



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 07:18 AM EDT

PDB ID : 7R1P / pdb_00007r1p
Title : X-ray structure of the adduct formed upon reaction of the gold(I) N-heterocyclic carbene complex Au1 with RNase A
Authors : Merlino, A.; Ferraro, G.
Deposited on : 2022-02-03
Resolution : 1.42 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

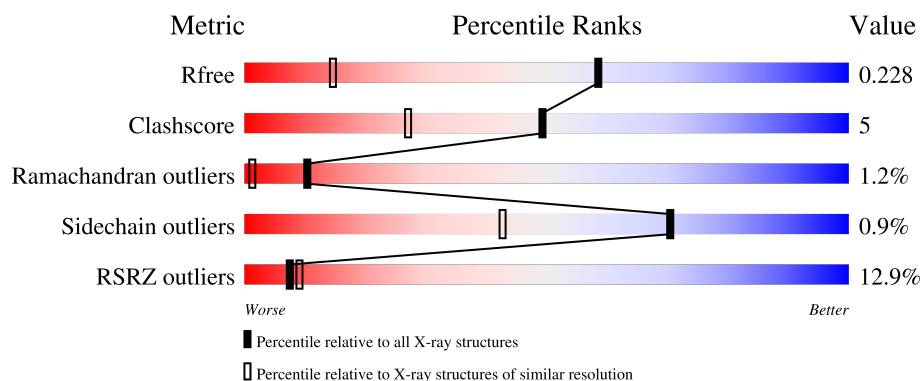
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.42 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}	180053	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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 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 $\leq 5\%$. 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	
1	BBB	124	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2259 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.

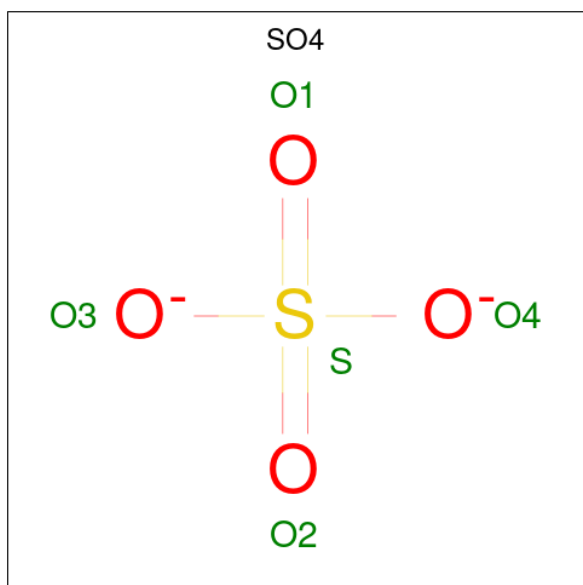
- Molecule 1 is a protein called Ribonuclease pancreatic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	124	Total	C	N	O	S	0	4	0
			985	594	178	201	12			
1	BBB	124	Total	C	N	O	S	0	7	0
			1009	609	183	204	13			

- Molecule 2 is GOLD ION (CCD ID: AU) (formula: Au) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Au	0	0
			1	1		
2	BBB	1	Total	Au	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	O	S	0	0
			5	4	1		

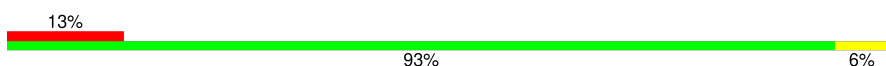
- Molecule 4 is water.

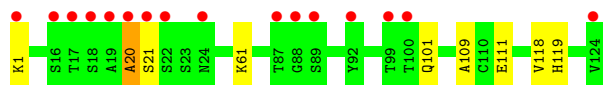
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	126	Total	O	0	2
			127	127		
4	BBB	131	Total	O	0	3
			131	131		

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.

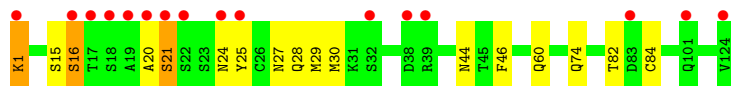
- Molecule 1: Ribonuclease pancreatic

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, α , β , γ	100.72Å 32.72Å 72.71Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	50.36 – 1.42 50.36 – 1.42	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.36-1.42) 96.1 (50.36-1.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.27Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.189 , 0.219 0.197 , 0.228	Depositor DCC
R_{free} test set	2704 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2259	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 8.92% 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: SO4, AU

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	1.04	0/1002	1.26	0/1351
1	BBB	1.09	1/1025 (0.1%)	1.19	0/1379
All	All	1.07	1/2027 (0.0%)	1.22	0/2730

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	60	GLN	N-CA	5.76	1.50	1.46

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	985	0	927	6	0
1	BBB	1009	0	960	15	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
3	AAA	5	0	0	0	0
4	AAA	127	0	0	2	0
4	BBB	131	0	0	3	0
All	All	2259	0	1887	21	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 5.

All (21) 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:BBB:30[B]:MET:HE1	1:BBB:44:ASN:HB3	1.67	0.75
1:BBB:30[B]:MET:HE3	1:BBB:84:CYS:CB	2.20	0.71
1:AAA:109:ALA:HB3	1:AAA:119[A]:HIS:HB3	1.73	0.70
1:AAA:101:GLN:HG3	4:AAA:342:HOH:O	1.96	0.65
1:BBB:30[B]:MET:HE2	1:BBB:46:PHE:HE2	1.61	0.65
1:AAA:111[A]:GLU:HG2	1:AAA:118:VAL:HG21	1.82	0.60
1:AAA:20:ALA:H	1:AAA:101:GLN:NE2	2.01	0.59
1:BBB:30[B]:MET:HE3	1:BBB:84:CYS:HB2	1.88	0.53
1:BBB:30[B]:MET:HE2	1:BBB:46:PHE:CE2	2.46	0.50
1:AAA:61:LYS:HE3	4:AAA:413:HOH:O	2.13	0.48
1:BBB:24:ASN:OD1	1:BBB:28:GLN:NE2	2.46	0.48
1:BBB:74[B]:GLN:NE2	4:BBB:308:HOH:O	2.45	0.47
1:BBB:1:LYS:HE2	4:BBB:311:HOH:O	2.16	0.45
1:BBB:24:ASN:ND2	1:BBB:27:ASN:HD22	2.14	0.45
1:BBB:20:ALA:O	1:BBB:21:SER:C	2.61	0.43
1:BBB:20:ALA:HB2	1:BBB:82:THR:OG1	2.18	0.43
1:BBB:1:LYS:CE	4:BBB:311:HOH:O	2.65	0.43
1:BBB:15:SER:O	1:BBB:16:SER:C	2.61	0.43
1:BBB:25:TYR:CZ	1:BBB:29:MET:HG3	2.54	0.43
1:AAA:20:ALA:O	1:AAA:21:SER:C	2.63	0.40
1:BBB:30[B]:MET:CE	1:BBB:44:ASN:HB3	2.44	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	126/124 (102%)	119 (94%)	6 (5%)	1 (1%)	16 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	129/124 (104%)	121 (94%)	6 (5%)	2 (2%)	7	1
All	All	255/248 (103%)	240 (94%)	12 (5%)	3 (1%)	10	1

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	20	ALA
1	BBB	21	SER
1	BBB	16	SER

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	113/109 (104%)	112 (99%)	1 (1%)	70	43
1	BBB	116/109 (106%)	115 (99%)	1 (1%)	70	43
All	All	229/218 (105%)	227 (99%)	2 (1%)	70	43

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

Mol	Chain	Res	Type
1	AAA	1	LYS
1	BBB	1	LYS

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 [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 3 ligands modelled in this entry, 2 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	SO4	AAA	202	-	4,4,4	0.43	0	6,6,6	0.22	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.

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, 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%)	0.80	16 (12%) 7 9	8, 22, 47, 64	4 (3%)
1	BBB	124/124 (100%)	0.69	16 (12%) 7 9	7, 20, 52, 83	7 (5%)
All	All	248/248 (100%)	0.74	32 (12%) 7 9	7, 21, 52, 83	11 (4%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	21	SER	7.1
1	AAA	19	ALA	6.0
1	BBB	20	ALA	6.0
1	BBB	19	ALA	5.2
1	AAA	20	ALA	5.0
1	BBB	17	THR	4.1
1	AAA	17	THR	3.9
1	BBB	21	SER	3.8
1	BBB	18	SER	3.6
1	AAA	18	SER	3.5
1	AAA	24	ASN	3.5
1	AAA	88	GLY	3.4
1	BBB	16	SER	3.4
1	AAA	1	LYS	3.2
1	AAA	16	SER	3.1
1	AAA	99	THR	3.1
1	BBB	1	LYS	2.9
1	AAA	22	SER	2.8
1	BBB	25	TYR	2.4
1	AAA	100	THR	2.4
1	BBB	22	SER	2.4
1	BBB	83	ASP	2.3
1	AAA	89	SER	2.3
1	AAA	124	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	92	TYR	2.2
1	BBB	38	ASP	2.1
1	BBB	124	VAL	2.1
1	BBB	101	GLN	2.1
1	BBB	39	ARG	2.1
1	AAA	87	THR	2.0
1	BBB	32	SER	2.0
1	BBB	24	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

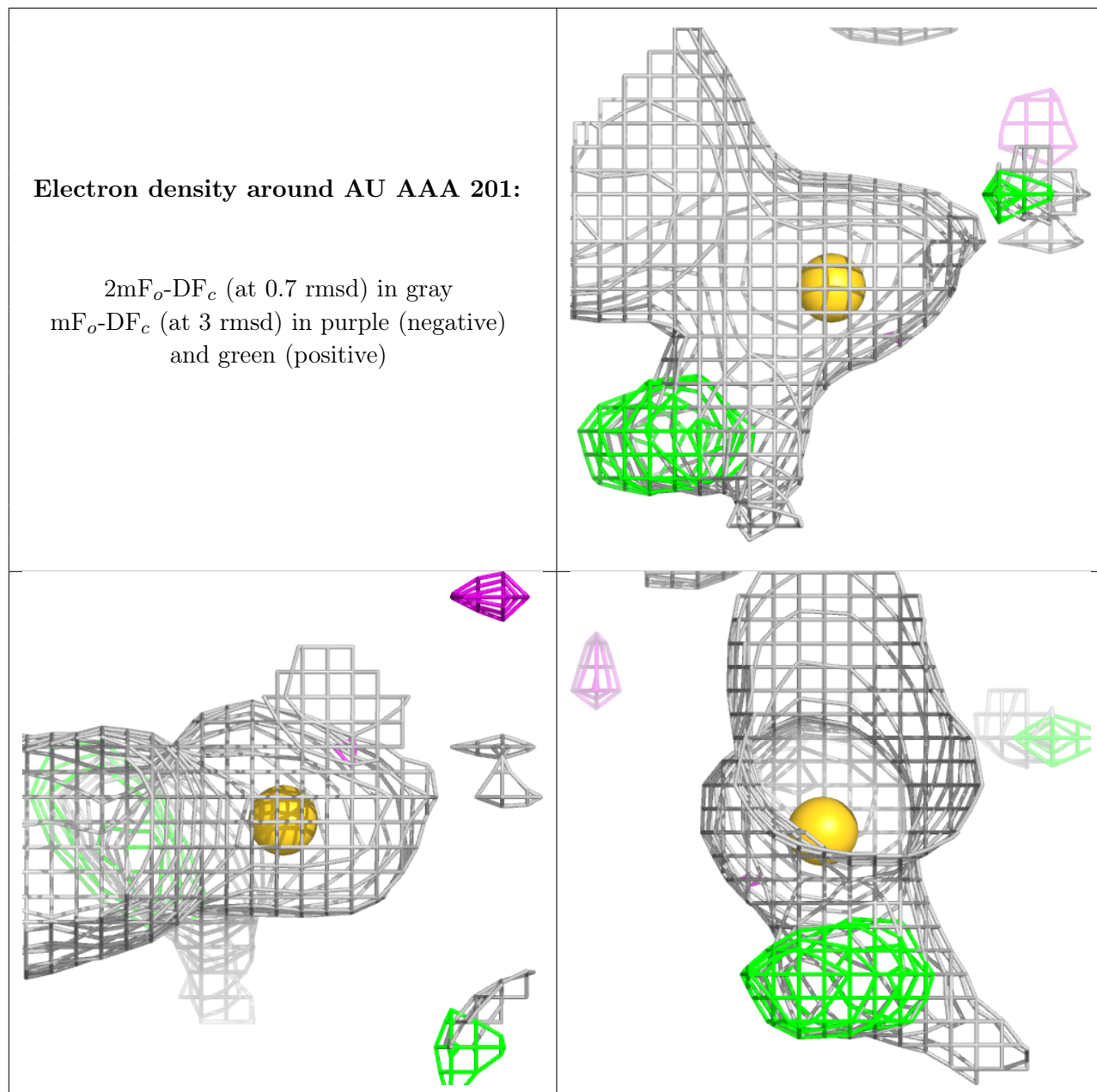
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	AAA	202	5/5	0.82	0.14	21,24,32,32	5
2	AU	AAA	201	1/1	0.85	0.18	65,65,65,65	1
2	AU	BBB	201	1/1	0.90	0.15	51,51,51,51	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.

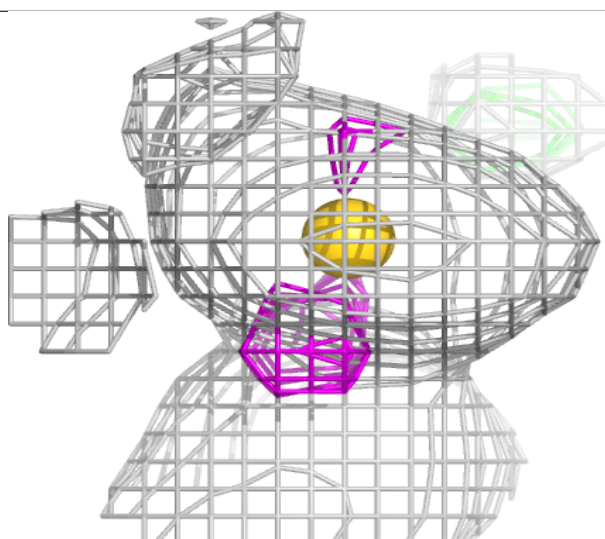
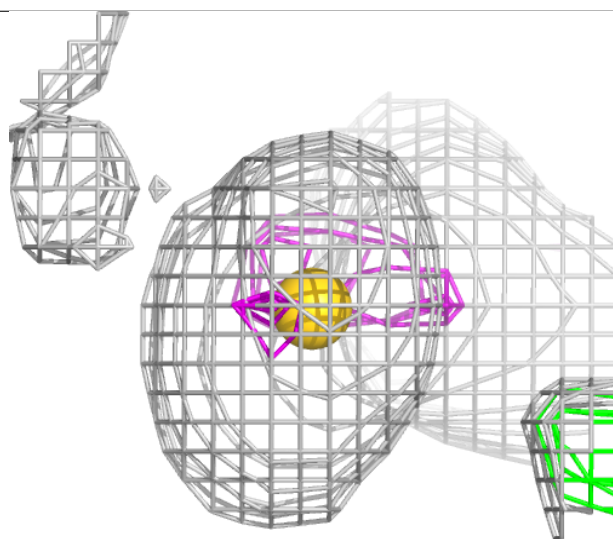
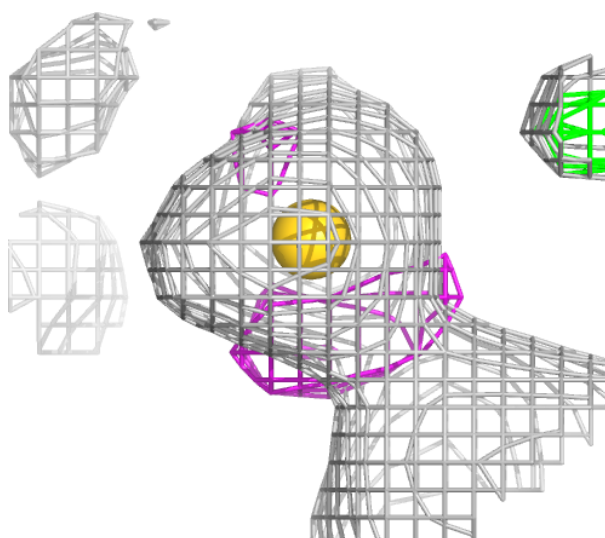
Electron density around AU AAA 201:

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



Electron density around AU 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.