

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

#### Nov 30, 2020 – 04:07 pm GMT

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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 following versions of software and data (see references (1)) were used in the production of this report:

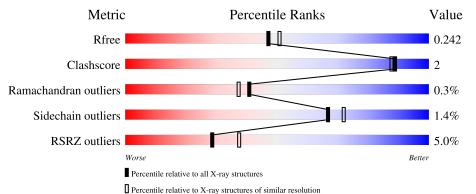
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac	· · · · · · · · · · · · · · · · · · ·	1.8.5 (274361), CSD as541be (2020) 1.13 2.14.6 1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001)
Validation Pipeline (wwPDB-VP)	:	2.14.6

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1479 (2.16-2.16)
Clashscore	141614	1585(2.16-2.16)
Ramachandran outliers	138981	$1560 \ (2.16-2.16)$
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 <=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	А	581	96%				
1	В	581	92%	7%			



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18134 atoms, of which 8807 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.

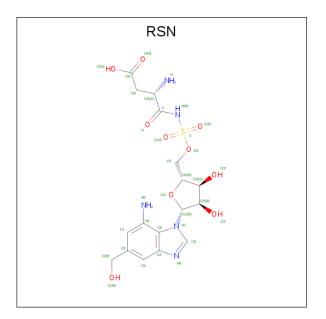
• Molecule 1 is a protein called Aspartate-tRNA(Asp) ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	Δ	573	Total	С	Η	Ν	Ο	S	0	0	0
	л	575	8944	2883	4447	797	806	11			
1	В	580	Total	С	Η	Ν	Ο	S	0	2	0
	Ъ	500	8783	2860	4316	797	799	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q5SKD2
В	0	GLY	-	expression tag	UNP Q5SKD2

• Molecule 2 is  $(3 \{S\})$ -3-azanyl-4-[[ $(2 \{R\}, 3 \{S\}, 4 \{R\}, 5 \{R\})$ -5-[7-azanyl-5-(hydroxymet hyl)benzimidazol-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxysulfonylamino]-4-oxidanylide ne-butanoic acid (three-letter code: RSN) (formula:  $C_{17}H_{23}N_5O_{10}S$ ) (labeled as "Ligand of Interest" by author).





7A	P4
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
0	Δ	1	Total	С	Η	Ν	Ο	S	0	0
		1	55	17	22	5	10	1	0	0
0	р	1	Total	С	Η	Ν	Ο	S	0	0
			55	17	22	5	10	1	0	0

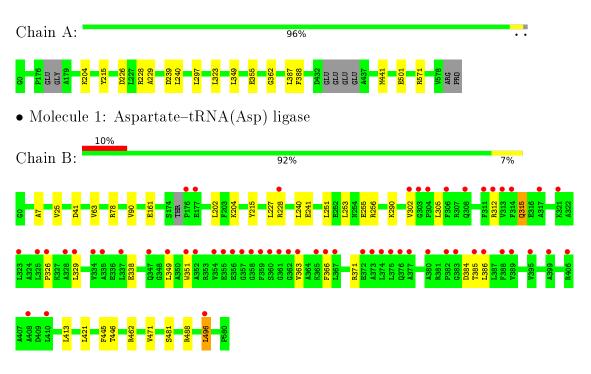
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	166	Total O 166 166	0	0
3	В	131	Total O 131 131	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.



 $\bullet$  Molecule 1: Aspartate–tRNA(Asp) ligase



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	82.28Å 112.53Å 88.25Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $104.86^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	79.53 - 2.15	Depositor
Resolution (A)	79.53 - 2.06	EDS
% Data completeness	98.8 (79.53-2.15)	Depositor
(in resolution range)	98.8(79.53-2.06)	EDS
R <sub>merge</sub>	0.07	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.53 (at 2.07 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
D D.	0.199 , $0.240$	Depositor
$R, R_{free}$	0.200 , $0.242$	DCC
$R_{free}$ test set	2340 reflections $(2.47%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	47.4	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 49.8	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18134	wwPDB-VP
Average B, all atoms $(Å^2)$	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.64% 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: RSN

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		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.25	0/4603	0.45	0/6243	
1	В	0.25	0/4585	0.46	0/6235	
All	All	0.25	0/9188	0.46	0/12478	

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	4497	4447	4447	7	0
1	В	4467	4316	4304	26	0
2	А	33	22	0	1	0
2	В	33	22	0	0	0
3	А	166	0	0	1	0
3	В	131	0	0	1	0
All	All	9327	8807	8751	34	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 2.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}~({ m \AA})$	overlap (Å)
1:B:302:VAL:HG13	1:B:305:LEU:HD12	1.56	0.88
2:A:601:RSN:N6	3:A:701:HOH:O	2.29	0.65
1:B:302:VAL:CG1	1:B:305:LEU:HD12	2.26	0.64
1:B:329:LEU:HG	1:B:385:THR:HG21	1.82	0.61
1:A:501:GLU:OE1	1:A:501:GLU:N	2.38	0.57
1:B:338:GLU:N	1:B:349:LEU:HD22	2.24	0.53
1:B:25:VAL:HG21	1:B:63:VAL:CG1	2.38	0.53
1:B:251:LEU:O	1:B:255:GLU:HG2	2.10	0.52
1:B:363:VAL:HG12	1:B:363:VAL:O	2.10	0.52
1:B:312:ARG:HA	1:B:315:GLN:HG3	1.92	0.51
1:B:421:LEU:HD12	1:B:421:LEU:C	2.30	0.51
1:A:349:LEU:HD11	1:A:387:LEU:HB3	1.92	0.51
1:A:349:LEU:HD12	1:A:388:PHE:O	2.12	0.50
1:B:302:VAL:HG13	1:B:305:LEU:CD1	2.35	0.50
1:B:161:GLU:OE2	1:B:256:ARG:NH2	2.40	0.49
1:B:228:ARG:NH2	3:B:708:HOH:O	2.45	0.48
1:B:326:PRO:HA	1:B:384:ASP:OD1	2.16	0.46
1:B:496:LEU:HD13	1:B:496:LEU:O	2.15	0.46
1:B:290:LYS:HA	1:B:471:VAL:HG21	1.98	0.45
1:B:202:LEU:HD21	1:B:445:PHE:CZ	2.51	0.45
1:B:363:VAL:HG12	1:B:366:PHE:HB2	1.99	0.44
1:B:446:THR:HG23	1:B:481:SER:HB2	1.98	0.44
1:B:7:ALA:N	1:B:41:ASP:OD2	2.41	0.44
1:A:204:LYS:HD3	1:A:239:ASP:OD1	2.17	0.43
1:B:240:LEU:HD12	1:B:240:LEU:C	2.39	0.43
1:A:228:ARG:O	1:A:229:ALA:HB3	2.19	0.43
1:B:351:TRP:HA	1:B:386:LEU:O	2.19	0.43
1:B:25:VAL:HG21	1:B:63:VAL:HG13	2.01	0.42
1:B:202:LEU:HD21	1:B:445:PHE:CE2	2.55	0.42
1:A:297:LEU:HB3	1:A:323:LEU:HD11	2.02	0.41
1:B:385:THR:O	1:B:385:THR:HG23	2.21	0.41
1:A:240:LEU:HD12	1:A:240:LEU:C	2.41	0.41
1:B:78:ARG:HD2	1:B:90:VAL:O	2.22	0.40
1:B:204:LYS:HD2	1:B:241:GLU:HB2	2.03	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	Percen	tiles
1	А	567/581~(98%)	544 (96%)	22~(4%)	1 (0%)	47	46
1	В	578/581~(100%)	558~(96%)	18 (3%)	2 (0%)	41	37
All	All	1145/1162~(98%)	1102 (96%)	40 (4%)	3~(0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	371	ARG
1	В	227	LEU
1	А	362	GLY

#### 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	А	454/483~(94%)	449~(99%)	5 (1%)	73 78
1	В	436/483~(90%)	429~(98%)	7 (2%)	62 67
All	All	890/966~(92%)	878~(99%)	12 (1%)	67 74

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	215	TYR
1	А	226	ASP
1	А	355	GLU

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Mol	Chain	$\mathbf{Res}$	Type
1	А	441	MET
1	А	571	ARG
1	В	215	TYR
1	В	253	LEU
1	В	315	GLN
1	В	413	LEU
1	В	462	ARG
1	В	488	ARG
1	В	496	LEU

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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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

2 ligands are 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	Tune	Chain	Res	Link	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
	Type	Cham	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	RSN	А	601	-	28,35,35	1.09	1 (3%)	$36,\!52,\!52$	0.83	1 (2%)
2	RSN	В	601	-	28,35,35	1.04	1 (3%)	36,52,52	0.83	1 (2%)



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.

$\mathbb{N}$	Лоl	Type	Chain	Res	Link	Chirals	Torsions	Rings
	2	RSN	А	601	-	-	6/18/41/41	0/3/3/3
	2	RSN	В	601	-	-	1/18/41/41	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	А	601	RSN	C-N3S	4.87	1.46	1.37
2	В	601	RSN	C-N3S	4.56	1.46	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	601	RSN	O-C-N3S	-3.22	116.80	123.00
2	А	601	RSN	O-C-N3S	-3.20	116.83	123.00

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
2	А	601	RSN	N-CA-CB-CG
2	А	601	RSN	O-C-CA-N
2	А	601	RSN	O-C-CA-CB
2	А	601	RSN	N3S-C-CA-CB
2	А	601	RSN	C-CA-CB-CG
2	А	601	RSN	C3'-C4'-C5'-O5'
2	В	601	RSN	C3'-C4'-C5'-O5'

There are no ring outliers.

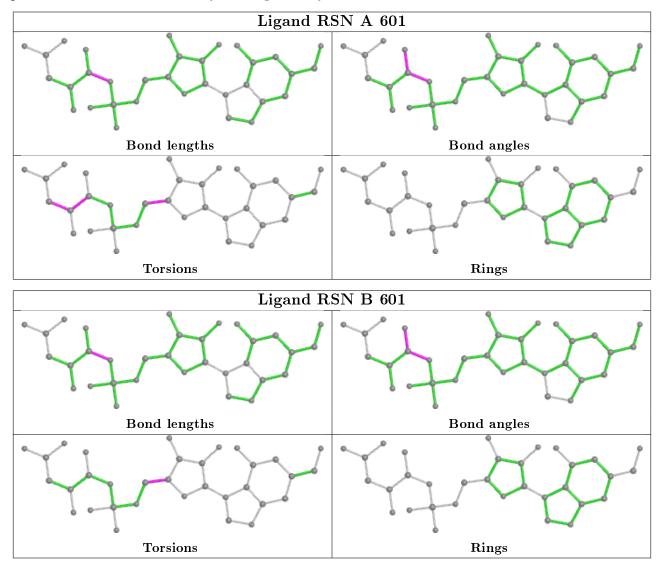
1 monomer is involved in 1 short contact:

Mol	Chain	$\mathbf{Res}$	Type	Clashes	Symm-Clashes
2	А	601	RSN	1	0

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 then 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 (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,  $95^{th}$  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 $>$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	573/581~(98%)	0.18	0 100 100	35,  55,  85,  113	0
1	В	580/581~(99%)	0.59	58 (10%) 7 11	37, 59, 160, 282	0
All	All	1153/1162~(99%)	0.39	58 (5%) 28 37	35, 57, 147, 282	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	365	LYS	7.7
1	В	303	GLY	7.4
1	В	375	LEU	7.4
1	В	360	SER	7.3
1	В	325	LEU	6.2
1	В	323	LEU	5.7
1	В	362	GLY	5.7
1	В	357	GLY	5.6
1	В	376	GLN	5.6
1	В	382	PRO	5.5
1	В	355	GLU	5.2
1	В	349	LEU	5.0
1	В	374	LEU	4.6
1	В	302	VAL	4.5
1	В	311	PHE	4.5
1	В	317	ALA	4.5
1	В	361	GLY	4.3
1	В	372	GLU	4.3
1	В	363	VAL	4.2
1	В	304	PRO	4.0
1	В	312	ARG	3.8
1	В	329	LEU	3.8
1	В	326	PRO	3.8
1	В	354	VAL	3.6

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Mol	Chain	Res	Type	RSRZ			
1	В	367	LEU	3.5			
1	В	356	GLU	3.5			
1	В	176	PRO	3.5			
1	В	385	THR	3.4			
1	В	306	PHE	3.4			
1	В	496	LEU	3.3			
1	В	321	LYS	3.3			
1	В	352	ALA	3.1			
1	В	366	PHE	3.1			
1	В	373	ALA	3.1			
1	В	177	GLU	3.1			
1	В	386	LEU	3.1			
1	В	399	ALA	3.0			
1	В	388	PHE	2.9			
1	В	335	ALA	2.9			
1	В	351	TRP	2.8			
1	В	389	VAL	2.8			
1	В	359	PHE	2.5			
1	В	395	VAL	2.5			
1	В	408	ALA	2.4			
1	В	358	GLY	2.4			
1	В	328	ALA	2.4			
1	В	406	ARG	2.4			
1	В	314	PHE	2.3			
1	В	383	GLY	2.3			
1	В	347	GLN	2.3			
1	В	337	LEU	2.2			
1	В	228	ARG	2.2			
1	В	308	GLN	2.2			
1	В	334	VAL	2.2			
1	В	377	ALA	2.1			
1	В	313	VAL	2.1			
1	В	380	ALA	2.0			
1	В	410	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)

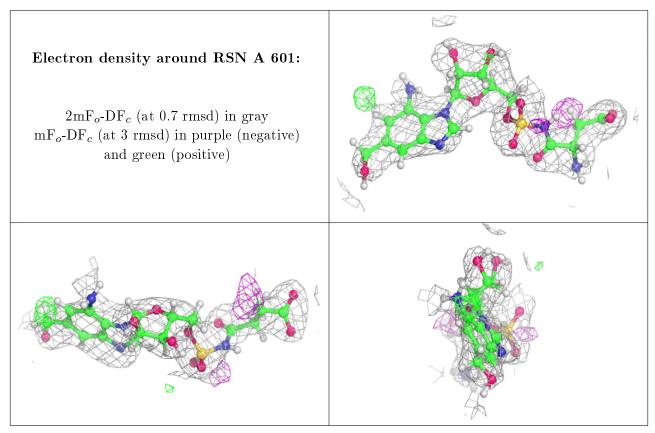
There are no monosaccharides in this entry.

## 6.4 Ligands (i)

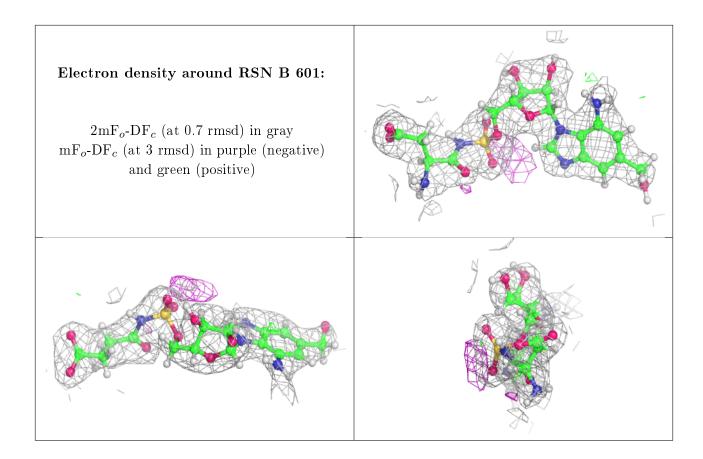
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$Q{<}0.9$
2	RSN	А	601	33/33	0.86	0.20	$53,\!82,\!98,\!114$	0
2	RSN	В	601	33/33	0.96	0.15	$50,\!62,\!75,\!93$	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.

