



# Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:20 am BST

PDB ID : 2MLY  
Title : NMR structure of E. coli Trigger Factor in complex with unfolded PhoA1-150  
Authors : Saio, T.; Guan, X.; Rossi, P.; Economou, A.; Kalodimos, C.G.  
Deposited on : 2014-03-05

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

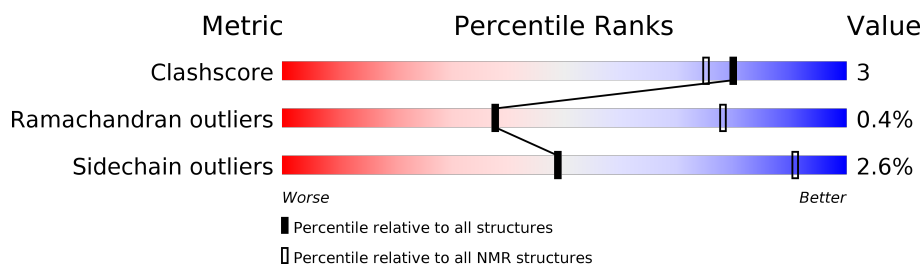
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 35%.

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  $\geq 3$ , 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	443	
2	B	151	

## 2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 7 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:1-A:373, A:392-A:429 (411)	0.82	7

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. No single-model clusters were found.

Cluster number	Models
1	2, 4, 5, 6, 7, 8, 9, 10
2	1, 3

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9012 atoms, of which 4519 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms						Trace
1	A	432	Total	C	H	N	O	S	0
			6789	2119	3403	582	674	11	

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP U6N325
A	-9	ASN	-	EXPRESSION TAG	UNP U6N325
A	-8	HIS	-	EXPRESSION TAG	UNP U6N325
A	-7	LYS	-	EXPRESSION TAG	UNP U6N325
A	-6	VAL	-	EXPRESSION TAG	UNP U6N325
A	-5	HIS	-	EXPRESSION TAG	UNP U6N325
A	-4	HIS	-	EXPRESSION TAG	UNP U6N325
A	-3	HIS	-	EXPRESSION TAG	UNP U6N325
A	-2	HIS	-	EXPRESSION TAG	UNP U6N325
A	-1	HIS	-	EXPRESSION TAG	UNP U6N325
A	0	HIS	-	EXPRESSION TAG	UNP U6N325

- Molecule 2 is a protein called Alkaline phosphatase.

Mol	Chain	Residues	Atoms						Trace
2	B	150	Total	C	H	N	O	S	0
			2223	694	1116	192	218	3	

There is a discrepancy between the modelled and reference sequences:

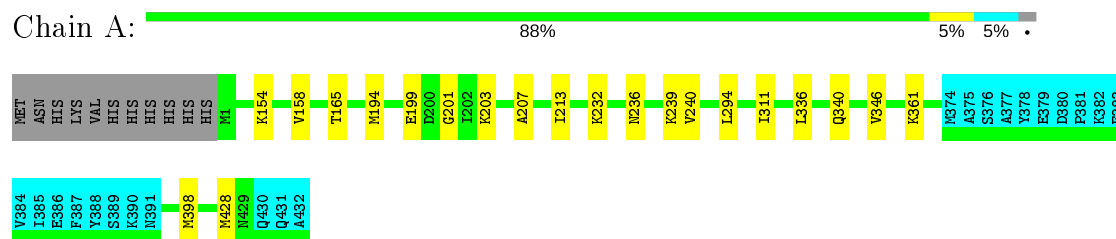
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	EXPRESSION TAG	UNP U6N3P1

## 4 Residue-property plots

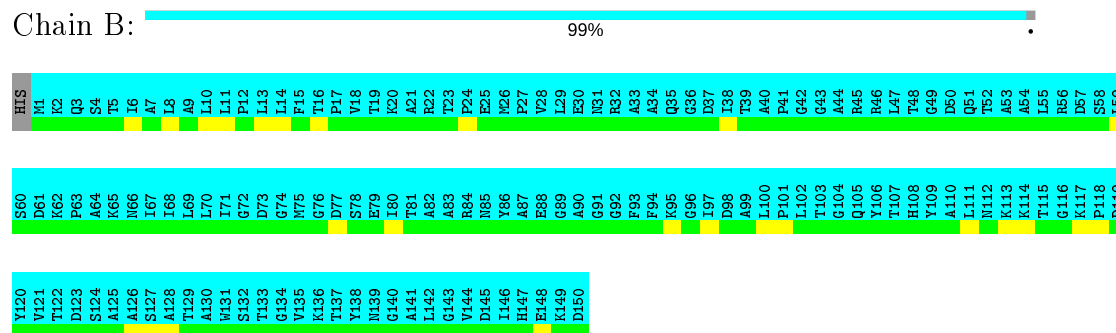
### 4.1 Average score per residue in the NMR ensemble

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: Trigger factor



- Molecule 2: Alkaline phosphatase

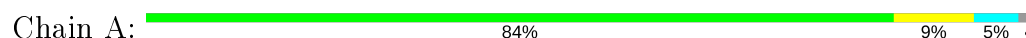


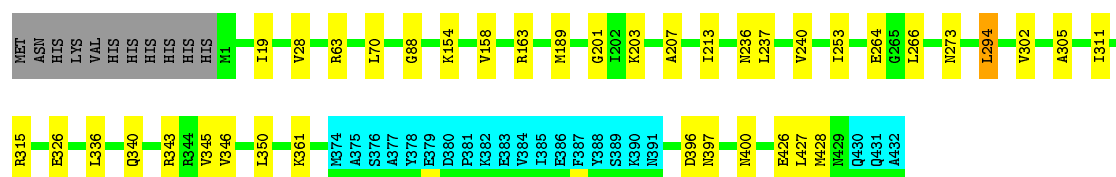
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

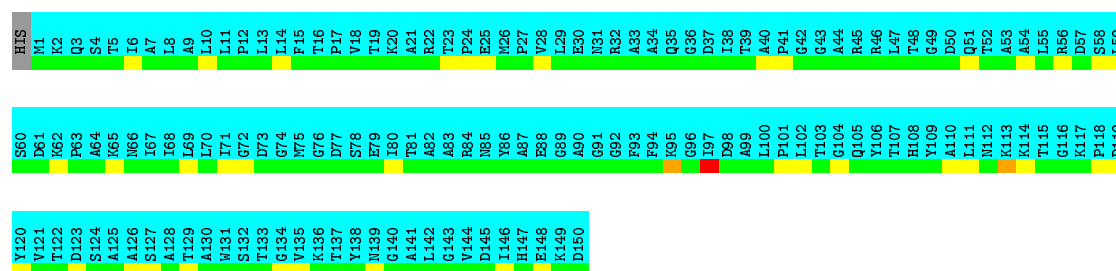
- Molecule 1: Trigger factor





- Molecule 2: Alkaline phosphatase

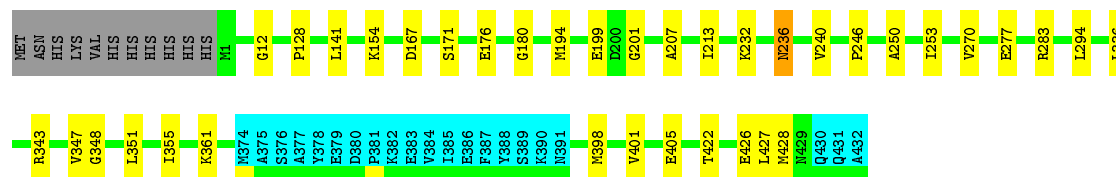
Chain B: 99%



#### 4.2.2 Score per residue for model 2

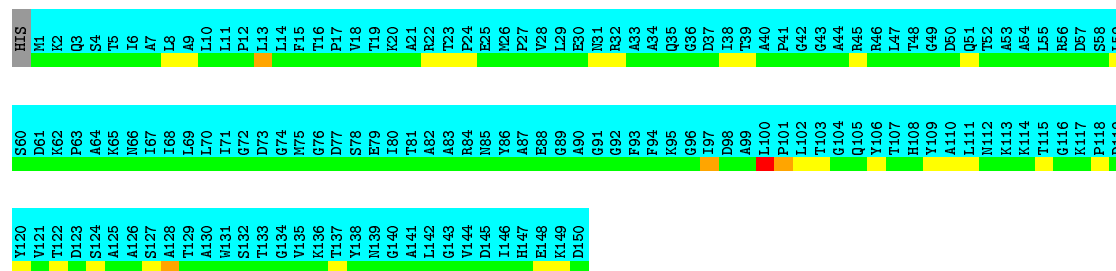
- Molecule 1: Trigger factor

Chain A: 84%



- Molecule 2: Alkaline phosphatase

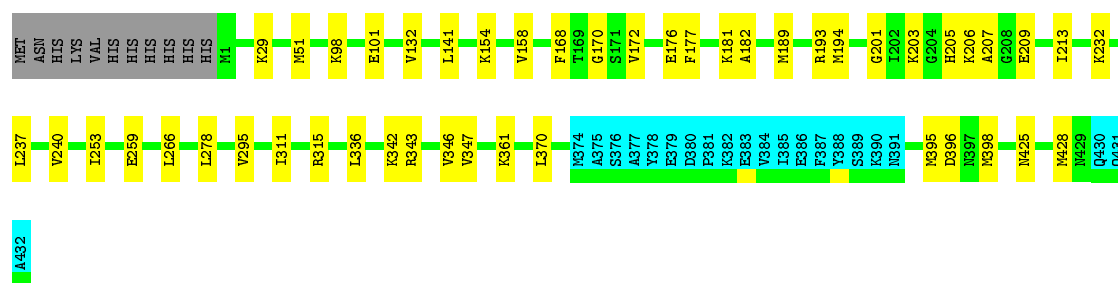
Chain B: 99%



#### 4.2.3 Score per residue for model 3

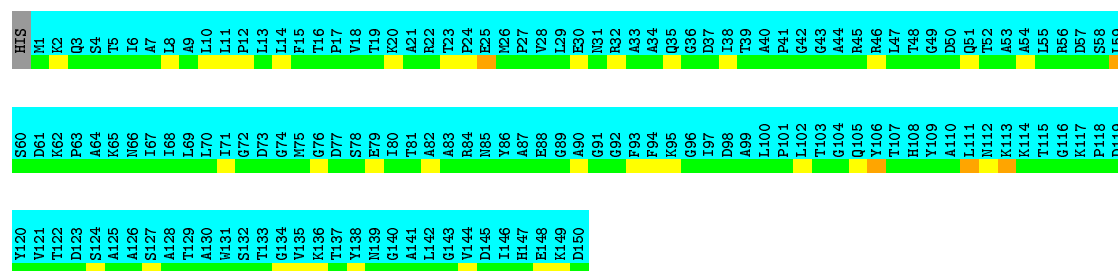
- Molecule 1: Trigger factor

Chain A: 82%



- Molecule 2: Alkaline phosphatase

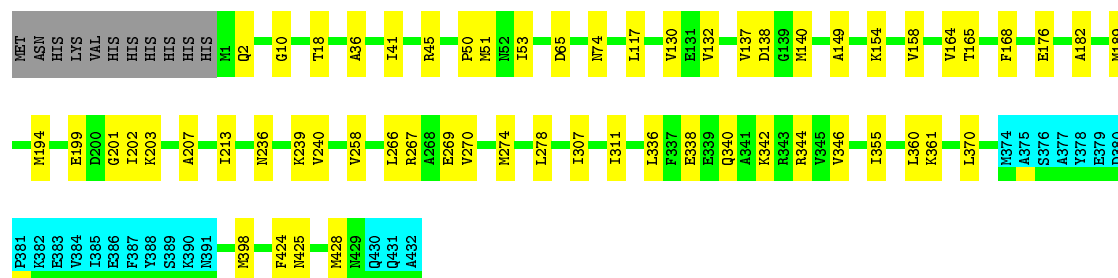
Chain B: 99%



#### 4.2.4 Score per residue for model 4

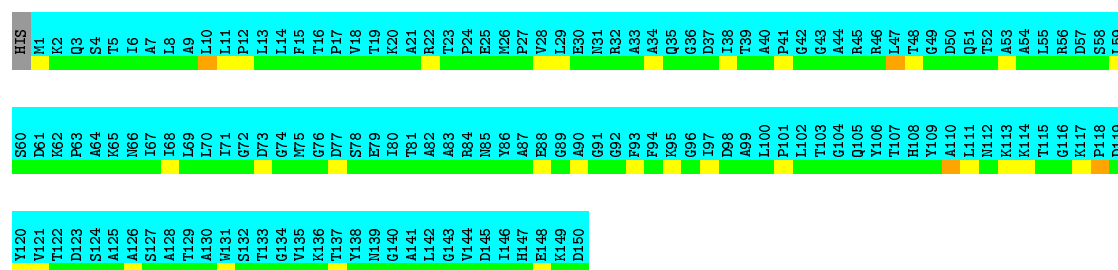
- Molecule 1: Trigger factor

Chain A: 79%



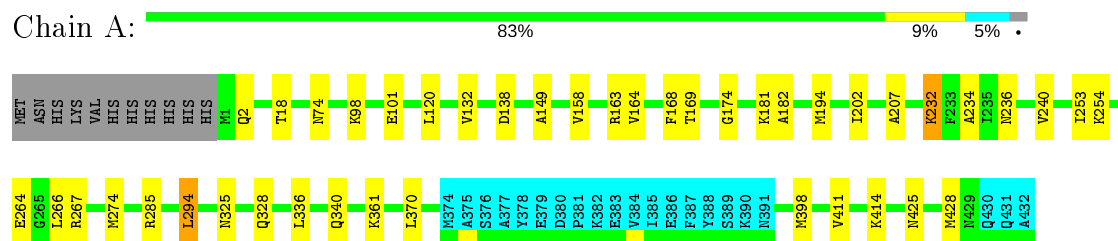
- Molecule 2: Alkaline phosphatase

Chain B: 99%

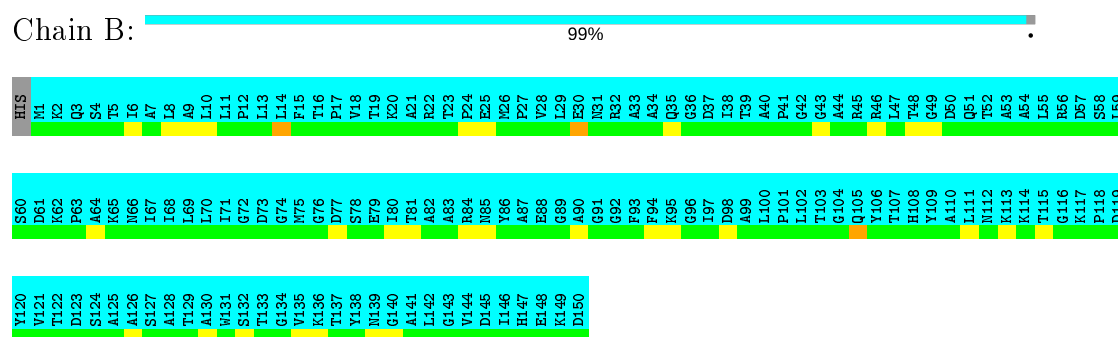


### 4.2.5 Score per residue for model 5

- Molecule 1: Trigger factor

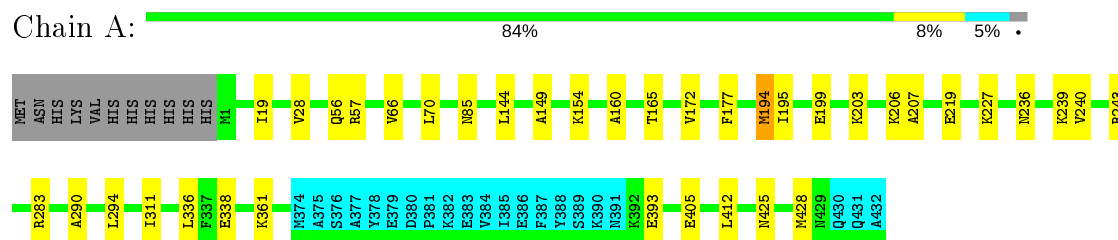


- Molecule 2: Alkaline phosphatase

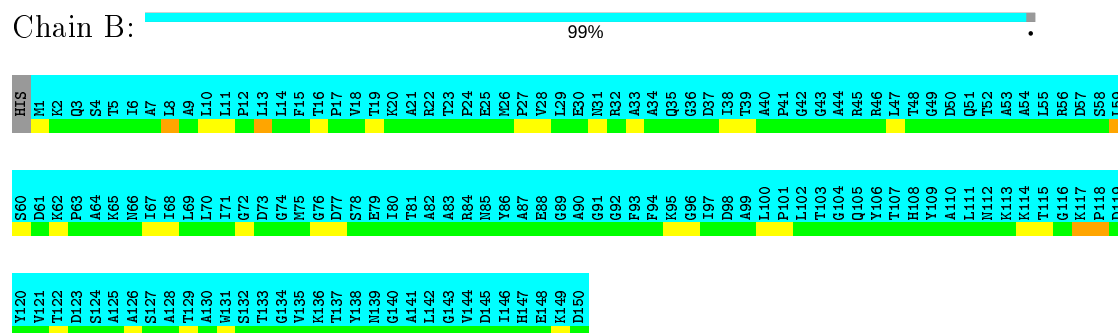


### 4.2.6 Score per residue for model 6

- Molecule 1: Trigger factor



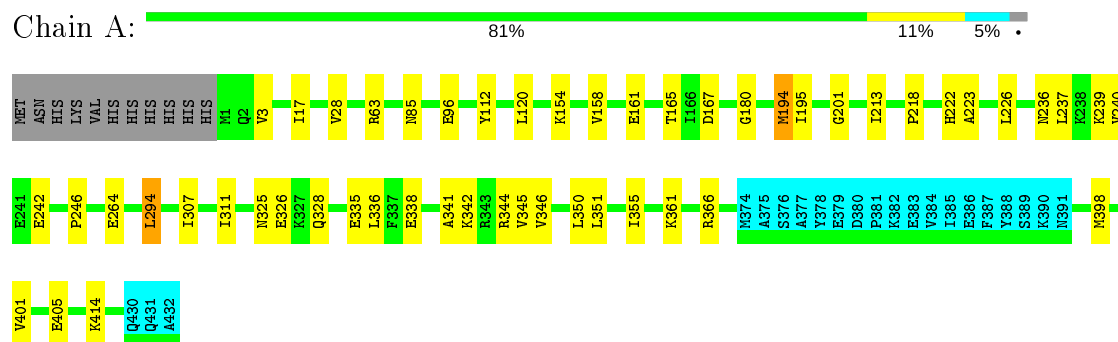
- Molecule 2: Alkaline phosphatase



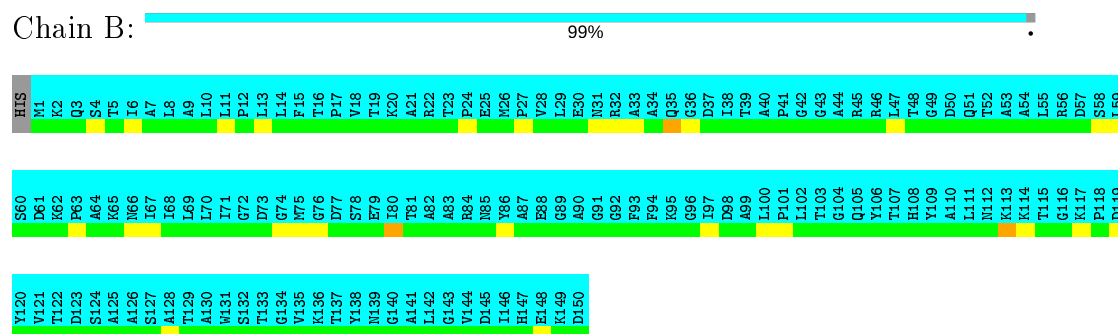


### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Trigger factor

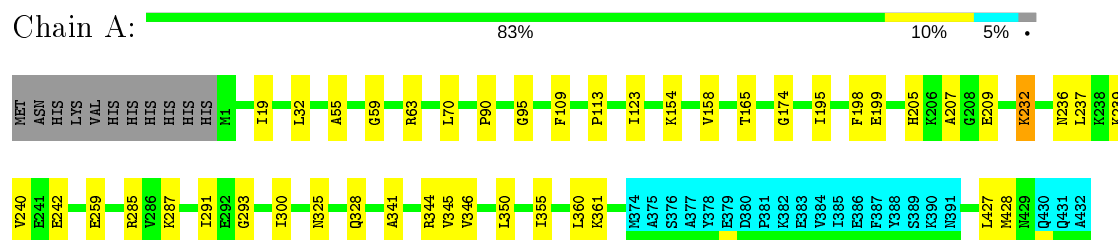


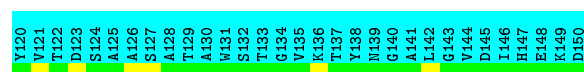
- Molecule 2: Alkaline phosphatase



### 4.2.8 Score per residue for model 8

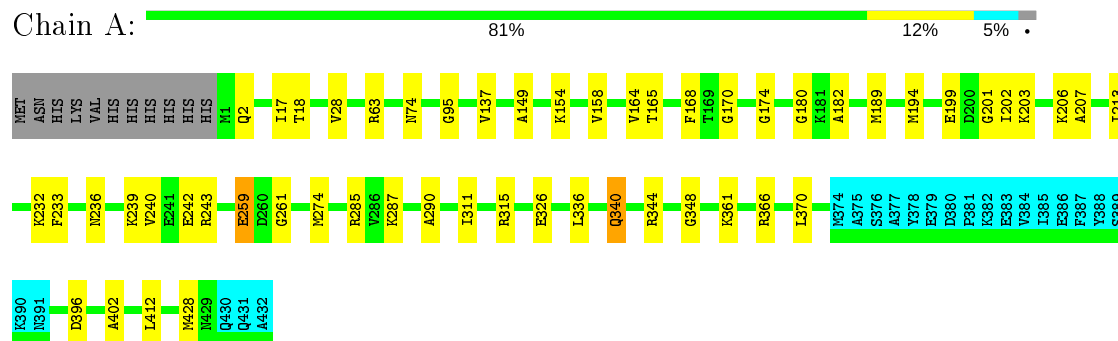
- Molecule 1: Trigger factor



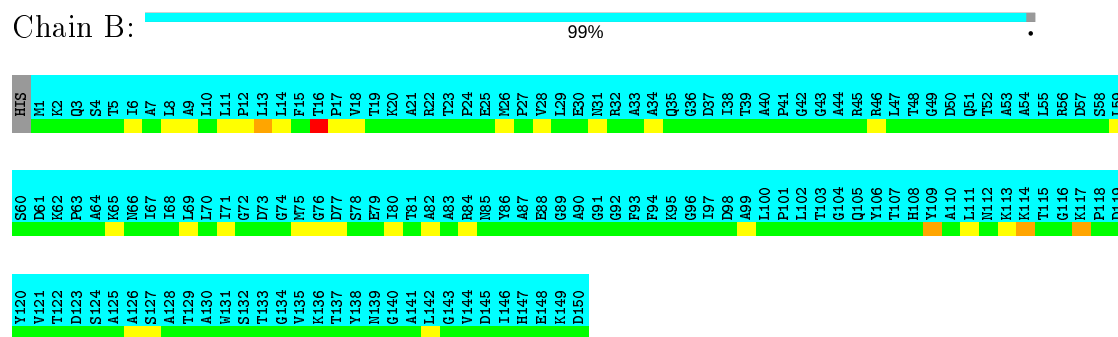


#### 4.2.9 Score per residue for model 9

- Molecule 1: Trigger factor

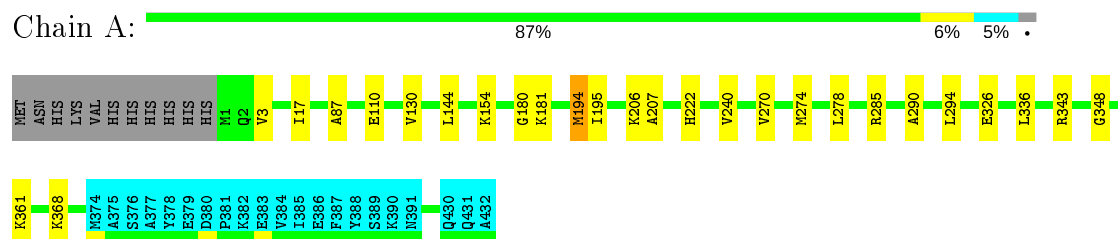


- Molecule 2: Alkaline phosphatase

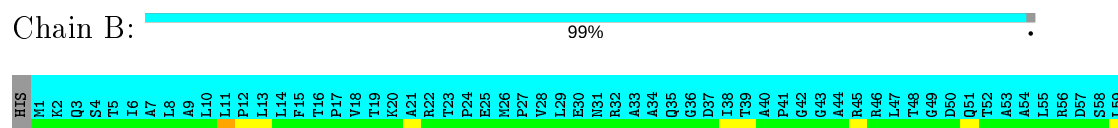


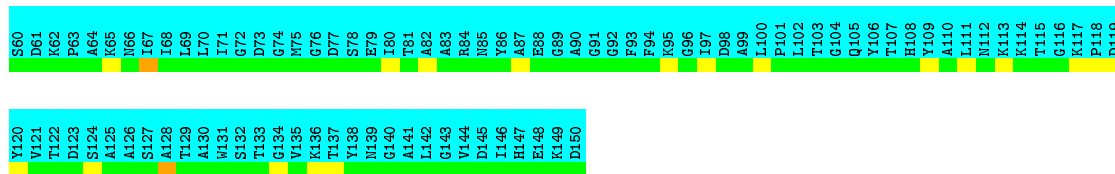
#### 4.2.10 Score per residue for model 10

- Molecule 1: Trigger factor



- Molecule 2: Alkaline phosphatase





## 5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure solution	3.0
X-PLOR NIH	structure solution	
TALOSN	geometry optimization	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	2
Total number of shifts	2632
Number of shifts mapped to atoms	2632
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	35%

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

COVALENT-GEOMETRY INFOmissingINFO

### 5.1 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	3214	3245	3245	18±5
2	B	0	0	0	0±0
All	All	32140	32450	32450	175

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:425:ASN:HA	1:A:428:MET:HB2	0.65	1.66	5	3
1:A:132:VAL:HG11	1:A:274:MET:SD	0.60	2.36	4	2
1:A:88:GLY:HA2	1:A:305:ALA:HB2	0.59	1.73	1	1
1:A:137:VAL:HA	1:A:274:MET:HE1	0.58	1.76	4	1
1:A:154:LYS:HG3	1:A:240:VAL:HG13	0.58	1.74	7	9
1:A:138:ASP:HB2	1:A:267:ARG:HH22	0.57	1.59	4	2
1:A:45:ARG:NH2	1:A:51:MET:SD	0.57	2.77	4	1
1:A:205:HIS:HB3	1:A:209:GLU:HG3	0.57	1.77	8	2
1:A:370:LEU:HD23	1:A:398:MET:SD	0.57	2.39	3	1
1:A:165:THR:HB	1:A:239:LYS:HB2	0.55	1.78	6	5
1:A:98:LYS:HB2	1:A:101:GLU:HB2	0.55	1.78	5	2
1:A:253:ILE:HG23	1:A:266:LEU:HD13	0.53	1.78	3	2
1:A:19:ILE:HD13	1:A:70:LEU:HB3	0.52	1.80	6	3
1:A:189:MET:SD	1:A:203:LYS:HG2	0.52	2.45	1	4
1:A:167:ASP:HB3	1:A:236:ASN:HB2	0.52	1.81	7	2
1:A:335:GLU:HA	1:A:338:GLU:HB2	0.52	1.81	7	1
1:A:370:LEU:HD11	1:A:398:MET:SD	0.52	2.45	5	1
1:A:2:GLN:HB3	1:A:18:THR:HB	0.51	1.80	4	3
1:A:141:LEU:HD21	1:A:270:VAL:HG21	0.51	1.81	2	1
1:A:207:ALA:HB2	1:A:240:VAL:HG12	0.51	1.81	5	9
1:A:140:MET:SD	1:A:424:PHE:CZ	0.51	3.03	4	1
1:A:158:VAL:HG21	1:A:237:LEU:HD21	0.51	1.83	1	4
1:A:194:MET:SD	1:A:195:ILE:N	0.51	2.84	6	3
1:A:294:LEU:HD22	1:A:350:LEU:HD13	0.50	1.81	1	2
1:A:355:ILE:HA	1:A:360:LEU:HB3	0.50	1.82	4	2
1:A:50:PRO:HG2	1:A:53:ILE:HD12	0.50	1.83	4	1
1:A:311:ILE:HD11	1:A:338:GLU:HA	0.50	1.83	4	2
1:A:123:ILE:HG23	1:A:293:GLY:HA3	0.50	1.82	8	1
1:A:164:VAL:HG21	1:A:202:ILE:HG21	0.50	1.83	9	3
1:A:120:LEU:HB2	1:A:414:LYS:HE3	0.50	1.82	5	2
1:A:201:GLY:HA3	1:A:213:ILE:HG21	0.49	1.84	3	6
1:A:164:VAL:HG12	1:A:240:VAL:HG23	0.49	1.83	4	1
1:A:28:VAL:HG21	1:A:63:ARG:HD3	0.49	1.84	1	1
1:A:154:LYS:HD3	1:A:242:GLU:HB2	0.49	1.84	7	3
1:A:130:VAL:HB	1:A:278:LEU:HD11	0.49	1.85	4	2
1:A:302:VAL:HG11	1:A:345:VAL:HG11	0.48	1.84	1	1
1:A:398:MET:HA	1:A:401:VAL:HG12	0.48	1.86	2	2
1:A:149:ALA:HB1	1:A:243:ARG:HB2	0.48	1.85	6	2
1:A:351:LEU:O	1:A:355:ILE:HD13	0.48	2.08	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:294:LEU:HG	1:A:411:VAL:HG11	0.48	1.86	5	1
1:A:28:VAL:HG11	1:A:63:ARG:NH2	0.47	2.24	7	1
1:A:174:GLY:HA2	1:A:232:LYS:HG3	0.47	1.87	9	3
1:A:113:PRO:HG2	1:A:300:ILE:HD11	0.47	1.85	8	1
1:A:426:GLU:HG3	1:A:427:LEU:HD12	0.47	1.87	1	1
1:A:325:ASN:HB3	1:A:328:GLN:HB2	0.46	1.87	7	3
1:A:137:VAL:HG22	1:A:274:MET:SD	0.46	2.50	9	1
1:A:283:ARG:NH2	1:A:405:GLU:HB3	0.46	2.25	6	2
1:A:158:VAL:HG11	1:A:202:ILE:HG22	0.46	1.86	5	3
1:A:172:VAL:HG23	1:A:177:PHE:CE1	0.46	2.45	3	2
1:A:168:PHE:CE1	1:A:182:ALA:HB3	0.46	2.45	9	4
1:A:28:VAL:HG11	1:A:63:ARG:HG2	0.46	1.85	9	1
1:A:341:ALA:O	1:A:345:VAL:HG23	0.46	2.10	8	2
1:A:253:ILE:HD11	1:A:266:LEU:HB2	0.45	1.87	5	1
1:A:290:ALA:O	1:A:294:LEU:HB2	0.45	2.12	10	1
1:A:3:VAL:HG12	1:A:17:ILE:HG12	0.45	1.87	10	2
1:A:169:THR:HA	1:A:181:LYS:HG3	0.45	1.88	5	1
1:A:366:ARG:HH12	1:A:370:LEU:HD12	0.44	1.72	9	1
1:A:128:PRO:HB2	1:A:427:LEU:HD11	0.44	1.88	2	1
1:A:295:VAL:HG21	1:A:347:VAL:HG22	0.44	1.90	3	1
1:A:346:VAL:O	1:A:350:LEU:HG	0.44	2.13	1	2
1:A:195:ILE:HB	1:A:198:PHE:HB2	0.44	1.89	8	1
1:A:311:ILE:O	1:A:315:ARG:HG3	0.44	2.13	1	3
1:A:287:LYS:O	1:A:291:ILE:HG12	0.44	2.13	8	1
1:A:87:ALA:HB3	1:A:110:GLU:HB2	0.43	1.90	10	1
1:A:290:ALA:HB2	1:A:412:LEU:HD21	0.43	1.89	6	2
1:A:422:THR:HG21	1:A:426:GLU:HG2	0.43	1.91	2	1
1:A:90:PRO:HA	1:A:109:PHE:HB3	0.43	1.89	8	1
1:A:266:LEU:O	1:A:270:VAL:HG23	0.43	2.13	4	1
1:A:141:LEU:HD13	1:A:266:LEU:HG	0.43	1.90	3	1
1:A:160:ALA:HB1	1:A:203:LYS:HE3	0.42	1.91	6	1
1:A:366:ARG:NE	1:A:405:GLU:HB3	0.42	2.29	7	1
1:A:366:ARG:NH1	1:A:402:ALA:HA	0.42	2.29	9	1
1:A:170:GLY:H	1:A:181:LYS:HG3	0.42	1.74	3	1
1:A:340:GLN:O	1:A:344:ARG:HG3	0.42	2.14	9	1
1:A:17:ILE:HG21	1:A:74:ASN:HB3	0.42	1.92	9	1
1:A:169:THR:HB	1:A:234:ALA:HB3	0.42	1.91	5	1
1:A:258:VAL:HG13	1:A:269:GLU:HG2	0.42	1.90	4	1
1:A:132:VAL:HG23	1:A:278:LEU:HD22	0.41	1.91	3	1
1:A:56:GLN:HG3	1:A:57:ARG:HG3	0.41	1.92	6	1
1:A:85:ASN:ND2	1:A:112:TYR:HB2	0.41	2.30	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:397:ASN:HA	1:A:400:ASN:ND2	0.41	2.29	1	1
1:A:158:VAL:HA	1:A:240:VAL:HG21	0.41	1.92	7	1
1:A:59:GLY:O	1:A:63:ARG:HG3	0.41	2.15	8	1
1:A:219:GLU:HA	1:A:227:LYS:HB2	0.41	1.91	6	1
1:A:270:VAL:O	1:A:274:MET:HG3	0.41	2.15	10	1
1:A:170:GLY:HA2	1:A:233:PHE:CD1	0.41	2.51	9	1
1:A:171:SER:HB2	1:A:232:LYS:HB2	0.41	1.92	2	1
1:A:250:ALA:HA	1:A:253:ILE:HG22	0.41	1.92	2	1
1:A:29:LYS:HG3	1:A:51:MET:HG3	0.41	1.92	3	1
1:A:370:LEU:HD22	1:A:398:MET:SD	0.41	2.56	4	1
1:A:307:ILE:O	1:A:311:ILE:HG12	0.41	2.15	7	2
1:A:32:LEU:HD21	1:A:55:ALA:HA	0.41	1.92	8	1
1:A:342:LYS:O	1:A:346:VAL:HG23	0.40	2.16	7	3
1:A:343:ARG:O	1:A:347:VAL:HG23	0.40	2.16	2	1
1:A:28:VAL:HA	1:A:66:VAL:HG21	0.40	1.93	6	1
1:A:195:ILE:HG12	1:A:218:PRO:HD3	0.40	1.92	7	1
1:A:223:ALA:HB3	1:A:226:LEU:HB2	0.40	1.93	7	1
1:A:36:ALA:HA	1:A:41:ILE:HB	0.40	1.92	4	1

## 5.2 Torsion angles ⓘ

### 5.2.1 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	410/443 (93%)	372±5 (91±1%)	36±5 (9±1%)	2±1 (0±0%)	38	78
2	B	0	-	-	-	-	-
All	All	4100/5940 (69%)	3724 (91%)	361 (9%)	15 (0%)	38	78

All 11 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	149	ALA	2
1	A	246	PRO	2
1	A	95	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	326	GLU	2
1	A	259	GLU	1
1	A	96	GLU	1
1	A	393	GLU	1
1	A	10	GLY	1
1	A	176	GLU	1
1	A	261	GLY	1
1	A	12	GLY	1

## 5.2.2 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	341/370 (92%)	332±2 (97±1%)	9±2 (3±1%)	49 91
2	B	0	-	-	-
All	All	3410/4840 (70%)	3322 (97%)	88 (3%)	49 91

All 29 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	361	LYS	10
1	A	336	LEU	9
1	A	194	MET	8
1	A	236	ASN	7
1	A	294	LEU	5
1	A	199	GLU	5
1	A	206	LYS	4
1	A	340	GLN	4
1	A	264	GLU	3
1	A	396	ASP	3
1	A	343	ARG	3
1	A	259	GLU	3
1	A	232	LYS	3
1	A	163	ARG	2
1	A	74	ASN	2
1	A	326	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	176	GLU	2
1	A	285	ARG	2
1	A	161	GLU	1
1	A	85	ASN	1
1	A	425	ASN	1
1	A	368	LYS	1
1	A	65	ASP	1
1	A	428	MET	1
1	A	273	ASN	1
1	A	181	LYS	1
1	A	222	HIS	1
1	A	254	LYS	1
1	A	117	LEU	1

### 5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.5 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.6 Other polymers [i](#)

There are no such molecules in this entry.

### 5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 35% for the well-defined parts and 30% for the entire structure.

### 6.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 6.1.1 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	2303
Number of shifts mapped to atoms	2303
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	37

#### 6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	91	$-0.09 \pm 0.32$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	106	$0.08 \pm 0.17$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	1	—	None (insufficient data)
$^{15}\text{N}$	392	$0.43 \pm 0.22$	None needed ( $< 0.5$ ppm)

#### 6.1.3 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 35%, i.e. 1792 atoms were assigned a chemical shift out of a possible 5066. 0 out of 72 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	929/2033 (46%)	464/811 (57%)	92/822 (11%)	373/400 (93%)
Sidechain	762/2813 (27%)	432/1630 (27%)	330/1043 (32%)	0/140 (0%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	101/220 (46%)	44/118 (37%)	56/97 (58%)	1/5 (20%)
Overall	1792/5066 (35%)	940/2559 (37%)	478/1962 (24%)	374/545 (69%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 26%, i.e. 1856 atoms were assigned a chemical shift out of a possible 7035. 0 out of 93 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	967/2870 (34%)	483/1144 (42%)	92/1164 (8%)	392/562 (70%)
Sidechain	776/3825 (20%)	439/2220 (20%)	337/1423 (24%)	0/182 (0%)
Aromatic	113/340 (33%)	44/180 (24%)	68/150 (45%)	1/10 (10%)
Overall	1856/7035 (26%)	966/3544 (27%)	497/2737 (18%)	393/754 (52%)

#### 6.1.4 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	387	PHE	CD2	41.95	137.34 – 125.84	-77.9
1	A	256	PHE	CD2	41.95	137.34 – 125.84	-77.9
1	A	424	PHE	CD2	41.95	137.34 – 125.84	-77.9
1	A	252	PHE	CD2	42.05	137.34 – 125.84	-77.9
1	A	337	PHE	CD2	42.22	137.34 – 125.84	-77.7
1	A	322	PHE	CD2	42.79	137.34 – 125.84	-77.2
1	A	337	PHE	CE2	40.88	136.81 – 124.71	-74.3
1	A	322	PHE	CE2	41.09	136.81 – 124.71	-74.1
1	A	252	PHE	CE2	41.30	136.81 – 124.71	-73.9
1	A	256	PHE	CE2	41.42	136.81 – 124.71	-73.8
1	A	387	PHE	CE2	41.43	136.81 – 124.71	-73.8
1	A	387	PHE	CD1	41.95	137.63 – 125.43	-73.4
1	A	256	PHE	CD1	41.95	137.63 – 125.43	-73.4
1	A	424	PHE	CD1	41.95	137.63 – 125.43	-73.4
1	A	424	PHE	CE2	41.95	136.81 – 124.71	-73.4
1	A	252	PHE	CD1	42.05	137.63 – 125.43	-73.3
1	A	337	PHE	CD1	42.22	137.63 – 125.43	-73.2
1	A	322	PHE	CD1	42.79	137.63 – 125.43	-72.7
1	A	378	TYR	CE1	28.15	124.14 – 111.74	-72.4
1	A	388	TYR	CE1	28.19	124.14 – 111.74	-72.4
1	A	388	TYR	CD1	43.26	139.11 – 126.41	-70.5
1	A	378	TYR	CD1	43.67	139.11 – 126.41	-70.1

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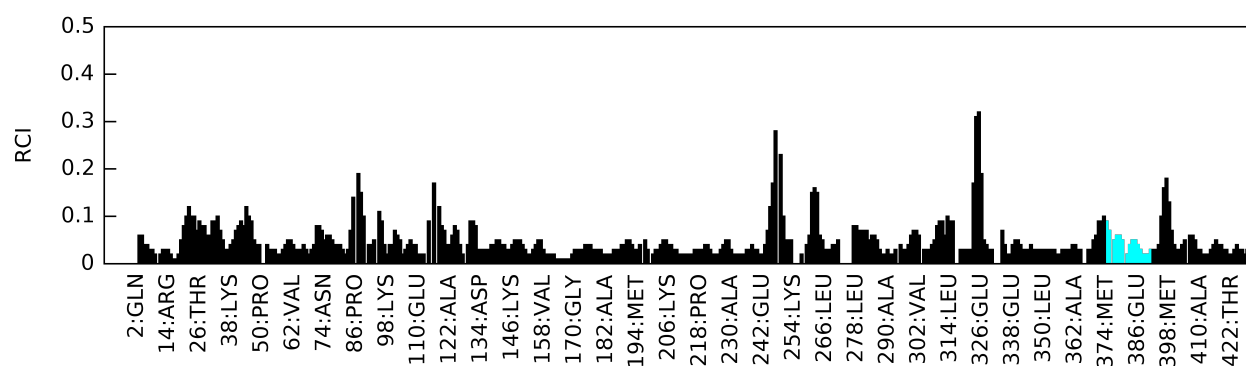
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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	378	TYR	CE2	28.15	124.68 – 111.18	-66.5
1	A	388	TYR	CE2	28.19	124.68 – 111.18	-66.5
1	A	337	PHE	CE1	40.88	137.92 – 123.42	-61.9
1	A	322	PHE	CE1	41.09	137.92 – 123.42	-61.8
1	A	252	PHE	CE1	41.30	137.92 – 123.42	-61.6
1	A	256	PHE	CE1	41.42	137.92 – 123.42	-61.6
1	A	387	PHE	CE1	41.43	137.92 – 123.42	-61.5
1	A	424	PHE	CE1	41.95	137.92 – 123.42	-61.2
1	A	388	TYR	CD2	43.26	140.11 – 125.31	-60.4
1	A	378	TYR	CD2	43.67	140.11 – 125.31	-60.2
1	A	337	PHE	CZ	39.15	137.04 – 121.44	-57.8
1	A	322	PHE	CZ	39.16	137.04 – 121.44	-57.7
1	A	424	PHE	CZ	39.81	137.04 – 121.44	-57.3
1	A	387	PHE	CZ	39.84	137.04 – 121.44	-57.3
1	A	163	ARG	HB2	0.21	3.15 – 0.45	-5.9

### 6.1.5 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:



## 6.2 Chemical shift list 2

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1\_dup*

### 6.2.1 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	329
Number of shifts mapped to atoms	329
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	16

### 6.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	4	—	None (insufficient data)
$^{13}\text{C}_\beta$	10	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	84	$-0.81 \pm 0.20$	Should be applied

### 6.2.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 5066. 0 out of 72 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	0/2033 (0%)	0/811 (0%)	0/822 (0%)	0/400 (0%)
Sidechain	0/2813 (0%)	0/1630 (0%)	0/1043 (0%)	0/140 (0%)
Aromatic	0/220 (0%)	0/118 (0%)	0/97 (0%)	0/5 (0%)
Overall	0/5066 (0%)	0/2559 (0%)	0/1962 (0%)	0/545 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 274 atoms were assigned a chemical shift out of a possible 7035. 0 out of 93 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	176/2870 (6%)	88/1144 (8%)	4/1164 (0%)	84/562 (15%)
Sidechain	63/3825 (2%)	33/2220 (1%)	30/1423 (2%)	0/182 (0%)
Aromatic	35/340 (10%)	18/180 (10%)	17/150 (11%)	0/10 (0%)
Overall	274/7035 (4%)	139/3544 (4%)	51/2737 (2%)	84/754 (11%)

### 6.2.4 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
2	B	100	LEU	HD12	25.30	2.16 – -0.64	87.6
2	B	100	LEU	HD13	25.30	2.16 – -0.64	87.6
2	B	100	LEU	HD11	25.30	2.16 – -0.64	87.6
2	B	102	LEU	HD13	25.30	2.16 – -0.64	87.6
2	B	102	LEU	HD11	25.30	2.16 – -0.64	87.6
2	B	102	LEU	HD12	25.30	2.16 – -0.64	87.6
2	B	100	LEU	HD23	23.55	2.14 – -0.66	81.5
2	B	100	LEU	HD22	23.55	2.14 – -0.66	81.5
2	B	100	LEU	HD21	23.55	2.14 – -0.66	81.5
2	B	102	LEU	HD23	23.55	2.14 – -0.66	81.5
2	B	102	LEU	HD22	23.55	2.14 – -0.66	81.5
2	B	102	LEU	HD21	23.55	2.14 – -0.66	81.5
2	B	100	LEU	CD1	0.82	32.77 – 16.57	-14.7
2	B	102	LEU	CD1	0.83	32.77 – 16.57	-14.7
2	B	102	LEU	CD2	0.78	32.60 – 15.60	-13.7
2	B	100	LEU	CD2	0.78	32.60 – 15.60	-13.7

### 6.2.5 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 B:

