

Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 11:31 pm BST

PDB ID 3ZE7

> Title 3D structure of the Ni-Fe-Se hydrogenase from D. vulgaris Hildenborough in

> > the reduced state at 1.95 Angstroms

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2012-12-03 Deposited on

1.95 Å(reported) Resolution

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

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.11

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

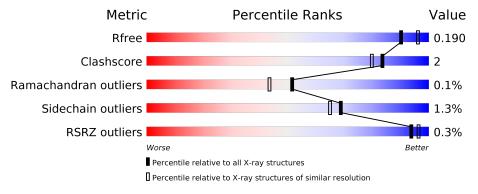
Validation Pipeline (wwPDB-VP) 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.95 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	283	91%	7%	-
2	В	484	92%	7%	



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6625 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.

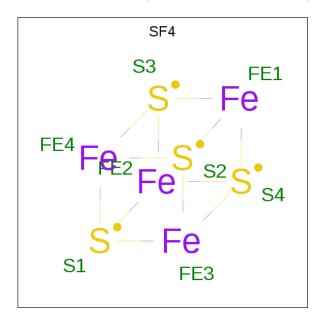
• Molecule 1 is a protein called PERIPLASMIC [NIFESE] HYDROGENASE, SMALL SUB-UNIT.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	277	Total 2112	C 1350	N 352	O 390	S 20	0	5	0

• Molecule 2 is a protein called PERIPLASMIC [NIFESE] HYDROGENASE, LARGE SUB-UNIT, SELENOCYSTEINE-CONTAINING.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
2	В	481	Total 3745	C 2391	N 653	O 683	S 17	Se 1	0	2	0

• Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	Λ	1	Total	Fe	S	0	0
)	Α	1	8	4	4		0

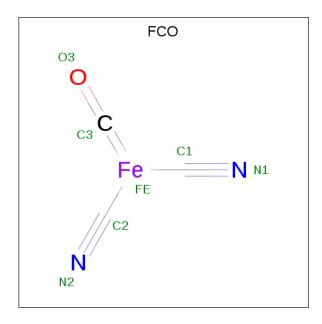
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	Δ	1	Total Fe S	0	0	
)	Λ	1	8 4 4	0		
2	Λ.	1	Total Fe S	0	0	
3	A	1	8 4 4	0	0	

• Molecule 4 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues		$\mathbf{A}\mathbf{t}$	oms			ZeroOcc	AltConf
1	R	1	Total	С	Fe	N	О	0	0
4	ע	1	7	3	1	2	1	0	U

• Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

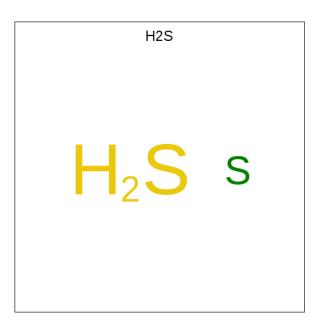
\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
5	В	1	Total Ni 1 1	0	0

 \bullet Molecule 6 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total Fe 1 1	0	0

• Molecule 7 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H₂S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	1	Total S 1 1	0	0

• Molecule 8 is water.

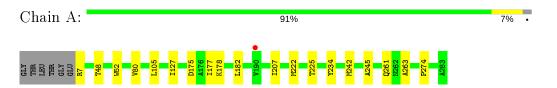
\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	$\mid \mathbf{AltConf} \mid$
8	A	280	Total O 280 280	0	0
8	В	454	Total O 454 454	0	0



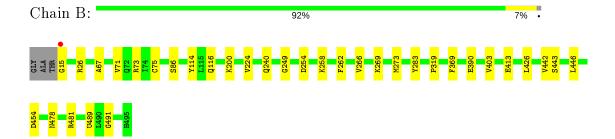
3 Residue-property plots (i)

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: PERIPLASMIC [NIFESE] HYDROGENASE, SMALL SUBUNIT



• Molecule 2: PERIPLASMIC [NIFESE] HYDROGENASE, LARGE SUBUNIT, SELENOCYST EINE-CONTAINING





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	72.30Å 96.99Å 103.86Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.78 - 1.95	Depositor
Resolution (A)	45.78 - 1.95	EDS
% Data completeness	99.0 (45.78-1.95)	Depositor
(in resolution range)	99.2 (45.78-1.95)	EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.31 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
P. P.	0.153 , 0.190	Depositor
R, R_{free}	0.151 , 0.190	DCC
R_{free} test set	2686 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 53.1	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6625	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: NI, SF4, H2S, SEC, FE2, OCS, FCO

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.39	0/2184	0.53	0/2968	
2	В	0.41	0/3821	0.55	0/5161	
All	All	0.40	0/6005	0.54	0/8129	

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	A	2112	0	2060	10	0
2	В	3745	0	3762	20	0
3	A	24	0	0	0	0
4	В	7	0	0	0	0
5	В	1	0	0	0	0
6	В	1	0	0	0	0
7	В	1	0	0	0	0
8	A	280	0	0	2	0
8	В	454	0	0	5	0
All	All	6625	0	5822	28	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 2.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
2:B:390:GLU:OE2	8:B:2397:HOH:O	2.02	0.77
1:A:175:ASP:HA	1:A:178:LYS:HE3	1.76	0.66
2:B:15:GLY:O	8:B:2004:HOH:O	2.14	0.64
2:B:319:PRO:HG3	2:B:446:LEU:HG	1.85	0.58
2:B:75:OCS:OD2	2:B:489:SEC:SE	2.73	0.56
1:A:207:ILE:HD11	1:A:245:ALA:HB3	1.90	0.52
1:A:7:ARG:HB2	8:A:2001:HOH:O	2.09	0.50
2:B:283:TYR:HB3	2:B:454:ASP:OD1	2.14	0.48
8:A:2012:HOH:O	2:B:491:GLY:HA3	2.13	0.47
1:A:127:ILE:HD12	2:B:73:ARG:HG2	1.97	0.47
2:B:200:LYS:HG2	8:B:2232:HOH:O	2.15	0.46
2:B:71:VAL:HG21	2:B:86:SER:HB2	1.97	0.45
2:B:443:SER:O	2:B:446:LEU:HB3	2.17	0.45
2:B:67:ALA:O	2:B:71:VAL:HG22	2.16	0.45
1:A:48:THR:O	2:B:26:ARG:HA	2.17	0.45
1:A:80:VAL:HG21	1:A:105:LEU:HD12	1.99	0.45
2:B:240:GLN:HA	2:B:369:PHE:O	2.17	0.45
1:A:175:ASP:O	1:A:178:LYS:HG2	2.18	0.44
1:A:127:ILE:HG12	1:A:274:PRO:HG3	2.00	0.44
2:B:478:ASN:HA	2:B:481:ARG:HB2	2.00	0.43
2:B:413:GLU:OE2	8:B:2334:HOH:O	2.22	0.42
1:A:177:ILE:HG23	1:A:182:LEU:HA	2.01	0.42
2:B:249:GLY:HA2	2:B:262:PHE:O	2.19	0.42
2:B:269[A]:LYS:HD2	8:B:2301:HOH:O	2.19	0.42
2:B:426:LEU:HG	2:B:442:VAL:HB	2.02	0.42
2:B:266:VAL:HB	2:B:273:MET:HG2	2.02	0.41
2:B:254:ASP:OD2	2:B:258:LYS:HG3	2.20	0.41
1:A:222[A]:MET:SD	1:A:234:TYR:HB3	2.61	0.41

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	Favoured Allowed		Percentiles	
1	A	$280/283 \ (99\%)$	271 (97%)	8 (3%)	1 (0%)	34	22
2	В	479/484 (99%)	466 (97%)	13 (3%)	0	100	100
All	All	759/767 (99%)	737 (97%)	21 (3%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ALA

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	227/226 (100%)	222 (98%)	5 (2%)	52 44
2	В	392/391 (100%)	388 (99%)	4 (1%)	76 74
All	All	619/617 (100%)	610 (98%)	9 (2%)	69 60

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	TRP
1	A	225	THR
1	A	242[A]	MET
1	A	242[B]	MET
1	A	261	GLN
2	В	114	TYR
2	В	116	GLN
2	В	224	VAL
2	В	403	VAL

Some 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)

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	B	ond leng	$_{ m gths}$	В	ond ang	gles
WIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OCS	В	75	2,5	3,7,9	3.30	1 (33%)	1,8,13	1.18	0

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	OCS	В	75	2,5	-	0/2/6/9	-

All (1) bond length outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	Z	${ m Observed}(m \AA)$	$\operatorname{Ideal}(ext{\AA})$
2	В	75	OCS	O-C	5.38	1.41	1.19

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

\mathbf{Mol}	Chain	${f Res}$	\mathbf{Type}	Clashes	Symm-Clashes
2	В	75	OCS	1	0



5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - 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	Tuno	Chain	Res	Link	В	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	$\mid \text{RMSZ} \mid \# Z > 2$		
3	SF4	A	284	1	0,12,12	0.00	-	_			
3	SF4	A	286	1	0,12,12	0.00	-	-			
3	SF4	A	285	1	0,12,12	0.00	-	-			
4	FCO	В	500	2,5	0,6,6	0.00	-	-			

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	A	284	1	-	-	0/6/5/5
3	SF4	A	286	1	-	-	0/6/5/5
3	SF4	A	285	1	=	-	0/6/5/5

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.



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)

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 $>$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q<0.9
1	A	277/283 (97%)	-0.29	1 (0%)	92 95	8, 13, 27, 46	6 (2%)
2	В	479/484 (98%)	-0.45	1 (0%)	95 97	7, 11, 23, 44	11 (2%)
All	All	756/767~(98%)	-0.39	2 (0%)	94 96	7, 12, 26, 46	17 (2%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	15	GLY	3.3
1	A	190	VAL	2.4

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

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. The B-factors column lists the minimum, median, 95^{th} 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	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	OCS	В	75	8/10	0.98	0.13	7,9,12,13	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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. The B-factors column lists the minimum,



median, 95^{th} 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	${f Res}$	Atoms	RSCC	RSR	$\operatorname{B-factors}({ ext{\AA}}^2)$	Q<0.9
7	H2S	В	503	1/1	1.00	0.07	8,8,8,8	0
3	SF4	A	285	8/8	1.00	0.04	11,11,12,12	0
6	FE2	В	502	1/1	1.00	0.06	11,11,11,11	0
3	SF4	A	286	8/8	1.00	0.06	10,10,10,11	0
5	NI	В	501	1/1	1.00	0.04	12,12,12,12	0
3	SF4	A	284	8/8	1.00	0.03	13,13,14,14	0
4	FCO	В	500	7/7	1.00	0.10	10,10,12,15	0

6.5 Other polymers (i)

There are no such residues in this entry.

