



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:58 pm BST

PDB ID : 2IA0
Title : Transcriptional Regulatory Protein PF0864 From *Pyrococcus Furiosus* a Member of the ASNC Family (PF0864)
Authors : Yang, H.; Chang, J.; Liu, Z.J.; Rose, J.P.; Wang, B.C.; Southeast Collaboratory for Structural Genomics; Southeast Collaboratory for Structural Genomics (SECSG)
Deposited on : 2006-09-06
Resolution : 2.37 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

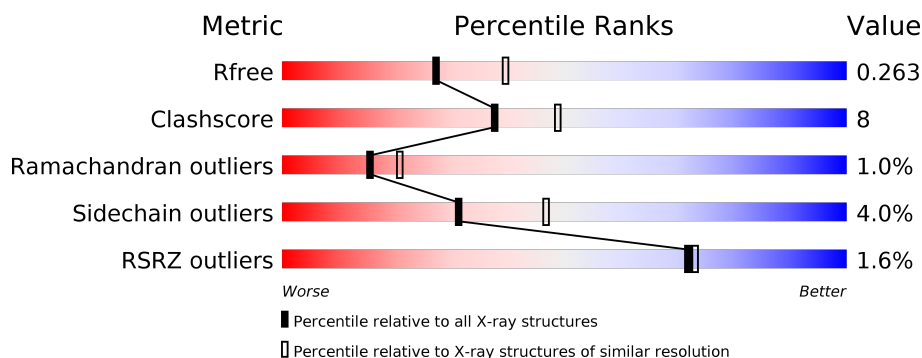
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 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	171	<div> <div> <div></div> <div>74%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> <div> <div>2%</div> <div>69%</div> <div>15%</div> <div>5%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	171	<div> <div> <div></div> <div>74%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> <div> <div>2%</div> <div>69%</div> <div>15%</div> <div>5%</div> <div>•</div> <div>11%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2572 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 HTH-type transcriptional regulator PF0864.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	15	0	0
			1249	807	210	232			
1	B	153	Total	C	N	O	2	0	0
			1224	793	204	227			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	CLONING ARTIFACT	UNP Q8U2H1
A	-7	ALA	-	CLONING ARTIFACT	UNP Q8U2H1
A	-6	HIS	-	EXPRESSION TAG	UNP Q8U2H1
A	-5	HIS	-	EXPRESSION TAG	UNP Q8U2H1
A	-4	HIS	-	EXPRESSION TAG	UNP Q8U2H1
A	-3	HIS	-	EXPRESSION TAG	UNP Q8U2H1
A	-2	HIS	-	EXPRESSION TAG	UNP Q8U2H1
A	-1	HIS	-	EXPRESSION TAG	UNP Q8U2H1
A	0	GLY	-	CLONING ARTIFACT	UNP Q8U2H1
A	1	SER	-	CLONING ARTIFACT	UNP Q8U2H1
B	-8	MET	-	CLONING ARTIFACT	UNP Q8U2H1
B	-7	ALA	-	CLONING ARTIFACT	UNP Q8U2H1
B	-6	HIS	-	EXPRESSION TAG	UNP Q8U2H1
B	-5	HIS	-	EXPRESSION TAG	UNP Q8U2H1
B	-4	HIS	-	EXPRESSION TAG	UNP Q8U2H1
B	-3	HIS	-	EXPRESSION TAG	UNP Q8U2H1
B	-2	HIS	-	EXPRESSION TAG	UNP Q8U2H1
B	-1	HIS	-	EXPRESSION TAG	UNP Q8U2H1
B	0	GLY	-	CLONING ARTIFACT	UNP Q8U2H1
B	1	SER	-	CLONING ARTIFACT	UNP Q8U2H1

- Molecule 2 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Au 1	0	0
2	A	1	Total 1	Au 1	0	0

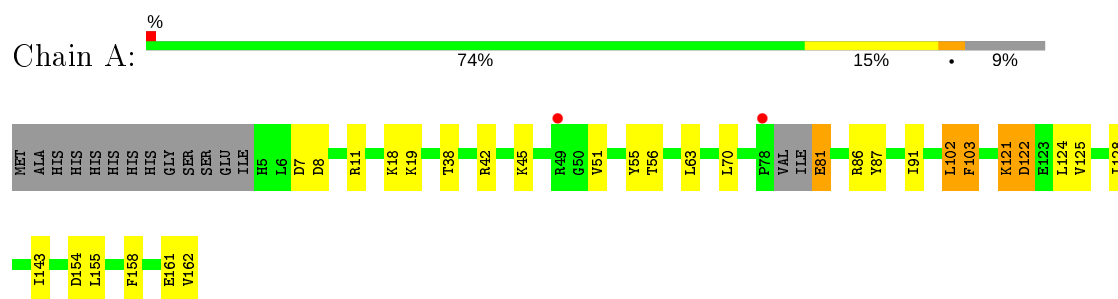
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total 53	O 53	0	0
3	B	44	Total 44	O 44	0	0

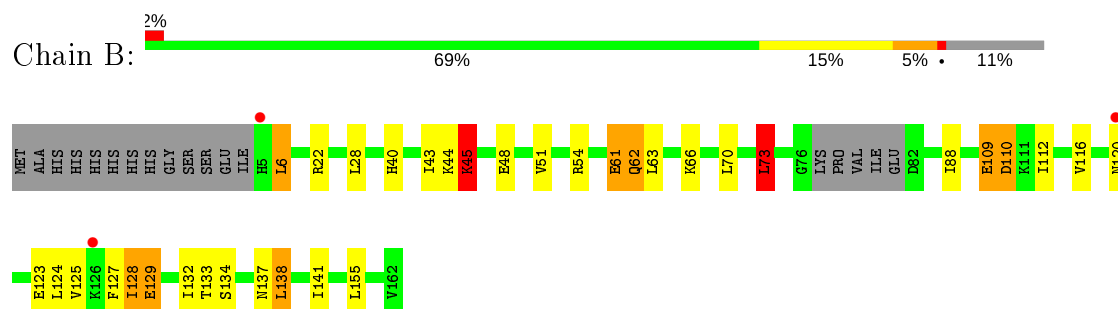
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Putative HTH-type transcriptional regulator PF0864



- Molecule 1: Putative HTH-type transcriptional regulator PF0864



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.07Å 70.37Å 96.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.89 – 2.37 48.27 – 2.37	Depositor EDS
% Data completeness (in resolution range)	91.7 (56.89-2.37) 91.7 (48.27-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.269 0.201 , 0.263	Depositor DCC
R_{free} test set	776 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2572	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AU

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	2.54	4/1265 (0.3%)	0.95	9/1701 (0.5%)
1	B	0.62	1/1240 (0.1%)	0.97	8/1668 (0.5%)
All	All	1.86	5/2505 (0.2%)	0.96	17/3369 (0.5%)

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	1
1	B	1	3
All	All	1	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	LYS	CE-NZ	86.81	3.66	1.49
1	A	81	GLU	CB-CG	6.99	1.65	1.52
1	A	161	GLU	CG-CD	5.80	1.60	1.51
1	B	45	LYS	N-CA	-5.74	1.34	1.46
1	A	19	LYS	N-CA	-5.20	1.35	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	LYS	CD-CE-NZ	11.53	138.22	111.70
1	A	19	LYS	N-CA-CB	11.13	130.63	110.60
1	B	73	LEU	CA-CB-CG	9.66	137.53	115.30
1	B	129	GLU	N-CA-C	-8.83	87.15	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	LYS	O-C-N	-8.32	109.39	122.70
1	A	18	LYS	O-C-N	-8.31	109.39	122.70
1	A	19	LYS	CD-CE-NZ	8.08	130.29	111.70
1	A	18	LYS	C-N-CA	7.56	140.61	121.70
1	B	138	LEU	N-CA-C	6.32	128.06	111.00
1	A	18	LYS	CA-C-N	5.99	130.37	117.20
1	B	44	LYS	CA-C-N	5.94	130.27	117.20
1	A	103	PHE	N-CA-CB	5.90	121.21	110.60
1	A	121	LYS	C-N-CA	5.24	134.79	121.70
1	B	44	LYS	C-N-CA	5.20	134.69	121.70
1	A	81	GLU	CA-CB-CG	-5.15	102.07	113.40
1	A	86	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	6	LEU	CA-CB-CG	5.05	126.91	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	138	LEU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	LEU	Peptide
1	B	109	GLU	Peptide
1	B	128	ILE	Peptide
1	B	137	ASN	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	1249	0	1316	19	0
1	B	1224	0	1296	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	53	0	0	3	0
3	B	44	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2572	0	2612	39	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 8.

All (39) 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:B:61:GLU:OE1	1:B:62:GLN:NE2	2.17	0.76
1:A:128:ILE:HD13	1:A:143:ILE:HD13	1.68	0.75
1:B:133:THR:HG22	1:B:141:ILE:HD13	1.75	0.69
1:A:122:ASP:H	1:A:125:VAL:H	1.42	0.65
1:B:124:LEU:O	1:B:128:ILE:HG13	1.98	0.62
1:A:63:LEU:HD11	1:B:6:LEU:HD11	1.85	0.59
1:B:141:ILE:HG13	1:B:141:ILE:O	2.03	0.57
1:A:63:LEU:CD1	1:B:51:VAL:HG13	2.35	0.57
1:B:116:VAL:HG11	1:B:127:PHE:CE2	2.40	0.57
1:A:8:ASP:OD1	1:A:11:ARG:NH1	2.38	0.56
1:B:155:LEU:HG	3:B:3041:HOH:O	2.04	0.56
1:B:73:LEU:HD22	1:B:112:ILE:HB	1.87	0.56
1:A:87:TYR:CE2	1:A:91:ILE:HD11	2.40	0.56
1:B:88:ILE:CD1	1:B:110:ASP:H	2.19	0.56
1:B:88:ILE:HD13	1:B:110:ASP:H	1.71	0.56
1:A:63:LEU:HD13	1:B:51:VAL:HG13	1.87	0.55
1:A:45:LYS:HE3	3:A:3050:HOH:O	2.06	0.55
1:A:38:THR:O	1:A:42:ARG:HG2	2.08	0.54
1:B:109:GLU:CA	1:B:110:ASP:HB2	2.39	0.53
1:A:56:THR:HG21	1:A:158:PHE:HE1	1.77	0.49
1:A:121:LYS:N	1:A:122:ASP:CB	2.76	0.48
1:A:121:LYS:N	1:A:122:ASP:HB3	2.29	0.48
1:B:125:VAL:O	1:B:129:GLU:HB2	2.15	0.47
1:B:45:LYS:HA	1:B:48:GLU:HG2	1.97	0.47
1:B:61:GLU:HB3	1:B:62:GLN:H	1.43	0.46
1:A:70:LEU:HD21	1:B:70:LEU:HD21	1.97	0.45
1:A:55:TYR:CD2	1:B:22:ARG:HD3	2.52	0.45
1:A:121:LYS:HG3	3:A:3051:HOH:O	2.18	0.43
1:B:109:GLU:N	1:B:110:ASP:HB2	2.33	0.43
1:B:120:ASN:HB3	1:B:123:GLU:HB2	2.01	0.43
1:A:154:ASP:OD2	1:B:54:ARG:NH1	2.49	0.43
1:B:28:LEU:CD1	1:B:43:ILE:HD11	2.49	0.42
1:B:132:ILE:C	1:B:134:SER:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:HG	1:B:138:LEU:HD11	2.02	0.41
1:A:7:ASP:HB2	3:A:3030:HOH:O	2.19	0.41
1:B:109:GLU:H	1:B:110:ASP:HB2	1.85	0.41
1:A:51:VAL:HG13	1:B:63:LEU:HD12	2.02	0.41
1:A:121:LYS:H	1:A:122:ASP:CB	2.34	0.41
1:B:54:ARG:NH2	3:B:3033:HOH:O	2.55	0.40

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	152/171 (89%)	146 (96%)	4 (3%)	2 (1%)	12	15
1	B	149/171 (87%)	146 (98%)	2 (1%)	1 (1%)	22	30
All	All	301/342 (88%)	292 (97%)	6 (2%)	3 (1%)	15	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	PHE
1	A	122	ASP
1	B	110	ASP

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	140/155 (90%)	135 (96%)	5 (4%)	35	51
1	B	138/155 (89%)	132 (96%)	6 (4%)	29	43
All	All	278/310 (90%)	267 (96%)	11 (4%)	31	47

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLU
1	A	102	LEU
1	A	124	LEU
1	A	155	LEU
1	A	162	VAL
1	B	40	HIS
1	B	45	LYS
1	B	61	GLU
1	B	62	GLN
1	B	66	LYS
1	B	73	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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, 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	156/171 (91%)	0.10	2 (1%) 77 78	7, 18, 24, 31	4 (2%)
1	B	153/171 (89%)	0.20	3 (1%) 65 66	10, 19, 27, 34	1 (0%)
All	All	309/342 (90%)	0.15	5 (1%) 72 73	7, 18, 26, 34	5 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	PRO	3.8
1	B	5	HIS	3.5
1	A	49	ARG	3.3
1	B	120	ASN	2.6
1	B	126	LYS	2.2

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 carbohydrates in this entry.

6.4 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(\AA^2)	Q<0.9
2	AU	A	3001	1/1	1.00	0.13	25,25,25,25	1
2	AU	B	3002	1/1	1.00	0.11	33,33,33,33	1

6.5 Other polymers [i](#)

There are no such residues in this entry.