



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:29 PM BST

PDB ID : 2JVV  
Title : Solution Structure of E. coli NusG carboxyterminal domain  
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Deposited on : 2007-09-26

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  
<http://wwpdb.org/validation/2016/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  
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

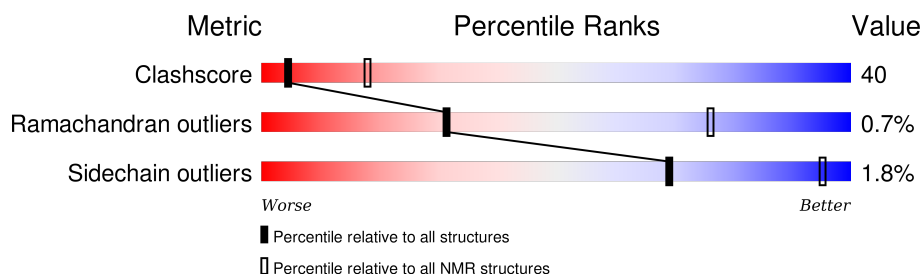
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment 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	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  $\geq 3$ , 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	181	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:128-A:163, A:167-A:181 (51)	0.27	2

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 4 clusters and 1 single-model cluster was found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 926 atoms, of which 459 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription antitermination protein nusG.

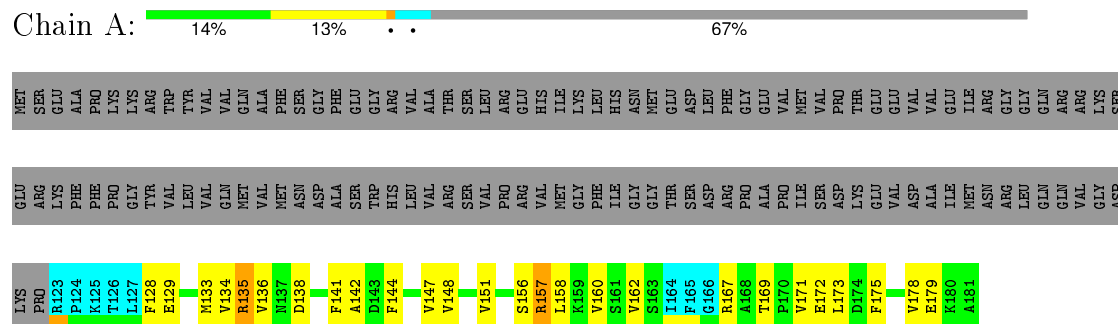
Mol	Chain	Residues	Atoms						Trace
1	A	59	Total	C	H	N	O	S	0
			926	297	459	78	91	1	

## 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: Transcription antitermination protein nusG

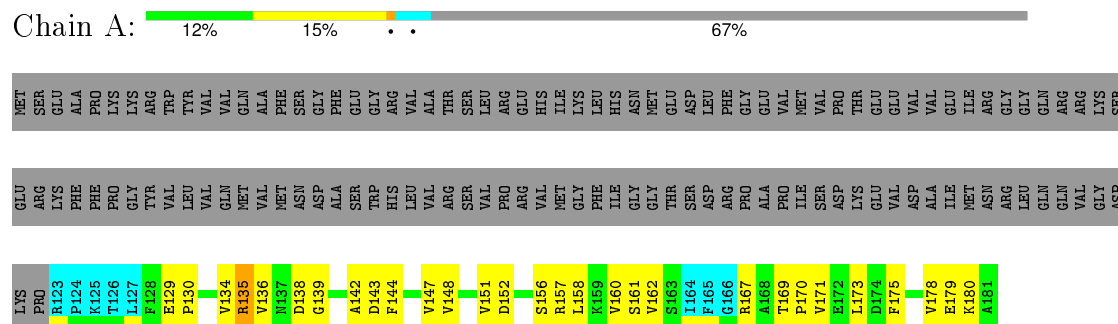


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

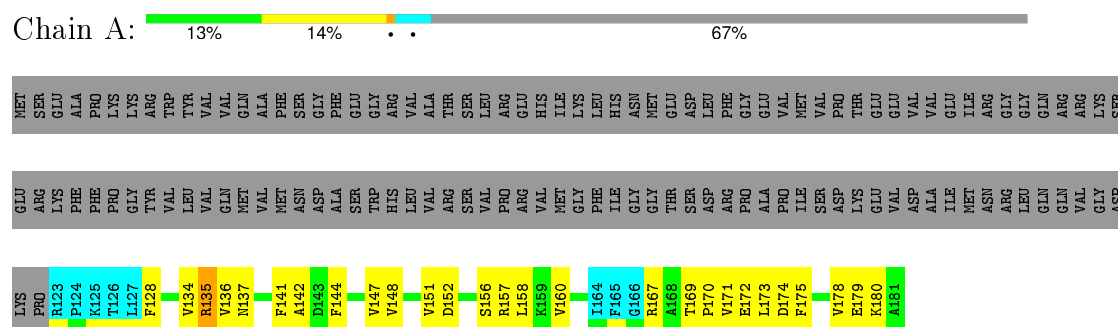
#### 4.2.1 Score per residue for model 1

- Molecule 1: Transcription antitermination protein nusG



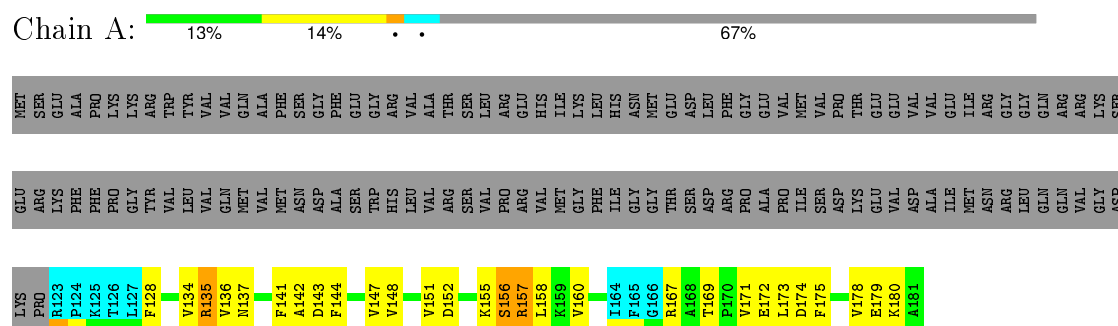
#### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Transcription antitermination protein nusG



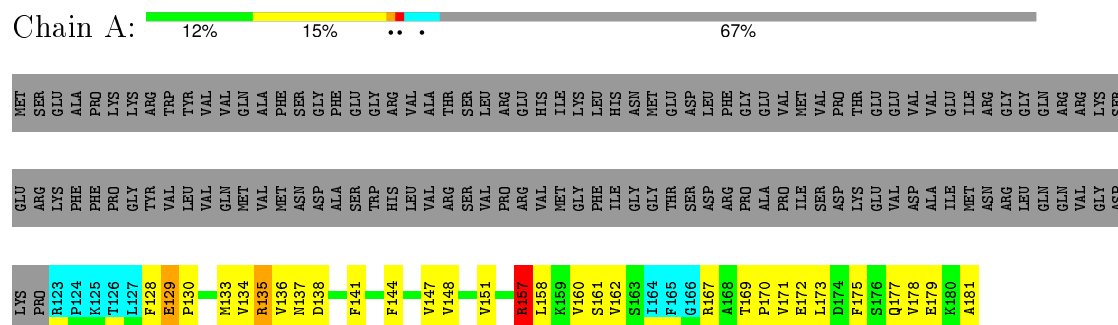
### 4.2.3 Score per residue for model 3

- Molecule 1: Transcription antitermination protein nusG



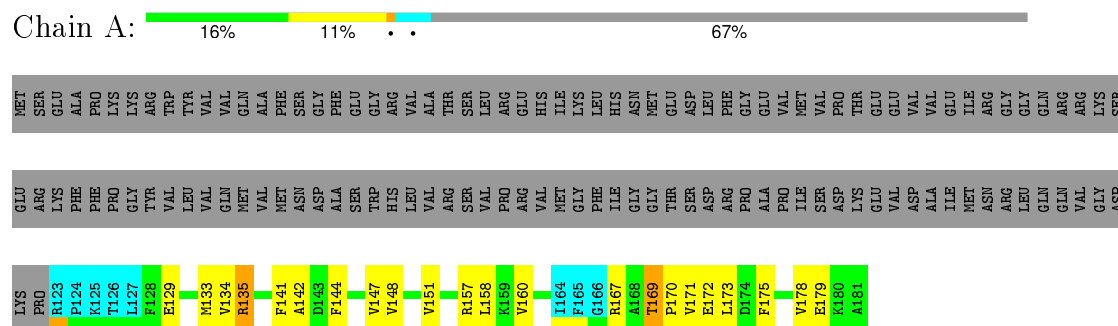
#### 4.2.4 Score per residue for model 4

- Molecule 1: Transcription antitermination protein nusG



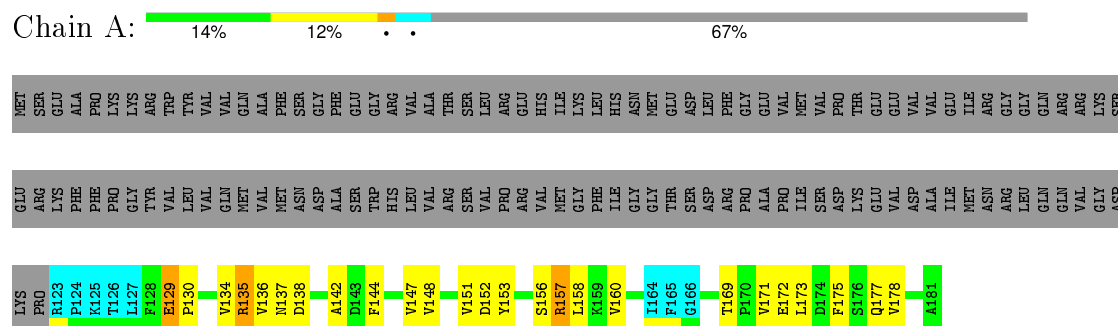
#### 4.2.5 Score per residue for model 5

- Molecule 1: Transcription antitermination protein nusG



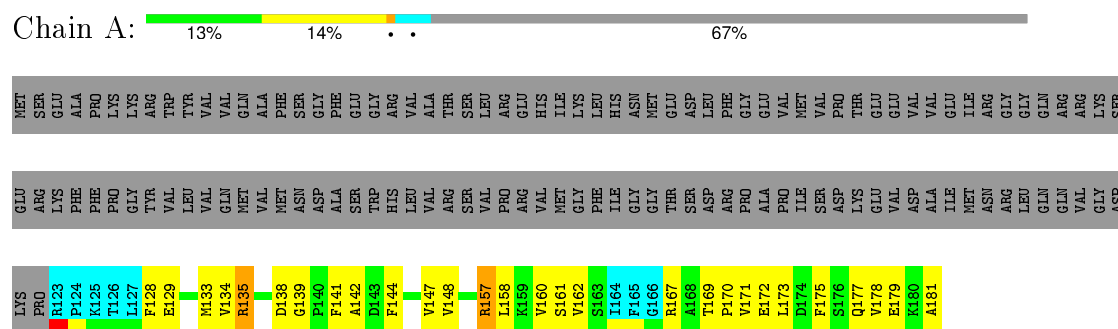
#### 4.2.6 Score per residue for model 6

- Molecule 1: Transcription antitermination protein nusG



#### 4.2.7 Score per residue for model 7

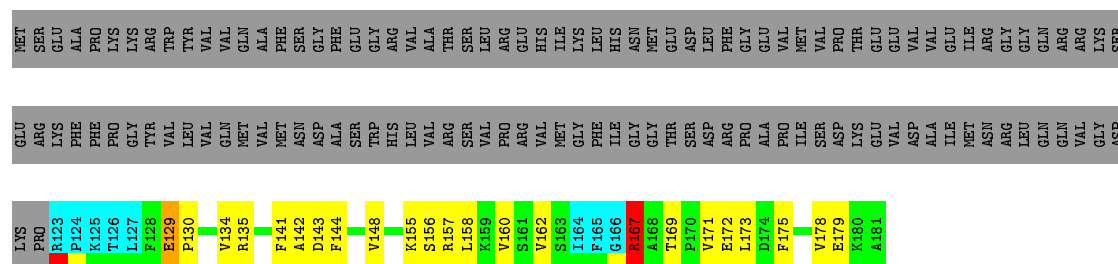
- Molecule 1: Transcription antitermination protein nusG



#### 4.2.8 Score per residue for model 8

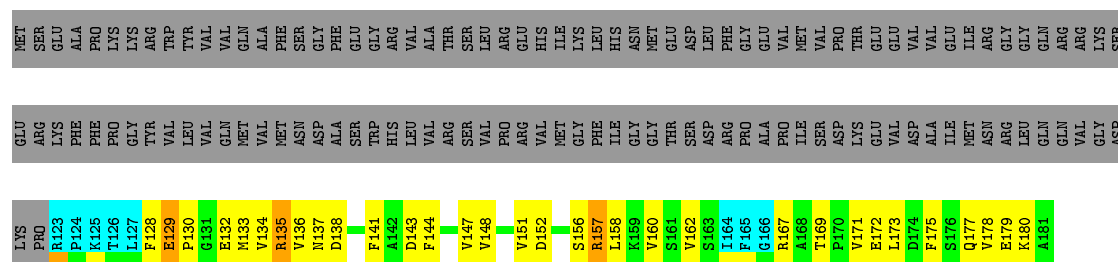
- Molecule 1: Transcription antitermination protein nusG





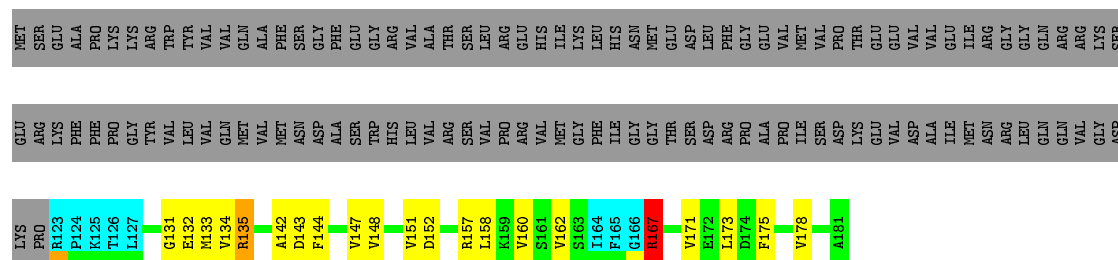
#### 4.2.9 Score per residue for model 9

- Molecule 1: Transcription antitermination protein nusG



#### 4.2.10 Score per residue for model 10

- Molecule 1: Transcription antitermination protein nusG

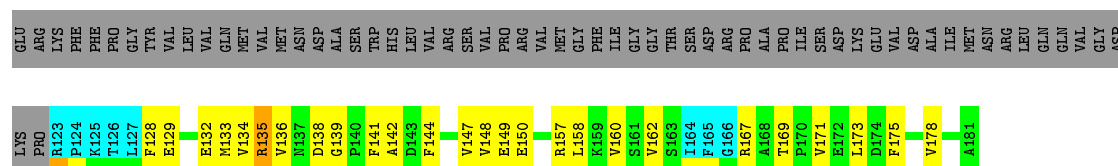


#### 4.2.11 Score per residue for model 11

- Molecule 1: Transcription antitermination protein nusG



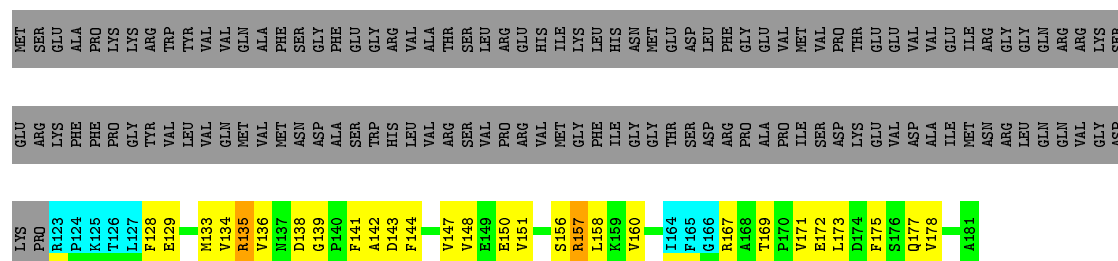




#### 4.2.12 Score per residue for model 12

- Molecule 1: Transcription antitermination protein nusG

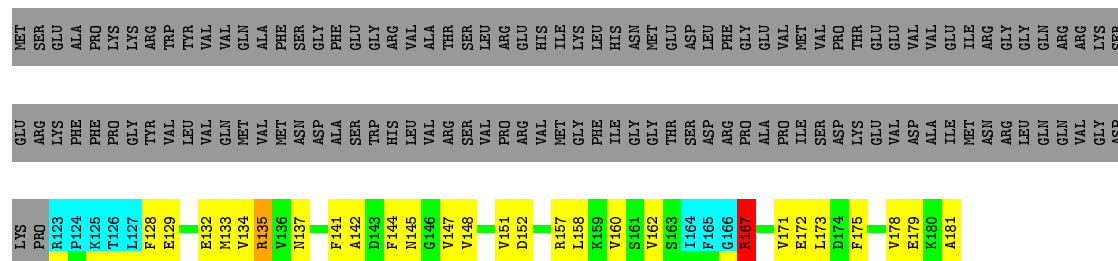
Chain A: 13% 14% 67%



#### 4.2.13 Score per residue for model 13

- Molecule 1: Transcription antitermination protein nusG

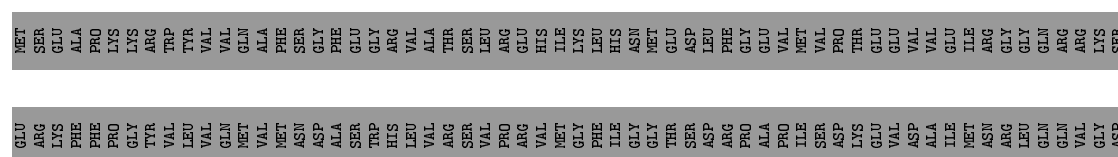
Chain A: 13% 14% 67%



#### 4.2.14 Score per residue for model 14

- Molecule 1: Transcription antitermination protein nusG

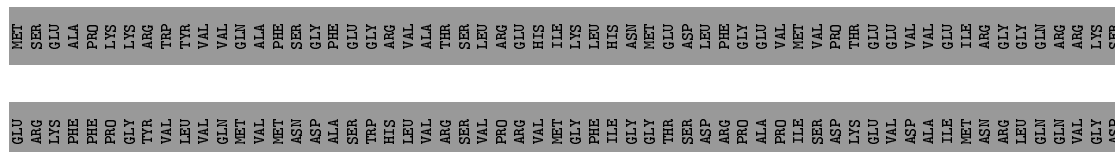
Chain A: 14% 13% 67%





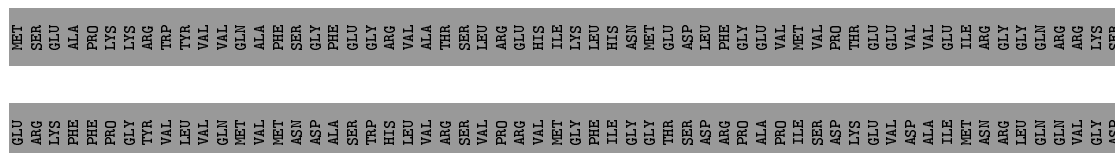
#### 4.2.15 Score per residue for model 15

- Molecule 1: Transcription antitermination protein nusG



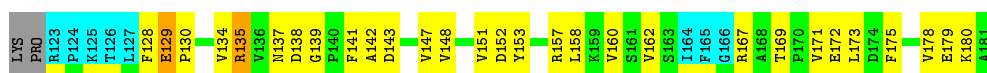
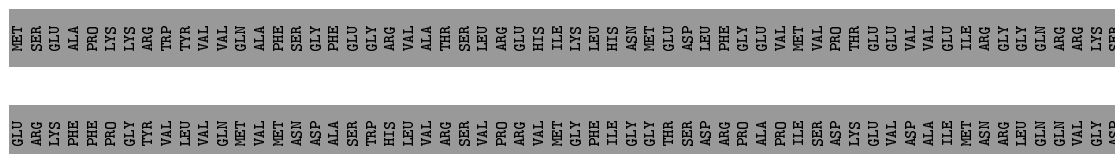
#### 4.2.16 Score per residue for model 16

- Molecule 1: Transcription antitermination protein nusG



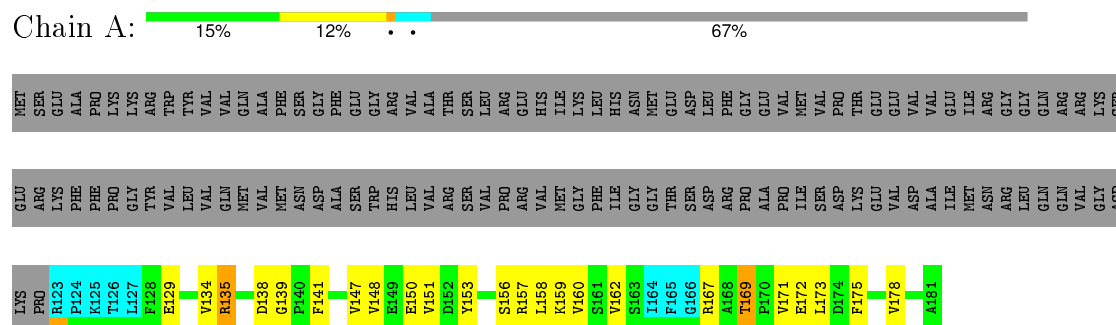
#### 4.2.17 Score per residue for model 17

- Molecule 1: Transcription antitermination protein nusG



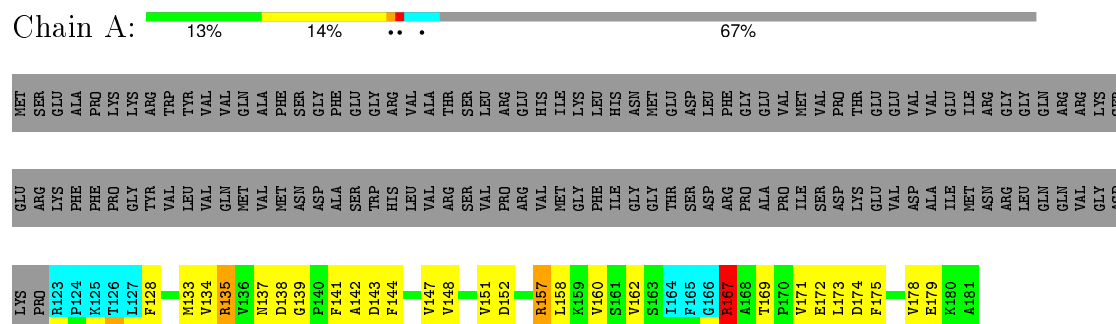
## 4.2.18 Score per residue for model 18

- Molecule 1: Transcription antitermination protein nusG



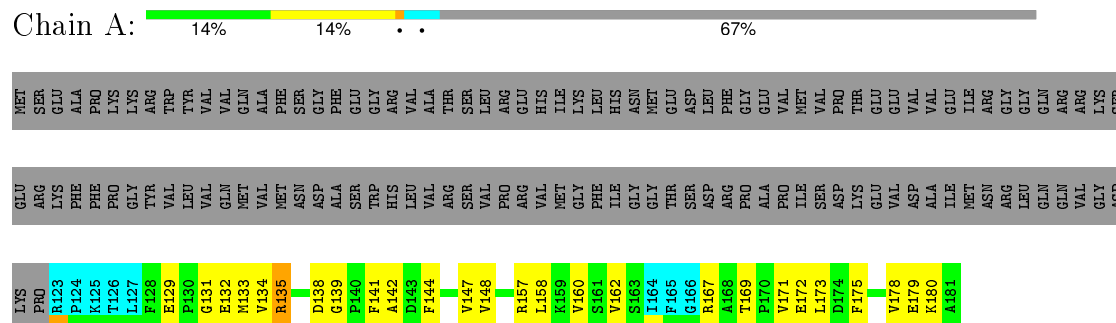
## 4.2.19 Score per residue for model 19

- Molecule 1: Transcription antitermination protein nusG



## 4.2.20 Score per residue for model 20

- Molecule 1: Transcription antitermination protein nusG



## 5 Refinement protocol and experimental data overview

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

Of the 120 calculated structures, 20 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
X-PLOR NIH	structure solution	1.2.1
X-PLOR NIH	refinement	1.2.1

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 15490
Number of chemical shift lists	1
Total number of shifts	708
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	708
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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](#)

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.9±0.4
All	All	0	57

There are no bond-length outliers.

There are no bond-angle outliers.

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	157	ARG	Sidechain	20
1	A	167	ARG	Sidechain	19
1	A	135	ARG	Sidechain	18

### 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	402	385	385	31±4
All	All	8040	7700	7700	625

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 40.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:171:VAL:HG23	1:A:173:LEU:HD21	1.07	1.22	13	8
1:A:141:PHE:CD1	1:A:162:VAL:HG21	1.06	1.86	8	4
1:A:158:LEU:HD11	1:A:175:PHE:CD1	1.05	1.85	12	11
1:A:151:VAL:HG13	1:A:158:LEU:CD2	0.95	1.91	16	7
1:A:133:MET:SD	1:A:147:VAL:HG22	0.90	2.06	15	5
1:A:147:VAL:O	1:A:160:VAL:HG13	0.87	1.69	9	16
1:A:134:VAL:CG2	1:A:148:VAL:HG23	0.83	2.03	11	9
1:A:134:VAL:HG21	1:A:148:VAL:HG23	0.82	1.51	11	6
1:A:158:LEU:HD12	1:A:158:LEU:N	0.81	1.91	12	2
1:A:141:PHE:CZ	1:A:171:VAL:HG11	0.80	2.12	11	8
1:A:128:PHE:O	1:A:151:VAL:HG21	0.79	1.76	16	2
1:A:171:VAL:HG23	1:A:173:LEU:CD2	0.79	2.06	13	7
1:A:171:VAL:CG2	1:A:173:LEU:HD21	0.78	2.07	13	3
1:A:173:LEU:HD22	1:A:173:LEU:N	0.78	1.93	19	3
1:A:158:LEU:HD11	1:A:175:PHE:CE1	0.78	2.13	4	7
1:A:158:LEU:N	1:A:158:LEU:HD12	0.78	1.93	14	4
1:A:147:VAL:C	1:A:160:VAL:HG13	0.77	1.99	13	11
1:A:173:LEU:N	1:A:173:LEU:HD22	0.77	1.93	15	5
1:A:172:GLU:C	1:A:173:LEU:HD22	0.77	1.99	2	8
1:A:132:GLU:O	1:A:147:VAL:HG13	0.77	1.80	20	5
1:A:169:THR:O	1:A:171:VAL:HG13	0.77	1.80	15	16
1:A:173:LEU:HD22	1:A:177:GLN:NE2	0.75	1.97	12	3
1:A:158:LEU:HD11	1:A:175:PHE:CG	0.74	2.16	14	1
1:A:148:VAL:HG11	1:A:151:VAL:HG22	0.74	1.58	4	3
1:A:136:VAL:HG22	1:A:173:LEU:CD1	0.71	2.15	6	5
1:A:148:VAL:HG22	1:A:160:VAL:HG22	0.70	1.61	7	5
1:A:148:VAL:HG21	1:A:151:VAL:HG22	0.70	1.61	1	7
1:A:134:VAL:HG21	1:A:148:VAL:CG2	0.69	2.18	6	8
1:A:172:GLU:O	1:A:173:LEU:HD23	0.68	1.88	5	9
1:A:128:PHE:CE2	1:A:134:VAL:HG13	0.65	2.26	16	1
1:A:158:LEU:CD1	1:A:175:PHE:CE1	0.65	2.79	7	5
1:A:148:VAL:HG22	1:A:160:VAL:CG2	0.65	2.22	4	2
1:A:148:VAL:CA	1:A:160:VAL:HG22	0.65	2.21	10	8
1:A:128:PHE:CD1	1:A:158:LEU:CD1	0.63	2.81	16	1
1:A:158:LEU:CD1	1:A:175:PHE:CD1	0.63	2.81	11	5
1:A:151:VAL:HG13	1:A:158:LEU:HD23	0.63	1.70	2	2
1:A:151:VAL:HG13	1:A:158:LEU:HD22	0.63	1.70	16	3
1:A:148:VAL:HA	1:A:160:VAL:HG22	0.62	1.69	10	9
1:A:173:LEU:HD12	1:A:178:VAL:CG1	0.61	2.25	9	3
1:A:133:MET:HG2	1:A:147:VAL:HG22	0.61	1.72	10	5
1:A:128:PHE:CE1	1:A:134:VAL:HG13	0.61	2.30	19	2
1:A:158:LEU:HD21	1:A:175:PHE:CE1	0.61	2.31	6	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:PHE:CE2	1:A:171:VAL:HG11	0.61	2.31	5	2
1:A:136:VAL:HG22	1:A:173:LEU:HD12	0.59	1.75	12	2
1:A:141:PHE:CZ	1:A:169:THR:HG21	0.59	2.32	15	3
1:A:148:VAL:HG11	1:A:151:VAL:CG2	0.59	2.28	5	2
1:A:162:VAL:HG12	1:A:169:THR:HB	0.59	1.74	18	3
1:A:141:PHE:CD1	1:A:162:VAL:HG11	0.58	2.32	18	2
1:A:132:GLU:C	1:A:147:VAL:HG13	0.58	2.17	10	2
1:A:175:PHE:N	1:A:175:PHE:CD1	0.58	2.70	17	8
1:A:173:LEU:N	1:A:173:LEU:CD2	0.58	2.67	2	3
1:A:158:LEU:N	1:A:158:LEU:CD1	0.58	2.67	9	3
1:A:173:LEU:CB	1:A:178:VAL:CG1	0.57	2.82	19	17
1:A:173:LEU:CD1	1:A:178:VAL:CG1	0.57	2.81	9	2
1:A:128:PHE:CD2	1:A:158:LEU:HD21	0.57	2.34	7	4
1:A:173:LEU:CD2	1:A:173:LEU:N	0.57	2.67	7	5
1:A:158:LEU:CD1	1:A:158:LEU:N	0.57	2.65	12	1
1:A:157:ARG:C	1:A:158:LEU:HD12	0.57	2.19	9	6
1:A:175:PHE:CD1	1:A:175:PHE:N	0.56	2.71	16	5
1:A:134:VAL:CG2	1:A:148:VAL:CG2	0.56	2.83	18	4
1:A:172:GLU:O	1:A:173:LEU:HD13	0.56	2.00	2	8
1:A:148:VAL:CG2	1:A:160:VAL:HG22	0.56	2.30	4	1
1:A:128:PHE:CE1	1:A:180:LYS:CG	0.56	2.88	2	1
1:A:128:PHE:CE1	1:A:180:LYS:HG3	0.56	2.36	2	1
1:A:136:VAL:CG2	1:A:173:LEU:CD1	0.56	2.83	6	3
1:A:148:VAL:HB	1:A:160:VAL:HG22	0.56	1.78	2	4
1:A:173:LEU:HB2	1:A:178:VAL:HG11	0.55	1.78	14	6
1:A:142:ALA:O	1:A:144:PHE:CD2	0.55	2.59	13	15
1:A:141:PHE:HZ	1:A:169:THR:HG21	0.55	1.62	15	1
1:A:158:LEU:CD2	1:A:175:PHE:CE1	0.54	2.90	6	4
1:A:173:LEU:HD12	1:A:178:VAL:HG11	0.54	1.79	4	2
1:A:158:LEU:HD11	1:A:175:PHE:CZ	0.53	2.38	11	1
1:A:132:GLU:O	1:A:148:VAL:HG12	0.53	2.03	9	1
1:A:158:LEU:HD12	1:A:175:PHE:CE1	0.52	2.39	11	1
1:A:128:PHE:CD1	1:A:158:LEU:HD11	0.52	2.40	16	1
1:A:152:ASP:O	1:A:156:SER:N	0.52	2.43	9	3
1:A:142:ALA:O	1:A:143:ASP:CB	0.52	2.58	19	7
1:A:135:ARG:N	1:A:179:GLU:O	0.51	2.43	2	6
1:A:128:PHE:CD2	1:A:158:LEU:HD11	0.51	2.41	13	2
1:A:134:VAL:HG12	1:A:135:ARG:H	0.51	1.66	6	20
1:A:132:GLU:OE2	1:A:180:LYS:NZ	0.51	2.43	20	1
1:A:151:VAL:HG13	1:A:158:LEU:HD21	0.51	1.78	16	1
1:A:141:PHE:HD1	1:A:162:VAL:HG21	0.50	1.52	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:162:VAL:HG13	1:A:162:VAL:O	0.50	2.06	20	1
1:A:141:PHE:CE1	1:A:169:THR:HG21	0.50	2.42	8	2
1:A:148:VAL:CG2	1:A:151:VAL:HG22	0.50	2.36	1	1
1:A:173:LEU:HD12	1:A:177:GLN:NE2	0.50	2.21	7	1
1:A:148:VAL:CB	1:A:160:VAL:HG22	0.50	2.36	13	4
1:A:173:LEU:HB2	1:A:178:VAL:CG1	0.49	2.36	3	13
1:A:147:VAL:HG12	1:A:148:VAL:N	0.49	2.22	6	3
1:A:148:VAL:HG13	1:A:148:VAL:O	0.49	2.07	12	2
1:A:135:ARG:O	1:A:179:GLU:N	0.49	2.44	16	8
1:A:131:GLY:C	1:A:147:VAL:CG1	0.49	2.81	10	2
1:A:138:ASP:OD1	1:A:139:GLY:N	0.49	2.46	18	9
1:A:173:LEU:CB	1:A:178:VAL:HG13	0.49	2.38	9	5
1:A:142:ALA:O	1:A:144:PHE:CD1	0.48	2.67	19	1
1:A:135:ARG:CZ	1:A:179:GLU:OE1	0.48	2.61	5	1
1:A:158:LEU:HD11	1:A:175:PHE:CE2	0.47	2.44	11	1
1:A:136:VAL:O	1:A:143:ASP:N	0.47	2.47	9	3
1:A:156:SER:O	1:A:157:ARG:CG	0.47	2.63	6	1
1:A:149:GLU:O	1:A:150:GLU:CG	0.47	2.63	15	1
1:A:133:MET:SD	1:A:147:VAL:CG2	0.47	2.98	12	3
1:A:129:GLU:CB	1:A:130:PRO:HD2	0.47	2.40	6	6
1:A:132:GLU:O	1:A:147:VAL:CG1	0.47	2.57	20	2
1:A:161:SER:OG	1:A:170:PRO:N	0.47	2.48	4	1
1:A:173:LEU:HB3	1:A:178:VAL:CG1	0.46	2.41	11	3
1:A:144:PHE:HB3	1:A:162:VAL:CG1	0.46	2.41	7	8
1:A:175:PHE:O	1:A:178:VAL:O	0.46	2.33	3	10
1:A:135:ARG:NH2	1:A:145:ASN:OD1	0.46	2.49	15	1
1:A:138:ASP:CB	1:A:177:GLN:OE1	0.46	2.64	9	1
1:A:135:ARG:O	1:A:178:VAL:CA	0.46	2.64	16	12
1:A:144:PHE:HB3	1:A:162:VAL:HG13	0.45	1.86	7	3
1:A:139:GLY:O	1:A:142:ALA:N	0.45	2.49	12	1
1:A:136:VAL:HG11	1:A:141:PHE:HB2	0.45	1.87	16	2
1:A:137:ASN:O	1:A:138:ASP:OD1	0.45	2.35	4	3
1:A:138:ASP:HB2	1:A:177:GLN:OE1	0.44	2.13	9	1
1:A:148:VAL:CG1	1:A:151:VAL:HG22	0.44	2.40	17	1
1:A:148:VAL:O	1:A:148:VAL:HG13	0.44	2.12	14	2
1:A:157:ARG:NH1	1:A:172:GLU:O	0.43	2.51	4	1
1:A:129:GLU:CG	1:A:130:PRO:HD2	0.43	2.43	4	2
1:A:141:PHE:CE1	1:A:162:VAL:HG11	0.43	2.48	17	1
1:A:173:LEU:HB3	1:A:178:VAL:HG13	0.43	1.91	1	3
1:A:174:ASP:O	1:A:178:VAL:HG22	0.43	2.13	2	1
1:A:156:SER:HA	1:A:175:PHE:CZ	0.43	2.49	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:ARG:O	1:A:178:VAL:HA	0.43	2.14	16	13
1:A:162:VAL:CG1	1:A:162:VAL:O	0.43	2.66	20	1
1:A:142:ALA:O	1:A:143:ASP:HB3	0.43	2.14	1	3
1:A:151:VAL:O	1:A:152:ASP:OD1	0.43	2.36	10	7
1:A:147:VAL:O	1:A:160:VAL:CG1	0.43	2.57	15	1
1:A:128:PHE:CE2	1:A:180:LYS:HD3	0.43	2.48	3	1
1:A:151:VAL:HG11	1:A:153:TYR:CZ	0.43	2.49	6	3
1:A:137:ASN:C	1:A:137:ASN:OD1	0.43	2.57	17	5
1:A:150:GLU:HG2	1:A:151:VAL:N	0.43	2.29	12	1
1:A:160:VAL:O	1:A:171:VAL:O	0.43	2.36	18	3
1:A:145:ASN:OD1	1:A:145:ASN:O	0.42	2.36	13	1
1:A:149:GLU:N	1:A:159:LYS:O	0.42	2.52	16	1
1:A:133:MET:O	1:A:181:ALA:HB3	0.42	2.15	4	2
1:A:136:VAL:HG12	1:A:142:ALA:HA	0.42	1.91	3	1
1:A:161:SER:CA	1:A:170:PRO:HA	0.42	2.44	1	1
1:A:173:LEU:CD1	1:A:178:VAL:HG12	0.42	2.44	9	1
1:A:149:GLU:O	1:A:150:GLU:CD	0.42	2.58	11	1
1:A:136:VAL:HG22	1:A:173:LEU:HD13	0.42	1.92	11	1
1:A:128:PHE:CG	1:A:158:LEU:HD21	0.42	2.49	11	1
1:A:133:MET:O	1:A:181:ALA:CB	0.42	2.67	7	1
1:A:129:GLU:O	1:A:132:GLU:CB	0.42	2.67	13	1
1:A:141:PHE:CZ	1:A:169:THR:CG2	0.42	3.02	5	1
1:A:155:LYS:O	1:A:156:SER:C	0.41	2.57	8	2
1:A:132:GLU:OE2	1:A:180:LYS:CE	0.41	2.68	20	1
1:A:155:LYS:O	1:A:156:SER:OG	0.41	2.39	14	1
1:A:157:ARG:HD2	1:A:174:ASP:OD1	0.41	2.15	3	1
1:A:128:PHE:CD2	1:A:158:LEU:CD1	0.41	3.04	17	1
1:A:129:GLU:O	1:A:132:GLU:HB2	0.41	2.15	13	1
1:A:135:ARG:O	1:A:178:VAL:HB	0.41	2.16	4	10
1:A:137:ASN:OD1	1:A:138:ASP:OD1	0.41	2.38	6	1
1:A:136:VAL:CG1	1:A:141:PHE:O	0.41	2.68	12	1
1:A:137:ASN:OD1	1:A:137:ASN:C	0.41	2.59	19	1
1:A:157:ARG:CD	1:A:174:ASP:OD1	0.41	2.68	19	2
1:A:129:GLU:O	1:A:132:GLU:HG2	0.41	2.15	11	2
1:A:157:ARG:HD3	1:A:174:ASP:OD1	0.41	2.16	19	1
1:A:162:VAL:CG1	1:A:169:THR:HB	0.41	2.44	17	1
1:A:149:GLU:O	1:A:150:GLU:HG3	0.41	2.16	15	1
1:A:135:ARG:NE	1:A:179:GLU:OE1	0.41	2.54	5	1
1:A:156:SER:OG	1:A:156:SER:O	0.40	2.35	1	1
1:A:128:PHE:CE2	1:A:180:LYS:CG	0.40	3.04	16	1
1:A:132:GLU:OE2	1:A:180:LYS:HE2	0.40	2.16	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:PHE:CE1	1:A:180:LYS:HG2	0.40	2.51	17	1
1:A:173:LEU:CB	1:A:178:VAL:HG11	0.40	2.46	19	1
1:A:128:PHE:CE2	1:A:180:LYS:HG2	0.40	2.50	16	1
1:A:158:LEU:HD11	1:A:175:PHE:CD2	0.40	2.52	11	1
1:A:150:GLU:HB2	1:A:159:LYS:CD	0.40	2.47	18	1
1:A:161:SER:CB	1:A:170:PRO:HA	0.40	2.47	7	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	50/181 (28%)	48±1 (95±2%)	2±1 (4±2%)	0±0 (1±1%)	31	76
All	All	1000/3620 (28%)	953 (95%)	40 (4%)	7 (1%)	31	76

All 2 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	167	ARG	4
1	A	170	PRO	3

### 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	45/158 (28%)	44±1 (98±2%)	1±1 (2±2%)	69	95
All	All	900/3160 (28%)	884 (98%)	16 (2%)	69	95

All 4 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	129	GLU	10
1	A	156	SER	3
1	A	169	THR	2
1	A	157	ARG	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 0% for the well-defined parts and 0% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 15490

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	708
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	708
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Chain not found in structure. All 708 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	162	VAL	HG22	0.47	0.03	2
UNMAPPED	166	GLY	C	173.8	0.2	1
UNMAPPED	155	LYS	HG2	1.29	0.03	2
UNMAPPED	164	ILE	CA	60.23	0.2	1
UNMAPPED	131	GLY	HA3	4.45	0.03	2
UNMAPPED	155	LYS	HD3	1.57	0.03	1
UNMAPPED	178	VAL	HG22	0.51	0.03	2
UNMAPPED	164	ILE	HG23	0.69	0.03	1
UNMAPPED	167	ARG	HB2	1.81	0.03	2
UNMAPPED	162	VAL	CB	33.63	0.2	1
UNMAPPED	165	PHE	HA	4.34	0.03	1
UNMAPPED	129	GLU	N	120.56	0.1	1
UNMAPPED	153	TYR	HE1	7.16	0.03	1
UNMAPPED	140	PRO	HG2	1.78	0.03	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	162	VAL	N	127.97	0.1	1
UNMAPPED	173	LEU	HB3	1.66	0.03	2
UNMAPPED	128	PHE	HB2	2.19	0.03	2
UNMAPPED	134	VAL	H	9.08	0.03	1
UNMAPPED	181	ALA	HB3	1.21	0.03	1
UNMAPPED	144	PHE	HD2	7.37	0.03	1
UNMAPPED	178	VAL	CA	58.57	0.2	1
UNMAPPED	150	GLU	C	173.74	0.2	1
UNMAPPED	131	GLY	C	174.25	0.2	1
UNMAPPED	171	VAL	HG22	0.61	0.03	2
UNMAPPED	154	GLU	H	8.47	0.03	1
UNMAPPED	159	LYS	HG2	1.16	0.03	2
UNMAPPED	165	PHE	CD2	131.8	0.2	1
UNMAPPED	134	VAL	HG23	0.67	0.03	2
UNMAPPED	150	GLU	HB2	1.88	0.03	2
UNMAPPED	144	PHE	HE2	7.13	0.03	1
UNMAPPED	129	GLU	HA	4.94	0.03	1
UNMAPPED	151	VAL	HG13	0.58	0.03	1
UNMAPPED	177	GLN	HB2	2.36	0.03	2
UNMAPPED	158	LEU	CA	53.39	0.2	1
UNMAPPED	177	GLN	HG2	2.52	0.03	2
UNMAPPED	133	MET	HG2	2.55	0.03	2
UNMAPPED	173	LEU	HD23	0.9	0.03	2
UNMAPPED	164	ILE	H	8.27	0.03	1
UNMAPPED	165	PHE	HD2	7.28	0.03	1
UNMAPPED	151	VAL	N	122.37	0.1	1
UNMAPPED	131	GLY	CA	44.89	0.2	1
UNMAPPED	178	VAL	HG12	0.66	0.03	2
UNMAPPED	168	ALA	N	130.96	0.1	1
UNMAPPED	151	VAL	CB	34.94	0.2	1
UNMAPPED	132	GLU	H	7.84	0.03	1
UNMAPPED	177	GLN	CG	36.25	0.2	1
UNMAPPED	168	ALA	CB	18.73	0.2	1
UNMAPPED	127	LEU	HD22	0.78	0.03	2
UNMAPPED	155	LYS	H	7.51	0.03	1
UNMAPPED	163	SER	CA	57.37	0.2	1
UNMAPPED	127	LEU	HB3	1.49	0.03	2
UNMAPPED	175	PHE	N	121.89	0.1	1
UNMAPPED	133	MET	N	121.97	0.1	1
UNMAPPED	149	GLU	HG3	2.23	0.03	2
UNMAPPED	136	VAL	CG2	21.06	0.2	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	162	VAL	HA	4.37	0.03	1
UNMAPPED	170	PRO	CB	31.63	0.2	1
UNMAPPED	143	ASP	HB3	3.0	0.03	2
UNMAPPED	150	GLU	H	7.66	0.03	1
UNMAPPED	179	GLU	CG	35.78	0.2	1
UNMAPPED	157	ARG	CG	26.57	0.2	1
UNMAPPED	167	ARG	HB3	1.89	0.03	2
UNMAPPED	125	LYS	CA	56.79	0.2	1
UNMAPPED	157	ARG	CA	53.33	0.2	1
UNMAPPED	125	LYS	HB2	1.74	0.03	2
UNMAPPED	125	LYS	CG	24.91	0.2	1
UNMAPPED	137	ASN	HB3	2.52	0.03	2
UNMAPPED	181	ALA	HA	4.19	0.03	1
UNMAPPED	155	LYS	HE3	3.03	0.03	2
UNMAPPED	128	PHE	H	7.62	0.03	1
UNMAPPED	131	GLY	H	9.36	0.03	1
UNMAPPED	137	ASN	CB	40.72	0.2	1
UNMAPPED	140	PRO	CD	49.56	0.2	1
UNMAPPED	154	GLU	C	175.96	0.2	1
UNMAPPED	175	PHE	HD2	7.07	0.03	1
UNMAPPED	155	LYS	HB2	1.29	0.03	2
UNMAPPED	180	LYS	CE	42.11	0.2	1
UNMAPPED	159	LYS	CD	29.45	0.2	1
UNMAPPED	149	GLU	CB	31.91	0.2	1
UNMAPPED	153	TYR	HB2	3.01	0.03	2
UNMAPPED	144	PHE	HB3	3.38	0.03	2
UNMAPPED	156	SER	HB2	3.22	0.03	2
UNMAPPED	158	LEU	HD23	0.39	0.03	2
UNMAPPED	143	ASP	HA	4.19	0.03	1
UNMAPPED	173	LEU	HD12	0.61	0.03	2
UNMAPPED	141	PHE	HE2	7.1	0.03	1
UNMAPPED	135	ARG	CG	27.67	0.2	1
UNMAPPED	159	LYS	HE3	2.85	0.03	1
UNMAPPED	171	VAL	HG23	0.61	0.03	2
UNMAPPED	135	ARG	CA	54.62	0.2	1
UNMAPPED	132	GLU	C	175.03	0.2	1
UNMAPPED	126	THR	CA	61.89	0.2	1
UNMAPPED	124	PRO	HG3	1.99	0.03	2
UNMAPPED	124	PRO	HB2	1.86	0.03	2
UNMAPPED	149	GLU	HB2	1.68	0.03	2
UNMAPPED	161	SER	H	9.0	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	136	VAL	H	8.75	0.03	1
UNMAPPED	173	LEU	CD2	23.95	0.2	2
UNMAPPED	139	GLY	HA3	4.37	0.03	2
UNMAPPED	144	PHE	HA	4.72	0.03	1
UNMAPPED	136	VAL	HG22	0.72	0.03	2
UNMAPPED	154	GLU	CB	29.4	0.2	1
UNMAPPED	133	MET	HE1	2.04	0.03	1
UNMAPPED	126	THR	C	172.84	0.2	1
UNMAPPED	178	VAL	CB	36.09	0.2	1
UNMAPPED	154	GLU	N	120.47	0.1	1
UNMAPPED	176	SER	CB	63.21	0.2	1
UNMAPPED	141	PHE	CD2	131.2	0.2	1
UNMAPPED	164	ILE	HD12	0.46	0.03	1
UNMAPPED	124	PRO	HA	4.43	0.03	1
UNMAPPED	164	ILE	N	127.59	0.1	1
UNMAPPED	167	ARG	HA	4.59	0.03	1
UNMAPPED	158	LEU	N	121.51	0.1	1
UNMAPPED	181	ALA	HB2	1.21	0.03	1
UNMAPPED	177	GLN	HB3	2.36	0.03	2
UNMAPPED	164	ILE	CB	38.24	0.2	1
UNMAPPED	131	GLY	HA2	3.48	0.03	2
UNMAPPED	165	PHE	HB2	3.12	0.03	2
UNMAPPED	147	VAL	HA	4.9	0.03	1
UNMAPPED	180	LYS	HG3	1.59	0.03	1
UNMAPPED	163	SER	N	120.41	0.1	1
UNMAPPED	147	VAL	CB	34.81	0.2	1
UNMAPPED	162	VAL	CA	60.91	0.2	1
UNMAPPED	143	ASP	H	8.93	0.03	1
UNMAPPED	132	GLU	CB	31.6	0.2	1
UNMAPPED	153	TYR	HE2	7.16	0.03	1
UNMAPPED	140	PRO	HG3	1.87	0.03	2
UNMAPPED	178	VAL	N	109.92	0.1	1
UNMAPPED	178	VAL	HG13	0.66	0.03	2
UNMAPPED	127	LEU	H	7.93	0.03	1
UNMAPPED	144	PHE	HD1	7.37	0.03	1
UNMAPPED	147	VAL	N	118.32	0.1	1
UNMAPPED	157	ARG	HB2	1.45	0.03	2
UNMAPPED	165	PHE	CD1	131.8	0.2	1
UNMAPPED	150	GLU	CB	34.58	0.2	1
UNMAPPED	167	ARG	CD	43.6	0.2	1
UNMAPPED	161	SER	C	175.06	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	141	PHE	CA	56.74	0.2	1
UNMAPPED	177	GLN	HA	4.72	0.03	1
UNMAPPED	177	GLN	HG3	2.52	0.03	2
UNMAPPED	154	GLU	HA	4.17	0.03	1
UNMAPPED	128	PHE	N	117.32	0.1	1
UNMAPPED	131	GLY	N	112.98	0.1	1
UNMAPPED	124	PRO	HD3	3.63	0.03	2
UNMAPPED	124	PRO	CD	50.6	0.2	1
UNMAPPED	126	THR	HG21	0.91	0.03	1
UNMAPPED	174	ASP	CB	42.87	0.2	1
UNMAPPED	168	ALA	HB1	1.25	0.03	1
UNMAPPED	124	PRO	CB	32.21	0.2	1
UNMAPPED	174	ASP	CA	54.33	0.2	1
UNMAPPED	176	SER	C	175.79	0.2	1
UNMAPPED	139	GLY	CA	45.27	0.2	1
UNMAPPED	149	GLU	H	9.57	0.03	1
UNMAPPED	142	ALA	HB2	1.23	0.03	1
UNMAPPED	127	LEU	HD23	0.78	0.03	2
UNMAPPED	165	PHE	HB3	3.42	0.03	2
UNMAPPED	153	TYR	HD2	7.46	0.03	1
UNMAPPED	134	VAL	HG13	0.43	0.03	2
UNMAPPED	127	LEU	HB2	1.38	0.03	2
UNMAPPED	133	MET	CE	16.6	0.2	1
UNMAPPED	164	ILE	CD1	13.17	0.2	1
UNMAPPED	142	ALA	CA	54.09	0.2	1
UNMAPPED	181	ALA	H	7.98	0.03	1
UNMAPPED	148	VAL	HG11	0.89	0.03	2
UNMAPPED	160	VAL	HG12	0.41	0.03	2
UNMAPPED	132	GLU	HA	4.4	0.03	1
UNMAPPED	142	ALA	CB	17.99	0.2	1
UNMAPPED	150	GLU	N	115.69	0.1	1
UNMAPPED	143	ASP	HB2	2.81	0.03	2
UNMAPPED	167	ARG	CG	27.2	0.2	1
UNMAPPED	160	VAL	CG1	21.35	0.2	2
UNMAPPED	157	ARG	CD	43.22	0.2	1
UNMAPPED	147	VAL	HG22	0.87	0.03	2
UNMAPPED	152	ASP	HB3	2.91	0.03	2
UNMAPPED	155	LYS	HA	4.31	0.03	1
UNMAPPED	166	GLY	CA	45.42	0.2	1
UNMAPPED	174	ASP	HB3	2.94	0.03	2
UNMAPPED	167	ARG	N	120.96	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	155	LYS	HE2	2.94	0.03	2
UNMAPPED	140	PRO	HD3	3.8	0.03	2
UNMAPPED	180	LYS	HB3	1.83	0.03	2
UNMAPPED	170	PRO	CG	27.16	0.2	1
UNMAPPED	175	PHE	HD1	7.07	0.03	1
UNMAPPED	155	LYS	HB3	1.83	0.03	2
UNMAPPED	148	VAL	HG21	0.57	0.03	2
UNMAPPED	161	SER	N	120.52	0.1	1
UNMAPPED	153	TYR	CB	38.52	0.2	1
UNMAPPED	172	GLU	N	126.17	0.1	1
UNMAPPED	142	ALA	C	178.01	0.2	1
UNMAPPED	128	PHE	CE2	130.7	0.2	1
UNMAPPED	169	THR	HB	3.88	0.03	1
UNMAPPED	144	PHE	CB	39.69	0.2	1
UNMAPPED	179	GLU	H	8.76	0.03	1
UNMAPPED	144	PHE	HB2	3.08	0.03	2
UNMAPPED	175	PHE	H	8.15	0.03	1
UNMAPPED	133	MET	H	8.68	0.03	1
UNMAPPED	127	LEU	HD13	0.85	0.03	2
UNMAPPED	156	SER	CA	58.28	0.2	1
UNMAPPED	176	SER	H	8.58	0.03	1
UNMAPPED	170	PRO	HA	4.96	0.03	1
UNMAPPED	178	VAL	CG2	19.93	0.2	2
UNMAPPED	173	LEU	HD13	0.61	0.03	2
UNMAPPED	135	ARG	N	121.68	0.1	1
UNMAPPED	130	PRO	CG	28.77	0.2	1
UNMAPPED	126	THR	N	116.37	0.1	1
UNMAPPED	171	VAL	CB	35.4	0.2	1
UNMAPPED	159	LYS	HE2	2.85	0.03	1
UNMAPPED	130	PRO	CA	63.78	0.2	1
UNMAPPED	126	THR	CB	69.84	0.2	1
UNMAPPED	155	LYS	CG	25.45	0.2	1
UNMAPPED	160	VAL	HA	4.69	0.03	1
UNMAPPED	126	THR	HB	4.0	0.03	1
UNMAPPED	143	ASP	N	113.7	0.1	1
UNMAPPED	134	VAL	C	173.77	0.2	1
UNMAPPED	175	PHE	CE1	131.8	0.2	1
UNMAPPED	143	ASP	CB	39.67	0.2	1
UNMAPPED	168	ALA	HA	4.52	0.03	1
UNMAPPED	128	PHE	HD2	6.38	0.03	1
UNMAPPED	139	GLY	HA2	3.85	0.03	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	127	LEU	CB	43.48	0.2	1
UNMAPPED	141	PHE	HB2	2.94	0.03	2
UNMAPPED	136	VAL	HG23	0.72	0.03	2
UNMAPPED	154	GLU	CA	59.38	0.2	1
UNMAPPED	165	PHE	C	176.27	0.2	1
UNMAPPED	171	VAL	CG1	20.4	0.2	2
UNMAPPED	178	VAL	HG21	0.51	0.03	2
UNMAPPED	176	SER	CA	60.29	0.2	1
UNMAPPED	158	LEU	HD13	0.04	0.03	2
UNMAPPED	128	PHE	CA	56.63	0.2	1
UNMAPPED	164	ILE	HD13	0.46	0.03	1
UNMAPPED	151	VAL	C	173.46	0.2	1
UNMAPPED	173	LEU	HB2	1.21	0.03	2
UNMAPPED	145	ASN	H	8.85	0.03	1
UNMAPPED	153	TYR	CD1	133.3	0.2	1
UNMAPPED	157	ARG	HG3	1.58	0.03	2
UNMAPPED	134	VAL	CB	36.09	0.2	1
UNMAPPED	135	ARG	HD2	3.19	0.03	2
UNMAPPED	180	LYS	HG2	1.59	0.03	1
UNMAPPED	160	VAL	H	9.19	0.03	1
UNMAPPED	128	PHE	CB	44.08	0.2	1
UNMAPPED	132	GLU	CG	36.7	0.2	1
UNMAPPED	164	ILE	HG21	0.69	0.03	1
UNMAPPED	168	ALA	HB3	1.25	0.03	1
UNMAPPED	170	PRO	HD3	3.62	0.03	2
UNMAPPED	163	SER	HB3	3.83	0.03	2
UNMAPPED	175	PHE	HB3	3.42	0.03	2
UNMAPPED	169	THR	N	122.74	0.1	1
UNMAPPED	132	GLU	CA	56.69	0.2	1
UNMAPPED	129	GLU	CB	32.0	0.2	1
UNMAPPED	158	LEU	HD21	0.39	0.03	2
UNMAPPED	176	SER	HB3	4.01	0.03	2
UNMAPPED	181	ALA	CB	20.36	0.2	1
UNMAPPED	157	ARG	HB3	1.73	0.03	2
UNMAPPED	150	GLU	CG	36.43	0.2	1
UNMAPPED	151	VAL	HA	4.24	0.03	1
UNMAPPED	128	PHE	C	174.32	0.2	1
UNMAPPED	141	PHE	N	116.14	0.1	1
UNMAPPED	151	VAL	HG11	0.58	0.03	1
UNMAPPED	150	GLU	CA	55.39	0.2	1
UNMAPPED	133	MET	HB2	2.1	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	140	PRO	C	177.81	0.2	1
UNMAPPED	158	LEU	H	9.45	0.03	1
UNMAPPED	173	LEU	H	8.89	0.03	1
UNMAPPED	150	GLU	HG2	2.18	0.03	2
UNMAPPED	156	SER	C	173.97	0.2	1
UNMAPPED	124	PRO	HD2	3.86	0.03	2
UNMAPPED	124	PRO	CG	27.5	0.2	1
UNMAPPED	126	THR	CG2	22.2	0.2	1
UNMAPPED	172	GLU	H	8.44	0.03	1
UNMAPPED	139	GLY	N	108.68	0.1	1
UNMAPPED	153	TYR	H	8.96	0.03	1
UNMAPPED	177	GLN	CA	56.64	0.2	1
UNMAPPED	138	ASP	C	174.63	0.2	1
UNMAPPED	155	LYS	C	175.6	0.2	1
UNMAPPED	180	LYS	HE2	2.69	0.03	2
UNMAPPED	144	PHE	H	8.28	0.03	1
UNMAPPED	141	PHE	HD1	6.76	0.03	1
UNMAPPED	129	GLU	HB3	2.02	0.03	2
UNMAPPED	134	VAL	HG12	0.43	0.03	2
UNMAPPED	175	PHE	CB	37.96	0.2	1
UNMAPPED	133	MET	CB	33.03	0.2	1
UNMAPPED	162	VAL	HG11	0.65	0.03	2
UNMAPPED	167	ARG	HG2	1.64	0.03	2
UNMAPPED	141	PHE	HA	4.58	0.03	1
UNMAPPED	148	VAL	HA	3.67	0.03	1
UNMAPPED	148	VAL	HG12	0.89	0.03	2
UNMAPPED	160	VAL	HG13	0.41	0.03	2
UNMAPPED	141	PHE	C	173.3	0.2	1
UNMAPPED	162	VAL	CG1	21.92	0.2	2
UNMAPPED	167	ARG	H	7.8	0.03	1
UNMAPPED	180	LYS	HE3	2.77	0.03	2
UNMAPPED	169	THR	HG22	1.03	0.03	1
UNMAPPED	147	VAL	HG23	0.87	0.03	2
UNMAPPED	130	PRO	HG3	2.33	0.03	2
UNMAPPED	152	ASP	HB2	2.44	0.03	2
UNMAPPED	126	THR	H	8.02	0.03	1
UNMAPPED	166	GLY	N	103.47	0.1	1
UNMAPPED	164	ILE	HB	1.69	0.03	1
UNMAPPED	127	LEU	CD2	23.76	0.2	2
UNMAPPED	128	PHE	CD2	131.5	0.2	1
UNMAPPED	163	SER	H	8.8	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	159	LYS	HD2	1.53	0.03	2
UNMAPPED	180	LYS	CA	58.04	0.2	1
UNMAPPED	161	SER	CA	56.95	0.2	1
UNMAPPED	140	PRO	HD2	3.5	0.03	2
UNMAPPED	170	PRO	CD	50.64	0.2	1
UNMAPPED	140	PRO	CB	31.61	0.2	1
UNMAPPED	178	VAL	HA	5.32	0.03	1
UNMAPPED	172	GLU	CA	55.23	0.2	1
UNMAPPED	153	TYR	CA	61.91	0.2	1
UNMAPPED	135	ARG	CD	43.5	0.2	1
UNMAPPED	153	TYR	HD1	7.46	0.03	1
UNMAPPED	146	GLY	H	8.95	0.03	1
UNMAPPED	153	TYR	HA	4.32	0.03	1
UNMAPPED	133	MET	CG	32.16	0.2	1
UNMAPPED	149	GLU	N	129.0	0.1	1
UNMAPPED	148	VAL	CG2	22.94	0.2	2
UNMAPPED	173	LEU	HG	1.36	0.03	1
UNMAPPED	144	PHE	CA	58.38	0.2	1
UNMAPPED	179	GLU	C	175.39	0.2	1
UNMAPPED	158	LEU	HB3	1.27	0.03	2
UNMAPPED	158	LEU	C	175.11	0.2	1
UNMAPPED	136	VAL	HG12	1.08	0.03	2
UNMAPPED	127	LEU	HD12	0.85	0.03	2
UNMAPPED	138	ASP	H	7.31	0.03	1
UNMAPPED	145	ASN	N	117.59	0.1	1
UNMAPPED	147	VAL	CG2	20.82	0.2	2
UNMAPPED	130	PRO	CD	50.83	0.2	1
UNMAPPED	145	ASN	CB	41.2	0.2	1
UNMAPPED	157	ARG	H	7.76	0.03	1
UNMAPPED	153	TYR	C	178.19	0.2	1
UNMAPPED	125	LYS	H	8.52	0.03	1
UNMAPPED	160	VAL	HB	1.61	0.03	1
UNMAPPED	156	SER	CB	61.03	0.2	1
UNMAPPED	128	PHE	HE2	6.49	0.03	1
UNMAPPED	160	VAL	CB	35.23	0.2	1
UNMAPPED	147	VAL	C	176.2	0.2	1
UNMAPPED	144	PHE	C	174.94	0.2	1
UNMAPPED	146	GLY	C	170.78	0.2	1
UNMAPPED	129	GLU	H	9.02	0.03	1
UNMAPPED	151	VAL	CA	61.78	0.2	1
UNMAPPED	141	PHE	HB3	3.23	0.03	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	167	ARG	C	175.62	0.2	1
UNMAPPED	128	PHE	HA	4.97	0.03	1
UNMAPPED	133	MET	HE3	2.04	0.03	1
UNMAPPED	160	VAL	HG23	0.58	0.03	2
UNMAPPED	175	PHE	CZ	128.6	0.2	1
UNMAPPED	177	GLN	C	174.53	0.2	1
UNMAPPED	162	VAL	HG21	0.47	0.03	2
UNMAPPED	160	VAL	CA	59.51	0.2	1
UNMAPPED	158	LEU	HD12	0.04	0.03	2
UNMAPPED	169	THR	CG2	19.6	0.2	1
UNMAPPED	170	PRO	HD2	3.83	0.03	2
UNMAPPED	138	ASP	HB3	2.99	0.03	2
UNMAPPED	135	ARG	H	9.03	0.03	1
UNMAPPED	172	GLU	HA	5.26	0.03	1
UNMAPPED	152	ASP	CB	41.68	0.2	1
UNMAPPED	150	GLU	HA	4.62	0.03	1
UNMAPPED	158	LEU	CB	46.43	0.2	1
UNMAPPED	153	TYR	CD2	133.3	0.2	1
UNMAPPED	157	ARG	HG2	1.53	0.03	2
UNMAPPED	149	GLU	C	176.01	0.2	1
UNMAPPED	152	ASP	N	126.68	0.1	1
UNMAPPED	157	ARG	HA	5.18	0.03	1
UNMAPPED	135	ARG	HD3	3.24	0.03	2
UNMAPPED	141	PHE	H	8.96	0.03	1
UNMAPPED	138	ASP	HA	4.99	0.03	1
UNMAPPED	129	GLU	CG	35.78	0.2	1
UNMAPPED	163	SER	HB2	3.68	0.03	2
UNMAPPED	167	ARG	HG3	1.54	0.03	2
UNMAPPED	175	PHE	HB2	3.42	0.03	2
UNMAPPED	140	PRO	HB3	2.06	0.03	2
UNMAPPED	130	PRO	C	177.35	0.2	1
UNMAPPED	129	GLU	CA	52.8	0.2	1
UNMAPPED	176	SER	HB2	4.17	0.03	2
UNMAPPED	139	GLY	H	8.27	0.03	1
UNMAPPED	157	ARG	N	117.59	0.1	1
UNMAPPED	171	VAL	HG21	0.61	0.03	2
UNMAPPED	171	VAL	CG2	21.17	0.2	2
UNMAPPED	173	LEU	CG	26.9	0.2	1
UNMAPPED	178	VAL	HG11	0.66	0.03	2
UNMAPPED	129	GLU	HG2	2.22	0.03	1
UNMAPPED	181	ALA	CA	53.58	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	142	ALA	N	121.25	0.1	1
UNMAPPED	165	PHE	CA	58.52	0.2	1
UNMAPPED	142	ALA	HB3	1.23	0.03	1
UNMAPPED	151	VAL	HB	1.8	0.03	1
UNMAPPED	171	VAL	CA	60.91	0.2	1
UNMAPPED	173	LEU	CB	47.16	0.2	1
UNMAPPED	174	ASP	HB2	2.63	0.03	2
UNMAPPED	167	ARG	CB	31.72	0.2	1
UNMAPPED	133	MET	HB3	2.1	0.03	1
UNMAPPED	171	VAL	H	9.08	0.03	1
UNMAPPED	175	PHE	C	177.71	0.2	1
UNMAPPED	152	ASP	HA	5.0	0.03	1
UNMAPPED	164	ILE	HA	4.06	0.03	1
UNMAPPED	150	GLU	HG3	2.27	0.03	2
UNMAPPED	166	GLY	H	8.18	0.03	1
UNMAPPED	142	ALA	HA	3.52	0.03	1
UNMAPPED	153	TYR	CE2	118.8	0.2	1
UNMAPPED	181	ALA	HB1	1.21	0.03	1
UNMAPPED	147	VAL	HG13	0.94	0.03	2
UNMAPPED	151	VAL	HG23	0.58	0.03	1
UNMAPPED	181	ALA	N	131.73	0.1	1
UNMAPPED	171	VAL	N	122.94	0.1	1
UNMAPPED	163	SER	C	173.93	0.2	1
UNMAPPED	156	SER	H	7.42	0.03	1
UNMAPPED	167	ARG	HD3	3.25	0.03	2
UNMAPPED	125	LYS	N	121.94	0.1	1
UNMAPPED	129	GLU	HB2	1.78	0.03	2
UNMAPPED	158	LEU	CD1	26.69	0.2	2
UNMAPPED	162	VAL	HB	1.75	0.03	1
UNMAPPED	137	ASN	C	175.26	0.2	1
UNMAPPED	175	PHE	CA	58.8	0.2	1
UNMAPPED	162	VAL	HG12	0.65	0.03	2
UNMAPPED	138	ASP	CB	45.99	0.2	1
UNMAPPED	136	VAL	CG1	22.9	0.2	2
UNMAPPED	148	VAL	HG13	0.89	0.03	2
UNMAPPED	179	GLU	N	117.55	0.1	1
UNMAPPED	138	ASP	N	117.2	0.1	1
UNMAPPED	143	ASP	C	176.18	0.2	1
UNMAPPED	157	ARG	HD2	3.04	0.03	2
UNMAPPED	179	GLU	CB	33.82	0.2	1
UNMAPPED	157	ARG	CB	35.1	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	165	PHE	CB	36.99	0.2	1
UNMAPPED	130	PRO	HG2	1.74	0.03	2
UNMAPPED	165	PHE	N	126.14	0.1	1
UNMAPPED	164	ILE	HG13	1.16	0.03	2
UNMAPPED	125	LYS	CB	32.66	0.2	1
UNMAPPED	169	THR	CB	72.27	0.2	1
UNMAPPED	127	LEU	C	175.75	0.2	1
UNMAPPED	135	ARG	HB2	1.61	0.03	2
UNMAPPED	140	PRO	CG	27.15	0.2	1
UNMAPPED	159	LYS	HD3	1.6	0.03	2
UNMAPPED	161	SER	CB	62.93	0.2	1
UNMAPPED	170	PRO	HB2	1.76	0.03	2
UNMAPPED	170	PRO	CA	62.15	0.2	1
UNMAPPED	137	ASN	CA	52.56	0.2	1
UNMAPPED	140	PRO	CA	64.49	0.2	1
UNMAPPED	148	VAL	HG23	0.57	0.03	2
UNMAPPED	159	LYS	CA	55.6	0.2	1
UNMAPPED	149	GLU	CA	57.46	0.2	1
UNMAPPED	159	LYS	CG	25.29	0.2	1
UNMAPPED	149	GLU	CG	36.01	0.2	1
UNMAPPED	180	LYS	N	122.53	0.1	1
UNMAPPED	158	LEU	HB2	1.52	0.03	2
UNMAPPED	136	VAL	HG11	1.08	0.03	2
UNMAPPED	166	GLY	HA3	4.22	0.03	2
UNMAPPED	179	GLU	HG3	2.22	0.03	2
UNMAPPED	171	VAL	HB	1.72	0.03	1
UNMAPPED	141	PHE	HE1	7.1	0.03	1
UNMAPPED	172	GLU	CB	31.5	0.2	1
UNMAPPED	176	SER	HA	4.42	0.03	1
UNMAPPED	153	TYR	N	122.73	0.1	1
UNMAPPED	173	LEU	HD11	0.61	0.03	2
UNMAPPED	135	ARG	CB	33.24	0.2	1
UNMAPPED	164	ILE	CG1	26.8	0.2	1
UNMAPPED	152	ASP	H	8.77	0.03	1
UNMAPPED	155	LYS	CA	55.12	0.2	1
UNMAPPED	179	GLU	HB2	2.12	0.03	2
UNMAPPED	174	ASP	C	178.15	0.2	1
UNMAPPED	173	LEU	CD1	27.99	0.2	2
UNMAPPED	159	LYS	H	8.46	0.03	1
UNMAPPED	156	SER	HA	2.46	0.03	1
UNMAPPED	145	ASN	HA	5.74	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	178	VAL	H	7.39	0.03	1
UNMAPPED	159	LYS	N	121.37	0.1	1
UNMAPPED	134	VAL	CA	58.65	0.2	1
UNMAPPED	151	VAL	CG2	21.17	0.2	2
UNMAPPED	173	LEU	HD22	0.9	0.03	2
UNMAPPED	141	PHE	CE2	131.2	0.2	1
UNMAPPED	136	VAL	HG21	0.72	0.03	2
UNMAPPED	159	LYS	CE	41.95	0.2	1
UNMAPPED	154	GLU	CG	36.68	0.2	1
UNMAPPED	133	MET	HE2	2.04	0.03	1
UNMAPPED	160	VAL	HG22	0.58	0.03	2
UNMAPPED	141	PHE	CD1	131.2	0.2	1
UNMAPPED	178	VAL	HG23	0.51	0.03	2
UNMAPPED	159	LYS	HA	5.02	0.03	1
UNMAPPED	142	ALA	H	7.4	0.03	1
UNMAPPED	178	VAL	C	173.95	0.2	1
UNMAPPED	158	LEU	CG	26.49	0.2	1
UNMAPPED	138	ASP	HB2	2.39	0.03	2
UNMAPPED	171	VAL	HA	4.26	0.03	1
UNMAPPED	152	ASP	CA	52.01	0.2	1
UNMAPPED	125	LYS	HG2	1.43	0.03	2
UNMAPPED	168	ALA	C	177.69	0.2	1
UNMAPPED	169	THR	HG23	1.03	0.03	1
UNMAPPED	173	LEU	HD21	0.9	0.03	2
UNMAPPED	128	PHE	HZ	6.97	0.03	1
UNMAPPED	170	PRO	HG3	2.2	0.03	2
UNMAPPED	147	VAL	HB	1.88	0.03	1
UNMAPPED	148	VAL	CB	32.05	0.2	1
UNMAPPED	156	SER	N	114.11	0.1	1
UNMAPPED	180	LYS	HD2	1.64	0.03	1
UNMAPPED	153	TYR	HB3	3.29	0.03	2
UNMAPPED	148	VAL	N	126.69	0.1	1
UNMAPPED	140	PRO	HB2	1.14	0.03	2
UNMAPPED	133	MET	C	176.67	0.2	1
UNMAPPED	161	SER	HB3	3.68	0.03	2
UNMAPPED	156	SER	HB3	3.92	0.03	2
UNMAPPED	159	LYS	HB2	1.67	0.03	2
UNMAPPED	147	VAL	CA	59.9	0.2	1
UNMAPPED	129	GLU	HG3	2.22	0.03	1
UNMAPPED	146	GLY	CA	45.76	0.2	1
UNMAPPED	134	VAL	HG21	0.67	0.03	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	180	LYS	C	175.84	0.2	1
UNMAPPED	159	LYS	C	175.51	0.2	1
UNMAPPED	175	PHE	HA	4.14	0.03	1
UNMAPPED	160	VAL	CG2	22.54	0.2	2
UNMAPPED	136	VAL	HG13	1.08	0.03	2
UNMAPPED	174	ASP	N	120.39	0.1	1
UNMAPPED	141	PHE	CB	37.0	0.2	1
UNMAPPED	167	ARG	CA	54.75	0.2	1
UNMAPPED	165	PHE	H	8.94	0.03	1
UNMAPPED	169	THR	H	9.06	0.03	1
UNMAPPED	126	THR	HG22	0.91	0.03	1
UNMAPPED	168	ALA	HB2	1.25	0.03	1
UNMAPPED	124	PRO	CA	62.93	0.2	1
UNMAPPED	153	TYR	CE1	118.8	0.2	1
UNMAPPED	146	GLY	HA3	4.72	0.03	2
UNMAPPED	147	VAL	HG12	0.94	0.03	2
UNMAPPED	160	VAL	C	174.11	0.2	1
UNMAPPED	151	VAL	HG22	0.58	0.03	1
UNMAPPED	145	ASN	HB3	2.81	0.03	2
UNMAPPED	180	LYS	HA	4.37	0.03	1
UNMAPPED	147	VAL	H	8.01	0.03	1
UNMAPPED	130	PRO	HD2	3.75	0.03	2
UNMAPPED	158	LEU	CD2	25.77	0.2	2
UNMAPPED	125	LYS	C	176.62	0.2	1
UNMAPPED	178	VAL	CG1	23.08	0.2	2
UNMAPPED	162	VAL	HG13	0.65	0.03	2
UNMAPPED	138	ASP	CA	54.03	0.2	1
UNMAPPED	134	VAL	CG1	17.96	0.2	2
UNMAPPED	160	VAL	HG11	0.41	0.03	2
UNMAPPED	135	ARG	HA	4.98	0.03	1
UNMAPPED	157	ARG	HD3	3.15	0.03	2
UNMAPPED	172	GLU	HG2	2.01	0.03	2
UNMAPPED	147	VAL	HG21	0.87	0.03	2
UNMAPPED	175	PHE	HE1	7.33	0.03	1
UNMAPPED	173	LEU	CA	53.4	0.2	1
UNMAPPED	164	ILE	HG12	0.55	0.03	2
UNMAPPED	125	LYS	CE	42.1	0.2	1
UNMAPPED	169	THR	CA	59.87	0.2	1
UNMAPPED	167	ARG	HD2	3.2	0.03	2
UNMAPPED	135	ARG	HB3	1.7	0.03	2
UNMAPPED	137	ASN	N	125.31	0.1	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	170	PRO	HB3	2.06	0.03	2
UNMAPPED	141	PHE	CE1	131.2	0.2	1
UNMAPPED	180	LYS	CG	26.06	0.2	1
UNMAPPED	164	ILE	CG2	17.01	0.2	1
UNMAPPED	132	GLU	HB3	2.06	0.03	1
UNMAPPED	132	GLU	HG2	2.39	0.03	1
UNMAPPED	172	GLU	CG	37.3	0.2	1
UNMAPPED	148	VAL	HG22	0.57	0.03	2
UNMAPPED	159	LYS	CB	34.38	0.2	1
UNMAPPED	127	LEU	HA	4.55	0.03	1
UNMAPPED	128	PHE	CE1	130.7	0.2	1
UNMAPPED	177	GLN	H	7.93	0.03	1
UNMAPPED	136	VAL	HA	4.24	0.03	1
UNMAPPED	127	LEU	HG	1.46	0.03	1
UNMAPPED	171	VAL	HG11	0.42	0.03	2
UNMAPPED	134	VAL	HB	2.05	0.03	1
UNMAPPED	169	THR	HA	4.74	0.03	1
UNMAPPED	125	LYS	HA	4.27	0.03	1
UNMAPPED	164	ILE	C	175.87	0.2	1
UNMAPPED	171	VAL	HG12	0.42	0.03	2
UNMAPPED	172	GLU	C	175.52	0.2	1
UNMAPPED	166	GLY	HA2	3.55	0.03	2
UNMAPPED	179	GLU	HG2	2.34	0.03	2
UNMAPPED	171	VAL	HG13	0.42	0.03	2
UNMAPPED	155	LYS	N	115.61	0.1	1
UNMAPPED	179	GLU	HA	4.86	0.03	1
UNMAPPED	136	VAL	HB	2.56	0.03	1
UNMAPPED	130	PRO	CB	31.45	0.2	1
UNMAPPED	130	PRO	HB2	1.93	0.03	2
UNMAPPED	175	PHE	CD1	129.6	0.2	1
UNMAPPED	155	LYS	CD	29.45	0.2	1
UNMAPPED	154	GLU	HB3	2.28	0.03	2
UNMAPPED	126	THR	HA	4.14	0.03	1
UNMAPPED	154	GLU	HG2	2.31	0.03	2
UNMAPPED	155	LYS	CB	33.0	0.2	1
UNMAPPED	148	VAL	H	9.05	0.03	1
UNMAPPED	180	LYS	H	8.87	0.03	1
UNMAPPED	178	VAL	HB	1.8	0.03	1
UNMAPPED	160	VAL	N	125.89	0.1	1
UNMAPPED	143	ASP	CA	57.21	0.2	1
UNMAPPED	173	LEU	HA	4.83	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	128	PHE	HD1	6.38	0.03	1
UNMAPPED	136	VAL	CA	63.22	0.2	1
UNMAPPED	134	VAL	N	116.28	0.1	1
UNMAPPED	127	LEU	CA	54.56	0.2	1
UNMAPPED	172	GLU	HB3	1.88	0.03	2
UNMAPPED	124	PRO	HB3	2.31	0.03	2
UNMAPPED	151	VAL	CG1	21.17	0.2	2
UNMAPPED	161	SER	HA	4.72	0.03	1
UNMAPPED	160	VAL	HG21	0.58	0.03	2
UNMAPPED	135	ARG	HG2	1.42	0.03	2
UNMAPPED	162	VAL	HG23	0.47	0.03	2
UNMAPPED	179	GLU	HB3	2.03	0.03	2
UNMAPPED	155	LYS	HG3	1.45	0.03	2
UNMAPPED	155	LYS	HD2	1.57	0.03	1
UNMAPPED	125	LYS	HG3	1.5	0.03	2
UNMAPPED	170	PRO	HG2	2.03	0.03	2
UNMAPPED	164	ILE	HG22	0.69	0.03	1
UNMAPPED	163	SER	CB	63.03	0.2	1
UNMAPPED	148	VAL	CA	64.99	0.2	1
UNMAPPED	175	PHE	CE2	131.8	0.2	1
UNMAPPED	180	LYS	HD3	1.64	0.03	1
UNMAPPED	132	GLU	N	120.83	0.1	1
UNMAPPED	180	LYS	HB2	1.78	0.03	2
UNMAPPED	158	LEU	HD22	0.39	0.03	2
UNMAPPED	128	PHE	HB3	2.6	0.03	2
UNMAPPED	161	SER	HB2	3.68	0.03	2
UNMAPPED	125	LYS	HD3	1.7	0.03	2
UNMAPPED	159	LYS	HB3	1.73	0.03	2
UNMAPPED	146	GLY	N	105.84	0.1	1
UNMAPPED	159	LYS	HG3	1.3	0.03	2
UNMAPPED	157	ARG	C	174.09	0.2	1
UNMAPPED	134	VAL	HG22	0.67	0.03	2
UNMAPPED	150	GLU	HB3	2.01	0.03	2
UNMAPPED	144	PHE	HE1	7.13	0.03	1
UNMAPPED	151	VAL	HG12	0.58	0.03	1
UNMAPPED	142	ALA	HB1	1.23	0.03	1
UNMAPPED	148	VAL	C	176.28	0.2	1
UNMAPPED	133	MET	HG3	2.65	0.03	2
UNMAPPED	141	PHE	HZ	7.33	0.03	1
UNMAPPED	128	PHE	CZ	129.7	0.2	1
UNMAPPED	165	PHE	HD1	7.28	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	126	THR	HG23	0.91	0.03	1
UNMAPPED	162	VAL	H	8.76	0.03	1
UNMAPPED	152	ASP	C	176.92	0.2	1
UNMAPPED	177	GLN	N	119.2	0.1	1
UNMAPPED	146	GLY	HA2	3.48	0.03	2
UNMAPPED	168	ALA	CA	52.83	0.2	1
UNMAPPED	130	PRO	HA	3.93	0.03	1
UNMAPPED	147	VAL	HG11	0.94	0.03	2
UNMAPPED	177	GLN	CB	31.63	0.2	1
UNMAPPED	151	VAL	HG21	0.58	0.03	1
UNMAPPED	127	LEU	HD21	0.78	0.03	2
UNMAPPED	145	ASN	HB2	2.75	0.03	2
UNMAPPED	141	PHE	HD2	6.76	0.03	1
UNMAPPED	134	VAL	HG11	0.43	0.03	2
UNMAPPED	170	PRO	C	177.05	0.2	1
UNMAPPED	130	PRO	HD3	3.83	0.03	2
UNMAPPED	135	ARG	C	175.54	0.2	1
UNMAPPED	149	GLU	HG2	2.13	0.03	2
UNMAPPED	125	LYS	HE3	2.99	0.03	2
UNMAPPED	148	VAL	HB	2.34	0.03	1
UNMAPPED	133	MET	CA	54.6	0.2	1
UNMAPPED	136	VAL	C	177.25	0.2	1
UNMAPPED	134	VAL	CG2	22.35	0.2	2
UNMAPPED	169	THR	HG21	1.03	0.03	1
UNMAPPED	176	SER	N	109.76	0.1	1
UNMAPPED	162	VAL	CG2	20.91	0.2	2
UNMAPPED	173	LEU	N	125.38	0.1	1
UNMAPPED	158	LEU	HG	1.34	0.03	1
UNMAPPED	172	GLU	HG3	2.17	0.03	2
UNMAPPED	125	LYS	HB3	1.83	0.03	2
UNMAPPED	175	PHE	HE2	7.33	0.03	1
UNMAPPED	163	SER	HA	4.61	0.03	1
UNMAPPED	158	LEU	HA	5.01	0.03	1
UNMAPPED	125	LYS	CD	29.21	0.2	1
UNMAPPED	137	ASN	HB2	2.93	0.03	2
UNMAPPED	180	LYS	CB	33.09	0.2	1
UNMAPPED	127	LEU	CD1	25.11	0.2	2
UNMAPPED	127	LEU	N	124.51	0.1	1
UNMAPPED	145	ASN	C	175.29	0.2	1
UNMAPPED	128	PHE	CD1	131.5	0.2	1
UNMAPPED	151	VAL	H	8.89	0.03	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	180	LYS	CD	28.99	0.2	1
UNMAPPED	127	LEU	CG	27.0	0.2	1
UNMAPPED	132	GLU	HB2	2.06	0.03	1
UNMAPPED	132	GLU	HG3	2.39	0.03	1
UNMAPPED	168	ALA	H	8.72	0.03	1
UNMAPPED	148	VAL	CG1	23.7	0.2	2
UNMAPPED	144	PHE	N	119.1	0.1	1
UNMAPPED	134	VAL	HA	5.06	0.03	1
UNMAPPED	124	PRO	C	176.76	0.2	1
UNMAPPED	127	LEU	HD11	0.85	0.03	2
UNMAPPED	179	GLU	CA	53.97	0.2	1
UNMAPPED	171	VAL	C	173.82	0.2	1
UNMAPPED	137	ASN	HA	5.14	0.03	1
UNMAPPED	145	ASN	CA	52.01	0.2	1
UNMAPPED	147	VAL	CG1	21.53	0.2	2
UNMAPPED	162	VAL	C	174.96	0.2	1
UNMAPPED	130	PRO	HB3	2.23	0.03	2
UNMAPPED	175	PHE	CD2	129.6	0.2	1
UNMAPPED	155	LYS	CE	42.24	0.2	1
UNMAPPED	154	GLU	HB2	2.19	0.03	2
UNMAPPED	154	GLU	HG3	2.41	0.03	2
UNMAPPED	175	PHE	HZ	6.75	0.03	1
UNMAPPED	124	PRO	HG2	2.04	0.03	2
UNMAPPED	135	ARG	HG3	1.46	0.03	2
UNMAPPED	172	GLU	HB2	1.83	0.03	2
UNMAPPED	133	MET	HA	5.28	0.03	1
UNMAPPED	149	GLU	HB3	2.03	0.03	2
UNMAPPED	128	PHE	HE1	6.49	0.03	1
UNMAPPED	174	ASP	H	9.03	0.03	1
UNMAPPED	137	ASN	H	9.16	0.03	1
UNMAPPED	136	VAL	N	127.25	0.1	1
UNMAPPED	173	LEU	C	175.73	0.2	1
UNMAPPED	136	VAL	CB	31.02	0.2	1
UNMAPPED	149	GLU	HA	4.66	0.03	1
UNMAPPED	174	ASP	HA	5.2	0.03	1
UNMAPPED	140	PRO	HA	4.19	0.03	1
UNMAPPED	164	ILE	HD11	0.46	0.03	1
UNMAPPED	158	LEU	HD11	0.04	0.03	2

### 7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	58	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	54	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	54	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{15}\text{N}$	54	0.00 $\pm$ 0.00	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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 619. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	0/249 (0%)	0/99 (0%)	0/102 (0%)	0/48 (0%)
Sidechain	0/326 (0%)	0/190 (0%)	0/121 (0%)	0/15 (0%)
Aromatic	0/44 (0%)	0/24 (0%)	0/20 (0%)	0/0 (—%)
Overall	0/619 (0%)	0/313 (0%)	0/243 (0%)	0/63 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 731. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	0/287 (0%)	0/114 (0%)	0/118 (0%)	0/55 (0%)
Sidechain	0/391 (0%)	0/229 (0%)	0/143 (0%)	0/19 (0%)
Aromatic	0/53 (0%)	0/29 (0%)	0/24 (0%)	0/0 (—%)
Overall	0/731 (0%)	0/372 (0%)	0/285 (0%)	0/74 (0%)

### 7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

### 7.1.5 Random Coil Index (RCI) plots ⓘ

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned\_chem\_shift\_list\_1). RCI is only applicable to proteins.