



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 27, 2021 – 03:00 pm BST

PDB ID : 7ATK
Title : Crystal structure of UipA in complex with Uranium
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Deposited on : 2020-10-30
Resolution : 2.85 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

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
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

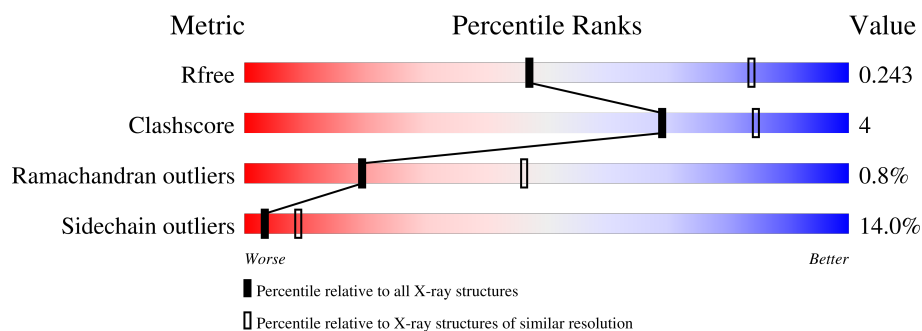
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AAA	206	<div> <div>55%</div> <div>10%</div> <div>34%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 971 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 UipA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	136	Total	C	N	O	S	0	0	0
			962	582	155	224	1			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	76	MET	-	initiating methionine	UNP A0A3Q9JIL7
AAA	77	GLY	-	expression tag	UNP A0A3Q9JIL7
AAA	78	SER	-	expression tag	UNP A0A3Q9JIL7
AAA	79	SER	-	expression tag	UNP A0A3Q9JIL7
AAA	80	HIS	-	expression tag	UNP A0A3Q9JIL7
AAA	81	HIS	-	expression tag	UNP A0A3Q9JIL7
AAA	82	HIS	-	expression tag	UNP A0A3Q9JIL7
AAA	83	HIS	-	expression tag	UNP A0A3Q9JIL7
AAA	84	HIS	-	expression tag	UNP A0A3Q9JIL7
AAA	85	HIS	-	expression tag	UNP A0A3Q9JIL7
AAA	86	SER	-	expression tag	UNP A0A3Q9JIL7
AAA	87	SER	-	expression tag	UNP A0A3Q9JIL7
AAA	88	GLY	-	expression tag	UNP A0A3Q9JIL7
AAA	89	GLU	-	expression tag	UNP A0A3Q9JIL7
AAA	90	ASN	-	expression tag	UNP A0A3Q9JIL7
AAA	91	LEU	-	expression tag	UNP A0A3Q9JIL7
AAA	92	TYR	-	expression tag	UNP A0A3Q9JIL7
AAA	93	PHE	-	expression tag	UNP A0A3Q9JIL7
AAA	94	GLN	-	expression tag	UNP A0A3Q9JIL7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	5	Total	Zn	0	0
			5	5		

- Molecule 3 is URANIUM ATOM (three-letter code: U1) (formula: U) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	4	Total	U	0	0
			4	4		

- Molecule 1: UipA

SER	ASN	GLY	ARG	GLY	PRO	VAL	T143	D151	E167	V200	T204	S205	T206	D207	G211	ASP	ASP	T214	D222	I225	R226	V229	T241	D248	D249	V250	S251	T259	S260	D261	R263	S264	V276	D279	I280	ASP
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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.16Å 95.16Å 52.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.00 – 2.85 47.58 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.00-2.85) 99.7 (47.58-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.207 , 0.234 0.216 , 0.243	Depositor DCC
R_{free} test set	298 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	87.1	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	971	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.95% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, U1

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	0.73	0/967	0.97	0/1322

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 [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	962	0	906	7	1
2	AAA	5	0	0	0	0
3	AAA	4	0	0	0	0
All	All	971	0	906	7	1

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.

The worst 5 of 7 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:225:ILE:O	1:AAA:229:VAL:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:251:SER:OG	1:AAA:251:SER:O	2.28	0.51
1:AAA:261:ASP:OD2	1:AAA:261:ASP:N	2.42	0.51
1:AAA:222:ASP:O	1:AAA:226:ARG:HG3	2.15	0.47
1:AAA:248:ASP:O	1:AAA:250:VAL:N	2.41	0.46

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:151:ASP:OD1	1:AAA:226:ARG:NH2[7_555]	1.95	0.25

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	132/206 (64%)	118 (89%)	13 (10%)	1 (1%)	19	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	261	ASP

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	100/157 (64%)	86 (86%)	14 (14%)	3 9

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	241	THR
1	AAA	251	SER
1	AAA	279	ASP
1	AAA	264	SER
1	AAA	276	VAL

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 9 ligands modelled in this entry, 9 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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

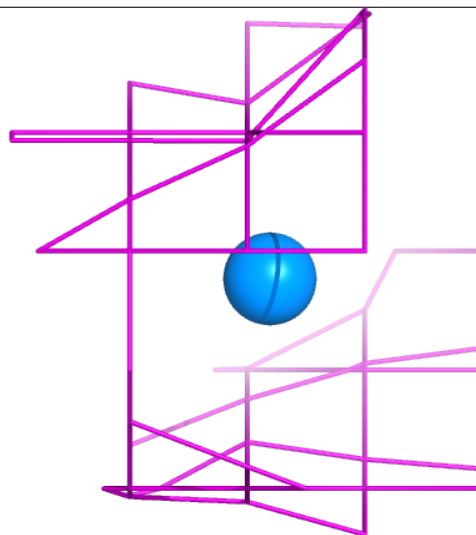
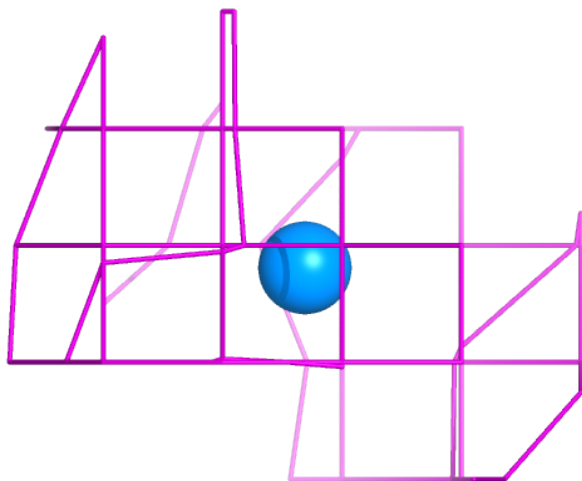
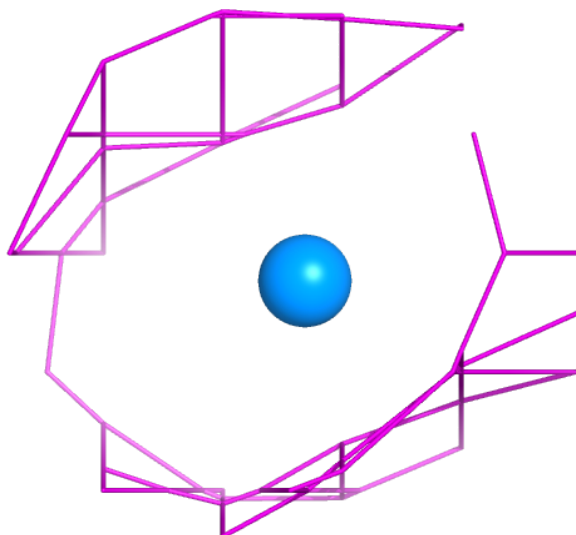
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

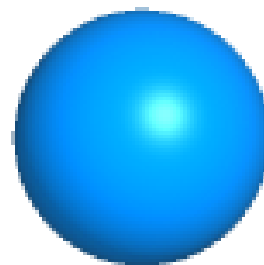
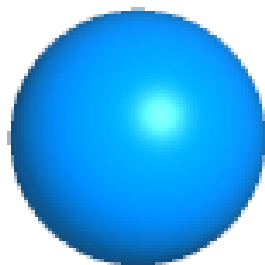
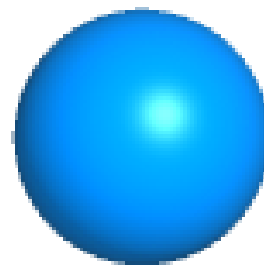
Electron density around U1 AAA 306:

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



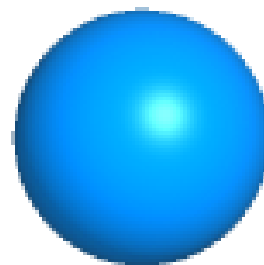
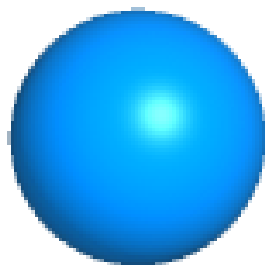
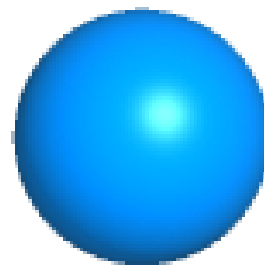
Electron density around U1 AAA 307:

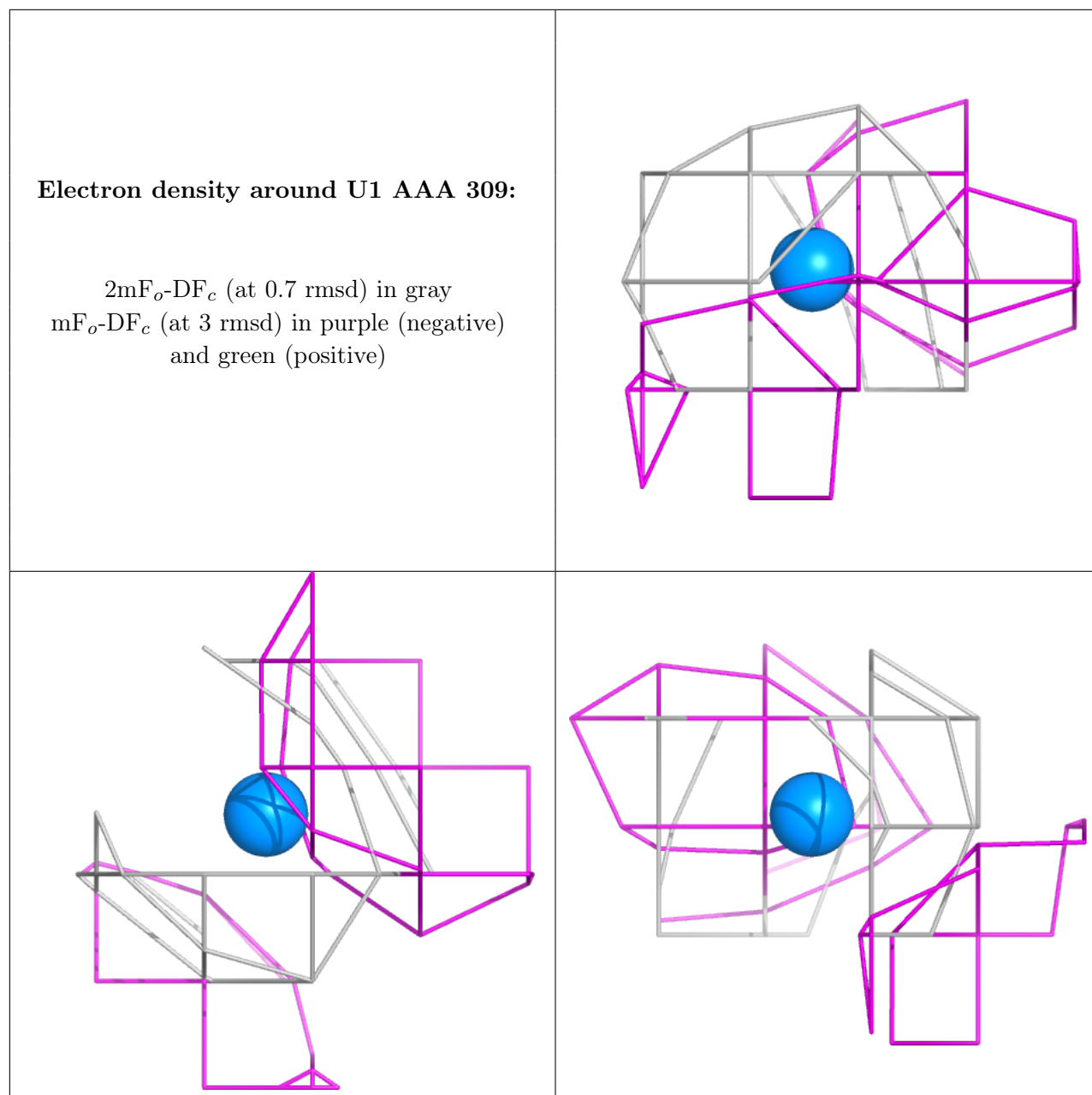
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around U1 AAA 308:

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





6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.