

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

#### Oct 12, 2021 - 05:36 pm BST

PDB ID	:	70EE
Title	:	Crystal structure of the human METTL3-METTL14 complex with compound
		UOZ019b
Authors	:	Bedi, R.K.; Huang, D.; Caflisch, A.
Deposited on		
Resolution	:	2.70  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 following versions of software and data (see references (1)) were used in the production of this report:

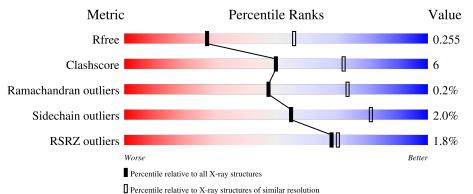
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins)	:::::::::::::::::::::::::::::::::::::::	<ul> <li>1.8.5 (274361), CSD as541be (2020)</li> <li>1.13</li> <li>2.23.2</li> <li>1.1.7 (2018)</li> <li>20191225.v01 (using entries in the PDB archive December 25th 2019)</li> <li>5.8.0267</li> <li>7.1.010 (Gargrove)</li> <li>Engh &amp; Huber (2001)</li> </ul>
		0
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.23.2

# 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 2.70 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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% 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	246	<sup>2%</sup> 65%	17%	18%			
2	В	290	% 72%	10%	18%			



#### 70EE

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3524 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 N6-adenosine-methyltransferase catalytic subunit.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	А	201	Total 1572	C 1006	N 274	0 283	${ m S} 9$	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	335	MET	-	initiating methionine	UNP Q86U44
А	336	GLY	-	expression tag	UNP Q86U44
А	337	HIS	-	expression tag	UNP Q86U44
А	338	HIS	-	expression tag	UNP Q86U44
А	339	HIS	-	expression tag	UNP Q86U44
А	340	HIS	-	expression tag	UNP Q86U44
А	341	HIS	-	expression tag	UNP Q86U44
А	342	HIS	-	expression tag	UNP Q86U44
А	343	SER	-	expression tag	UNP Q86U44
А	344	SER	-	expression tag	UNP Q86U44
А	345	GLY	-	expression tag	UNP Q86U44
А	346	ARG	-	expression tag	UNP Q86U44
А	347	GLU	-	expression tag	UNP Q86U44
А	348	ASN	-	expression tag	UNP Q86U44
А	349	LEU	-	expression tag	UNP Q86U44
А	350	TYR	-	expression tag	UNP Q86U44
А	351	PHE	-	expression tag	UNP Q86U44
А	352	GLN	-	expression tag	UNP Q86U44
А	353	GLY	-	expression tag	UNP Q86U44

There are 19 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called N6-adenosine-methyltransferase non-catalytic subunit.

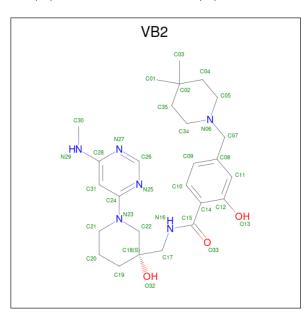
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	238	Total 1859	C 1193	N 316	O 337	S 13	0	2	0



There is a discrepancy between the modelled and reference sequences:

ſ	Chain	Residue	Modelled	Actual	Comment	Reference
	В	106	MET	-	initiating methionine	UNP Q9HCE5

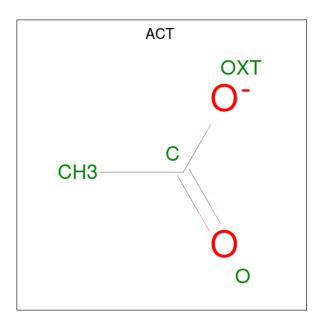
• Molecule 3 is 4-[(4,4-dimethylpiperidin-1-yl)methyl]- {N}-[[(3 {S})-1-[6-(methylamino)p yrimidin-4-yl]-3-oxidanyl-piperidin-3-yl]methyl]-2-oxidanyl-benzamide (three-letter code: VB2) (formula: C<sub>26</sub>H<sub>38</sub>N<sub>6</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
3	А	1	Total 35	C 26	N 6	O 3	0	0

• Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	В	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	O 2	0	0

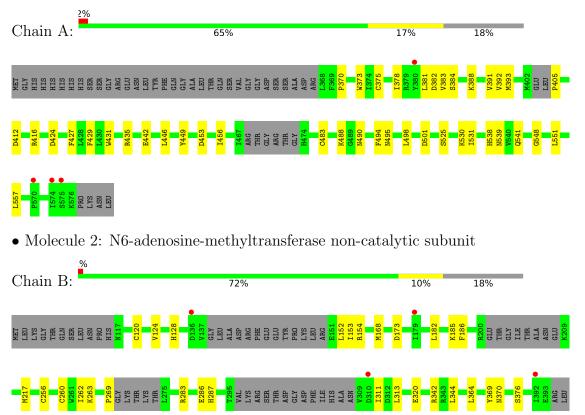
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	20	TotalO2020	0	0
5	В	34	Total O 34 34	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: N6-adenosine-methyltransferase catalytic subunit



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	63.80Å 63.80Å 224.73Å	Denesiten
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	49.58 - 2.70	Depositor
Resolution (A)	49.58 - 2.70	EDS
% Data completeness	99.9 (49.58-2.70)	Depositor
(in resolution range)	99.9 (49.58 - 2.70)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.17 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
B B.	0.194 , $0.258$	Depositor
$R, R_{free}$	0.191 , $0.255$	DCC
$R_{free}$ test set	762 reflections $(4.98\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	54.2	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3524	wwPDB-VP
Average B, all atoms $(Å^2)$	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.82% 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: VB2, ACT

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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.46	0/1611	0.66	1/2194~(0.0%)	
2	В	0.48	0/1909	0.64	0/2596	
All	All	0.47	0/3520	0.65	1/4790~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	405	PRO	N-CA-CB	6.13	110.66	103.30

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	1572	0	1490	24	0
2	В	1859	0	1728	17	0
3	А	35	0	0	1	0
4	В	4	0	3	0	0
5	А	20	0	0	0	0
5	В	34	0	0	1	0
All	All	3524	0	3221	39	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 6.

All (39) 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:391:VAL:HB	1:A:530:LYS:HG2	1.67	0.77
2:B:168:MET:HE3	2:B:369:TYR:HA	1.77	0.67
2:B:320:GLU:H	2:B:320:GLU:CD	2.00	0.65
2:B:152:LEU:C	2:B:154:ARG:H	2.01	0.63
1:A:495:ASN:HB3	1:A:498:LEU:HD23	1.80	0.62
1:A:382:ASP:OD1	1:A:384:SER:OG	2.21	0.57
1:A:381:LEU:HD23	1:A:383:VAL:HG12	1.85	0.56
1:A:456:ILE:HD11	2:B:262:ILE:HD11	1.86	0.56
2:B:120:CYS:O	2:B:124:VAL:HG23	2.06	0.55
1:A:373:TRP:HB2	1:A:551:LEU:HD13	1.88	0.55
2:B:128:HIS:CD2	2:B:269:PRO:HB3	2.43	0.54
1:A:539:ASN:O	1:A:541:GLN:HG2	2.09	0.52
2:B:256:CYS:HB3	5:B:529:HOH:O	2.09	0.52
1:A:412:ASP:HB3	1:A:416:ARG:NH1	2.24	0.52
1:A:431:TRP:CE3	1:A:483:CYS:HB2	2.46	0.50
1:A:378:ILE:HD12	3:A:601:VB2:C26	2.42	0.50
1:A:370:PRO:HG2	1:A:557:LEU:HD12	1.93	0.49
1:A:393:MET:HG3	1:A:429:PHE:HB2	1.94	0.49
2:B:185:LYS:O	2:B:342[B]:ARG:NH1	2.47	0.47
1:A:449:TYR:CD2	1:A:488:LYS:HB2	2.50	0.46
1:A:498:LEU:HD13	1:A:498:LEU:HA	1.80	0.45
1:A:392:VAL:HG22	1:A:531:ILE:HG22	1.98	0.45
2:B:311:ILE:HG23	2:B:313:LEU:H	1.81	0.45
1:A:388:LYS:HD2	1:A:424:ASP:OD2	2.16	0.45
2:B:263:LYS:HE2	2:B:286:GLU:HG3	1.98	0.44
2:B:152:LEU:C	2:B:154:ARG:N	2.70	0.44
1:A:495:ASN:HB3	1:A:498:LEU:CD2	2.47	0.44
1:A:442:GLU:O	1:A:446:LEU:HG	2.19	0.43
1:A:501:ASP:OD2	2:B:283:ARG:HA	2.19	0.43
1:A:449:TYR:CE2	1:A:488:LYS:HB2	2.55	0.42
2:B:168:MET:HE1	2:B:370:ASN:H	1.86	0.41
1:A:538:HIS:HD2	1:A:539:ASN:ND2	2.19	0.41
1:A:427:PHE:HE2	1:A:494:PHE:CD1	2.38	0.41
2:B:152:LEU:O	2:B:154:ARG:N	2.53	0.41
2:B:182:LEU:HD23	2:B:182:LEU:HA	1.94	0.41
2:B:186:PHE:CD1	2:B:344:LEU:HB2	2.55	0.41
2:B:260[B]:CYS:SG	2:B:287:HIS:CE1	3.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:CYS:HA	1:A:548:GLY:O	2.21	0.40
1:A:525:SER:O	1:A:530:LYS:NZ	2.52	0.40

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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	А	195/246~(79%)	186~(95%)	9~(5%)	0	100 100
2	В	230/290~(79%)	220~(96%)	9~(4%)	1 (0%)	34 60
All	All	425/536~(79%)	406 (96%)	18 (4%)	1 (0%)	47 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type	
2	В	153	ILE	

#### 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	162/215~(75%)	159~(98%)	3~(2%)	57 82		
2	В	189/259~(73%)	185~(98%)	4 (2%)	53 80		
All	All	351/474 (74%)	344 (98%)	7 (2%)	55 81		



Mol	Chain	Res	Type
1	А	435	ARG
1	А	453	ASP
1	А	490	ASN
2	В	173	ASP
2	В	217	MET
2	В	364	LEU
2	В	376	SER

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	512	HIS
1	А	538	HIS
1	А	543	ASN
1	А	550	GLN

#### 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).



Mal	Mol Type Chair		hain Res Link		B	Bond lengths			ond ang	les
IVIOI	Type	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	VB2	А	601	-	36,38,38	2.50	8 (22%)	48,55,55	1.87	8 (16%)
4	ACT	В	401	-	1,3,3	7.20	1 (100%)	0,3,3	-	-

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
3	VB2	А	601	-	-	5/20/44/44	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
3	А	601	VB2	C07-N06	-7.85	1.32	1.47
4	В	401	ACT	CH3-C	7.20	1.57	1.48
3	А	601	VB2	C15-N16	5.56	1.46	1.33
3	А	601	VB2	C05-N06	-5.29	1.32	1.46
3	А	601	VB2	C34-N06	-5.12	1.32	1.46
3	А	601	VB2	C28-N29	4.67	1.46	1.36
3	А	601	VB2	C24-N23	4.18	1.46	1.37
3	А	601	VB2	C22-N23	-2.46	1.43	1.46
3	А	601	VB2	O13-C12	2.29	1.41	1.36

All $(8)$	bond	angle	outliers	are	listed	below:	
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Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
3	А	601	VB2	C26-N25-C24	6.43	120.56	114.94
3	А	601	VB2	N27-C26-N25	-5.99	119.24	128.60
3	А	601	VB2	C21-N23-C22	4.78	122.50	114.00
3	А	601	VB2	C20-C21-N23	3.35	117.59	111.05
3	А	601	VB2	C20-C19-C18	-2.41	109.73	112.96
3	А	601	VB2	C01-C02-C04	-2.41	106.42	110.05
3	А	601	VB2	C17-N16-C15	-2.41	118.92	122.89
3	А	601	VB2	C35-C02-C04	2.38	111.97	108.71

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	601	VB2	C31-C28-N29-C30

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Mol	Chain	Res	Type	Atoms
3	А	601	VB2	N27-C28-N29-C30
3	А	601	VB2	C12-C14-C15-O33
3	А	601	VB2	C12-C14-C15-N16
3	А	601	VB2	N16-C17-C18-O32

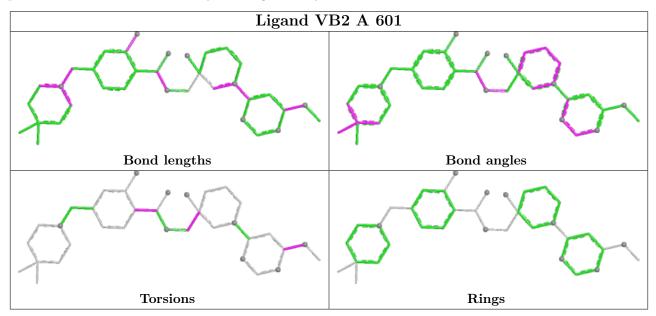
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There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	601	VB2	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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	201/246~(81%)	0.08	4 (1%) 65 67	30, 48, 81, 96	0
2	В	238/290~(82%)	-0.06	4 (1%) 70 72	31, 44, 77, 96	0
All	All	439/536~(81%)	0.00	8 (1%) 68 70	30, 46, 81, 96	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	392	ILE	4.3
1	А	570	PRO	3.9
1	А	575	SER	2.9
1	А	574	ILE	2.4
2	В	310	ASP	2.4
1	А	380	TYR	2.3
2	В	179	ILE	2.1
2	В	136	ASP	2.1

## 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)

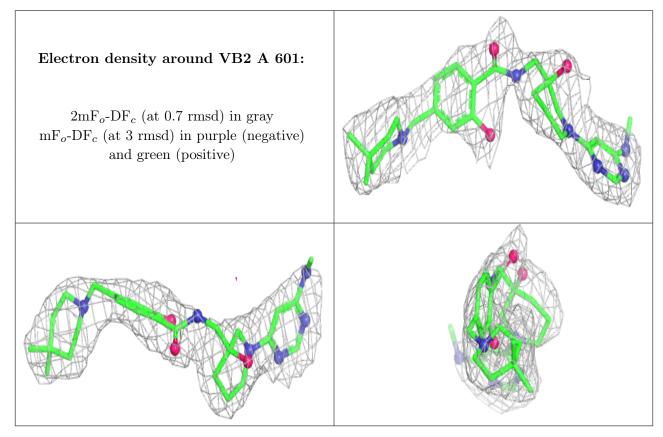
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
3	VB2	А	601	35/35	0.89	0.26	43,56,77,83	0
4	ACT	В	401	4/4	0.99	0.16	40,41,41,41	0

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.

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.

