



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2021 – 06:41 pm BST

PDB ID : 7PNI  
Title : X-ray structure of the adduct formed upon reaction of Pt(II) complex 2c with ribonuclease A  
Authors : Ferraro, G.; Merlino, A.  
Deposited on : 2021-09-07  
Resolution : 2.13 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

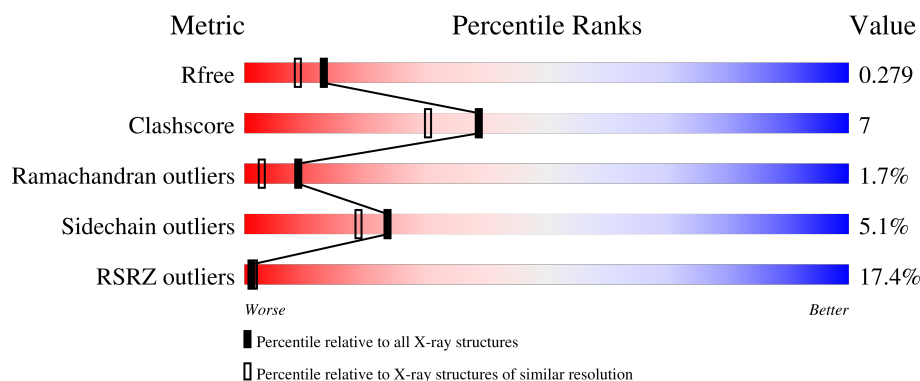
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	124	<div> <div>11%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	BBB	124	<div> <div>23%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2073 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	124	Total	C	N	O	S	0	3	0
			971	586	175	197	13			
1	BBB	123	Total	C	N	O	S	0	2	0
			952	574	171	195	12			

- Molecule 2 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is water.

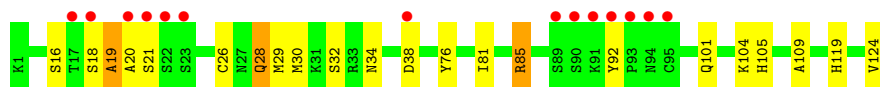
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	75	Total	O	0	5
			78	78		
3	BBB	64	Total	O	0	3
			67	67		

### 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.

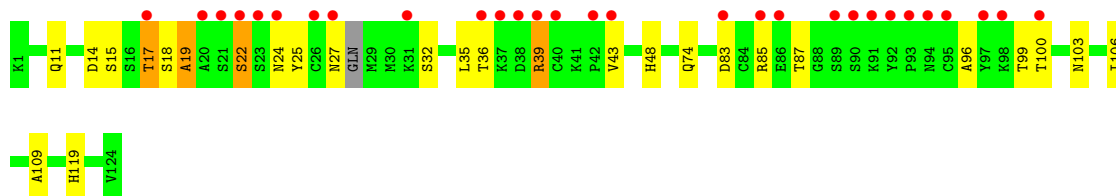
- Molecule 1: Ribonuclease pancreatic

Chain AAA: 



- Molecule 1: Ribonuclease pancreatic

Chain BBB: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.14Å 31.79Å 73.74Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	28.04 – 2.13 28.04 – 2.13	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.04-2.13) 98.2 (28.04-2.13)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.192 , 0.275 0.198 , 0.279	Depositor DCC
$R_{free}$ test set	674 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.74	0/988	0.95	1/1333 (0.1%)
1	BBB	0.73	0/967	0.89	0/1304
All	All	0.74	0/1955	0.92	1/2637 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	85	ARG	NE-CZ-NH2	-6.68	116.96	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	971	0	912	14	0
1	BBB	952	0	894	14	0
2	AAA	3	0	0	0	0
2	BBB	2	0	0	0	0
3	AAA	78	0	0	4	0
3	BBB	67	0	0	3	0
All	All	2073	0	1806	28	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 7.

All (28) 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:119[A]:HIS:HE1	3:AAA:339[A]:HOH:O	1.42	1.00
1:AAA:28:GLN:NE2	3:AAA:301:HOH:O	2.15	0.79
1:AAA:119[A]:HIS:CE1	3:AAA:339[A]:HOH:O	2.27	0.74
1:BBB:87:THR:OG1	1:BBB:96:ALA:HB3	1.95	0.67
1:AAA:29[B]:MET:HA	1:AAA:29[B]:MET:CE	2.26	0.64
1:BBB:14:ASP:O	1:BBB:48:HIS:HA	2.06	0.56
1:BBB:11:GLN:HG2	1:BBB:35:LEU:HD21	1.88	0.56
1:AAA:18:SER:O	1:AAA:19:ALA:HB2	2.11	0.51
1:BBB:27:ASN:C	3:BBB:321:HOH:O	2.50	0.49
1:AAA:29[B]:MET:HA	1:AAA:29[B]:MET:HE2	1.92	0.49
1:BBB:36:THR:OG1	3:BBB:301:HOH:O	2.20	0.48
1:BBB:17:THR:OG1	1:BBB:19:ALA:O	2.31	0.46
1:AAA:76:TYR:O	1:AAA:105:HIS:HE1	1.99	0.46
1:BBB:43:VAL:HG12	1:BBB:85:ARG:HG2	1.99	0.45
1:BBB:103:ASN:ND2	3:BBB:307:HOH:O	2.48	0.45
1:BBB:36:THR:HA	1:BBB:39:ARG:O	2.16	0.45
1:AAA:81:ILE:HD11	1:AAA:104:LYS:HD3	2.00	0.44
1:AAA:109:ALA:HB3	1:AAA:119[A]:HIS:HB3	1.98	0.43
1:AAA:29[B]:MET:HA	1:AAA:29[B]:MET:HE3	1.99	0.43
1:BBB:18:SER:O	1:BBB:19:ALA:HB2	2.18	0.43
1:AAA:20:ALA:H	1:AAA:101:GLN:NE2	2.18	0.42
1:BBB:25:TYR:HB3	1:BBB:99:THR:HG21	2.01	0.42
1:BBB:109:ALA:HB3	1:BBB:119:HIS:HB3	2.01	0.42
1:AAA:34:ASN:HA	3:AAA:325:HOH:O	2.22	0.40
1:AAA:26:CYS:O	1:AAA:30:MET:HG2	2.22	0.40
1:BBB:22:SER:CB	1:BBB:24:ASN:HD22	2.33	0.40
1:BBB:74:GLN:HA	1:BBB:106:ILE:O	2.21	0.40
1:AAA:38:ASP:O	1:AAA:92:TYR:CZ	2.75	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	125/124 (101%)	116 (93%)	7 (6%)	2 (2%)	9	3
1	BBB	121/124 (98%)	113 (93%)	6 (5%)	2 (2%)	9	3
All	All	246/248 (99%)	229 (93%)	13 (5%)	4 (2%)	9	3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	19	ALA
1	AAA	16	SER
1	AAA	19	ALA
1	BBB	39	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	111/109 (102%)	106 (96%)	5 (4%)	27	23
1	BBB	109/109 (100%)	103 (94%)	6 (6%)	21	16
All	All	220/218 (101%)	209 (95%)	11 (5%)	24	20

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	21	SER
1	AAA	28	GLN
1	AAA	32	SER
1	AAA	85	ARG
1	AAA	124	VAL
1	BBB	15	SER
1	BBB	17	THR
1	BBB	22	SER

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Mol	Chain	Res	Type
1	BBB	32	SER
1	BBB	83	ASP
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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	124/124 (100%)	0.81	14 (11%) 5 6	18, 33, 70, 87	0
1	BBB	123/124 (99%)	1.44	29 (23%) 0 0	19, 46, 92, 118	0
All	All	247/248 (99%)	1.12	43 (17%) 1 1	18, 37, 87, 118	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	22	SER	10.0
1	BBB	94	ASN	9.1
1	BBB	92	TYR	8.4
1	BBB	43	VAL	4.9
1	BBB	93	PRO	4.6
1	BBB	97	TYR	4.5
1	AAA	23	SER	4.3
1	BBB	91	LYS	4.3
1	AAA	21	SER	4.3
1	BBB	90	SER	4.1
1	BBB	42	PRO	4.0
1	AAA	92	TYR	3.9
1	BBB	21	SER	3.9
1	BBB	39	ARG	3.8
1	BBB	24	ASN	3.8
1	BBB	38	ASP	3.7
1	BBB	36	THR	3.6
1	AAA	22	SER	3.6
1	AAA	20	ALA	3.4
1	BBB	17	THR	3.4
1	AAA	38	ASP	3.4
1	BBB	37	LYS	3.3
1	BBB	98	LYS	3.3
1	AAA	91	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	31	LYS	3.2
1	BBB	86	GLU	3.2
1	BBB	40	CYS	3.1
1	AAA	18	SER	3.1
1	BBB	23	SER	3.1
1	BBB	95	CYS	3.0
1	BBB	27	ASN	3.0
1	BBB	20	ALA	2.7
1	AAA	94	ASN	2.7
1	BBB	26	CYS	2.7
1	BBB	85	ARG	2.6
1	AAA	17	THR	2.5
1	BBB	89	SER	2.5
1	AAA	93	PRO	2.4
1	AAA	89	SER	2.4
1	BBB	100	THR	2.1
1	AAA	90	SER	2.1
1	BBB	83	ASP	2.0
1	AAA	95	CYS	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<sup>th</sup> 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.

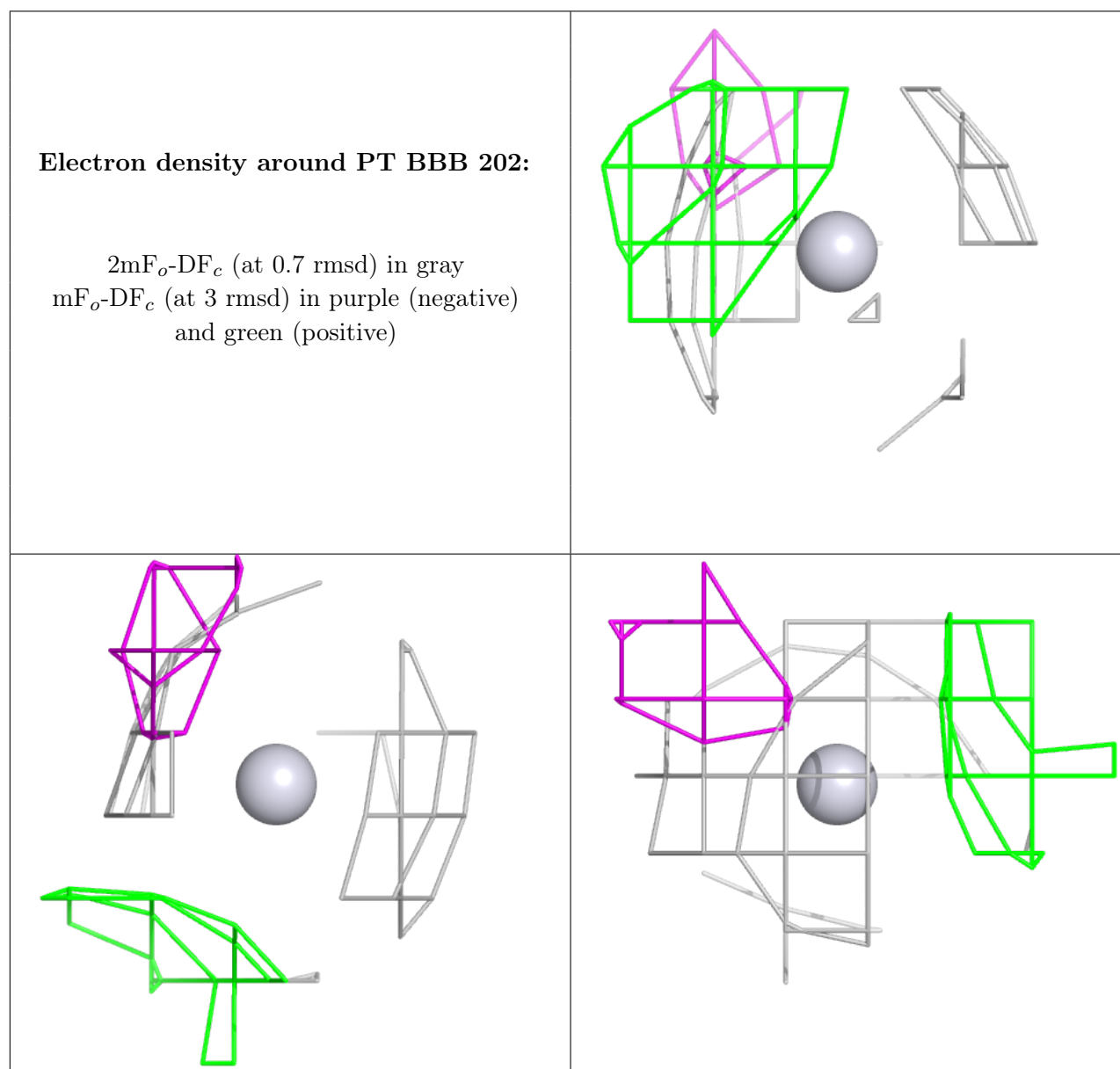
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	PT	BBB	202	1/1	0.77	0.09	68,68,68,68	1
2	PT	AAA	203[A]	1/1	0.90	0.09	59,59,59,59	1
2	PT	AAA	201	1/1	0.91	0.05	60,60,60,60	1
2	PT	BBB	201	1/1	0.96	0.04	61,61,61,61	1

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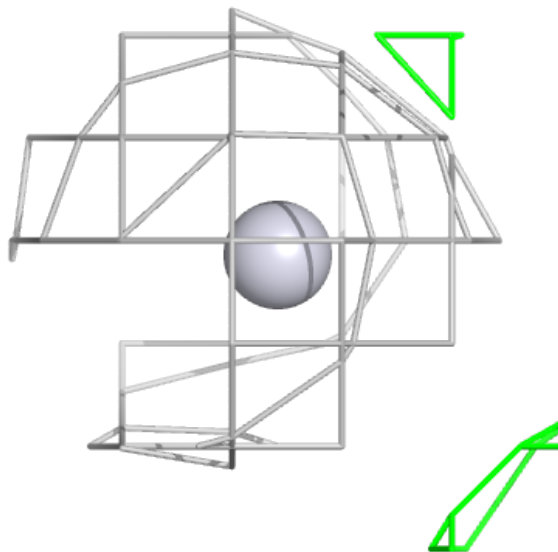
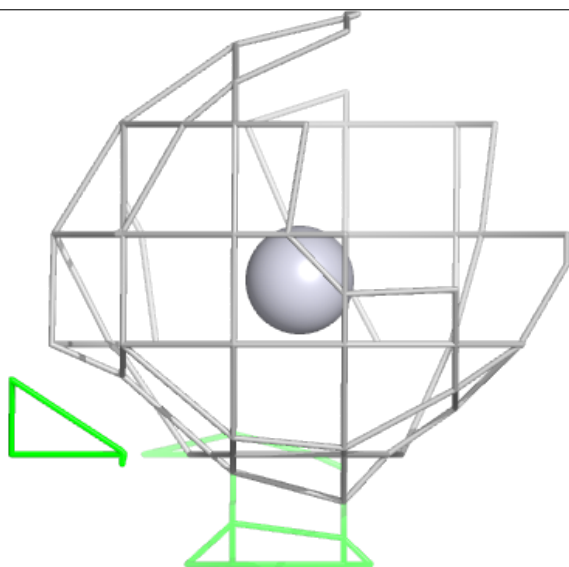
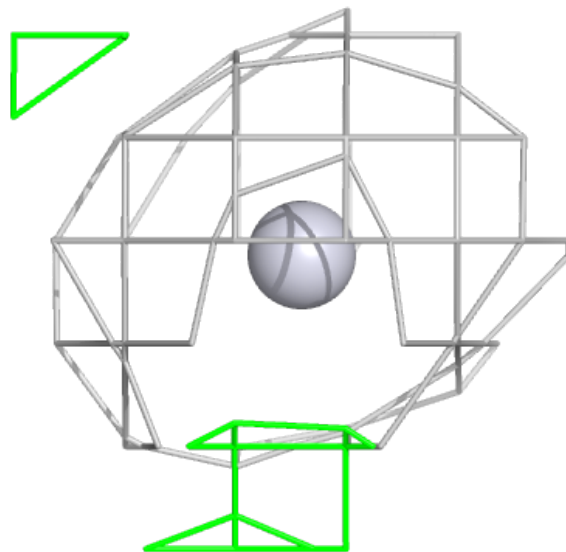
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PT	AAA	202[B]	1/1	0.97	0.17	56,56,56,56	1

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.



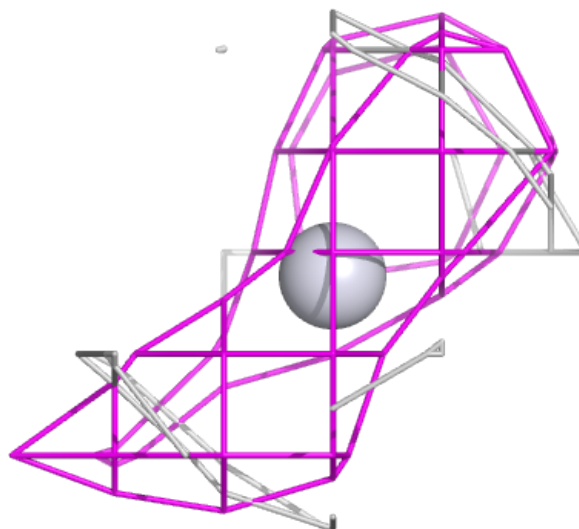
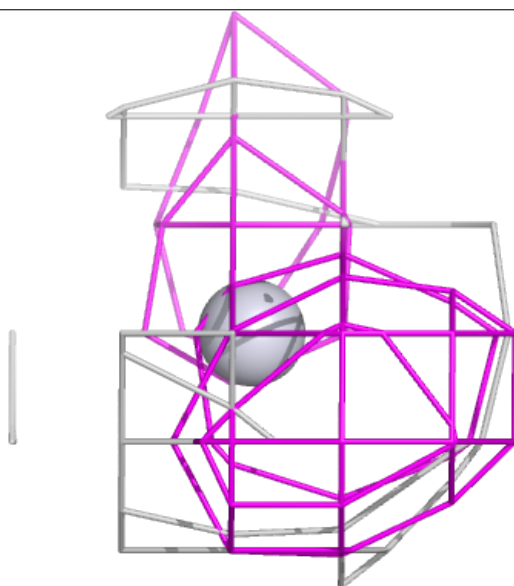
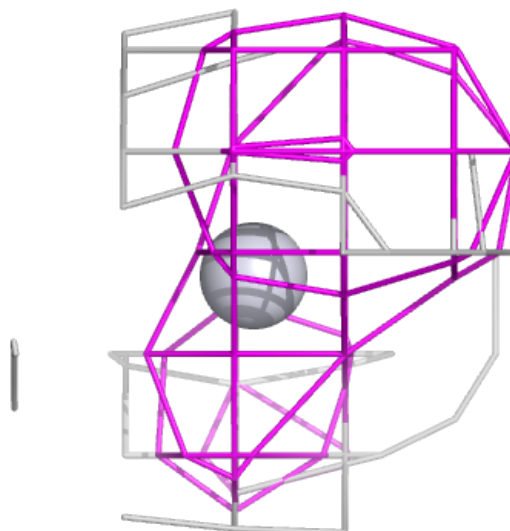
**Electron density around PT AAA 203 (A):**

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



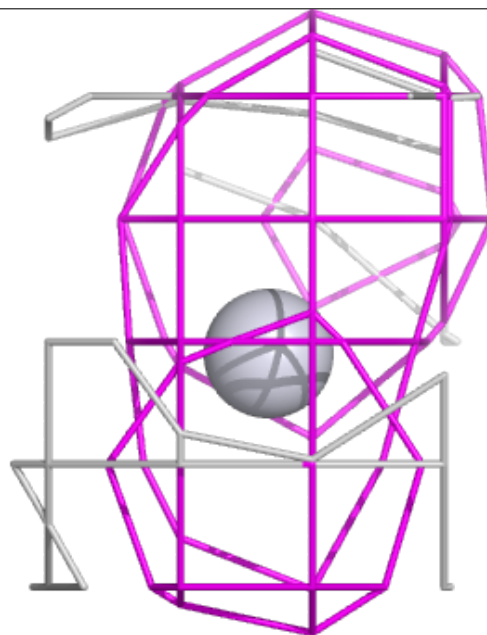
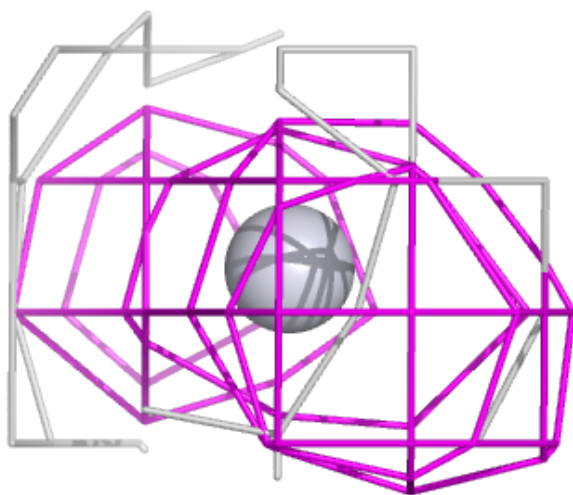
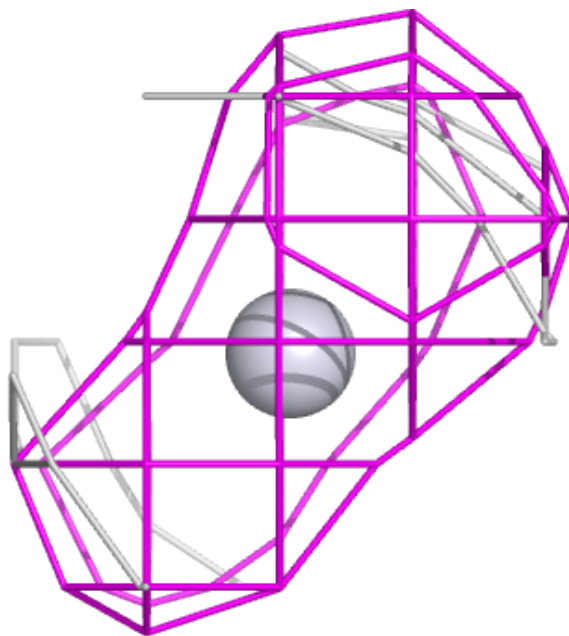
**Electron density around PT AAA 201:**

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



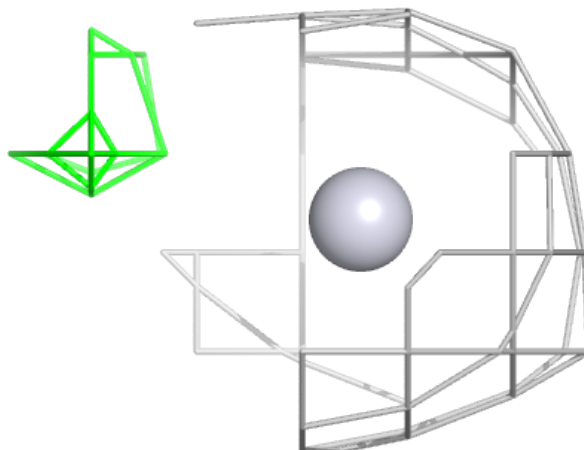
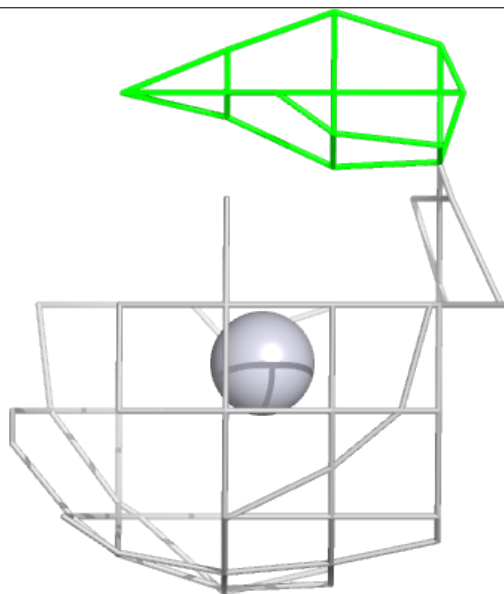
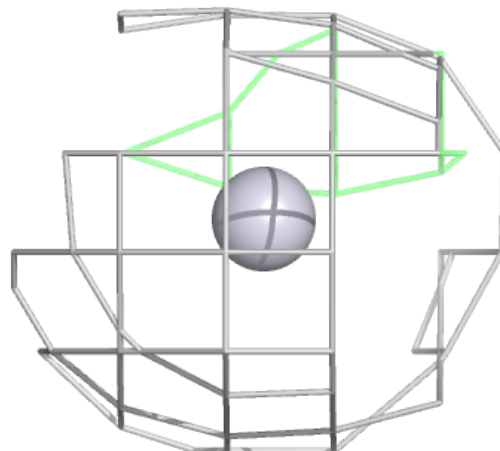
**Electron density around PT BBB 201:**

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



**Electron density around PT AAA 202 (B):**

$2mF_o-DF_c$  (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.