

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 7, 2023 - 05:05 am GMT

PDB ID	:	7QLO
Title	:	rsKiiro pump dump probe structure by TR-SFX
Authors	:	van Thor, J.J.
Deposited on		
Resolution	:	1.31 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 (i) 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 (1)) were used in the production of this report:

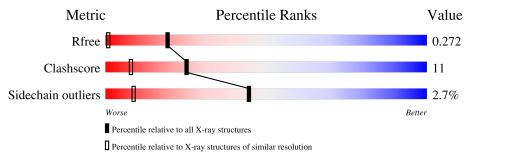
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as $541$ be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.31 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1611(1.34-1.30)
Clashscore	141614	1667 (1.34-1.30)
Sidechain outliers	138945	1615 (1.34-1.30)

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 <=5%

Mol	Chain	Length	Quality of chain		
1	А	220	81%	17%	

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
1	PIA	А	62	-	-	Х	-



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## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2074 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 rsKiiro.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	217	Total 1913	C 1231	N 320	O 350	S 12	0	32	1

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	11	LYS	ASN	engineered mutation	UNP Q5S6Z9
А	62	PIA	HIS	chromophore	UNP Q5S6Z9
А	62	PIA	TYR	chromophore	UNP Q5S6Z9
А	62	PIA	GLY	chromophore	UNP Q5S6Z9
A	68	LYS	GLU	engineered mutation	UNP Q5S6Z9
А	72	ASN	HIS	engineered mutation	UNP Q5S6Z9
А	100	ASN	ILE	engineered mutation	UNP Q5S6Z9
А	119	TYR	HIS	engineered mutation	UNP Q5S6Z9
А	121	THR	VAL	engineered mutation	UNP Q5S6Z9
A	155	VAL	ILE	engineered mutation	UNP Q5S6Z9
А	156	GLU	THR	engineered mutation	UNP Q5S6Z9
А	157	THR	MET	engineered mutation	UNP Q5S6Z9
А	187	ALA	TYR	engineered mutation	UNP Q5S6Z9
А	220	ASN	ASP	engineered mutation	UNP Q5S6Z9

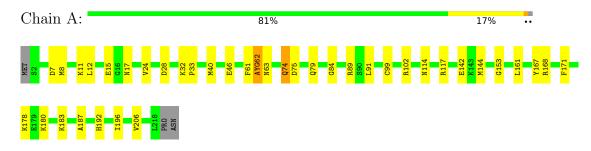
• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	161	Total O 161 161	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. 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. 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: rsKiiro



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	39.34Å 74.01Å 78.62Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	11.99 - 1.31	Depositor
Resolution (A)	19.00 - 1.31	EDS
% Data completeness	88.6 (11.99-1.31)	Depositor
(in resolution range)	88.3 (19.00-1.31)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$6.40 (at 1.31 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
D D.	0.417 , $0.452$	Depositor
$R, R_{free}$	0.267 , $0.272$	DCC
$R_{free}$ test set	2462 reflections $(4.94%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	13.8	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , $32.6$	EDS
L-test for twinning <sup>2</sup>	$ \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	0.94	EDS
Total number of atoms	2074	wwPDB-VP
Average B, all atoms $(Å^2)$	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: PIA

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	
IVI01	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.61	0/2029	0.84	0/2727

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	А	1913	0	1925	41	0
2	А	161	0	0	5	2
All	All	2074	0	1925	41	2

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 11.

All (41) 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:PHE:C	1:A:62:PIA:HN12	1.16	1.50
1:A:62:PIA:C3	1:A:63:ASN:N	1.86	1.36

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Continued from previou		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:61:PHE:C	1:A:62:PIA:N1	1.92	1.21
1:A:62:PIA:HD2	1:A:62:PIA:O2	1.83	0.79
1:A:15[B]:GLU:HG3	1:A:24:VAL:HG22	1.74	0.69
1:A:62:PIA:HD1	1:A:192[B]:HIS:CE1	2.29	0.67
1:A:102[B]:ARG:HD3	1:A:117[B]:ARG:HE	1.60	0.66
1:A:61:PHE:CA	1:A:62:PIA:HN12	2.08	0.65
1:A:102[B]:ARG:CZ	1:A:102[B]:ARG:HB2	2.28	0.64
1:A:12[B]:LEU:C	1:A:12[B]:LEU:HD12	2.21	0.60
1:A:17[B]:ASN:ND2	2:A:404:HOH:O	2.34	0.59
1:A:102[B]:ARG:HH11	1:A:102[B]:ARG:HG3	1.67	0.59
1:A:7:ASP:OD1	1:A:32:LYS:HE2	2.05	0.56
1:A:61:PHE:O	1:A:62:PIA:N1	2.38	0.56
1:A:102[B]:ARG:HD3	1:A:117[B]:ARG:NE	2.23	0.53
1:A:12[B]:LEU:HD21	1:A:40[B]:MET:HE2	1.89	0.53
1:A:8[B]:MET:HG3	1:A:33:PRO:CG	2.39	0.52
1:A:8[B]:MET:HG3	1:A:33:PRO:HG2	1.93	0.51
1:A:61:PHE:C	1:A:62:PIA:CA1	2.79	0.51
1:A:196:ILE:HG23	1:A:206:VAL:HG13	1.93	0.50
1:A:102[B]:ARG:HH11	1:A:102[B]:ARG:CG	2.24	0.49
1:A:161:LEU:HD11	1:A:167:TYR:HB2	1.94	0.48
1:A:74:GLN:HE22	1:A:79[B]:GLN:HE22	1.61	0.47
1:A:75:ASP:O	1:A:79[B]:GLN:HG3	2.15	0.47
1:A:144:MET:O	1:A:187:ALA:HA	2.15	0.46
1:A:11:LYS:HE2	1:A:28:ASP:OD1	2.15	0.46
1:A:40[B]:MET:HB2	1:A:40[B]:MET:HE3	1.79	0.46
1:A:84:GLY:C	1:A:178:LYS:HD2	2.36	0.45
1:A:102[B]:ARG:CD	1:A:117[B]:ARG:HE	2.29	0.45
1:A:168:ARG:NH2	2:A:410:HOH:O	2.49	0.45
1:A:74:GLN:NE2	2:A:413:HOH:O	2.51	0.44
1:A:142:GLU:OE2	2:A:401:HOH:O	2.21	0.43
1:A:102[B]:ARG:CG	1:A:102[B]:ARG:NH1	2.81	0.43
1:A:91:LEU:HB2	1:A:99:CYS:HB2	2.01	0.43
1:A:62:PIA:HD2	1:A:62:PIA:C2	2.50	0.42
1:A:24:VAL:HB	1:A:46:GLU:HG3	2.00	0.42
1:A:117[B]:ARG:CD	2:A:436:HOH:O	2.68	0.41
1:A:102[A]:ARG:HG2	1:A:117[A]:ARG:HB2	2.02	0.41
1:A:12[B]:LEU:HB2	1:A:114:ASN:HB2	2.01	0.41

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All (2) 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)
2:A:454:HOH:O	2:A:485:HOH:O[4_555]	2.10	0.10
2:A:450:HOH:O	2:A:547:HOH:O[3_554]	2.18	0.02

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

#### 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	Analysed Rotameric		Percentiles	
1	А	215/187~(115%)	210~(98%)	5(2%)	50 13	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	74	GLN
1	А	89	ARG
1	А	171	PHE
1	А	180	LYS
1	А	183	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type	
1	А	74	GLN	
1	А	199	HIS	

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue 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	Bo	ond leng	ths	B	ond ang	les
	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
1	PIA	А	62	-	21,21,22	4.29	9 (42%)	27,29,31	4.58	8 (29%)

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
1	PIA	А	62	-	-	4/8/27/28	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	62	PIA	CB2-CA2	13.57	1.46	1.35
1	А	62	PIA	O2-C2	10.84	1.46	1.23
1	А	62	PIA	OH-CZ	-5.34	1.24	1.37
1	А	62	PIA	O3-C3	3.83	1.41	1.19
1	А	62	PIA	C2-N3	-3.17	1.32	1.39
1	А	62	PIA	CA2-N2	-2.91	1.32	1.38
1	А	62	PIA	CA1-C1	-2.82	1.47	1.51
1	А	62	PIA	CA2-C2	-2.46	1.46	1.48
1	А	62	PIA	C1-N2	2.42	1.35	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	62	PIA	CB2-CA2-C2	13.57	138.48	122.28
1	А	62	PIA	CA2-C2-N3	12.46	109.26	103.37
1	А	62	PIA	CB2-CA2-N2	-9.83	115.19	128.83
1	А	62	PIA	C2-N3-C1	-6.36	104.75	107.97

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	62	PIA	CG2-CB2-CA2	-4.80	124.06	129.94
1	А	62	PIA	C2-CA2-N2	-4.50	105.78	108.93
1	А	62	PIA	O2-C2-CA2	-4.20	128.60	130.96
1	А	62	PIA	CA1-C1-N2	-2.28	121.13	124.05

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There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	62	PIA	C3-CA3-N3-C2
1	А	62	PIA	C2-CA2-CB2-CG2
1	А	62	PIA	N2-CA2-CB2-CG2
1	А	62	PIA	C3-CA3-N3-C1

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	62	PIA	9	0

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

There are no ligands in this entry.

#### 5.7 Other polymers (i)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	А	2



All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	А	61:PHE	С	62:PIA	N1	1.92
1	А	62:PIA	C3	63:ASN	Ν	1.86



## 6 Fit of model and data (i)

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

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

### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

#### 6.3 Carbohydrates (i)

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

#### 6.4 Ligands (i)

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

#### 6.5 Other polymers (i)

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

