

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

#### May 16, 2020 – 12:23 pm BST

PDB ID : 6MJG

Title: Structure of dbOphMA in Complex with SAH and Methylated Peptide

Authors: Ongpipattanakul, C.; Nair, S.K.

Deposited on : 2018-09-20

Resolution : 2.12 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:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.11

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)

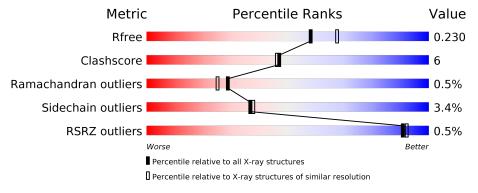
Validation Pipeline (wwPDB-VP) : 2.11

## 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 2.12 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	A	420	78%	12%	•	8%



# 2 Entry composition (i)

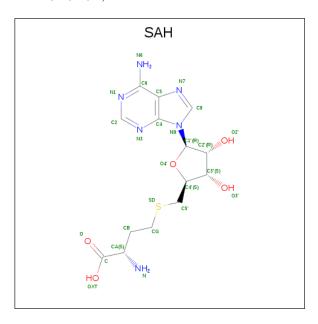
There are 4 unique types of molecules in this entry. The entry contains 3210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 fusion protein of dbOphMA and methylated peptide.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	386	Total	С	N	О	S	0	0	0
1	11	300	2996	1909	502	567	18		0	

• Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



M	ol	Chain	Residues	Atoms			ZeroOcc	AltConf		
6	2	A	1	Total 26		N 6	O 5	S 1	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

• Molecule 4 is water.



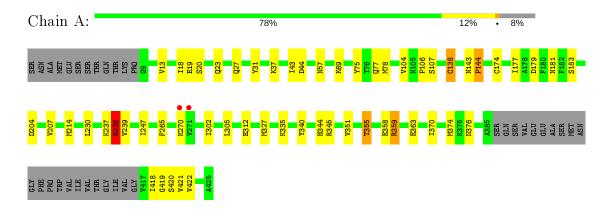
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	187	Total O 187 187	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: fusion protein of dbOphMA and methylated peptide





# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	C 2 2 21	Depositor	
Cell constants	106.41Å 107.97Å 79.34Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	_	
Resolution (Å)	25.00 - 2.12	Depositor	
` ′	54.80 - 2.12	EDS	
% Data completeness	$96.2\ (25.00 - 2.12)$	Depositor	
(in resolution range)	96.2 (54.80-2.12)	EDS	
$R_{merge}$	0.06	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.43 (at 2.12Å)	Xtriage	
Refinement program	REFMAC 5.8.0158	Depositor	
$R, R_{free}$	0.186 , $0.227$	Depositor	
10, 10 free	0.189 , $0.230$	DCC	
$R_{free}$ test set	1220 reflections $(4.84\%)$	wwPDB-VP	
Wilson B-factor $(A^2)$	34.6	Xtriage	
Anisotropy	0.692	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	$0.35 \; ,  42.2$	EDS	
L-test for twinning <sup>2</sup>	$< L > = 0.49, < L^2> = 0.32$	Xtriage	
Estimated twinning fraction	$\begin{array}{c} 0.013 \text{ for } -1/2*\text{h-}1/2*\text{k+}\text{l}, -1/2*\text{h-}1/2*\text{k-}\text{l}, 1/2 \\ *\text{h-}1/2*\text{k} \\ 0.013 \text{ for } -1/2*\text{h-}1/2*\text{k-}\text{l}, -1/2*\text{h-}1/2*\text{k+}\text{l}, -1/2 \\ 2*\text{h-}1/2*\text{k} \\ 0.011 \text{ for } -1/2*\text{h-}1/2*\text{k-}\text{l}, 1/2*\text{h-}1/2*\text{k-}\text{l}, -1/2 \\ *\text{h-}1/2*\text{k} \\ 0.000 \text{ for } -1/2*\text{h+}1/2*\text{k+}\text{l}, 1/2*\text{h-}1/2*\text{k+}\text{l}, 1 \\ /2*\text{h-}1/2*\text{k} \\ 0.027 \text{ for } -\text{k}, -\text{h}, -\text{l} \end{array}$	Xtriage	
$F_o, F_c$ correlation	0.96	EDS	
Total number of atoms	3210	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  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: MVA, ZN, SAH, IML, SAR

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).

Mal	Chain	Bond	lengths	Bo	nd angles
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5
1	A	0.52	0/3036	0.71	1/4130 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	A	238	ARG	NE-CZ-NH1	5.79	123.20	120.30

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2996	0	2962	37	0
2	A	26	0	19	1	0
3	A	1	0	0	0	0
4	A	187	0	0	1	1
All	All	3210	0	2981	37	1

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 (37) 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	${f distance}({ m \AA})$	$ m overlap~(\AA)$
1:A:78:MET:HE3	1:A:106:PRO:HG3	1.24	1.13
1:A:78:MET:CE	1:A:106:PRO:HG3	1.85	1.04
1:A:78:MET:HE3	1:A:106:PRO:CG	2.09	0.79
1:A:104:VAL:HG13	1:A:421:MVA:HG13	1.64	0.78
1:A:238:ARG:HH11	1:A:238:ARG:HG3	1.49	0.76
1:A:355:THR:HG22	1:A:358:GLU:H	1.58	0.68
1:A:20:SER:HB2	1:A:44:ASP:OD2	1.99	0.63
1:A:75:TYR:HA	1:A:78:MET:HE2	1.80	0.62
1:A:181:ASN:HD22	1:A:183:SER:H	1.45	0.62
1:A:370:ILE:HG23	1:A:374:MET:HE3	1.84	0.59
1:A:69:LYS:NZ	1:A:77:GLN:HE22	2.01	0.58
1:A:340:TYR:O	1:A:344:HIS:HD2	1.90	0.54
1:A:69:LYS:HZ1	1:A:77:GLN:HE22	1.56	0.53
1:A:238:ARG:HH11	1:A:238:ARG:CG	2.21	0.53
1:A:207:VAL:HG23	1:A:247:ILE:HD13	1.91	0.52
1:A:421:MVA:HN3	1:A:422:VAL:N	2.24	0.51
1:A:351:VAL:O	1:A:359:ARG:NH2	2.42	0.48
1:A:37:LYS:HG2	1:A:57:ASN:ND2	2.29	0.48
1:A:327:MET:HG3	1:A:374:MET:HE2	1.96	0.47
1:A:420:SER:HA	1:A:421:MVA:HN1	1.69	0.47
1:A:207:VAL:HG11	1:A:230:LEU:HD11	1.96	0.47
1:A:418:IML:HA	1:A:419:SAR:HN1	1.71	0.46
1:A:174:CYS:HA	1:A:177:ILE:HD12	1.98	0.46
1:A:302:ILE:O	1:A:305:LEU:HB2	2.16	0.45
1:A:421:MVA:CN	2:A:500:SAH:SD	3.05	0.45
1:A:327:MET:HG3	1:A:374:MET:CE	2.46	0.45
1:A:312:GLU:HG2	4:A:759:HOH:O	2.16	0.44
1:A:143:ASN:HA	1:A:144:PRO:HA	1.76	0.43
1:A:421:MVA:HN3	1:A:422:VAL:H	1.83	0.43
1:A:19:GLU:H	1:A:23:GLN:NE2	2.17	0.42
1:A:18:ILE:H	1:A:23:GLN:HE21	1.67	0.42
1:A:138:CYS:SG	1:A:138:CYS:O	2.77	0.42
1:A:43:ILE:HD11	1:A:214:MET:HE1	2.01	0.42
1:A:27:GLN:O	1:A:31:TYR:HD1	2.03	0.42
1:A:345:ARG:HA	1:A:363:GLU:HG2	2.02	0.41
1:A:78:MET:HE1	1:A:106:PRO:HG3	1.90	0.40
1:A:13:VAL:HG11	1:A:107:SER:HB2	2.04	0.40

All (1) 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	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
4:A:607:HOH:O	4:A:607:HOH:O[4_555]	1.96	0.24

## 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	A	379/420 (90%)	367 (97%)	10 (3%)	2 (0%)	29 25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	CYS
1	A	144	PRO

#### 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	A	322/351 (92%)	311 (97%)	11 (3%)	37 38	

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	${f Res}$	$\mathbf{Type}$
1	A	179	ASP
1	A	204	ASP
1	A	237	LYS
1	A	238	ARG

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	A	239	VAL
1	A	265	PHE
1	A	270	LYS
1	A	335	LYS
1	A	355	THR
1	A	359	ARG
1	A	376	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	${f Res}$	Type
1	A	23	GLN
1	A	27	GLN
1	A	77	GLN
1	A	171	GLN
1	A	181	ASN
1	A	277	GLN
1	A	344	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)

4 non-standard protein/DNA/RNA residues 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	В	ond leng	$\operatorname{gths}$	Е	ond ang	gles
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SAR	A	419	1	4,4,5	0.50	0	1,3,5	1.99	0
1	MVA	A	417	1	6,7,8	0.93	0	7,8,10	2.05	2 (28%)
1	IML	A	418	1	7,8,9	0.63	0	7,9,11	1.29	1 (14%)
1	MVA	A	421	1	6,7,8	0.96	1 (16%)	7,8,10	4.99	3 (42%)



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	SAR	A	419	1	-	1/1/2/3	-
1	MVA	A	417	1	-	1/6/8/10	_
1	IML	A	418	1	-	4/8/10/12	_
1	MVA	A	421	1	-	4/6/8/10	-

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${ m Observed}({ m \AA})$	$\mathbf{Ideal}( exttt{\AA})$
1	Α	421	MVA	CB-CA	2.07	1.57	1.54

#### All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	421	MVA	CB-CA-C	11.65	127.66	113.04
1	A	421	MVA	CG1-CB-CA	4.64	118.31	111.21
1	A	421	MVA	CG2-CB-CA	3.78	117.00	111.21
1	A	417	MVA	CG2-CB-CA	3.47	116.53	111.21
1	A	417	MVA	CB-CA-N	3.05	115.14	111.17
1	A	418	IML	CG1-CB-CA	2.03	116.22	111.17

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	418	IML	CB-CA-N-CN
1	A	421	MVA	N-CA-CB-CG2
1	A	421	MVA	C-CA-CB-CG1
1	A	421	MVA	C-CA-CB-CG2
1	A	418	IML	CA-CB-CG1-CD1
1	A	418	IML	CG2-CB-CG1-CD1
1	A	418	IML	N-CA-CB-CG1
1	A	417	MVA	CB-CA-N-CN
1	A	421	MVA	CB-CA-N-CN
1	A	419	SAR	C-CA-N-CN

There are no ring outliers.

3 monomers are involved in 6 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	419	SAR	1	0
1	A	418	IML	1	0
1	A	421	MVA	5	0

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	nd leng	ths	В	ond ang	les
	WIOI	Type	Chain	res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
	2	SAH	A	500	-	21,28,28	0.96	1 (4%)	20,40,40	1.48	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	SAH	A	500	-	_	0/7/31/31	0/3/3/3

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	Ideal(A)
2	A	500	SAH	C5-C4	2.31	1.47	1.40

#### All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
2	A	500	SAH	N3-C2-N1	-3.25	123.60	128.68
2	A	500	SAH	C4-C5-N7	-2.71	106.57	109.40

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
2	A	500	SAH	C2-N1-C6	2.39	122.83	118.75

There are no chirality outliers.

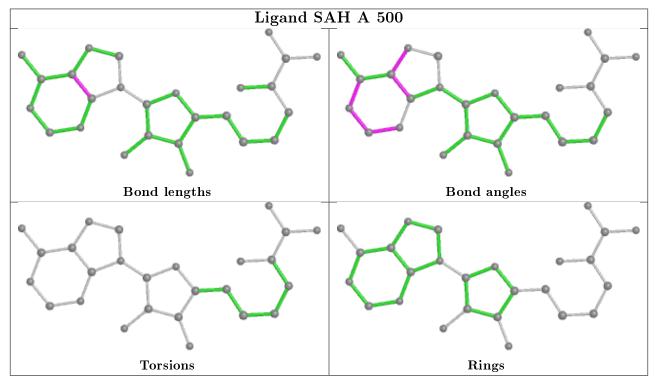
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	$\operatorname{Res}$	Type	Clashes	Symm-Clashes
2	A	500	SAH	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	Mol Chain Analysed		<rsrz></rsrz>	$\#\mathrm{RSRZ}{>}2$		$OWAB(\AA^2)$	Q < 0.9
1	A	382/420 (90%)	-0.23	2 (0%)	91 92	25, 40, 60, 89	0

All (2) RSRZ outliers are listed below:

Mol	Chain	${f Res}$	Type	RSRZ
1	A	271	VAL	5.3
1	A	270	LYS	2.2

## 6.2 Non-standard residues in protein, DNA, RNA chains (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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	MVA	A	417	8/9	0.90	0.15	50,54,57,59	0
1	MVA	A	421	8/9	0.94	0.15	38,41,43,44	0
1	IML	A	418	9/10	0.95	0.14	47,49,51,52	0
1	SAR	A	419	5/6	0.97	0.13	41,44,45,46	0

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

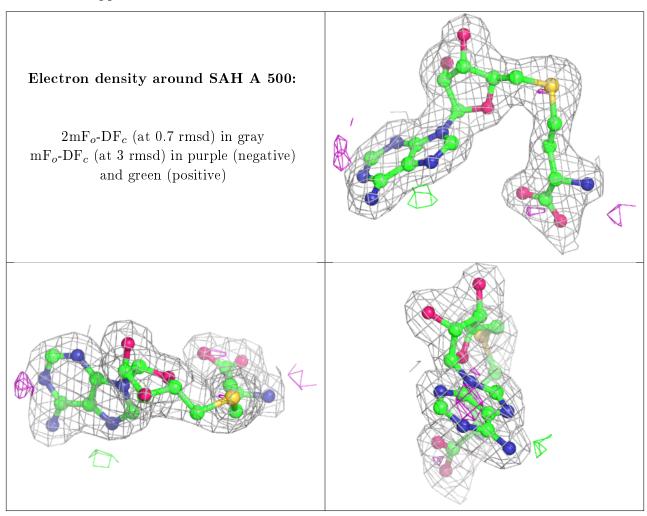
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



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	${f B-factors(\AA^2)}$	Q < 0.9
2	SAH	A	500	26/26	0.98	0.09	26,28,33,34	0
3	ZN	A	501	1/1	0.99	0.35	63,63,63,63	1

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.

