



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 08:33 PM GMT

PDB ID : 1G21
Title : MGATP-BOUND AND NUCLEOTIDE-FREE STRUCTURES OF A NITROGENASE PROTEIN COMPLEX BETWEEN LEU127DEL-FE PROTEIN AND THE MOFE PROTEIN
Authors : Chiu, H.-J.; Peters, J.W.; Lanzilotta, W.N.; Ryle, M.J.; Seefeldt, L.C.; Howard, J.B.; Rees, D.C.
Deposited on : 2000-10-16
Resolution : 3.00 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

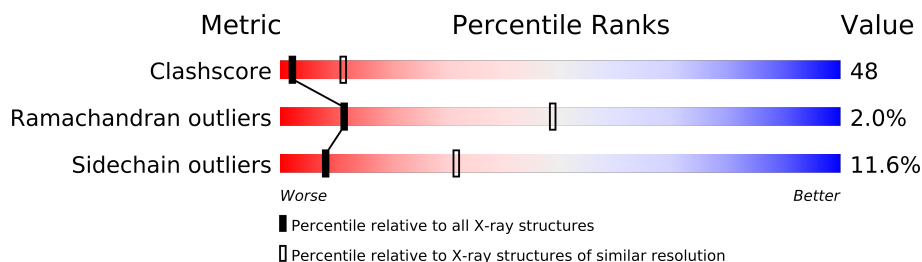
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)

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	A	492	
1	C	492	
2	B	523	
2	D	523	
3	E	289	
3	F	289	
3	G	289	
3	H	289	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 24237 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 NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3776	2402	642	708	24			
1	C	476	Total	C	N	O	S	0	0	0
			3776	2402	642	708	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4170	2663	704	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4170	2663	704	775	28			

- Molecule 3 is a protein called NITROGENASE IRON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	268	Total	C	N	O	S	109	0	0
			2029	1265	347	397	20			
3	F	267	Total	C	N	O	S	71	0	0
			2020	1260	346	394	20			
3	G	268	Total	C	N	O	S	130	0	0
			2029	1265	347	397	20			
3	H	268	Total	C	N	O	S	116	0	0
			2029	1265	347	397	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	DELETION	UNP P00459
F	?	-	LEU	DELETION	UNP P00459
G	?	-	LEU	DELETION	UNP P00459

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	LEU	DELETION	UNP P00459

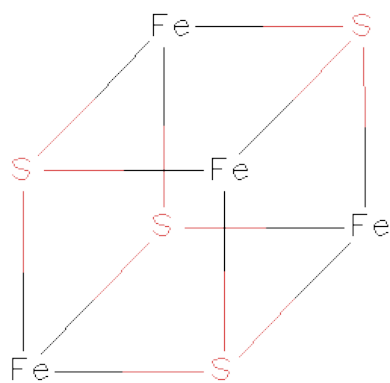
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

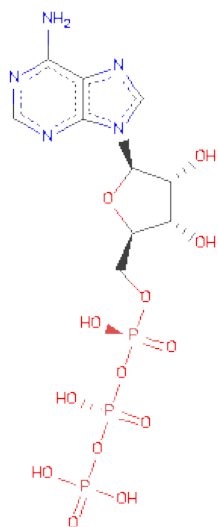
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



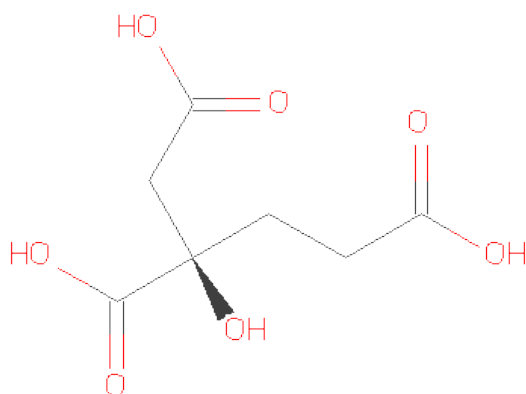
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	Fe	S	0	0
			8	4	4		
6	G	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



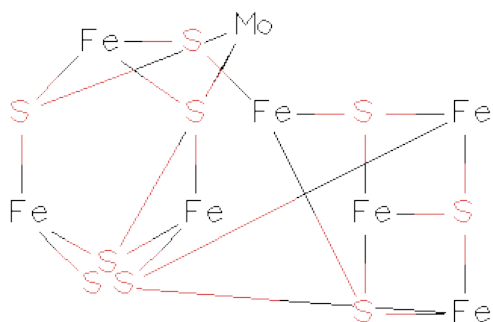
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 8 is 3-HYDROXY-3-CARBOXY-ADIPIACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$).



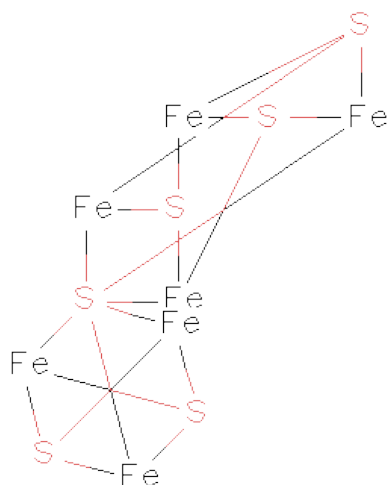
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			14	7	7		
8	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 9 is FE-MO-S CLUSTER (three-letter code: CFM) (formula: Fe_7MoS_9).



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

- Molecule 10 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	Fe	S	0	0
			15	8	7		
10	D	1	Total	Fe	S	0	0
			15	8	7		

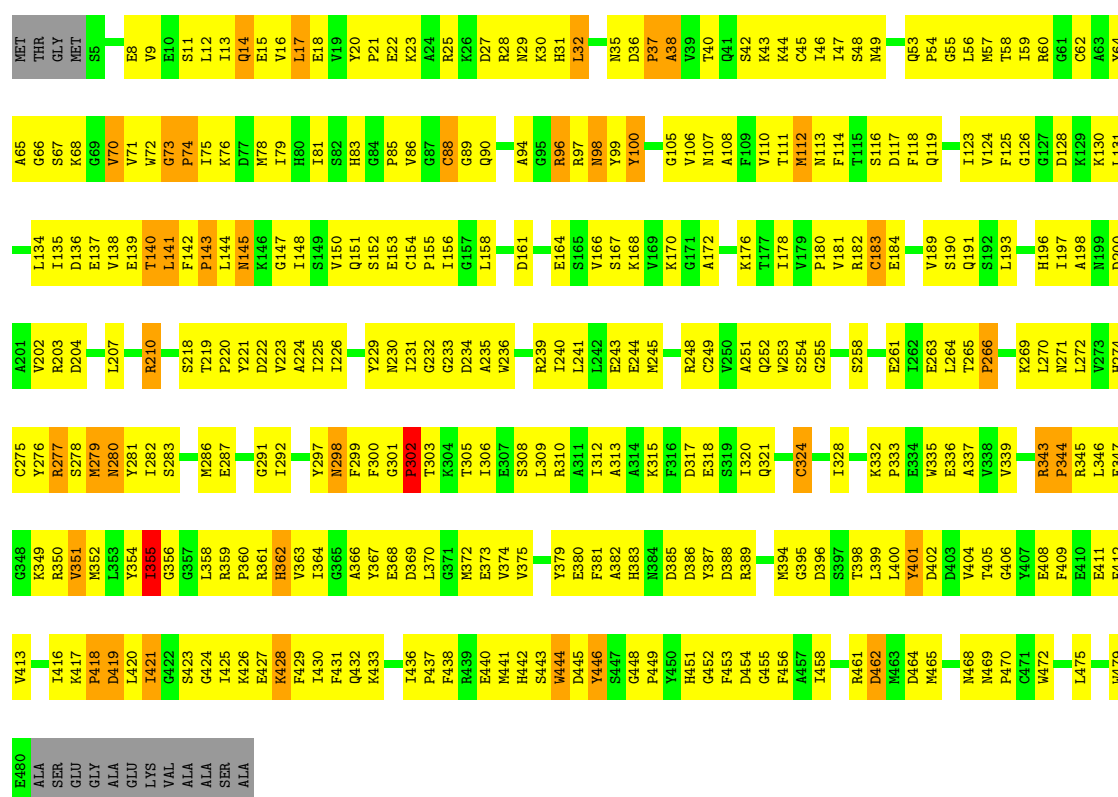
3 Residue-property plots

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.

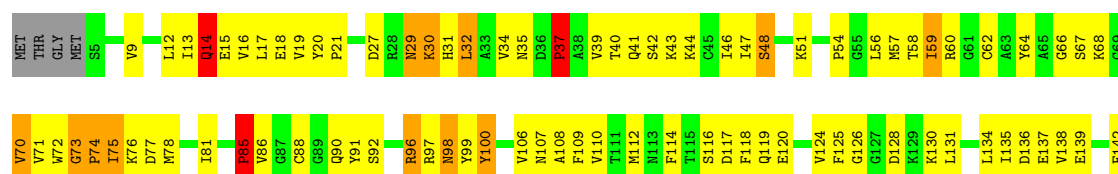
• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN

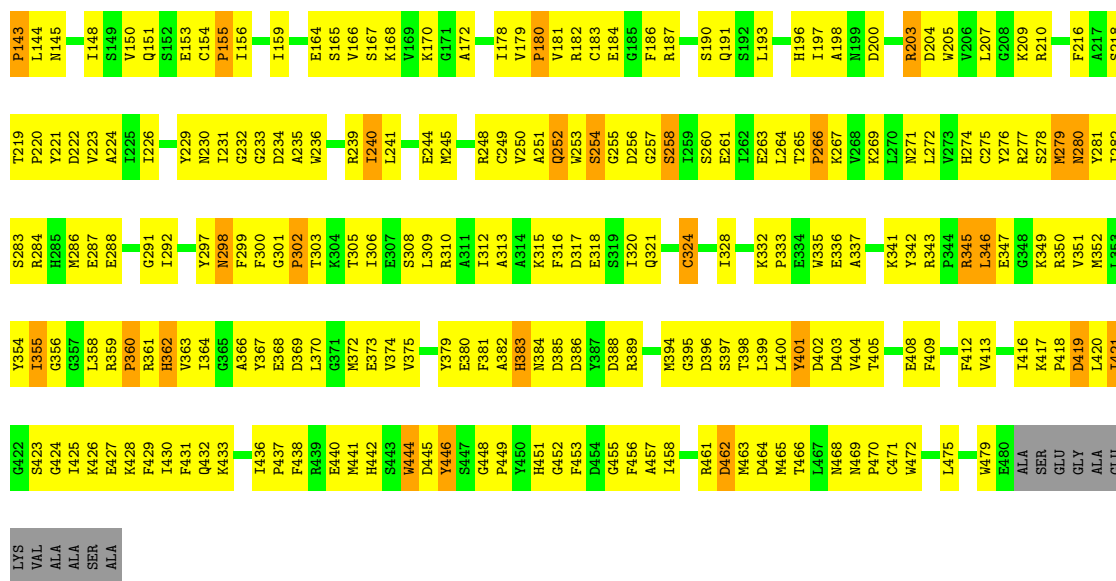
Chain A:



• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN

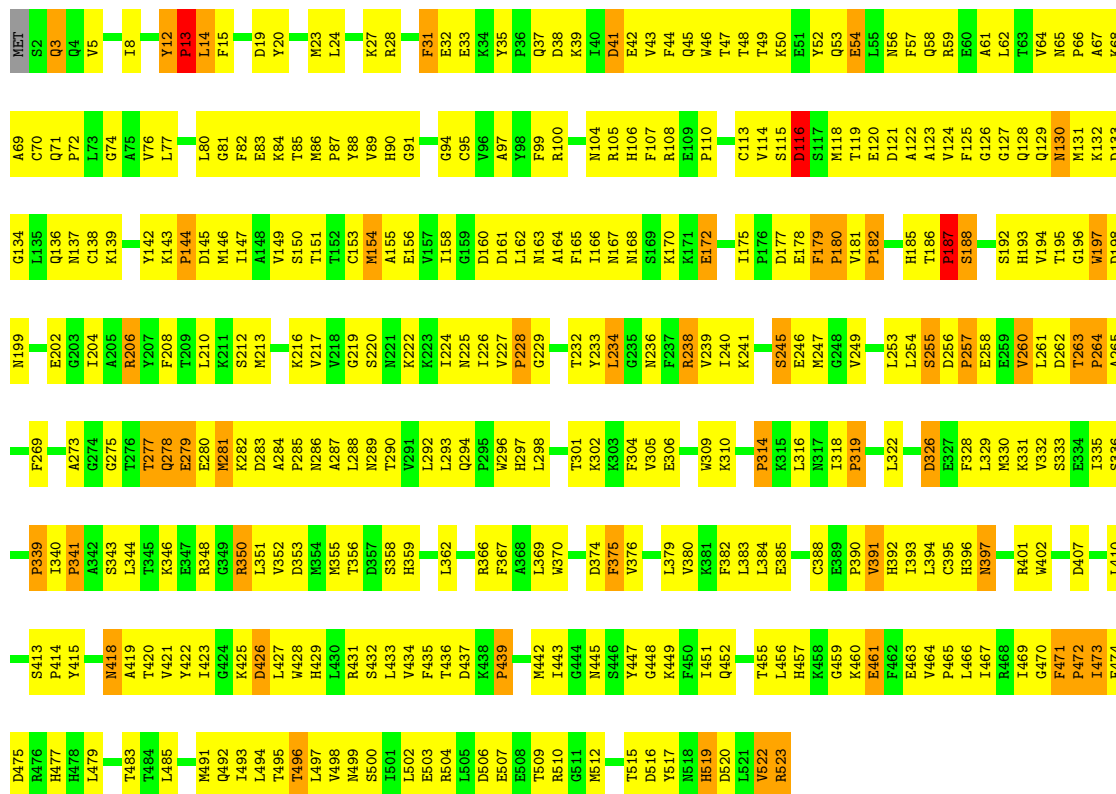
Chain C:





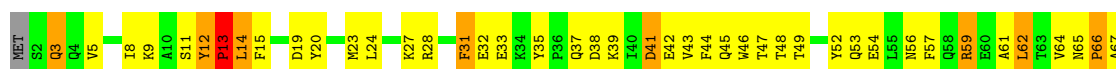
• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

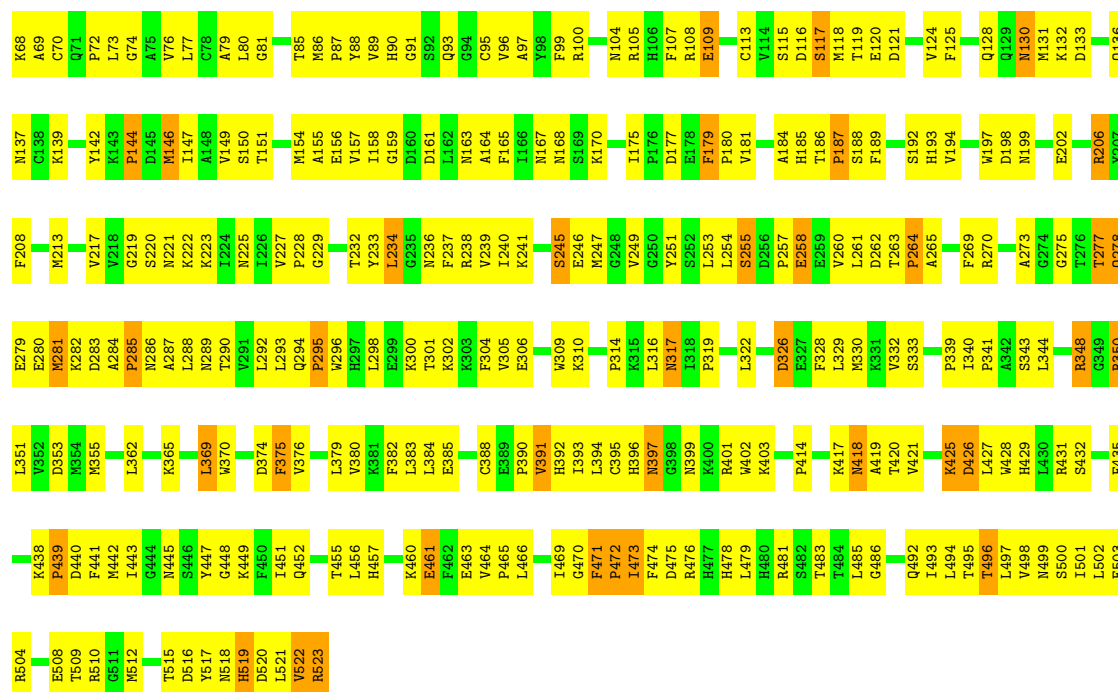
Chain B:



• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

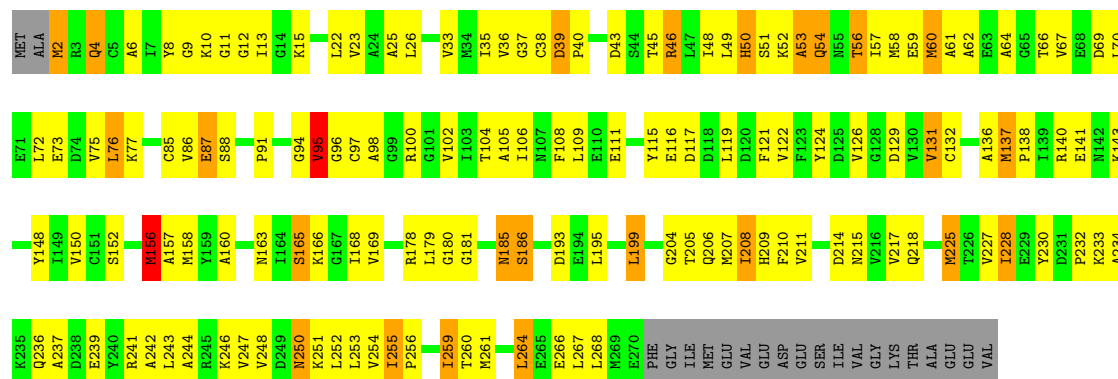
Chain D:





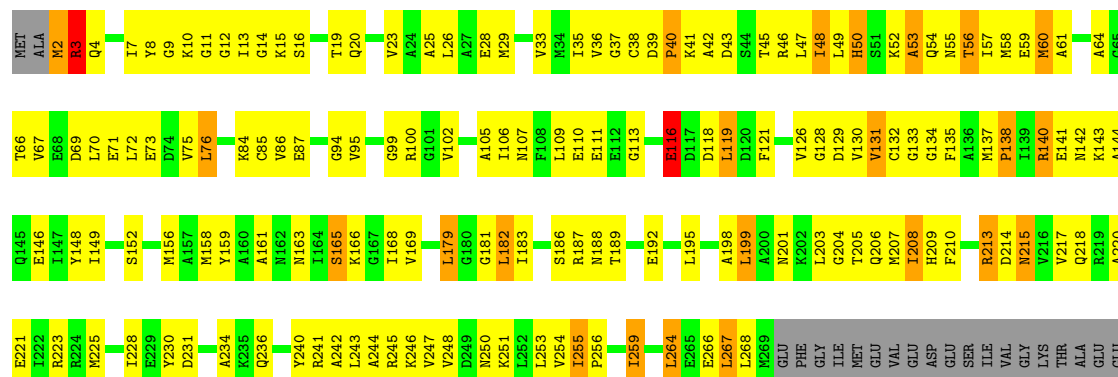
• Molecule 3: NITROGENASE IRON PROTEIN

Chain E:



• Molecule 3: NITROGENASE IRON PROTEIN

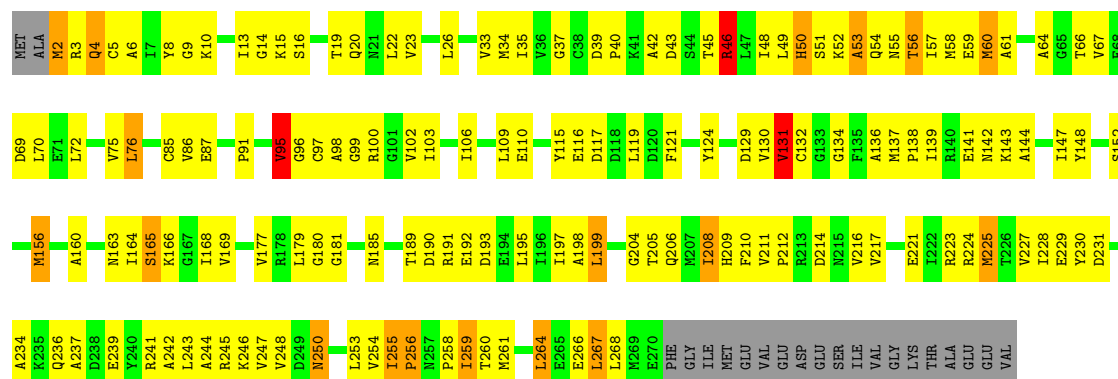
Chain F:



VAL

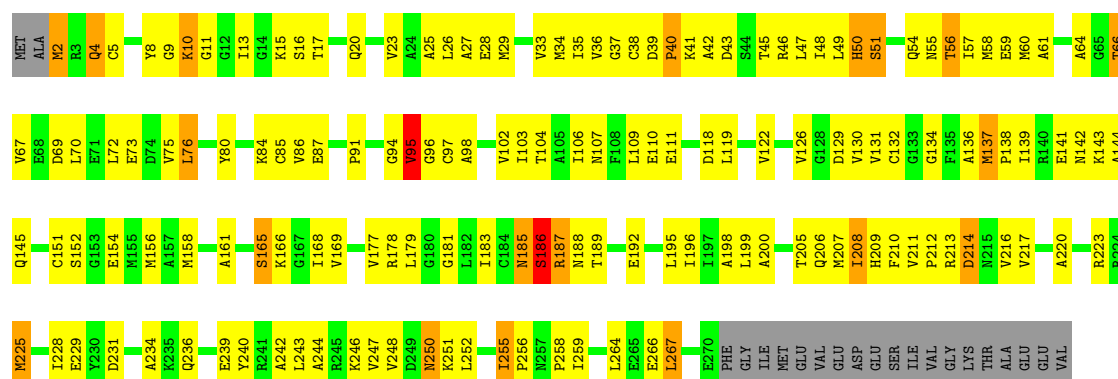
• Molecule 3: NITROGENASE IRON PROTEIN

Chain G:



• Molecule 3: NITROGENASE IRON PROTEIN

Chain H:



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	110.50Å 121.50Å 264.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	71.6 (20.00-3.00)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24237	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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, CFM, CLF, HCA, ATP, CA, 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	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.50	0/3864	0.73	2/5212 (0.0%)
1	C	0.48	0/3864	0.73	2/5212 (0.0%)
2	B	0.54	0/4276	0.82	7/5782 (0.1%)
2	D	0.50	1/4276 (0.0%)	0.88	15/5782 (0.3%)
3	E	0.51	0/2052	0.80	2/2764 (0.1%)
3	F	0.55	1/2043 (0.0%)	0.84	4/2752 (0.1%)
3	G	0.47	0/2052	0.75	0/2764
3	H	0.54	1/2052 (0.0%)	0.81	1/2764 (0.0%)
All	All	0.51	3/24479 (0.0%)	0.80	33/33032 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	40	PRO	N-CD	5.37	1.55	1.47
3	F	40	PRO	N-CD	5.31	1.55	1.47
2	D	109	GLU	C-N	-5.08	1.24	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	TYR	C-N-CD	-21.77	72.71	120.60
2	B	12	TYR	C-N-CD	-20.40	75.71	120.60
2	B	12	TYR	C-N-CA	13.32	177.95	122.00
2	D	12	TYR	C-N-CA	12.49	174.45	122.00
1	A	88	CYS	CA-CB-SG	-10.83	94.51	114.00

There are no chirality outliers.

There are no planarity outliers.

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	A	3776	0	3709	452	0
1	C	3776	0	3709	490	0
2	B	4170	0	4076	441	0
2	D	4170	0	4076	461	0
3	E	2029	0	2040	150	0
3	F	2020	0	2034	166	0
3	G	2029	0	2041	158	0
3	H	2029	0	2041	153	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	F	8	0	0	0	0
6	G	8	0	0	0	0
7	E	31	0	12	4	0
7	F	31	0	12	6	0
7	G	31	0	12	11	0
7	H	31	0	12	6	0
8	A	14	0	6	1	0
8	C	14	0	6	2	0
9	A	17	0	0	4	0
9	C	17	0	0	7	0
10	A	15	0	0	1	0
10	D	15	0	0	3	0
All	All	24237	0	23786	2236	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 48.

The worst 5 of 2236 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:39:ASP:OD1	3:F:40:PRO:HD2	1.28	1.29

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:91:GLY:HA2	2:D:118:MET:CE	1.62	1.28
1:C:124:VAL:HG21	3:H:58:MET:CE	1.70	1.21
1:A:355:ILE:HG23	1:A:356:GLY:H	0.99	1.15
3:F:39:ASP:OD1	3:F:40:PRO:CD	1.95	1.13

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	A	474/492 (96%)	420 (89%)	47 (10%)	7 (2%)	15	58
1	C	474/492 (96%)	415 (88%)	52 (11%)	7 (2%)	15	58
2	B	520/523 (99%)	470 (90%)	43 (8%)	7 (1%)	18	62
2	D	520/523 (99%)	450 (86%)	60 (12%)	10 (2%)	12	51
3	E	266/289 (92%)	232 (87%)	29 (11%)	5 (2%)	12	51
3	F	265/289 (92%)	232 (88%)	25 (9%)	8 (3%)	7	34
3	G	266/289 (92%)	225 (85%)	33 (12%)	8 (3%)	7	34
3	H	266/289 (92%)	234 (88%)	24 (9%)	8 (3%)	7	34
All	All	3051/3186 (96%)	2678 (88%)	313 (10%)	60 (2%)	11	48

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	13	PRO
2	B	391	VAL
2	D	13	PRO
2	D	439	PRO
3	E	53	ALA

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	A	405/415 (98%)	362 (89%)	43 (11%)	10	36
1	C	405/415 (98%)	357 (88%)	48 (12%)	8	30
2	B	453/455 (100%)	398 (88%)	55 (12%)	7	29
2	D	453/455 (100%)	411 (91%)	42 (9%)	13	45
3	E	216/233 (93%)	186 (86%)	30 (14%)	5	23
3	F	215/233 (92%)	190 (88%)	25 (12%)	8	31
3	G	216/233 (93%)	188 (87%)	28 (13%)	6	26
3	H	216/233 (93%)	189 (88%)	27 (12%)	7	28
All	All	2579/2672 (96%)	2281 (88%)	298 (12%)	8	31

5 of 298 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	346	LEU
2	D	281	MET
3	H	17	THR
1	C	398	THR
2	D	41	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	362	HIS
2	D	130	ASN
3	H	54	GLN
1	C	384	ASN
2	D	18	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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$
8	HCA	A	1494	9	13,13,13	2.30	4 (30%)	18,18,18	2.45	7 (38%)
9	CFM	A	1496	1,8	18,24,24	8.09	15 (83%)	0,45,45	0.00	-
10	CLF	A	1498	1,2	18,24,24	73.78	17 (94%)	0,57,57	0.00	-
8	HCA	C	3494	9	13,13,13	2.16	3 (23%)	18,18,18	2.55	6 (33%)
9	CFM	C	3496	1,8	18,24,24	4.48	10 (55%)	0,45,45	0.00	-
10	CLF	D	3498	1,2	18,24,24	74.02	16 (88%)	0,57,57	0.00	-
7	ATP	E	5292	4	33,33,33	1.28	3 (9%)	52,52,52	1.28	6 (11%)
6	SF4	F	5290	3	12,12,12	6.54	8 (66%)	0,24,24	0.00	-
7	ATP	F	6292	4	33,33,33	1.37	4 (12%)	52,52,52	1.37	6 (11%)
6	SF4	G	7290	3	12,12,12	3.05	8 (66%)	0,24,24	0.00	-
7	ATP	G	7292	4	33,33,33	1.69	7 (21%)	52,52,52	1.38	5 (9%)
7	ATP	H	8292	4	33,33,33	1.32	4 (12%)	52,52,52	1.33	7 (13%)

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
8	HCA	A	1494	9	-	0/17/17/17	0/0/0/0
9	CFM	A	1496	1,8	-	0/0/84/84	0/0/8/8
10	CLF	A	1498	1,2	-	0/0/132/132	0/0/10/10
8	HCA	C	3494	9	-	0/17/17/17	0/0/0/0
9	CFM	C	3496	1,8	-	0/0/84/84	0/0/8/8
10	CLF	D	3498	1,2	-	0/0/132/132	0/0/10/10
7	ATP	E	5292	4	-	0/22/38/38	0/1/3/3
6	SF4	F	5290	3	-	0/0/48/48	0/0/5/5
7	ATP	F	6292	4	-	0/22/38/38	0/1/3/3
6	SF4	G	7290	3	-	0/0/48/48	0/0/5/5
7	ATP	G	7292	4	-	0/22/38/38	0/1/3/3
7	ATP	H	8292	4	-	0/22/38/38	0/1/3/3

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1498	CLF	S4A-FE2	235.04	3.91	2.33
10	D	3498	CLF	S4A-FE2	231.19	3.88	2.33
10	D	3498	CLF	S3A-FE1	210.23	3.74	2.33
10	A	1498	CLF	S3A-FE1	202.59	3.69	2.33
9	A	1496	CFM	S1B-FE5	-22.57	2.18	2.33

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	3494	HCA	O6-C7-C3	7.38	123.62	112.89
8	A	1494	HCA	O6-C7-C3	6.17	121.86	112.89
8	A	1494	HCA	O5-C7-C3	-4.90	115.44	122.20
7	E	5292	ATP	O4'-C1'-C2'	-4.42	99.99	106.77
7	G	7292	ATP	C8-N9-C4	-4.37	103.56	106.90

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.