



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 10:55 AM UTC

PDB ID : 1H1L / pdb_00001h1l
Title : NITROGENASE MO-FE PROTEIN FROM KLEBSIELLA PNEUMONIAE,
NIFV MUTANT
Authors : Mayer, S.M.; Gormal, C.A.; Smith, B.E.; Lawson, D.M.
Deposited on : 2002-07-18
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

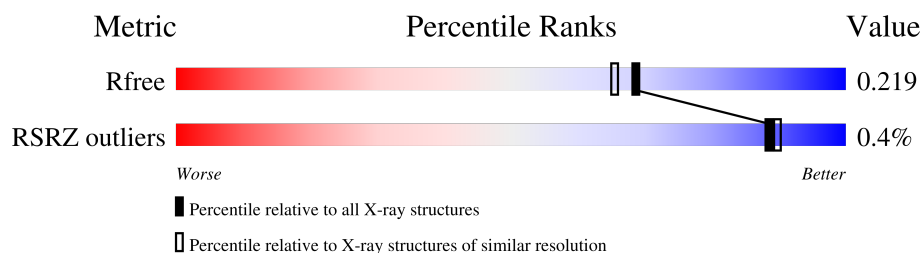
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17025 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 NITROGENASE MOLYBDENUM IRON PROTEIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3664	2331	627	682	24			
1	C	478	Total	C	N	O	S	0	0	0
			3674	2335	629	686	24			

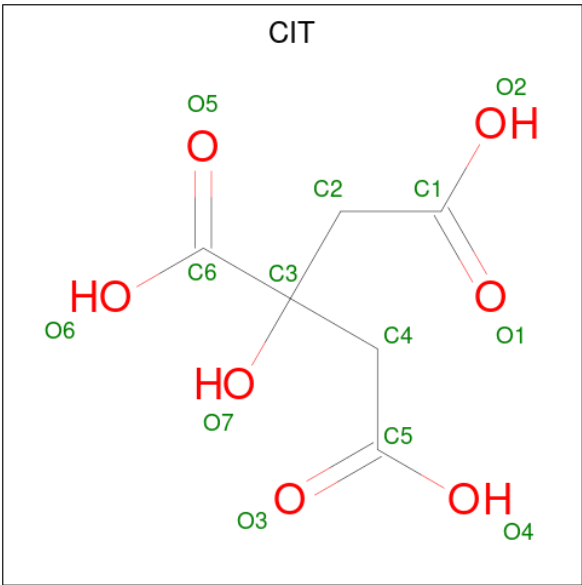
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	VAL	ALA	conflict	UNP P00466
A	94	GLY	GLU	conflict	UNP P00466
C	85	VAL	ALA	conflict	UNP P00466
C	94	GLY	GLU	conflict	UNP P00466

- Molecule 2 is a protein called NITROGENASE MOLYBDENUM IRON PROTEIN BETA CHAIN.

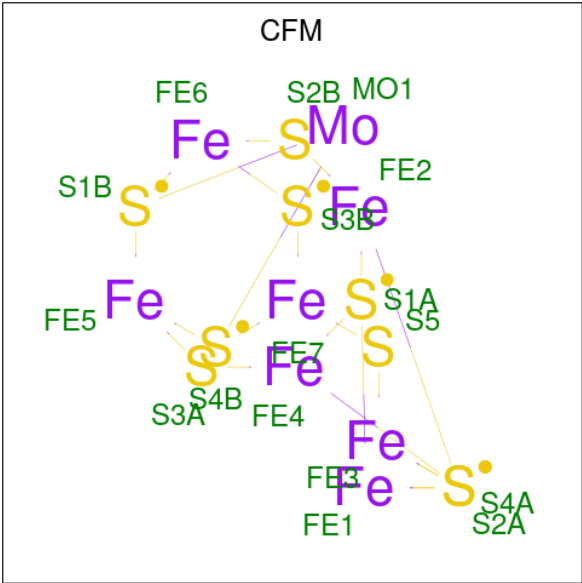
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	519	Total	C	N	O	S	0	0	0
			4026	2567	679	752	28			
2	D	519	Total	C	N	O	S	0	0	0
			4028	2568	678	754	28			

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is FE-MO-S CLUSTER (CCD ID: CFM) (formula: Fe₇MoS₉).

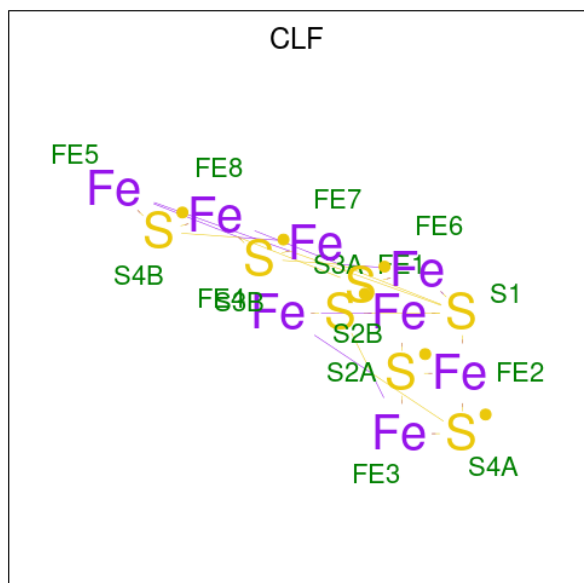


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
4	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	B	2	Total	Mg	0	0
			2	2		

- Molecule 6 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe₈S₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			15	8	7		
6	D	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	309	Total 309	O 309	0	0
8	B	474	Total 474	O 474	0	0
8	C	283	Total 283	O 283	0	0
8	D	471	Total 471	O 471	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.06Å 75.06Å 164.26Å 90.00° 123.95° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 40.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.2 (40.00-1.90) 94.3 (40.00-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.236 0.164 , 0.219	Depositor DCC
R_{free} test set	7646 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17025	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	CLF	B	1520	2,1	0,24,24	-	-	-		
4	CFM	C	1480	1	0,24,24	-	-	-		
4	CFM	A	1480	1	0,24,24	-	-	-		
6	CLF	D	1521	2,1	0,24,24	-	-	-		
3	CIT	C	1479	-	12,12,12	1.54	1 (8%)	17,17,17	2.10	6 (35%)
3	CIT	A	1479	-	12,12,12	1.52	1 (8%)	17,17,17	1.76	3 (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
3	CIT	A	1479	-	-	2/16/16/16	-
6	CLF	B	1520	2,1	-	-	0/12/10/10
6	CLF	D	1521	2,1	-	-	0/12/10/10
3	CIT	C	1479	-	-	5/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1479	CIT	C3-C6	-3.82	1.49	1.53
3	C	1479	CIT	C3-C6	-3.06	1.50	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1479	CIT	O4-C5-O3	-3.96	113.15	123.33
3	C	1479	CIT	C3-C4-C5	3.93	124.66	113.92
3	C	1479	CIT	O5-C6-C3	-3.24	115.82	122.09
3	C	1479	CIT	C4-C3-C6	-3.13	103.12	110.03
3	A	1479	CIT	O5-C6-C3	-2.98	116.32	122.09
3	A	1479	CIT	O6-C6-C3	2.96	118.81	113.14
3	C	1479	CIT	O1-C1-C2	-2.73	115.22	122.95
3	C	1479	CIT	O6-C6-C3	2.64	118.20	113.14
3	C	1479	CIT	O4-C5-C4	2.53	122.37	114.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1479	CIT	C1-C2-C3-C4
3	C	1479	CIT	C1-C2-C3-C6
3	C	1479	CIT	C1-C2-C3-O7
3	C	1479	CIT	O2-C1-C2-C3
3	C	1479	CIT	O1-C1-C2-C3
3	A	1479	CIT	C1-C2-C3-C6
3	A	1479	CIT	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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, 95th 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	478/481 (99%)	-0.21	0	100 100	14, 23, 35, 44	0
1	C	478/481 (99%)	-0.04	3 (0%)	85 87	15, 26, 39, 50	0
2	B	519/519 (100%)	-0.36	3 (0%)	85 87	13, 20, 34, 46	0
2	D	519/519 (100%)	-0.38	2 (0%)	88 90	12, 20, 34, 44	0
All	All	1994/2000 (99%)	-0.25	8 (0%)	88 90	12, 22, 35, 50	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	315	ASP	3.3
2	B	122	VAL	3.2
2	B	120	ALA	3.0
2	D	4	ILE	2.6
1	C	251	TRP	2.5
2	B	4	ILE	2.4
2	D	5	ASP	2.1
1	C	41	VAL	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	A	3003	1/1	0.82	0.18	37,37,37,37	0
3	CIT	C	1479	13/13	0.85	0.16	14,16,21,22	13
3	CIT	A	1479	13/13	0.87	0.15	12,16,17,18	13
5	MG	A	3001	1/1	0.88	0.09	28,28,28,28	0
5	MG	B	1522	1/1	0.98	0.07	23,23,23,23	0
5	MG	B	1523	1/1	0.98	0.02	21,21,21,21	0
6	CLF	B	1520	15/15	0.98	0.04	14,16,19,22	0
7	CL	B	1521	1/1	0.98	0.10	26,26,26,26	0
4	CFM	A	1480	17/17	0.99	0.03	12,15,17,17	0
6	CLF	D	1521	15/15	0.99	0.03	14,16,18,20	0
4	CFM	C	1480	17/17	0.99	0.04	13,18,19,20	0
7	CL	D	1520	1/1	1.00	0.11	23,23,23,23	0

5.5 Other polymers [i](#)

There are no such residues in this entry.