



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 08:59 PM BST

PDB ID : 2IFE
Title : TRANSLATION INITIATION FACTOR IF3 FROM ESCHERICHIA COLI
RIBOSOME BINDING DOMAIN (RESIDUES 84-180)
Authors : De Cock, E.; Garcia, C.; Dardel, F.
Deposited on : 1998-12-16

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

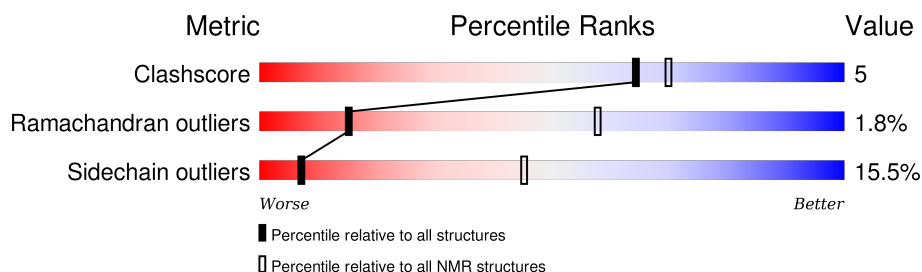
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	100	

2 Ensemble composition and analysis

This entry contains 24 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 2 as representative.

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:92-A:99, A:106-A:130, A:140-A:161, A:169-A:177 (64)	0.23	19

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 1 single-model cluster was found.

Cluster number	Models
1	2, 5, 8, 10, 12, 14, 15, 16, 17, 20, 21, 22, 23
2	1, 3, 4, 6, 7, 9, 13, 18, 19, 24
Single-model clusters	11

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1527 atoms, of which 784 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (TRANSLATION INITIATION FACTOR IF3).

Mol	Chain	Residues	Atoms						Trace
1	A	91	Total	C	H	N	O	S	0
			1527	470	784	135	134	4	

There are 3 discrepancies between the modelled and reference sequences:

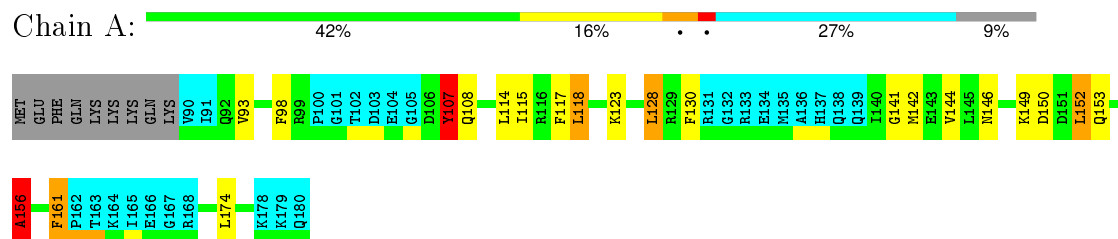
Chain	Residue	Modelled	Actual	Comment	Reference
A	81	MET	SER	SEE REMARK 999	UNP P0A707
A	82	GLU	LYS	SEE REMARK 999	UNP P0A707
A	83	PHE	GLU	SEE REMARK 999	UNP P0A707

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: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

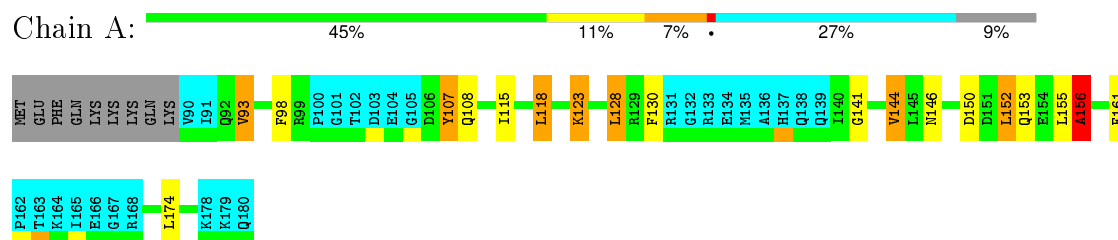


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

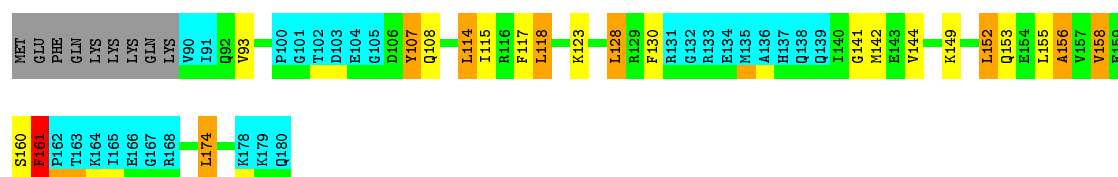
- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



4.2.2 Score per residue for model 2

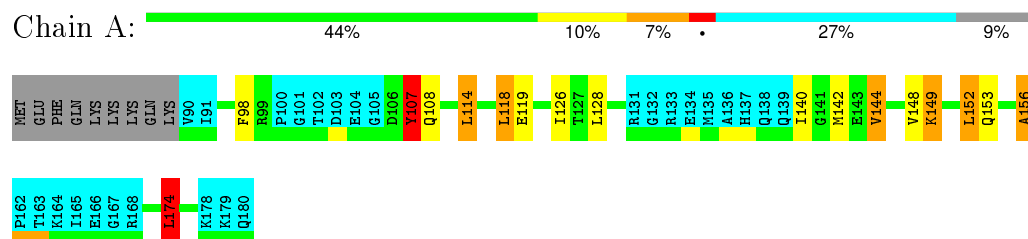
- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)





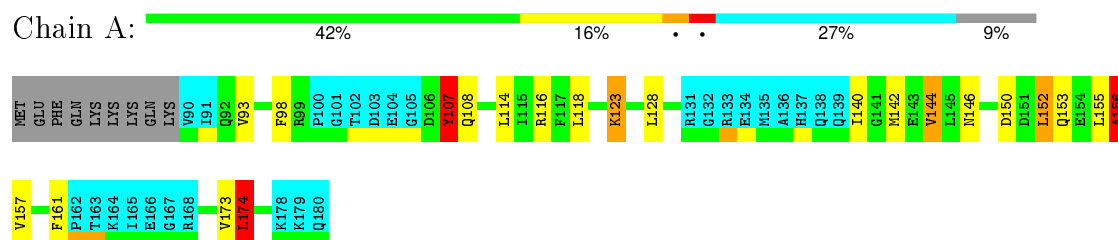
4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



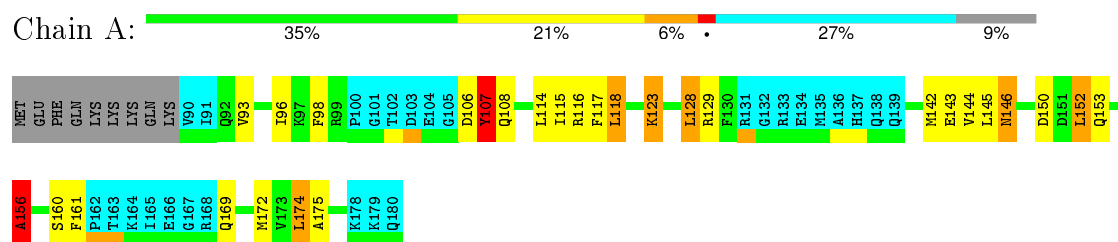
4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



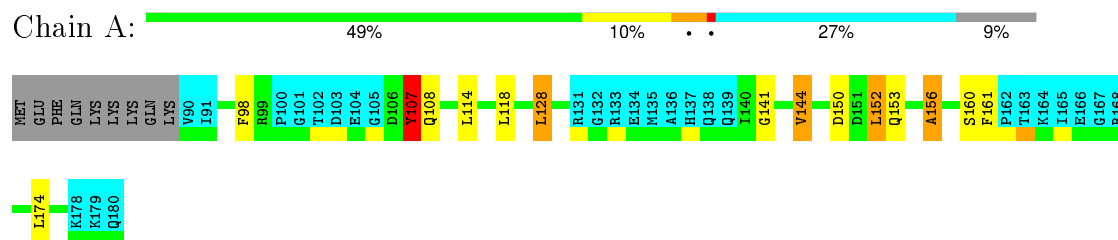
4.2.5 Score per residue for model 5

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



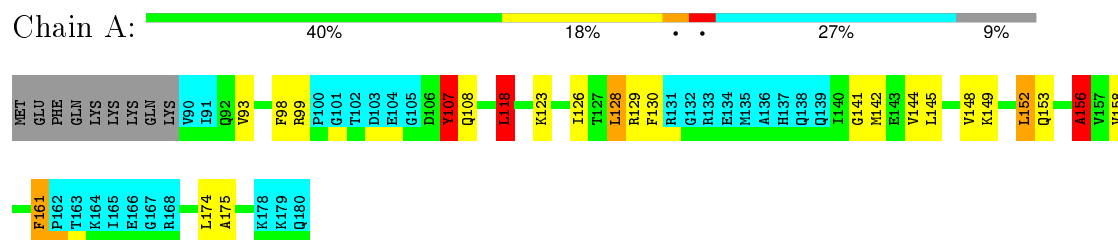
4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



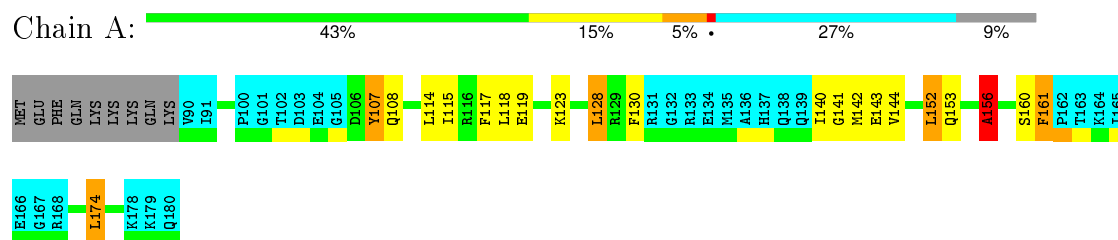
4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



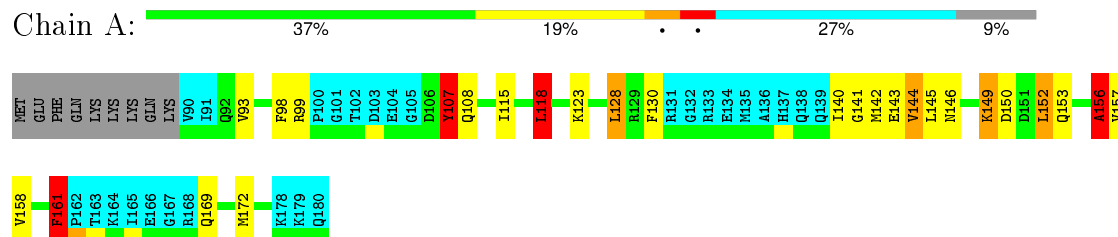
4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



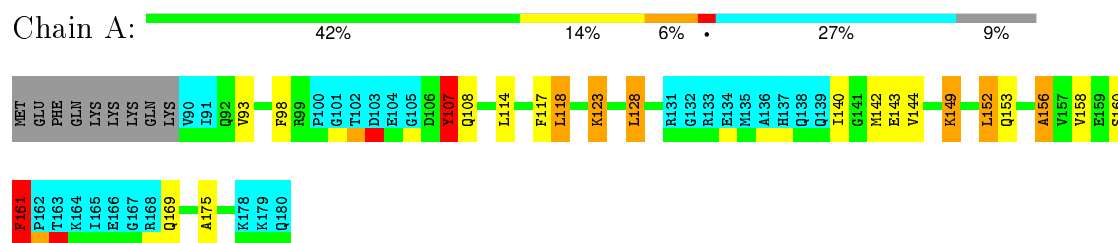
4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



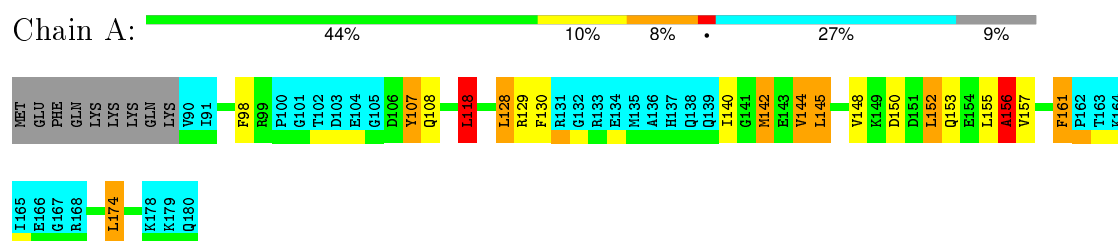
4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



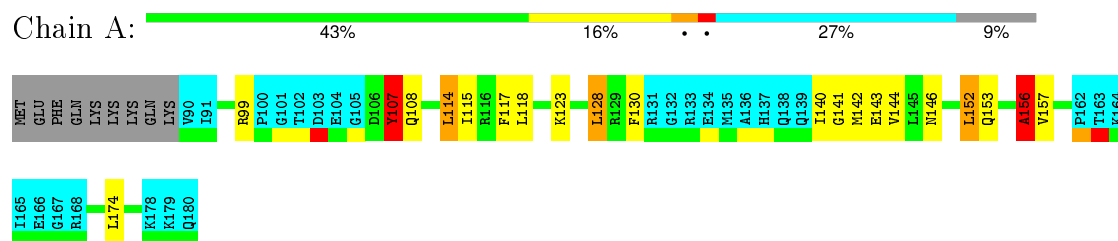
4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



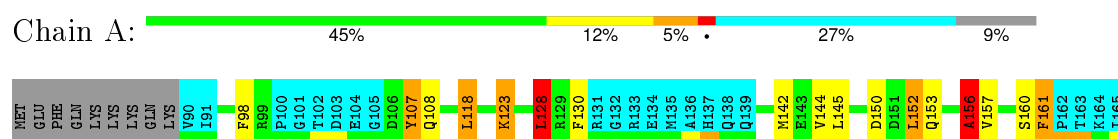
4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

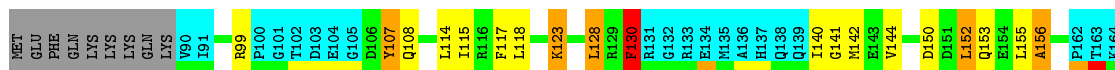




4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

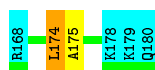
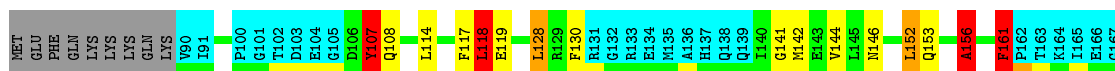
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

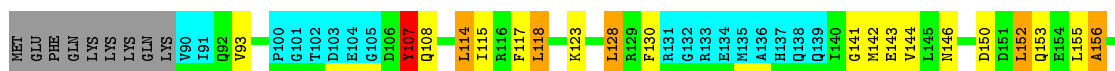
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

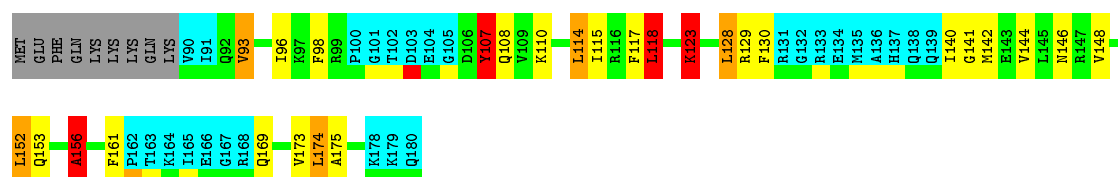
Chain A:



4.2.17 Score per residue for model 17

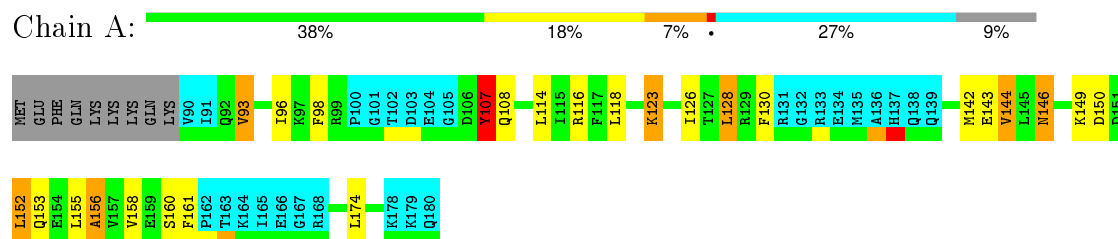
- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

Chain A:



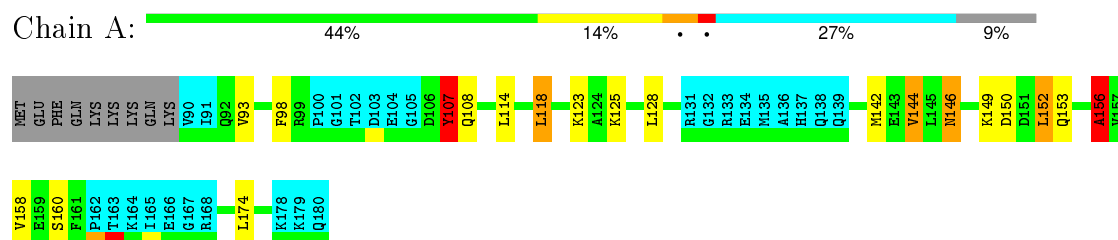
4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



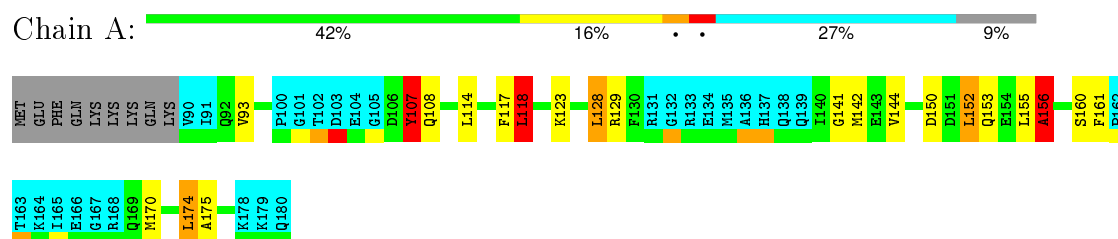
4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



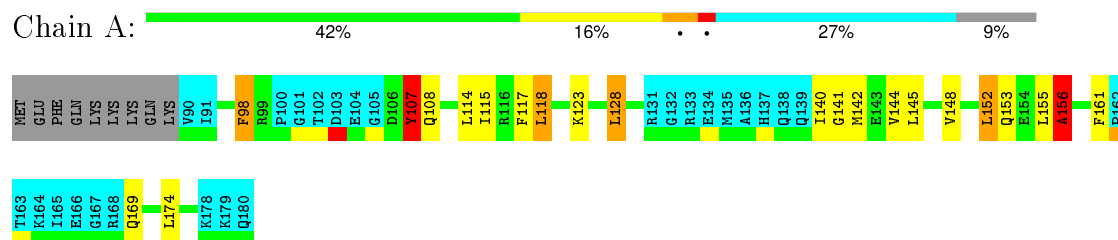
4.2.20 Score per residue for model 20

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



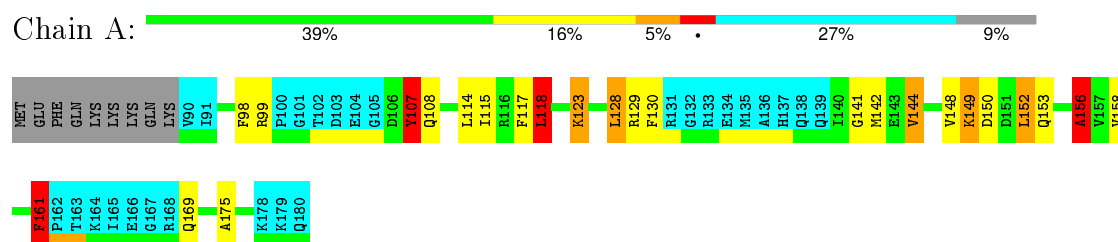
4.2.21 Score per residue for model 21

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



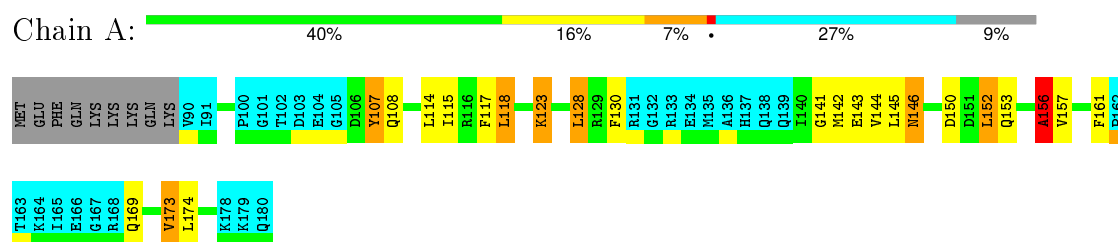
4.2.22 Score per residue for model 22

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



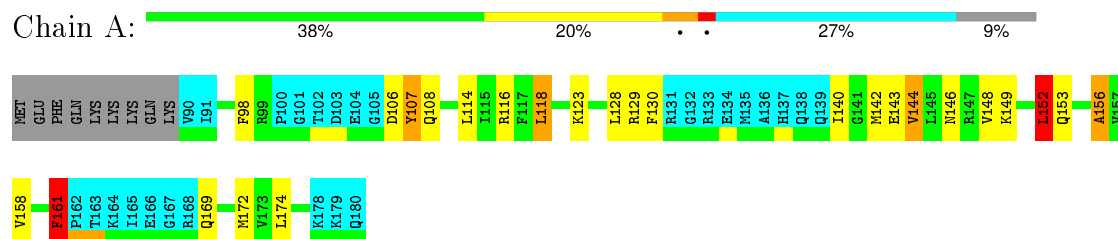
4.2.23 Score per residue for model 23

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



4.2.24 Score per residue for model 24

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY AND RESTRAINED SIMULATED ANNEALING*.

Of the 200 calculated structures, 24 were deposited, based on the following criterion: *LOWEST TARGET FUNCTION*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
DIANA	structure solution	
X-PLOR	structure solution	3.1

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 4394
Number of chemical shift lists	1
Total number of shifts	985
Number of shifts mapped to atoms	985
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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

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	1.19±0.01	0±0/536 (0.0±0.0%)	1.77±0.09	13±3/718 (1.8±0.4%)
All	All	1.19	0/12864 (0.0%)	1.77	310/17232 (1.8%)

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	3.7±0.9
All	All	0	88

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	107	TYR	CB-CG-CD2	-16.36	111.19	121.00	21	17
1	A	98	PHE	CB-CG-CD2	-14.22	110.84	120.80	13	4
1	A	98	PHE	CB-CG-CD1	14.16	130.71	120.80	13	4
1	A	117	PHE	CB-CG-CD2	-12.79	111.84	120.80	21	13
1	A	117	PHE	CB-CG-CD1	11.42	128.79	120.80	10	13
1	A	161	PHE	CB-CG-CD1	-8.96	114.53	120.80	22	8
1	A	175	ALA	CB-CA-C	-8.61	97.19	110.10	10	7
1	A	156	ALA	CB-CA-C	-8.46	97.42	110.10	5	24
1	A	144	VAL	CA-CB-CG2	-7.83	99.16	110.90	6	24
1	A	107	TYR	CB-CG-CD1	7.76	125.65	121.00	21	5
1	A	156	ALA	N-CA-CB	7.12	120.06	110.10	18	18
1	A	123	LYS	N-CA-CB	7.12	123.41	110.60	13	3
1	A	152	LEU	CB-CA-C	-6.85	97.19	110.20	7	24
1	A	114	LEU	CB-CA-C	-6.76	97.36	110.20	21	13
1	A	157	VAL	CB-CA-C	-6.29	99.44	111.40	23	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	114	LEU	N-CA-CB	-6.24	97.92	110.40	23	5
1	A	140	ILE	N-CA-C	-6.24	94.15	111.00	11	2
1	A	128	LEU	CB-CG-CD2	-6.19	100.48	111.00	14	5
1	A	128	LEU	CB-CA-C	-6.15	98.51	110.20	10	3
1	A	152	LEU	C-N-CA	6.15	137.07	121.70	24	22
1	A	93	VAL	CG1-CB-CG2	-6.06	101.20	110.90	5	11
1	A	140	ILE	C-N-CA	5.99	134.89	122.30	9	1
1	A	146	ASN	CA-CB-CG	5.89	126.37	113.40	18	9
1	A	130	PHE	CB-CG-CD1	-5.80	116.74	120.80	22	3
1	A	169	GLN	CB-CA-C	-5.70	99.00	110.40	24	6
1	A	115	ILE	CB-CA-C	-5.68	100.23	111.60	23	12
1	A	140	ILE	CA-C-N	-5.66	104.88	116.20	9	1
1	A	129	ARG	N-CA-C	-5.65	95.74	111.00	22	7
1	A	123	LYS	N-CA-C	-5.63	95.80	111.00	21	7
1	A	118	LEU	CA-CB-CG	-5.60	102.42	115.30	11	10
1	A	161	PHE	CB-CG-CD2	5.60	124.72	120.80	13	1
1	A	107	TYR	CA-CB-CG	5.54	123.94	113.40	12	8
1	A	158	VAL	CA-CB-CG2	5.54	119.22	110.90	2	2
1	A	174	LEU	CB-CG-CD1	-5.26	102.06	111.00	14	4
1	A	149	LYS	CB-CG-CD	5.21	125.14	111.60	22	3
1	A	143	GLU	N-CA-CB	5.10	119.79	110.60	8	1
1	A	173	VAL	CA-CB-CG1	-5.08	103.28	110.90	4	2
1	A	142	MET	CB-CA-C	-5.05	100.31	110.40	11	1
1	A	125	LYS	CB-CA-C	-5.02	100.36	110.40	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	107	TYR	Sidechain	24
1	A	156	ALA	Peptide	21
1	A	161	PHE	Sidechain,Peptide	18
1	A	142	MET	Peptide	17
1	A	160	SER	Peptide	2
1	A	130	PHE	Peptide	1

6.2 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 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	530	569	569	6±2
All	All	12720	13656	13656	138

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:ALA:HB1	1:A:174:LEU:HD11	0.93	1.38	3	6
1:A:128:LEU:HD21	1:A:141:GLY:HA2	0.72	1.62	14	5
1:A:128:LEU:HD13	1:A:130:PHE:CZ	0.66	2.26	11	2
1:A:128:LEU:HD11	1:A:141:GLY:HA2	0.64	1.69	6	8
1:A:156:ALA:CB	1:A:174:LEU:HD11	0.63	2.24	8	7
1:A:118:LEU:HD13	1:A:156:ALA:HB2	0.63	1.69	7	11
1:A:128:LEU:HD12	1:A:145:LEU:HD11	0.59	1.75	21	3
1:A:149:LYS:NZ	1:A:174:LEU:HD13	0.57	2.14	3	1
1:A:145:LEU:HD13	1:A:172:MET:HB2	0.55	1.79	5	2
1:A:128:LEU:HD23	1:A:130:PHE:CZ	0.54	2.37	16	4
1:A:128:LEU:HD21	1:A:141:GLY:CA	0.53	2.32	14	5
1:A:128:LEU:HD23	1:A:145:LEU:HD11	0.52	1.79	13	2
1:A:118:LEU:CD1	1:A:174:LEU:HD13	0.52	2.34	15	4
1:A:110:LYS:O	1:A:114:LEU:HD22	0.52	2.05	17	1
1:A:118:LEU:HD11	1:A:174:LEU:HD23	0.51	1.81	7	1
1:A:126:ILE:HD11	1:A:174:LEU:HD22	0.49	1.84	18	2
1:A:118:LEU:HD22	1:A:156:ALA:HB2	0.48	1.85	3	6
1:A:118:LEU:HD11	1:A:174:LEU:CD2	0.48	2.39	7	1
1:A:144:VAL:O	1:A:148:VAL:HG23	0.48	2.08	24	2
1:A:142:MET:O	1:A:146:ASN:HB2	0.48	2.09	18	4
1:A:149:LYS:HE3	1:A:158:VAL:HG21	0.48	1.86	10	4
1:A:98:PHE:HB3	1:A:144:VAL:HG11	0.48	1.86	6	9
1:A:128:LEU:HD11	1:A:141:GLY:CA	0.48	2.39	23	3
1:A:96:ILE:HG21	1:A:114:LEU:HD21	0.48	1.86	17	1
1:A:114:LEU:HD11	1:A:174:LEU:HD12	0.47	1.84	2	2
1:A:152:LEU:HG	1:A:156:ALA:HB3	0.47	1.86	24	1
1:A:128:LEU:CD2	1:A:141:GLY:HA2	0.47	2.40	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:LEU:HD12	1:A:145:LEU:CD2	0.46	2.41	11	1
1:A:149:LYS:HB2	1:A:158:VAL:HG21	0.46	1.88	22	2
1:A:123:LYS:HD3	1:A:173:VAL:HG12	0.46	1.87	23	2
1:A:118:LEU:HD13	1:A:156:ALA:CB	0.45	2.41	7	6
1:A:128:LEU:HD23	1:A:130:PHE:CE2	0.45	2.46	12	1
1:A:118:LEU:HD11	1:A:174:LEU:HD13	0.45	1.89	20	2
1:A:93:VAL:HG22	1:A:123:LYS:HD3	0.45	1.89	1	2
1:A:128:LEU:CD2	1:A:130:PHE:CZ	0.45	3.00	8	3
1:A:128:LEU:HD22	1:A:130:PHE:CE1	0.45	2.47	15	2
1:A:161:PHE:CZ	1:A:172:MET:SD	0.43	3.11	24	1
1:A:98:PHE:CE2	1:A:148:VAL:HG21	0.43	2.48	7	5
1:A:128:LEU:CD1	1:A:141:GLY:HA2	0.43	2.43	15	4
1:A:114:LEU:HD11	1:A:126:ILE:HD12	0.43	1.91	18	2
1:A:142:MET:HG2	1:A:161:PHE:CE1	0.42	2.49	11	1
1:A:114:LEU:O	1:A:118:LEU:HD12	0.42	2.14	12	1
1:A:93:VAL:HG22	1:A:123:LYS:HE3	0.41	1.91	17	1
1:A:161:PHE:CE1	1:A:172:MET:SD	0.41	3.14	9	1
1:A:93:VAL:HG22	1:A:123:LYS:HE2	0.41	1.93	4	1
1:A:146:ASN:HA	1:A:161:PHE:CZ	0.40	2.51	24	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	64/100 (64%)	57±1 (89±2%)	6±1 (9±2%)	1±0 (2±1%)	15	58
All	All	1536/2400 (64%)	1370 (89%)	139 (9%)	27 (2%)	15	58

All 4 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	153	GLN	24
1	A	144	VAL	1
1	A	169	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	106	ASP	1

6.3.2 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 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	59/90 (66%)	50±2 (84±4%)	9±2 (16±4%)	7	45
All	All	1416/2160 (66%)	1196 (84%)	220 (16%)	7	45

All 23 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	108	GLN	24
1	A	152	LEU	24
1	A	107	TYR	22
1	A	118	LEU	21
1	A	128	LEU	19
1	A	123	LYS	16
1	A	174	LEU	15
1	A	150	ASP	14
1	A	161	PHE	10
1	A	155	LEU	9
1	A	160	SER	9
1	A	143	GLU	8
1	A	99	ARG	5
1	A	116	ARG	4
1	A	149	LYS	3
1	A	169	GLN	3
1	A	158	VAL	3
1	A	119	GLU	3
1	A	145	LEU	2
1	A	146	ASN	2
1	A	96	ILE	2
1	A	170	MET	1
1	A	106	ASP	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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 70% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4394

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	985
Number of shifts mapped to atoms	985
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 \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	83	-0.15 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	70	0.39 ± 0.34	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	86	2.77 ± 0.21	Should be applied

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 79%, i.e. 685 atoms were assigned a chemical shift out of a possible 871. 10 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	254/318 (80%)	127/127 (100%)	64/128 (50%)	63/63 (100%)
Sidechain	410/509 (81%)	263/297 (89%)	141/185 (76%)	6/27 (22%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	21/44 (48%)	21/24 (88%)	0/20 (0%)	0/0 (—%)
Overall	685/871 (79%)	411/448 (92%)	205/333 (62%)	69/90 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 848 atoms were assigned a chemical shift out of a possible 1220. 11 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	340/449 (76%)	173/179 (97%)	82/182 (45%)	85/88 (97%)
Sidechain	485/720 (67%)	312/423 (74%)	167/255 (65%)	6/42 (14%)
Aromatic	23/51 (45%)	23/28 (82%)	0/22 (0%)	0/1 (0%)
Overall	848/1220 (70%)	508/630 (81%)	249/459 (54%)	91/131 (69%)

7.1.4 Statistically unusual chemical shifts ⓘ

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	149	LYS	CE	36.30	46.00 – 37.80	-6.8
1	A	154	GLU	CG	29.40	42.24 – 29.94	-5.4
1	A	155	LEU	CG	32.80	32.55 – 21.05	5.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

