



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:57 PM BST

PDB ID : 4CI0
EMDB ID: : EMD-2513
Title : Electron cryo-microscopy of F420-reducing NiFe hydrogenase Frh
Authors : Allegretti, M.; Mills, D.J.; McMullan, G.; Kuehlbrandt, W.; Vonck, J.
Deposited on : 2013-12-05
Resolution : 3.36 Å(reported)
Based on PDB ID : 3ZFS

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

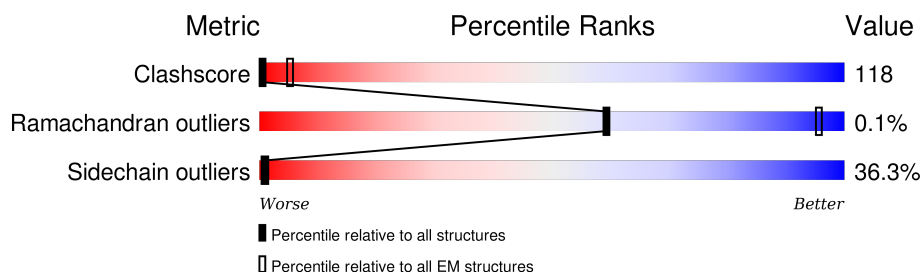
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	386	17% 53% 28% .
2	B	275	14% 44% 24% . 17%
3	C	281	16% 52% 31% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SF4	B	1274	-	-	X	-
7	SF4	B	1275	-	-	X	-
7	SF4	B	1276	-	-	X	-
7	SF4	C	1282	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6956 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 F420-REDUCING HYDROGENASE, SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	385	Total	C	N	O	S	0	0
			2985	1875	532	561	17		

- Molecule 2 is a protein called F420-REDUCING HYDROGENASE, SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	228	Total	C	N	O	S	0	0
			1737	1085	290	338	24		

- Molecule 3 is a protein called F420-REDUCING HYDROGENASE, SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	280	Total	C	N	O	S	0	0
			2145	1376	347	407	15		

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Fe	0
			1	1	

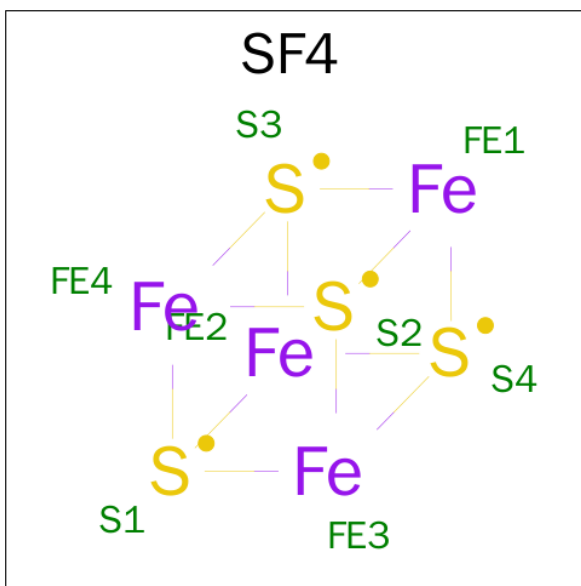
- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ni	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Fe	0
			1	1	

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

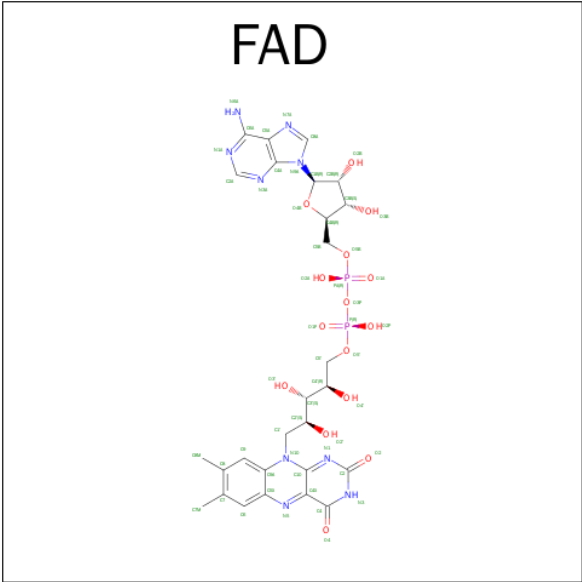


Mol	Chain	Residues	Atoms			AltConf
7	B	1	Total	Fe	S	0
			24	12	12	
7	B	1	Total	Fe	S	0
			24	12	12	
7	B	1	Total	Fe	S	0
			24	12	12	
7	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total	Zn	0
			1	1	

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH IMAGE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

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, ZN, SF4, FE2, FE, FAD

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.69	9/3048 (0.3%)	0.82	19/4133 (0.5%)
2	B	0.67	2/1768 (0.1%)	0.83	6/2400 (0.2%)
3	C	0.70	3/2184 (0.1%)	0.82	8/2946 (0.3%)
All	All	0.69	14/7000 (0.2%)	0.82	33/9479 (0.3%)

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	A	0	2
2	B	0	1
3	C	0	3
All	All	0	6

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	249	PRO	N-CD	5.54	1.55	1.47
1	A	9	PRO	N-CD	5.44	1.55	1.47
1	A	360	PRO	N-CD	5.42	1.55	1.47
3	C	280	PRO	N-CD	5.27	1.55	1.47
1	A	379	PRO	N-CD	5.26	1.55	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	PRO	CA-N-CD	-8.71	99.31	111.50
1	A	55	ALA	C-N-CD	6.01	141.01	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	115	TYR	C-N-CD	5.98	140.96	128.40
2	B	194	GLN	C-N-CD	5.98	140.96	128.40
3	C	102	ILE	C-N-CD	5.95	140.90	128.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	ARG	Sidechain
1	A	328	ARG	Sidechain
2	B	248	ARG	Sidechain
3	C	222	ARG	Sidechain
3	C	265	ALA	Peptide

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	2985	0	2970	712	0
2	B	1737	0	1699	468	0
3	C	2145	0	2192	576	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	B	24	0	0	7	0
7	C	8	0	0	5	0
8	B	1	0	0	0	0
9	C	53	0	31	13	0
All	All	6956	0	6892	1636	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 118.

The worst 5 of 1636 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)
3:C:164:GLY:HA3	3:C:169:TRP:CZ3	1.46	1.48
2:B:101:VAL:HG21	2:B:158:ILE:CD1	1.54	1.35
1:A:18:GLU:HG2	1:A:35:PHE:CZ	1.61	1.35
2:B:195:PRO:HG3	3:C:115:TYR:CE2	1.62	1.34
2:B:219:LEU:CD1	3:C:272:ARG:HH21	1.40	1.33

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 PDB entries followed by that with respect to all EM entries.

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	383/386 (99%)	369 (96%)	13 (3%)	1 (0%)	46	82
2	B	226/275 (82%)	216 (96%)	10 (4%)	0	100	100
3	C	278/281 (99%)	271 (98%)	7 (2%)	0	100	100
All	All	887/942 (94%)	856 (96%)	30 (3%)	1 (0%)	59	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	PRO

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 PDB entries followed by that with respect to all EM entries.

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	321/322 (100%)	213 (66%)	108 (34%)	0	1
2	B	194/232 (84%)	122 (63%)	72 (37%)	0	1
3	C	229/230 (100%)	139 (61%)	90 (39%)	0	0
All	All	744/784 (95%)	474 (64%)	270 (36%)	1	1

5 of 270 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	85	GLN
2	B	178	ILE
3	C	220	ILE
2	B	92	GLU
2	B	127	CYS

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

Mol	Chain	Res	Type
2	B	146	GLN
2	B	187	ASN
3	C	185	HIS
2	B	147	GLN
2	B	188	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 ⓘ

Of 9 ligands modelled in this entry, 4 are 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$
7	SF4	B	1274	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	1275	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	1276	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	C	1282	3	0,12,12	0.00	-	0,24,24	0.00	-
9	FAD	C	1283	-	52,58,58	1.24	9 (17%)	52,89,89	2.11	9 (17%)

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
7	SF4	B	1274	2	-	0/0/48/48	0/6/5/5
7	SF4	B	1275	2	-	0/0/48/48	0/6/5/5
7	SF4	B	1276	2	-	0/0/48/48	0/6/5/5
7	SF4	C	1282	3	-	0/0/48/48	0/6/5/5
9	FAD	C	1283	-	-	0/30/50/50	0/6/6/6

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1283	FAD	C1'-N10	-2.57	1.45	1.48
9	C	1283	FAD	C2B-C1B	-2.35	1.49	1.53
9	C	1283	FAD	C6-C5X	-2.17	1.38	1.41
9	C	1283	FAD	C2-N3	-2.04	1.33	1.38
9	C	1283	FAD	C8-C7	2.15	1.46	1.41

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1283	FAD	N3A-C2A-N1A	-6.59	123.69	128.87
9	C	1283	FAD	C4-C4X-C10	-5.92	116.15	119.94
9	C	1283	FAD	C4X-C4-N3	-3.40	119.08	123.52
9	C	1283	FAD	N3-C2-N1	-3.06	122.53	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1283	FAD	C1'-N10-C9A	2.73	122.00	118.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1274	SF4	2	0
7	B	1275	SF4	2	0
7	B	1276	SF4	3	0
7	C	1282	SF4	5	0
9	C	1283	FAD	13	0

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.