



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:02 pm BST

PDB ID : 6XW0
Title : X-ray structure obtained upon reaction of dirhodium tetraacetate with RNase A (low resolution)
Authors : Merlino, A.; Ferraro, G.
Deposited on : 2020-01-22
Resolution : 1.80 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 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

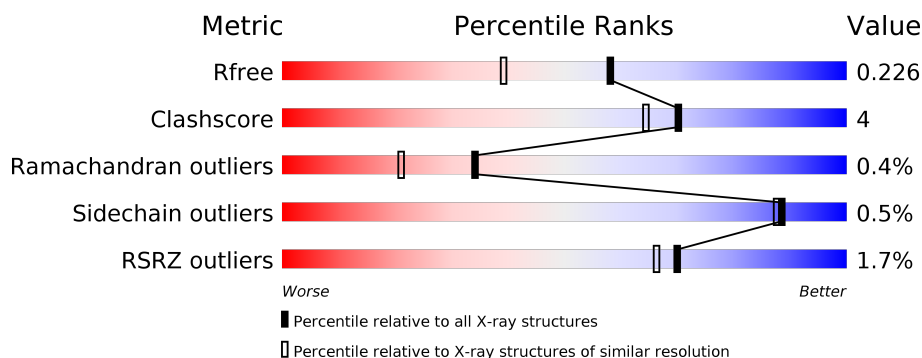
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 ≥ 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>3%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div></div> </div> </div>
1	BBB	124	<div> <div></div> <div> <div>89%</div> <div>6%</div> <div>5%</div> </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
3	ACT	AAA	205	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2306 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.

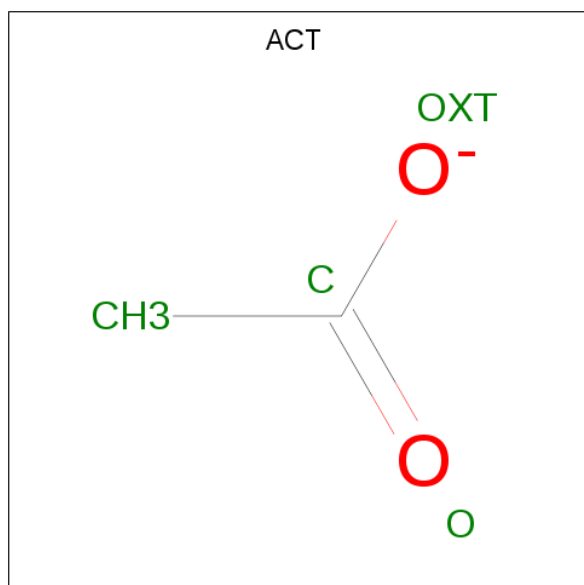
- Molecule 1 is a protein called Ribonuclease pancreatic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	124	Total	C	N	O	S	0	3	0
			972	586	175	199	12			
1	BBB	118	Total	C	N	O	S	0	5	0
			959	579	176	192	12			

- Molecule 2 is RHODIUM(III) ION (three-letter code: RH3) (formula: Rh) (labeled as "Ligand of Interest" by author).

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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

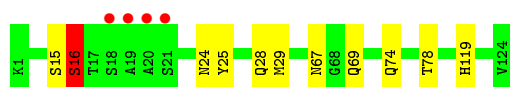
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	169	Total O 170 170	0	1
4	BBB	149	Total O 149 149	0	1

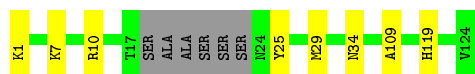
3 Residue-property plots [i](#)

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



- Molecule 1: Ribonuclease pancreatic



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.66Å 32.44Å 68.02Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	67.93 – 1.80 41.16 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (67.93-1.80) 94.1 (41.16-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.169 , 0.218 0.178 , 0.226	Depositor DCC
R_{free} test set	993 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2306	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.72	0/988	0.90	0/1332
1	BBB	0.71	0/974	0.82	0/1310
All	All	0.72	0/1962	0.86	0/2642

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	972	0	920	8	0
1	BBB	959	0	905	5	0
2	AAA	4	0	0	0	0
2	BBB	4	0	0	0	0
3	AAA	32	0	24	3	0
3	BBB	16	0	12	0	0
4	AAA	170	0	0	3	0
4	BBB	149	0	0	2	0
All	All	2306	0	1861	14	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 4.

All (14) 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)
3:AAA:205:ACT:H3	4:AAA:418:HOH:O	2.05	0.57
1:AAA:25:TYR:CZ	1:AAA:29:MET:HG3	2.39	0.56
1:AAA:74:GLN:HG2	4:AAA:301:HOH:O	2.05	0.56
1:BBB:10:ARG:HD2	1:BBB:34[A]:ASN:HD22	1.78	0.48
1:AAA:67:ASN:ND2	1:AAA:69[A]:GLN:OE1	2.44	0.48
1:BBB:25:TYR:CZ	1:BBB:29:MET:HG3	2.49	0.47
1:AAA:15:SER:O	1:AAA:16:SER:C	2.55	0.45
1:AAA:119:HIS:HB2	3:AAA:206:ACT:O	2.17	0.45
1:AAA:78:THR:HG21	3:AAA:205:ACT:H1	1.99	0.44
1:AAA:69[A]:GLN:NE2	4:AAA:309:HOH:O	2.52	0.42
1:BBB:109:ALA:HB3	1:BBB:119:HIS:HB3	2.00	0.42
1:BBB:1:LYS:N	4:BBB:317:HOH:O	2.53	0.42
1:AAA:24:ASN:ND2	1:AAA:28:GLN:HG3	2.36	0.41
1:BBB:7:LYS:NZ	4:BBB:301:HOH:O	2.15	0.41

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%)	120 (96%)	4 (3%)	1 (1%)	19	7
1	BBB	119/124 (96%)	115 (97%)	4 (3%)	0	100	100
All	All	244/248 (98%)	235 (96%)	8 (3%)	1 (0%)	34	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	16	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	112/109 (103%)	111 (99%)	1 (1%)	78	75
1	BBB	110/109 (101%)	110 (100%)	0	100	100
All	All	222/218 (102%)	221 (100%)	1 (0%)	88	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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 [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	BBB	205	2	1,3,3	3.91	1 (100%)	0,3,3	0.00	-
3	ACT	AAA	208	2	1,3,3	4.22	1 (100%)	0,3,3	0.00	-
3	ACT	AAA	210	2	1,3,3	3.08	1 (100%)	0,3,3	0.00	-
3	ACT	AAA	207	2	1,3,3	5.17	1 (100%)	0,3,3	0.00	-
3	ACT	AAA	209	2	1,3,3	7.57	1 (100%)	0,3,3	0.00	-
3	ACT	BBB	207	2	1,3,3	3.96	1 (100%)	0,3,3	0.00	-
3	ACT	AAA	206	2	1,3,3	3.58	1 (100%)	0,3,3	0.00	-
3	ACT	BBB	206	2	1,3,3	4.53	1 (100%)	0,3,3	0.00	-
3	ACT	AAA	205	2	1,3,3	4.04	1 (100%)	0,3,3	0.00	-
3	ACT	BBB	208	2	1,3,3	2.06	1 (100%)	0,3,3	0.00	-
3	ACT	AAA	211	2	1,3,3	3.87	1 (100%)	0,3,3	0.00	-
3	ACT	AAA	212	2	1,3,3	3.23	1 (100%)	0,3,3	0.00	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	209	ACT	CH3-C	7.57	1.58	1.48
3	AAA	207	ACT	CH3-C	5.17	1.55	1.48
3	BBB	206	ACT	CH3-C	4.53	1.54	1.48
3	AAA	208	ACT	CH3-C	4.22	1.54	1.48
3	AAA	205	ACT	CH3-C	4.04	1.53	1.48
3	BBB	207	ACT	CH3-C	3.96	1.53	1.48
3	BBB	205	ACT	CH3-C	3.91	1.53	1.48
3	AAA	211	ACT	CH3-C	3.87	1.53	1.48
3	AAA	206	ACT	CH3-C	3.58	1.53	1.48
3	AAA	212	ACT	CH3-C	3.23	1.52	1.48
3	AAA	210	ACT	CH3-C	3.08	1.52	1.48
3	BBB	208	ACT	CH3-C	2.06	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	206	ACT	1	0
3	AAA	205	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 [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, 95th 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	124/124 (100%)	-0.17	4 (3%) 47 41	11, 20, 50, 83	0
1	BBB	118/124 (95%)	-0.26	0 100 100	12, 21, 40, 63	0
All	All	242/248 (97%)	-0.21	4 (1%) 70 66	11, 21, 44, 83	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	20	ALA	6.0
1	AAA	18	SER	4.6
1	AAA	19	ALA	2.2
1	AAA	21	SER	2.2

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, 95th 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
3	ACT	AAA	209	4/4	0.82	0.23	21,24,26,26	4

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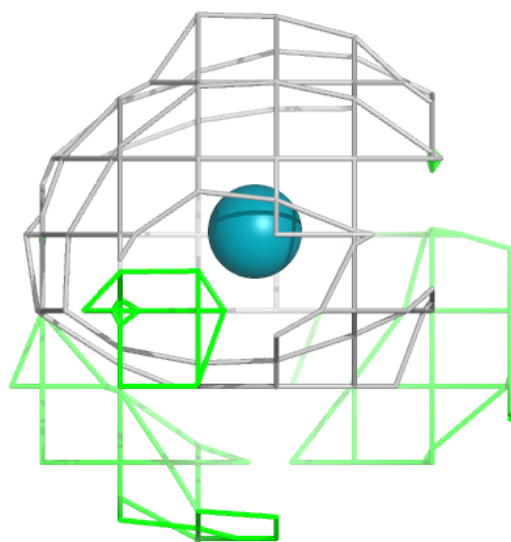
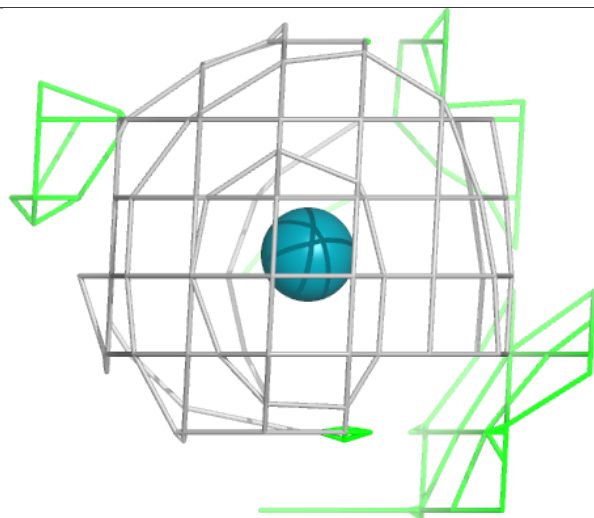
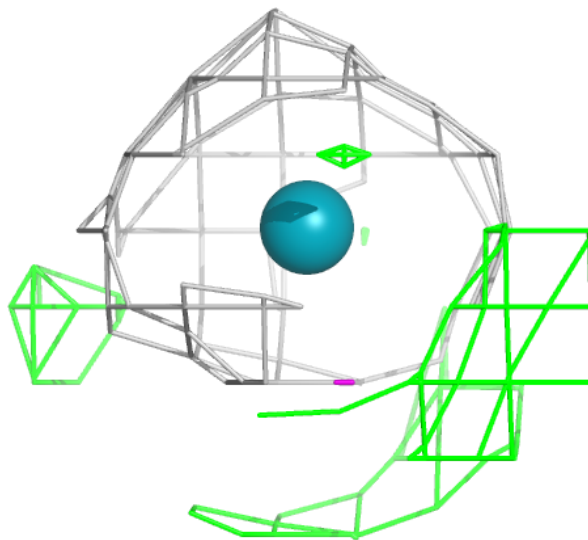
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACT	AAA	207	4/4	0.86	0.18	33,38,39,39	4
3	ACT	AAA	206	4/4	0.87	0.18	26,29,30,33	4
3	ACT	AAA	210	4/4	0.89	0.18	26,29,30,33	4
3	ACT	AAA	208	4/4	0.92	0.20	33,35,35,35	4
3	ACT	BBB	206	4/4	0.92	0.13	22,22,23,26	4
3	ACT	AAA	211	4/4	0.92	0.21	35,38,38,39	4
3	ACT	BBB	205	4/4	0.96	0.13	28,33,34,37	4
3	ACT	BBB	208	4/4	0.97	0.12	22,24,25,26	4
3	ACT	AAA	205	4/4	0.97	0.21	17,21,24,24	4
2	RH3	BBB	204	1/1	0.98	0.04	36,36,36,36	1
2	RH3	AAA	204	1/1	0.98	0.04	36,36,36,36	1
2	RH3	AAA	202	1/1	0.98	0.04	30,30,30,30	1
2	RH3	AAA	201	1/1	0.98	0.04	24,24,24,24	1
3	ACT	BBB	207	4/4	0.99	0.08	25,32,33,35	4
2	RH3	BBB	203	1/1	0.99	0.06	19,19,19,19	1
2	RH3	BBB	201	1/1	0.99	0.03	28,28,28,28	1
2	RH3	AAA	203	1/1	0.99	0.04	29,29,29,29	1
3	ACT	AAA	212	4/4	0.99	0.07	18,22,23,24	4
2	RH3	BBB	202	1/1	1.00	0.03	20,20,20,20	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.

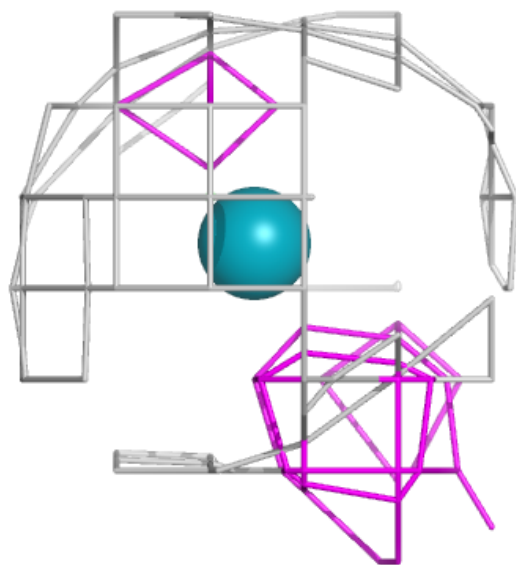
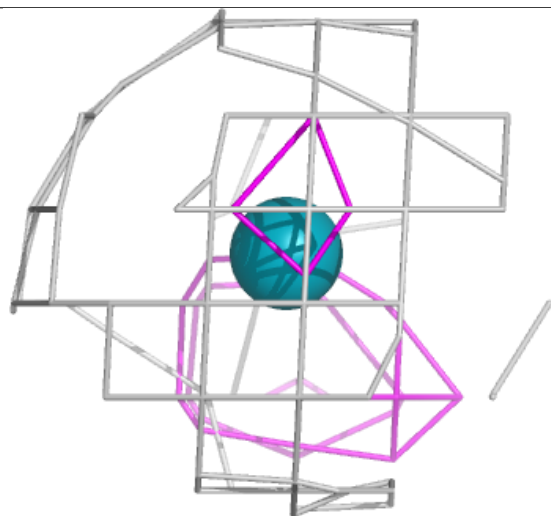
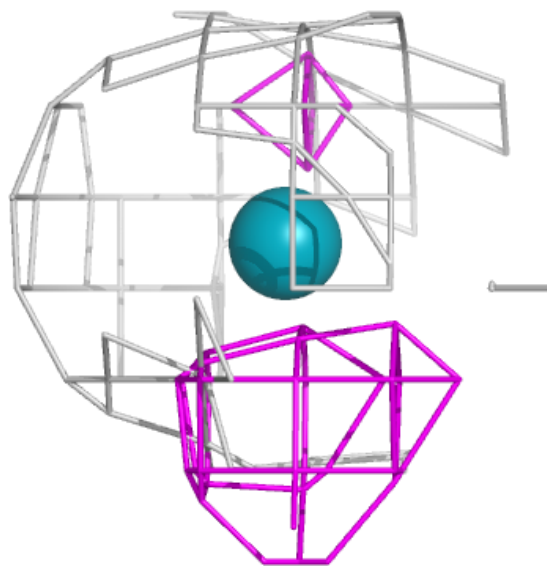
Electron density around RH3 BBB 204:

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



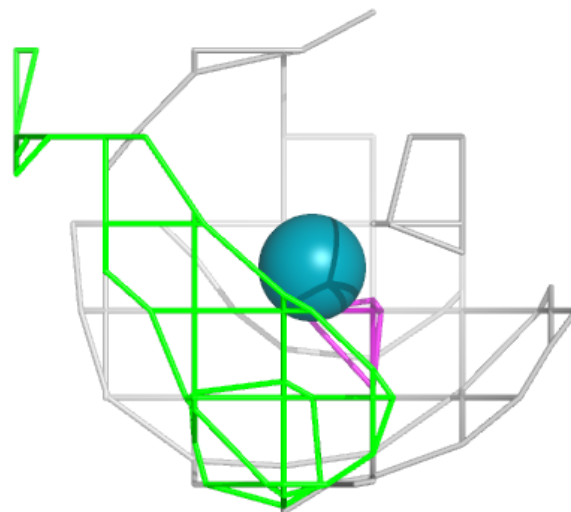
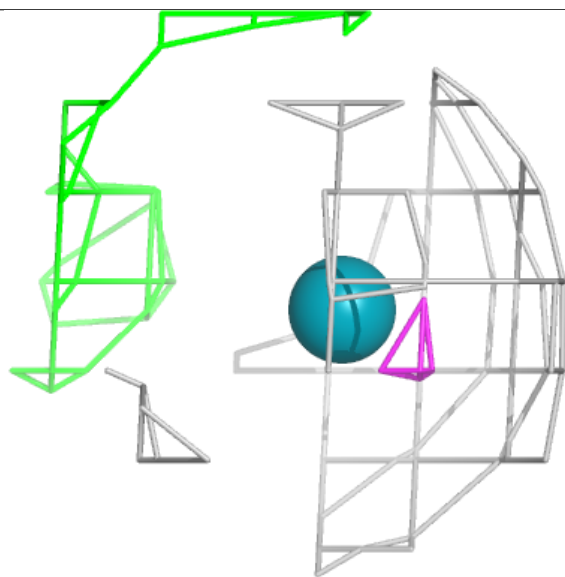
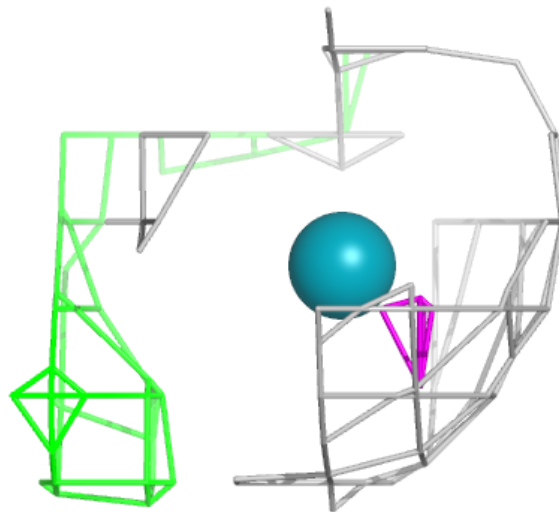
Electron density around RH3 AAA 204:

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



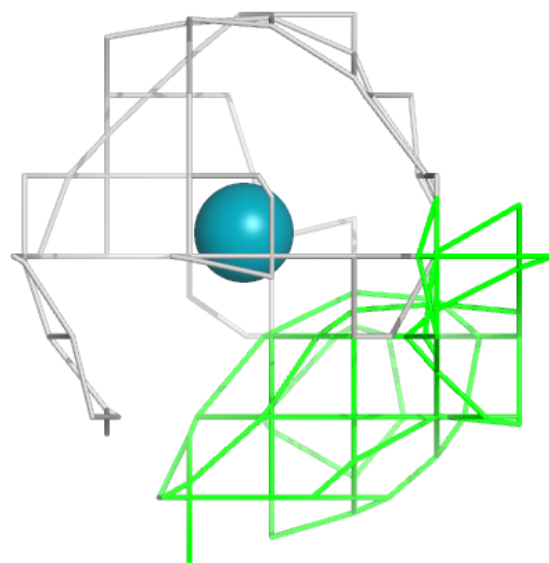
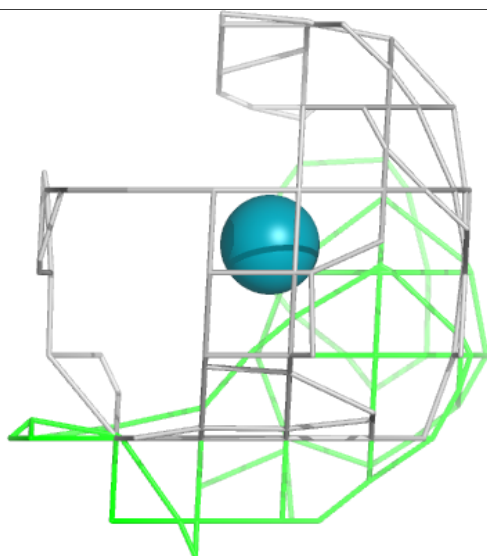
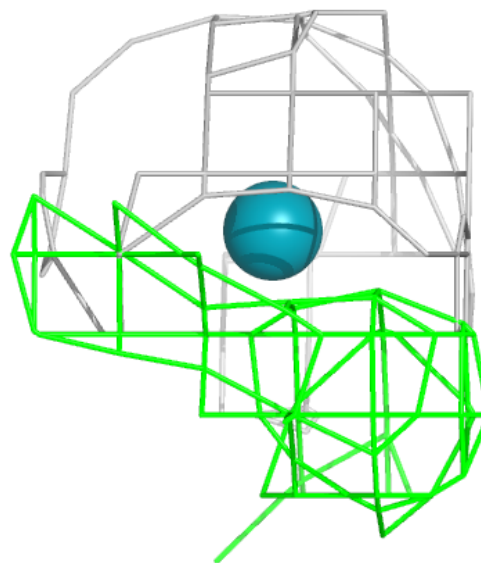
Electron density around RH3 AAA 202:

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



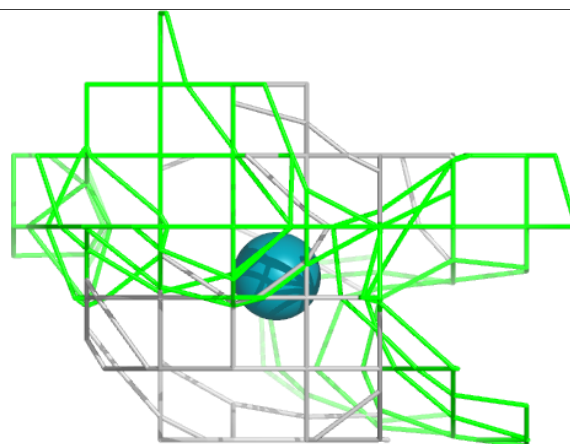
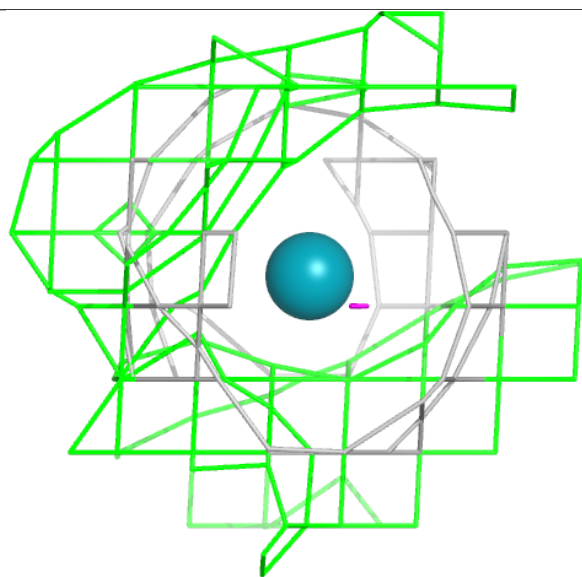
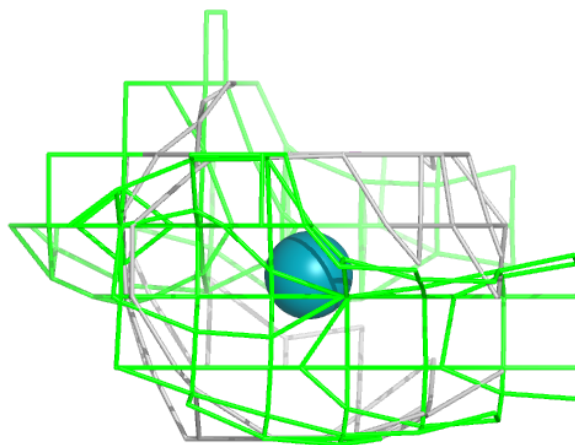
Electron density around RH3 AAA 201:

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



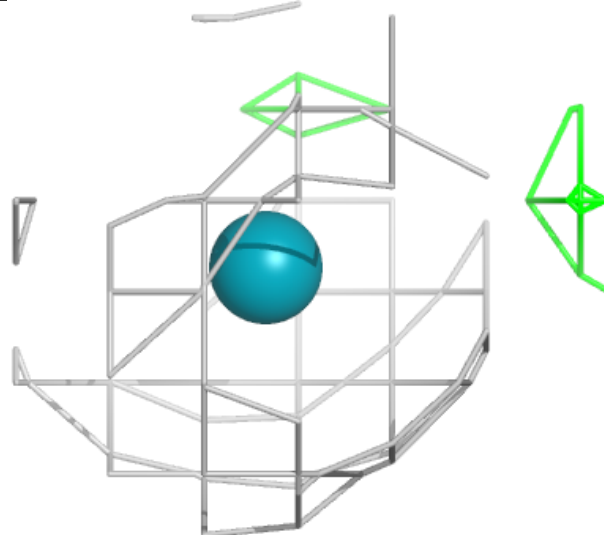
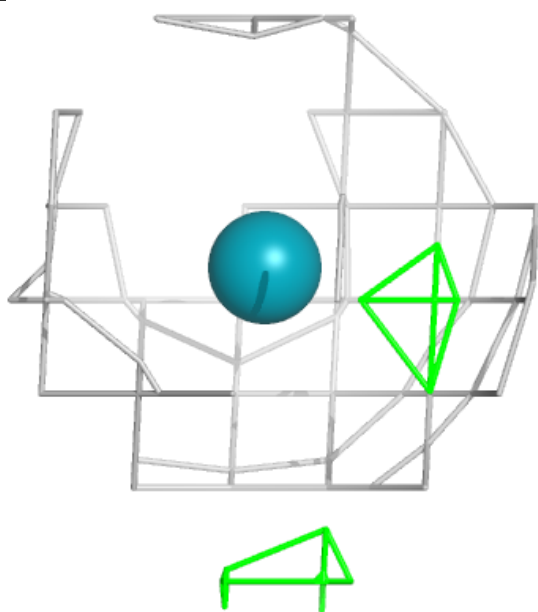
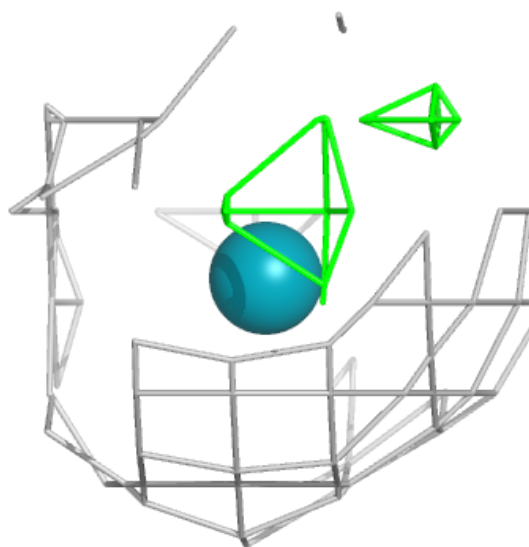
Electron density around RH3 BBB 203:

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



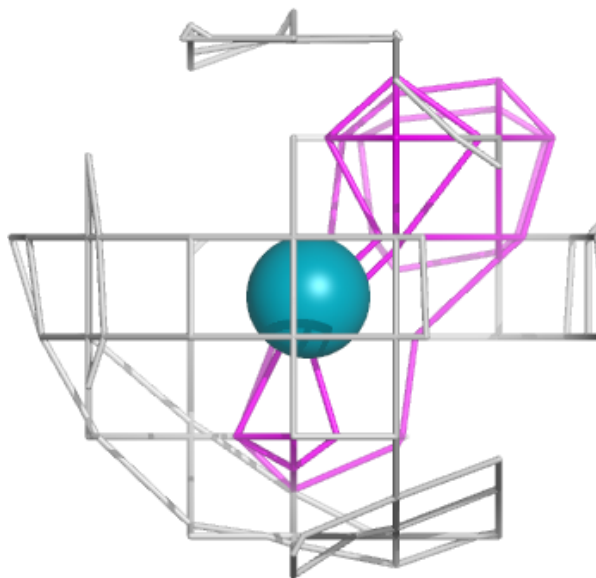
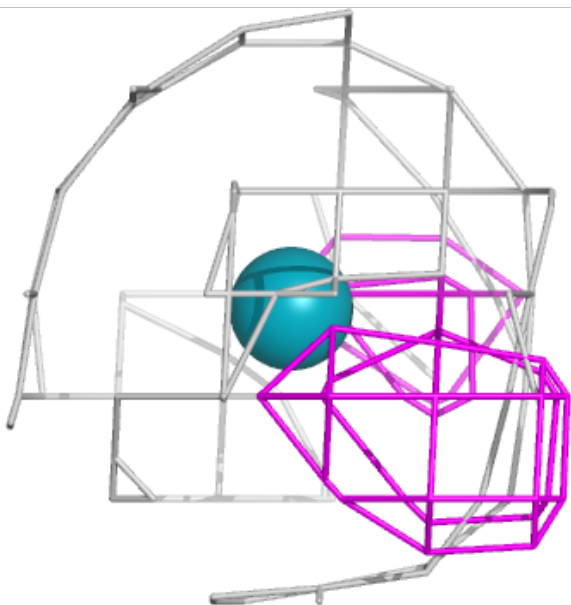
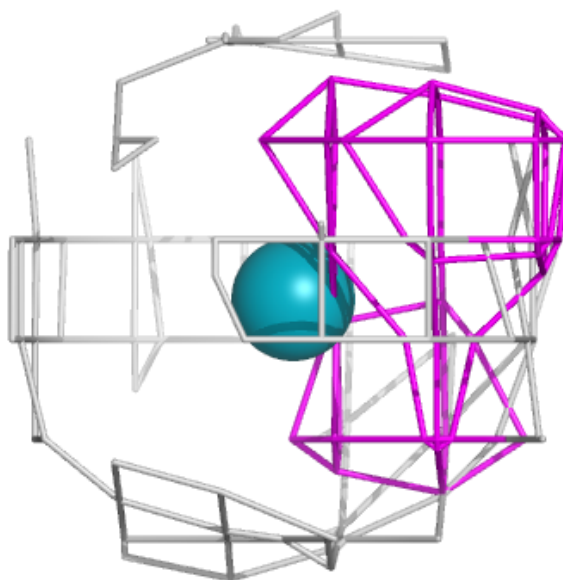
Electron density around RH3 BBB 201:

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



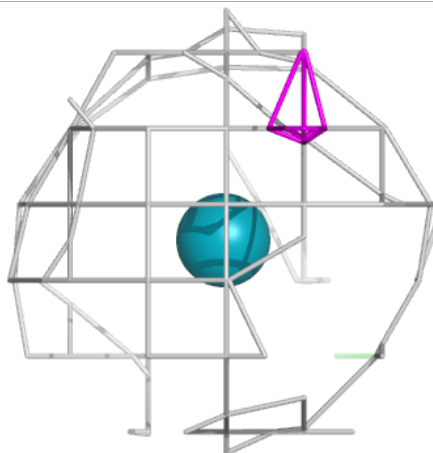
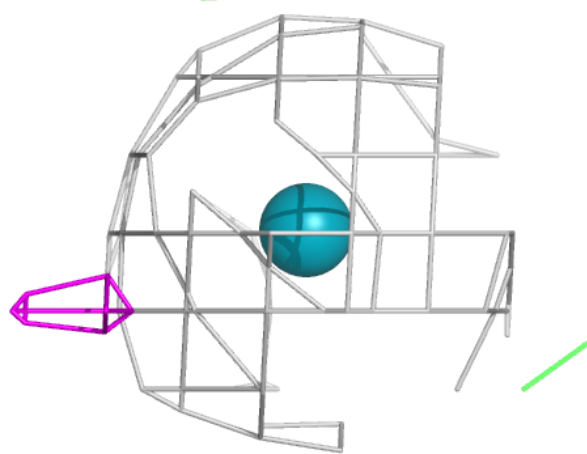
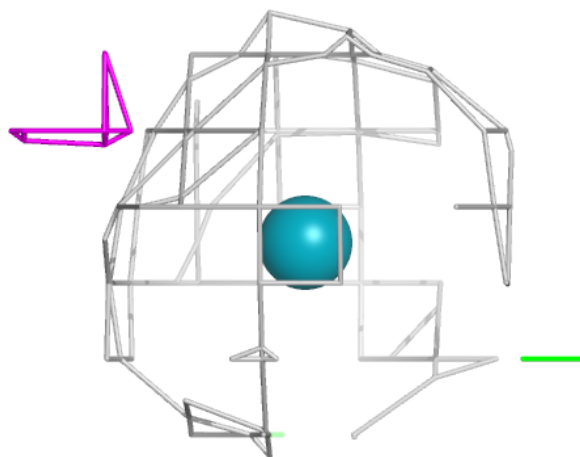
Electron density around RH3 AAA 203:

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



Electron density around RH3 BBB 202:

$2mF_o-DF_c$ (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.