

wwPDB X-ray Structure Validation Summary Report (i)

Oct 18, 2023 – 06:25 PM EDT

PDB ID	:	1UBU
Title	:	Three-dimensional Structure of The Carbon Monoxide Complex of
		[NiFe]hydrogenase From Desulufovibrio vulgaris Miyazaki F
Authors	:	Ogata, H.; Mizoguchi, Y.; Mizuno, N.; Miki, K.; Adachi, S.; Yasuoka, N.; Yagi,
		T.; Yamauchi, O.; Hirota, S.; Higuchi, Y.
Deposited on	:	2003-04-04
Resolution	:	1.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

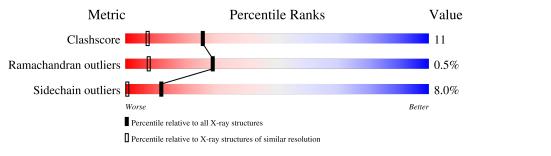
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.35 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	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	S	267	75%	18%	5%•
2	L	534	79%	15%	5%•



1UBU

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7157 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 Periplasmic [NiFe] hydrogenase Small subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	S	267	Total 2019	C 1282	N 342	O 378	S 17	0	0	0

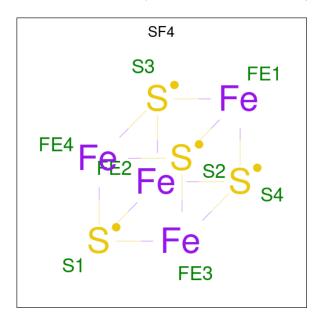
• Molecule 2 is a protein called Periplasmic [NiFe] hydrogenase Large subunit.

Μ	ol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	2	L	534	Total 4177	С 2674	N 725	O 763	S 15	0	0	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

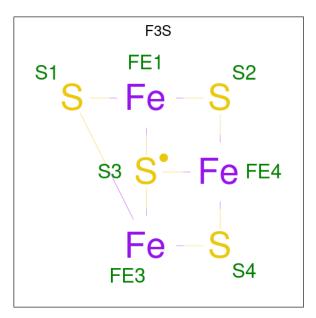
• Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	S	1	TotalFeS844	0	0
3	S	1	TotalFeS844	0	0

• Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



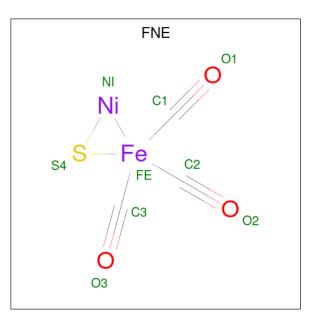
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total 7	Fe 3	$\frac{S}{4}$	0	0

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

• Molecule 6 is (MU-SULPHIDO)-BIS(MU-CYS,S)-[TRICARBONYLIRON-DI-(CYS,S)NIC KEL(II)](FE-NI) (three-letter code: FNE) (formula: C₃FeNiO₃S).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
6	т	1	Total	С	Fe	Ni	0	0	0
0		1	8	3	1	1	3	0	U

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	S	317	Total O 317 317	0	0
7	L	612	Total O 612 612	0	0

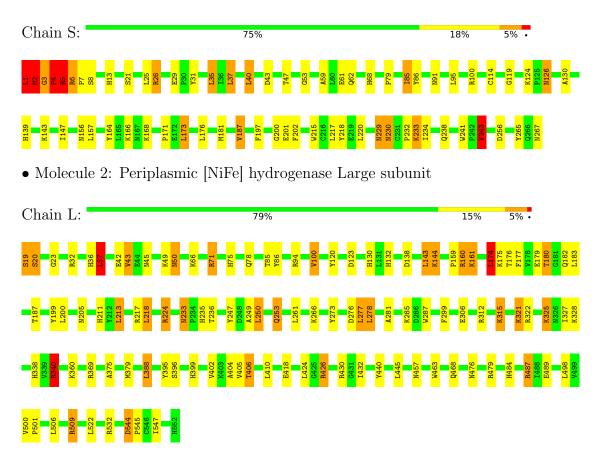


3 Residue-property plots (i)

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.

Note EDS was not executed.

• Molecule 1: Periplasmic [NiFe] hydrogenase Small subunit





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	98.01Å 126.02Å 66.57Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 - 1.35	Depositor
% Data completeness	91.9 (10.00-1.35)	Depositor
(in resolution range)	51.5 (10.00-1.50)	Depositor
R_{merge}	0.10	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	CNS, SHELXL-97	Depositor
R, R_{free}	0.121 , 0.186	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7157	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP



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: FNE, F3S, MG, SF4 $\,$

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		Bo	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	S	0.68	1/2075~(0.0%)	1.47	21/2830~(0.7%)	
2	L	0.62	0/4288	1.33	45/5831~(0.8%)	
All	All	0.64	1/6363~(0.0%)	1.38	66/8661~(0.8%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	267	ASN	C-O	6.93	1.36	1.23

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	S	6	ARG	CD-NE-CZ	27.92	162.69	123.60
1	S	100	ARG	NE-CZ-NH1	14.17	127.38	120.30
1	S	5	ARG	NE-CZ-NH1	-12.47	114.06	120.30
2	L	217	ARG	NE-CZ-NH1	-11.59	114.50	120.30
2	L	273	TYR	CB-CG-CD1	10.67	127.40	121.00

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	S	2019	0	1949	73	0
2	L	4177	0	4129	78	0
3	S	16	0	0	0	0
4	S	7	0	0	0	0
5	L	1	0	0	0	0
6	L	8	0	0	0	0
7	L	612	0	0	19	0
7	S	317	0	0	9	0
All	All	7157	0	6078	130	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 11.

The worst 5 of 130 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:S:26:ARG:HH21	2:L:233:ASN:HD21	1.16	0.93
1:S:230:ASN:HB2	1:S:233:LYS:HE2	1.52	0.90
1:S:126:ASN:HD21	1:S:130:ALA:H	1.19	0.84
1:S:2:MET:HA	2:L:182:GLN:HG2	1.61	0.81
1:S:238:GLN:HE21	2:L:224:ARG:HH21	1.29	0.80

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	\mathbf{S}	265/267~(99%)	257~(97%)	5(2%)	3~(1%)	14 1
2	L	532/534~(100%)	518 (97%)	13~(2%)	1 (0%)	47 21
All	All	797/801~(100%)	775 (97%)	18 (2%)	4 (0%)	29 8

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	S	4	PRO
2	L	20	SER
1	S	5	ARG
1	S	3	GLY

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		Percentiles		
1	S	213/213~(100%)	192~(90%)	21 (10%)	8 0		
2	L	438/438 (100%)	407~(93%)	31 (7%)	14 1		
All	All	651/651~(100%)	599~(92%)	52 (8%)	12 1		

 $5~{\rm of}~52$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	L	143	LEU
2	L	233	ASN
2	L	445	LEU
2	L	144	LYS
2	L	183	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	113	ASN
2	L	457	ASN
2	L	205	ASN
2	L	476	ASN
2	L	399	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)

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)

Of 5 ligands modelled in this entry, 1 is 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	e Chain Res Link		Bond lengths			Bond angles		
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ # Z > 2
3	SF4	S	1002	1	$0,\!12,\!12$	-	-	-	
6	FNE	L	1004	2	3,7,9	2.35	1 (33%)	-	
4	F3S	S	1003	1	0,9,9	-	-	-	
3	SF4	S	1001	1	0,12,12	-	-	-	

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	SF4	S	1002	1	-	-	0/6/5/5
4	F3S	S	1003	1	-	-	0/3/3/3
3	SF4	S	1001	1	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1004	FNE	O2-C2	-3.75	1.10	1.16

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.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

