Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2JMR
Title	:	NMR structure of the E. coli type 1 pilus subunit FimF
Authors	:	Gossert, A.D.; Bettendorff, P.; Puorger, C.; Vetsch, M.; Herrmann, T.; Fiorito, F.; Hiller, S.; Glockshuber, R.; Wuthrich, K.
Deposited on	:	2006-11-29

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

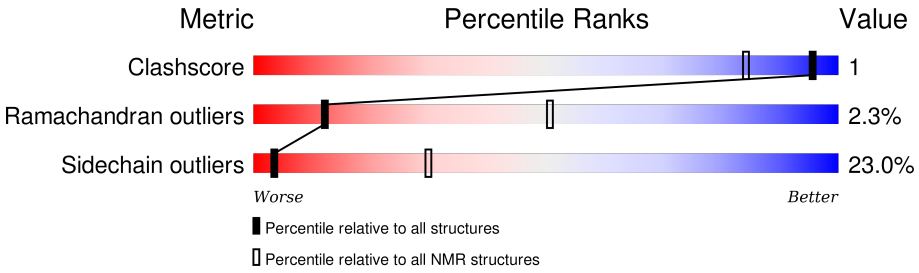
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 is 91%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	179	70% 15% 15%

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:16-A:155, A:167-A:179 (153)	0.53	6

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 3 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 6, 8, 10, 11, 13, 16, 18
2	17, 19
3	4, 7
Single-model clusters	9; 12; 14; 15; 20

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2669 atoms, of which 1321 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called fimF.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	179	2669	837	1321	243	263	5	0

There are 25 discrepancies between the modelled and reference sequences:

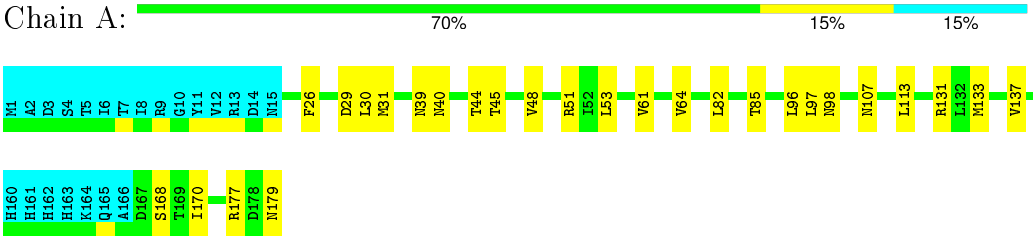
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P08189
A	156	ASP	-	SEE REMARK 999	UNP P08189
A	157	ASN	-	SEE REMARK 999	UNP P08189
A	158	HIS	-	SEE REMARK 999	UNP P08189
A	159	HIS	-	SEE REMARK 999	UNP P08189
A	160	HIS	-	SEE REMARK 999	UNP P08189
A	161	HIS	-	SEE REMARK 999	UNP P08189
A	162	HIS	-	SEE REMARK 999	UNP P08189
A	163	HIS	-	SEE REMARK 999	UNP P08189
A	164	LYS	-	SEE REMARK 999	UNP P08189
A	165	GLN	-	SEE REMARK 999	UNP P08189
A	166	ALA	-	SEE REMARK 999	UNP P08189
A	167	ASP	-	SEE REMARK 999	UNP P08189
A	168	SER	-	SEE REMARK 999	UNP P08189
A	169	THR	-	SEE REMARK 999	UNP P08189
A	170	ILE	-	SEE REMARK 999	UNP P08189
A	171	THR	-	SEE REMARK 999	UNP P08189
A	172	ILE	-	SEE REMARK 999	UNP P08189
A	173	ARG	-	SEE REMARK 999	UNP P08189
A	174	GLY	-	SEE REMARK 999	UNP P08189
A	175	TYR	-	SEE REMARK 999	UNP P08189
A	176	VAL	-	SEE REMARK 999	UNP P08189
A	177	ARG	-	SEE REMARK 999	UNP P08189
A	178	ASP	-	SEE REMARK 999	UNP P08189
A	179	ASN	-	SEE REMARK 999	UNP P08189

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: fimF

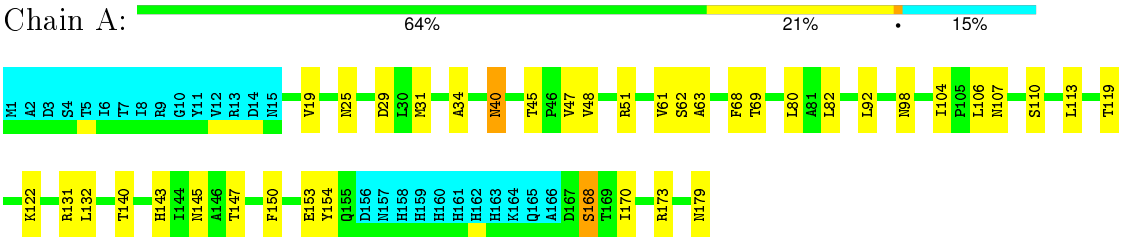
Chain A: 

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

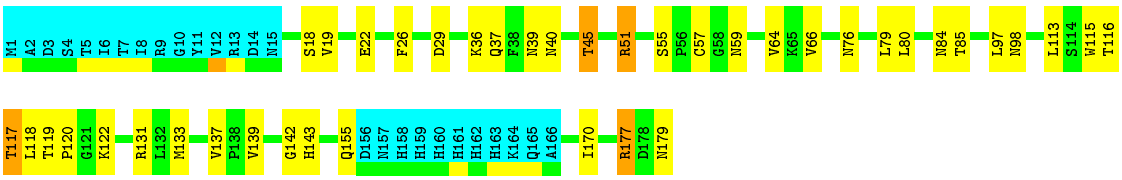
- Molecule 1: fimF

Chain A: 

4.2.2 Score per residue for model 2

- Molecule 1: fimF

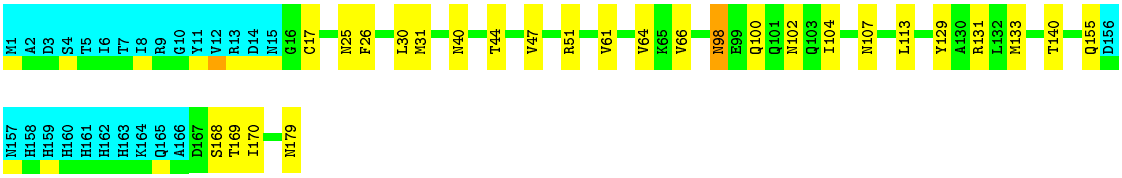
Chain A: 



4.2.3 Score per residue for model 3

- Molecule 1: fimF

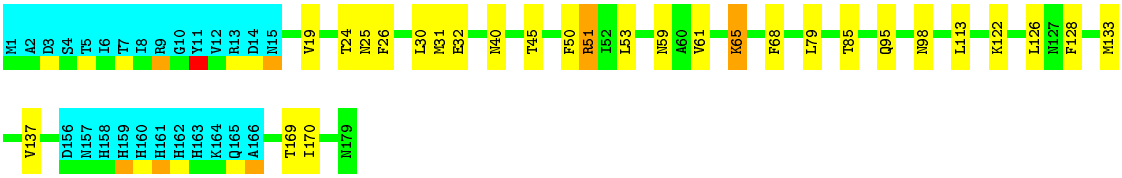
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: fimF

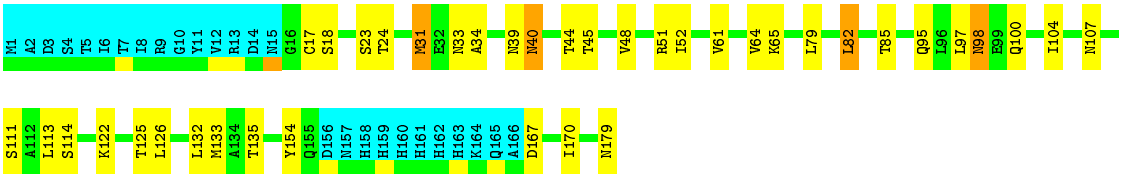
Chain A:



4.2.5 Score per residue for model 5

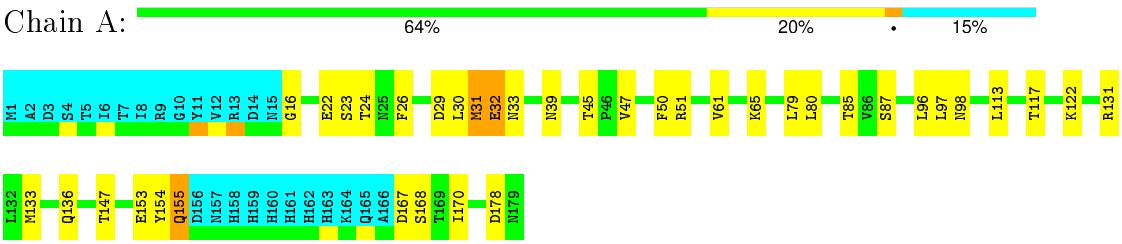
- Molecule 1: fimF

Chain A:



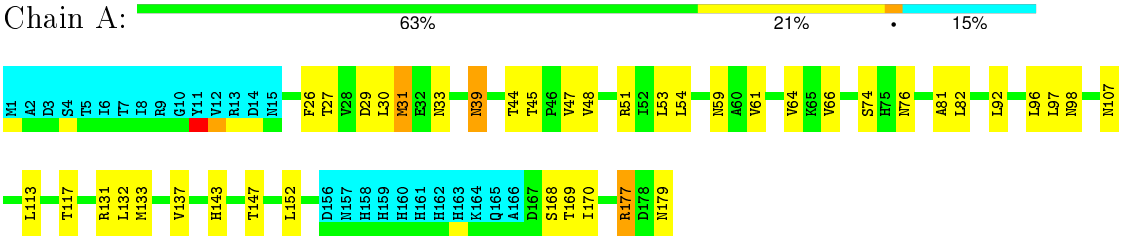
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: fimF



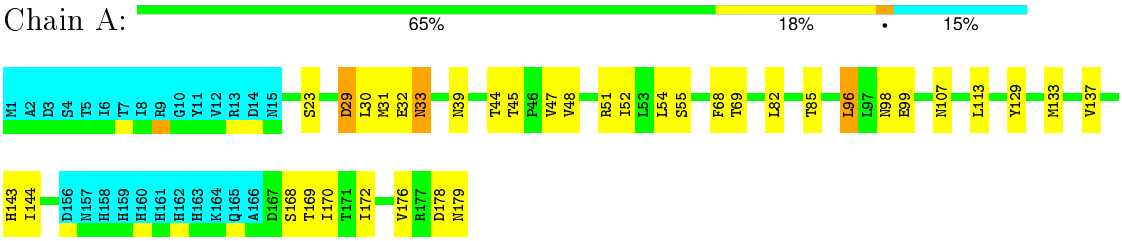
4.2.7 Score per residue for model 7

- Molecule 1: fimF



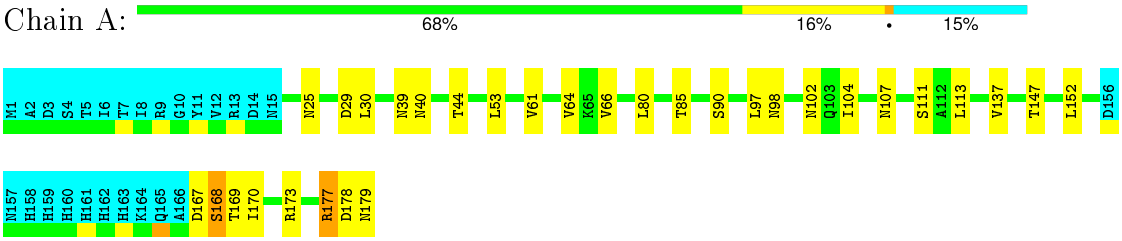
4.2.8 Score per residue for model 8

- Molecule 1: fimF



4.2.9 Score per residue for model 9

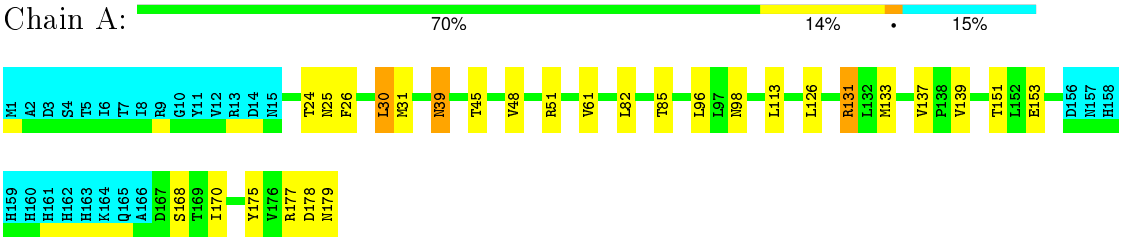
- Molecule 1: fimF



4.2.10 Score per residue for model 10

- Molecule 1: fimF

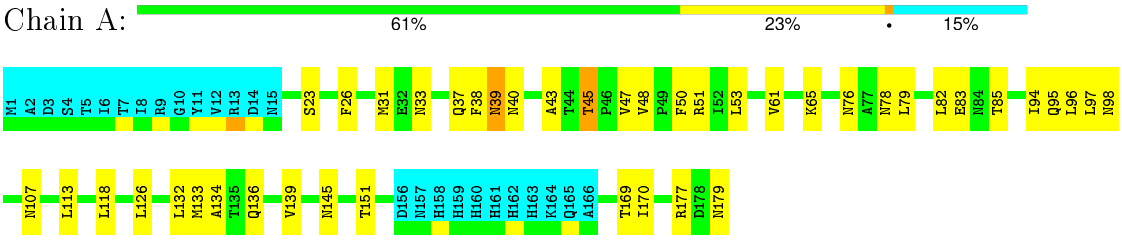
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: fimF

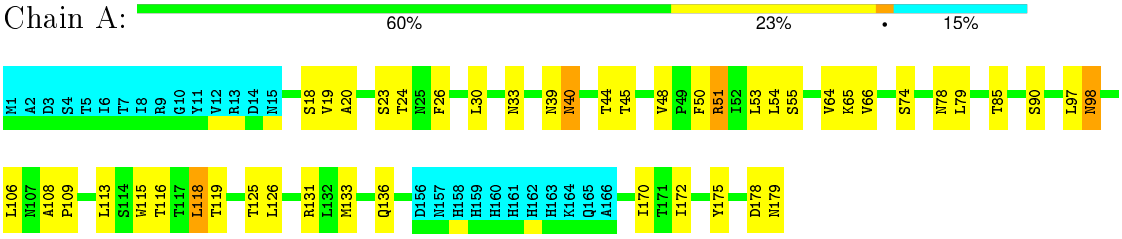
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: fimF

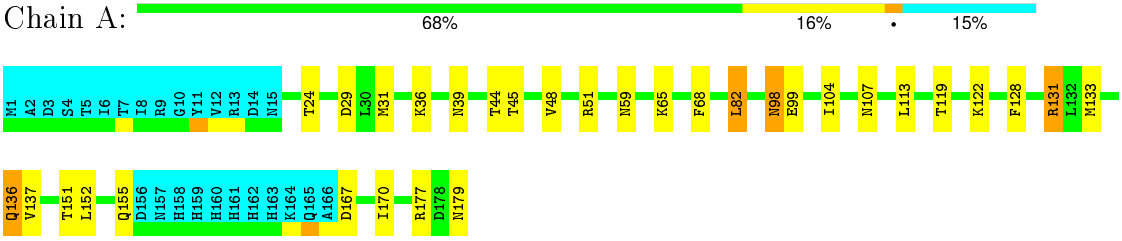
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: fimF

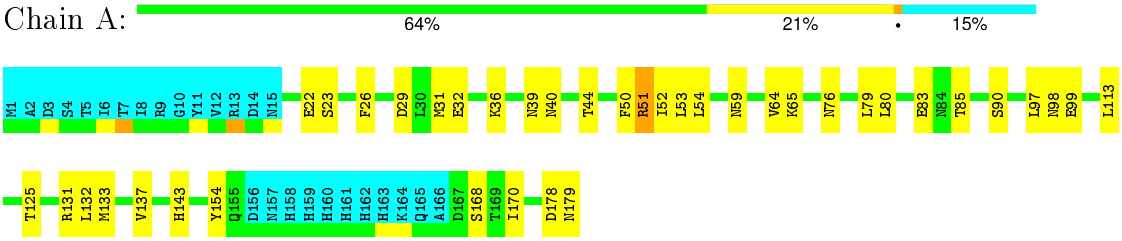
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: fimF

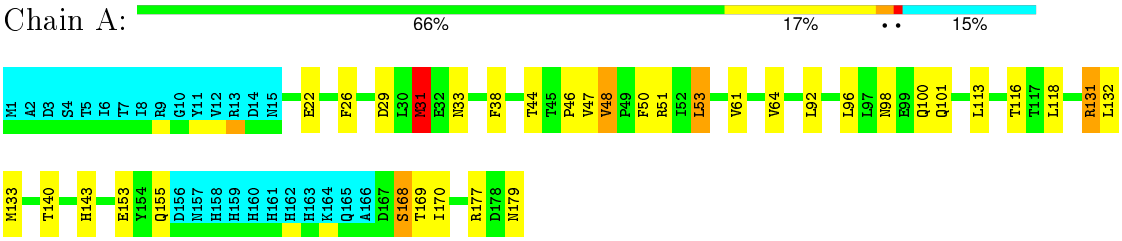
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: fimF

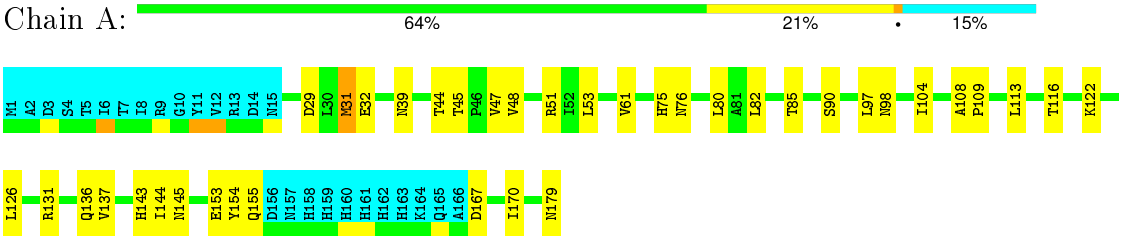
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: fimF

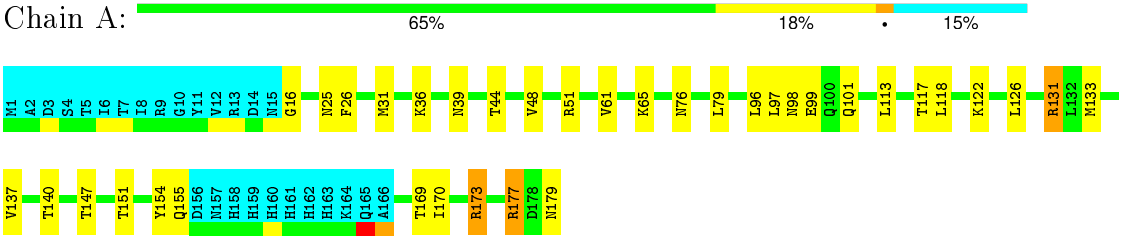
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: fimF

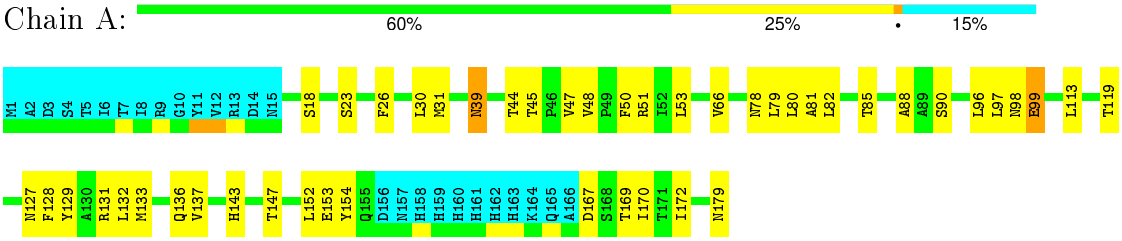
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: fimF

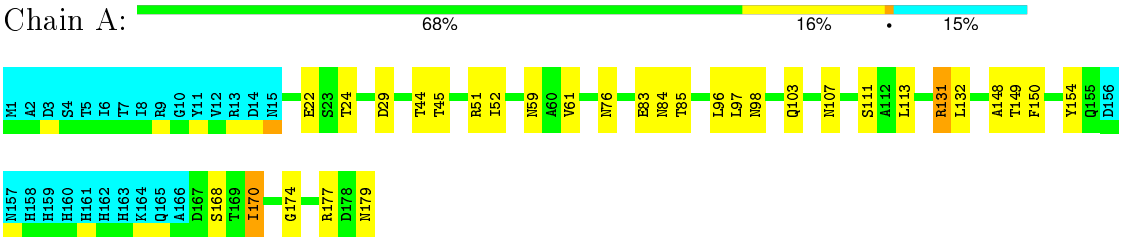
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: fimF

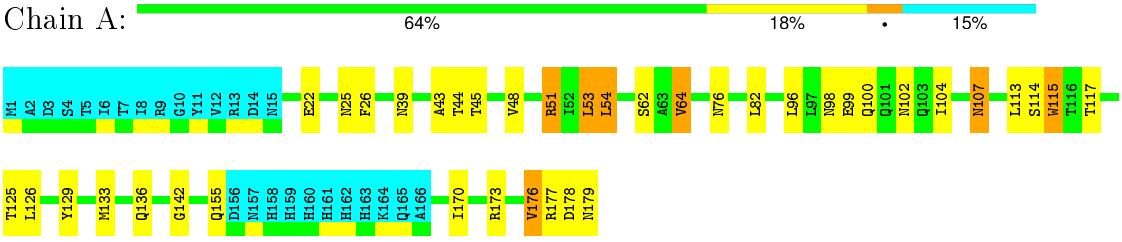
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: fimF

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
OPAL	refinement	p

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 15032
Number of chemical shift lists	1
Total number of shifts	2019
Number of shifts mapped to atoms	2019
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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	0.57±0.01	0±0/1151 (0.0±0.0%)	1.12±0.02	1±1/1577 (0.1±0.1%)
All	All	0.57	0/23020 (0.0%)	1.12	18/31540 (0.1%)

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	1.6±1.2
All	All	0	31

There are no bond-length outliers.

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	51	ARG	NE-CZ-NH1	7.59	124.09	120.30	4	1
1	A	177	ARG	NE-CZ-NH2	-6.56	117.02	120.30	7	2
1	A	129	TYR	CB-CG-CD1	-6.54	117.08	121.00	20	2
1	A	51	ARG	NE-CZ-NH2	-6.28	117.16	120.30	12	1
1	A	51	ARG	CD-NE-CZ	6.04	132.06	123.60	4	2
1	A	131	ARG	NE-CZ-NH2	5.95	123.28	120.30	13	1
1	A	137	VAL	CA-CB-CG2	5.89	119.74	110.90	4	1
1	A	85	THR	N-CA-CB	-5.80	99.28	110.30	18	1
1	A	122	LYS	CB-CA-C	5.36	121.12	110.40	16	1
1	A	31	MET	CG-SD-CE	-5.31	91.71	100.20	15	1
1	A	64	VAL	CA-CB-CG1	5.18	118.68	110.90	7	3
1	A	154	TYR	CB-CG-CD1	-5.10	117.94	121.00	1	1
1	A	131	ARG	NE-CZ-NH1	5.10	122.85	120.30	19	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	154	TYR	Sidechain	6
1	A	177	ARG	Sidechain	4
1	A	173	ARG	Sidechain	3
1	A	131	ARG	Sidechain	3
1	A	29	ASP	Peptide	2
1	A	175	TYR	Sidechain	2
1	A	65	LYS	Peptide	1
1	A	88	ALA	Peptide	1
1	A	17	CYS	Peptide	1
1	A	152	LEU	Peptide	1
1	A	155	GLN	Peptide	1
1	A	31	MET	Peptide	1
1	A	51	ARG	Sidechain	1
1	A	129	TYR	Sidechain	1
1	A	30	LEU	Peptide	1
1	A	59	ASN	Peptide	1
1	A	150	PHE	Peptide	1

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	1131	1121	1119	3±2
All	All	22620	22420	22380	58

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ASN:HA	1:A:137:VAL:HG13	0.72	1.61	2	10
1:A:96:LEU:HD11	1:A:172:ILE:HD11	0.66	1.66	8	1
1:A:64:VAL:HG13	1:A:115:TRP:CD1	0.66	2.26	20	1
1:A:38:PHE:HA	1:A:43:ALA:HB1	0.63	1.68	11	1
1:A:92:LEU:HB3	1:A:132:LEU:HD11	0.61	1.72	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:ALA:HB1	1:A:109:PRO:CD	0.55	2.31	16	1
1:A:144:ILE:HD11	1:A:176:VAL:HG13	0.54	1.79	8	1
1:A:30:LEU:HD13	1:A:172:ILE:CG2	0.54	2.33	12	1
1:A:107:ASN:ND2	1:A:107:ASN:H	0.51	2.02	20	1
1:A:108:ALA:HB1	1:A:109:PRO:HD2	0.50	1.83	12	2
1:A:33:ASN:O	1:A:176:VAL:HG12	0.49	2.07	8	1
1:A:51:ARG:HG2	1:A:125:THR:HG23	0.48	1.85	20	2
1:A:64:VAL:HG13	1:A:118:LEU:CD2	0.48	2.38	12	1
1:A:37:GLN:HE22	1:A:45:THR:CG2	0.48	2.22	2	1
1:A:17:CYS:SG	1:A:61:VAL:HG11	0.47	2.49	5	1
1:A:98:ASN:ND2	1:A:100:GLN:H	0.47	2.07	3	2
1:A:64:VAL:HG12	1:A:154:TYR:CD1	0.47	2.44	5	1
1:A:98:ASN:ND2	1:A:98:ASN:H	0.47	2.06	12	1
1:A:149:THR:HG22	1:A:168:SER:O	0.47	2.10	19	1
1:A:116:THR:HG23	1:A:126:LEU:CD2	0.45	2.41	12	1
1:A:20:ALA:HB3	1:A:53:LEU:HD22	0.45	1.88	12	1
1:A:142:GLY:H	1:A:176:VAL:CG2	0.45	2.25	20	1
1:A:52:ILE:O	1:A:54:LEU:HD22	0.44	2.11	8	2
1:A:53:LEU:HD23	1:A:54:LEU:N	0.44	2.27	12	1
1:A:52:ILE:HG12	1:A:150:PHE:CE2	0.44	2.47	19	1
1:A:116:THR:HG23	1:A:126:LEU:HD21	0.44	1.90	12	1
1:A:43:ALA:HB3	1:A:134:ALA:HB3	0.43	1.90	11	1
1:A:99:GLU:HA	1:A:129:TYR:CE2	0.43	2.48	18	1
1:A:98:ASN:HA	1:A:128:PHE:CD2	0.43	2.48	13	1
1:A:148:ALA:HB3	1:A:170:ILE:CG2	0.43	2.43	19	1
1:A:37:GLN:NE2	1:A:45:THR:HG22	0.42	2.29	11	1
1:A:39:ASN:CA	1:A:137:VAL:HG13	0.42	2.40	2	1
1:A:48:VAL:H	1:A:131:ARG:HD2	0.42	1.75	15	1
1:A:33:ASN:HD21	1:A:132:LEU:HD12	0.42	1.75	5	1
1:A:119:THR:HG21	1:A:122:LYS:HD3	0.42	1.92	1	1
1:A:30:LEU:HD12	1:A:131:ARG:HE	0.41	1.75	10	1
1:A:98:ASN:HA	1:A:128:PHE:CD1	0.41	2.50	18	1
1:A:64:VAL:HG22	1:A:115:TRP:CD1	0.41	2.50	2	1
1:A:119:THR:HG23	1:A:122:LYS:HB2	0.41	1.92	13	1
1:A:53:LEU:HD13	1:A:54:LEU:N	0.41	2.30	20	1
1:A:136:GLN:HA	1:A:136:GLN:HE21	0.41	1.75	13	1
1:A:30:LEU:HD21	1:A:131:ARG:HA	0.41	1.92	6	1
1:A:38:PHE:CG	1:A:92:LEU:HD21	0.41	2.51	15	1
1:A:148:ALA:HB3	1:A:170:ILE:HG22	0.40	1.92	19	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	152/179 (85%)	125±4 (82±3%)	23±3 (15±2%)	3±2 (2±1%)	12 51
All	All	3040/3580 (85%)	2503 (82%)	468 (15%)	69 (2%)	12 51

All 30 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	31	MET	13
1	A	168	SER	8
1	A	40	ASN	4
1	A	139	VAL	3
1	A	19	VAL	3
1	A	47	VAL	3
1	A	117	THR	3
1	A	81	ALA	2
1	A	34	ALA	2
1	A	155	GLN	2
1	A	53	LEU	2
1	A	82	LEU	2
1	A	83	GLU	2
1	A	16	GLY	2
1	A	22	GLU	2
1	A	107	ASN	2
1	A	120	PRO	1
1	A	43	ALA	1
1	A	66	VAL	1
1	A	32	GLU	1
1	A	142	GLY	1
1	A	174	GLY	1
1	A	99	GLU	1
1	A	131	ARG	1
1	A	63	ALA	1
1	A	103	GLN	1
1	A	111	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	46	PRO	1
1	A	39	ASN	1
1	A	169	THR	1

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	124/147 (84%)	95±5 (77±4%)	29±5 (23±4%)	3 30
All	All	2480/2940 (84%)	1909 (77%)	571 (23%)	3 30

All 97 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	170	ILE	20
1	A	113	LEU	20
1	A	51	ARG	19
1	A	98	ASN	19
1	A	179	ASN	18
1	A	133	MET	16
1	A	45	THR	15
1	A	44	THR	14
1	A	26	PHE	13
1	A	48	VAL	13
1	A	61	VAL	12
1	A	97	LEU	12
1	A	85	THR	12
1	A	131	ARG	10
1	A	96	LEU	10
1	A	29	ASP	10
1	A	82	LEU	10
1	A	79	LEU	9
1	A	143	HIS	8
1	A	53	LEU	8
1	A	76	ASN	8
1	A	65	LYS	8

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Mol	Chain	Res	Type	Models (Total)
1	A	39	ASN	8
1	A	169	THR	8
1	A	177	ARG	8
1	A	40	ASN	8
1	A	107	ASN	8
1	A	136	GLN	7
1	A	80	LEU	7
1	A	178	ASP	7
1	A	126	LEU	7
1	A	23	SER	7
1	A	24	THR	7
1	A	25	ASN	7
1	A	104	ILE	7
1	A	50	PHE	7
1	A	153	GLU	6
1	A	155	GLN	6
1	A	167	ASP	6
1	A	33	ASN	6
1	A	47	VAL	6
1	A	30	LEU	6
1	A	31	MET	6
1	A	147	THR	6
1	A	118	LEU	5
1	A	99	GLU	5
1	A	132	LEU	5
1	A	122	LYS	5
1	A	90	SER	5
1	A	66	VAL	5
1	A	32	GLU	5
1	A	59	ASN	5
1	A	168	SER	4
1	A	18	SER	4
1	A	22	GLU	4
1	A	140	THR	4
1	A	36	LYS	4
1	A	68	PHE	4
1	A	78	ASN	3
1	A	64	VAL	3
1	A	116	THR	3
1	A	145	ASN	3
1	A	102	ASN	3
1	A	95	GLN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	119	THR	3
1	A	117	THR	3
1	A	55	SER	3
1	A	151	THR	2
1	A	69	THR	2
1	A	152	LEU	2
1	A	115	TRP	2
1	A	101	GLN	2
1	A	106	LEU	2
1	A	54	LEU	2
1	A	62	SER	2
1	A	125	THR	2
1	A	74	SER	2
1	A	100	GLN	2
1	A	173	ARG	2
1	A	84	ASN	2
1	A	114	SER	2
1	A	111	SER	2
1	A	57	CYS	1
1	A	52	ILE	1
1	A	128	PHE	1
1	A	19	VAL	1
1	A	176	VAL	1
1	A	172	ILE	1
1	A	83	GLU	1
1	A	87	SER	1
1	A	135	THR	1
1	A	144	ILE	1
1	A	27	THR	1
1	A	94	ILE	1
1	A	110	SER	1
1	A	127	ASN	1
1	A	75	HIS	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 15032

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2019
Number of shifts mapped to atoms	2019
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	169	0.62 ± 0.14	Should be applied
$^{13}C_{\beta}$	158	0.17 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	150	0.90 ± 0.15	Should be applied
^{15}N	161	0.14 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1572 atoms were assigned a chemical shift out of a possible 1731. 27 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	733/749 (98%)	298/298 (100%)	290/306 (95%)	145/145 (100%)
Sidechain	761/876 (87%)	459/505 (91%)	277/334 (83%)	25/37 (68%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	78/106 (74%)	49/56 (88%)	26/45 (58%)	3/5 (60%)
Overall	1572/1731 (91%)	806/859 (94%)	593/685 (87%)	173/187 (93%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1734 atoms were assigned a chemical shift out of a possible 2070. 28 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	810/879 (92%)	330/350 (94%)	319/358 (89%)	161/171 (94%)
Sidechain	840/1029 (82%)	507/595 (85%)	305/387 (79%)	28/47 (60%)
Aromatic	84/162 (52%)	53/84 (63%)	28/61 (46%)	3/17 (18%)
Overall	1734/2070 (84%)	890/1029 (86%)	652/806 (81%)	192/235 (82%)

7.1.4 Statistically unusual chemical shifts (i)

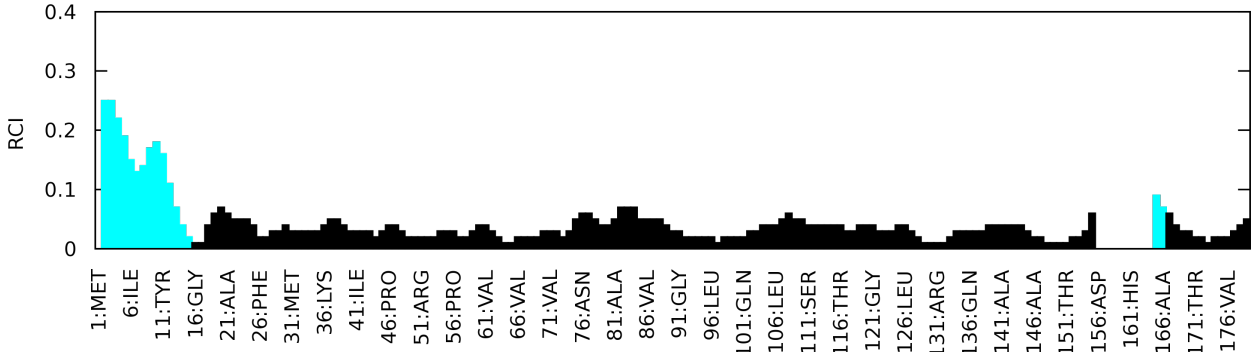
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	36	LYS	NZ	67.80	49.86 – 18.16	10.7
1	A	177	ARG	NE	95.80	92.63 – 76.73	7.0
1	A	128	PHE	HB3	0.31	4.85 – 1.05	-6.9

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:


RCI
0.4
0.3
0.2
0.1
0
1:MET
6:ILE
11:TYR
16:GLY
21:ALA
26:PHE
31:MET
36:LYS
41:ILE
46:PRO
51:ARG
56:PRO
61:VAL
66:VAL
71:VAL
76:ASN
81:ALA
86:VAL
91:GLY
96:LEU
101:GLN
106:LEU
111:SER
116:THR
121:GLY
126:LEU
131:ARG
136:GLN
141:ALA
146:ALA
151:THR
156:ASP
161:HIS
166:ALA
171:THR
176:VAL