



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 07:26 AM UTC

PDB ID : 2IFE / pdb_00002ife
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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

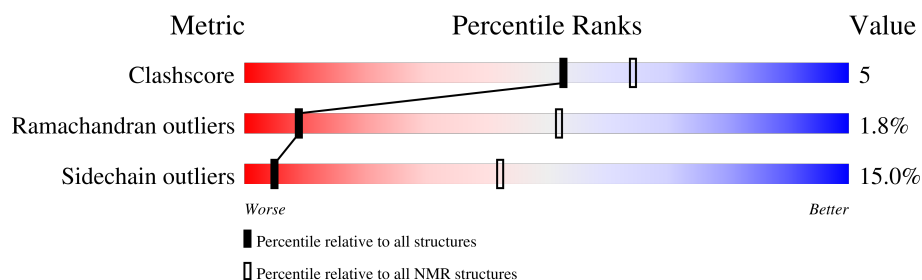
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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)	0.41	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, 13, 14, 15, 16, 17, 20, 21, 22, 23
2	1, 3, 4, 6, 7, 9, 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:

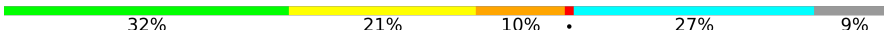
Chain	Residue	Modelled	Actual	Comment	Reference
A	81	MET	SER	SEE REMARK 999	UNP P0A707
A	82	GLU	LYS	SEE REMARK 999	UNP P0A707
A	83	PHE	GLU	SEE REMARK 999	UNP P0A707

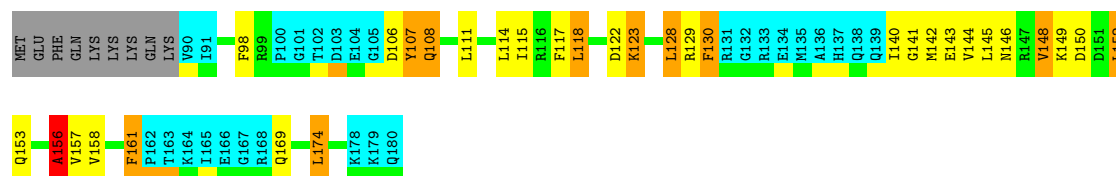
4 Residue-property plots

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: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

Chain A: 

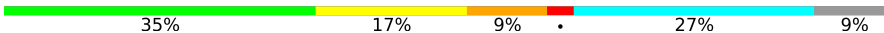


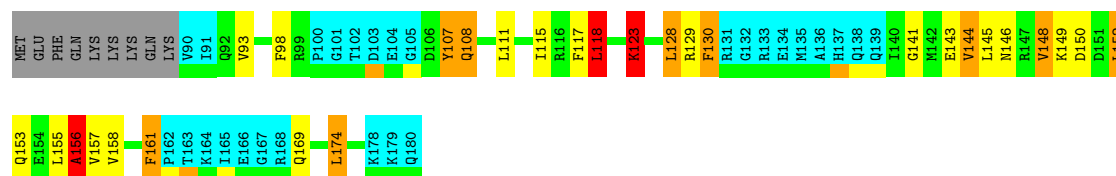
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

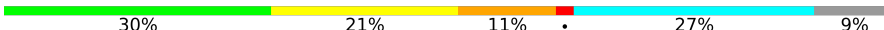
- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

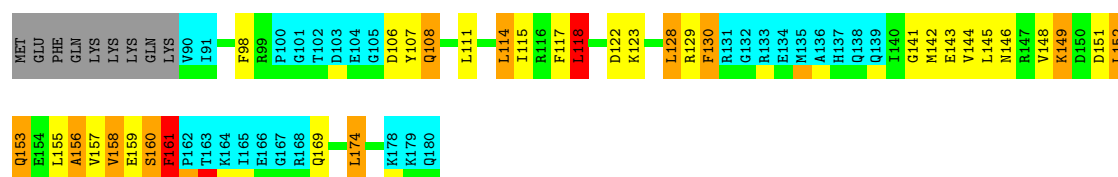
Chain A: 



4.2.2 Score per residue for model 2

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

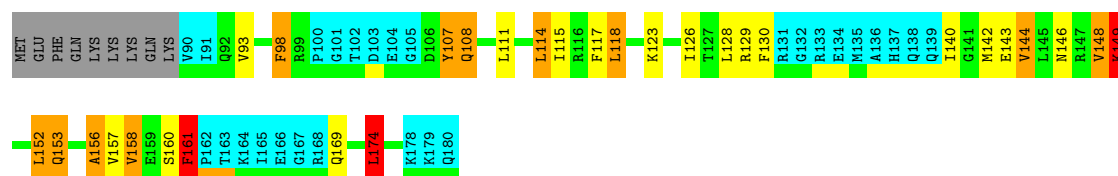
Chain A: 



4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

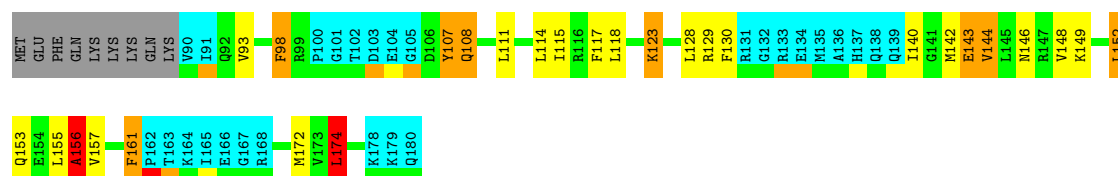
Chain A: 34% 16% 11% • 27% 9%



4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

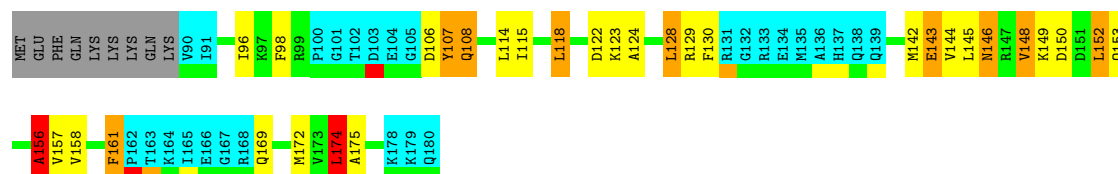
Chain A: 36% 18% 8% • 27% 9%



4.2.5 Score per residue for model 5

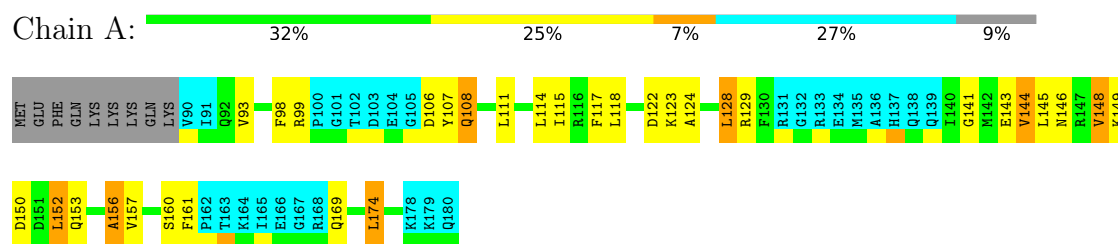
- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

Chain A: 32% 21% 9% • 27% 9%



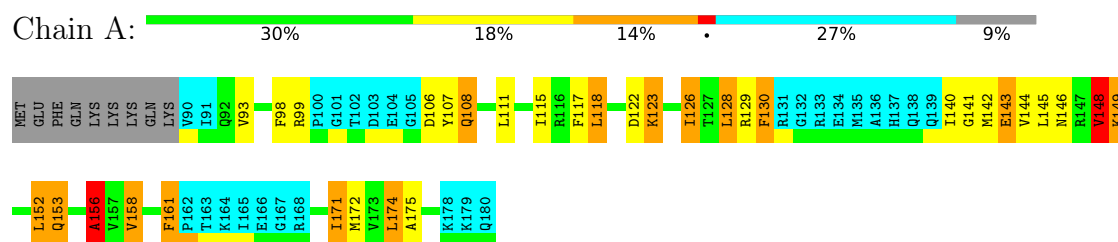
4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



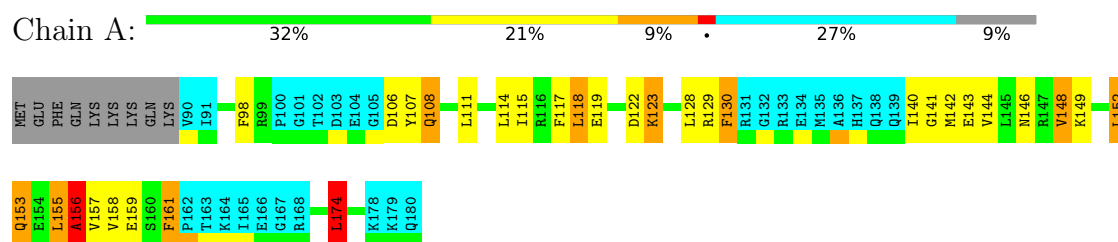
4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



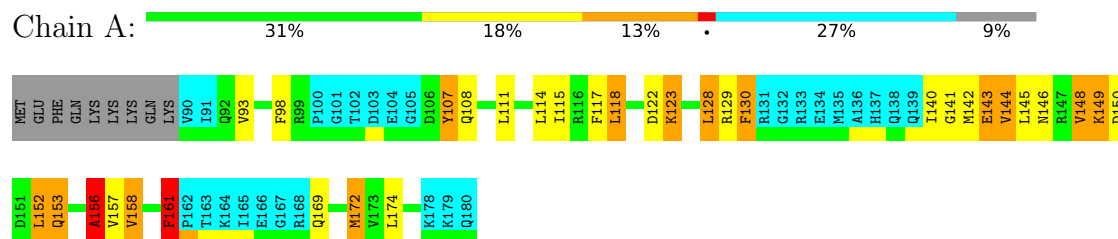
4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



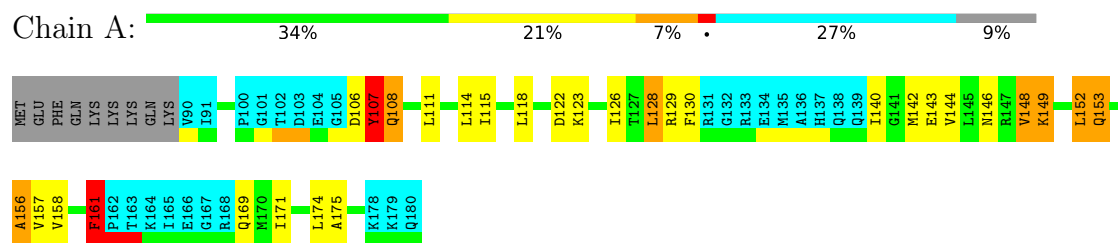
4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



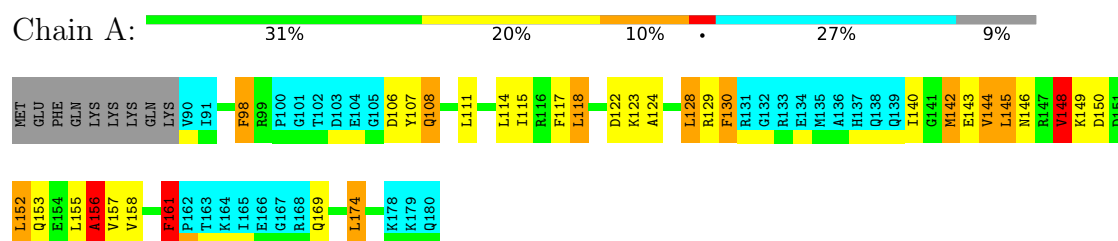
4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



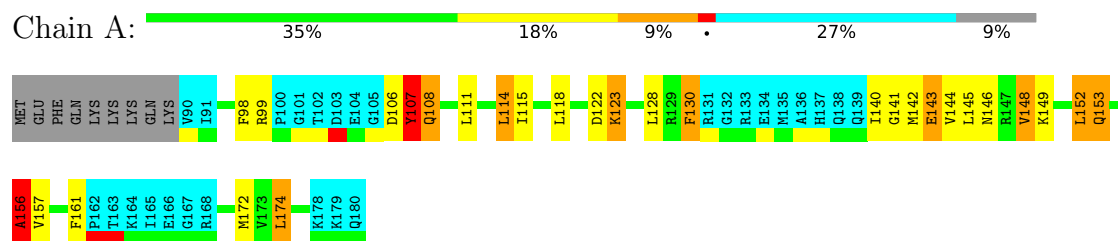
4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



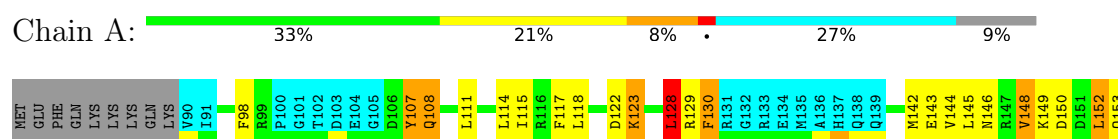
4.2.12 Score per residue for model 12

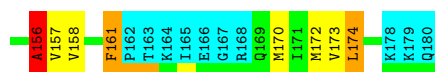
- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

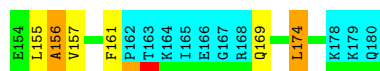




4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

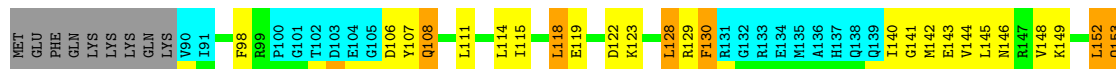
Chain A: 33% 25% 6% 27% 9%



4.2.15 Score per residue for model 15

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

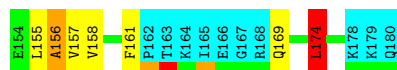
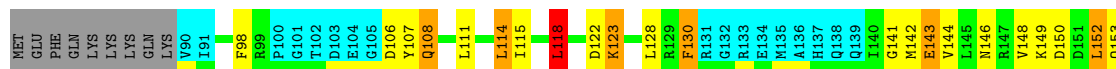
Chain A: 32% 23% 6% 27% 9%



4.2.16 Score per residue for model 16

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

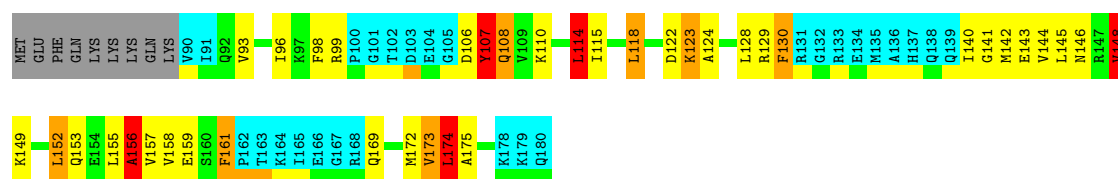
Chain A: 35% 20% 7% 27% 9%



4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

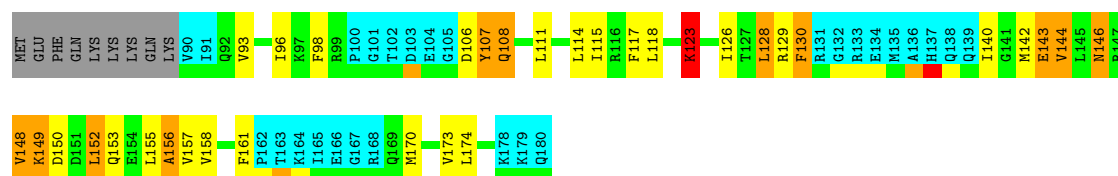
Chain A: 25% 27% 7% 5% 27% 9%



4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

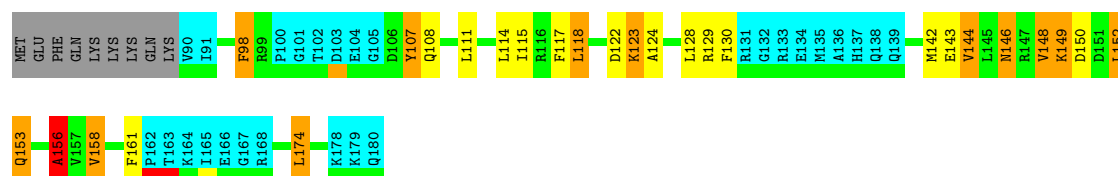
Chain A: 30% 22% 11% • 27% 9%



4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

Chain A: 37% 14% 12% • 27% 9%



4.2.20 Score per residue for model 20

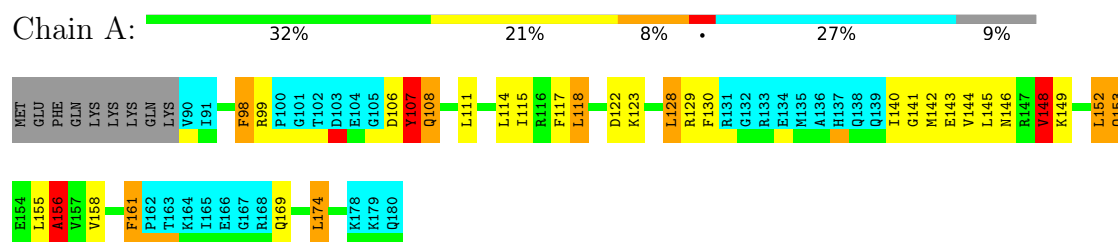
- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)

Chain A: 32% 22% 7% • 27% 9%



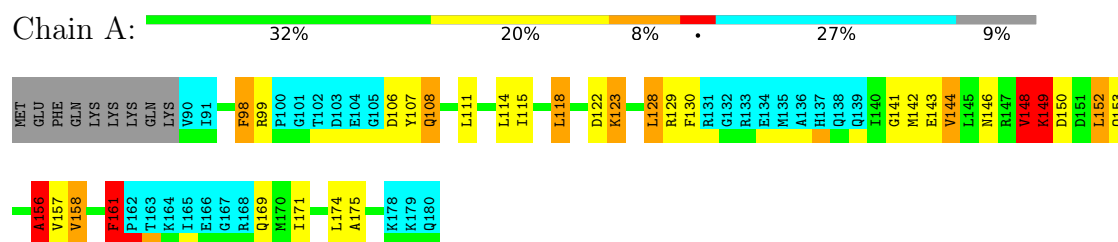
4.2.21 Score per residue for model 21

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



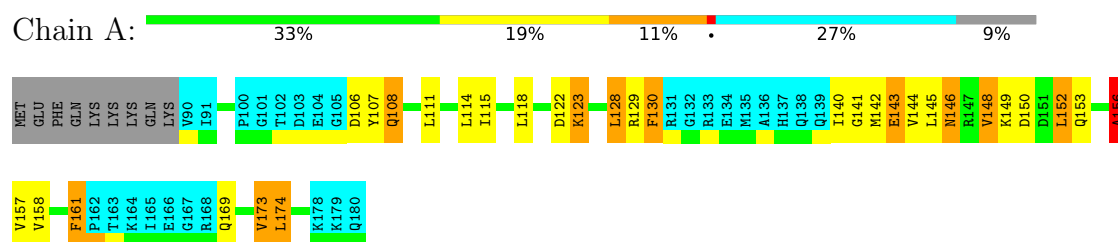
4.2.22 Score per residue for model 22

- Molecule 1: PROTEIN (TRANSLATION INITIATION FACTOR IF3)



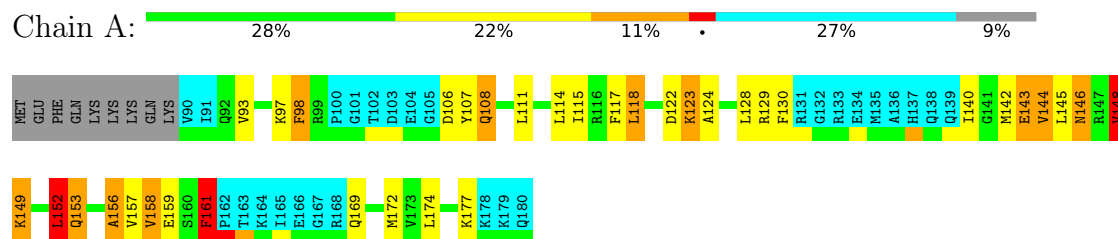
4.2.23 Score per residue for model 23

- 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

No chemical shift data was provided.

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	1.76±0.03	8±2/536 (1.5± 0.4%)	2.25±0.03	32±3/718 (4.5± 0.5%)
All	All	1.76	192/12864 (1.5%)	2.25	769/17232 (4.5%)

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	Planarity
1	A	0.0±0.0	3.7±0.9
All	All	0	88

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	140	ILE	N-CA	-7.67	1.38	1.46	9	2
1	A	144	VAL	CA-C	-7.41	1.43	1.52	9	24
1	A	129	ARG	CA-C	-7.36	1.45	1.53	22	22
1	A	143	GLU	CA-C	-7.05	1.43	1.52	11	23
1	A	156	ALA	CA-C	-6.83	1.44	1.52	7	21
1	A	122	ASP	CA-C	-6.28	1.45	1.52	17	18
1	A	140	ILE	CA-C	-6.21	1.46	1.53	9	1
1	A	107	TYR	CA-C	-6.21	1.47	1.53	9	6
1	A	123	LYS	CA-C	-6.03	1.45	1.52	14	12
1	A	149	LYS	CA-C	-5.90	1.45	1.52	24	4
1	A	157	VAL	CA-C	-5.79	1.45	1.52	15	12
1	A	158	VAL	N-CA	-5.73	1.39	1.46	24	16
1	A	123	LYS	N-CA	-5.58	1.39	1.46	19	9
1	A	124	ALA	CA-C	-5.52	1.46	1.52	11	1
1	A	129	ARG	N-CA	-5.52	1.39	1.46	22	10
1	A	148	VAL	CA-CB	-5.47	1.47	1.54	11	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	128	LEU	CA-C	-5.36	1.45	1.52	10	2
1	A	158	VAL	CA-CB	-5.33	1.47	1.54	7	3
1	A	144	VAL	CA-CB	-5.24	1.48	1.54	12	2
1	A	115	ILE	CA-C	-5.10	1.46	1.52	5	1
1	A	140	ILE	CA-CB	-5.04	1.48	1.54	20	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(°)	Ideal(°)	Models	
								Worst	Total
1	A	146	ASN	CA-CB-CG	13.77	126.37	112.60	18	24
1	A	117	PHE	CA-CB-CG	-11.20	102.60	113.80	9	11
1	A	161	PHE	CA-CB-CG	-11.15	102.65	113.80	10	23
1	A	130	PHE	CA-CB-CG	-9.58	104.22	113.80	20	22
1	A	115	ILE	N-CA-CB	9.34	121.48	110.55	2	24
1	A	115	ILE	CB-CA-C	-9.17	100.23	111.97	23	24
1	A	157	VAL	N-CA-C	9.11	119.93	108.82	3	15
1	A	140	ILE	N-CA-C	-8.49	94.15	107.15	11	2
1	A	175	ALA	N-CA-C	8.24	119.60	110.13	5	6
1	A	152	LEU	CA-C-N	8.13	137.07	121.54	24	24
1	A	152	LEU	C-N-CA	8.13	137.07	121.54	24	24
1	A	158	VAL	CB-CA-C	-8.04	102.75	111.59	3	2
1	A	114	LEU	N-CA-CB	-7.97	97.92	110.28	23	6
1	A	174	LEU	N-CA-C	7.97	119.78	108.54	20	17
1	A	123	LYS	N-CA-C	-7.93	95.80	108.73	21	24
1	A	123	LYS	N-CA-CB	7.88	123.41	110.17	13	4
1	A	122	ASP	N-CA-C	-7.87	97.78	109.81	5	18
1	A	157	VAL	CB-CA-C	-7.67	99.47	110.82	13	11
1	A	175	ALA	CB-CA-C	-7.66	97.19	108.91	10	6
1	A	161	PHE	N-CA-C	-7.50	97.63	109.04	16	2
1	A	98	PHE	CA-CB-CG	-7.25	106.55	113.80	16	12
1	A	144	VAL	CA-C-N	6.94	129.91	120.54	11	14
1	A	144	VAL	C-N-CA	6.94	129.91	120.54	11	14
1	A	114	LEU	CB-CA-C	-6.93	97.36	110.67	21	13
1	A	129	ARG	N-CA-C	-6.88	95.74	107.23	22	14
1	A	140	ILE	CA-C-N	6.88	134.89	121.41	9	1
1	A	140	ILE	C-N-CA	6.88	134.89	121.41	9	1
1	A	156	ALA	CB-CA-C	-6.87	97.94	109.48	19	22
1	A	111	LEU	N-CA-C	-6.85	103.60	112.23	9	22
1	A	140	ILE	CB-CA-C	6.78	121.57	112.22	23	4
1	A	148	VAL	N-CA-C	-6.71	103.94	110.72	2	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	157	VAL	CA-C-N	6.70	130.52	120.95	18	3
1	A	157	VAL	C-N-CA	6.70	130.52	120.95	18	3
1	A	144	VAL	CA-CB-CG2	-6.61	99.16	110.40	6	24
1	A	161	PHE	CA-C-N	-6.49	111.73	119.84	9	1
1	A	161	PHE	C-N-CA	-6.49	111.73	119.84	9	1
1	A	108	GLN	N-CA-C	6.48	120.65	112.87	22	22
1	A	152	LEU	CB-CA-C	-6.47	97.19	110.38	7	24
1	A	143	GLU	N-CA-CB	6.45	119.33	109.91	14	22
1	A	107	TYR	CB-CG-CD2	-6.41	111.19	120.80	21	4
1	A	153	GLN	CA-C-N	6.38	129.15	120.54	21	12
1	A	153	GLN	C-N-CA	6.38	129.15	120.54	21	12
1	A	169	GLN	CB-CA-C	-6.37	99.47	109.72	22	12
1	A	149	LYS	CB-CA-C	-6.33	100.67	110.81	20	22
1	A	148	VAL	N-CA-CB	6.25	118.56	110.57	17	15
1	A	156	ALA	CA-C-N	-6.23	114.11	122.77	16	4
1	A	156	ALA	C-N-CA	-6.23	114.11	122.77	16	4
1	A	149	LYS	CB-CG-CD	6.02	125.14	111.30	22	4
1	A	115	ILE	CA-C-N	6.01	128.65	120.54	1	7
1	A	115	ILE	C-N-CA	6.01	128.65	120.54	1	7
1	A	146	ASN	N-CA-C	6.00	118.61	111.71	8	6
1	A	140	ILE	CA-C-O	6.00	128.13	120.76	9	1
1	A	128	LEU	CB-CA-C	-5.95	98.51	109.46	10	3
1	A	156	ALA	N-CA-CB	5.92	120.06	110.41	18	6
1	A	130	PHE	CB-CA-C	-5.90	101.67	111.41	16	1
1	A	124	ALA	N-CA-C	-5.90	102.59	110.55	19	6
1	A	98	PHE	CB-CG-CD1	5.89	130.71	120.70	13	2
1	A	123	LYS	CB-CA-C	5.83	119.64	110.19	18	2
1	A	126	ILE	CB-CA-C	-5.82	103.69	110.91	10	2
1	A	98	PHE	CB-CG-CD2	-5.80	110.84	120.70	13	3
1	A	118	LEU	CA-C-N	5.79	129.12	120.31	2	1
1	A	118	LEU	C-N-CA	5.79	129.12	120.31	2	1
1	A	93	VAL	N-CA-CB	5.78	117.59	111.00	24	5
1	A	118	LEU	CB-CA-C	-5.77	100.88	110.68	1	3
1	A	173	VAL	CB-CA-C	-5.70	103.17	110.98	13	1
1	A	155	LEU	N-CA-C	-5.66	105.47	112.72	8	1
1	A	99	ARG	CA-C-N	5.66	125.61	119.78	21	5
1	A	99	ARG	C-N-CA	5.66	125.61	119.78	21	5
1	A	142	MET	CB-CA-C	-5.65	100.31	110.37	11	1
1	A	106	ASP	N-CA-C	-5.65	106.43	113.55	22	15
1	A	149	LYS	CG-CD-CE	5.60	124.17	111.30	7	13
1	A	114	LEU	N-CA-C	5.59	118.14	111.71	6	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	107	TYR	CA-CB-CG	5.58	123.94	113.90	12	8
1	A	171	ILE	CB-CA-C	-5.55	102.27	110.82	7	2
1	A	159	GLU	N-CA-C	-5.55	104.86	111.69	2	4
1	A	149	LYS	CA-C-N	5.53	127.69	120.28	2	3
1	A	149	LYS	C-N-CA	5.53	127.69	120.28	2	3
1	A	123	LYS	CA-C-N	-5.44	115.33	123.00	11	1
1	A	123	LYS	C-N-CA	-5.44	115.33	123.00	11	1
1	A	117	PHE	CA-C-N	5.42	127.80	120.38	18	1
1	A	117	PHE	C-N-CA	5.42	127.80	120.38	18	1
1	A	160	SER	CB-CA-C	-5.39	101.32	109.99	3	2
1	A	148	VAL	CB-CA-C	-5.38	105.04	112.24	24	4
1	A	145	LEU	CB-CA-C	-5.36	101.94	110.84	2	3
1	A	146	ASN	CB-CG-ND2	-5.29	108.47	116.40	23	7
1	A	143	GLU	CB-CA-C	-5.29	102.55	110.90	6	2
1	A	170	MET	CB-CA-C	-5.26	101.43	110.16	13	1
1	A	130	PHE	N-CA-C	-5.24	101.42	109.76	11	1
1	A	117	PHE	CB-CG-CD2	-5.21	111.84	120.70	21	3
1	A	158	VAL	CA-CB-CG2	5.19	119.22	110.40	2	1
1	A	145	LEU	CA-C-N	5.19	127.23	120.28	15	1
1	A	145	LEU	C-N-CA	5.19	127.23	120.28	15	1
1	A	149	LYS	N-CA-CB	5.16	117.67	109.82	22	1
1	A	106	ASP	N-CA-CB	-5.15	102.61	110.33	15	1
1	A	170	MET	N-CA-C	-5.14	102.45	110.42	18	1
1	A	172	MET	CA-C-N	-5.11	116.49	122.93	4	1
1	A	172	MET	C-N-CA	-5.11	116.49	122.93	4	1
1	A	151	ASP	N-CA-C	5.08	116.90	111.36	2	1
1	A	173	VAL	CA-C-N	5.08	130.21	122.65	18	1
1	A	173	VAL	C-N-CA	5.08	130.21	122.65	18	1
1	A	115	ILE	CA-CB-CG2	-5.05	101.91	110.50	24	1
1	A	174	LEU	CB-CA-C	5.01	119.20	109.33	8	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
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	140

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:144:VAL:O	1:A:148:VAL:HG23	0.48	2.08	24	2
1:A:118:LEU:HD11	1:A:174:LEU:CD2	0.48	2.39	7	1
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:128:LEU:HD12	1:A:145:LEU:CD2	0.46	2.41	11	1
1:A:145:LEU:O	1:A:172:MET:HE1	0.46	2.11	17	2
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 ⓘ

6.3.1 Protein backbone ⓘ

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%)	9	52
All	All	1536/2400 (64%)	1370 (89%)	139 (9%)	27 (2%)	9	52

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
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±1 (85±2%)	9±1 (15±2%)	5	42
All	All	1416/2160 (66%)	1204 (85%)	212 (15%)	5	42

All 26 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	148	VAL	22
1	A	118	LEU	21
1	A	128	LEU	19
1	A	174	LEU	19
1	A	150	ASP	13
1	A	123	LYS	12
1	A	155	LEU	11
1	A	143	GLU	9
1	A	161	PHE	7
1	A	149	LYS	4
1	A	158	VAL	3
1	A	145	LEU	3
1	A	172	MET	3
1	A	169	GLN	3
1	A	96	ILE	2
1	A	99	ARG	2
1	A	171	ILE	2
1	A	119	GLU	2
1	A	173	VAL	2
1	A	160	SER	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	106	ASP	1
1	A	114	LEU	1
1	A	97	LYS	1
1	A	177	LYS	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 oligosaccharides 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

No chemical shift data were provided