Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2GMG
Title	:	Solution NMR Structure of protein PF0610 from Pyrococcus furiosus, Northeast Structural Genomics Consortium Target PfG3
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Deposited on	:	2006-04-06

This is a Full wwPDB NMR 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

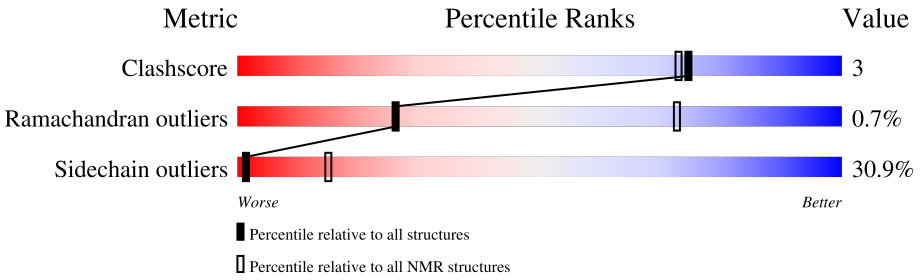
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	105	53% 27% • 18%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:9-A:34, A:41-A:87, A:93-A:105 (86)	0.54	4

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	2, 4, 5, 6, 8, 10
2	1, 3
Single-model clusters	7; 9

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1757 atoms, of which 906 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called hypothetical protein Pf0610.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	105	1757	539	906	161	145	6	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP Q8U362
A	2	HIS	-	expression tag	UNP Q8U362
A	3	HIS	-	expression tag	UNP Q8U362
A	4	HIS	-	expression tag	UNP Q8U362
A	5	HIS	-	expression tag	UNP Q8U362
A	6	HIS	-	expression tag	UNP Q8U362
A	7	HIS	-	expression tag	UNP Q8U362
A	8	GLY	-	expression tag	UNP Q8U362
A	9	SER	-	expression tag	UNP Q8U362

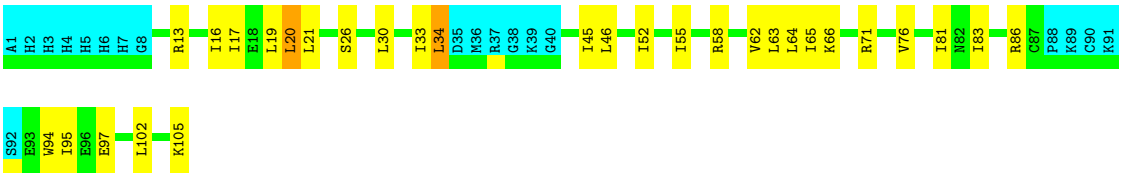
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: hypothetical protein Pf0610

Chain A:

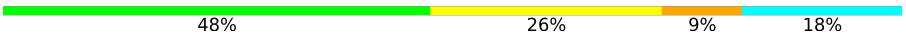


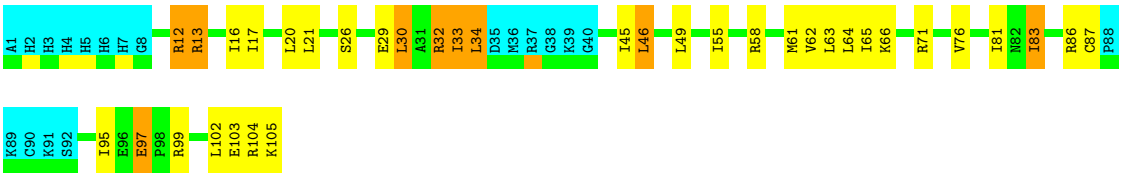
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: hypothetical protein Pf0610

Chain A: 



4.2.2 Score per residue for model 2

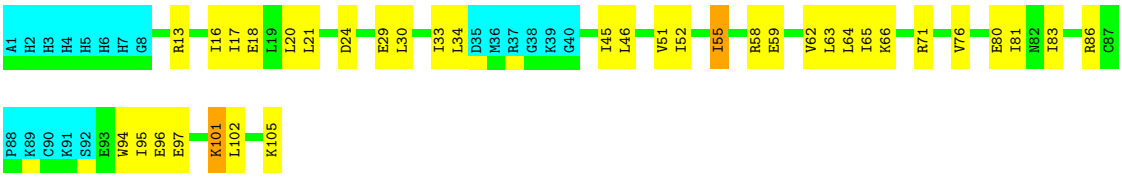
• Molecule 1: hypothetical protein Pf0610

Chain A:

4.2.3 Score per residue for model 3

- Molecule 1: hypothetical protein Pf0610

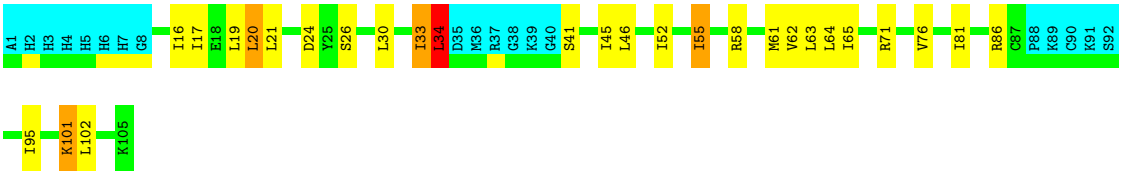
Chain A: 48% 32% • 18%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: hypothetical protein Pf0610

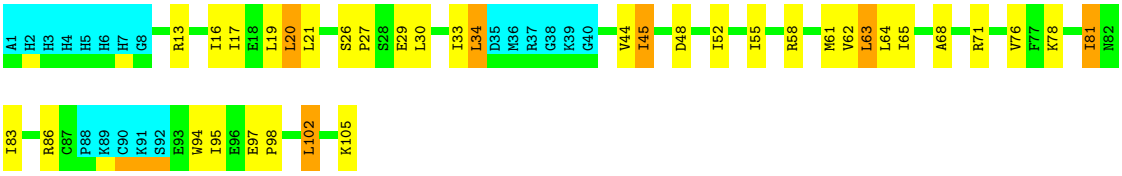
Chain A: 55% 22% • • 18%



4.2.5 Score per residue for model 5

- Molecule 1: hypothetical protein Pf0610

Chain A: 48% 29% 6% 18%



4.2.6 Score per residue for model 6

- Molecule 1: hypothetical protein Pf0610

Chain A: 50% 30% • 18%

A1 H2 H3 H4 H5 H6 H7 G8 S9 R12 R13 I16 I17 E18 L19 L20 L21 D24 L30 A31 R32 I33 L34 D35 M36 R37 G38 K39 G40 K43 V44 I45 L46 E47 D48 V51 I52 S53 K54 I55 R58 V62 L63 L64 I65 R71 K72 V76 I81

N82 I83 R86 C87 P88 K89 C90 K91 S92 I95 L102 K105

4.2.7 Score per residue for model 7

- Molecule 1: hypothetical protein Pf0610

Chain A: 50% 29% • • 18%

A1 H2 H3 H4 H5 H6 H7 G8 S9 R12 R13 I16 I17 E18 L19 L20 L21 S26 L30 I33 L34 D35 M36 R37 G38 K39 G40 I45 L49 I52 I55 A56 K57 R58 M61 V62 L63 L64 I65 Q69 C70 R71 V76 I81 N82 I83

R86 C87 P88 K89 C90 K91 S92 E93 W94 I95 L102 K105

4.2.8 Score per residue for model 8

- Molecule 1: hypothetical protein Pf0610

Chain A: 51% 26% 5% 18%

A1 H2 H3 H4 H5 H6 H7 G8 I16 I17 E18 L19 L20 L21 E22 P27 L30 A31 R32 I33 L34 D35 M36 R37 G38 K39 G40 S41 I45 R58 E59 V62 L63 L64 I65 Q69 C70 R71 V76 F77 K78 I81 N82 I83 P84 S85 R86 C87 P88 K89 C90

K91 S92 E93 W94 I95 E96 E97 L102 E103 R104 K105

4.2.9 Score per residue for model 9

- Molecule 1: hypothetical protein Pf0610

Chain A: 47% 31% • 18%

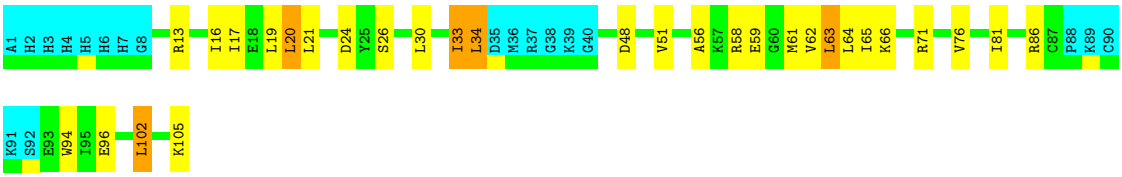
A1 H2 H3 H4 H5 H6 H7 G8 R12 R13 I16 I17 E18 L19 L20 L21 S26 L30 A31 R32 I33 L34 D35 M36 R37 G38 K39 G40 S41 I45 L46 L49 K50 V51 K57 R58 V62 L63 L64 I65 K66 Q69 C70 R71 F75 I81 N82 I83

R86 C87 P88 K89 C90 K91 S92 E93 W94 I95 E96 E97 P98 R99 L102 E103 R104 K105

4.2.10 Score per residue for model 10

- Molecule 1: hypothetical protein Pf0610

Chain A: 53% 24% 5% 18%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing using torsion angle dynamics*.

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	2.15
XPLOR-NIH	refinement	2.14

No chemical shift data was provided.

6 Model quality (i)

6.1 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 (average) 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	1.31±0.26	2±3/710 (0.3± 0.4%)	0.88±0.23	2±3/947 (0.2± 0.4%)
All	All	1.33	21/7100 (0.3%)	0.91	17/9470 (0.2%)

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	Planarity
1	A	0.0±0.0	2.4±1.2
All	All	0	24

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	87	CYS	C-N	7.17	1.47	1.34	9	2
1	A	26	SER	C-N	6.79	1.47	1.34	9	2
1	A	83	ILE	C-N	6.51	1.46	1.34	9	2
1	A	105	LYS	N-CA	6.45	1.59	1.46	1	6
1	A	97	GLU	C-N	6.42	1.46	1.34	1	2
1	A	104	ARG	C-N	6.12	1.48	1.34	1	1
1	A	66	LYS	C-N	6.07	1.45	1.34	9	2
1	A	105	LYS	CA-CB	5.50	1.66	1.53	1	1
1	A	33	ILE	CA-CB	5.30	1.67	1.54	9	2
1	A	103	GLU	CG-CD	5.11	1.59	1.51	1	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	13	ARG	NE-CZ-NH1	8.62	124.61	120.30	9	2
1	A	32	ARG	NE-CZ-NH1	8.44	124.52	120.30	1	2
1	A	12	ARG	NE-CZ-NH1	8.36	124.48	120.30	9	2
1	A	86	ARG	NE-CZ-NH1	8.00	124.30	120.30	9	2
1	A	71	ARG	NE-CZ-NH1	7.82	124.21	120.30	9	2
1	A	99	ARG	NE-CZ-NH1	7.61	124.10	120.30	9	2
1	A	58	ARG	NE-CZ-NH1	7.33	123.96	120.30	9	2
1	A	104	ARG	NE-CZ-NH1	6.61	123.60	120.30	9	2
1	A	86	ARG	NE-CZ-NH2	-5.59	117.50	120.30	1	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	58	ARG	Sidechain	8
1	A	71	ARG	Sidechain	8
1	A	86	ARG	Sidechain	8

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	701	760	760	5±2
All	All	7010	7600	7600	47

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 3.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ILE:O	1:A:34:LEU:HB2	0.68	1.88	7	2
1:A:13:ARG:HA	1:A:16:ILE:HD12	0.59	1.74	9	8
1:A:68:ALA:HB2	1:A:98:PRO:HG3	0.56	1.75	5	1
1:A:52:ILE:HA	1:A:55:ILE:HD12	0.53	1.80	6	4
1:A:43:LYS:HA	1:A:46:LEU:HD12	0.49	1.84	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:O	1:A:33:ILE:HG22	0.49	2.06	8	1
1:A:27:PRO:HB3	1:A:45:ILE:HG21	0.49	1.84	8	2
1:A:69:GLN:HG3	1:A:76:VAL:HG13	0.47	1.85	7	2
1:A:16:ILE:O	1:A:20:LEU:HB2	0.47	2.10	5	7
1:A:20:LEU:HD21	1:A:30:LEU:HD11	0.45	1.89	1	1
1:A:33:ILE:O	1:A:33:ILE:HG23	0.44	2.12	10	3
1:A:63:LEU:HG	1:A:102:LEU:HG	0.43	1.91	10	2
1:A:33:ILE:O	1:A:34:LEU:CB	0.43	2.62	7	1
1:A:24:ASP:HB3	1:A:101:LYS:HG3	0.42	1.91	4	2
1:A:46:LEU:HA	1:A:49:LEU:HD12	0.42	1.92	9	2
1:A:56:ALA:O	1:A:61:MET:O	0.42	2.37	7	2
1:A:69:GLN:HG3	1:A:76:VAL:HG23	0.42	1.89	8	1
1:A:48:ASP:O	1:A:52:ILE:HG12	0.42	2.14	6	2
1:A:81:ILE:H	1:A:81:ILE:HG13	0.41	1.60	5	1
1:A:27:PRO:HB3	1:A:45:ILE:HB	0.41	1.91	2	1
1:A:41:SER:O	1:A:45:ILE:HG12	0.40	2.17	2	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	85/105 (81%)	81±1 (95±1%)	4±1 (4±1%)	1±0 (1±1%)	26	73
All	All	850/1050 (81%)	807 (95%)	37 (4%)	6 (1%)	26	73

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	34	LEU	6

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	78/93 (84%)	54±2 (69±2%)	24±2 (31±2%)	1 15
All	All	780/930 (84%)	539 (69%)	241 (31%)	1 15

All 51 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	17	ILE	10
1	A	21	LEU	10
1	A	30	LEU	10
1	A	34	LEU	10
1	A	62	VAL	10
1	A	64	LEU	10
1	A	65	ILE	10
1	A	81	ILE	10
1	A	102	LEU	10
1	A	63	LEU	9
1	A	95	ILE	9
1	A	33	ILE	8
1	A	45	ILE	8
1	A	19	LEU	8
1	A	20	LEU	8
1	A	94	TRP	7
1	A	55	ILE	6
1	A	76	VAL	6
1	A	83	ILE	6
1	A	97	GLU	6
1	A	26	SER	5
1	A	51	VAL	5
1	A	46	LEU	4
1	A	59	GLU	4
1	A	66	LYS	4
1	A	12	ARG	3
1	A	29	GLU	3
1	A	32	ARG	3
1	A	61	MET	3
1	A	24	ASP	3
1	A	48	ASP	3
1	A	41	SER	3
1	A	49	LEU	2
1	A	57	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	96	GLU	2
1	A	101	LYS	2
1	A	78	LYS	2
1	A	9	SER	2
1	A	87	CYS	2
1	A	103	GLU	2
1	A	52	ILE	1
1	A	18	GLU	1
1	A	80	GLU	1
1	A	44	VAL	1
1	A	53	SER	1
1	A	72	LYS	1
1	A	82	ASN	1
1	A	22	GLU	1
1	A	85	SER	1
1	A	69	GLN	1
1	A	75	PHE	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided