



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 11:21 am GMT

PDB ID : 8CJU  
Title : PBP AccA from *A. vitis* S4 in complex with agrocin84  
Authors : Morera, S.; Vigouroux, A.  
Deposited on : 2023-02-13  
Resolution : 1.35 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

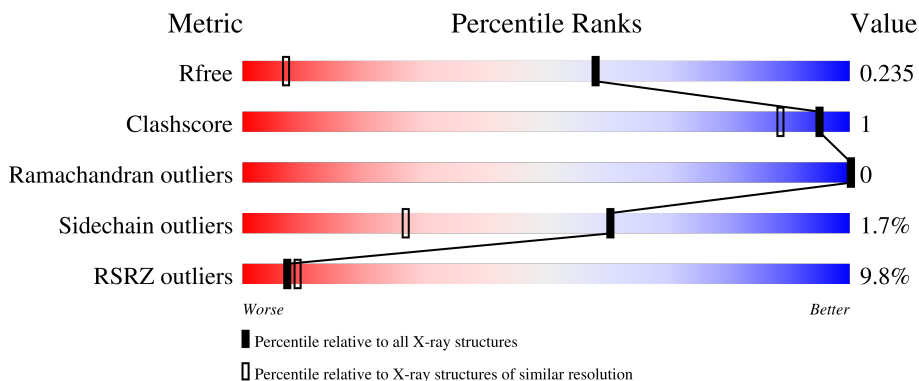
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 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	1385 (1.36-1.32)
Clashscore	141614	1417 (1.36-1.32)
Ramachandran outliers	138981	1397 (1.36-1.32)
Sidechain outliers	138945	1397 (1.36-1.32)
RSRZ outliers	127900	1369 (1.36-1.32)

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	A	499	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 8234 atoms, of which 3837 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.

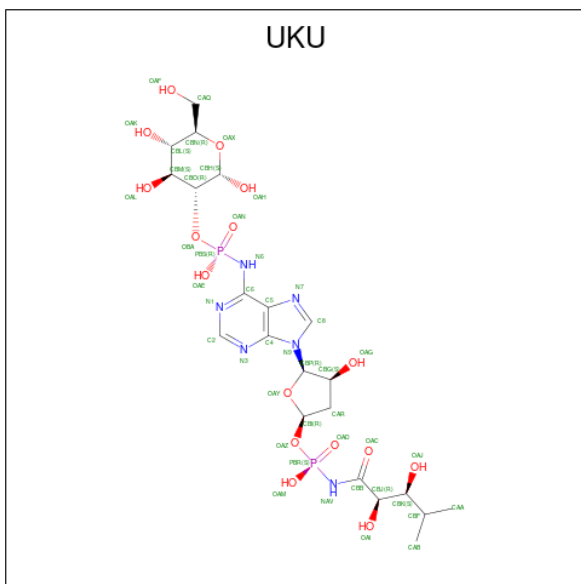
- Molecule 1 is a protein called ABC transporter substrate binding protein (Agrocinopine).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	478	7663	2476	3807	652	706	22	0	7	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	522	HIS	-	expression tag	UNP B9JXG4
A	523	HIS	-	expression tag	UNP B9JXG4
A	524	HIS	-	expression tag	UNP B9JXG4
A	525	HIS	-	expression tag	UNP B9JXG4
A	526	HIS	-	expression tag	UNP B9JXG4
A	527	HIS	-	expression tag	UNP B9JXG4

- Molecule 2 is [(2S,3R,4S,5S,6R)-6-(hydroxymethyl)-2,4,5-tris(oxidanyl)oxan-3-yl]oxy-N-[9-[(2R,3S,5R)-5-[[[(2R,3S)-4-methyl-2,3-bis(oxidanyl)pentanoyl]amino]-oxidanyl-phosphoryl]oxy-3-oxidanyl-oxolan-2-yl]purin-6-yl]phosphonamidic acid (three-letter code: UKU) (formula: C<sub>21</sub>H<sub>34</sub>N<sub>6</sub>O<sub>16</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	75	21	30	6	16	2	0	0

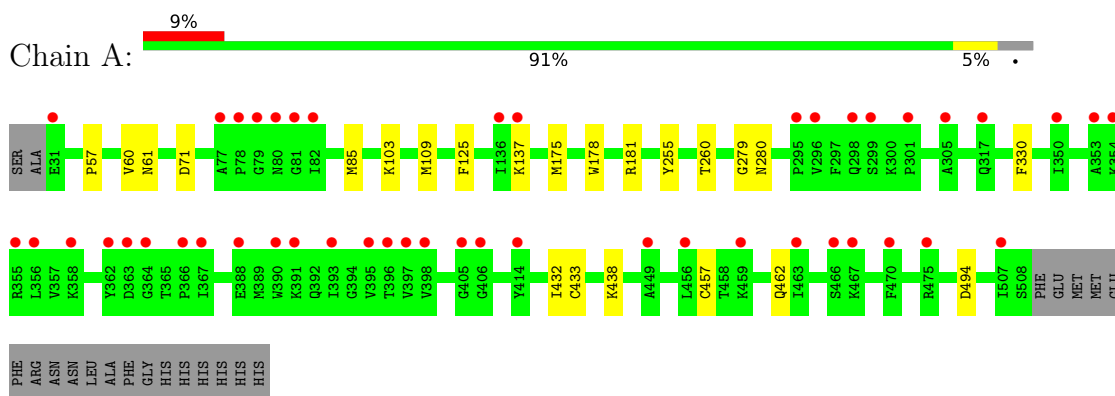
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	496	Total 496	O 496	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: ABC transporter substrate binding protein (Agrocinopine)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.01Å 60.74Å 151.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.89 – 1.35 38.89 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.89-1.35) 99.8 (38.89-1.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 1.35Å)	Xtrriage
Refinement program	BUSTER 2.10.4	Depositor
R, $R_{free}$	0.218 , 0.244 0.217 , 0.235	Depositor DCC
$R_{free}$ test set	4821 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtrriage
Anisotropy	0.377	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: UKU

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	A	0.60	1/3967 (0.0%)	0.73	0/5397

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	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	MET	SD-CE	-6.07	1.43	1.77

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	TYR	Sidechain
1	A	433	CYS	Mainchain

### 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	A	3856	3807	3803	9	0
2	A	45	30	0	0	0
3	A	496	0	0	1	0
All	All	4397	3837	3803	9	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 1.

All (9) 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:A:61:ASN:OD1	1:A:181[B]:ARG:CZ	2.28	0.81
1:A:61:ASN:OD1	1:A:181[B]:ARG:NH1	2.23	0.72
1:A:61:ASN:OD1	1:A:181[B]:ARG:NH2	2.34	0.60
1:A:103:LYS:HG3	3:A:995:HOH:O	2.06	0.55
1:A:71:ASP:HB2	1:A:85[B]:MET:CE	2.38	0.53
1:A:125:PHE:CZ	1:A:175[A]:MET:SD	3.11	0.43
1:A:57:PRO:HA	1:A:60:VAL:HG22	2.02	0.41
1:A:432:ILE:HD12	1:A:457:CYS:SG	2.60	0.41
1:A:279:GLY:HA2	1:A:494:ASP:O	2.22	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	A	483/499 (97%)	467 (97%)	16 (3%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.



### 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	A	414/425 (97%)	407 (98%)	7 (2%)	60 27

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LYS
1	A	178	TRP
1	A	260	THR
1	A	280	ASN
1	A	330	PHE
1	A	438	LYS
1	A	462	GLN

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](#)

1 ligand is modelled in this entry.

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	UKU	A	601	-	42,48,48	2.73	11 (26%)	51,73,73	2.63	12 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UKU	A	601	-	-	6/27/70/70	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	UKU	C2-N3	9.81	1.47	1.32
2	A	601	UKU	C6-N6	-9.02	1.33	1.40
2	A	601	UKU	C2-N1	7.12	1.47	1.33
2	A	601	UKU	CBH-CBO	-3.07	1.50	1.52
2	A	601	UKU	PBR-OAM	-3.07	1.48	1.56
2	A	601	UKU	CBF-CBK	2.77	1.57	1.53
2	A	601	UKU	CAR-CBI	2.69	1.56	1.52
2	A	601	UKU	C5-C4	-2.58	1.34	1.40
2	A	601	UKU	PBS-OAE	-2.49	1.50	1.56
2	A	601	UKU	OAY-CBI	2.43	1.47	1.42
2	A	601	UKU	PBS-N6	2.22	1.67	1.63

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	UKU	N3-C2-N1	-11.31	110.99	128.68
2	A	601	UKU	OAZ-PBR-OAD	-7.87	101.45	115.36
2	A	601	UKU	C2-N1-C6	6.43	122.11	116.59
2	A	601	UKU	OBA-PBS-OAN	-5.77	105.16	115.36
2	A	601	UKU	N6-C6-N1	3.86	122.24	115.86
2	A	601	UKU	CBP-N9-C4	-3.29	120.87	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	UKU	OAE-PBS-OAN	3.13	116.49	109.92
2	A	601	UKU	CBI-OAY-CBP	-2.92	101.65	106.28
2	A	601	UKU	OAY-CBI-OAZ	2.44	113.85	109.10
2	A	601	UKU	OAD-PBR-NAV	2.29	115.59	111.17
2	A	601	UKU	OAM-PBR-OAD	2.26	114.67	109.92
2	A	601	UKU	C4-C5-N7	-2.25	107.06	109.40

There are no chirality outliers.

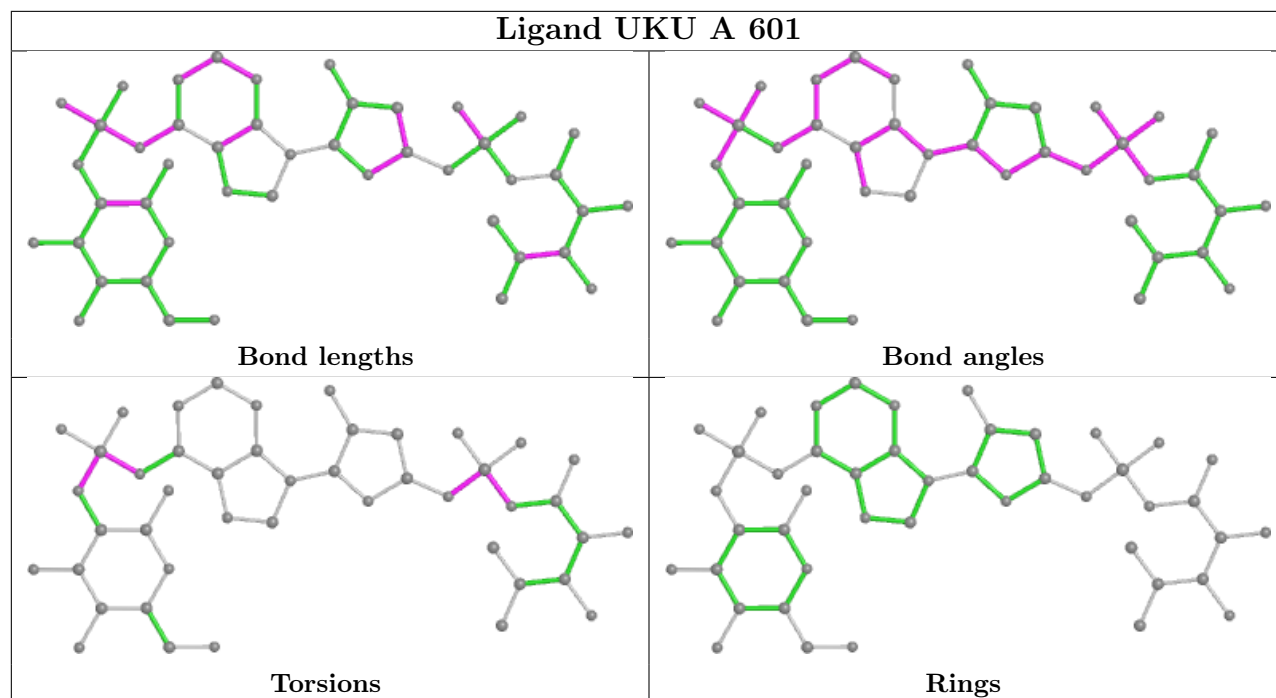
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	UKU	CBI-OAZ-PBR-OAD
2	A	601	UKU	C6-N6-PBS-OAN
2	A	601	UKU	CBB-NAV-PBR-OAD
2	A	601	UKU	C6-N6-PBS-OBA
2	A	601	UKU	CBB-NAV-PBR-OAZ
2	A	601	UKU	CBO-OBA-PBS-OAE

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	A	478/499 (95%)	0.48	47 (9%) <b>7</b> <b>9</b>	13, 27, 49, 64	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	ILE	6.1
1	A	367	ILE	5.6
1	A	414	TYR	5.6
1	A	350	ILE	5.3
1	A	397	VAL	4.9
1	A	463	ILE	4.8
1	A	78	PRO	4.7
1	A	467	LYS	4.5
1	A	366	PRO	4.5
1	A	80	ASN	4.1
1	A	137	LYS	4.1
1	A	363	ASP	4.0
1	A	405	GLY	4.0
1	A	358	LYS	3.9
1	A	82	ILE	3.5
1	A	81	GLY	3.3
1	A	398	VAL	3.3
1	A	393	ILE	3.2
1	A	77	ALA	3.1
1	A	475	ARG	3.1
1	A	456	LEU	3.1
1	A	507	ILE	3.0
1	A	79	GLY	3.0
1	A	362	TYR	2.9
1	A	466	SER	2.9
1	A	355	ARG	2.7
1	A	390	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	295	PRO	2.7
1	A	31	GLU	2.6
1	A	406	GLY	2.6
1	A	301	PRO	2.6
1	A	305	ALA	2.6
1	A	353	ALA	2.6
1	A	354	LYS	2.5
1	A	298	GLN	2.4
1	A	395	VAL	2.3
1	A	470	PHE	2.3
1	A	449	ALA	2.3
1	A	388	GLU	2.2
1	A	296	VAL	2.2
1	A	299	SER	2.2
1	A	391	LYS	2.2
1	A	396	THR	2.1
1	A	317	GLN	2.0
1	A	459	LYS	2.0
1	A	364	GLY	2.0
1	A	356	LEU	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.

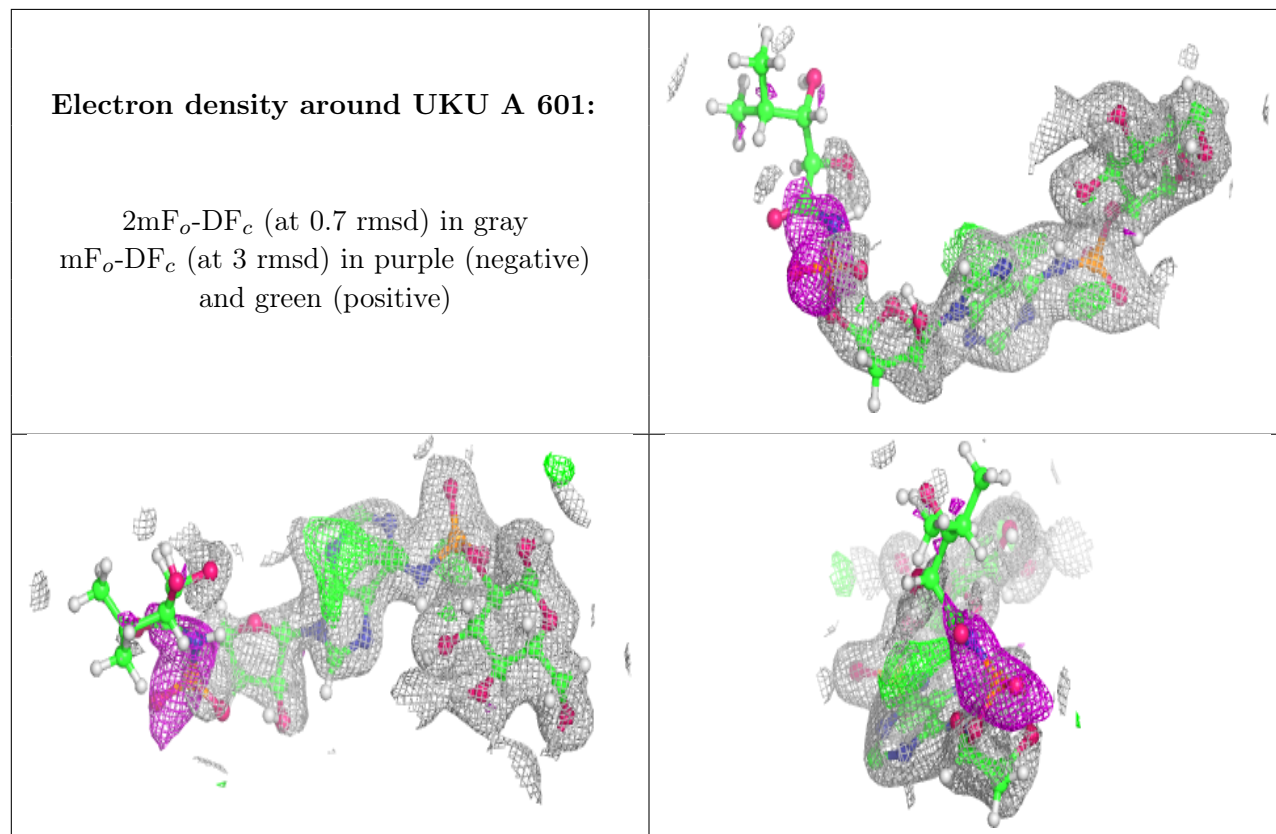
## 6.4 Ligands [i](#)

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	UKU	A	601	45/45	0.88	0.20	20,44,66,66	0

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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.