



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 03:57 PM BST

PDB ID : 6Z17  
Title : PqsR (MvfR) in complex with antagonist 6  
Authors : Richardson, W.K.; Emsley, J.  
Deposited on : 2020-05-12  
Resolution : 3.15 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 : 2.14.4.dev1  
buster-report : 1.1.7 (2018)  
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) : 2.14.4.dev1

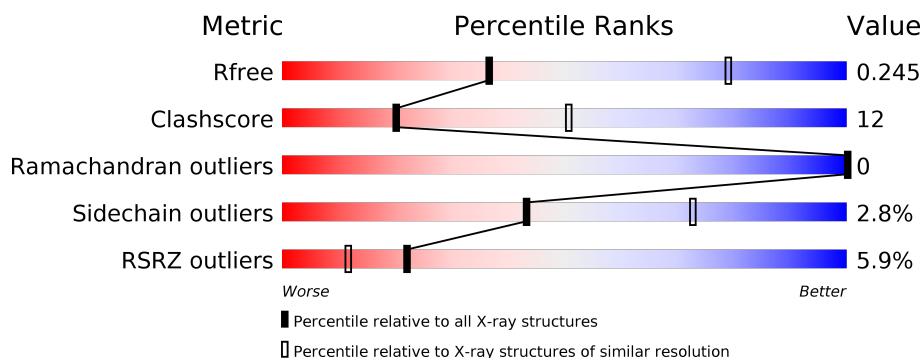
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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  $\geq 3$ , 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	AAA	239	<div> <div>5%</div> <div>67%</div> <div>17%</div> <div>15%</div> </div>

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
2	Q4W	AAA	401	X	-	-	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3229 atoms, of which 1610 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.

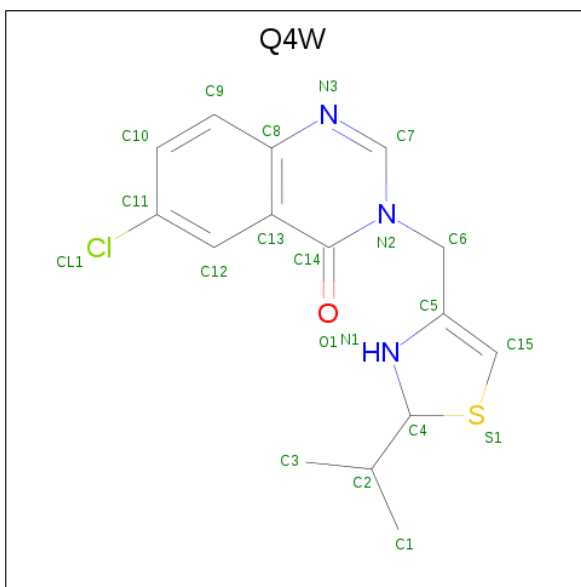
- Molecule 1 is a protein called Transcriptional regulator MvfR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	203	Total	C	H	N	O	S	81	0	0
			3194	1011	1596	277	304	6			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	71	MET	-	initiating methionine	UNP A0A0H2Z7A6
AAA	72	GLY	-	expression tag	UNP A0A0H2Z7A6
AAA	73	SER	-	expression tag	UNP A0A0H2Z7A6
AAA	74	SER	-	expression tag	UNP A0A0H2Z7A6
AAA	75	HIS	-	expression tag	UNP A0A0H2Z7A6
AAA	76	HIS	-	expression tag	UNP A0A0H2Z7A6
AAA	77	HIS	-	expression tag	UNP A0A0H2Z7A6
AAA	78	HIS	-	expression tag	UNP A0A0H2Z7A6
AAA	79	HIS	-	expression tag	UNP A0A0H2Z7A6
AAA	80	HIS	-	expression tag	UNP A0A0H2Z7A6
AAA	81	SER	-	expression tag	UNP A0A0H2Z7A6
AAA	82	SER	-	expression tag	UNP A0A0H2Z7A6
AAA	83	GLY	-	expression tag	UNP A0A0H2Z7A6
AAA	84	LEU	-	expression tag	UNP A0A0H2Z7A6
AAA	85	VAL	-	expression tag	UNP A0A0H2Z7A6
AAA	86	PRO	-	expression tag	UNP A0A0H2Z7A6
AAA	87	ARG	-	expression tag	UNP A0A0H2Z7A6
AAA	88	GLY	-	expression tag	UNP A0A0H2Z7A6
AAA	89	SER	-	expression tag	UNP A0A0H2Z7A6
AAA	90	HIS	-	expression tag	UNP A0A0H2Z7A6
AAA	91	MET	-	expression tag	UNP A0A0H2Z7A6
AAA	92	ALA	-	expression tag	UNP A0A0H2Z7A6
AAA	93	SER	-	expression tag	UNP A0A0H2Z7A6

- Molecule 2 is 6-chloranyl-3-[(2-propan-2-yl-2,3-dihydro-1,3-thiazol-4-yl)methyl]quinazolin-4-one (three-letter code: Q4W) (formula: C<sub>15</sub>H<sub>16</sub>ClN<sub>3</sub>OS) (labeled as "Ligand of Interest" by author).

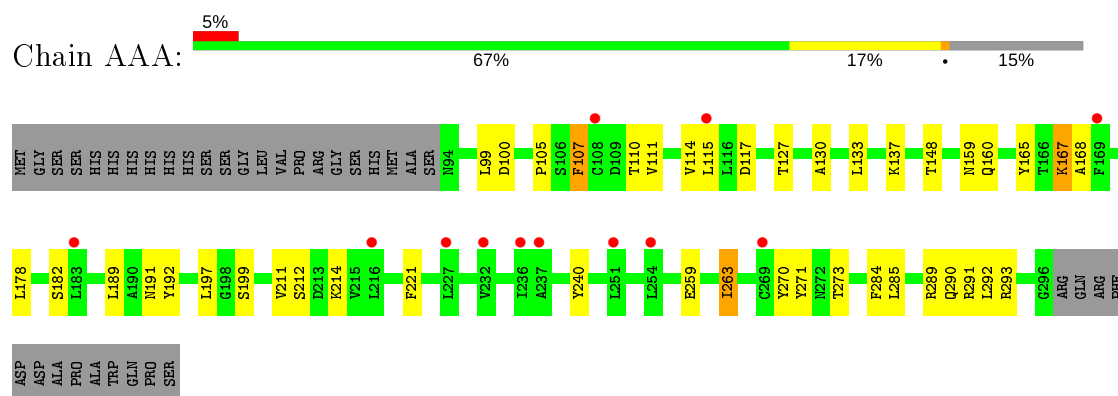


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	H	N	O	S		
2	AAA	1	35	15	1	14	3	1	1	0	0

### 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: Transcriptional regulator MvfR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.27Å 120.27Å 115.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.13 – 3.15 60.13 – 3.15	Depositor EDS
% Data completeness (in resolution range)	94.5 (60.13-3.15) 94.6 (60.13-3.15)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.195 , 0.241 0.201 , 0.245	Depositor DCC
$R_{free}$ test set	406 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	136.5	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 104.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	143.0	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>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: Q4W

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	0.70	0/1628	0.91	0/2210

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	1598	1596	1590	40	0
2	AAA	21	14	0	1	0
All	All	1619	1610	1590	40	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 12.

All (40) 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:110:THR:HG23	1:AAA:291:ARG:HD2	1.56	0.86
1:AAA:111:VAL:HG12	1:AAA:284:PHE:HE1	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:110:THR:HA	1:AAA:291:ARG:HH11	1.47	0.78
1:AAA:259:GLU:OE1	1:AAA:263:ILE:HG23	1.92	0.69
1:AAA:285:LEU:O	1:AAA:289:ARG:HG3	1.94	0.68
1:AAA:130:ALA:HB1	1:AAA:199:SER:HB3	1.79	0.65
1:AAA:107:PHE:CE1	1:AAA:111:VAL:HG13	2.34	0.62
1:AAA:107:PHE:CD1	1:AAA:107:PHE:C	2.74	0.61
1:AAA:110:THR:CG2	1:AAA:291:ARG:HD2	2.28	0.60
1:AAA:110:THR:HG21	1:AAA:291:ARG:HB2	1.85	0.58
1:AAA:107:PHE:CE1	1:AAA:111:VAL:CG1	2.88	0.57
1:AAA:111:VAL:CG1	1:AAA:284:PHE:HE1	2.17	0.56
1:AAA:160:GLN:HG3	1:AAA:270:TYR:CE2	2.42	0.54
1:AAA:168:ALA:O	1:AAA:263:ILE:HG13	2.07	0.54
1:AAA:197:LEU:HD11	1:AAA:221:PHE:CZ	2.44	0.52
1:AAA:167:LYS:NZ	1:AAA:167:LYS:HB3	2.25	0.50
1:AAA:110:THR:CG2	1:AAA:291:ARG:HB2	2.41	0.50
1:AAA:111:VAL:HB	1:AAA:115:LEU:HD12	1.92	0.50
1:AAA:167:LYS:HZ3	1:AAA:167:LYS:HB3	1.77	0.49
1:AAA:211:VAL:HG11	2:AAA:401:Q4W:C3	2.43	0.48
1:AAA:110:THR:CB	1:AAA:291:ARG:HD2	2.44	0.48
1:AAA:290:GLN:O	1:AAA:293:ARG:HB2	2.13	0.48
1:AAA:110:THR:HG23	1:AAA:291:ARG:CD	2.35	0.46
1:AAA:159:ASN:HB2	1:AAA:271:TYR:CZ	2.51	0.46
1:AAA:133:LEU:O	1:AAA:137:LYS:HG3	2.17	0.45
1:AAA:105:PRO:HD3	1:AAA:240:TYR:CE2	2.52	0.45
1:AAA:100:ASP:C	1:AAA:100:ASP:OD1	2.55	0.45
1:AAA:107:PHE:O	1:AAA:110:THR:N	2.50	0.45
1:AAA:114:VAL:HG11	1:AAA:284:PHE:HA	2.00	0.44
1:AAA:191:ASN:O	1:AAA:214:LYS:HE3	2.18	0.43
1:AAA:165:TYR:CD1	1:AAA:165:TYR:N	2.87	0.42
1:AAA:178:LEU:HD21	1:AAA:192:TYR:CE1	2.54	0.42
1:AAA:189:LEU:O	1:AAA:212:SER:HB3	2.19	0.42
1:AAA:111:VAL:HG12	1:AAA:284:PHE:CE1	2.38	0.41
1:AAA:114:VAL:O	1:AAA:117:ASP:HB2	2.20	0.41
1:AAA:197:LEU:HD11	1:AAA:221:PHE:CE1	2.55	0.41
1:AAA:99:LEU:N	1:AAA:99:LEU:HD12	2.36	0.41
1:AAA:159:ASN:OD1	1:AAA:273:THR:HG22	2.22	0.40
1:AAA:100:ASP:OD2	1:AAA:148:THR:HA	2.21	0.40
1:AAA:100:ASP:HA	1:AAA:127:THR:O	2.21	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	Percentiles	
1	AAA	201/239 (84%)	196 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	178/208 (86%)	173 (97%)	5 (3%)	43	73

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

Mol	Chain	Res	Type
1	AAA	107	PHE
1	AAA	167	LYS
1	AAA	182	SER
1	AAA	263	ILE
1	AAA	292	LEU

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](#)

1 ligand 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	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	Q4W	AAA	401	-	21,23,23	1.30	2 (9%)	20,33,33	1.62	3 (15%)

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
2	Q4W	AAA	401	-	1/1/4/5	2/6/17/17	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	401	Q4W	C4-S1	-4.70	1.73	1.83
2	AAA	401	Q4W	C14-C13	2.48	1.46	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	401	Q4W	C2-C4-N1	6.33	121.81	113.61
2	AAA	401	Q4W	C3-C2-C4	-2.26	106.44	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	401	Q4W	C13-C14-N2	-2.00	114.78	116.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	AAA	401	Q4W	C4

All (2) torsion outliers are listed below:

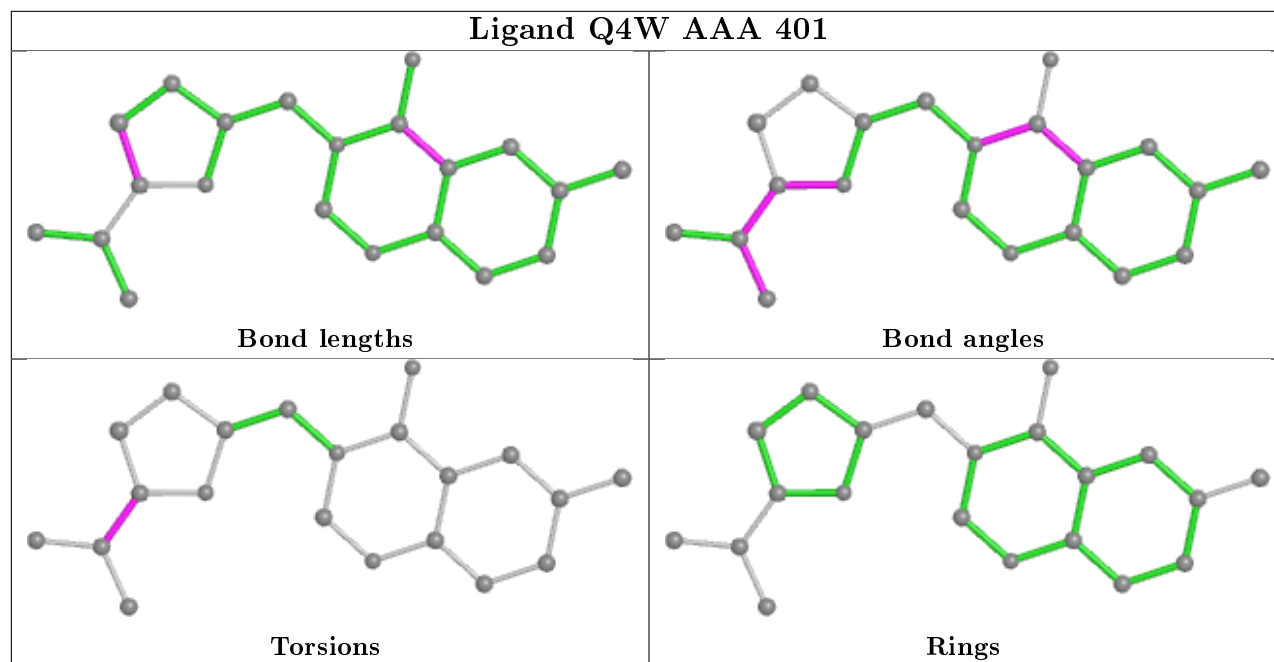
Mol	Chain	Res	Type	Atoms
2	AAA	401	Q4W	C1-C2-C4-N1
2	AAA	401	Q4W	C3-C2-C4-N1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	401	Q4W	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 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 [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<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	AAA	203/239 (84%)	0.54	12 (5%)	22 12	105, 137, 188, 246	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	108	CYS	3.7
1	AAA	251	LEU	3.4
1	AAA	115	LEU	2.9
1	AAA	183	LEU	2.7
1	AAA	169	PHE	2.6
1	AAA	236	ILE	2.5
1	AAA	216	LEU	2.4
1	AAA	269	CYS	2.2
1	AAA	227	LEU	2.1
1	AAA	237	ALA	2.1
1	AAA	232	VAL	2.1
1	AAA	254	LEU	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.

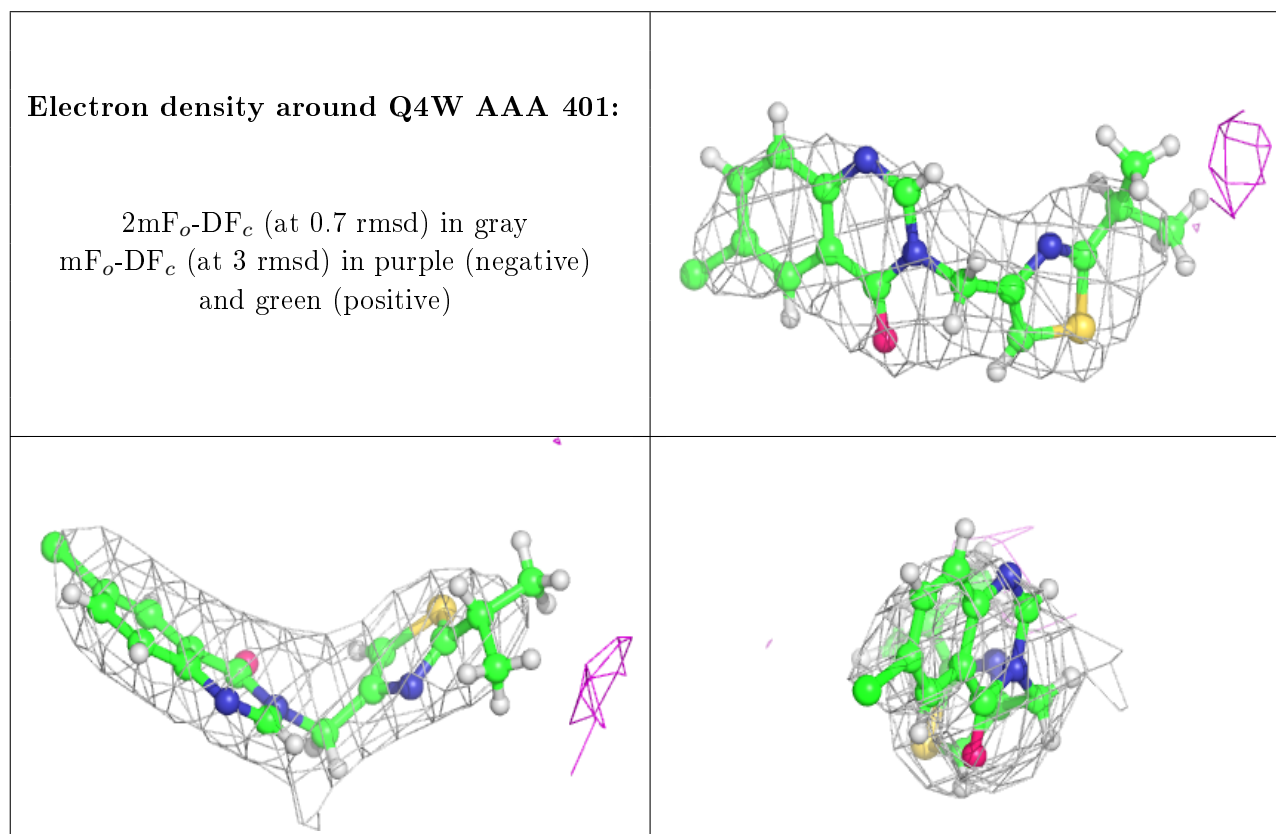
### 6.4 Ligands [i](#)

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
2	Q4W	AAA	401	21/21	0.92	0.46	110,130,146,152	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 ⓘ

There are no such residues in this entry.