



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:55 AM GMT

PDB ID : 3NTA  
Title : Structure of the Shewanella loihica PV-4 NADH-dependent persulfide reductase  
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Deposited on : 2010-07-03  
Resolution : 2.01 Å(reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

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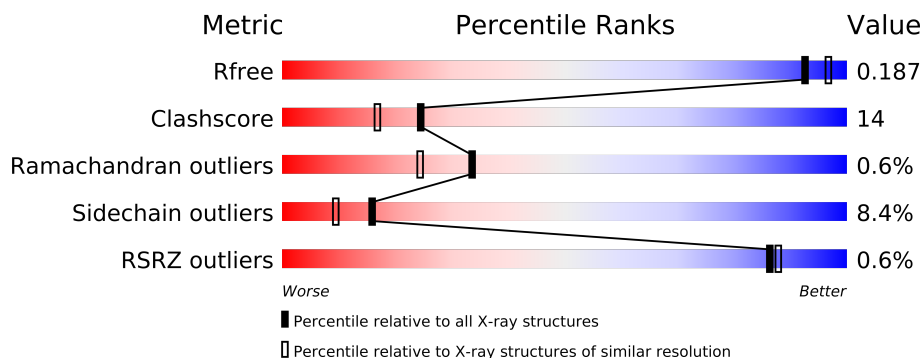
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.01 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	574	
1	B	574	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9344 atoms, of which 0 are hydrogen and 0 are deuterium.

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 FAD-dependent pyridine nucleotide-disulphideoxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	Se	0	1	0
			4301	2698	762	821	4	16			
1	B	565	Total	C	N	O	S	Se	0	0	0
			4294	2694	763	818	4	15			

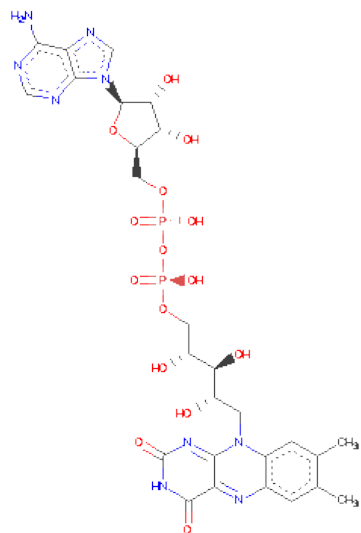
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	567	LEU	-	EXPRESSION TAG	UNP A3QAV3
A	568	GLU	-	EXPRESSION TAG	UNP A3QAV3
A	569	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	570	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	571	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	572	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	573	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	574	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	567	LEU	-	EXPRESSION TAG	UNP A3QAV3
B	568	GLU	-	EXPRESSION TAG	UNP A3QAV3
B	569	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	570	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	571	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	572	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	573	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	574	HIS	-	EXPRESSION TAG	UNP A3QAV3

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

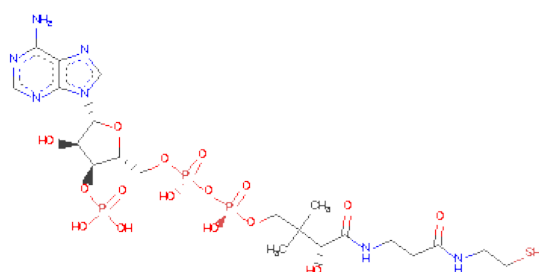
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
4	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	264	Total 264	O 264	0	0
5	B	281	Total 281	O 281	0	0



SE46	SE47	SE48	Y549	SE55	VAL	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.34Å 134.34Å 81.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	116.37 – 2.01 40.62 – 2.01	Depositor EDS
% Data completeness (in resolution range)	97.8 (116.37-2.01) 98.7 (40.62-2.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.137 , 0.173 0.167 , 0.187	Depositor DCC
$R_{free}$ test set	5481 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.9	EDS
Estimated twinning fraction	0.479 for H, K, L 0.521 for H, -H-K, -L 0.012 for -h,-k,l 0.018 for h,-h-k,-l 0.008 for -k,-h,-l	Xtriage
Reported twinning fraction	0.479 for H, K, L 0.521 for H, -H-K, -L	Depositor
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 108118 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: COA, FAD, CL

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	1.60	34/4359 (0.8%)	1.34	51/5877 (0.9%)
1	B	1.55	21/4349 (0.5%)	1.32	42/5863 (0.7%)
All	All	1.58	55/8708 (0.6%)	1.33	93/11740 (0.8%)

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	378	VAL	CB-CG2	-6.77	1.38	1.52
1	A	306	GLU	CD-OE2	-6.49	1.18	1.25
1	B	154	ALA	CA-CB	5.96	1.65	1.52
1	A	47	TYR	CE1-CZ	-5.90	1.30	1.38
1	A	107	ASP	CB-CG	5.89	1.64	1.51

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	ASP	CB-CG-OD1	-14.59	105.17	118.30
1	A	138	ASP	CB-CG-OD1	-12.34	107.20	118.30
1	B	257	ASP	CB-CG-OD1	-11.32	108.11	118.30
1	B	191	ASP	CB-CG-OD1	-10.42	108.92	118.30
1	B	138	ASP	CB-CG-OD1	-9.55	109.71	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4301	0	4303	120	1
1	B	4294	0	4300	133	1
2	A	1	0	0	1	0
2	B	1	0	0	2	0
3	A	53	0	31	6	0
3	B	53	0	31	3	0
4	A	48	0	32	3	0
4	B	48	0	32	4	0
5	A	264	0	0	4	0
5	B	281	0	0	13	0
All	All	9344	0	8729	246	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 246 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:290:MSE:HE3	1:A:339:GLU:HA	1.17	1.14
1:A:475:ILE:HG23	1:A:552:ARG:HD3	1.31	1.11
1:A:474:PRO:HB3	1:A:555:ILE:HD11	1.34	1.10
1:B:243:HIS:CE1	1:B:255:GLU:HG3	1.93	1.03
1:B:243:HIS:HE1	1:B:255:GLU:HG3	1.24	1.01

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	Distance(Å)	Clash(Å)
1:A:482:ASN:OD1	1:B:482:ASN:ND2[1_554]	2.15	0.05

## 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	564/574 (98%)	537 (95%)	24 (4%)	3 (0%)	38	29
1	B	563/574 (98%)	535 (95%)	24 (4%)	4 (1%)	30	20
All	All	1127/1148 (98%)	1072 (95%)	48 (4%)	7 (1%)	33	24

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	MSE
1	B	10	VAL
1	B	482	ASN
1	A	10	VAL
1	A	294	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	450/443 (102%)	416 (92%)	34 (8%)	19	12
1	B	449/443 (101%)	408 (91%)	41 (9%)	14	8
All	All	899/886 (102%)	824 (92%)	75 (8%)	16	10

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	ASP
1	B	98	ASP
1	B	482	ASN
1	B	34	ARG
1	B	67	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	543	GLN
1	A	547	ASN
1	B	440	GLN

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Mol	Chain	Res	Type
1	A	546	ASN
1	B	62	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	FAD	A	900	-	58,58,58	1.46	9 (15%)	85,89,89	1.90	18 (21%)
4	COA	A	901	-	50,50,50	1.62	8 (16%)	75,75,75	2.10	18 (24%)
3	FAD	B	900	-	58,58,58	1.54	9 (15%)	85,89,89	2.27	22 (25%)
4	COA	B	901	-	50,50,50	1.58	7 (14%)	75,75,75	2.30	22 (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	FAD	A	900	-	-	0/34/50/50	0/1/6/6
4	COA	A	901	-	-	0/48/64/64	0/1/3/3
3	FAD	B	900	-	-	0/34/50/50	0/1/6/6
4	COA	B	901	-	-	0/48/64/64	0/1/3/3

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	COA	O9P-C9P	5.98	1.35	1.23
3	B	900	FAD	C5X-N5	5.89	1.44	1.35
4	B	901	COA	O9P-C9P	5.18	1.33	1.23
4	B	901	COA	CBP-CAP	4.37	1.60	1.55
3	B	900	FAD	C1'-C2'	4.19	1.55	1.51

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	COA	N3A-C2A-N1A	-12.93	117.90	128.71
4	A	901	COA	N3A-C2A-N1A	-10.98	119.53	128.71
3	B	900	FAD	N3A-C2A-N1A	-10.71	119.76	128.71
3	A	900	FAD	N3A-C2A-N1A	-9.18	121.03	128.71
3	B	900	FAD	C2-N1-C10	6.38	121.41	114.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	565/574 (98%)	-0.32	5 (0%)	81 82	26, 36, 54, 73	0
1	B	565/574 (98%)	-0.31	2 (0%)	90 91	27, 36, 52, 66	0
All	All	1130/1148 (98%)	-0.31	7 (0%)	86 88	26, 36, 53, 73	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	LEU	3.0
1	A	499	GLN	2.6
1	B	342	TYR	2.6
1	A	475	ILE	2.6
1	A	10	VAL	2.4

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

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	575	1/1	0.12	1.49	57,57,57,57	0
4	COA	A	901	48/48	0.14	0.32	29,34,39,54	0
4	COA	B	901	48/48	0.14	0.25	24,35,42,55	0
3	FAD	B	900	53/53	0.12	0.03	24,32,36,37	0
2	CL	B	575	1/1	0.12	0.00	53,53,53,53	0
3	FAD	A	900	53/53	0.11	-0.25	27,33,39,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.