



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:35 AM UTC

PDB ID : 3LRX / pdb\_00003lrx  
Title : Crystal Structure of the C-terminal domain (residues 78-226) of PF1911 hydro-  
genase from *Pyrococcus furiosus*, Northeast Structural Genomics Consortium  
Target Pfr246A  
Authors : Forouhar, F.; Abashidze, M.; Seetharaman, J.; Mao, M.; Xiao, R.; Ciccocanti,  
C.; Foote, E.L.; Belote, R.L.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost,  
B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics  
Consortium (NESG)  
Deposited on : 2010-02-11  
Resolution : 2.60 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
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)

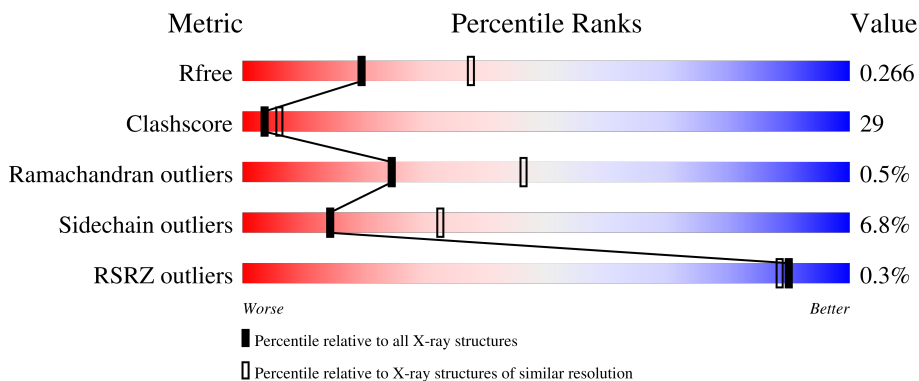
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)


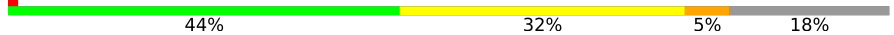

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ . 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	158	
1	B	158	
1	C	158	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	158	 41% 37% 5% 17%
1	E	158	%  44% 32% 6% 18%
1	F	158	 43% 34% 3% 20%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6291 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 Putative hydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	132	1045	679	168	193	5	0	0	0
1	B	132	1045	679	168	193	5	0	0	0
1	C	129	1026	669	165	187	5	0	0	0
1	D	131	1037	673	167	192	5	0	0	0
1	E	129	1026	671	167	183	5	0	0	0
1	F	127	1005	655	160	185	5	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MSE	-	initiating methionine	UNP Q8TZS3
A	227	LEU	-	expression tag	UNP Q8TZS3
A	228	GLU	-	expression tag	UNP Q8TZS3
A	229	HIS	-	expression tag	UNP Q8TZS3
A	230	HIS	-	expression tag	UNP Q8TZS3
A	231	HIS	-	expression tag	UNP Q8TZS3
A	232	HIS	-	expression tag	UNP Q8TZS3
A	233	HIS	-	expression tag	UNP Q8TZS3
A	234	HIS	-	expression tag	UNP Q8TZS3
B	77	MSE	-	initiating methionine	UNP Q8TZS3
B	227	LEU	-	expression tag	UNP Q8TZS3
B	228	GLU	-	expression tag	UNP Q8TZS3
B	229	HIS	-	expression tag	UNP Q8TZS3
B	230	HIS	-	expression tag	UNP Q8TZS3
B	231	HIS	-	expression tag	UNP Q8TZS3
B	232	HIS	-	expression tag	UNP Q8TZS3
B	233	HIS	-	expression tag	UNP Q8TZS3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	234	HIS	-	expression tag	UNP Q8TZS3
C	77	MSE	-	initiating methionine	UNP Q8TZS3
C	227	LEU	-	expression tag	UNP Q8TZS3
C	228	GLU	-	expression tag	UNP Q8TZS3
C	229	HIS	-	expression tag	UNP Q8TZS3
C	230	HIS	-	expression tag	UNP Q8TZS3
C	231	HIS	-	expression tag	UNP Q8TZS3
C	232	HIS	-	expression tag	UNP Q8TZS3
C	233	HIS	-	expression tag	UNP Q8TZS3
C	234	HIS	-	expression tag	UNP Q8TZS3
D	77	MSE	-	initiating methionine	UNP Q8TZS3
D	227	LEU	-	expression tag	UNP Q8TZS3
D	228	GLU	-	expression tag	UNP Q8TZS3
D	229	HIS	-	expression tag	UNP Q8TZS3
D	230	HIS	-	expression tag	UNP Q8TZS3
D	231	HIS	-	expression tag	UNP Q8TZS3
D	232	HIS	-	expression tag	UNP Q8TZS3
D	233	HIS	-	expression tag	UNP Q8TZS3
D	234	HIS	-	expression tag	UNP Q8TZS3
E	77	MSE	-	initiating methionine	UNP Q8TZS3
E	227	LEU	-	expression tag	UNP Q8TZS3
E	228	GLU	-	expression tag	UNP Q8TZS3
E	229	HIS	-	expression tag	UNP Q8TZS3
E	230	HIS	-	expression tag	UNP Q8TZS3
E	231	HIS	-	expression tag	UNP Q8TZS3
E	232	HIS	-	expression tag	UNP Q8TZS3
E	233	HIS	-	expression tag	UNP Q8TZS3
E	234	HIS	-	expression tag	UNP Q8TZS3
F	77	MSE	-	initiating methionine	UNP Q8TZS3
F	227	LEU	-	expression tag	UNP Q8TZS3
F	228	GLU	-	expression tag	UNP Q8TZS3
F	229	HIS	-	expression tag	UNP Q8TZS3
F	230	HIS	-	expression tag	UNP Q8TZS3
F	231	HIS	-	expression tag	UNP Q8TZS3
F	232	HIS	-	expression tag	UNP Q8TZS3
F	233	HIS	-	expression tag	UNP Q8TZS3
F	234	HIS	-	expression tag	UNP Q8TZS3

- Molecule 2 is water.

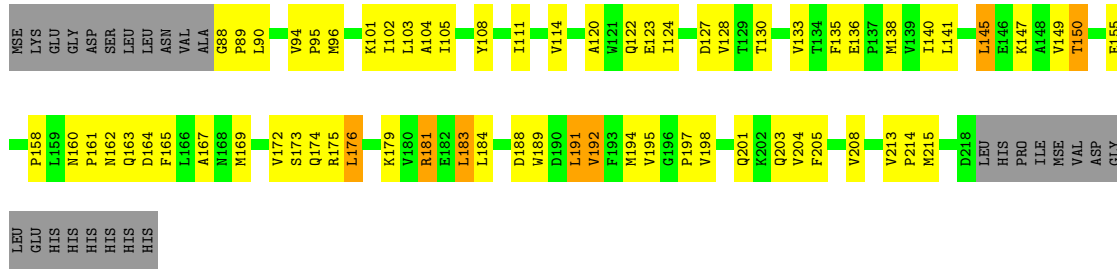
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	21	Total O 21 21	0	0

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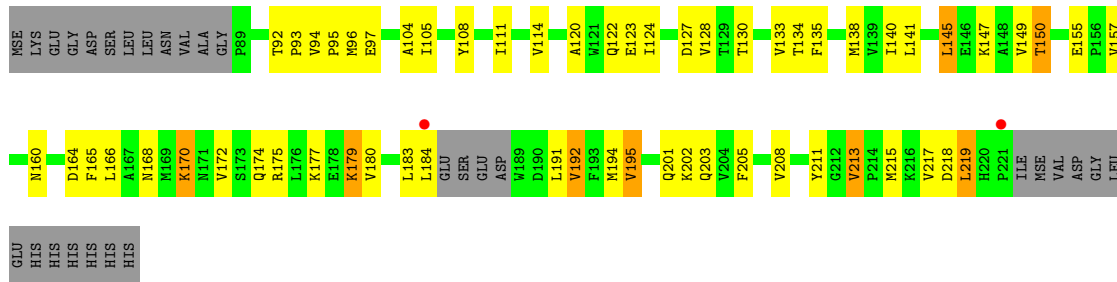
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
2	B	28	Total O 28 28	0	0
2	C	17	Total O 17 17	0	0
2	D	21	Total O 21 21	0	0
2	E	12	Total O 12 12	0	0
2	F	8	Total O 8 8	0	0

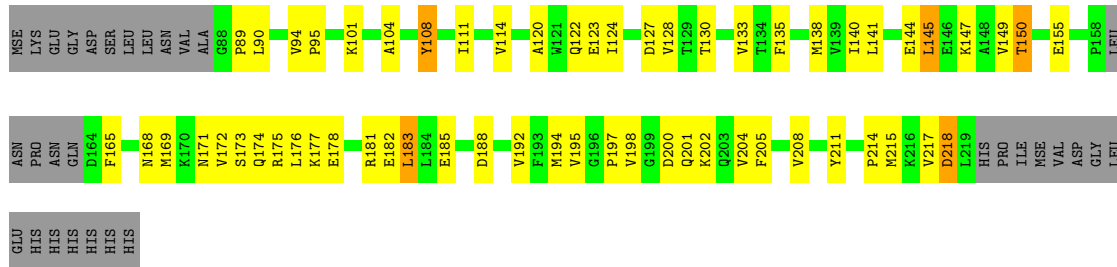




● Molecule 1: Putative hydrogenase



● Molecule 1: Putative hydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.20Å 77.20Å 110.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.30 – 2.60 19.30 – 2.60	Depositor EDS
% Data completeness (in resolution range)	78.6 (19.30-2.60) 92.9 (19.30-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2 & XtalView, REFMAC	Depositor
R, $R_{free}$	0.195 , 0.252 0.214 , 0.266	Depositor DCC
$R_{free}$ test set	4100 reflections (9.48%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.5	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.047 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6291	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5072e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.60	0/1063	0.91	1/1436 (0.1%)
1	B	0.60	0/1063	1.06	4/1436 (0.3%)
1	C	0.57	0/1043	0.88	1/1407 (0.1%)
1	D	0.56	0/1055	0.90	1/1425 (0.1%)
1	E	0.54	0/1045	0.89	1/1411 (0.1%)
1	F	0.57	0/1021	0.93	1/1376 (0.1%)
All	All	0.57	0/6290	0.93	9/8491 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	ARG	NE-CZ-NH2	13.72	131.54	119.20
1	B	151	ARG	NE-CZ-NH1	-12.66	108.84	121.50
1	B	151	ARG	CD-NE-CZ	10.87	139.61	124.40
1	B	108	TYR	CB-CA-C	-6.71	108.85	116.63
1	D	108	TYR	CB-CA-C	-6.56	109.02	116.63

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	1045	0	1069	63	0
1	B	1045	0	1069	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1026	0	1055	54	0
1	D	1037	0	1058	75	0
1	E	1026	0	1059	66	0
1	F	1005	0	1030	63	0
2	A	21	0	0	1	0
2	B	28	0	0	2	0
2	C	17	0	0	1	0
2	D	21	0	0	5	0
2	E	12	0	0	2	0
2	F	8	0	0	1	0
All	All	6291	0	6340	367	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 29.

The worst 5 of 367 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)
1:F:192:VAL:HG11	1:F:208:VAL:HG21	1.45	0.96
1:B:192:VAL:HG11	1:B:208:VAL:HG21	1.49	0.95
1:D:160:ASN:HD22	1:D:163:GLN:HG3	1.33	0.94
1:A:194:MSE:HE2	1:A:201:GLN:HG2	1.54	0.90
1:A:127:ASP:OD1	1:A:150:THR:HG21	1.72	0.89

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	Allowed	Outliers	Percentiles
1	A	130/158 (82%)	117 (90%)	13 (10%)	0	100 100
1	B	130/158 (82%)	117 (90%)	11 (8%)	2 (2%)	8 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	125/158 (79%)	115 (92%)	10 (8%)	0	100	100
1	D	129/158 (82%)	115 (89%)	13 (10%)	1 (1%)	16	34
1	E	125/158 (79%)	112 (90%)	13 (10%)	0	100	100
1	F	123/158 (78%)	112 (91%)	10 (8%)	1 (1%)	16	34
All	All	762/948 (80%)	688 (90%)	70 (9%)	4 (0%)	24	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	SER
1	B	174	GLN
1	F	218	ASP
1	D	161	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 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	117/133 (88%)	109 (93%)	8 (7%)	14	32
1	B	117/133 (88%)	108 (92%)	9 (8%)	12	27
1	C	115/133 (86%)	108 (94%)	7 (6%)	17	37
1	D	116/133 (87%)	107 (92%)	9 (8%)	11	26
1	E	115/133 (86%)	106 (92%)	9 (8%)	11	26
1	F	112/133 (84%)	107 (96%)	5 (4%)	24	50
All	All	692/798 (87%)	645 (93%)	47 (7%)	14	32

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	181	ARG
1	E	150	THR
1	D	183	LEU

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Mol	Chain	Res	Type
1	D	195	VAL
1	E	179	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	122	GLN
1	D	203	GLN
1	D	201	GLN
1	E	122	GLN
1	B	163	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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<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	127/158 (80%)	-0.19	0	100   100	12, 30, 51, 60	0
1	B	127/158 (80%)	-0.12	0	100   100	12, 33, 52, 65	0
1	C	124/158 (78%)	-0.03	0	100   100	19, 36, 56, 65	0
1	D	126/158 (79%)	0.01	0	100   100	13, 35, 61, 79	0
1	E	124/158 (78%)	0.13	2 (1%)	70   66	18, 39, 59, 70	0
1	F	122/158 (77%)	-0.11	0	100   100	16, 33, 54, 67	0
All	All	750/948 (79%)	-0.05	2 (0%)	90   88	12, 34, 56, 79	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	184	LEU	2.4
1	E	221	PRO	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.