Full wwPDB X-ray Structure Validation Report ⓘ

May 6, 2025 – 01:06 pm BST

PDB ID	:	9HLK / pdb_00009hlk
Title	:	X-ray structure of the adduct formed upon reaction of the diiodido analogue of picoplatin with lysozyme (structure A)
Authors	:	Ferraro, G.; Merlino, A.
Deposited on	:	2024-12-05
Resolution	:	1.96 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:

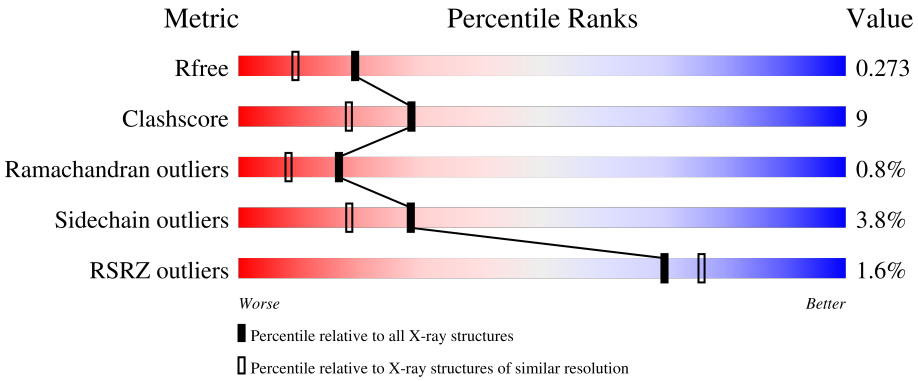
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 1.96 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	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

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	129	2% 82% 16%

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
3	ACT	AAA	203	-	-	X	-

2 Entry composition (i)

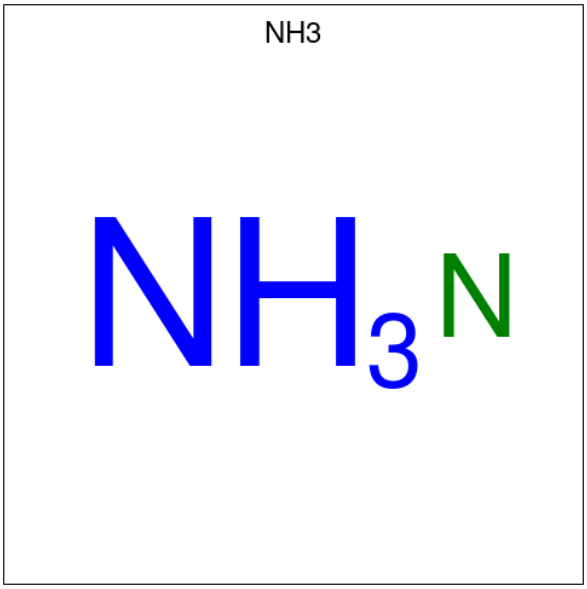
There are 7 unique types of molecules in this entry. The entry contains 1133 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysozyme C.

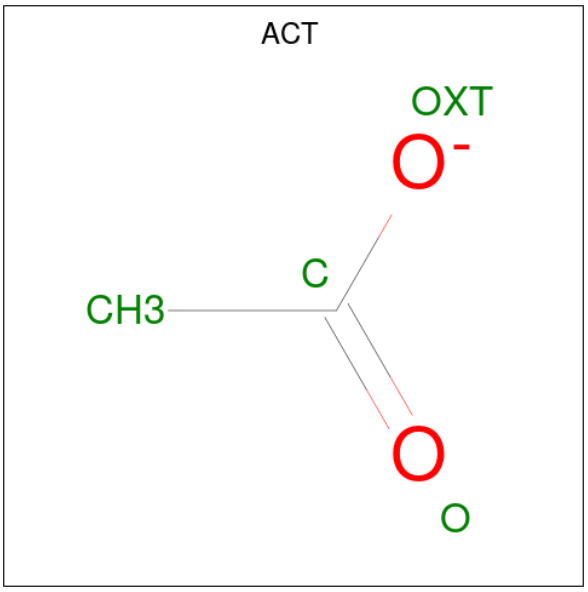
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	129	1047	638	206	193	10	0	7	0

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



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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 4 2 2	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	3	Total Pt 3 3	0	0

- Molecule 6 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	4	Total I 4 4	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	72	Total O 72 72	0	0

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: Lysozyme C

Chain AAA:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	78.40Å 78.40Å 36.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.44 – 1.96 55.44 – 1.96	Depositor EDS
% Data completeness (in resolution range)	98.2 (55.44-1.96) 98.2 (55.44-1.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.21 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.206 , 0.269 0.215 , 0.273	Depositor DCC
R_{free} test set	417 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 29.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	1133	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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, ACT, IOD, CL, NH3

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	1.12	0/1080	1.36	0/1458

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1047	0	1000	16	0
2	AAA	2	0	0	0	0
3	AAA	4	0	3	2	0
4	AAA	1	0	0	0	0
5	AAA	3	0	0	0	0
6	AAA	4	0	0	1	0
7	AAA	72	0	0	1	0
All	All	1133	0	1003	18	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 9.

All (18) 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:61[B]:ARG:HD2	1:AAA:61[B]:ARG:O	1.90	0.71
1:AAA:109[A]:VAL:HG22	1:AAA:112:ARG:HH22	1.67	0.60
1:AAA:10:ALA:HA	1:AAA:129:LEU:HD22	1.84	0.59
1:AAA:122:ALA:O	1:AAA:125:ARG:HG3	2.08	0.54
1:AAA:78:ILE:CD1	1:AAA:83:LEU:HD21	2.43	0.49
1:AAA:40:THR:O	1:AAA:84:LEU:HA	2.14	0.47
1:AAA:30:CYS:HB2	1:AAA:123:TRP:CD1	2.49	0.47
1:AAA:10:ALA:HA	1:AAA:129:LEU:CD2	2.47	0.45
1:AAA:111:TRP:CD1	1:AAA:115:CYS:HB2	2.52	0.44
1:AAA:109[A]:VAL:HG22	1:AAA:112:ARG:NH2	2.32	0.44
1:AAA:61[B]:ARG:O	1:AAA:72:SER:HB2	2.19	0.42
1:AAA:15:HIS:HB3	6:AAA:209:IOD:I	2.90	0.41
1:AAA:30:CYS:O	1:AAA:33:LYS:HB3	2.21	0.41
1:AAA:128:ARG:CD	7:AAA:369:HOH:O	2.69	0.41
1:AAA:33:LYS:HG2	1:AAA:123:TRP:CH2	2.56	0.40
1:AAA:59[A]:ASN:OD1	1:AAA:61[A]:ARG:CB	2.69	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	AAA	134/129 (104%)	128 (96%)	5 (4%)	1 (1%)	19 10

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	128	ARG

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AAA	112/105 (107%)	108 (96%)	4 (4%)	30 20

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

Mol	Chain	Res	Type
1	AAA	14	ARG
1	AAA	21	ARG
1	AAA	55	ILE
1	AAA	125	ARG

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 2 are modelled with single atom and 8 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
3	ACT	AAA	203	-	3,3,3	0.75	0	3,3,3	1.01	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	203	ACT	2	0

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	129/129 (100%)	0.40	2 (1%) 70 76	16, 39, 64, 125	7 (5%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	129	LEU	5.3
1	AAA	17	LEU	2.5

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	1/1	0.19	0.20	46,46,46,46	1
2	NH3	AAA	202	1/1	0.60	0.14	65,65,65,65	1
6	IOD	AAA	211	1/1	0.63	0.17	77,77,77,77	1
3	ACT	AAA	203	4/4	0.83	0.13	43,53,56,57	0
6	IOD	AAA	210	1/1	0.87	0.22	75,75,75,75	1

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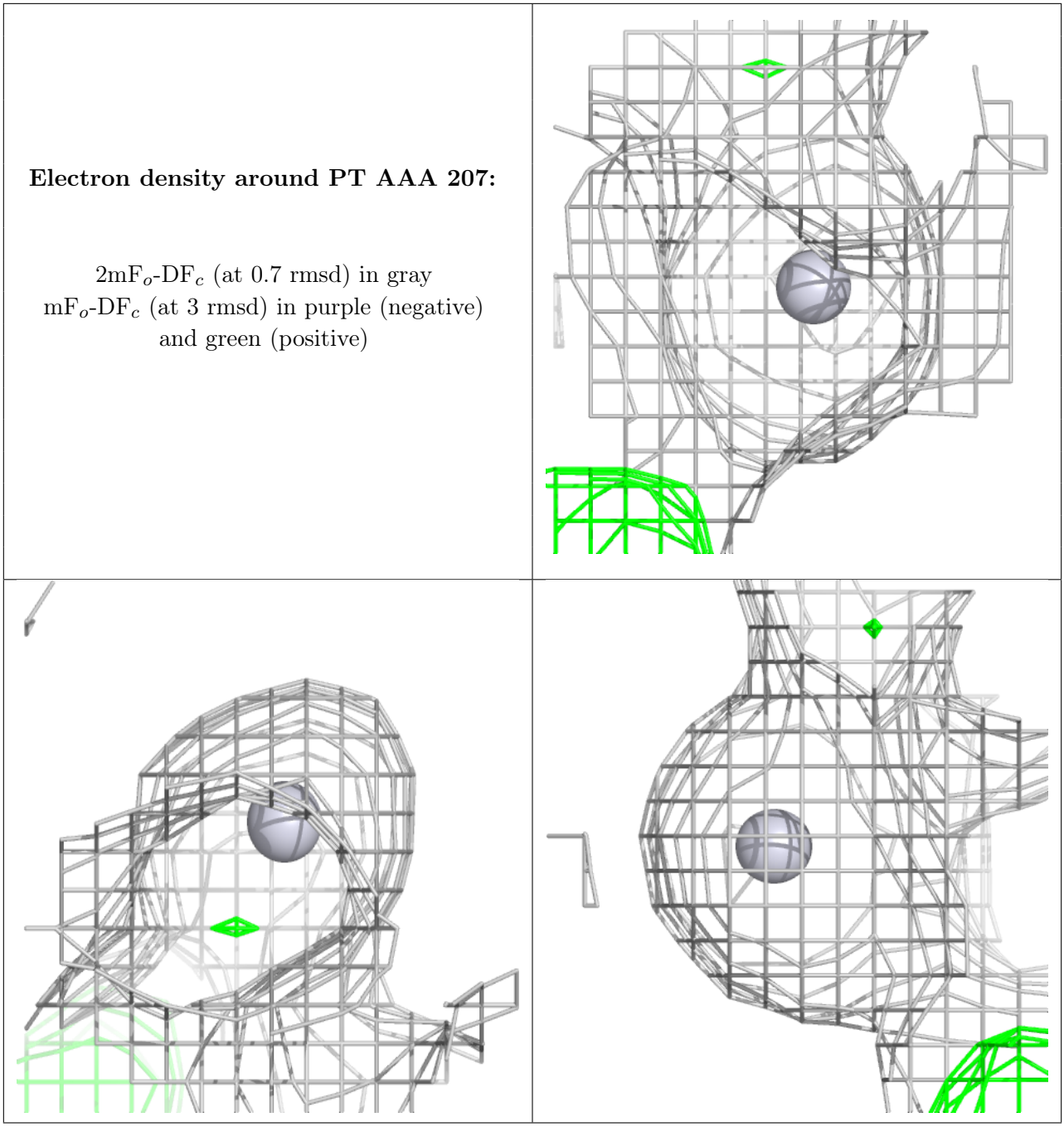
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	IOD	AAA	208	1/1	0.92	0.10	105,105,105,105	1
6	IOD	AAA	209	1/1	0.92	0.14	78,78,78,78	1
5	PT	AAA	207	1/1	0.94	0.08	75,75,75,75	1
5	PT	AAA	205	1/1	0.97	0.05	76,76,76,76	1
4	CL	AAA	204	1/1	0.97	0.07	48,48,48,48	0
5	PT	AAA	206	1/1	0.98	0.06	73,73,73,73	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.

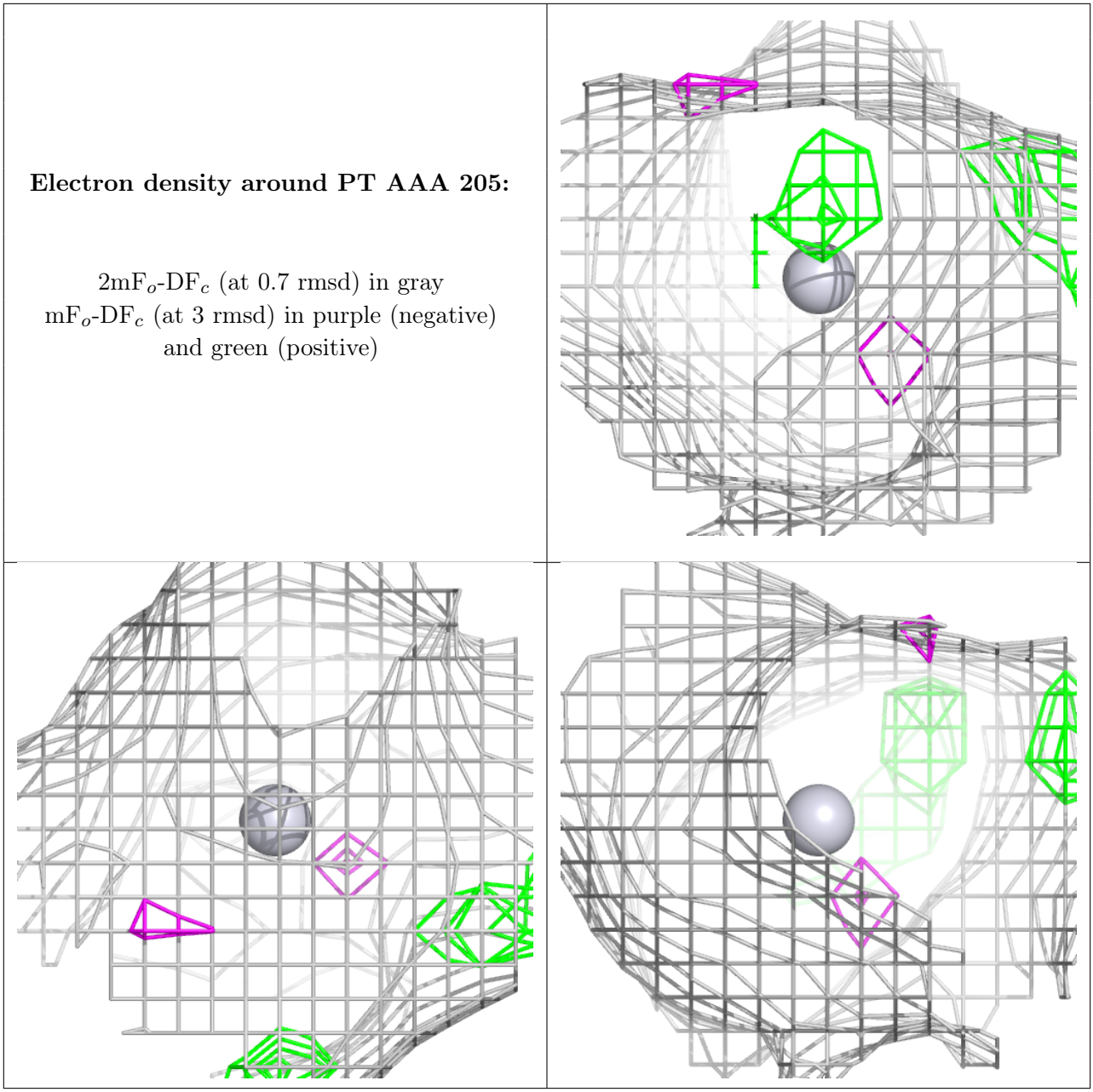
Electron density around PT AAA 207:

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



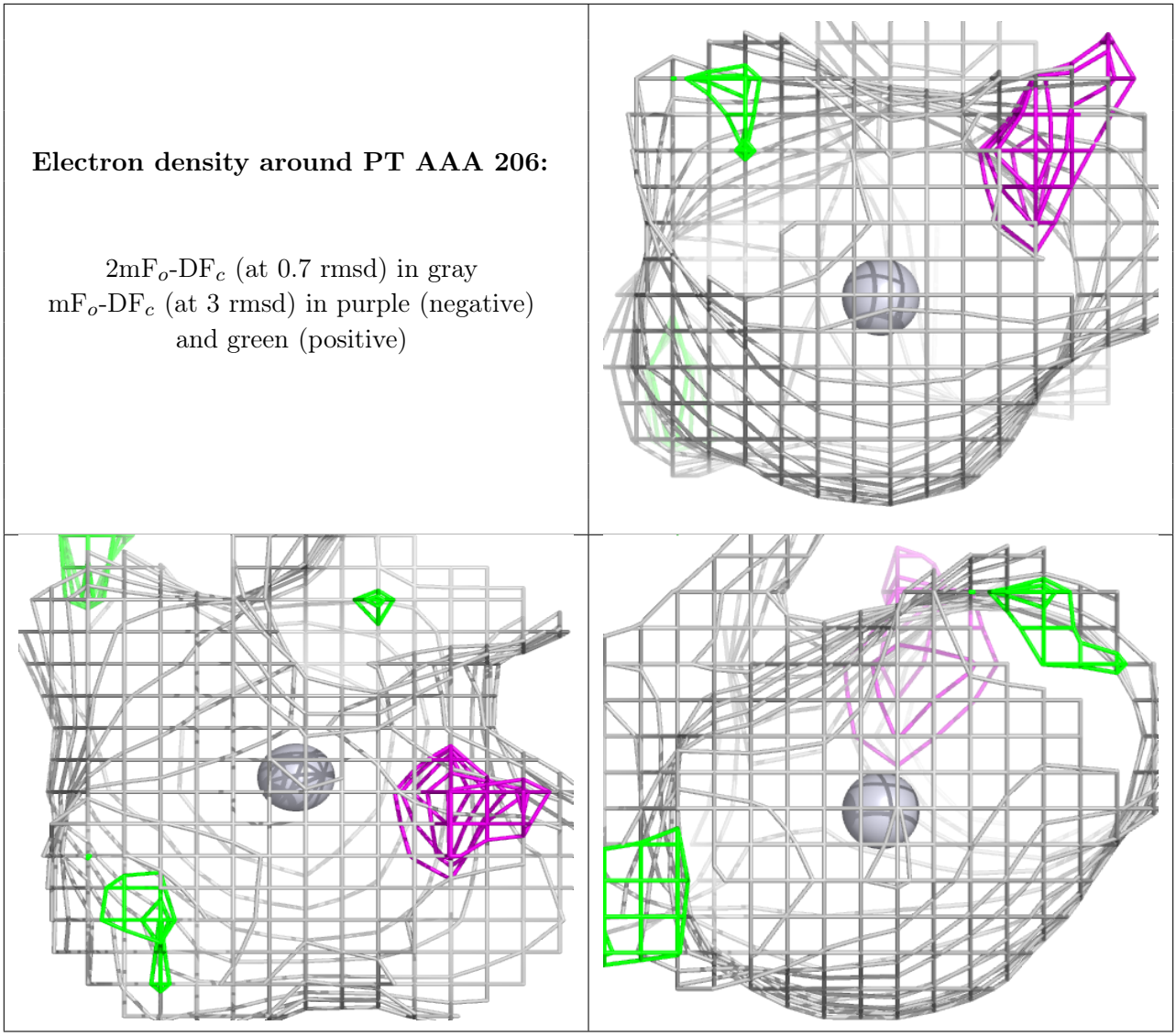
Electron density around PT AAA 205:

$2mF_o$-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)



6.5 Other polymers

There are no such residues in this entry.