

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

#### Jul 21, 2022 - 01:37 AM JST

PDB ID	:	7EEW
Title	:	Crystal structure of the intact MTase from Vibrio vulnificus YJ016 in complex
		with the DNA-mimicking Ocr protein and the S-adenosyl-L-homocysteine
		(SAH)
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Deposited on	:	2021-03-19
Resolution	:	2.90 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	?.? (???), CSD ??CSD?? (????)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

# 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 2.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 >=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%

Mol	Chain	Length	Quality of chain		
1	А	638	68%	24%	•••
2	В	117	65%	26%	• 6%



#### $7 \mathrm{EEW}$

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5829 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 Type I restriction-modification system methyltransferase subunit.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	610	Total 4840	C 3094	N 805	0 924	S 17	0	0	0

• Molecule 2 is a protein called Overcome classical restriction gp0.3.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	110	Total 903	C 565	N 141	0 191	S 6	0	0	0

• Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ato	$\mathbf{ms}$			ZeroOcc	AltConf
3	А	1	Total 26	C 14	N 6	O 5	S 1	0	0



• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0
4	В	6	Total O 6 6	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. 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. 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: Type I restriction-modification system methyltransferase subunit

 $\bullet$  Molecule 2: Overcome classical restriction gp0.3





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants	133.28Å 133.28Å 236.81Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Bosolution(A)	14.96 - 2.90	Depositor
Resolution (A)	14.96 - 2.90	EDS
% Data completeness	93.9 (14.96-2.90)	Depositor
(in resolution range)	93.9(14.96-2.90)	EDS
$R_{merge}$	0.19	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.95 (at 2.91 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
B B.	0.272 , $0.293$	Depositor
$n, n_{free}$	0.272 , $0.293$	DCC
$R_{free}$ test set	1312 reflections $(4.96\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	58.4	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.16 , -10.0	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.36, < L^2>=0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	5829	wwPDB-VP
Average B, all atoms $(Å^2)$	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.33% 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: SAH

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	Bond angles		
WIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.24	0/4929	0.42	0/6654	
2	В	0.23	0/920	0.37	0/1249	
All	All	0.24	0/5849	0.41	0/7903	

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	4840	0	4861	79	1
2	В	903	0	825	17	0
3	А	26	0	19	5	0
4	А	54	0	0	1	0
4	В	6	0	0	0	0
All	All	5829	0	5705	95	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 8.

All (95) 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:309:LEU:HB2	1.A.416.LEU.HB2	1.67	0.76
1:A:175:LEU:O	$1 \cdot A \cdot 299 \cdot ABG \cdot NH2$	2.19	0.75
1:A:310:PHE:O	1:A:320:LYS:NZ	2.23	0.71
1:A:51:ILE:HD11	1·A·86·ASN·HD22	1.60	0.66
1·A·340·LEU·HD13	1.A.348.VAL:HG21	1.80	0.64
1:A:215:ASN:HD21	1:A:242:SEB:HB3	1.60	0.64
1.A.155.SEB.O	4·A·801·HOH·O	2.15	0.63
1:A:216:ASP:OD2	3:A:700:SAH:O3'	2.18	0.61
2·B·26·ASP·O	2·B·28·ILE·N	2.36	0.59
1:A:19:ASN:HD21	1:A:22:ILE:HG13	1.67	0.59
1:A:189:GLY:HA3	3:A:700:SAH:HA	1.85	0.58
1.A.334.SEB.HB3	1·A·366·GLU·HA	1.85	0.58
1:A:71:ILE:HG13	1:A:121:THR:HG22	1.84	0.58
1:A:470:LEU:HD12	1:A:585:VAL:HB	1.86	0.57
1:A:371:LYS:HD3	1:A:372:PRO:HD2	1.86	0.57
2·B·23·ILE·HA	$2 \cdot B \cdot 28 \cdot ILE \cdot HD11$	1.86	0.57
1:A:35:ABG:HD2	1·A·131·LEU·HB3	1.88	0.55
1:A:54:PHE:HB2	1:A:57:LEU:HD12	1.89	0.55
1:A:186:PRO:HD2	1:A:258:SEB:HB2	1.88	0.53
1:A:263:GLY:HA2	1:A:282:LEU:H	1.72	0.54
2:B:56:VAL:HG11	2:B:86:ILE:HD12	1.89	0.53
1:A:509:ASN:HB2	1:A:535:TRP:CD1	2 44	0.53
2:B:57:MET:HG3	2:B:82:LEU:HD13	1.90	0.53
1:A:431:LYS:HG2	1:A:432:GLN:H	1.74	0.53
1:A:160:ALA:O	3:A:700:SAH:H5'1	2.09	0.52
1:A:361:ASP:O	1·A·394·ABG·NH2	2 41	0.52
2:B:73:PRO:HB2	2:B:75:THB:HG22	1.91	0.52
2:B:100:ASP:0	2·B·104·GLU·HG3	2 09	0.52
1.A.290.THB.HG21	1:A:302:ILE:HG12	1.92	0.52
1:A:520:VAL:HG23	1:A:576:PHE:HD1	1.75	0.52
1:A:7:ASN:HB3	1:A:130:ARG:HH21	1.76	0.51
1:A:177:PRO:HD2	1:A:200:HIS:CD2	2.46	0.51
2:B:29:ARG:HH22	2:B:109:VAL:HG11	1.76	0.51
1:A:58:PHE:HA	1:A:61:LEU:HD12	1.93	0.50
1:A:324:LEU:HD23	1:A:409:LEU:HD23	1.94	0.50
2:B:11:VAL:HG11	2:B:86:ILE:HD11	1.94	0.50
1:A:71:ILE:HD11	1:A:121:THR:HA	1.94	0.49
1:A:283:GLU·HG3	1:A:308:ILE·HG12	1.93	0.49
1:A:478:SEB:HA	1:A:541:MET:HA	1.94	0.49
1:A:556:LEU:HA	1.A.559.VAL.HG12	1.93	0.49
1:A:551:VAL:HG12	1:A:589:LEU·HG	1.95	0.49
1·A·381·ASP·OD1	1.A.381.ASP.N	2 41	0.49



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:448:SER:HB3	1:A:612:ILE:HD11	1.95	0.49	
1:A:299:ARG:HA	1:A:354:ASP:HA	1.95	0.48	
1:A:304:ILE:HB	1:A:308:ILE:HD11	1.95	0.48	
1:A:367:LEU:HD11	1:A:383:ASP:HB3	1.95	0.48	
1:A:374:SER:OG	1:A:375:LYS:N	2.46	0.48	
1:A:187:ALA:O	3:A:700:SAH:N	2.46	0.48	
1:A:5:LEU:HD21	1:A:140:ILE:HD11	1.96	0.47	
1:A:390:LEU:HD13	1:A:396:VAL:HG21	1.95	0.47	
2:B:7:THR:OG1	2:B:8:TYR:N	2.47	0.47	
1:A:337:LYS:HA	1:A:338:GLY:HA2	1.53	0.47	
1:A:30:LEU:HD22	1:A:114:ILE:HG22	1.97	0.47	
1:A:35:ARG:HE	1:A:132:GLU:HA	1.80	0.46	
1:A:145:ASP:OD1	1:A:146:HIS:N	2.49	0.46	
1:A:161:TYR:HA	3:A:700:SAH:H5'1	1.97	0.46	
1:A:19:ASN:O	1:A:23:ASP:HB2	2.15	0.46	
1:A:278:TYR:HE2	1:A:319:LEU:HD12	1.80	0.46	
1:A:601:TRP:O	1:A:605:ILE:HG22	2.15	0.46	
1:A:45:ILE:HG21	1:A:87:CYS:HA	1.99	0.45	
2:B:20:LYS:HG2	2:B:101:LEU:HD21	1.98	0.45	
1:A:8:ILE:HG23	1:A:127:VAL:HG23	1.98	0.45	
1:A:536:LEU:HD22	1:A:542:SER:HB3	1.98	0.45	
1:A:446:VAL:HA	1:A:449:ILE:HG12	2.00	0.44	
1:A:101:ARG:N	1:A:101:ARG:HD2	2.32	0.44	
1:A:519:LYS:NZ	1:A:541:MET:SD	2.89	0.43	
1:A:58:PHE:HB2	1:A:76:LEU:HB2	2.00	0.43	
1:A:370:ASN:N	1:A:370:ASN:OD1	2.51	0.43	
2:B:104:GLU:HG3	2:B:104:GLU:H	1.67	0.43	
1:A:263:GLY:CA	1:A:282:LEU:H	2.32	0.43	
1:A:505:ASN:OD1	1:A:506:VAL:N	2.51	0.43	
1:A:175:LEU:HD12	1:A:255:PHE:CE2	2.53	0.43	
1:A:183:VAL:HA	1:A:255:PHE:HB2	2.01	0.43	
1:A:582:LEU:HD23	1:A:582:LEU:HA	1.87	0.42	
1:A:558:HIS:CD2	1:A:602:PHE:HB3	2.55	0.42	
1:A:569:ALA:HB2	1:A:577:ILE:HG13	2.01	0.42	
1:A:19:ASN:ND2	1:A:22:ILE:HG13	2.33	0.42	
1:A:628:THR:O	1:A:632:THR:HG23	2.20	0.42	
1:A:81:ASN:O	1:A:85:VAL:HG23	2.19	0.42	
1:A:493:PHE:HB3	1:A:505:ASN:O	2.19	0.42	
1:A:493:PHE:CE1	1:A:508:PRO:HB3	2.55	0.42	
1:A:42:SER:O	1:A:46:SER:HB2	2.20	0.42	
2:B:83:GLN:HA	2:B:86:ILE:HG22	2.02	0.41	



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:459:ASN:O	1:A:459:ASN:ND2	2.53	0.41
1:A:552:TYR:CE2	1:A:596:ARG:HG2	2.56	0.41
1:A:15:ASP:OD2	1:A:119:ARG:HG3	2.19	0.41
1:A:165:ARG:N	1:A:166:PRO:HD2	2.36	0.41
1:A:476:LEU:HD21	1:A:543:LEU:HD12	2.02	0.41
1:A:574:GLN:HG3	2:B:87:TYR:CD2	2.55	0.41
2:B:40:MET:O	2:B:44:ASN:ND2	2.53	0.41
1:A:445:LEU:HD13	1:A:449:ILE:HD13	2.02	0.41
2:B:29:ARG:HG3	2:B:106:LEU:HD11	2.03	0.41
2:B:4:SER:HB3	2:B:55:SER:OG	2.21	0.40
1:A:329:LEU:O	1:A:362:ILE:HG12	2.22	0.40
2:B:2:ALA:O	2:B:4:SER:N	2.53	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:TYR:OH	1:A:489:ASP:OD2[6_554]	2.15	0.05

#### Torsion angles (i) 5.3

#### 5.3.1Protein 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	600/638~(94%)	551 (92%)	43 (7%)	6 (1%)	15 45
2	В	108/117~(92%)	105~(97%)	1 (1%)	2(2%)	8 28
All	All	708/755~(94%)	656 (93%)	44 (6%)	8 (1%)	14 42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type	
1	А	473	ILE	
Continued on next page				



Continued from previous page...

Mol	Chain	Res	Type
1	А	590	PRO
2	В	27	ASP
1	А	341	ALA
1	А	398	GLU
1	А	261	PRO
2	В	28	ILE
1	А	18	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	548/573~(96%)	484 (88%)	64 (12%)	5	16
2	В	98/105~(93%)	88 (90%)	10 (10%)	7	22
All	All	646/678~(95%)	572~(88%)	74 (12%)	5	17

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	22	ILE
1	А	43	ASN
1	А	51	ILE
1	А	52	ASP
1	А	55	LYS
1	А	58	PHE
1	А	61	LEU
1	А	70	VAL
1	А	72	ASP
1	А	74	TYR
1	А	76	LEU
1	А	77	ARG
1	А	80	LEU
1	А	99	PHE
1	А	101	ARG
1	А	132	GLU



Mol	Chain	Res	Type
1	А	161	TYR
1	А	167	LEU
1	А	175	LEU
1	А	180	LEU
1	А	188	MET
1	А	217	LEU
1	А	249	ASP
1	А	272	GLU
1	А	287	LEU
1	А	293	LYS
1	А	299	ARG
1	А	319	LEU
1	А	346	VAL
1	A	348	VAL
1	A	370	ASN
1	A	371	LYS
1	А	373	LEU
1	А	376	VAL
1	А	386	ASP
1	А	395	GLU
1	А	396	VAL
1	А	398	GLU
1	А	409	LEU
1	А	415	ASN
1	А	433	GLU
1	А	435	ILE
1	А	443	LEU
1	А	445	LEU
1	A	453	PHE
1	A	460	LEU
1	A	461	GLU
1	A	472	ASP
1	A	486	GLU
1	A	493	PHE
1	A	510	ARG
1	A	511	HIS
1	A	516	VAL
1	A	537	THR
1	A	546	LEU
1	A	566	ASN
1	А	582	LEU
1	А	587	VAL



Mol	Chain	Res	Type
1	А	589	LEU
1	А	594	LYS
1	А	600	GLU
1	А	605	ILE
1	А	607	GLU
1	А	628	THR
2	В	7	THR
2	В	32	ASP
2	В	35	HIS
2	В	36	ASP
2	В	40	MET
2	В	63	ASP
2	В	64	LEU
2	В	78	VAL
2	В	104	GLU
2	В	108	GLU

Sometimes 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)

ligand is modelled in this entry.
 There are no bond length outliers.
 There are no bond angle outliers.
 There are no chirality outliers.



There are no torsion outliers.

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 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

