



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:16 AM GMT

PDB ID : 3HRD  
Title : Crystal structure of nicotinate dehydrogenase  
Authors : Wagener, N.; Pierik, A.J.; Hille, R.; Dobbek, H.  
Deposited on : 2009-06-09  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

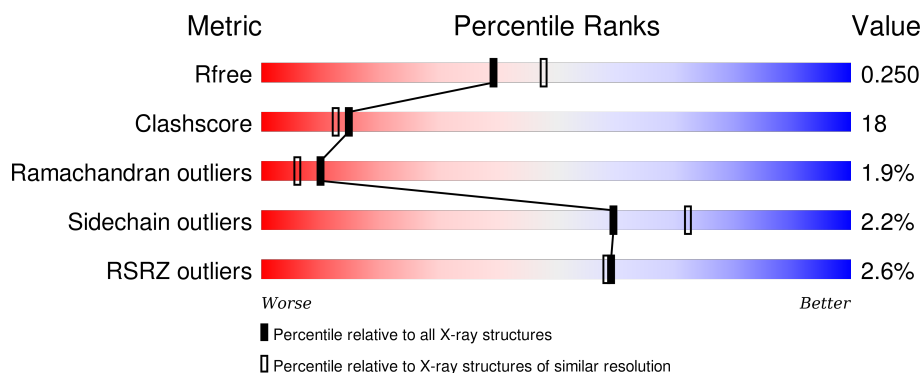
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	425	
1	E	425	
2	B	330	
2	F	330	
3	C	296	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	G	296	
4	D	160	
4	H	160	

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
10	NIO	B	5661	-	-	-	X
10	NIO	E	5660	-	-	-	X
12	FES	D	907	-	-	-	X
5	SE	A	922	-	-	X	X
5	SE	E	922	-	-	-	X

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 19284 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 Nicotinate dehydrogenase large molybdopterin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3213	2019	558	614	22			
1	E	420	Total	C	N	O	S	0	0	0
			3213	2019	558	614	22			

- Molecule 2 is a protein called Nicotinate dehydrogenase medium molybdopterin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	4	0	0
			2410	1506	405	481	18			
2	F	330	Total	C	N	O	S	0	0	0
			2410	1506	405	481	18			

- Molecule 3 is a protein called Nicotinate dehydrogenase FAD-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	291	Total	C	N	O	S	0	0	0
			2246	1425	385	424	12			
3	G	292	Total	C	N	O	S	0	0	0
			2250	1427	386	425	12			

- Molecule 4 is a protein called Nicotinate dehydrogenase small FeS subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	160	Total	C	N	O	S	0	0	0
			1176	724	200	237	15			
4	H	157	Total	C	N	O	S	0	0	0
			1161	715	197	234	15			

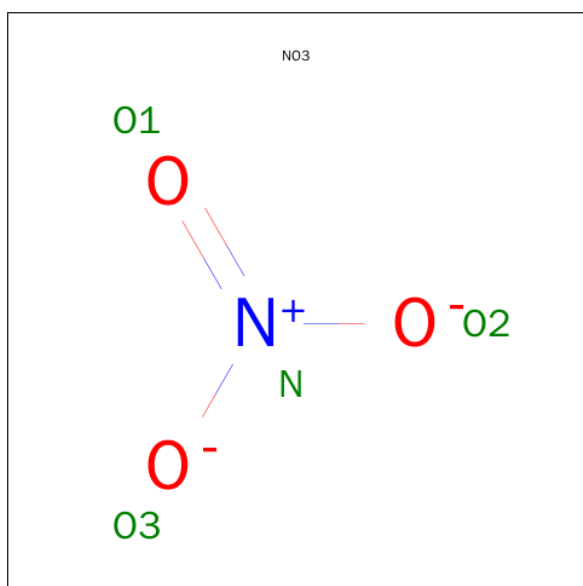
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	158	ALA	-	EXPRESSION TAG	UNP Q0QLF3
D	159	ALA	-	EXPRESSION TAG	UNP Q0QLF3
D	160	ALA	-	EXPRESSION TAG	UNP Q0QLF3
H	158	ALA	-	EXPRESSION TAG	UNP Q0QLF3
H	159	ALA	-	EXPRESSION TAG	UNP Q0QLF3
H	160	ALA	-	EXPRESSION TAG	UNP Q0QLF3

- Molecule 5 is SELENIUM ATOM (three-letter code: SE) (formula: Se).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Se	0	0
			1	1		
5	E	1	Total	Se	0	0
			1	1		

- Molecule 6 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).

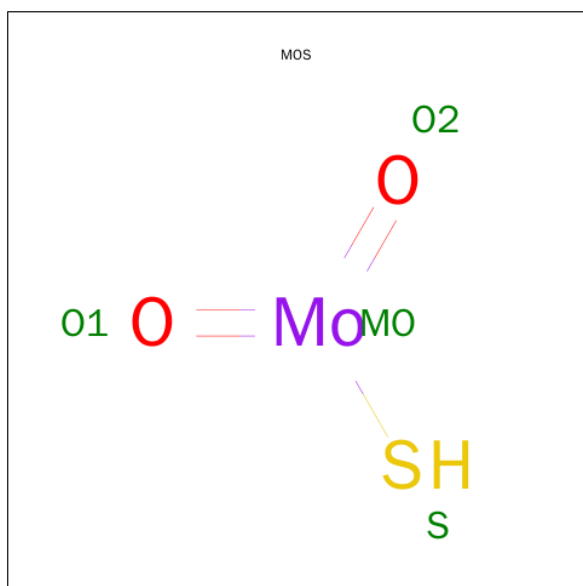


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	N	O	0	0
			4	1	3		
6	C	1	Total	N	O	0	0
			4	1	3		
6	E	1	Total	N	O	0	0
			4	1	3		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

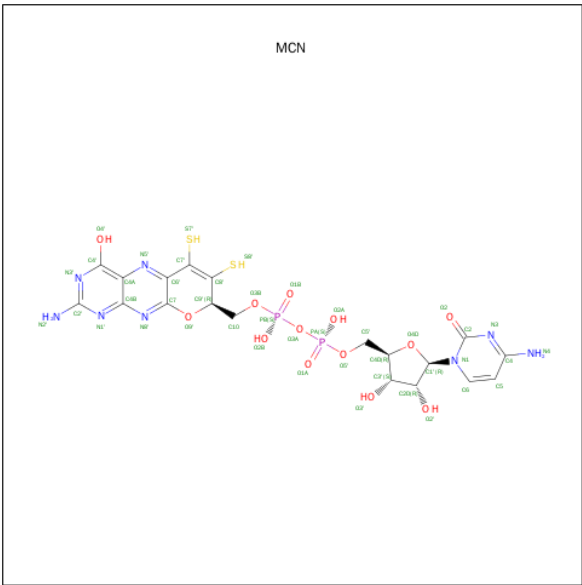
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Mg	0	0
			2	2		

- Molecule 8 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula:  $\text{HMoO}_2\text{S}$ ).



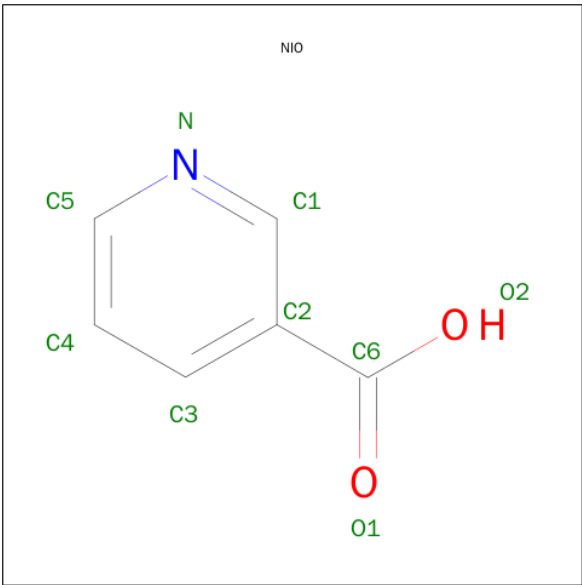
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Mo	O	0	0
			3	1	2		
8	F	1	Total	Mo	O	0	0
			3	1	2		

- Molecule 9 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula:  $\text{C}_{19}\text{H}_{22}\text{N}_8\text{O}_{13}\text{P}_2\text{S}_2$ ).



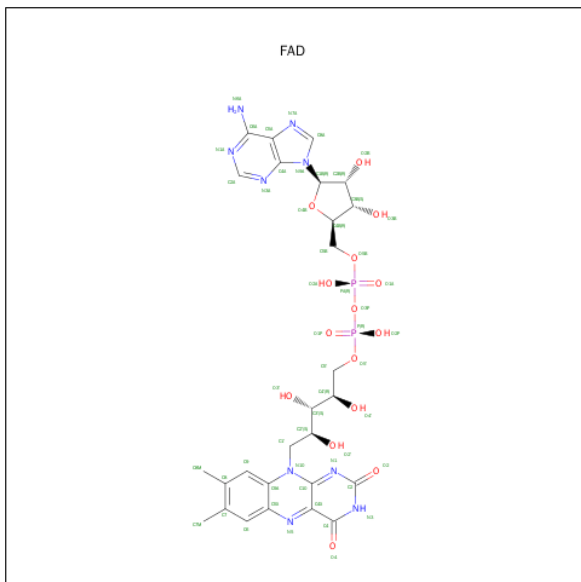
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	S	0	0
			44	19	8	13	2	2		
9	F	1	Total	C	N	O	P	S	0	0
			44	19	8	13	2	2		

- Molecule 10 is NICOTINIC ACID (three-letter code: NIO) (formula: C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub>).



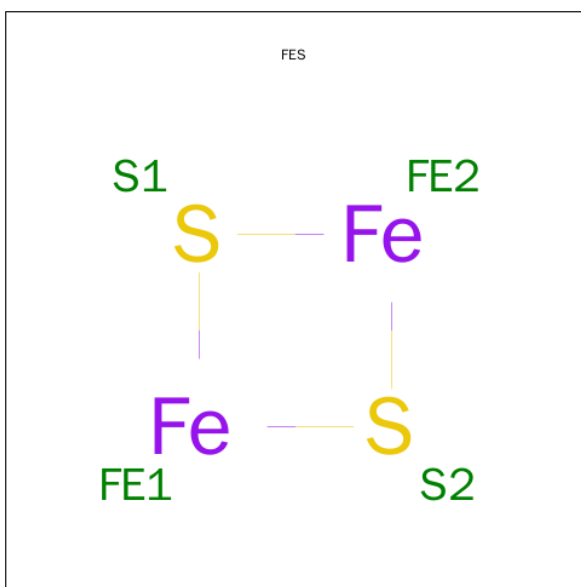
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			9	6	1	2		
10	E	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 11 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	D	1	Total 4	Fe 2	S 2	0	0
12	D	1	Total 4	Fe 2	S 2	0	0
12	H	1	Total 4	Fe 2	S 2	0	0
12	H	1	Total 4	Fe 2	S 2	0	0

- Molecule 13 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	E	1	Total 1	Ca 1	0	0

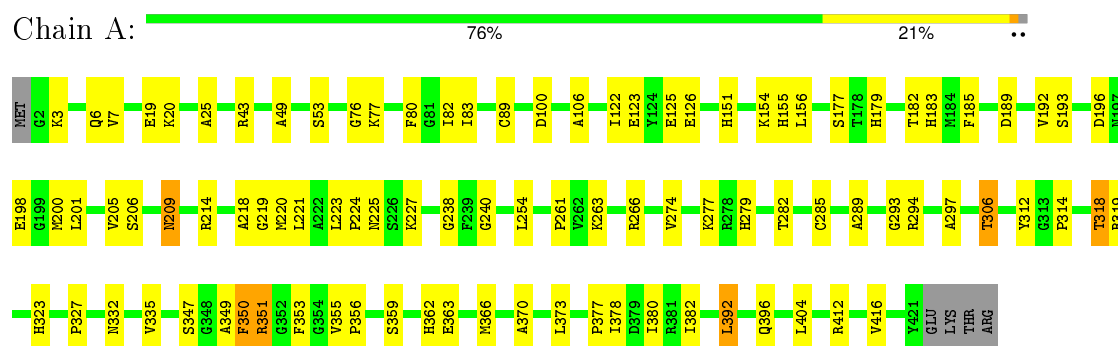
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	258	Total 258	O 258	0	0
14	B	170	Total 170	O 170	0	0
14	C	209	Total 209	O 209	0	0
14	D	112	Total 112	O 112	0	0
14	E	95	Total 95	O 95	0	0
14	F	59	Total 59	O 59	0	0
14	G	25	Total 25	O 25	0	0
14	H	26	Total 26	O 26	0	0

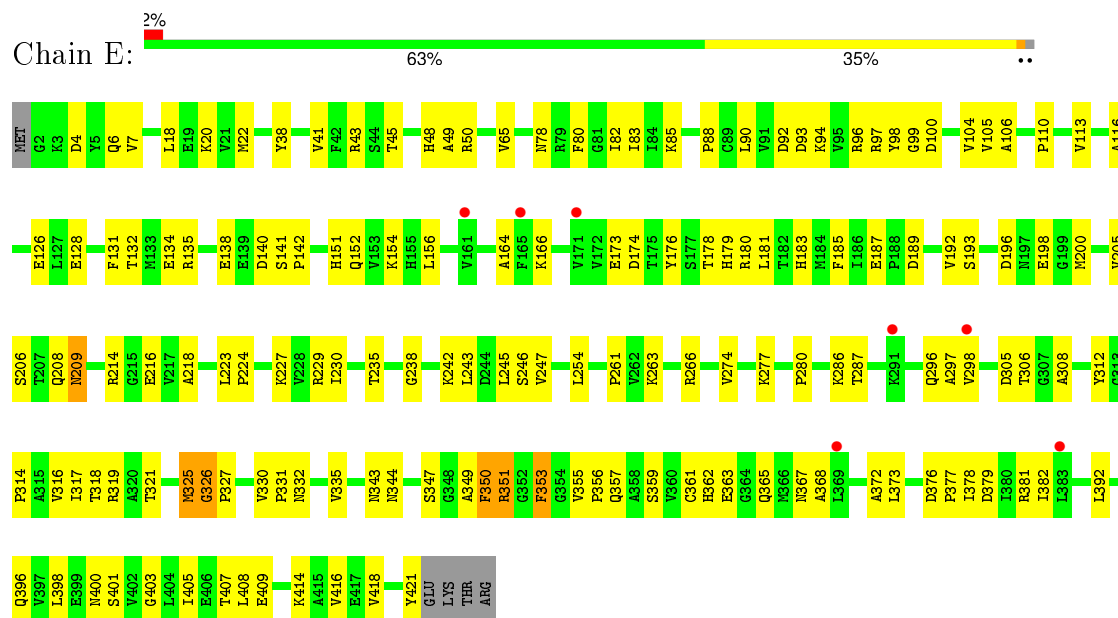
### 3 Residue-property plots

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.

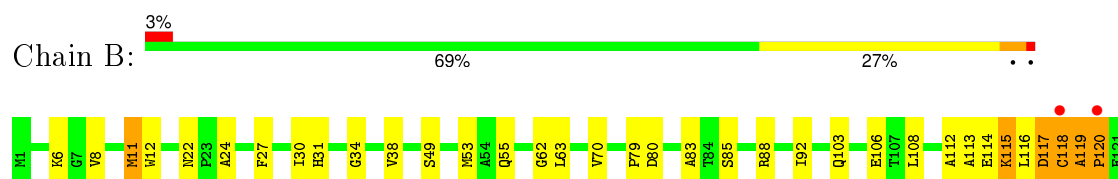
- Molecule 1: Nicotinate dehydrogenase large molybdopterin subunit

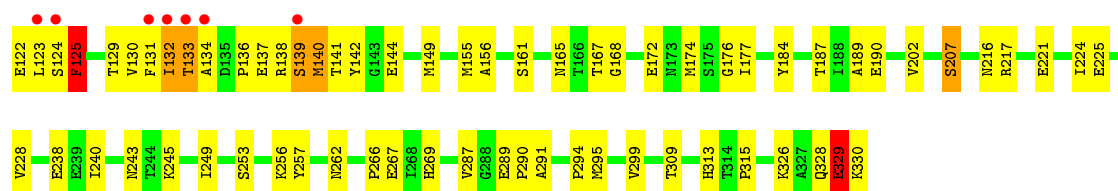


- Molecule 1: Nicotinate dehydrogenase large molybdopterin subunit

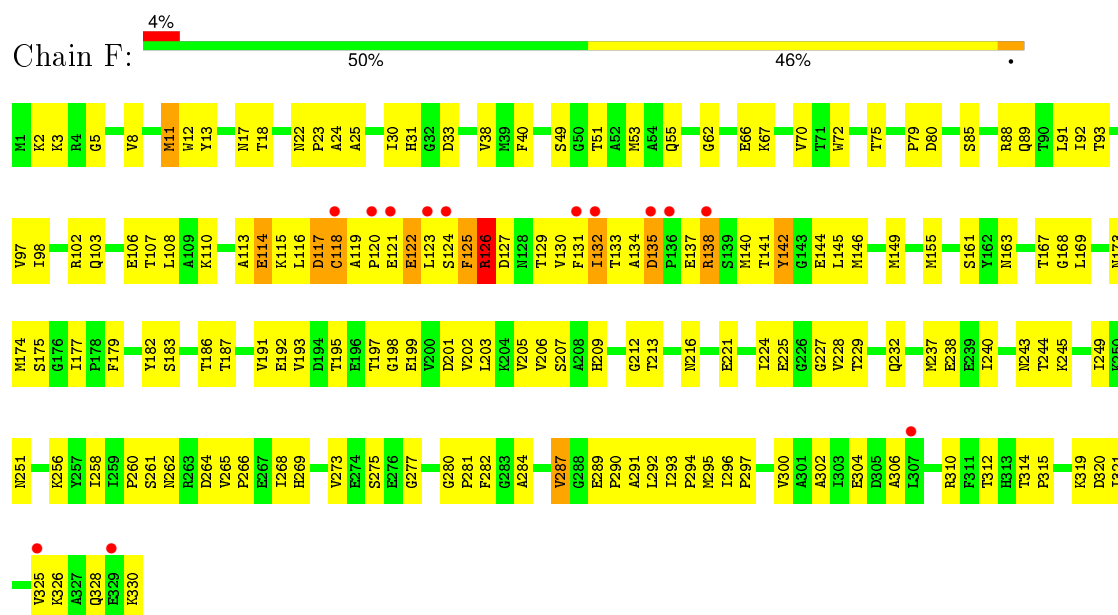


- Molecule 2: Nicotinate dehydrogenase medium molybdopterin subunit

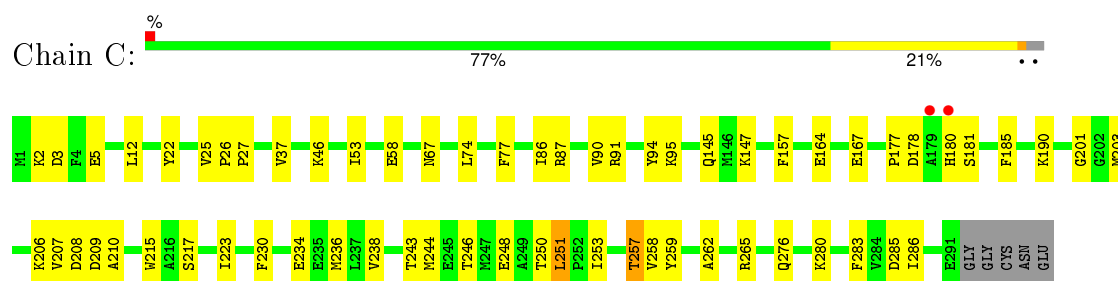




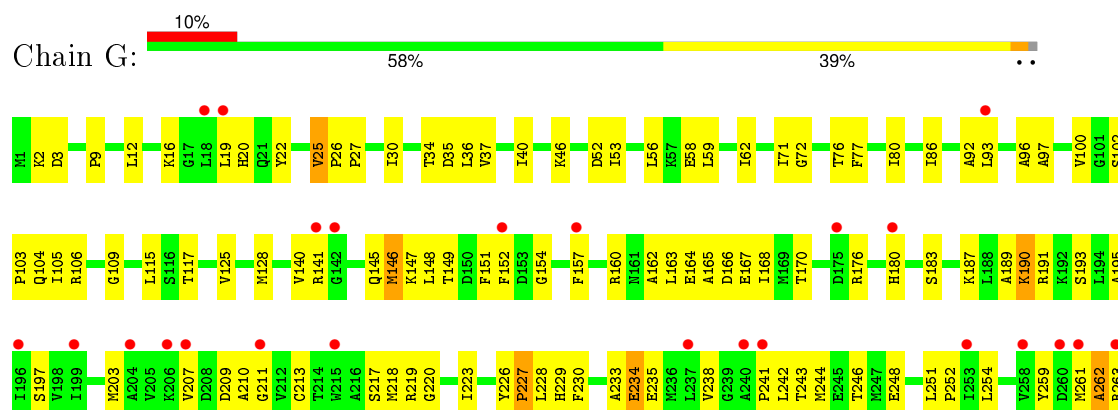
• Molecule 2: Nicotinate dehydrogenase medium molybdopterin subunit

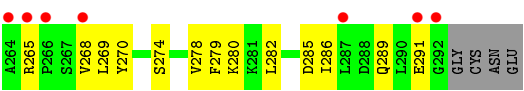


• Molecule 3: Nicotinate dehydrogenase FAD-subunit

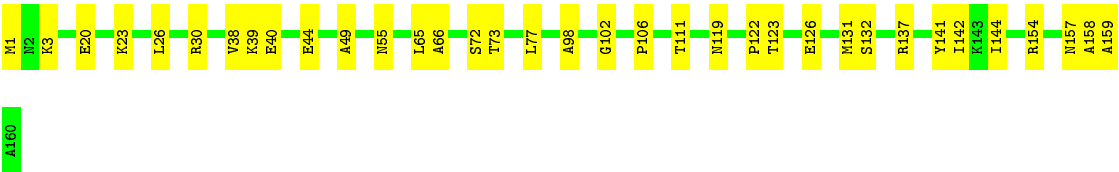
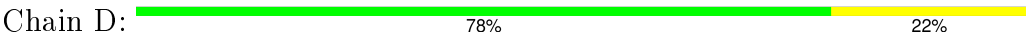


• Molecule 3: Nicotinate dehydrogenase FAD-subunit

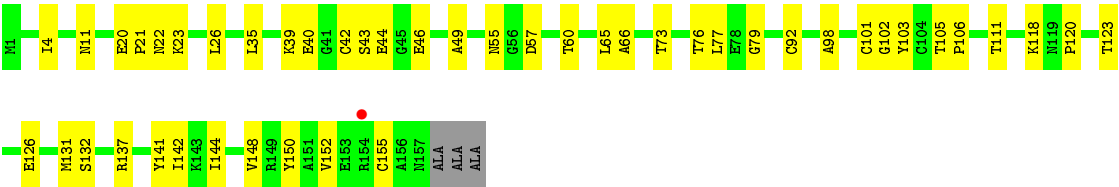




● Molecule 4: Nicotinate dehydrogenase small FeS subunit



● Molecule 4: Nicotinate dehydrogenase small FeS subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.07 Å 71.70 Å 214.49 Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	29.43 – 2.20 29.43 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.43-2.20) 98.9 (29.43-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.20 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.213 , 0.251 0.213 , 0.250	Depositor DCC
$R_{free}$ test set	7408 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 26.1	EDS
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 148159 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19284	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 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: MCN, MG, NIO, MOS, CA, FES, FAD, SE, NO3

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	0.36	0/3273	0.65	1/4432 (0.0%)
1	E	0.29	0/3273	0.57	0/4432
2	B	0.34	0/2452	0.67	0/3327
2	F	0.29	0/2452	0.60	0/3327
3	C	0.36	0/2284	0.63	0/3083
3	G	0.26	0/2288	0.51	0/3088
4	D	0.35	0/1188	0.65	0/1609
4	H	0.29	0/1173	0.60	0/1588
All	All	0.32	0/18383	0.61	1/24886 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	GLU	N-CA-C	-5.34	96.59	111.00

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	A	3213	0	3193	81	0
1	E	3213	0	3194	136	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2410	0	2391	114	0
2	F	2410	0	2391	166	0
3	C	2246	0	2281	53	0
3	G	2250	0	2284	101	0
4	D	1176	0	1168	23	0
4	H	1161	0	1153	32	0
5	A	1	0	0	2	0
5	E	1	0	0	1	0
6	A	4	0	0	0	0
6	C	4	0	0	1	0
6	E	4	0	0	0	0
7	A	2	0	0	0	0
8	B	3	0	0	1	0
8	F	3	0	0	1	0
9	B	44	0	17	1	0
9	F	44	0	17	1	0
10	B	9	0	4	0	0
10	E	9	0	4	2	0
11	C	53	0	31	1	0
11	G	53	0	31	2	0
12	D	8	0	0	0	0
12	H	8	0	0	0	0
13	E	1	0	0	0	0
14	A	258	0	0	8	0
14	B	170	0	0	5	0
14	C	209	0	0	8	1
14	D	112	0	0	2	0
14	E	95	0	0	3	0
14	F	59	0	0	6	0
14	G	25	0	0	1	0
14	H	26	0	0	0	0
All	All	19284	0	18159	644	1

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 18.

The worst 5 of 644 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)
2:B:108:LEU:HA	2:B:149:MET:HE1	1.40	1.04
1:A:19:GLU:HG2	1:E:198:GLU:HA	1.39	1.03

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:PRO:HB3	2:B:12:TRP:HB2	1.44	1.00
2:B:119:ALA:HB3	2:B:120:PRO:HD3	1.43	0.99
2:B:132:ILE:HD13	2:B:136:PRO:HG3	1.46	0.97

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:299:HOH:O	14:C:300:HOH:O[2_455]	2.07	0.13

## 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	A	418/425 (98%)	399 (96%)	16 (4%)	3 (1%)	26	25
1	E	418/425 (98%)	383 (92%)	30 (7%)	5 (1%)	16	12
2	B	328/330 (99%)	300 (92%)	15 (5%)	13 (4%)	4	1
2	F	328/330 (99%)	289 (88%)	27 (8%)	12 (4%)	4	1
3	C	289/296 (98%)	275 (95%)	13 (4%)	1 (0%)	46	50
3	G	290/296 (98%)	255 (88%)	27 (9%)	8 (3%)	6	3
4	D	158/160 (99%)	152 (96%)	4 (2%)	2 (1%)	15	11
4	H	155/160 (97%)	145 (94%)	9 (6%)	1 (1%)	30	29
All	All	2384/2422 (98%)	2198 (92%)	141 (6%)	45 (2%)	10	6

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	114	GLU
2	B	115	LYS

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	117	ASP
2	B	125	PHE
2	B	133	THR

### 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	344/349 (99%)	337 (98%)	7 (2%)	63	76
1	E	344/349 (99%)	338 (98%)	6 (2%)	68	81
2	B	252/252 (100%)	245 (97%)	7 (3%)	51	63
2	F	252/252 (100%)	246 (98%)	6 (2%)	57	69
3	C	241/246 (98%)	231 (96%)	10 (4%)	37	45
3	G	241/246 (98%)	236 (98%)	5 (2%)	61	74
4	D	129/129 (100%)	129 (100%)	0	100	100
4	H	129/129 (100%)	128 (99%)	1 (1%)	86	93
All	All	1932/1952 (99%)	1890 (98%)	42 (2%)	60	72

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	147	LYS
3	C	285	ASP
3	G	35	ASP
3	C	157	PHE
3	C	257	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	232	GLN
1	E	108	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	G	232	GLN
4	D	55	ASN
1	E	6	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 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	NO3	A	5658	-	3,3,3	0.28	0	3,3,3	0.15	0
10	NIO	B	5661	-	6,9,9	2.43	3 (50%)	8,11,11	1.38	1 (12%)
8	MOS	B	920	9,5	0,2,3	0.00	-	0,1,3	0.00	-
9	MCN	B	921	8	32,48,48	2.83	7 (21%)	39,74,74	1.68	7 (17%)
6	NO3	C	5659	-	3,3,3	0.34	0	3,3,3	0.12	0
11	FAD	C	900	-	48,58,58	2.24	14 (29%)	54,89,89	1.77	10 (18%)
12	FES	D	907	4	0,4,4	0.00	-	0,4,4	0.00	-
12	FES	D	908	4	0,4,4	0.00	-	0,4,4	0.00	-
10	NIO	E	5660	-	6,9,9	2.47	4 (66%)	8,11,11	1.32	1 (12%)
6	NO3	E	5662	-	3,3,3	0.45	0	3,3,3	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MOS	F	920	9,5	0,2,3	0.00	-	0,1,3	0.00	-
9	MCN	F	921	8	32,48,48	2.90	6 (18%)	39,74,74	1.59	7 (17%)
11	FAD	G	900	-	48,58,58	2.29	17 (35%)	54,89,89	1.80	10 (18%)
12	FES	H	907	4	0,4,4	0.00	-	0,4,4	0.00	-
12	FES	H	908	4	0,4,4	0.00	-	0,4,4	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
6	NO3	A	5658	-	-	0/0/0/0	0/0/0/0
10	NIO	B	5661	-	-	0/0/4/4	0/1/1/1
8	MOS	B	920	9,5	-	0/0/0/0	0/0/0/0
9	MCN	B	921	8	-	0/18/54/54	0/5/5/5
6	NO3	C	5659	-	-	0/0/0/0	0/0/0/0
11	FAD	C	900	-	-	0/30/50/50	0/6/6/6
12	FES	D	907	4	-	0/0/4/4	0/1/1/1
12	FES	D	908	4	-	0/0/4/4	0/1/1/1
10	NIO	E	5660	-	-	0/0/4/4	0/1/1/1
6	NO3	E	5662	-	-	0/0/0/0	0/0/0/0
8	MOS	F	920	9,5	-	0/0/0/0	0/0/0/0
9	MCN	F	921	8	-	0/18/54/54	0/5/5/5
11	FAD	G	900	-	-	0/30/50/50	0/6/6/6
12	FES	H	907	4	-	0/0/4/4	0/1/1/1
12	FES	H	908	4	-	0/0/4/4	0/1/1/1

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	900	FAD	PA-O2A	-4.86	1.34	1.54
11	C	900	FAD	PA-O2A	-4.83	1.34	1.54
9	F	921	MCN	O4D-C1'	-4.49	1.35	1.41
9	B	921	MCN	O4D-C1'	-4.22	1.35	1.41
11	G	900	FAD	P-O2P	-3.55	1.39	1.54

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	921	MCN	N1'-C2'-N3'	-5.30	119.36	127.44
9	F	921	MCN	N1'-C2'-N3'	-5.18	119.56	127.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	900	FAD	C4X-C4-N3	-4.70	117.16	123.59
11	C	900	FAD	C4X-C4-N3	-4.48	117.46	123.59
11	G	900	FAD	C4-C4X-C10	-4.17	117.27	119.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	920	MOS	1	0
9	B	921	MCN	1	0
6	C	5659	NO3	1	0
11	C	900	FAD	1	0
10	E	5660	NIO	2	0
8	F	920	MOS	1	0
9	F	921	MCN	1	0
11	G	900	FAD	2	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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	420/425 (98%)	-0.70	0 100 100	8, 20, 32, 69	1 (0%)
1	E	420/425 (98%)	-0.16	7 (1%) 73 72	20, 42, 72, 85	0
2	B	330/330 (100%)	-0.48	9 (2%) 58 57	9, 20, 77, 115	1 (0%)
2	F	330/330 (100%)	-0.03	13 (3%) 43 42	20, 42, 81, 101	0
3	C	291/296 (98%)	-0.63	2 (0%) 89 88	9, 20, 43, 62	1 (0%)
3	G	292/296 (98%)	0.64	31 (10%) 8 7	35, 63, 89, 123	1 (0%)
4	D	160/160 (100%)	-0.69	0 100 100	10, 17, 38, 52	0
4	H	157/160 (98%)	-0.30	1 (0%) 90 90	26, 37, 56, 70	0
All	All	2400/2422 (99%)	-0.29	63 (2%) 59 58	8, 30, 75, 123	4 (0%)

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	131	PHE	6.6
3	G	264	ALA	5.8
3	G	266	PRO	5.0
2	B	134	ALA	4.8
2	B	123	LEU	4.8

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SE	A	922	1/1	0.98	0.29	14.12	21,21,21,21	1
10	NIO	B	5661	9/9	0.81	0.25	6.98	24,25,26,26	9
5	SE	E	922	1/1	0.94	0.22	5.26	38,38,38,38	1
10	NIO	E	5660	9/9	0.86	0.15	3.27	42,42,44,44	0
12	FES	D	907	4/4	1.00	0.11	2.12	10,11,13,13	0
8	MOS	B	920	3/4	1.00	0.13	1.96	9,9,14,17	0
7	MG	A	426	1/1	0.99	0.11	1.87	21,21,21,21	0
12	FES	D	908	4/4	1.00	0.10	1.83	11,12,15,15	0
9	MCN	B	921	44/44	0.98	0.10	0.56	11,15,21,23	0
9	MCN	F	921	44/44	0.97	0.11	0.18	24,31,35,37	0
12	FES	H	908	4/4	0.99	0.11	-0.09	36,36,37,37	0
8	MOS	F	920	3/4	0.99	0.10	-0.13	34,34,35,37	0
11	FAD	C	900	53/53	0.98	0.09	-0.46	1,12,18,20	0
11	FAD	G	900	53/53	0.94	0.11	-0.60	36,41,44,49	0
13	CA	E	5663	1/1	0.96	0.08	-0.68	48,48,48,48	0
7	MG	A	427	1/1	0.99	0.08	-0.77	23,23,23,23	0
6	NO3	C	5659	4/4	0.96	0.09	-0.89	29,31,32,32	0
12	FES	H	907	4/4	0.99	0.08	-0.93	27,29,30,31	0
6	NO3	E	5662	4/4	0.98	0.07	-1.86	44,44,44,45	0
6	NO3	A	5658	4/4	0.98	0.06	-2.52	20,20,21,23	0

## 6.5 Other polymers

There are no such residues in this entry.