Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:07 pm BST

PDB ID	:	5I5J
Title	:	Shewanella denitrificans nitrous oxide reductase, reduced apo form
Authors	:	Schneider, L.K.; Einsle, O.
Deposited on	:	2016-02-15
Resolution	:	2.55 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 ⓘ symbol.

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

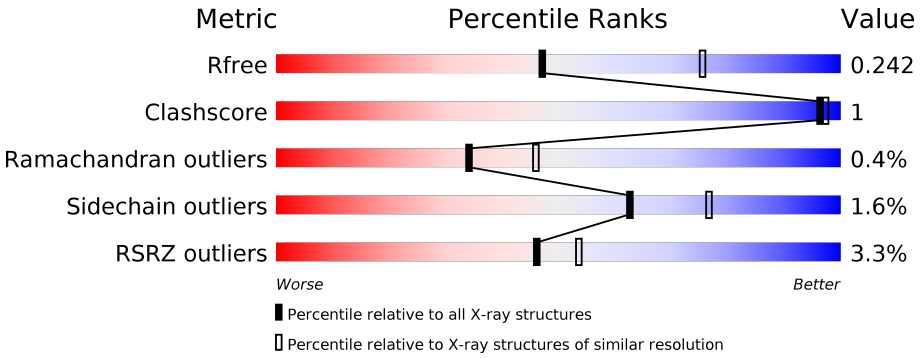
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	636	2% 79% 17%
1	B	636	4% 79% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8450 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 Nitrous-oxide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	2	0
			4193	2648	734	784	27			
1	B	529	Total	C	N	O	S	0	1	0
			4169	2635	728	779	27			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	629	LEU	-	expression tag	UNP Q12M27
A	630	GLU	-	expression tag	UNP Q12M27
A	631	HIS	-	expression tag	UNP Q12M27
A	632	HIS	-	expression tag	UNP Q12M27
A	633	HIS	-	expression tag	UNP Q12M27
A	634	HIS	-	expression tag	UNP Q12M27
A	635	HIS	-	expression tag	UNP Q12M27
A	636	HIS	-	expression tag	UNP Q12M27
B	629	LEU	-	expression tag	UNP Q12M27
B	630	GLU	-	expression tag	UNP Q12M27
B	631	HIS	-	expression tag	UNP Q12M27
B	632	HIS	-	expression tag	UNP Q12M27
B	633	HIS	-	expression tag	UNP Q12M27
B	634	HIS	-	expression tag	UNP Q12M27
B	635	HIS	-	expression tag	UNP Q12M27
B	636	HIS	-	expression tag	UNP Q12M27

- Molecule 2 is water.

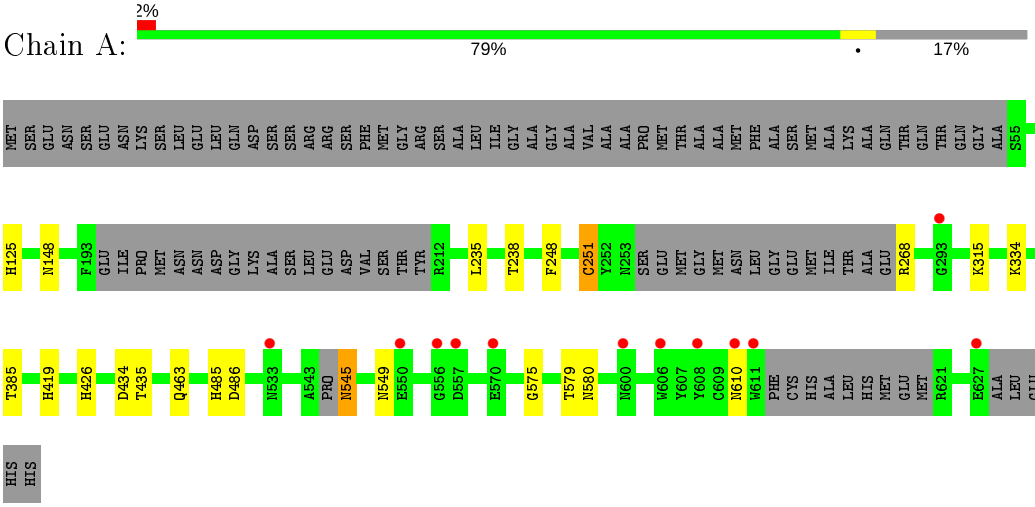
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	59	Total	O	0	0
			59	59		
2	B	29	Total	O	0	0
			29	29		

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.

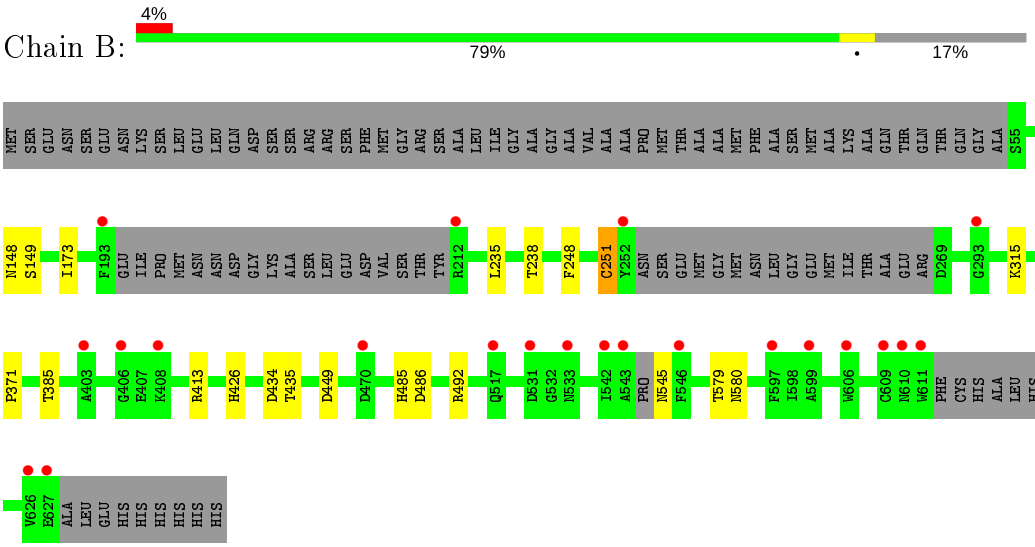
- Molecule 1: Nitrous-oxide reductase

Chain A:



- Molecule 1: Nitrous-oxide reductase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.10Å 121.46Å 172.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.29 – 2.55 70.30 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.29-2.55) 100.0 (70.30-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.188 , 0.228 0.215 , 0.242	Depositor DCC
R_{free} test set	1964 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 25.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8450	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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.

5 Model quality

5.1 Standard geometry

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	0.53	0/4293	0.75	3/5809 (0.1%)
1	B	0.51	0/4266	0.73	3/5773 (0.1%)
All	All	0.52	0/8559	0.74	6/11582 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	358	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	A	111	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	449	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	413	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	492	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4193	0	4108	10	0
1	B	4169	0	4085	9	0
2	A	59	0	0	0	0
2	B	29	0	0	0	0
All	All	8450	0	8193	17	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 1.

All (17) 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:125:HIS:CD2	1:A:485:HIS:HB2	2.28	0.67
1:A:426[B]:HIS:CE1	1:A:486:ASP:OD1	2.53	0.62
1:B:426[B]:HIS:NE2	1:B:486:ASP:OD1	2.36	0.58
1:A:419:HIS:HD2	1:A:463:GLN:HE22	1.63	0.46
1:A:235:LEU:HD23	1:A:251:CYS:HB2	1.98	0.46
1:B:235:LEU:HD23	1:B:251:CYS:HB2	1.97	0.46
1:A:580:ASN:HD22	1:B:148:ASN:HA	1.83	0.44
1:A:148:ASN:HA	1:B:580:ASN:HD22	1.82	0.44
1:B:426[B]:HIS:CE1	1:B:486:ASP:OD1	2.71	0.43
1:A:434:ASP:O	1:A:435:THR:C	2.57	0.43
1:B:125:HIS:ND1	1:B:485:HIS:HB2	2.35	0.42
1:A:371:PRO:HA	1:A:385:THR:O	2.20	0.41
1:A:575:GLY:HA3	1:A:610:ASN:OD1	2.20	0.41
1:B:371:PRO:HA	1:B:385:THR:O	2.21	0.41
1:B:149:SER:HA	1:B:173:ILE:HG12	2.02	0.41
1:A:545:ASN:N	1:A:545:ASN:OD1	2.53	0.40
1:B:434:ASP:O	1:B:435:THR:C	2.60	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	A	523/636 (82%)	502 (96%)	19 (4%)	2 (0%)	34	46
1	B	520/636 (82%)	500 (96%)	18 (4%)	2 (0%)	34	46
All	All	1043/1272 (82%)	1002 (96%)	37 (4%)	4 (0%)	34	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	LYS
1	B	315	LYS
1	A	334	LYS
1	B	334	LYS

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	460/541 (85%)	452 (98%)	8 (2%)	60	75
1	B	457/541 (84%)	450 (98%)	7 (2%)	65	77
All	All	917/1082 (85%)	902 (98%)	15 (2%)	62	77

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	TRP
1	A	238	THR
1	A	248	PHE
1	A	251	CYS
1	A	268	ARG
1	A	545	ASN
1	A	549	ASN
1	A	579	THR
1	B	70	TRP
1	B	238	THR
1	B	248	PHE
1	B	251	CYS
1	B	358	ARG
1	B	545	ASN
1	B	579	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	125	HIS
1	A	419	HIS
1	A	545	ASN
1	B	580	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{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	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	531/636 (83%)	0.33	12 (2%)	60	67	22, 36, 58, 86	0
1	B	529/636 (83%)	0.38	23 (4%)	35	42	25, 37, 57, 95	0
All	All	1060/1272 (83%)	0.36	35 (3%)	46	53	22, 36, 59, 95	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	GLY	5.9
1	B	543	ALA	5.2
1	B	611	TRP	3.9
1	B	408	LYS	3.6
1	A	610	ASN	3.5
1	B	533	ASN	3.4
1	A	557	ASP	3.1
1	B	293	GLY	3.1
1	B	609	CYS	3.1
1	B	606	TRP	3.0
1	B	610	ASN	2.9
1	A	533	ASN	2.9
1	B	531	ASP	2.8
1	B	599	ALA	2.7
1	B	406	GLY	2.7
1	A	627	GLU	2.6
1	A	570	GLU	2.6
1	B	212	ARG	2.6
1	A	611	TRP	2.5
1	B	193	PHE	2.5
1	B	358	ARG	2.4
1	B	252	TYR	2.3
1	A	556	GLY	2.2
1	B	627	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	608	TYR	2.2
1	A	600	ASN	2.2
1	B	470	ASP	2.2
1	B	542	ILE	2.2
1	B	597	PHE	2.1
1	B	626	VAL	2.1
1	B	403	ALA	2.1
1	B	517	GLN	2.1
1	A	606	TRP	2.1
1	A	550	GLU	2.0
1	B	546	PHE	2.0

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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.