



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 06:01 pm BST

PDB ID : 7OEK  
Title : Crystal structure of the human METTL3-METTL14 complex with compound UOZ091  
Authors : Bedi, R.K.; Huang, D.; Caflisch, A.  
Deposited on : 2021-05-03  
Resolution : 1.90 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
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

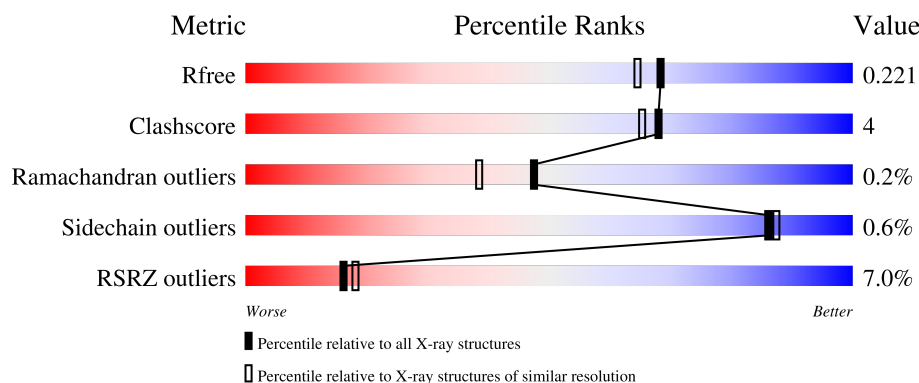
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	246	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>9%</div> <div>19%</div> </div> </div>
2	B	290	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>6%</div> <div>17%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3816 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	A	200	Total	C	N	O	S	0	1	0
			1587	1018	277	282	10			

There are 19 discrepancies between the modelled and reference sequences:

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

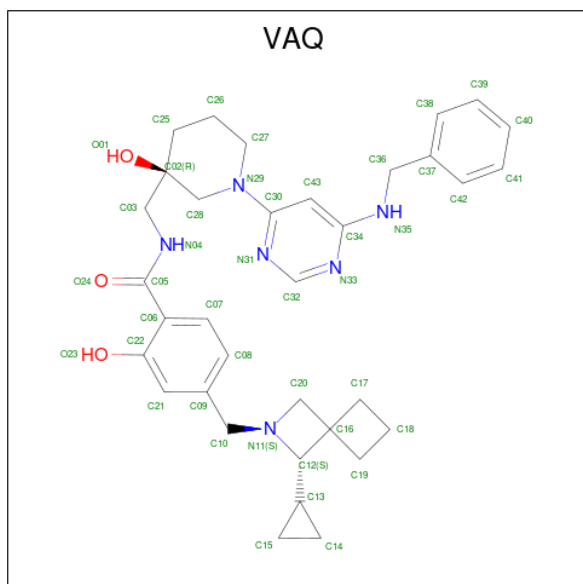
- Molecule 2 is a protein called N6-adenosine-methyltransferase non-catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	0	1	1
			1886	1211	314	348	13			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is 4-[[[(3S)-3-cyclopropyl-2-azaspiro[3.3]heptan-2-yl]methyl]-2-oxidanyl-N-[[[(3R)-3-oxidanyl-1-[6-[(phenylmethyl)amino]pyrimidin-4-yl]piperidin-3-yl]methyl]benzamide (three-letter code: VAQ) (formula: C<sub>34</sub>H<sub>42</sub>N<sub>6</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

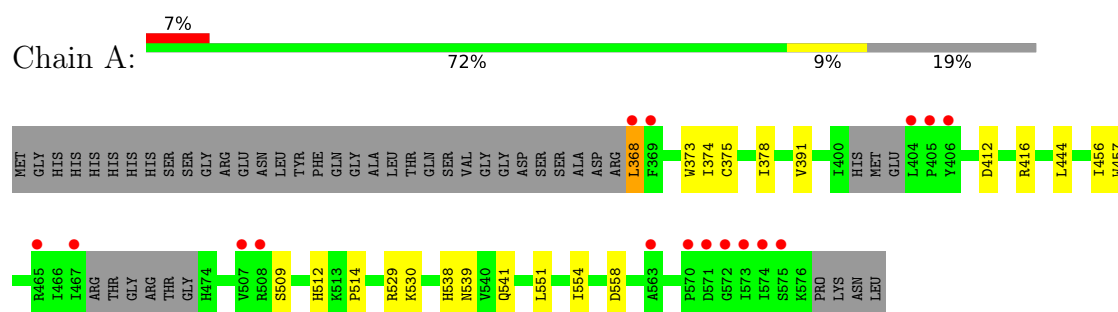
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	116	Total	O	0	0
			116	116		
5	B	180	Total	O	0	0
			180	180		

### 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



- Molecule 2: N6-adenosine-methyltransferase non-catalytic subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.90Å 63.90Å 225.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.68 – 1.90 49.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.68-1.90) 99.8 (49.68-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122+SVN	Depositor
R, $R_{free}$	0.191 , 0.223 0.189 , 0.221	Depositor DCC
$R_{free}$ test set	2162 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3816	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: VAQ, 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	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.41	0/1630	0.69	2/2218 (0.1%)
2	B	0.44	0/1933	0.66	2/2629 (0.1%)
All	All	0.43	0/3563	0.67	4/4847 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	LEU	CB-CG-CD2	-8.05	97.31	111.00
1	A	444	LEU	CA-CB-CG	5.51	127.97	115.30
2	B	276	ASP	CB-CG-OD1	5.44	123.20	118.30
2	B	248	LEU	CB-CG-CD2	-5.29	102.01	111.00

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	A	1587	0	1533	14	0
2	B	1886	0	1763	13	0
3	A	43	0	0	0	0
4	B	4	0	3	0	0
5	A	116	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	180	0	0	5	0
All	All	3816	0	3299	26	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 4.

All (26) 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:456:ILE:HD11	2:B:262:ILE:HD11	1.41	1.03
1:A:375:CYS:SG	5:A:803:HOH:O	2.29	0.89
1:A:368:LEU:HD22	1:A:558:ASP:HA	1.68	0.74
2:B:390:GLU:OE1	5:B:501:HOH:O	2.10	0.69
1:A:539:ASN:O	1:A:541:GLN:HG2	2.01	0.61
1:A:391:VAL:HB	1:A:530:LYS:HG2	1.82	0.61
2:B:293:LYS:NZ	5:B:506:HOH:O	2.32	0.59
1:A:529:ARG:HG3	5:A:741:HOH:O	2.06	0.56
1:A:512:HIS:CE1	1:A:538:HIS:CE1	2.96	0.54
2:B:275:LEU:N	5:B:509:HOH:O	2.43	0.51
2:B:173:ASP:HB3	2:B:175:GLU:OE2	2.13	0.48
2:B:254:ARG:NH1	5:B:505:HOH:O	2.30	0.48
2:B:191:LEU:HG	2:B:193:PRO:HD3	1.97	0.46
1:A:457:TRP:CE3	1:A:514:PRO:HD3	2.50	0.46
2:B:311:ILE:HG23	2:B:313:LEU:H	1.81	0.45
1:A:373:TRP:HB2	1:A:551:LEU:HD13	1.98	0.45
1:A:412:ASP:HB3	1:A:416:ARG:NH1	2.31	0.45
2:B:230:PHE:CE1	2:B:339:LEU:HD22	2.53	0.44
1:A:368:LEU:HD22	1:A:558:ASP:CA	2.45	0.43
1:A:412:ASP:O	1:A:416:ARG:HG3	2.19	0.43
2:B:325:GLU:CD	2:B:349:ARG:HH21	2.22	0.43
2:B:321:ILE:HD13	2:B:321:ILE:HA	1.88	0.42
2:B:320:GLU:H	2:B:320:GLU:HG3	1.62	0.42
1:A:374:ILE:HG23	1:A:554:ILE:HG12	2.01	0.42
1:A:378:ILE:O	5:A:701:HOH:O	2.21	0.41
2:B:214:ASP:HB2	5:B:567:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	195/246 (79%)	189 (97%)	5 (3%)	1 (0%)	29	18
2	B	231/290 (80%)	228 (99%)	3 (1%)	0	100	100
All	All	426/536 (80%)	417 (98%)	8 (2%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	SER

### 5.3.2 Protein sidechains

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	168/215 (78%)	168 (100%)	0	100	100
2	B	196/259 (76%)	194 (99%)	2 (1%)	76	76
All	All	364/474 (77%)	362 (100%)	2 (0%)	86	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	175	GLU
2	B	320	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ACT	B	401	-	1,3,3	8.82	1 (100%)	0,3,3	-	-
3	VAQ	A	601	-	44,49,49	3.01	21 (47%)	55,72,72	2.11	16 (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
3	VAQ	A	601	-	-	1/23/64/64	0/7/7/7

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	VAQ	C36-C37	9.01	1.70	1.51
4	B	401	ACT	CH3-C	8.82	1.60	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	VAQ	C34-N35	8.62	1.49	1.36
3	A	601	VAQ	C30-N29	5.99	1.49	1.37
3	A	601	VAQ	C28-N29	4.95	1.50	1.46
3	A	601	VAQ	C36-N35	4.04	1.58	1.45
3	A	601	VAQ	C27-N29	3.95	1.52	1.46
3	A	601	VAQ	C05-N04	3.81	1.42	1.33
3	A	601	VAQ	C32-N31	3.39	1.40	1.33
3	A	601	VAQ	O23-C22	3.09	1.42	1.36
3	A	601	VAQ	C08-C07	3.06	1.44	1.38
3	A	601	VAQ	C21-C09	3.04	1.44	1.39
3	A	601	VAQ	C32-N33	2.87	1.39	1.33
3	A	601	VAQ	C41-C42	2.78	1.44	1.38
3	A	601	VAQ	C26-C27	2.50	1.59	1.51
3	A	601	VAQ	C10-N11	2.32	1.51	1.47
3	A	601	VAQ	C43-C34	2.22	1.45	1.39
3	A	601	VAQ	C40-C39	2.22	1.43	1.38
3	A	601	VAQ	C41-C40	2.18	1.43	1.38
3	A	601	VAQ	C15-C13	2.10	1.56	1.49
3	A	601	VAQ	O24-C05	2.05	1.27	1.23
3	A	601	VAQ	C42-C37	2.01	1.43	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	VAQ	C32-N31-C30	5.78	119.99	114.94
3	A	601	VAQ	N33-C32-N31	-5.66	119.75	128.60
3	A	601	VAQ	C43-C30-N29	-4.42	117.04	122.29
3	A	601	VAQ	C06-C05-N04	3.95	125.12	117.36
3	A	601	VAQ	C15-C13-C12	3.89	127.29	119.22
3	A	601	VAQ	C07-C08-C09	-3.69	115.95	121.03
3	A	601	VAQ	C43-C34-N33	-3.54	117.82	122.75
3	A	601	VAQ	C09-C10-N11	-3.42	107.15	112.75
3	A	601	VAQ	N31-C30-N29	3.33	121.78	116.79
3	A	601	VAQ	C27-N29-C30	2.89	127.09	120.39
3	A	601	VAQ	C08-C09-C21	2.83	122.50	118.54
3	A	601	VAQ	O24-C05-C06	-2.74	116.00	121.01
3	A	601	VAQ	C36-N35-C34	2.68	128.68	123.40
3	A	601	VAQ	O23-C22-C06	-2.59	116.94	121.70
3	A	601	VAQ	N35-C34-N33	2.51	120.73	116.95
3	A	601	VAQ	C32-N33-C34	2.15	122.39	115.25

There are no chirality outliers.

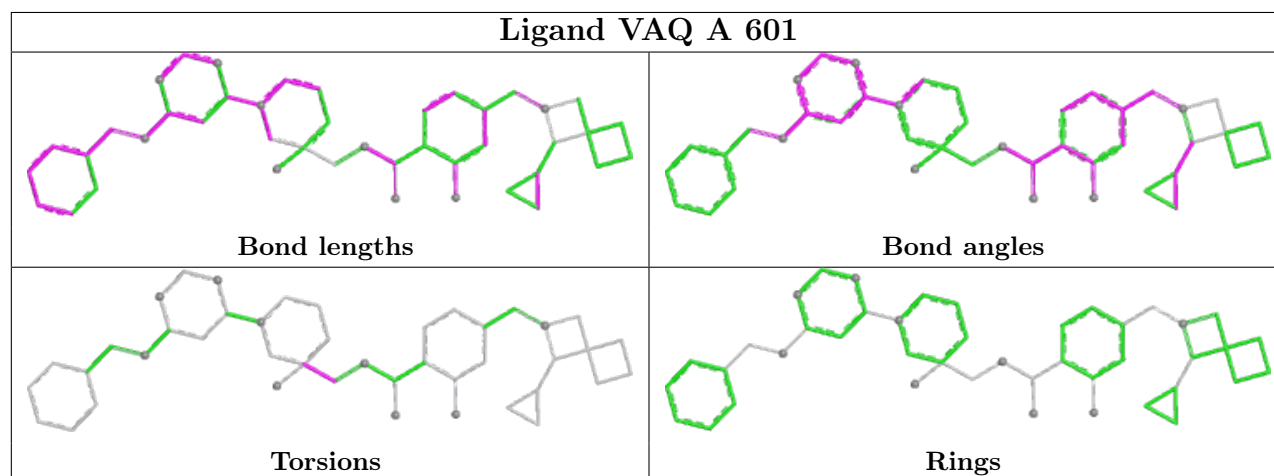
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	VAQ	O01-C02-C03-N04

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	200/246 (81%)	0.12	16 (8%) 12 13	21, 34, 62, 74	0
2	B	240/290 (82%)	0.13	15 (6%) 20 22	20, 32, 65, 74	0
All	All	440/536 (82%)	0.12	31 (7%) 16 18	20, 33, 63, 74	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	395	LEU	6.1
2	B	392	ILE	5.7
2	B	155	LEU	5.5
2	B	309	VAL	5.0
1	A	368	LEU	4.7
1	A	404	LEU	4.7
2	B	136	ASP	4.2
1	A	574	ILE	4.2
1	A	467	ILE	4.0
2	B	390	GLU	3.8
2	B	393	GLU	3.8
1	A	465	ARG	3.6
1	A	573	ILE	3.6
1	A	405	PRO	3.3
1	A	563	ALA	3.3
2	B	275	LEU	3.1
2	B	270	GLY	3.1
2	B	394	ARG	3.0
1	A	575	SER	3.0
2	B	153	ILE	2.9
1	A	369	PHE	2.9
1	A	570	PRO	2.7
1	A	571	ASP	2.4
1	A	508	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	384	TYR	2.3
1	A	572	GLY	2.3
2	B	154	ARG	2.3
2	B	391	GLU	2.3
1	A	507	VAL	2.2
2	B	137	VAL	2.2
1	A	406	TYR	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](#)

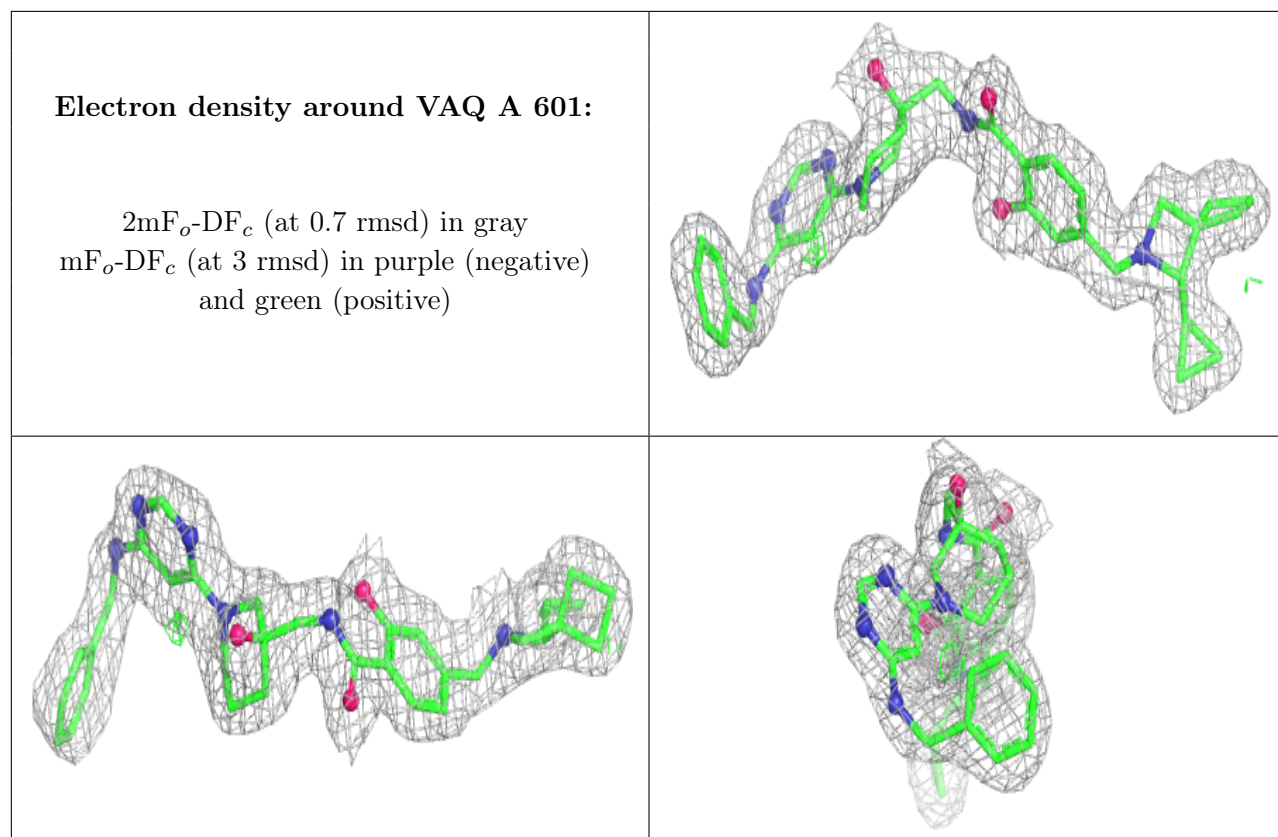
There are no monosaccharides in this entry.

## 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, 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( $\text{\AA}^2$ )	Q<0.9
3	VAQ	A	601	43/43	0.91	0.11	27,33,42,48	0
4	ACT	B	401	4/4	0.97	0.10	22,25,27,29	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.