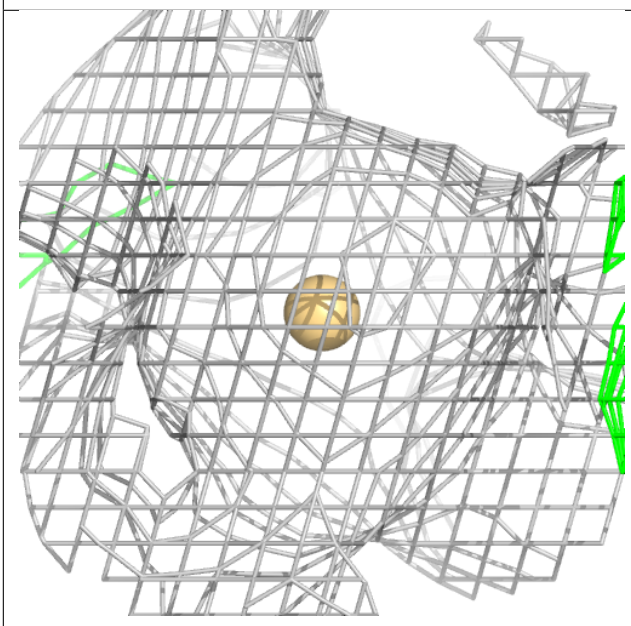
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

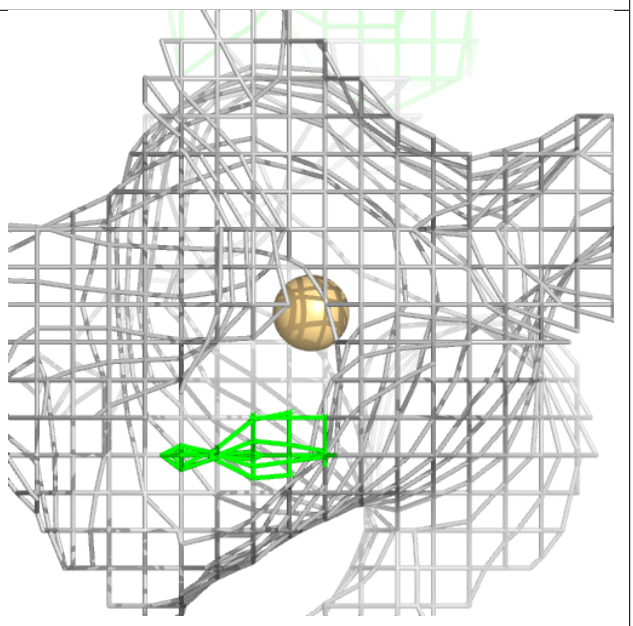


Electron density around CD A 512:

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

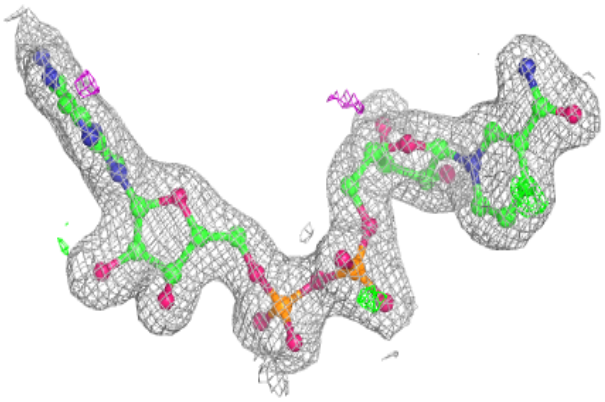


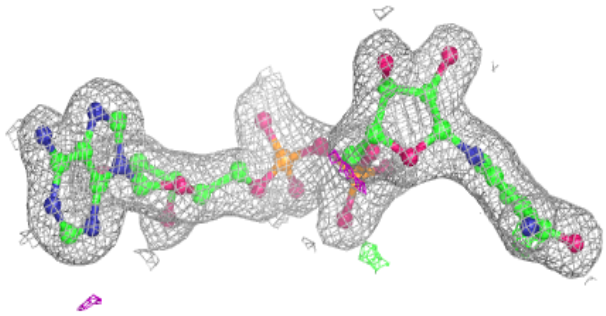


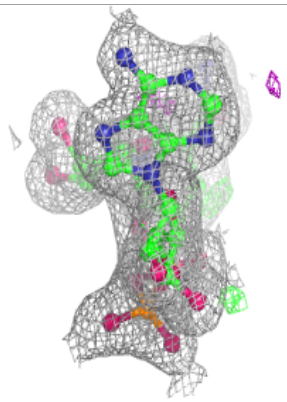


Electron density around NAD A 501:

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

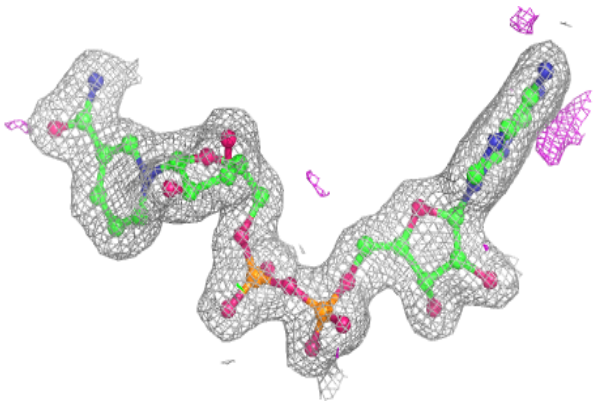


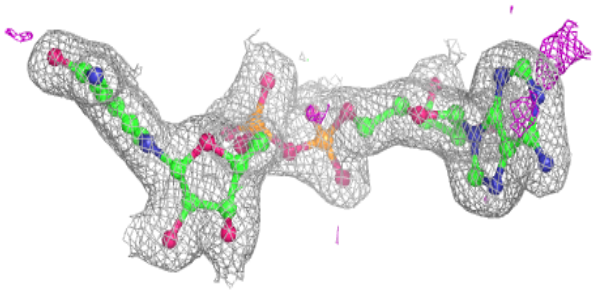


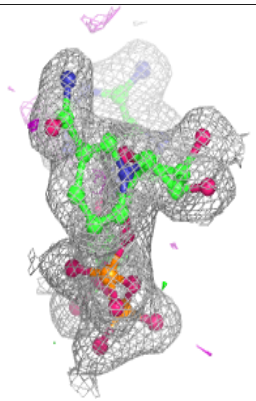


Electron density around NAD D 501:

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

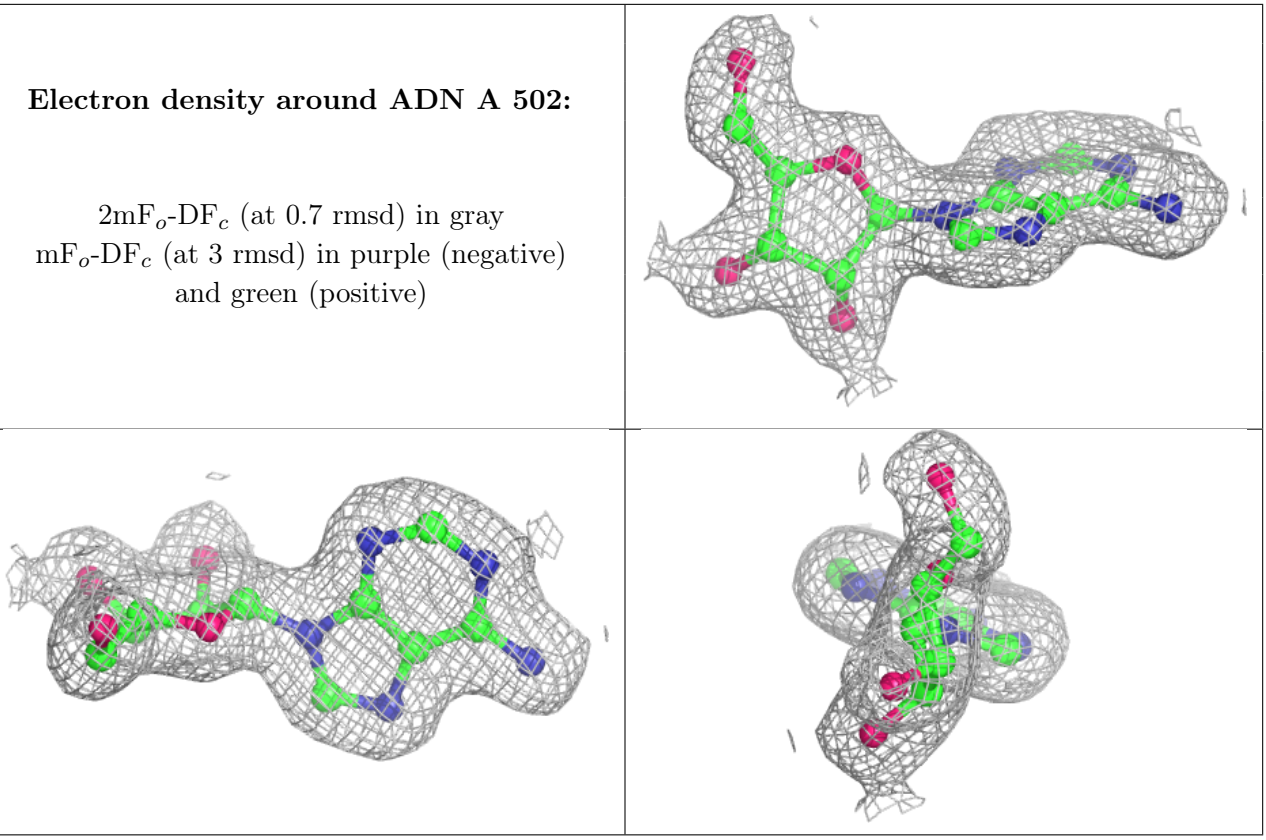






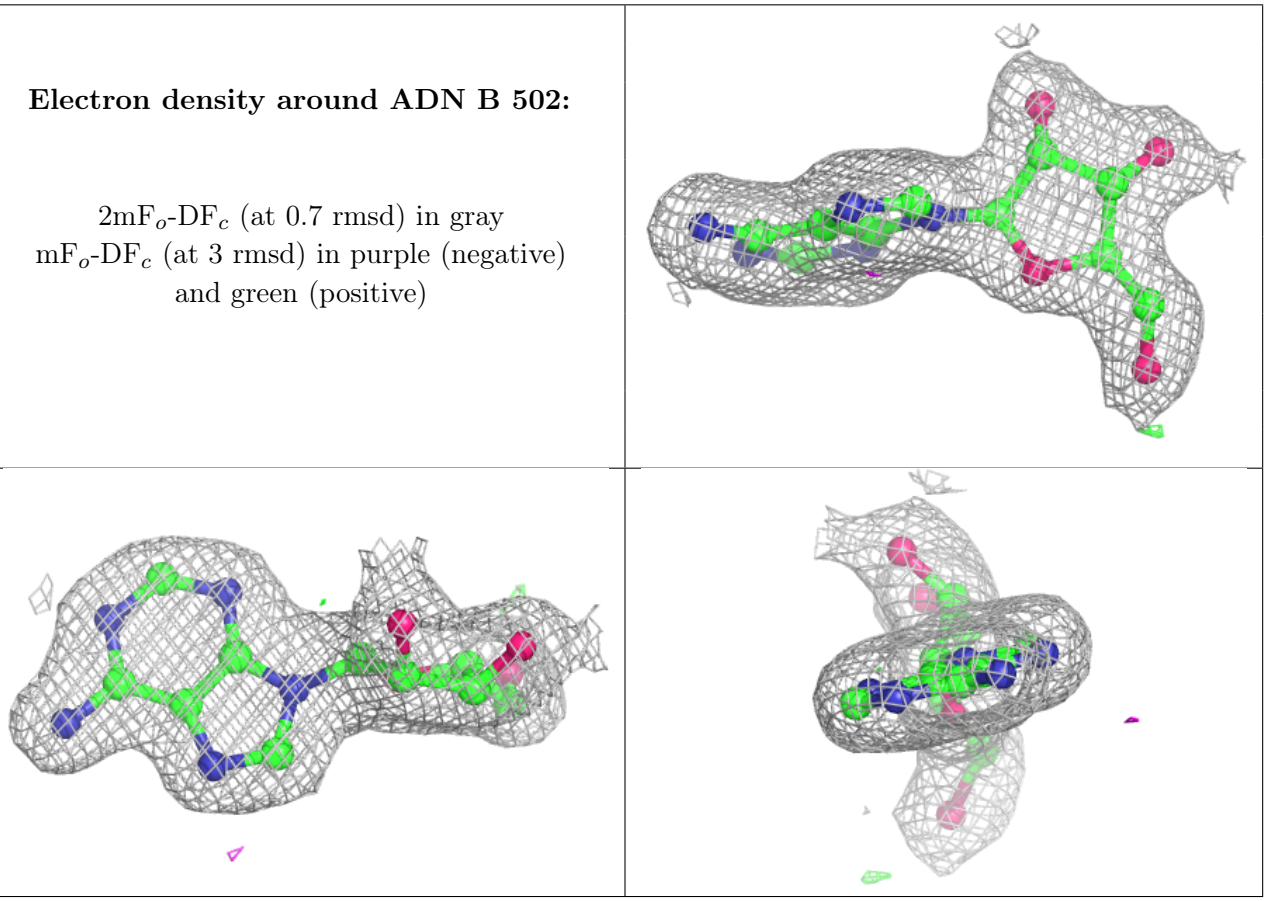
Electron density around ADN A 502:

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



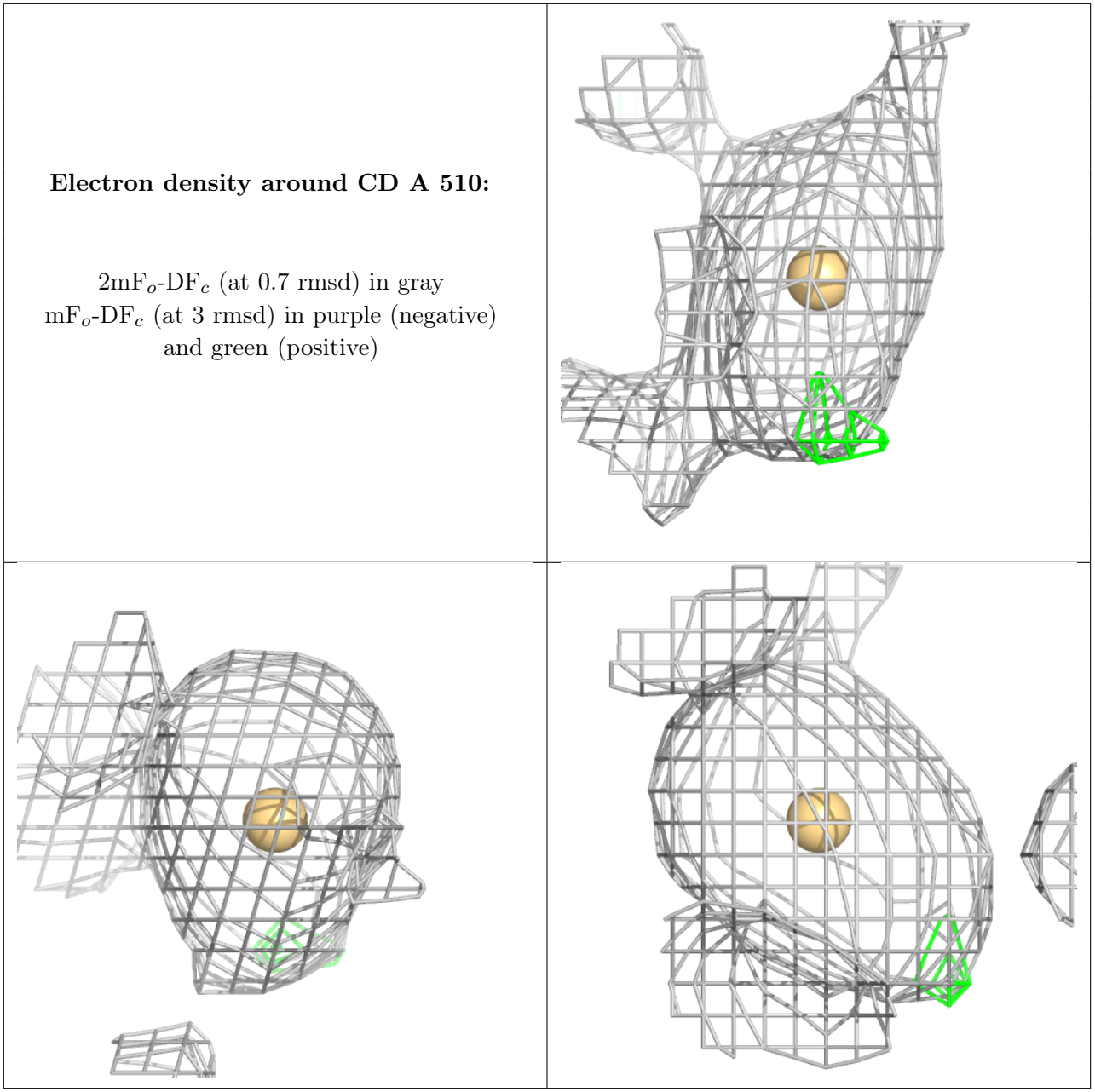
Electron density around ADN B 502:

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



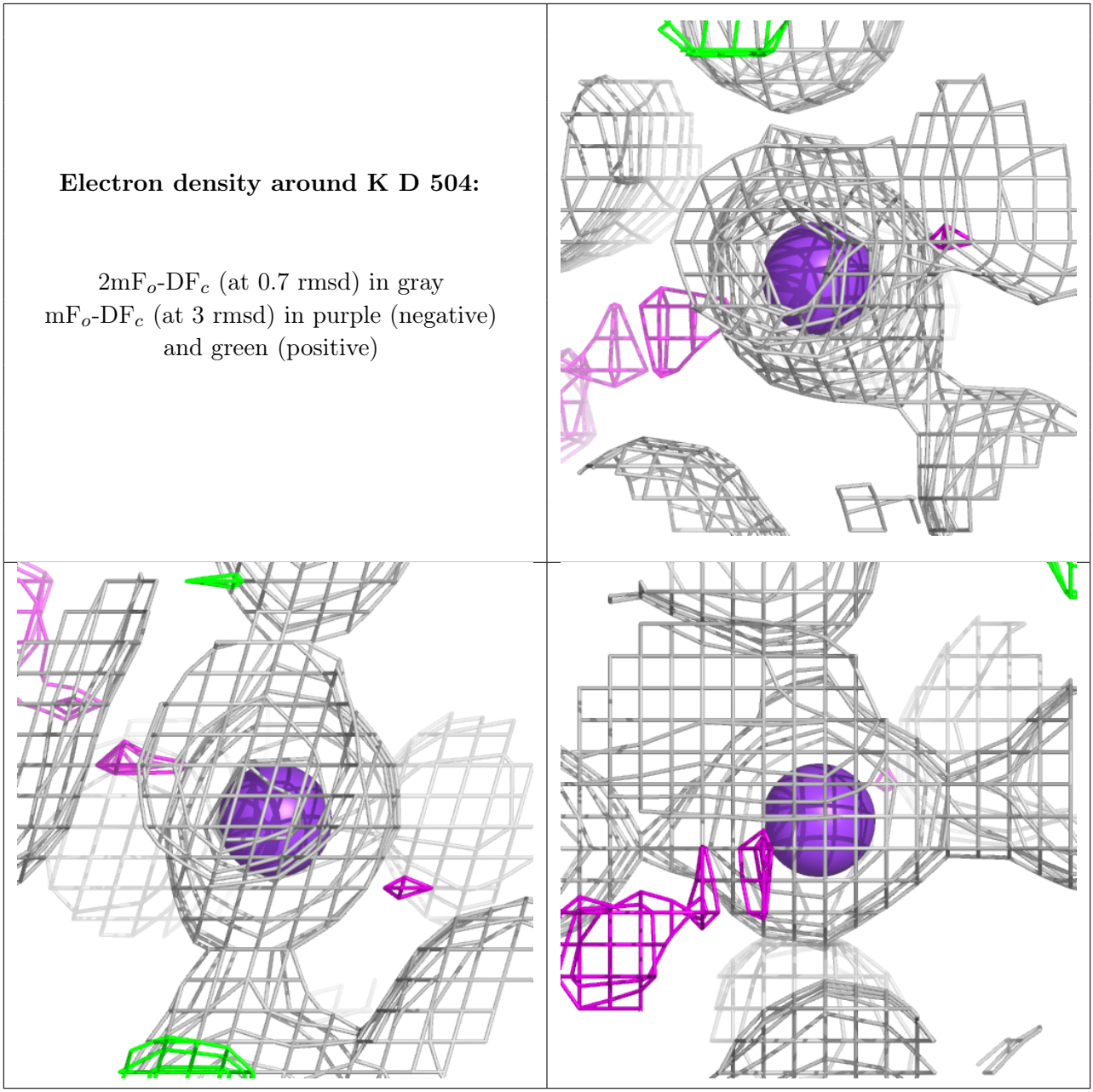
Electron density around CD A 510:

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



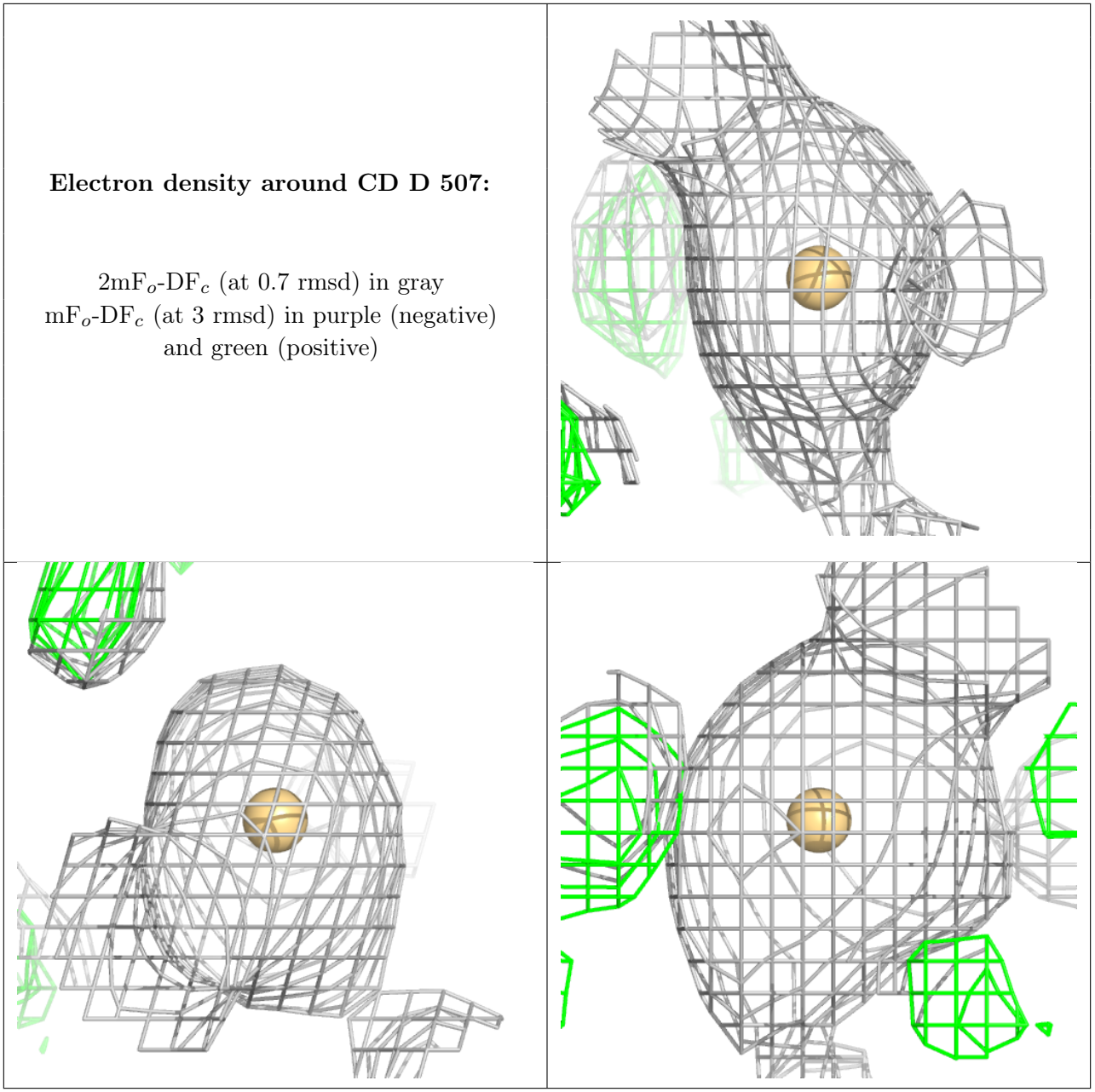
Electron density around K D 504:

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



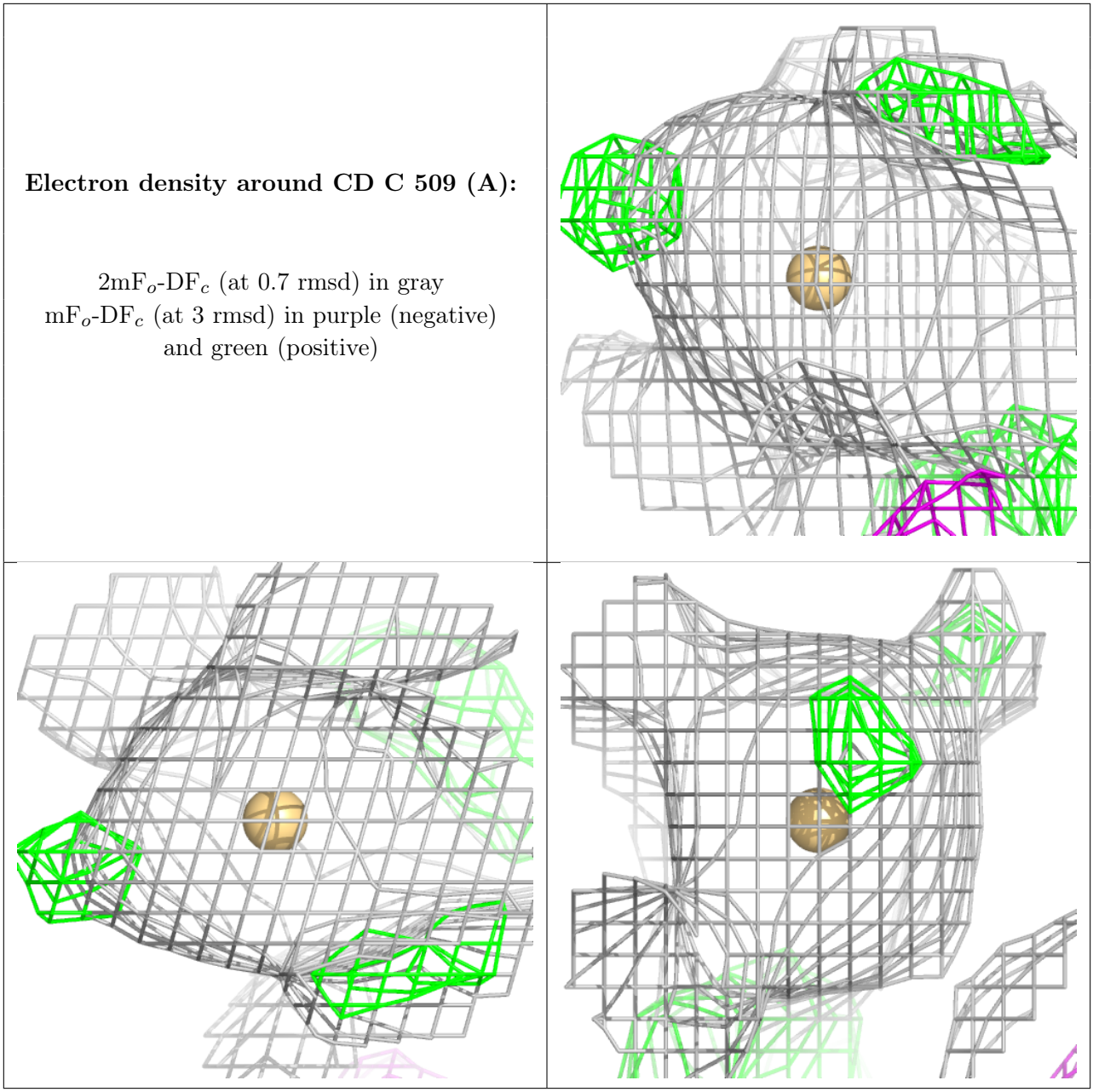
Electron density around CD D 507:

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



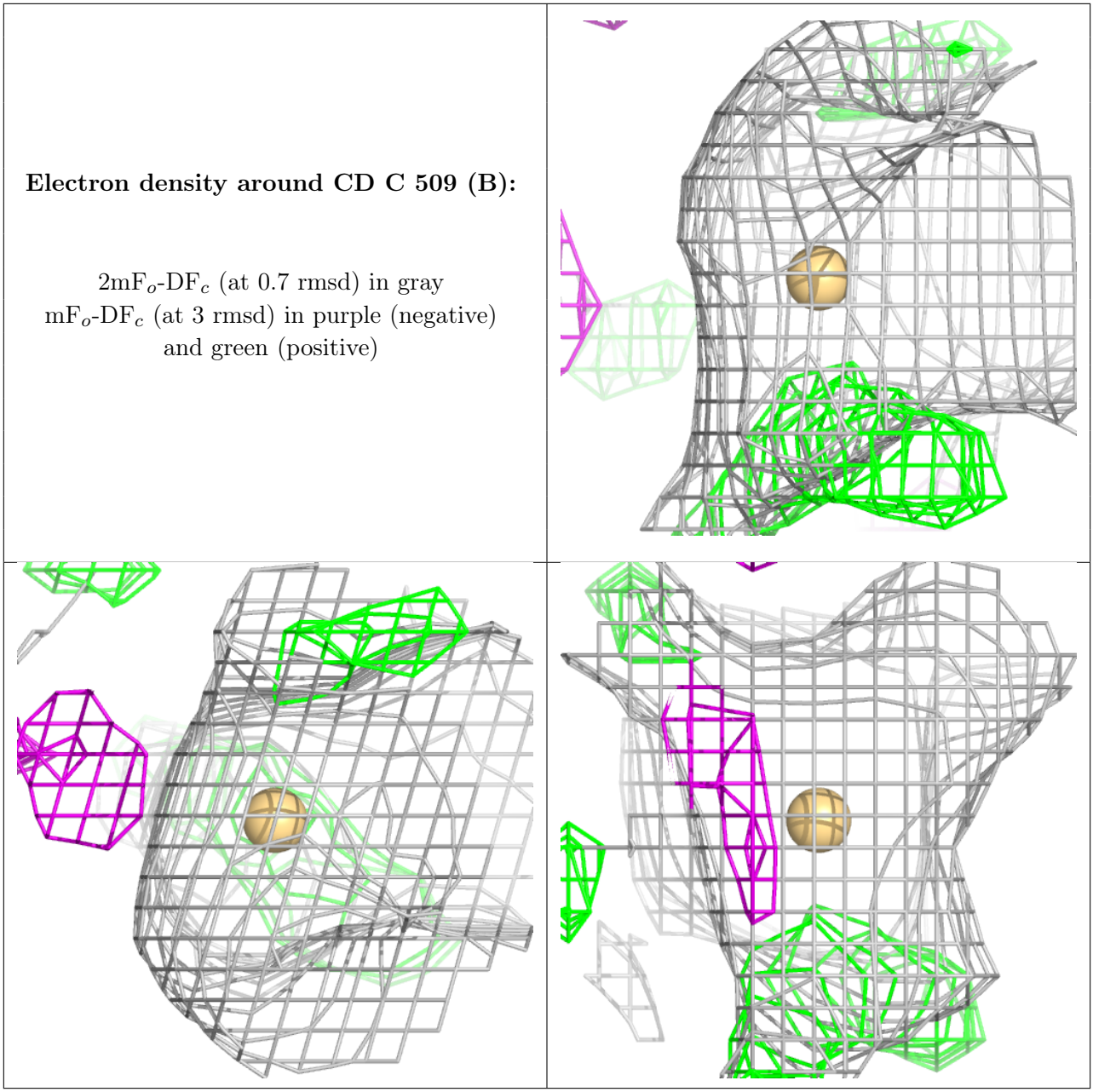
Electron density around CD C 509 (A):

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



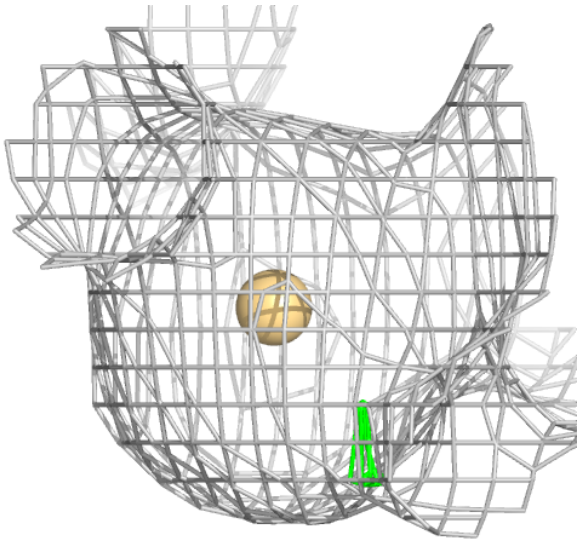
Electron density around CD C 509 (B):

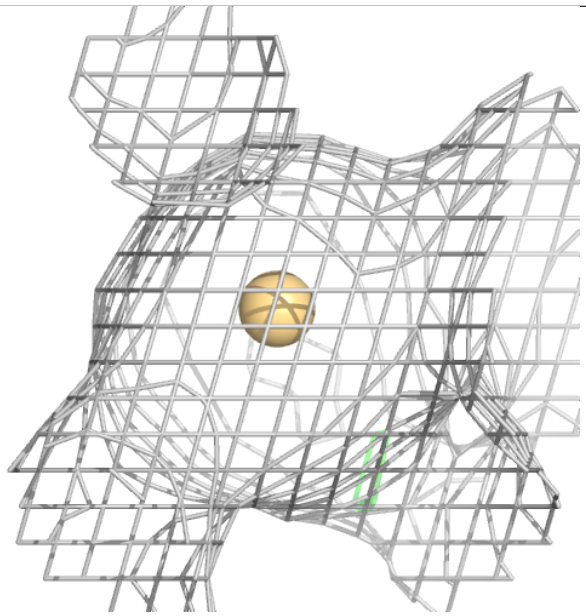
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

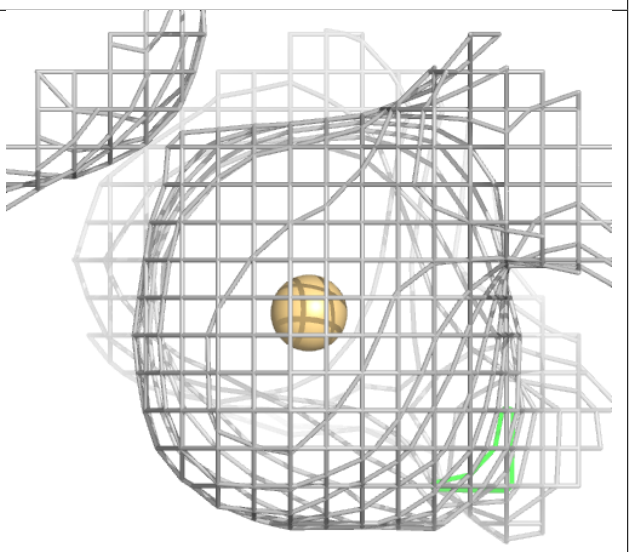


Electron density around CD B 507 (A):

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

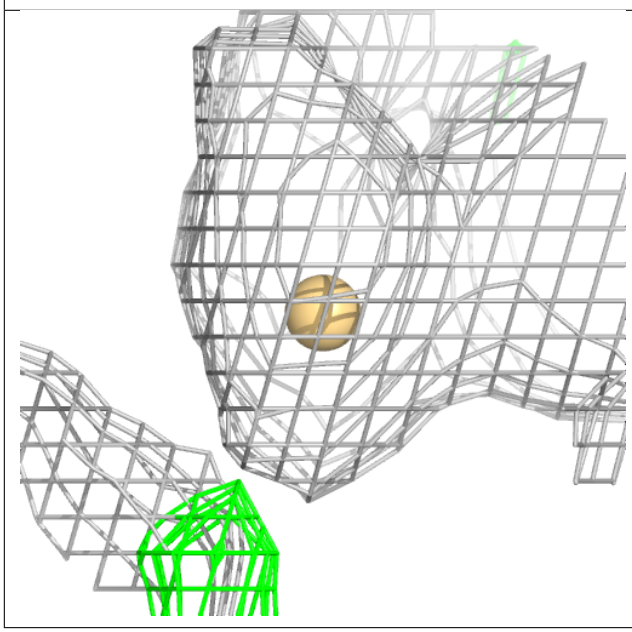


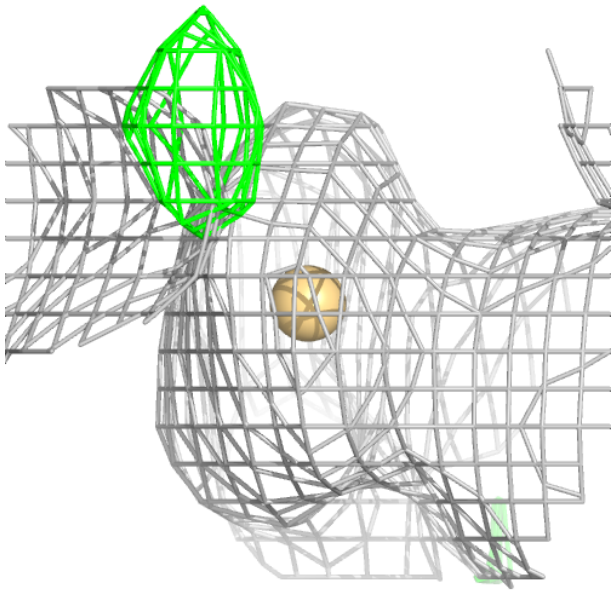


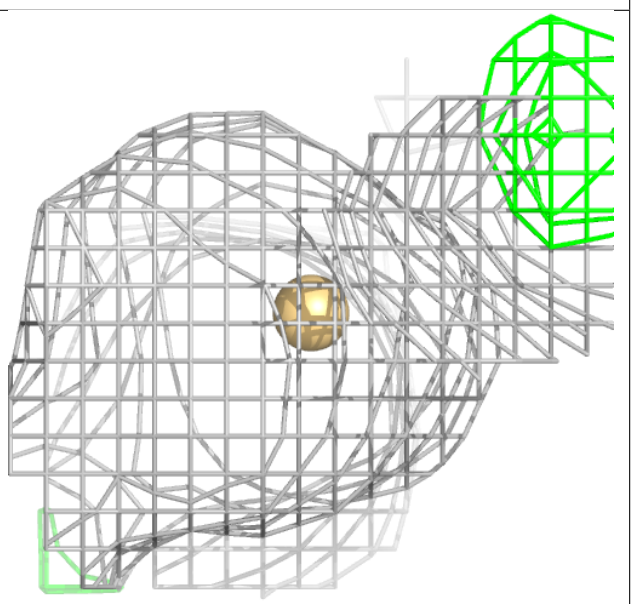


Electron density around CD B 507 (B):

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

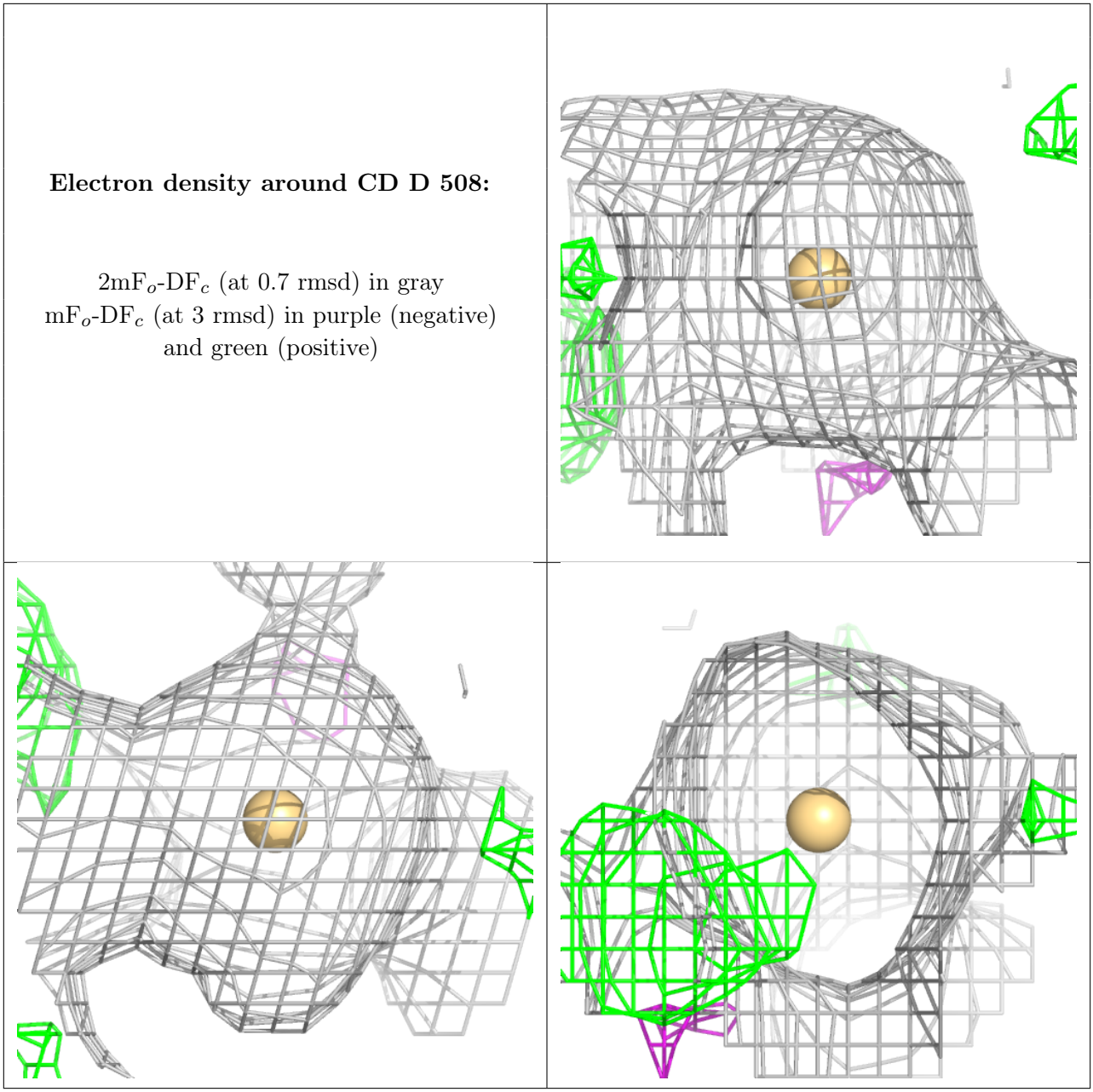






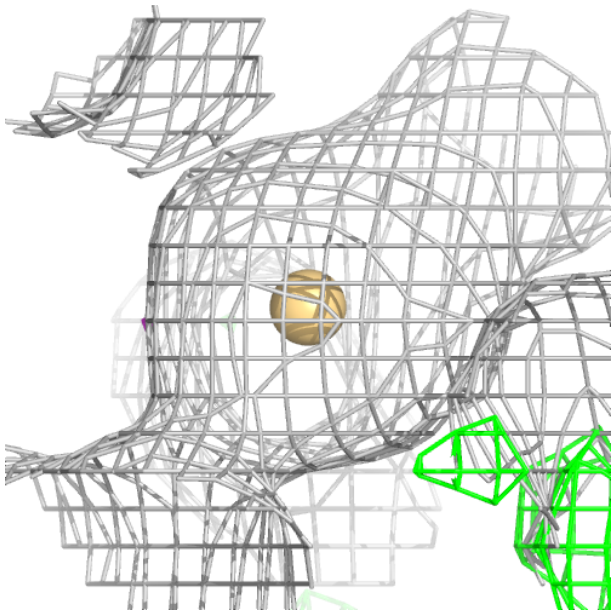
Electron density around CD D 508:

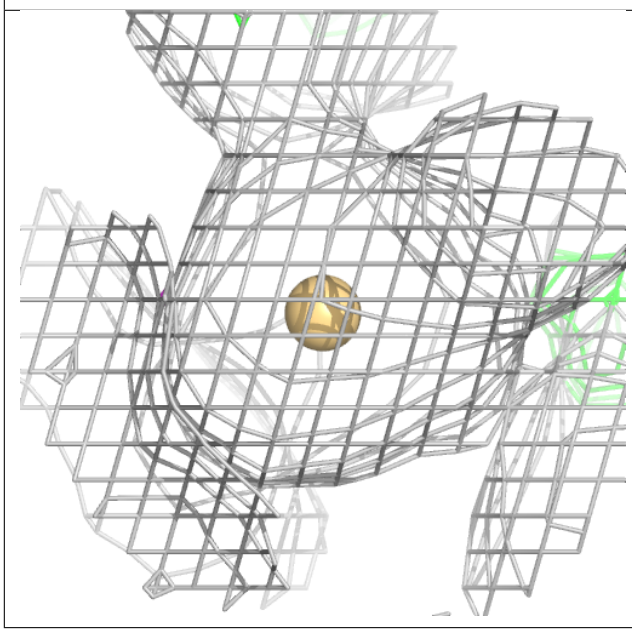
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

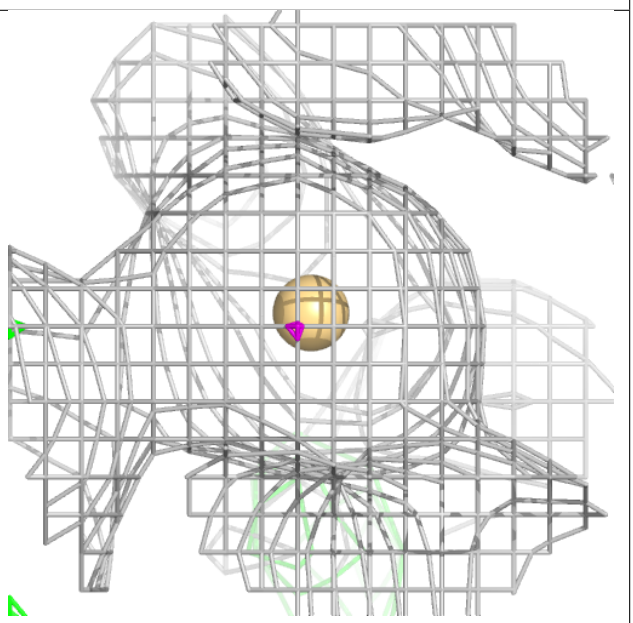


Electron density around CD B 509:

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

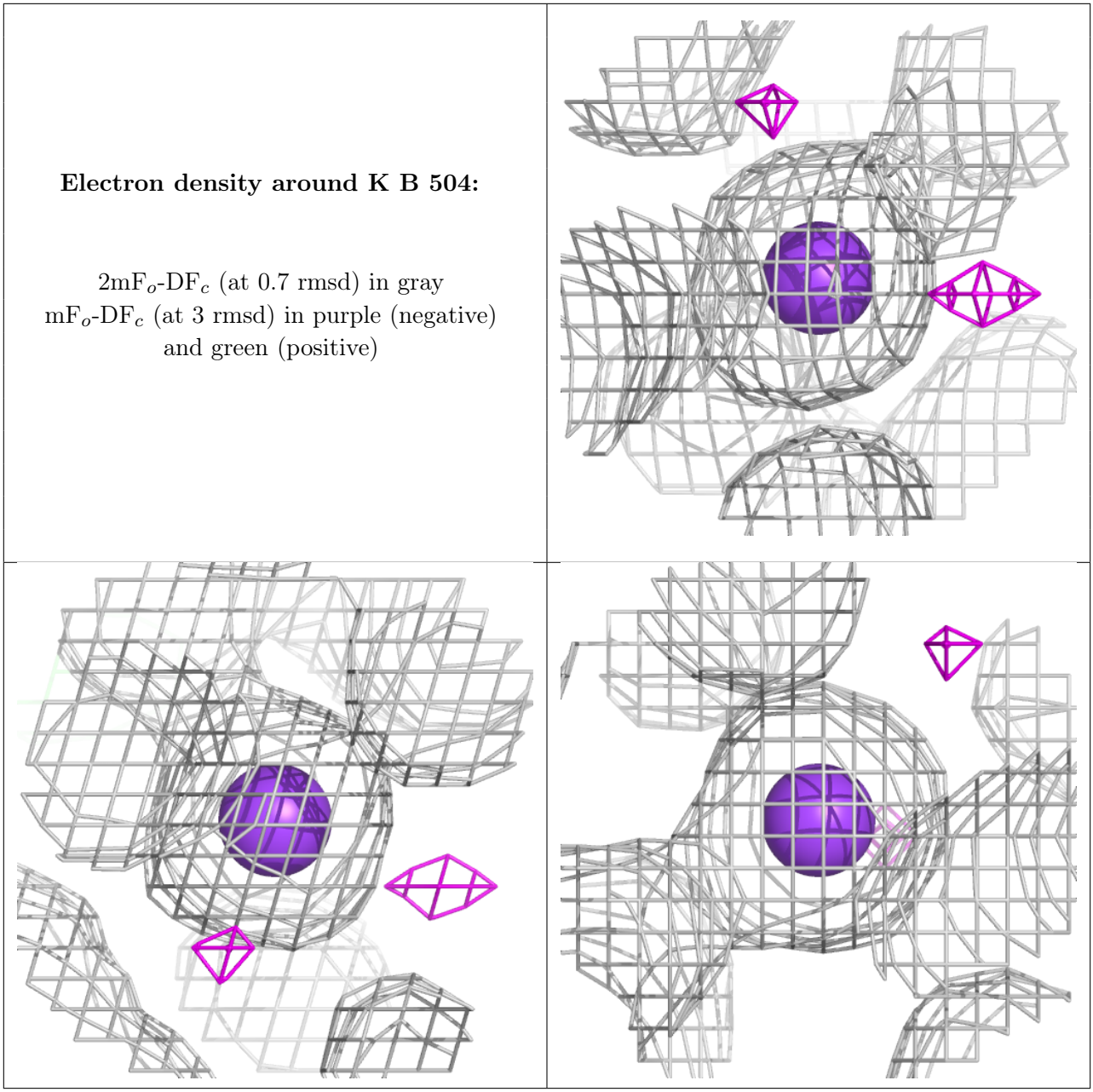






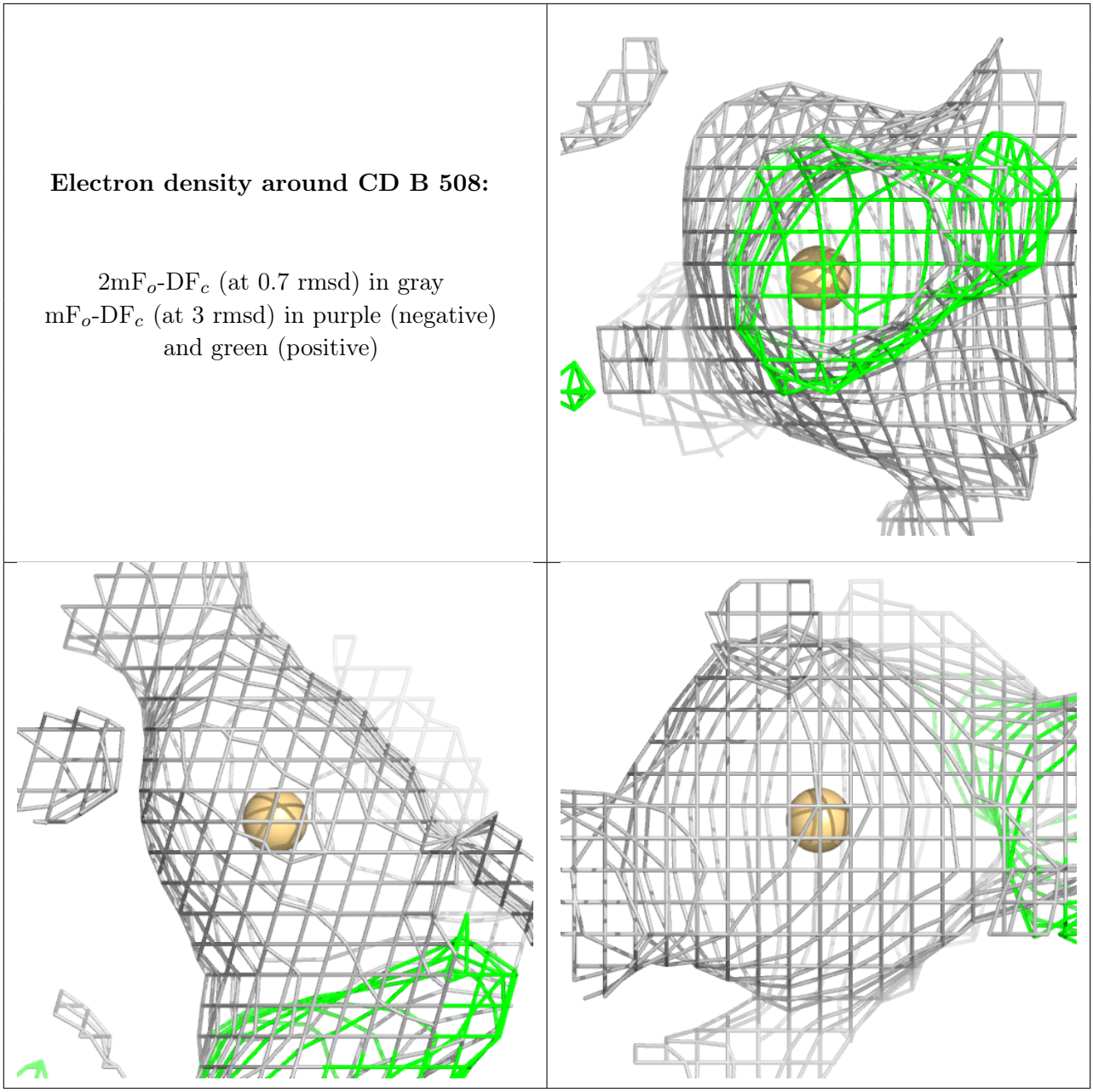
Electron density around K B 504:

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



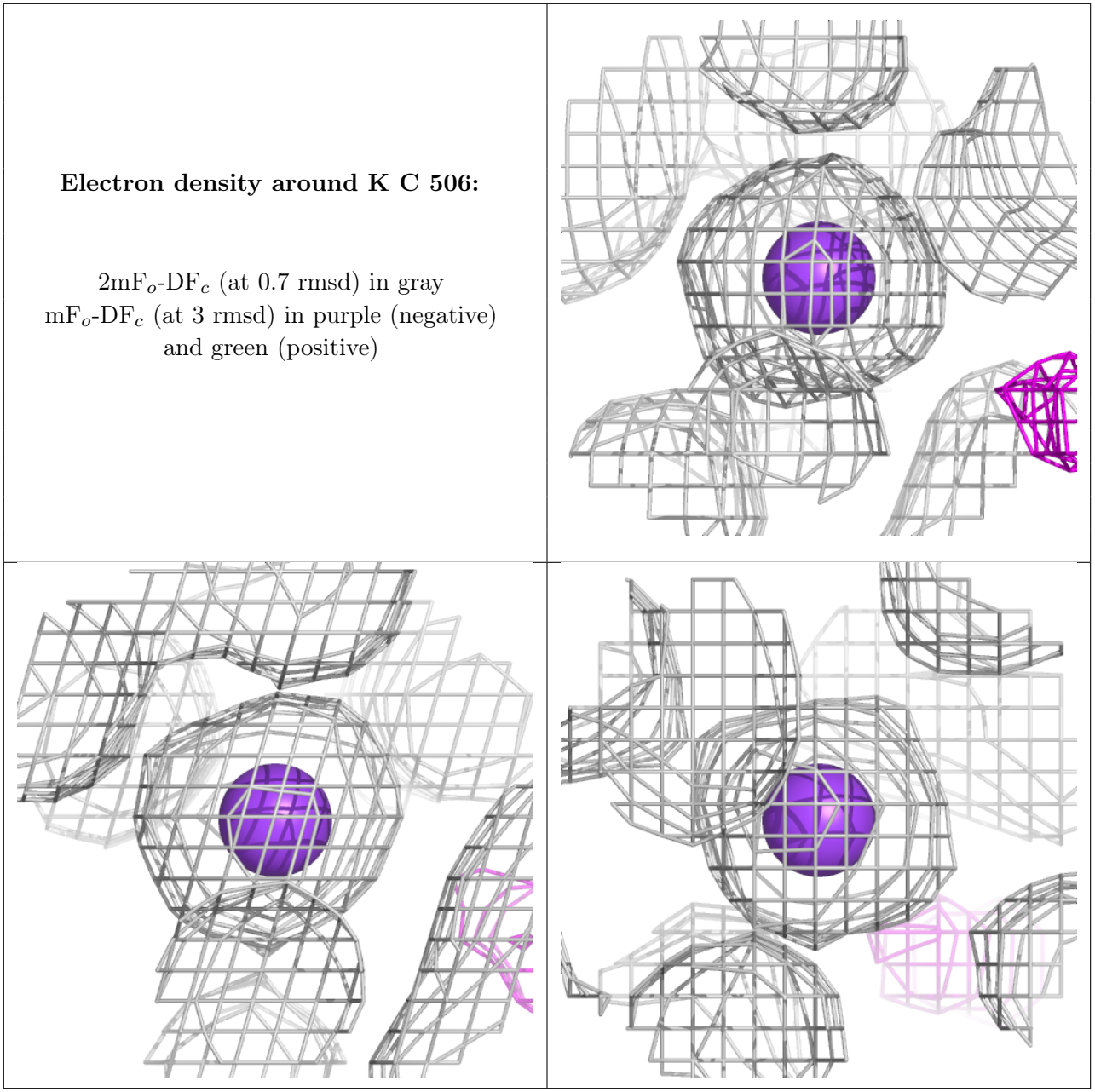
Electron density around CD B 508:

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



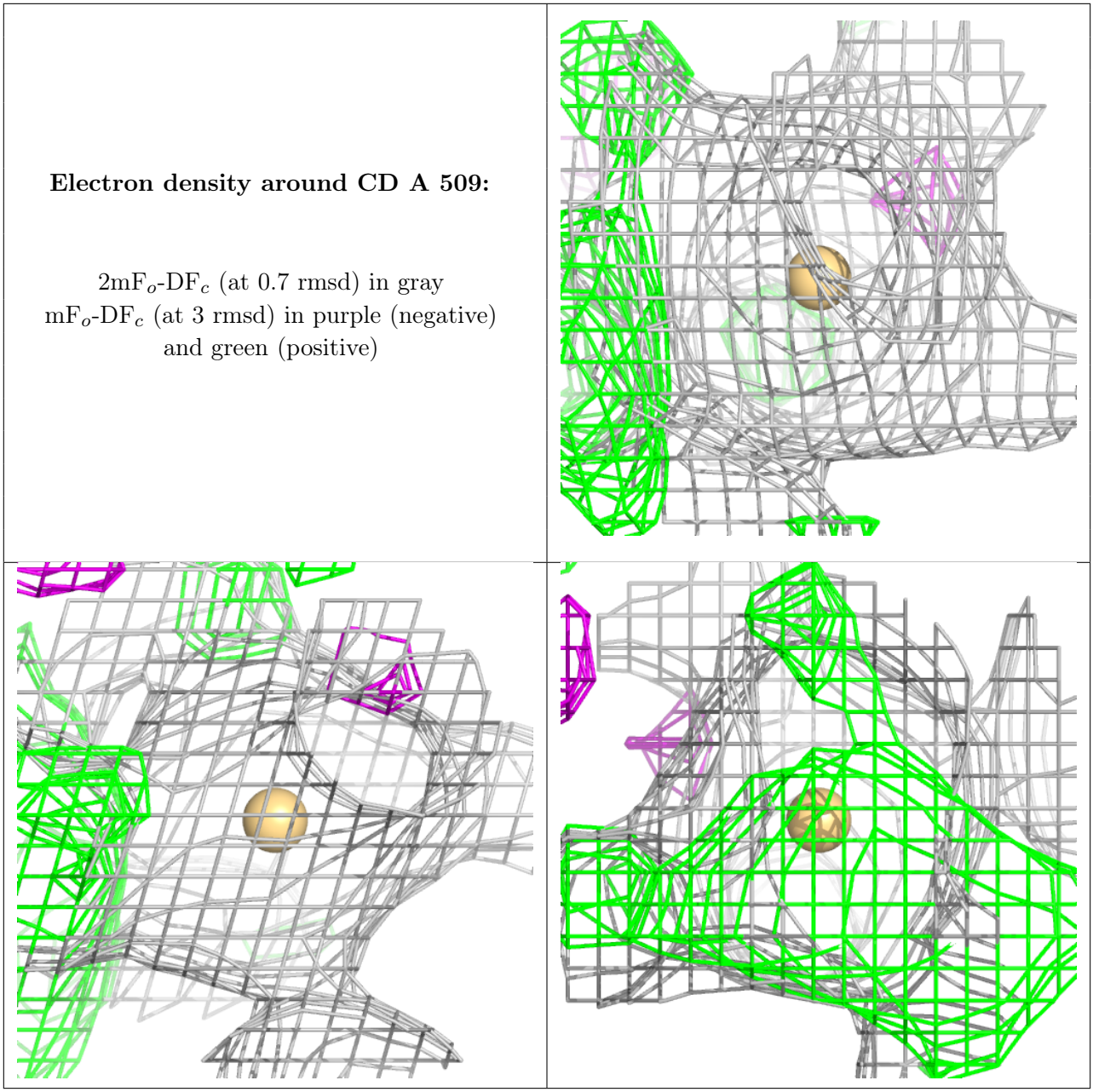
Electron density around K C 506:

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



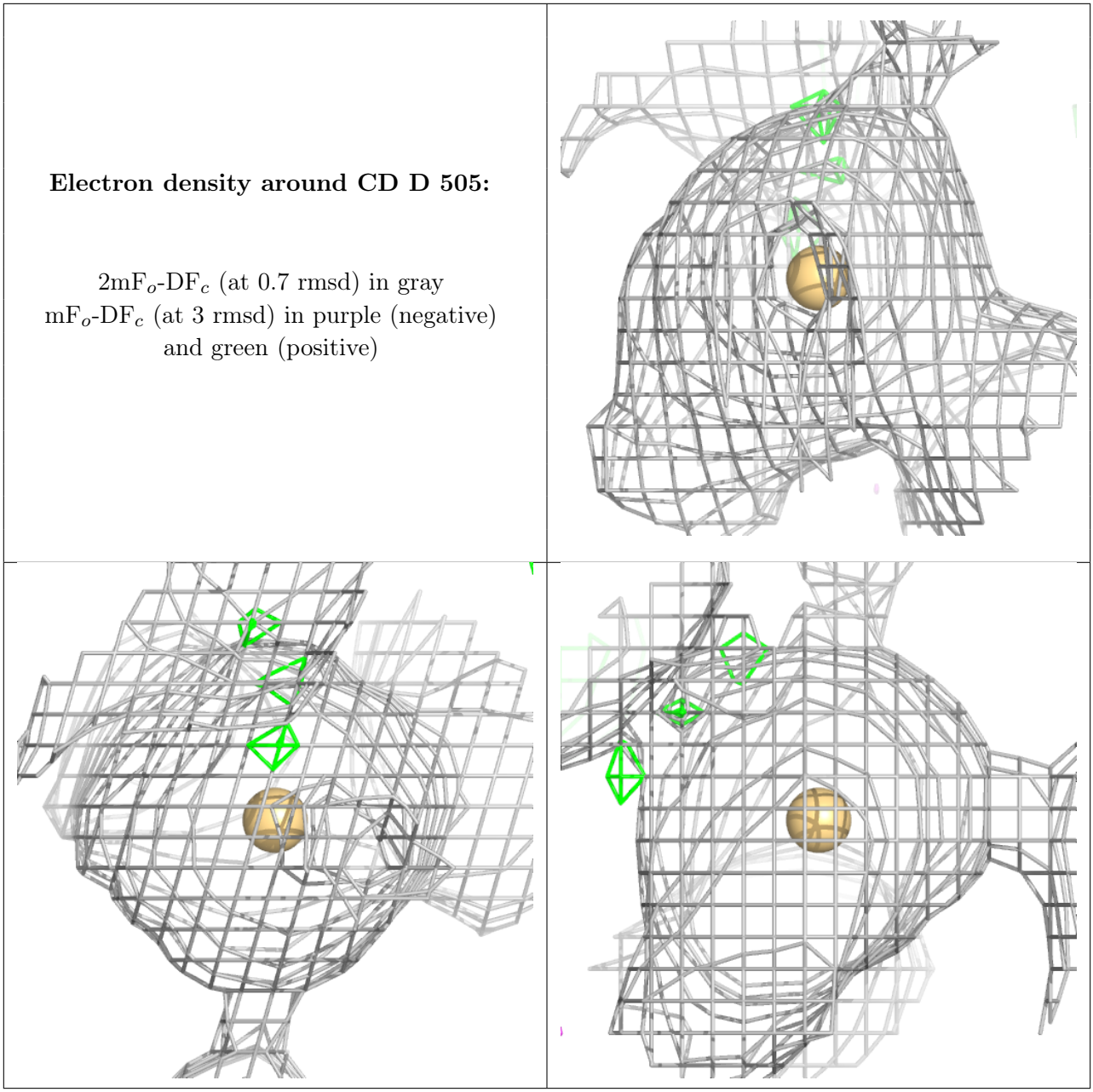
Electron density around CD A 509:

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



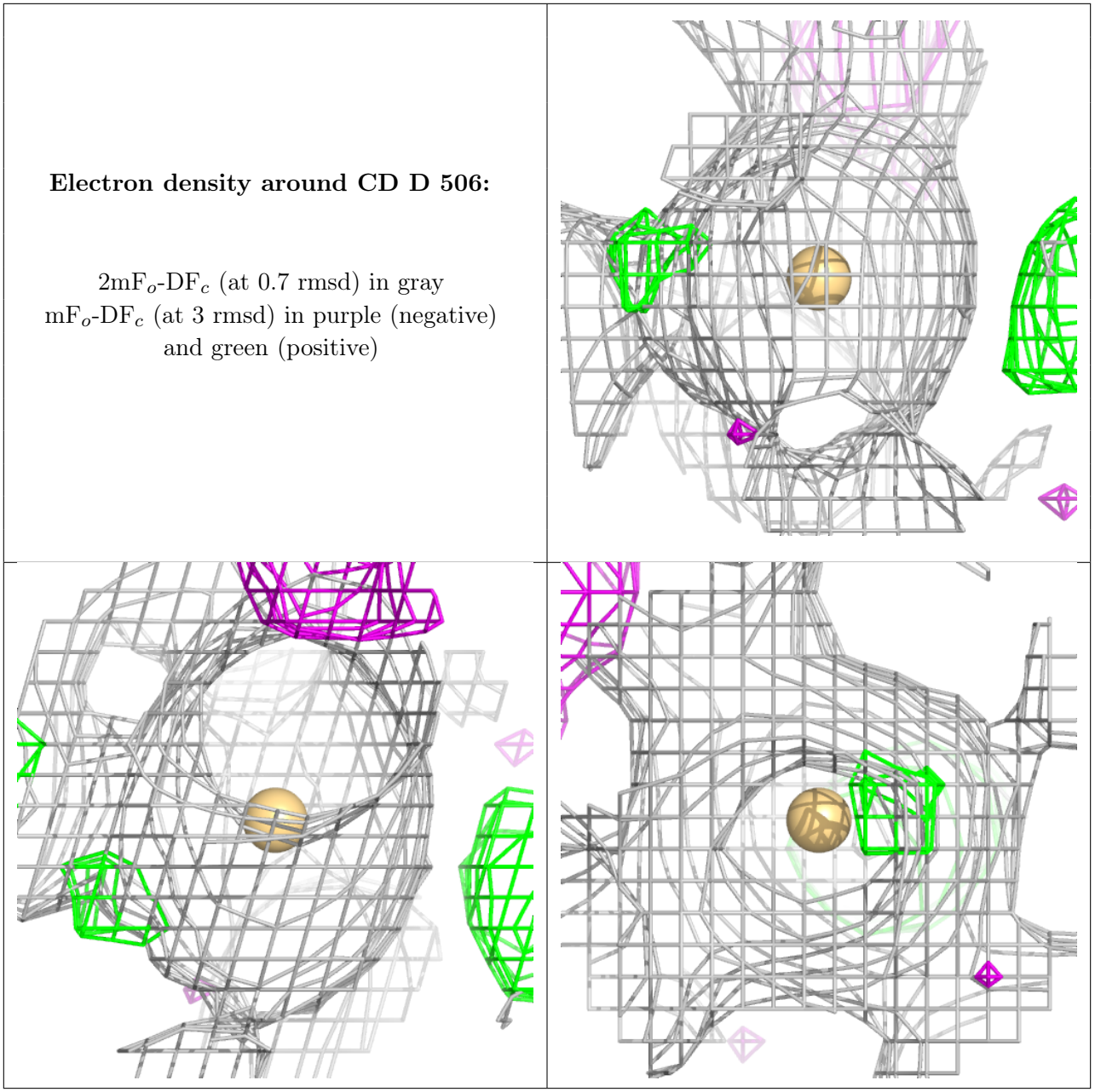
Electron density around CD D 505:

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



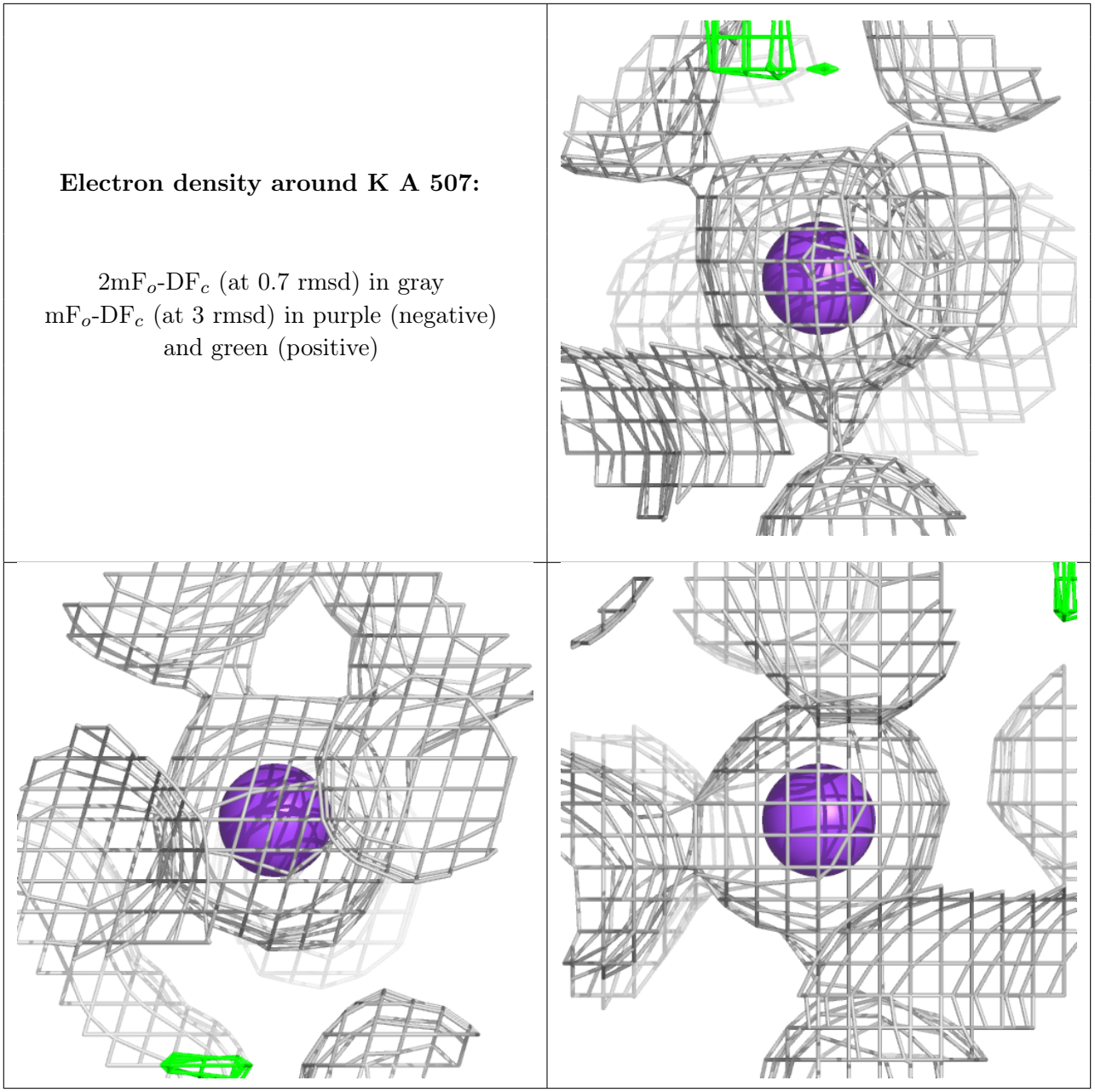
Electron density around CD D 506:

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



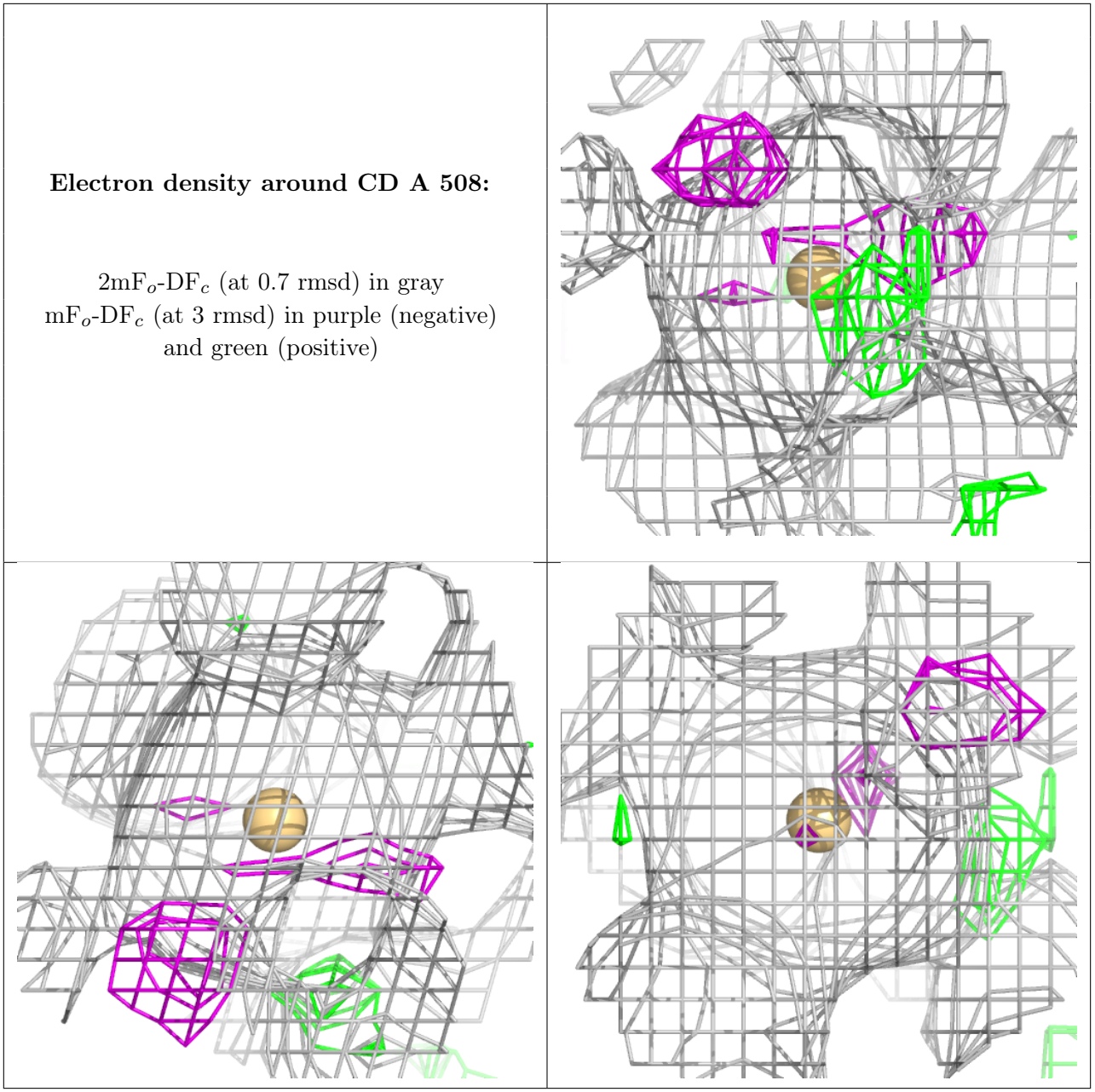
Electron density around K A 507:

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



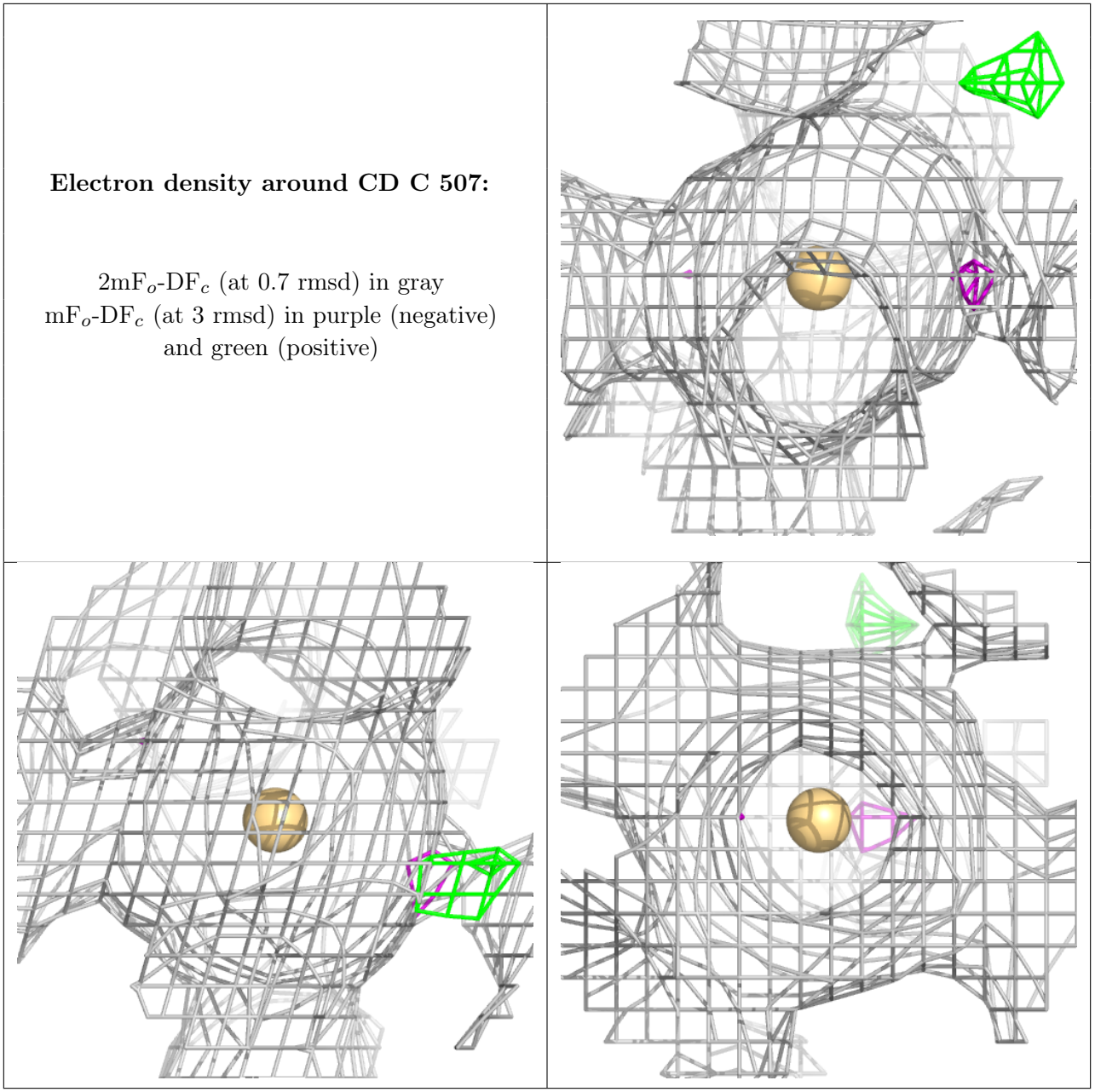
Electron density around CD A 508:

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



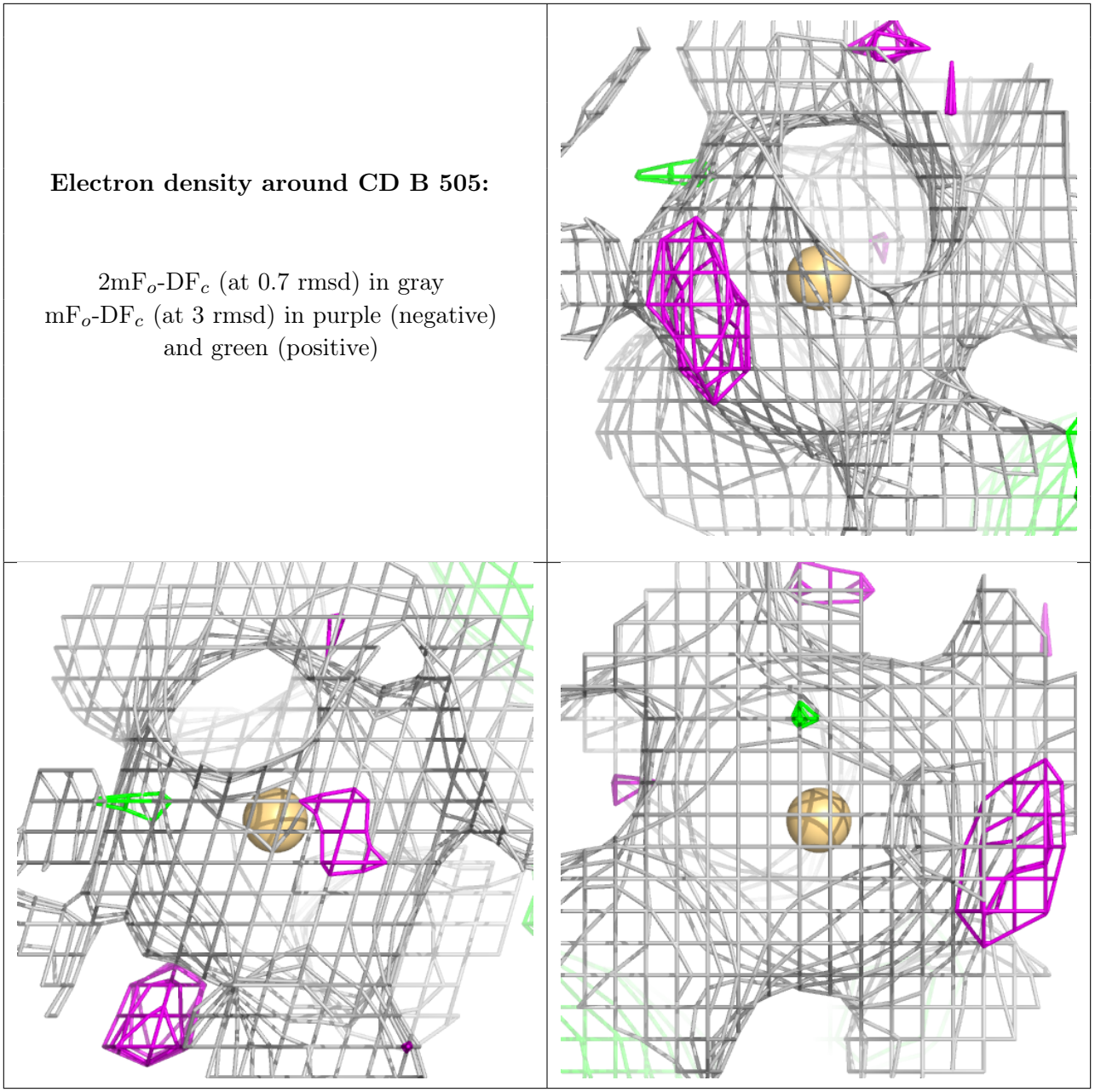
Electron density around CD C 507:

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



Electron density around CD B 505:

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



6.5 Other polymers (i)

There are no such residues in this entry.