Full wwPDB X-ray Structure Validation Report ⓘ

May 6, 2025 – 04:11 pm BST

PDB ID	:	9HN6 / pdb_00009hn6
Title	:	X-ray structure of the adduct formed upon reaction of the diiodido analogue of picoplatin with ribonuclease A
Authors	:	Ferraro, G.; Merlino, A.
Deposited on	:	2024-12-10
Resolution	:	1.77 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:

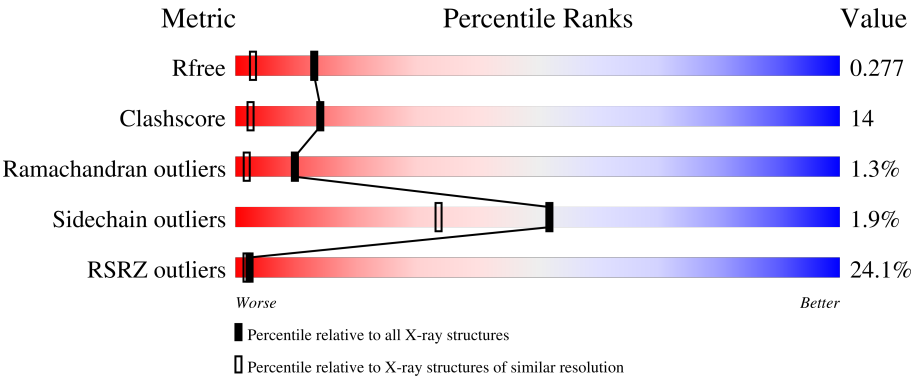
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 1.77 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}	164625	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

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	AAA	124	11% 81% 16%
1	BBB	124	35% 85% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NH3	AAA	202	-	-	-	X
2	NH3	BBB	201	-	-	-	X
4	IOD	AAA	212	-	-	X	-
4	IOD	AAA	214[B]	-	-	X	-
4	IOD	AAA	215	-	-	X	-
4	IOD	BBB	210	-	-	X	-
4	IOD	BBB	211	-	-	X	-

2 Entry composition (i)

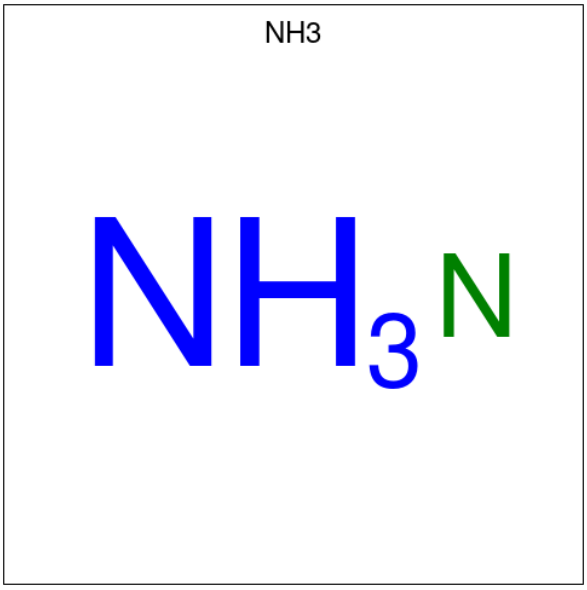
There are 6 unique types of molecules in this entry. The entry contains 2053 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribonuclease pancreatic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	121	Total	C	N	O	S	0	1	0
			939	568	170	189	12			
1	BBB	120	Total	C	N	O	S	0	3	0
			945	571	171	191	12			

- Molecule 2 is AMMONIA (CCD ID: NH3) (formula: H_3N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	N	0	1
			1	1		
2	AAA	1	Total	N	0	0
			1	1		
2	AAA	1	Total	N	0	0
			1	1		
2	AAA	1	Total	N	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	BBB	1	Total N 1 1	0	0
2	BBB	1	Total N 1 1	0	0

- Molecule 3 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	6	Total Pt 6 6	0	2
3	BBB	7	Total Pt 7 7	0	2

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	5	Total I 5 5	0	3
4	BBB	5	Total I 5 5	0	2

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total Cl 1 1	0	0

- Molecule 6 is water.

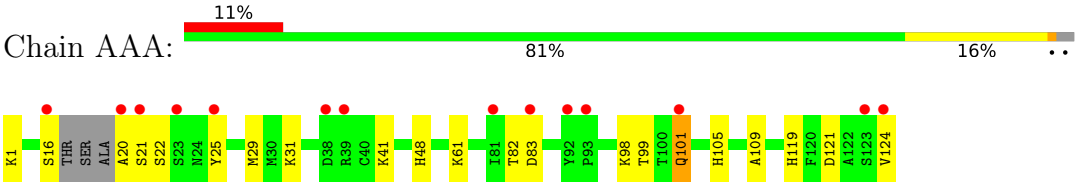
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	88	Total O 89 89	0	4
6	BBB	49	Total O 50 50	0	1

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.

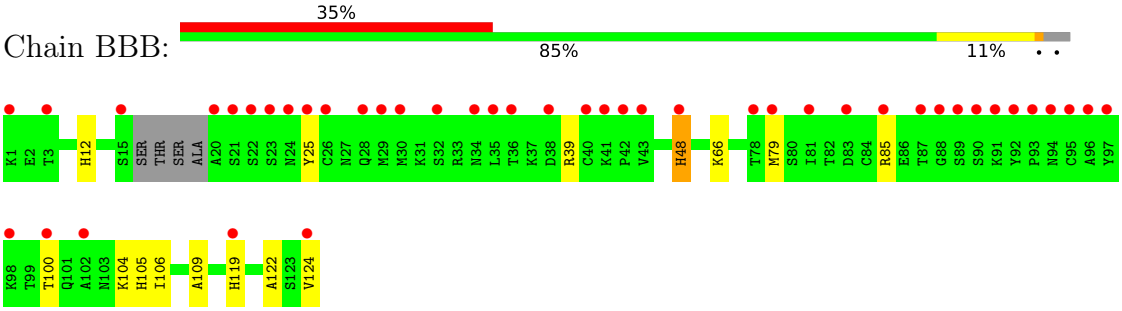
• Molecule 1: Ribonuclease pancreatic

Chain AAA:



• Molecule 1: Ribonuclease pancreatic

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	100.04Å 32.64Å 73.45Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	73.45 – 1.77 73.45 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.3 (73.45-1.77) 99.3 (73.45-1.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.208 , 0.276 0.215 , 0.277	Depositor DCC
R_{free} test set	1106 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2053	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.74% 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: PT, CL, NH3, IOD

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	AAA	1.02	0/955	1.25	2/1287 (0.2%)
1	BBB	1.04	0/961	1.32	1/1295 (0.1%)
All	All	1.03	0/1916	1.29	3/2582 (0.1%)

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	BBB	48	HIS	CA-CB-CG	-5.42	108.39	113.80
1	AAA	31	LYS	CA-C-N	5.12	127.65	120.28
1	AAA	31	LYS	C-N-CA	5.12	127.65	120.28

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	AAA	939	0	882	25	0
1	BBB	945	0	885	25	0
2	AAA	4	0	0	1	0
2	BBB	2	0	0	0	0
3	AAA	6	0	0	0	0
3	BBB	7	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AAA	5	0	0	10	0
4	BBB	5	0	0	6	0
5	AAA	1	0	0	0	0
6	AAA	89	0	0	9	0
6	BBB	50	0	0	10	0
All	All	2053	0	1767	52	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 14.

All (52) 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:AAA:105:HIS:NE2	4:AAA:212:IOD:I	2.26	1.38
1:AAA:119[A]:HIS:HE1	4:AAA:211[A]:IOD:I	1.75	1.31
1:BBB:105:HIS:HD2	6:BBB:301:HOH:O	1.28	1.14
1:BBB:119[A]:HIS:HE1	4:BBB:213[A]:IOD:I	1.99	1.10
4:AAA:215:IOD:I	6:AAA:367:HOH:O	2.45	1.03
1:BBB:105:HIS:NE2	4:BBB:210:IOD:I	2.63	1.01
1:BBB:48:HIS:HE1	6:BBB:332:HOH:O	1.44	1.00
1:AAA:121:ASP:OD1	2:AAA:201[A]:NH3:N	2.03	0.90
1:AAA:105:HIS:CD2	4:AAA:212:IOD:I	2.95	0.90
1:BBB:48:HIS:CE1	6:BBB:332:HOH:O	2.24	0.87
1:AAA:99:THR:OG1	6:AAA:301:HOH:O	1.92	0.87
1:BBB:105:HIS:CE1	4:BBB:210:IOD:I	2.98	0.87
1:AAA:48:HIS:CG	4:AAA:215:IOD:I	3.00	0.85
1:AAA:1:LYS:CB	6:AAA:383:HOH:O	2.23	0.84
3:BBB:204:PT:PT	4:BBB:210:IOD:I	1.89	0.83
1:AAA:20:ALA:HB1	4:AAA:215:IOD:I	2.55	0.76
1:BBB:48:HIS:CD2	1:BBB:48:HIS:C	2.69	0.71
1:BBB:79:MET:HE2	1:BBB:106:ILE:HG12	1.74	0.69
1:AAA:109:ALA:HB3	1:AAA:119[A]:HIS:HB3	1.77	0.65
1:BBB:66:LYS:HE3	1:BBB:122:ALA:HB2	1.78	0.64
1:AAA:20:ALA:HB2	1:AAA:82:THR:OG1	1.98	0.64
1:AAA:25:TYR:N	6:AAA:301:HOH:O	2.31	0.63
1:BBB:12:HIS:NE2	4:BBB:211:IOD:I	3.01	0.62
1:BBB:124:VAL:O	6:BBB:301:HOH:O	2.15	0.62
1:BBB:124:VAL:C	6:BBB:301:HOH:O	2.43	0.60
1:AAA:16:SER:HB3	6:BBB:322:HOH:O	2.03	0.59
1:AAA:25:TYR:CZ	1:AAA:29:MET:HG3	2.39	0.58
1:AAA:101:GLN:NE2	6:AAA:304:HOH:O	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:85:ARG:NH1	6:BBB:302:HOH:O	2.37	0.56
1:AAA:41:LYS:NZ	6:AAA:303:HOH:O	2.14	0.55
1:AAA:119[B]:HIS:HB3	4:AAA:214[B]:IOD:I	2.76	0.55
1:AAA:48:HIS:CB	4:AAA:215:IOD:I	3.26	0.53
1:BBB:104:LYS:NZ	6:BBB:304:HOH:O	2.41	0.53
1:BBB:105:HIS:CD2	6:BBB:301:HOH:O	2.19	0.52
1:BBB:48:HIS:C	1:BBB:48:HIS:HD2	2.18	0.52
1:BBB:124:VAL:OXT	6:BBB:301:HOH:O	2.18	0.50
1:BBB:12:HIS:CD2	4:BBB:211:IOD:I	3.34	0.50
1:BBB:105:HIS:HB2	1:BBB:124:VAL:HG23	1.94	0.49
1:AAA:16:SER:C	6:AAA:314:HOH:O	2.56	0.48
1:AAA:101:GLN:HE21	1:AAA:101:GLN:H	1.60	0.48
1:AAA:61:LYS:NZ	6:AAA:305:HOH:O	2.42	0.48
1:BBB:79:MET:HE1	1:BBB:106:ILE:CD1	2.44	0.47
1:AAA:105:HIS:HB2	1:AAA:124:VAL:HG23	1.97	0.47
1:BBB:79:MET:CE	1:BBB:106:ILE:CD1	2.93	0.47
1:AAA:29:MET:HE2	1:AAA:29:MET:HA	1.96	0.46
1:BBB:79:MET:HE2	1:BBB:106:ILE:CG1	2.42	0.46
1:AAA:98:LYS:HE3	6:AAA:351:HOH:O	2.16	0.46
1:BBB:79:MET:CE	1:BBB:106:ILE:HD13	2.46	0.46
1:AAA:119[B]:HIS:CG	4:AAA:214[B]:IOD:I	3.42	0.43
1:AAA:119[B]:HIS:CB	4:AAA:214[B]:IOD:I	3.36	0.43
1:BBB:79:MET:HE1	1:BBB:106:ILE:HD13	2.00	0.42
1:BBB:109:ALA:HB3	1:BBB:119[A]:HIS:HB3	2.02	0.41

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	AAA	118/124 (95%)	115 (98%)	2 (2%)	1 (1%)	16 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	BBB	119/124 (96%)	111 (93%)	6 (5%)	2 (2%)	7 1
All	All	237/248 (96%)	226 (95%)	8 (3%)	3 (1%)	10 2

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	21	SER
1	BBB	25	TYR
1	BBB	39	ARG

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	AAA	107/109 (98%)	104 (97%)	3 (3%)	38 18
1	BBB	108/109 (99%)	107 (99%)	1 (1%)	75 65
All	All	215/218 (99%)	211 (98%)	4 (2%)	52 33

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	22	SER
1	AAA	83	ASP
1	AAA	101	GLN
1	BBB	100	THR

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

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 6 are modelled with single atom and 24 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, 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	AAA	121/124 (97%)	0.75	14 (11%)	11	12	13, 27, 55, 100	1 (0%)
1	BBB	120/124 (96%)	1.46	44 (36%)	1	1	11, 40, 85, 124	3 (2%)
All	All	241/248 (97%)	1.10	58 (24%)	2	2	11, 31, 82, 124	4 (1%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	20	ALA	9.6
1	BBB	20	ALA	5.7
1	BBB	88	GLY	4.6
1	BBB	124	VAL	4.5
1	BBB	96	ALA	4.1
1	BBB	1	LYS	3.8
1	BBB	21	SER	3.8
1	BBB	93	PRO	3.8
1	BBB	23	SER	3.8
1	BBB	92	TYR	3.6
1	BBB	15	SER	3.6
1	BBB	22	SER	3.5
1	BBB	91	LYS	3.5
1	AAA	124	VAL	3.4
1	BBB	32	SER	3.3
1	BBB	25	TYR	3.2
1	AAA	93	PRO	3.0
1	BBB	29	MET	3.0
1	BBB	100	THR	2.9
1	BBB	35	LEU	2.9
1	AAA	25	TYR	2.9
1	BBB	97	TYR	2.9
1	BBB	28	GLN	2.8
1	BBB	90	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BBB	41	LYS	2.7
1	AAA	83	ASP	2.7
1	BBB	87	THR	2.7
1	AAA	21	SER	2.7
1	BBB	98	LYS	2.7
1	BBB	38	ASP	2.6
1	BBB	83	ASP	2.6
1	AAA	38	ASP	2.5
1	AAA	92	TYR	2.5
1	BBB	26	CYS	2.5
1	BBB	36	THR	2.5
1	BBB	119[A]	HIS	2.4
1	BBB	95	CYS	2.4
1	BBB	34	ASN	2.4
1	AAA	101	GLN	2.4
1	BBB	85	ARG	2.4
1	BBB	40	CYS	2.3
1	BBB	94	ASN	2.3
1	BBB	30	MET	2.3
1	BBB	43	VAL	2.3
1	AAA	23	SER	2.3
1	AAA	123	SER	2.3
1	BBB	24	ASN	2.2
1	AAA	16	SER	2.2
1	BBB	89	SER	2.2
1	BBB	102	ALA	2.2
1	AAA	39	ARG	2.2
1	BBB	48	HIS	2.2
1	BBB	3	THR	2.1
1	BBB	79	MET	2.1
1	BBB	81	ILE	2.1
1	BBB	78	THR	2.0
1	BBB	42	PRO	2.0
1	AAA	81	ILE	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.

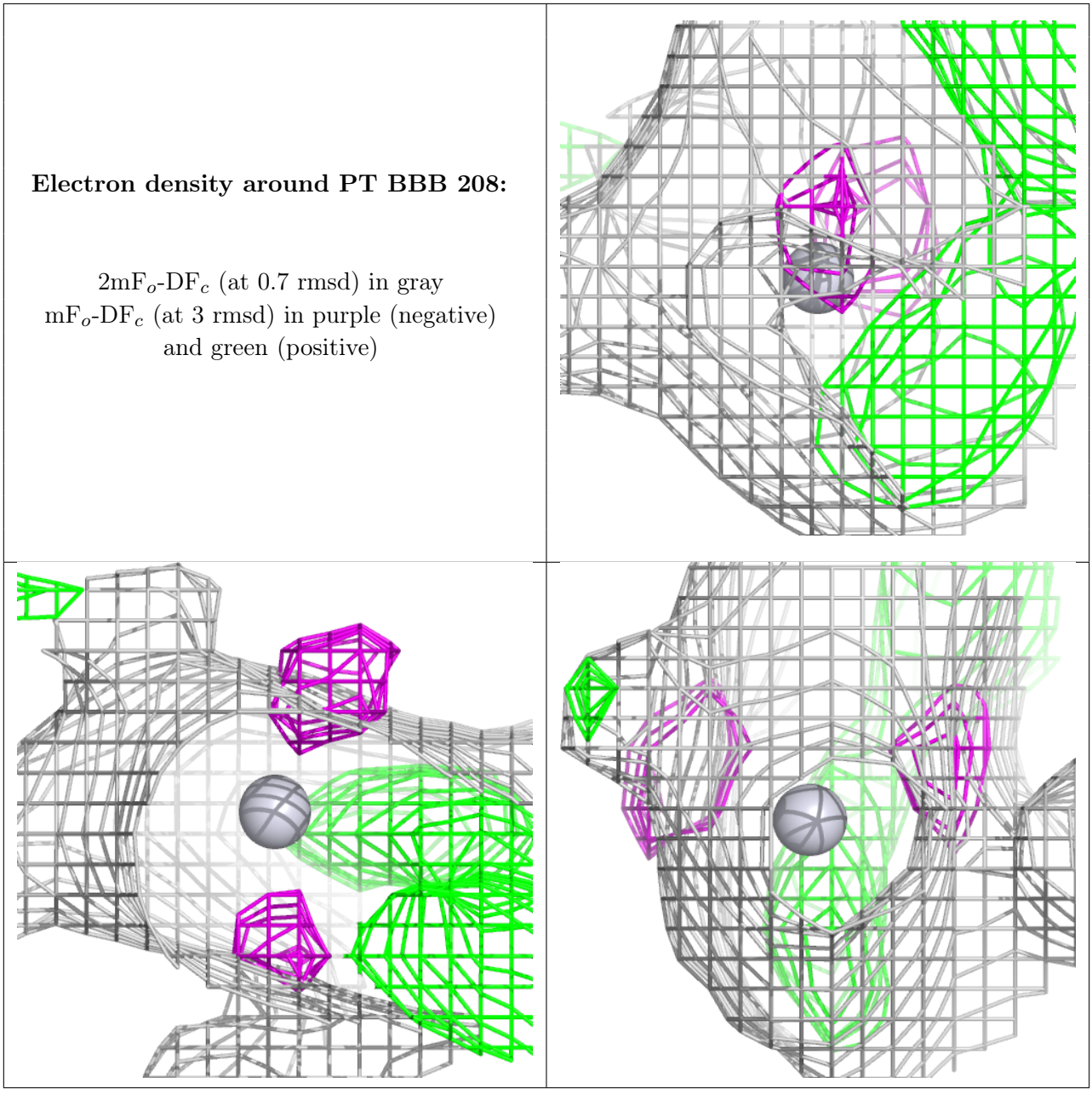
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NH3	AAA	201[A]	1/1	0.36	0.36	43,43,43,43	1
2	NH3	AAA	202	1/1	0.56	0.49	20,20,20,20	1
2	NH3	AAA	210	1/1	0.69	0.25	48,48,48,48	1
2	NH3	BBB	201	1/1	0.69	0.46	29,29,29,29	1
4	IOD	BBB	212	1/1	0.77	0.15	75,75,75,75	1
4	IOD	BBB	213[A]	1/1	0.78	0.12	80,80,80,80	1
3	PT	BBB	208	1/1	0.80	0.13	81,81,81,81	1
2	NH3	BBB	202	1/1	0.81	0.26	40,40,40,40	1
4	IOD	BBB	214[B]	1/1	0.82	0.13	54,54,54,54	1
3	PT	BBB	203	1/1	0.83	0.13	67,67,67,67	1
4	IOD	BBB	211	1/1	0.85	0.13	58,58,58,58	1
3	PT	AAA	208[B]	1/1	0.87	0.15	43,43,43,43	1
2	NH3	AAA	203	1/1	0.89	0.39	19,19,19,19	1
4	IOD	BBB	210	1/1	0.89	0.14	69,69,69,69	1
4	IOD	AAA	214[B]	1/1	0.90	0.08	31,31,31,31	1
3	PT	AAA	206	1/1	0.91	0.10	66,66,66,66	1
3	PT	BBB	209[B]	1/1	0.91	0.09	56,56,56,56	1
3	PT	BBB	206	1/1	0.92	0.08	46,46,46,46	1
3	PT	BBB	207[A]	1/1	0.93	0.10	64,64,64,64	1
4	IOD	AAA	215	1/1	0.94	0.08	35,35,35,35	1
4	IOD	AAA	213[B]	1/1	0.94	0.08	32,32,32,32	1
3	PT	AAA	209	1/1	0.94	0.08	37,37,37,37	1
3	PT	AAA	205[A]	1/1	0.95	0.07	48,48,48,48	1
3	PT	AAA	204	1/1	0.96	0.05	40,40,40,40	1
4	IOD	AAA	212	1/1	0.96	0.07	34,34,34,34	1
5	CL	AAA	216	1/1	0.96	0.08	44,44,44,44	0
3	PT	AAA	207	1/1	0.97	0.05	30,30,30,30	1
4	IOD	AAA	211[A]	1/1	0.97	0.05	45,45,45,45	1
3	PT	BBB	204	1/1	0.97	0.04	37,37,37,37	1
3	PT	BBB	205	1/1	0.97	0.05	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.

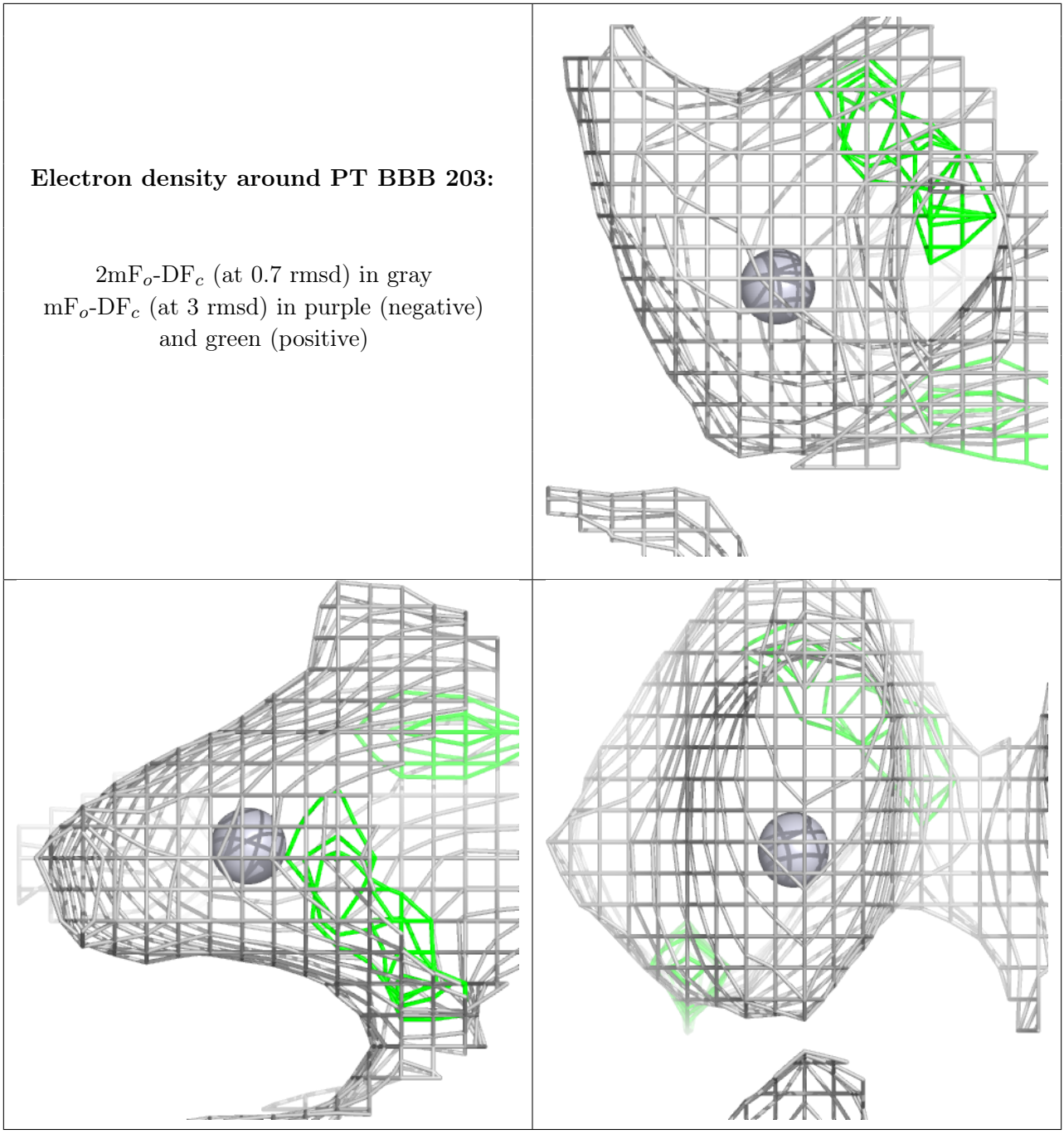
Electron density around PT BBB 208:

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



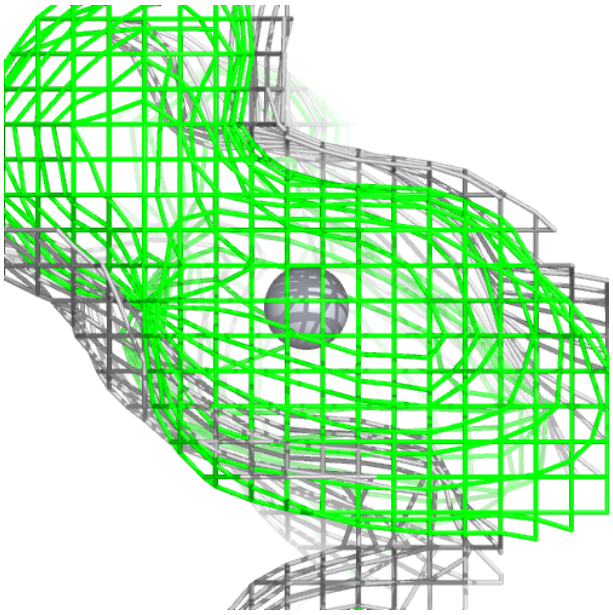
Electron density around PT BBB 203:

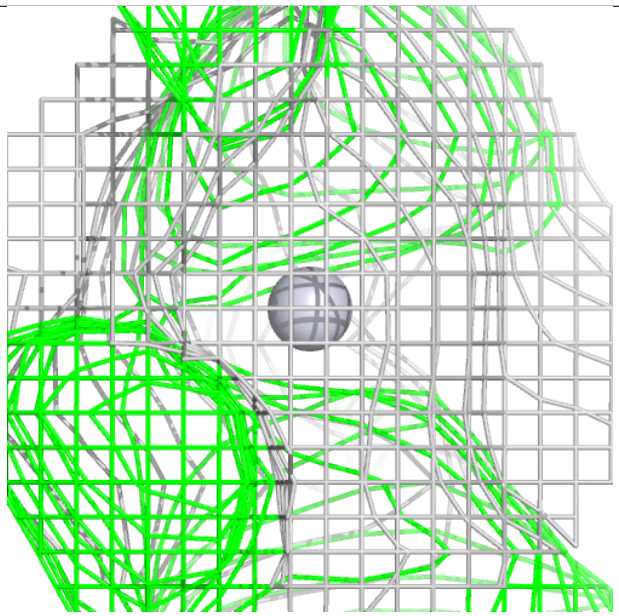
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

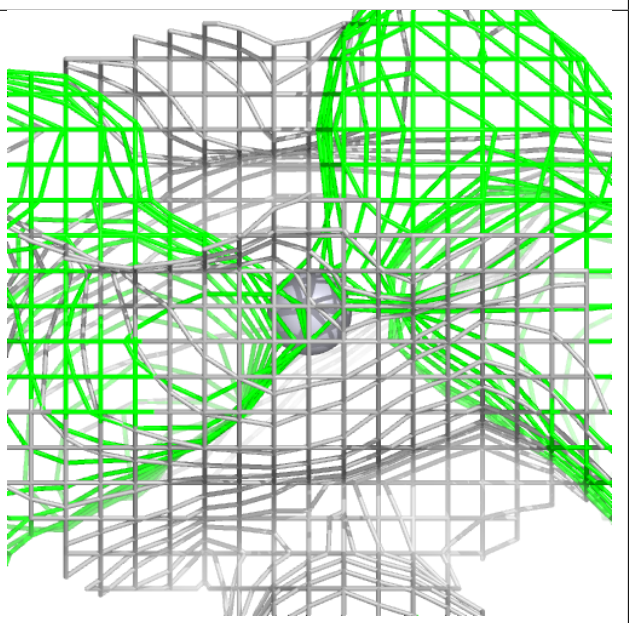


Electron density around PT AAA 208 (B):

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

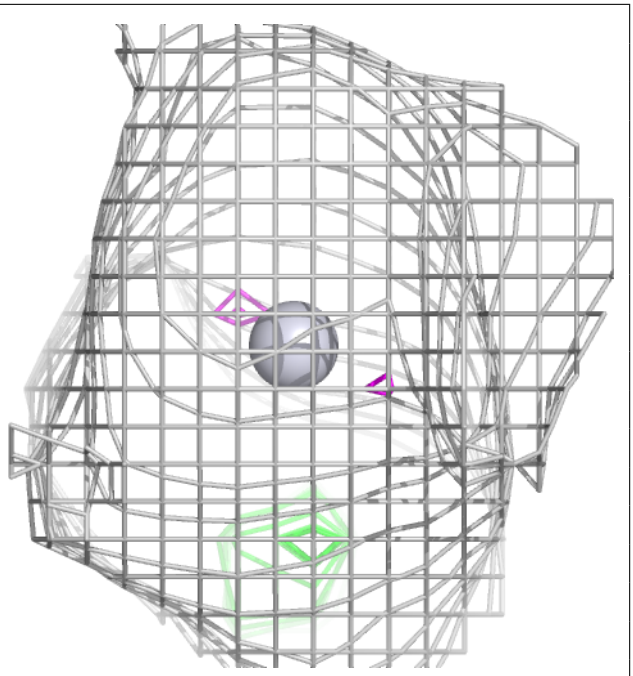


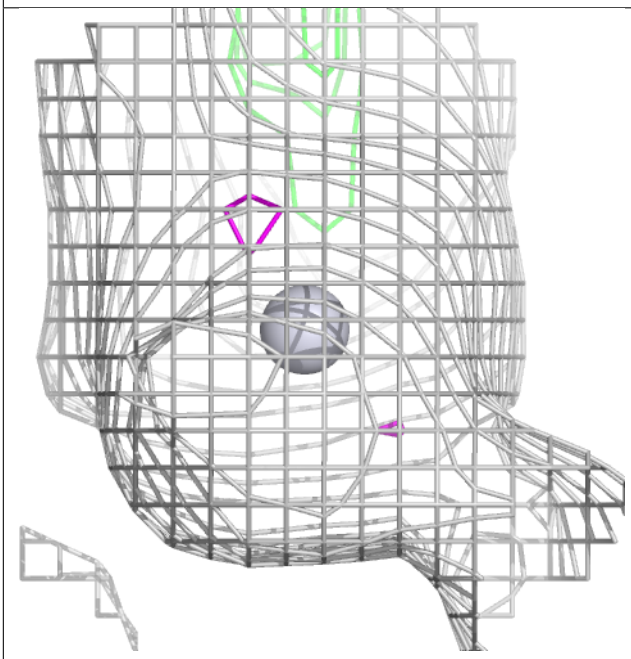


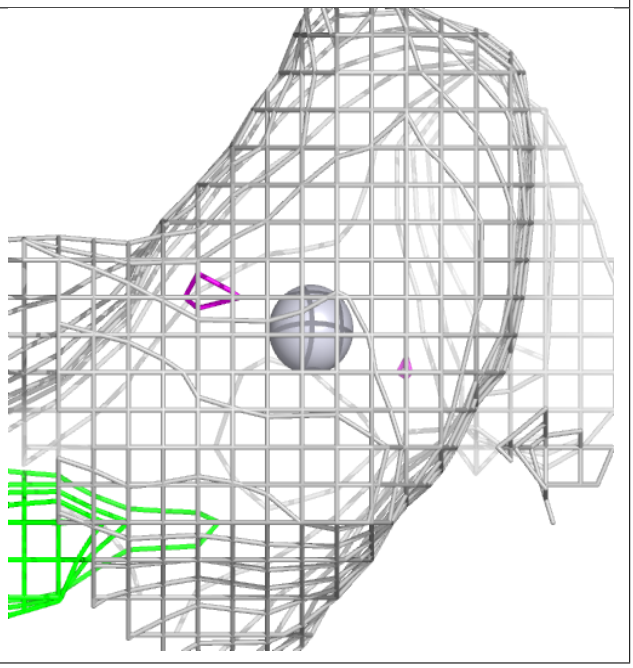


Electron density around PT AAA 206:

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

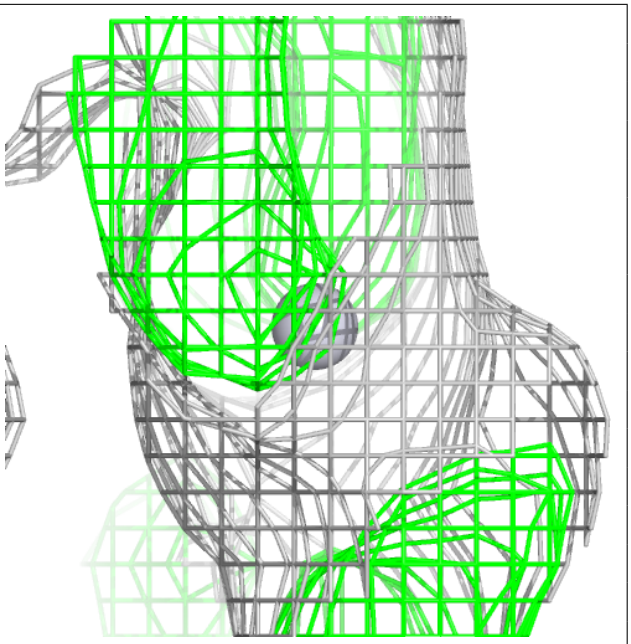


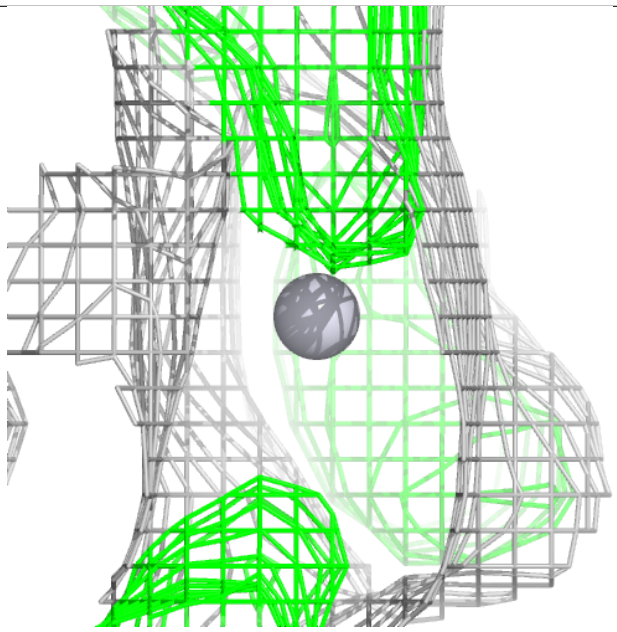


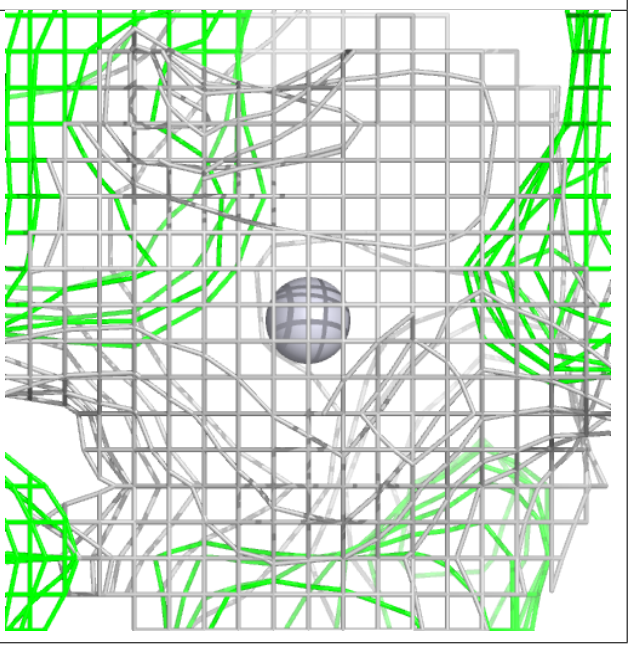


Electron density around PT BBB 209 (B):

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

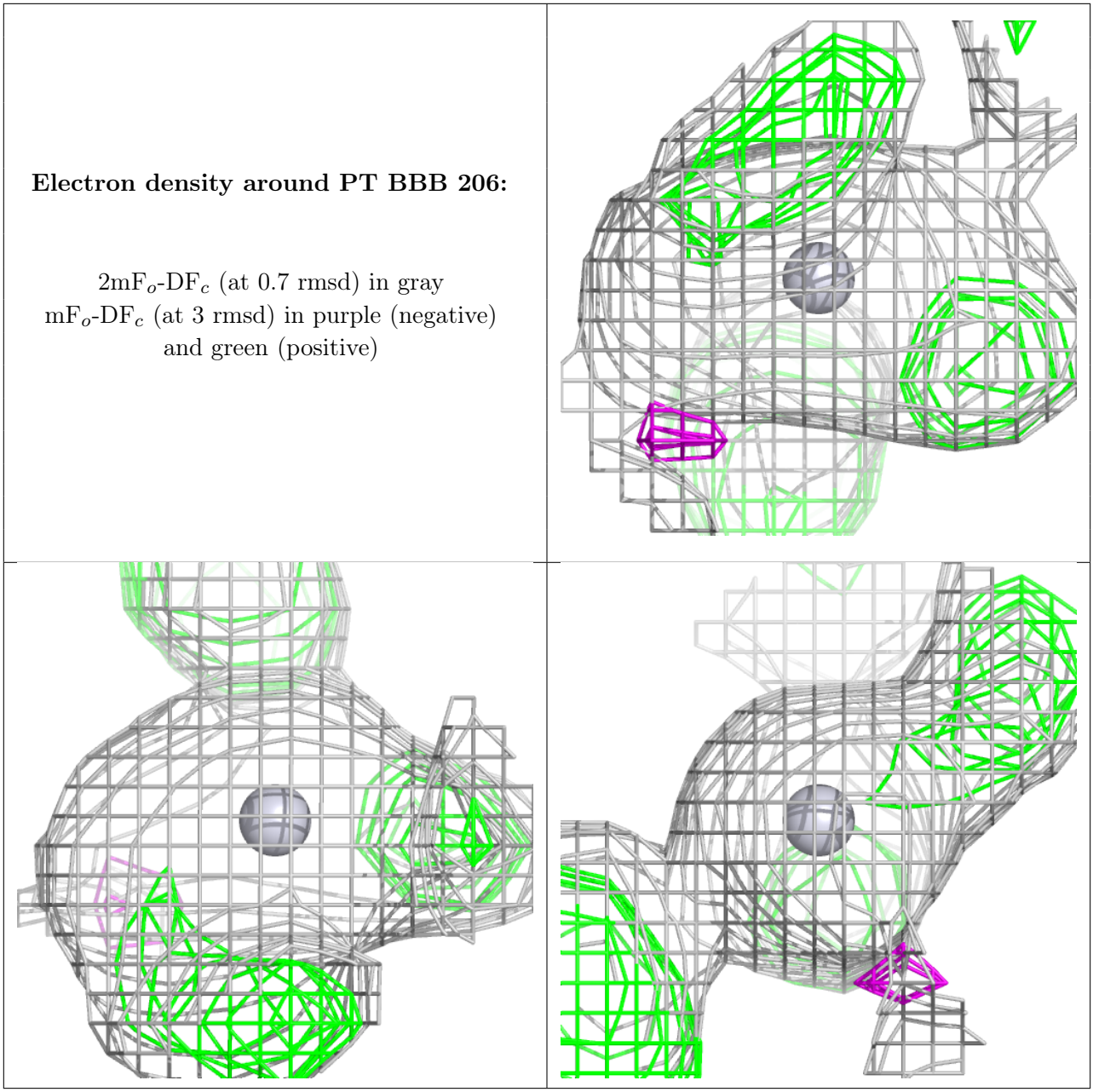






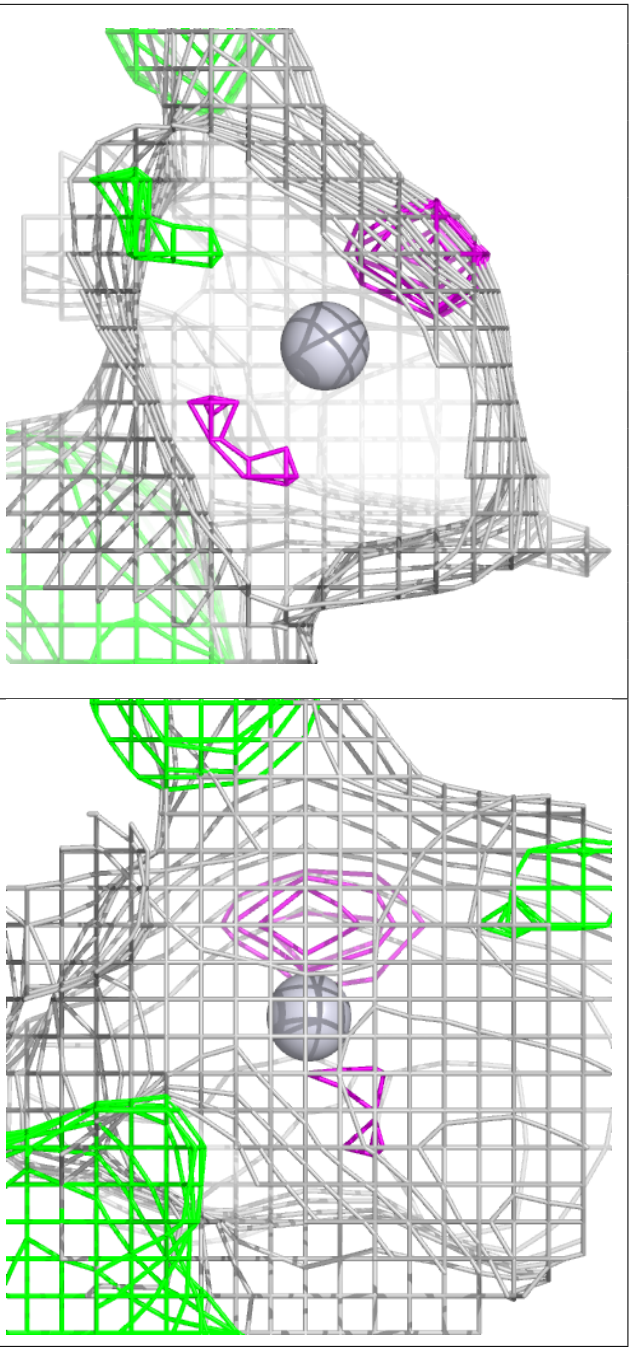
Electron density around PT BBB 206:

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



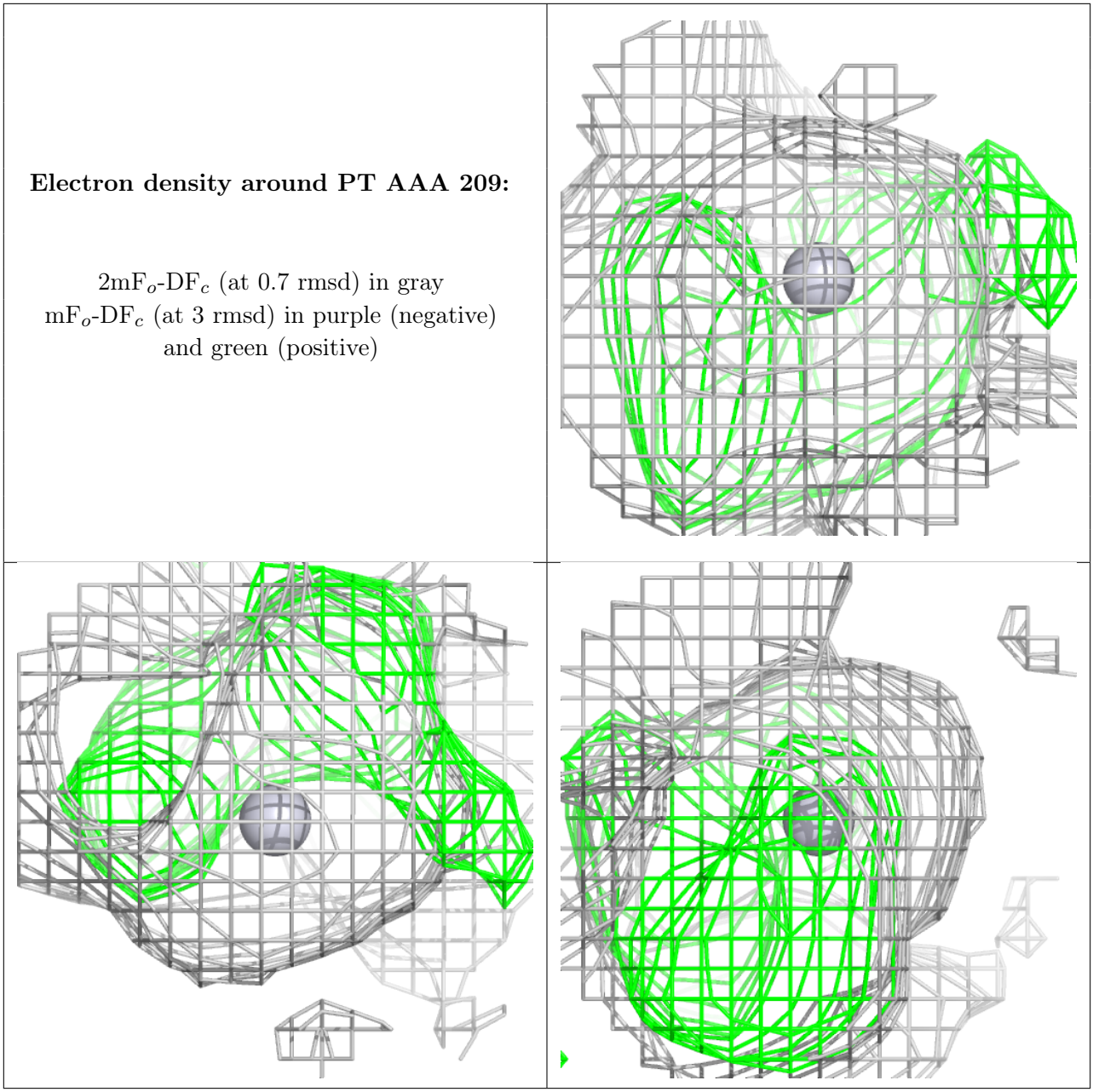
Electron density around PT BBB 207 (A):

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



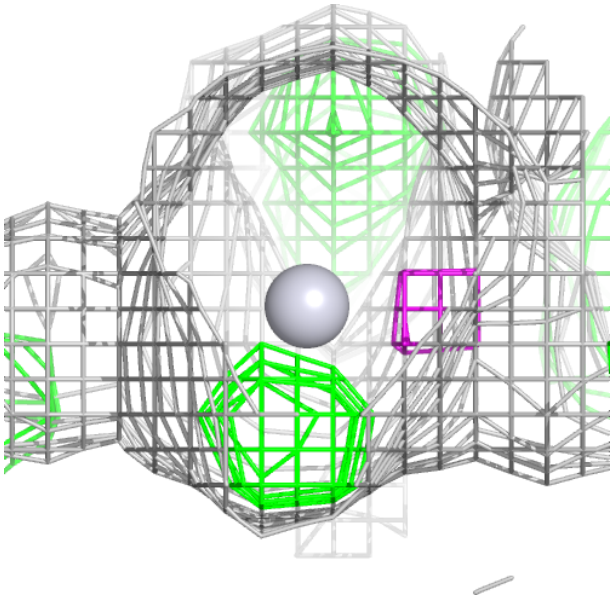
Electron density around PT AAA 209:

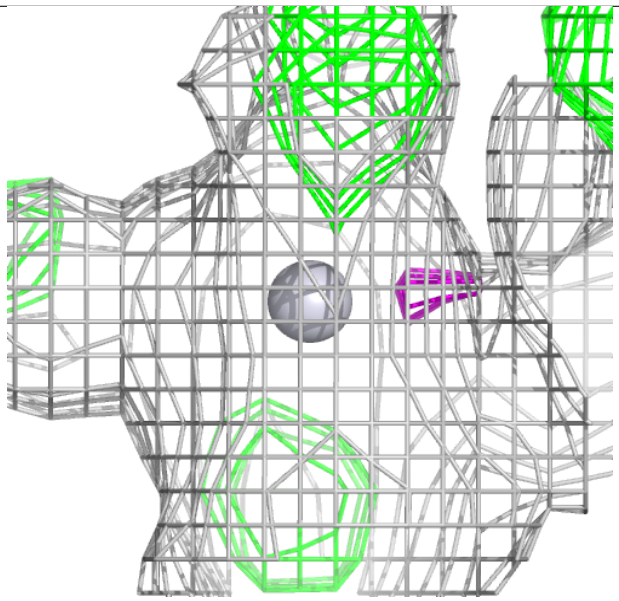
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

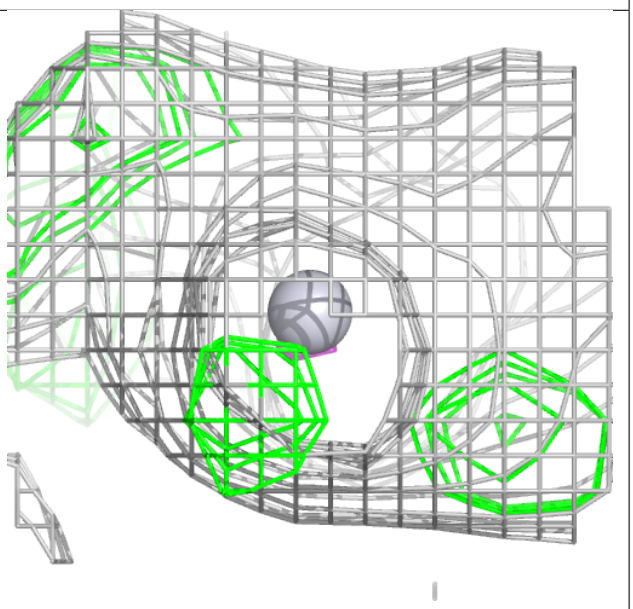


Electron density around PT AAA 205 (A):

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

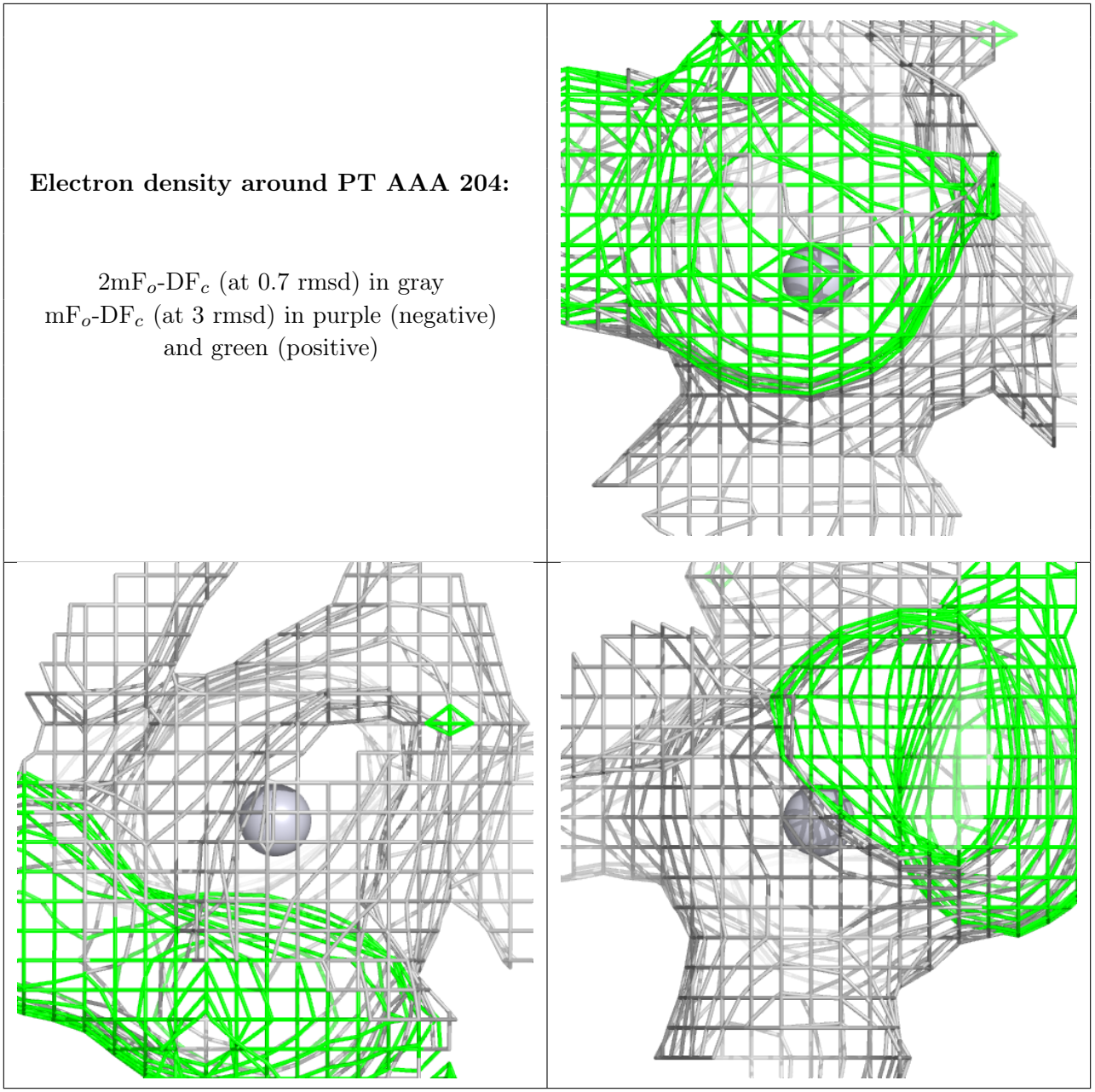






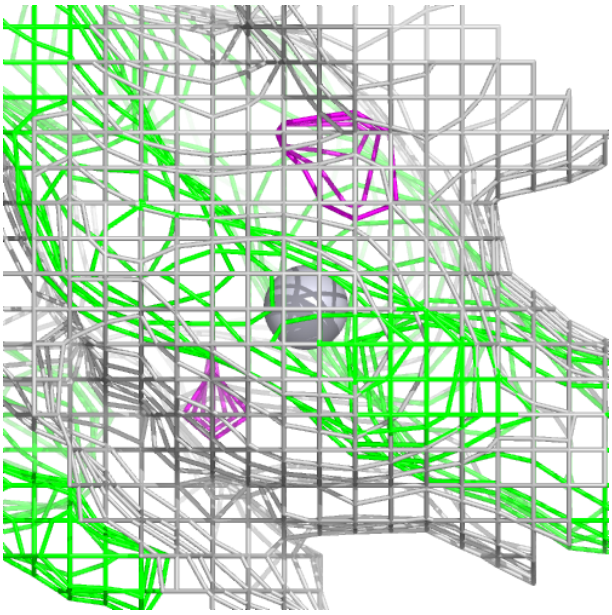
Electron density around PT AAA 204:

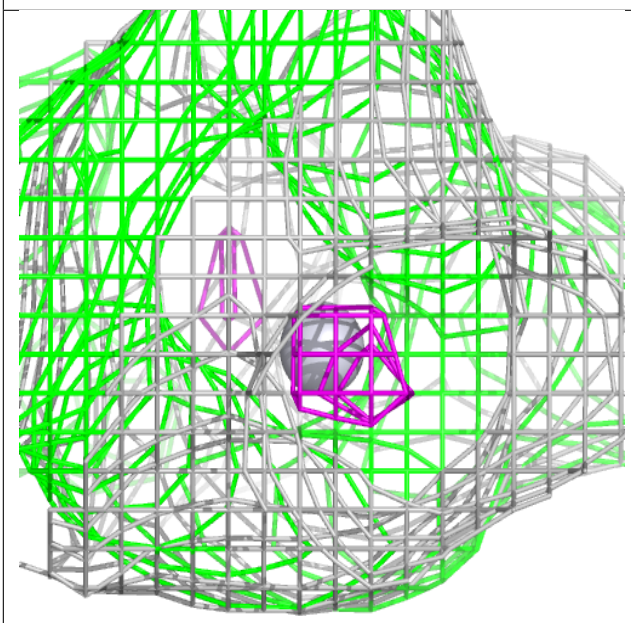
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

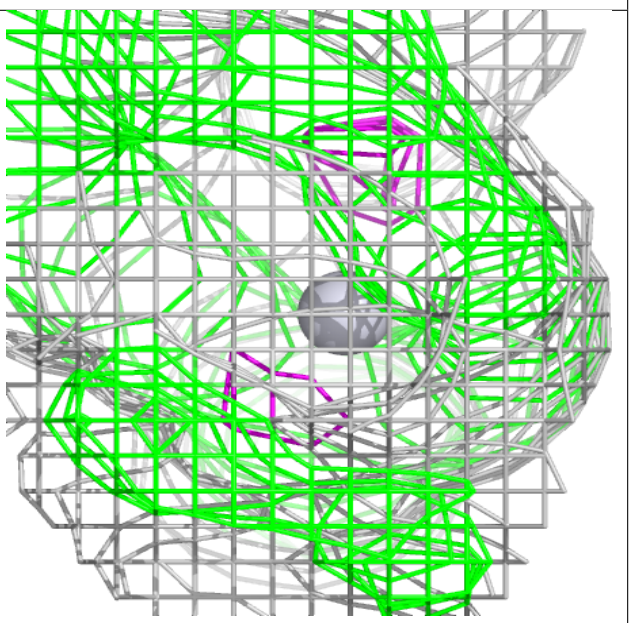


Electron density around PT AAA 207:

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

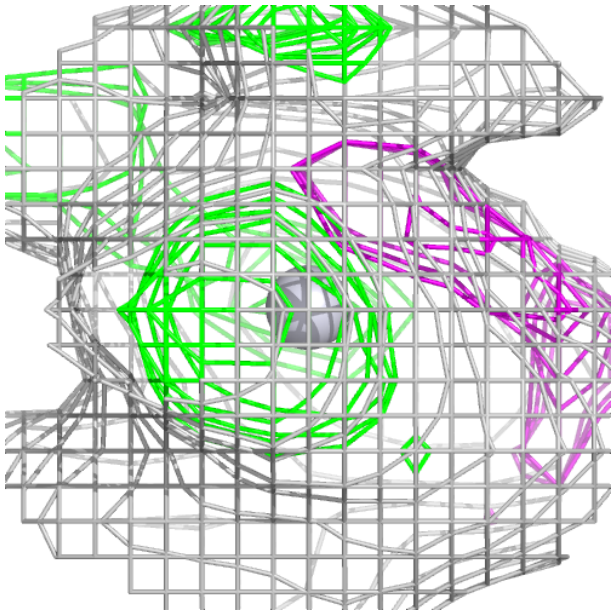


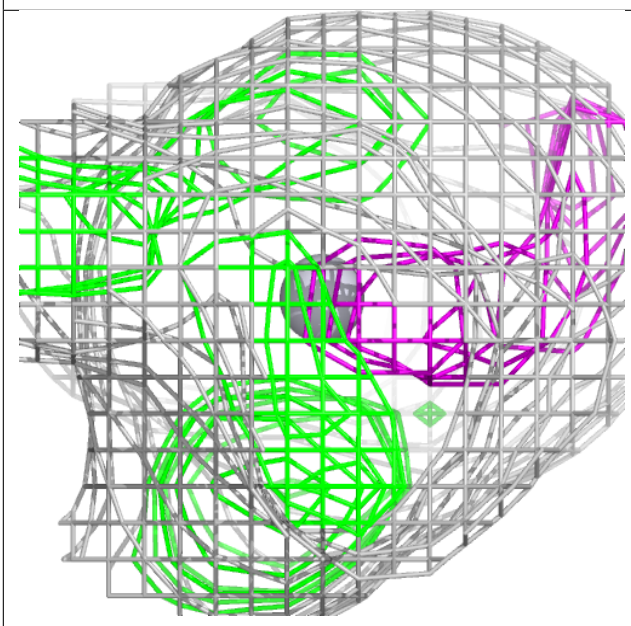


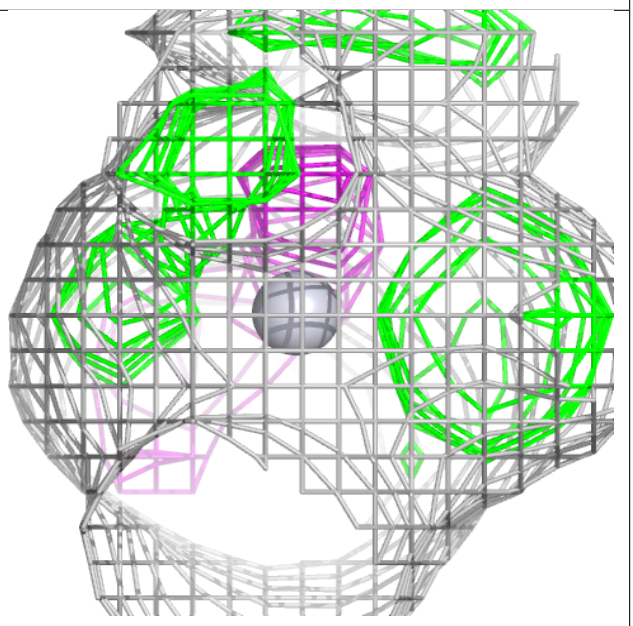


Electron density around PT BBB 204:

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

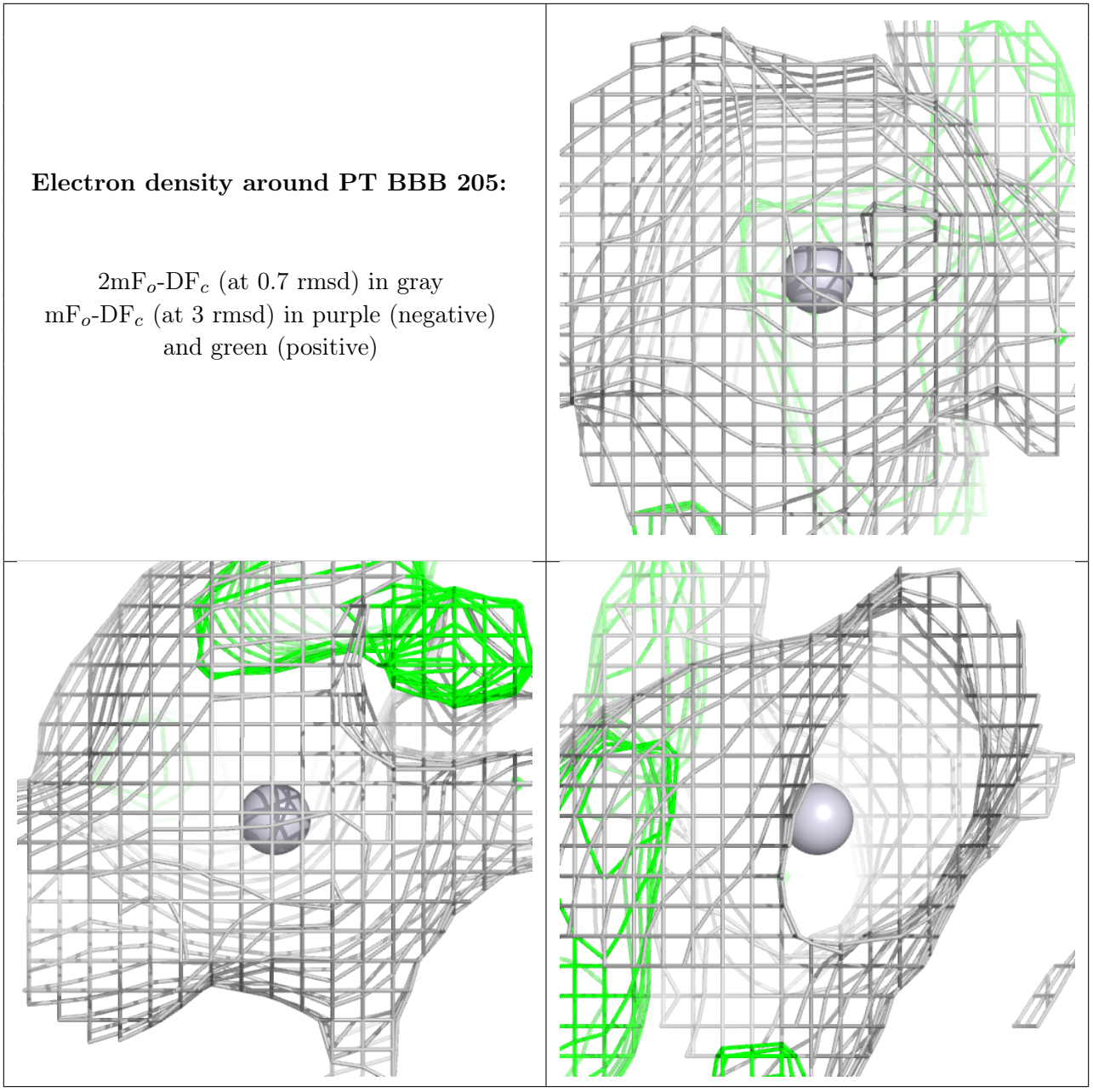






Electron density around PT BBB 205:

$2mF_o$-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.