



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 06:11 am BST

PDB ID : 6XVX  
Title : X-ray structure obtained upon reaction of dirhodium tetraacetate with RNase A (high resolution)  
Authors : Merlino, A.; Ferraro, G.  
Deposited on : 2020-01-22  
Resolution : 1.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

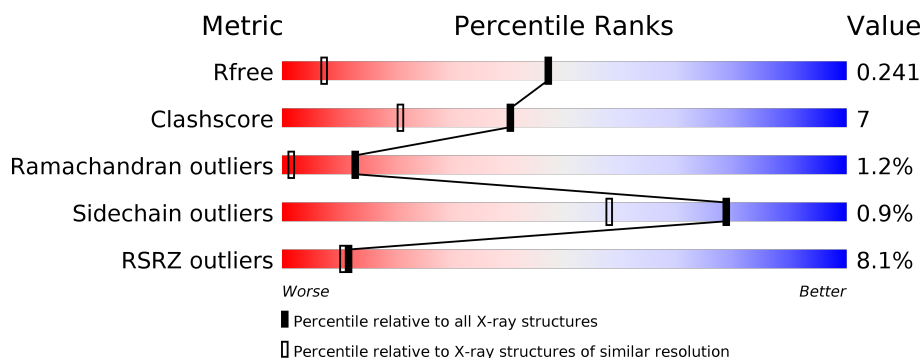
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 on 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>6%</div> <div>85%</div> <div>14%</div> </div>
1	BBB	124	<div> <div>10%</div> <div>92%</div> <div>7%</div> </div>

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	ACT	AAA	207	-	-	X	-
2	ACT	AAA	208	-	-	X	-
2	ACT	BBB	207	-	-	X	-
3	RH3	AAA	211	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2385 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	8	0
			1015	610	184	208	13			
1	BBB	124	Total	C	N	O	S	0	5	0
			989	596	177	203	13			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

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

- Molecule 3 is RHODIUM(III) ION (three-letter code: RH3) (formula: Rh) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	BBB	4	Total 4	Rh 4	0	0
3	AAA	4	Total 4	Rh 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	155	Total 162	O 162	0	9
4	BBB	140	Total 143	O 143	0	5

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

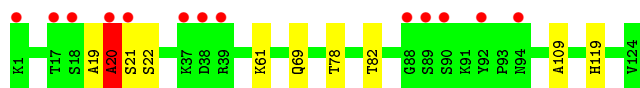
- Molecule 1: Ribonuclease pancreatic

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, $\alpha$ , $\beta$ , $\gamma$	100.43Å 32.75Å 72.69Å 90.00° 90.38° 90.00°	Depositor
Resolution (Å)	72.69 – 1.40 41.19 – 1.40	Depositor EDS
% Data completeness (in resolution range)	92.7 (72.69-1.40) 92.7 (41.19-1.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.188 , 0.233 0.196 , 0.241	Depositor DCC
$R_{free}$ test set	2317 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2385	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.86% 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: RH3, ACT

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	0.80	0/1032	0.93	0/1391
1	BBB	0.79	0/1005	0.89	0/1354
All	All	0.80	0/2037	0.91	0/2745

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	BBB	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	20	ALA	Peptide

### 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	1015	0	949	17	0
1	BBB	989	0	933	7	0
2	AAA	32	0	24	6	0
2	BBB	36	0	27	2	0
3	AAA	4	0	0	2	0
3	BBB	4	0	0	0	0
4	AAA	162	0	0	2	0
4	BBB	143	0	0	2	0
All	All	2385	0	1933	29	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.

The worst 5 of 29 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)
2:AAA:207:ACT:OXT	3:AAA:211:RH3:RH	1.18	0.98
2:AAA:208:ACT:OXT	3:AAA:211:RH3:RH	1.24	0.89
1:AAA:24[A]:ASN:HD22	1:AAA:28:GLN:HE21	1.32	0.75
1:AAA:29[A]:MET:HA	1:AAA:29[A]:MET:HE3	1.77	0.67
1:AAA:29[A]:MET:CE	1:AAA:29[A]:MET:HA	2.28	0.63

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	130/124 (105%)	127 (98%)	2 (2%)	1 (1%)	19 4
1	BBB	127/124 (102%)	117 (92%)	8 (6%)	2 (2%)	9 1
All	All	257/248 (104%)	244 (95%)	10 (4%)	3 (1%)	13 1

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	16	SER
1	BBB	20	ALA
1	BBB	22	SER

### 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	117/109 (107%)	115 (98%)	2 (2%)	60	31
1	BBB	114/109 (105%)	114 (100%)	0	100	100
All	All	231/218 (106%)	229 (99%)	2 (1%)	78	58

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	1	LYS
1	AAA	16	SER

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 25 ligands modelled in this entry, 8 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
2	ACT	AAA	207	3	1,3,3	4.42	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	201	3	1,3,3	2.60	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	205	3	1,3,3	4.87	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	207	3	1,3,3	4.27	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	206	3	1,3,3	2.90	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	203	3	1,3,3	3.54	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	203	3	1,3,3	4.61	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	206	3	1,3,3	5.14	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	202	3	1,3,3	3.25	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	208	3	1,3,3	6.19	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	205	3	1,3,3	3.57	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	204	3	1,3,3	5.80	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	209	3	1,3,3	3.39	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	208	-	1,3,3	5.38	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	201	3	1,3,3	3.30	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	202	3	1,3,3	3.66	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	204	3	1,3,3	4.21	1 (100%)	0,3,3	0.00	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	208	ACT	CH3-C	6.19	1.56	1.48
2	AAA	204	ACT	CH3-C	5.80	1.56	1.48
2	BBB	208	ACT	CH3-C	5.38	1.55	1.48
2	BBB	206	ACT	CH3-C	5.14	1.55	1.48
2	BBB	205	ACT	CH3-C	4.87	1.54	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	207	ACT	2	0
2	BBB	207	ACT	2	0
2	AAA	206	ACT	1	0
2	BBB	206	ACT	1	0
2	AAA	208	ACT	3	0
2	AAA	205	ACT	1	0
2	AAA	204	ACT	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	0.39	7 (5%) 24 22	9, 17, 44, 95	0
1	BBB	124/124 (100%)	0.38	13 (10%) 6 5	9, 19, 43, 60	0
All	All	248/248 (100%)	0.38	20 (8%) 12 11	9, 18, 44, 95	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	20	ALA	13.8
1	AAA	19	ALA	11.2
1	AAA	18	SER	8.6
1	AAA	21	SER	7.4
1	BBB	89	SER	4.3

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

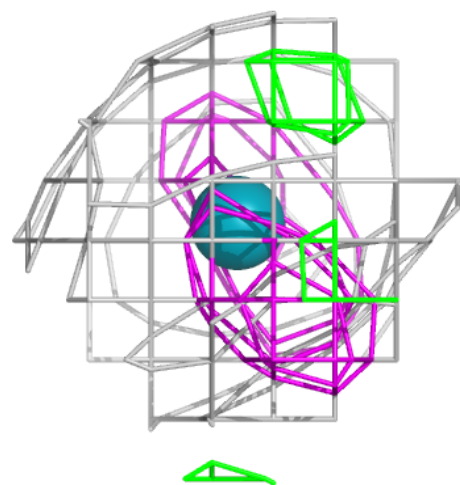
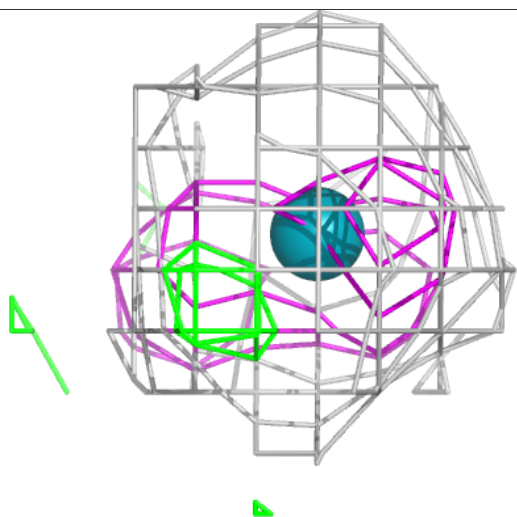
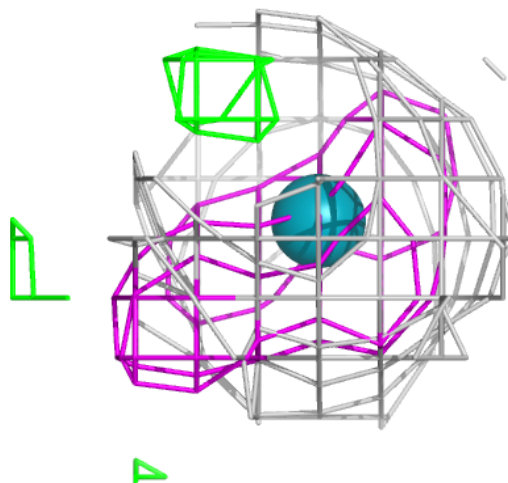
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACT	BBB	208	4/4	0.49	0.21	25,29,32,33	0
2	ACT	BBB	209	4/4	0.61	0.23	29,31,31,32	4
2	ACT	AAA	205	4/4	0.70	0.18	18,22,22,23	4
2	ACT	BBB	207	4/4	0.76	0.30	33,38,39,39	4
2	ACT	BBB	205	4/4	0.77	0.22	22,24,24,27	4
2	ACT	BBB	206	4/4	0.77	0.22	22,25,25,26	4
2	ACT	AAA	204	4/4	0.79	0.17	13,14,15,15	4
2	ACT	AAA	202	4/4	0.79	0.16	24,26,27,29	4
2	ACT	AAA	203	4/4	0.82	0.14	24,25,25,26	4
2	ACT	BBB	204	4/4	0.85	0.12	15,17,17,20	4
2	ACT	AAA	206	4/4	0.91	0.15	24,27,28,28	4
2	ACT	BBB	201	4/4	0.92	0.13	21,23,23,25	4
2	ACT	AAA	201	4/4	0.92	0.12	14,15,17,18	4
2	ACT	BBB	202	4/4	0.93	0.10	23,26,27,27	4
2	ACT	BBB	203	4/4	0.95	0.12	23,26,26,26	4
3	RH3	AAA	212	1/1	0.95	0.07	28,28,28,28	1
3	RH3	AAA	210	1/1	0.97	0.04	22,22,22,22	1
2	ACT	AAA	208	4/4	0.97	0.12	17,22,27,27	4
3	RH3	BBB	211	1/1	0.97	0.06	24,24,24,24	1
3	RH3	BBB	213	1/1	0.98	0.07	27,27,27,27	1
2	ACT	AAA	207	4/4	0.98	0.09	10,21,21,24	4
3	RH3	BBB	212	1/1	0.98	0.07	18,18,18,18	1
3	RH3	AAA	211	1/1	0.98	0.04	20,20,20,20	1
3	RH3	AAA	209	1/1	0.99	0.04	16,16,16,16	1
3	RH3	BBB	210	1/1	0.99	0.05	18,18,18,18	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.

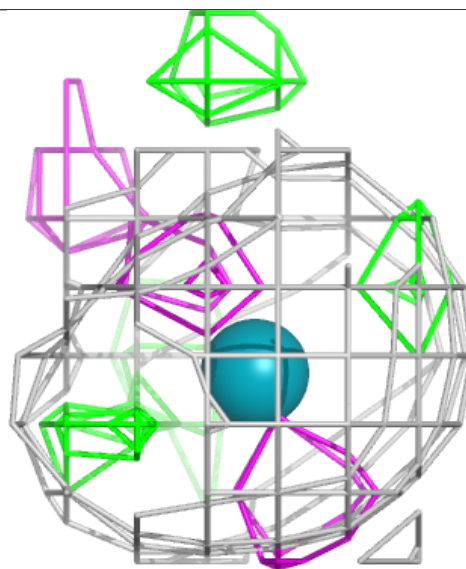
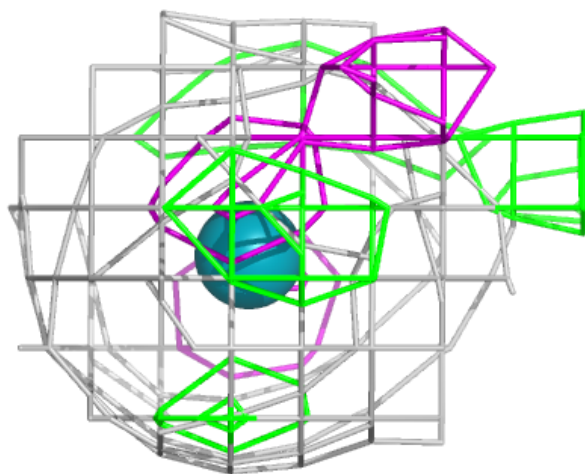
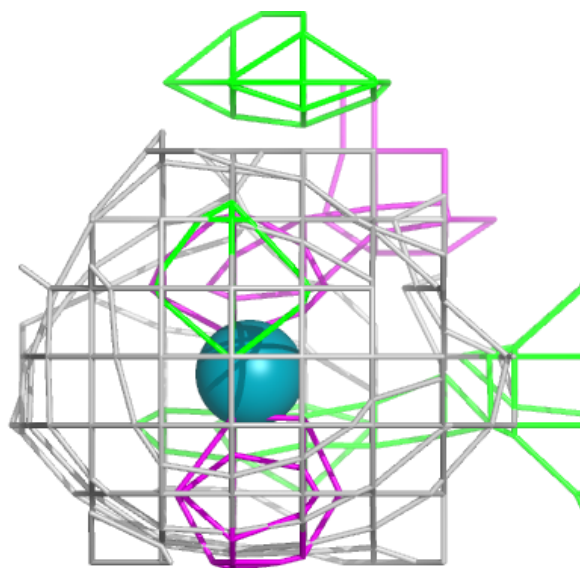
**Electron density around RH3 AAA 212:**

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



**Electron density around RH3 AAA 210:**

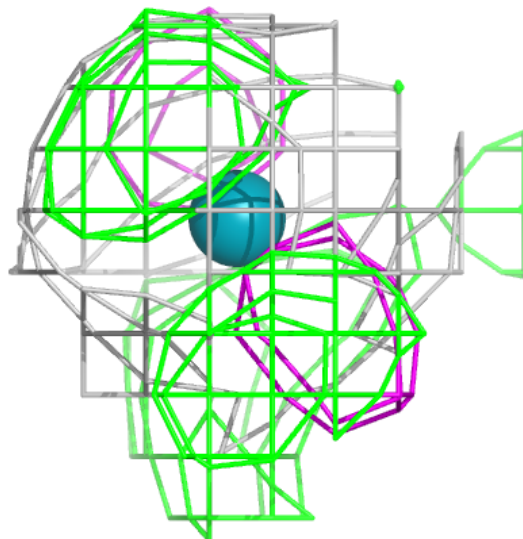
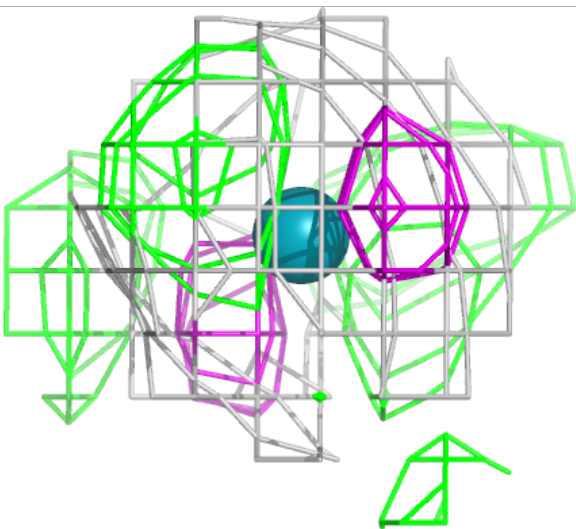
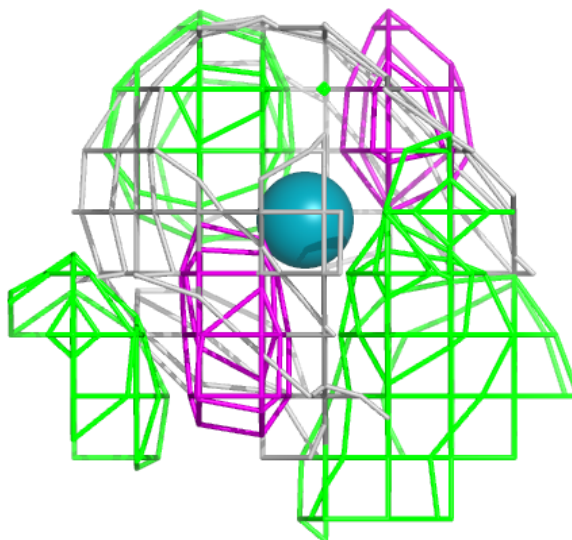
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





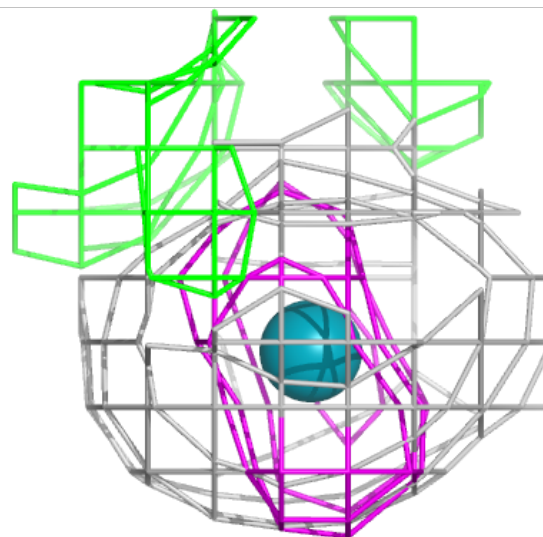
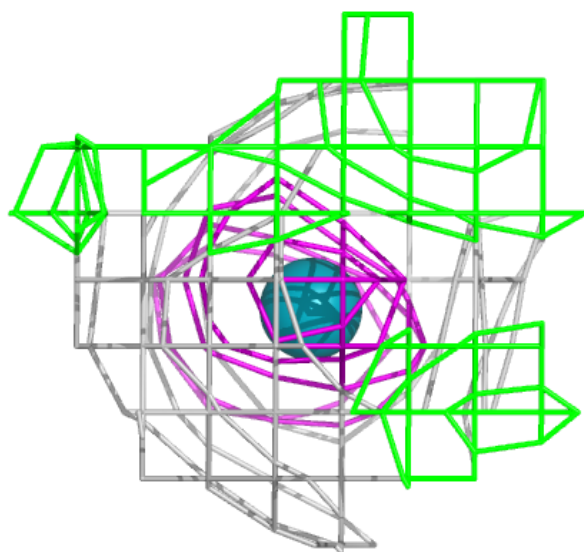
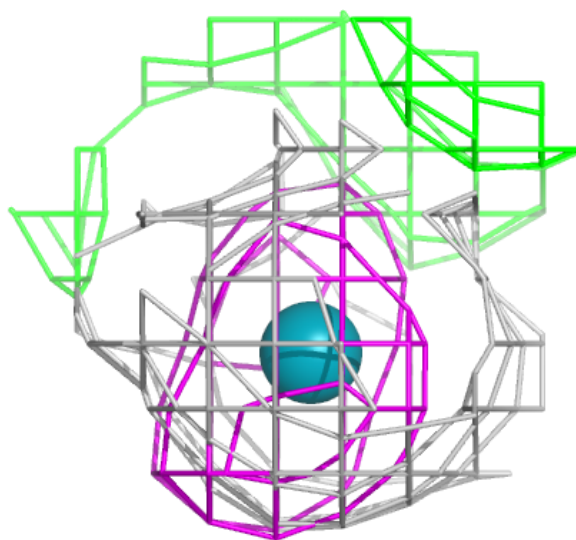
**Electron density around RH3 BBB 211:**

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



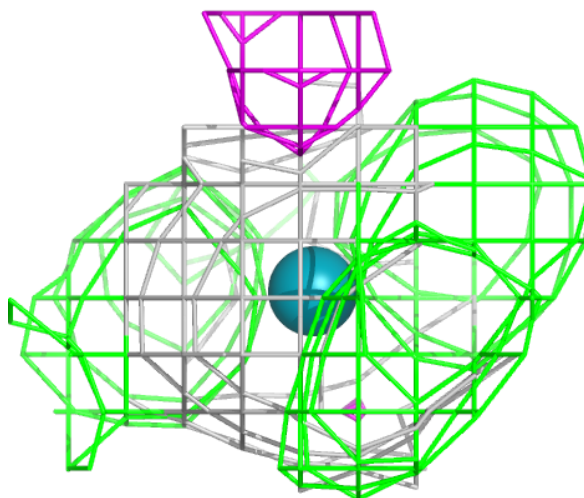
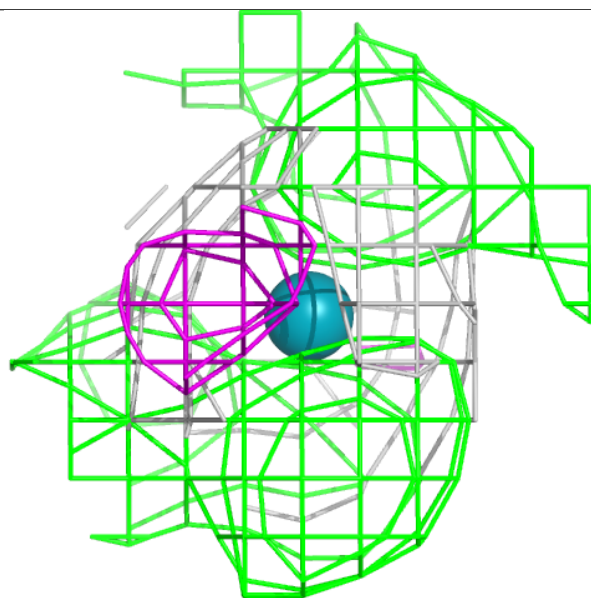
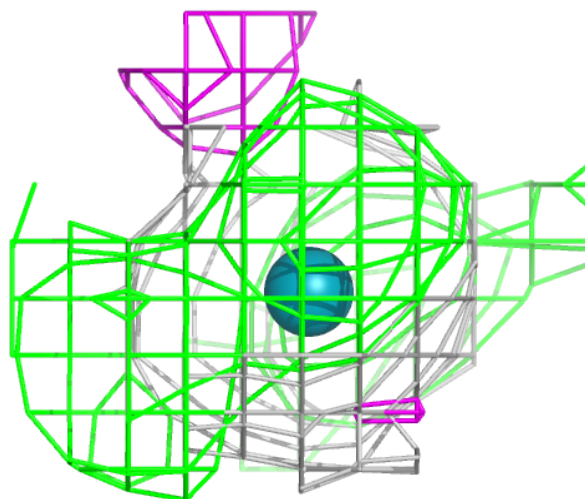
**Electron density around RH3 BBB 213:**

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



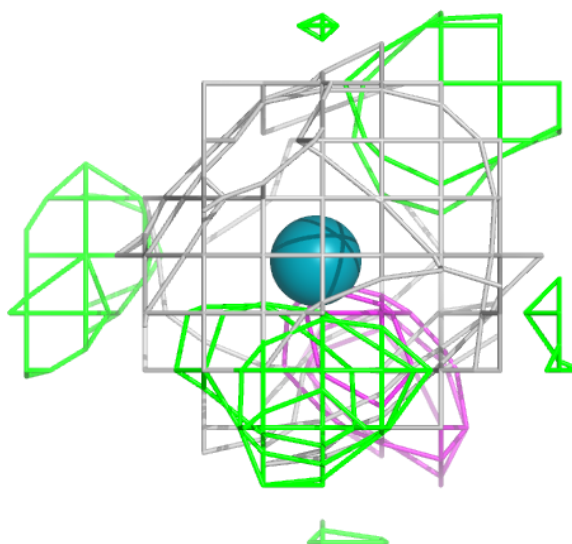
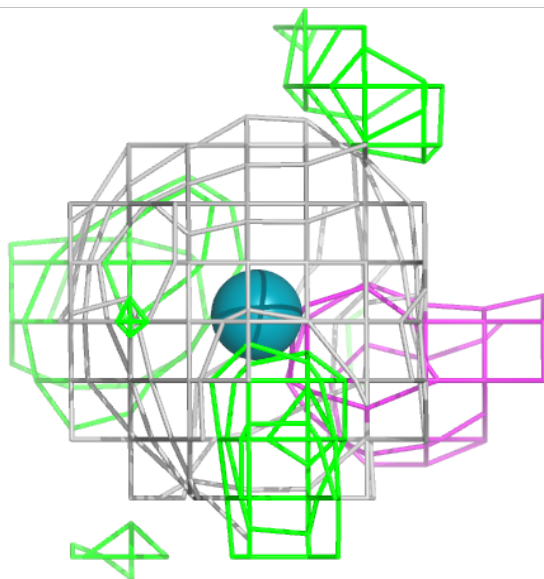
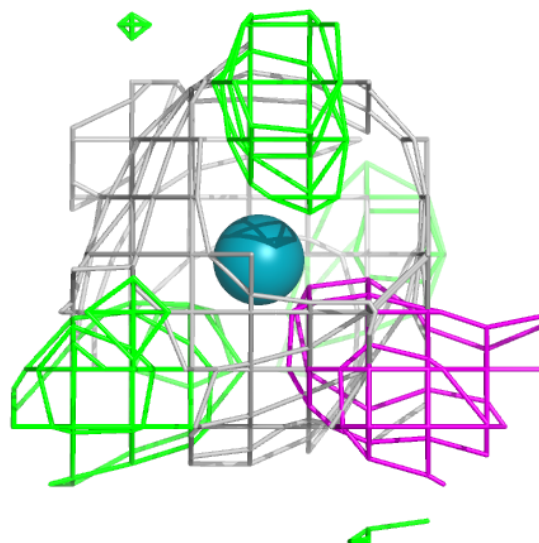
**Electron density around RH3 BBB 212:**

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



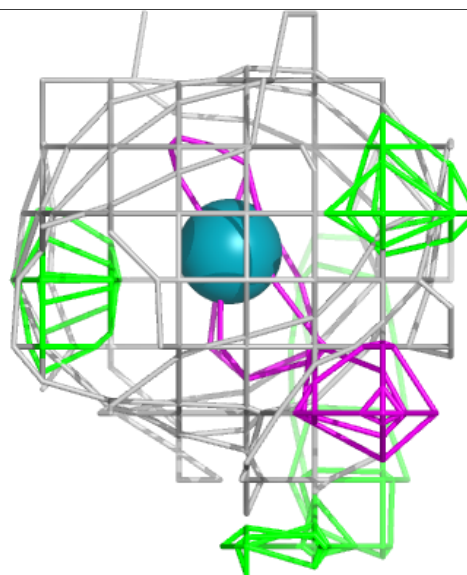
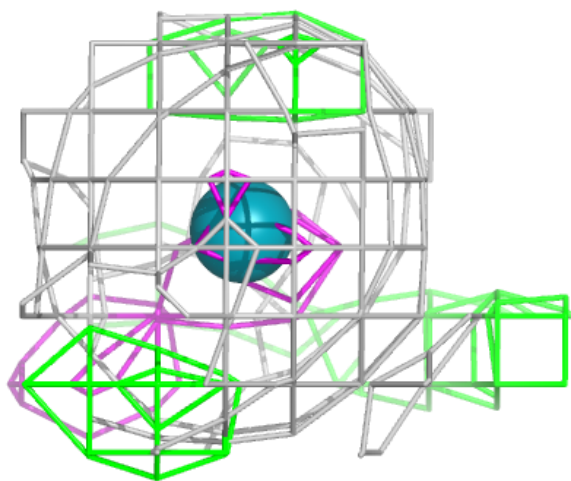
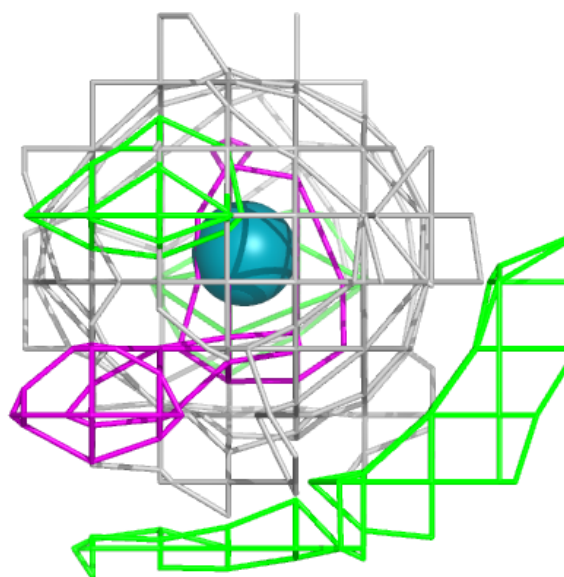
**Electron density around RH3 AAA 211:**

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



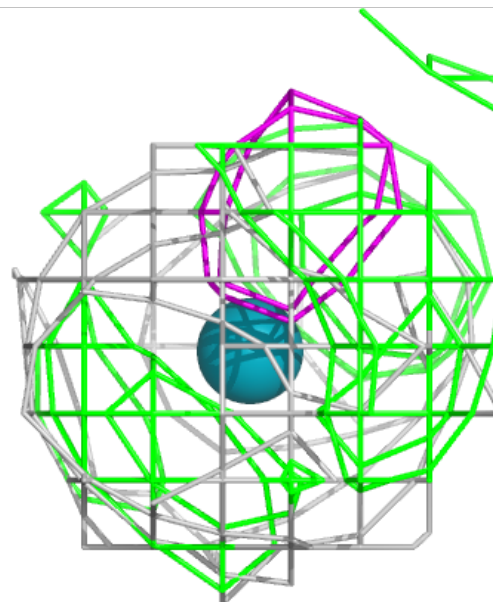
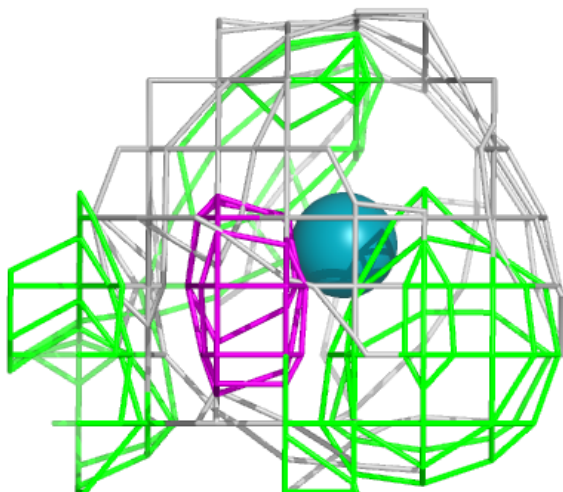
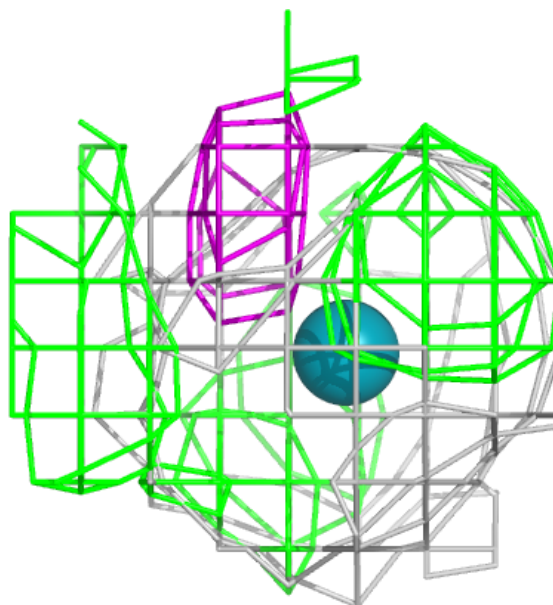
**Electron density around RH3 AAA 209:**

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



**Electron density around RH3 BBB 210:**

$2mF_o-DF_c$  (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.