W O R L D W I D E

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wwPDB X-ray Structure Validation Summary Report (i)

Mar 1, 2014 – 12:18 AM GMT

PDB ID	:	1WUK
Title	:	High resolution Structure Of The Oxidized State Of [Nife]Hydrogenase From Desulufovibrio Vulgaris Miyazaki F
Authors	:	Ogata, H.; Hirota, S.; Nakahara, A.; Komori, H.; Shibata, N.; Kato, T.; Kano, K.; Higuchi, Y.
Deposited on	:	2004-12-07
Resolution	:	1.10 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
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 1.10 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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.3%
Sidechain outliers		2.5%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
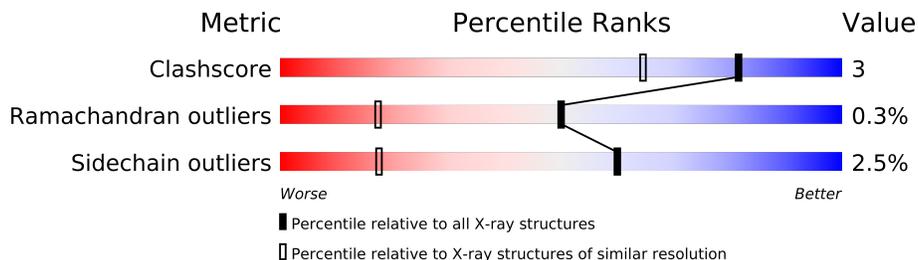
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1559 (1.20-1.00)
Ramachandran outliers	78287	1474 (1.20-1.00)
Sidechain outliers	78261	1472 (1.20-1.00)

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 >=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	S	267	
2	L	534	

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 7122 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 Periplasmic [NiFe] hydrogenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	S	267	2022	1284	342	378	18	0	3	0

- Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	534	4187	2681	726	765	15	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	514	LYS	ASN	SEE REMARK 999	UNP P21852
L	515	LEU	VAL	SEE REMARK 999	UNP P21852

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	L	1	1	1	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).
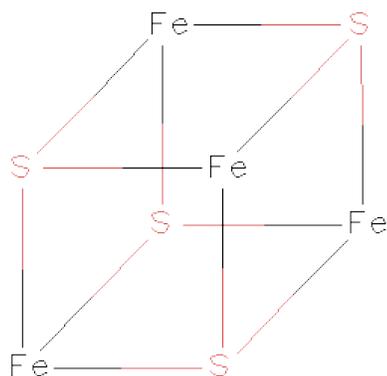
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total 8	Fe 4	S 4	0	0
4	S	1	Total 8	Fe 4	S 4	0	0

- Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).
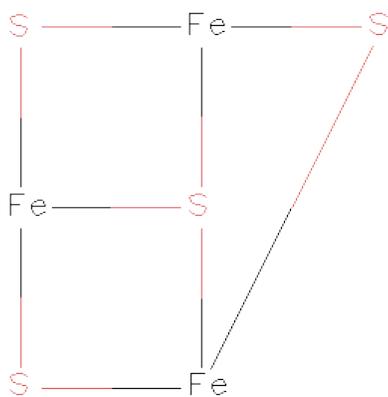
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total 7	Fe 3	S 4	0	0

- Molecule 6 is NI-FE OXIDIZED ACTIVE CENTER (three-letter code: NFO) (formula:

$C_3H_2FeNNiO_3$).
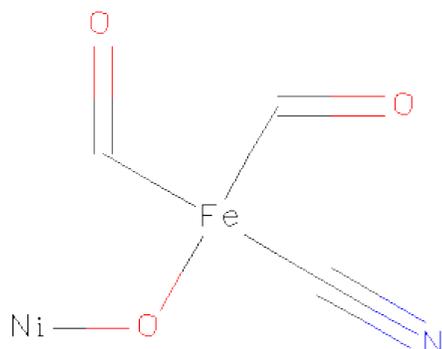
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	N	Ni	O		
6	L	1	9	3	1	1	1	3	0	0

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).
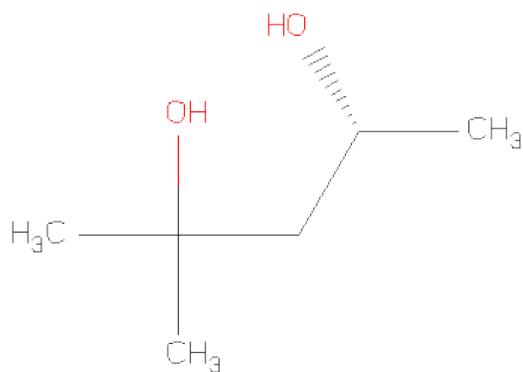
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	S	1	8	6	2	0	0

- Molecule 8 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	570	Total O 570 570	0	0
8	S	302	Total O 302 302	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: Periplasmic [NiFe] hydrogenase small subunit

Chain S:
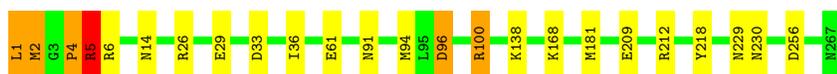
• Molecule 2: Periplasmic [NiFe] hydrogenase large subunit

Chain L:
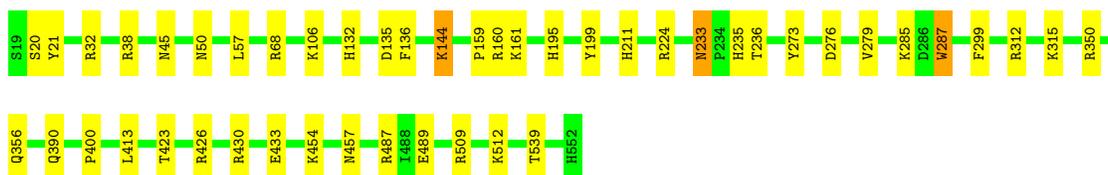
4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.29Å 125.84Å 66.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.094 , 0.123	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7122	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NFO, SF4, CSO, F3S, MRD

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	S	0.82	0/2099	1.32	24/2862 (0.8%)
2	L	0.78	1/4302 (0.0%)	1.21	35/5848 (0.6%)
All	All	0.79	1/6401 (0.0%)	1.24	59/8710 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	509	ARG	CZ-NH2	-5.99	1.25	1.33

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	224	ARG	NE-CZ-NH2	17.47	129.04	120.30
1	S	100	ARG	CD-NE-CZ	16.86	147.20	123.60
1	S	1	LEU	O-C-N	14.98	146.67	122.70
1	S	2	MET	C-N-CA	14.03	151.76	122.30
1	S	209	GLU	OE1-CD-OE2	-9.91	111.40	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	4	PRO	Peptide

5.2 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 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	S	2022	0	0	4	0
2	L	4187	0	0	16	0
3	L	1	0	0	0	0
4	S	16	0	0	0	0
5	S	7	0	0	0	0
6	L	9	0	0	0	0
7	S	8	0	0	0	0
8	L	570	0	0	11	0
8	S	302	0	0	5	0
All	All	7122	0	0	20	0

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 3.

The worst 5 of 20 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:539:THR:N	8:L:5622:HOH:O	2.34	0.61
2:L:287:TRP:CZ3	8:L:5622:HOH:O	2.52	0.60
8:S:5589:HOH:O	2:L:57:LEU:CD1	2.58	0.51
2:L:390:GLN:CA	8:L:5636:HOH:O	2.59	0.49
1:S:29:GLU:N	8:S:5658:HOH:O	2.46	0.48

There are no symmetry-related clashes.

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	S	268/267 (100%)	261 (97%)	5 (2%)	2 (1%)	30	5
2	L	533/534 (100%)	518 (97%)	15 (3%)	0	100	100
All	All	801/801 (100%)	779 (97%)	20 (2%)	2 (0%)	50	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	5	ARG
1	S	4	PRO

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	S	216/213 (101%)	207 (96%)	9 (4%)	40	6
2	L	439/437 (100%)	432 (98%)	7 (2%)	75	38
All	All	655/650 (101%)	639 (98%)	16 (2%)	60	19

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	229	ASN
1	S	230	ASN
2	L	161	LYS
1	S	168	LYS
2	L	233	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA   ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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	CSO	L	546	2,6	6,6,7	7.39	4 (66%)	3,6,8	4.54	1 (33%)

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	CSO	L	546	2,6	-	0/2/5/7	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	546	CSO	O-C	16.80	1.23	1.11
2	L	546	CSO	CB-SG	-4.84	1.76	1.82
2	L	546	CSO	OD-SG	-3.85	1.46	1.62
2	L	546	CSO	CA-C	2.71	1.53	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	546	CSO	C-CA-N	-7.83	106.01	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\#|Z| > 2$
6	NFO	L	1004	2	3,8,8	1.31	0	0,10,10	0.00	-
4	SF4	S	1001	1	12,12,12	135.04	8 (66%)	0,24,24	0.00	-
4	SF4	S	1002	1	12,12,12	136.36	9 (75%)	0,24,24	0.00	-
5	F3S	S	1003	1	3,9,9	3.79	3 (100%)	0,15,15	0.00	-
7	MRD	S	2001	-	7,7,7	0.90	0	10,10,10	2.11	1 (10%)

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
6	NFO	L	1004	2	-	0/0/12/12	0/0/0/0
4	SF4	S	1001	1	-	0/0/48/48	0/0/5/5
4	SF4	S	1002	1	-	0/0/48/48	0/0/5/5
5	F3S	S	1003	1	-	0/0/24/24	0/0/3/3
7	MRD	S	2001	-	-	0/5/5/5	0/0/0/0

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	1002	SF4	S2-FE4	242.54	3.96	2.33
4	S	1001	SF4	S2-FE4	240.65	3.95	2.33
4	S	1002	SF4	S3-FE2	239.42	3.94	2.33
4	S	1002	SF4	S1-FE3	233.44	3.90	2.33
4	S	1001	SF4	S1-FE3	232.26	3.89	2.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	2001	MRD	C2-C3-C4	6.01	149.65	116.70

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.