



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 01:07 am GMT

PDB ID : 2ML8  
Title : NMR structure of Saccharomyces cerevisiae Acyl Carrier Protein.  
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Deposited on : 2014-02-20

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  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

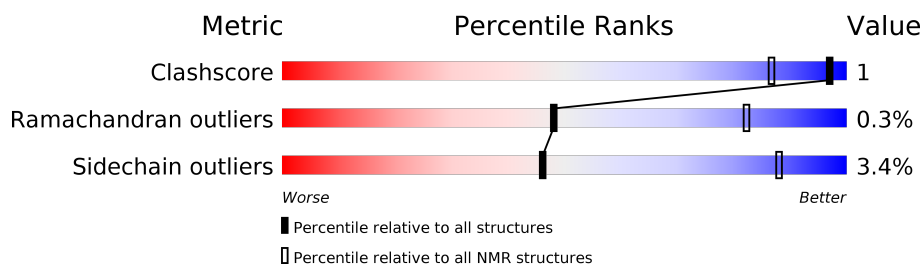
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*


The overall completeness of chemical shifts assignment is 94%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	183	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:140-A:302 (163)	0.39	1

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2793 atoms, of which 1401 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms						Trace
1	A	183	Total	C	H	N	O	S	0
			2793	877	1401	240	271	4	

There are 18 discrepancies between the modelled and reference sequences:

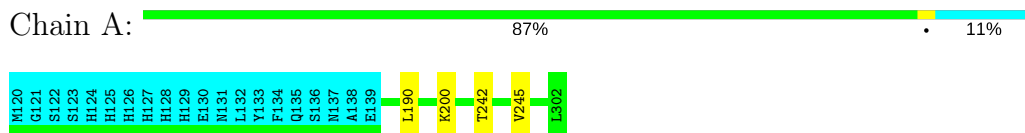
Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	-	EXPRESSION TAG	UNP P19097
A	121	GLY	-	EXPRESSION TAG	UNP P19097
A	122	SER	-	EXPRESSION TAG	UNP P19097
A	123	SER	-	EXPRESSION TAG	UNP P19097
A	124	HIS	-	EXPRESSION TAG	UNP P19097
A	125	HIS	-	EXPRESSION TAG	UNP P19097
A	126	HIS	-	EXPRESSION TAG	UNP P19097
A	127	HIS	-	EXPRESSION TAG	UNP P19097
A	128	HIS	-	EXPRESSION TAG	UNP P19097
A	129	HIS	-	EXPRESSION TAG	UNP P19097
A	130	GLU	-	EXPRESSION TAG	UNP P19097
A	131	ASN	-	EXPRESSION TAG	UNP P19097
A	132	LEU	-	EXPRESSION TAG	UNP P19097
A	133	TYR	-	EXPRESSION TAG	UNP P19097
A	134	PHE	-	EXPRESSION TAG	UNP P19097
A	135	GLN	-	EXPRESSION TAG	UNP P19097
A	136	SER	-	EXPRESSION TAG	UNP P19097
A	137	ASN	-	EXPRESSION TAG	UNP P19097

## 4 Residue-property plots [i](#)

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

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Fatty acid synthase subunit alpha

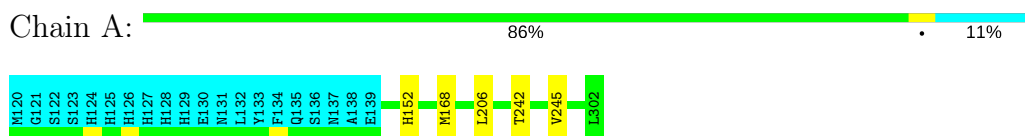


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

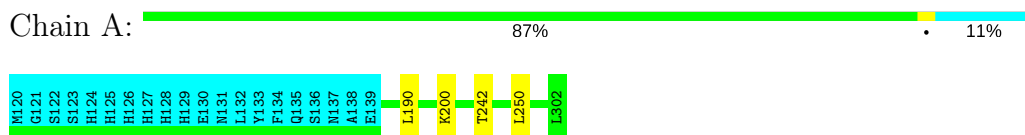
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Fatty acid synthase subunit alpha



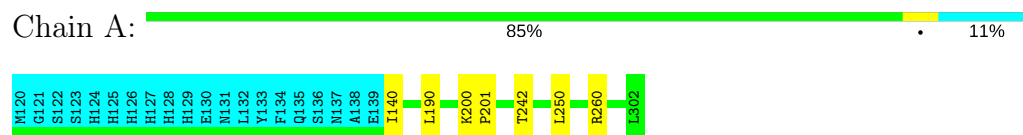
#### 4.2.2 Score per residue for model 2

- Molecule 1: Fatty acid synthase subunit alpha



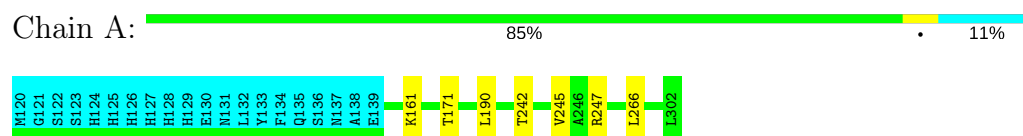
### 4.2.3 Score per residue for model 3

- Molecule 1: Fatty acid synthase subunit alpha



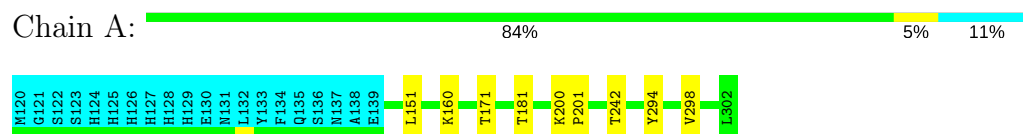
### 4.2.4 Score per residue for model 4

- Molecule 1: Fatty acid synthase subunit alpha



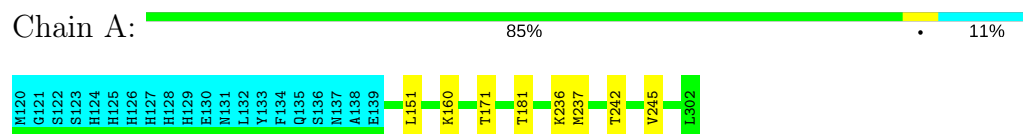
### 4.2.5 Score per residue for model 5

- Molecule 1: Fatty acid synthase subunit alpha



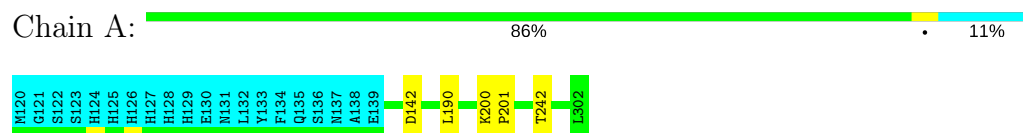
### 4.2.6 Score per residue for model 6

- Molecule 1: Fatty acid synthase subunit alpha



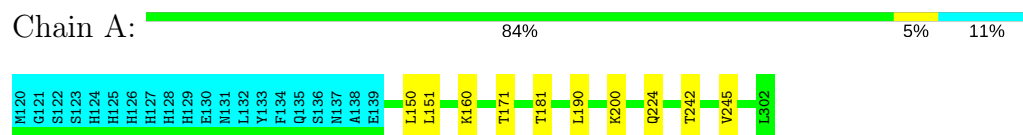
### 4.2.7 Score per residue for model 7

- Molecule 1: Fatty acid synthase subunit alpha



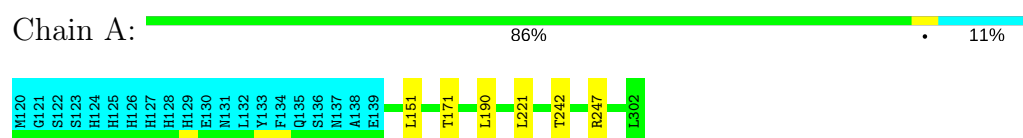
### 4.2.8 Score per residue for model 8

- Molecule 1: Fatty acid synthase subunit alpha



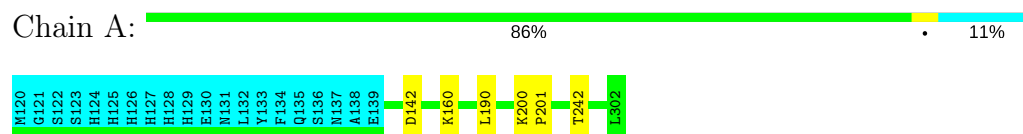
### 4.2.9 Score per residue for model 9

- Molecule 1: Fatty acid synthase subunit alpha



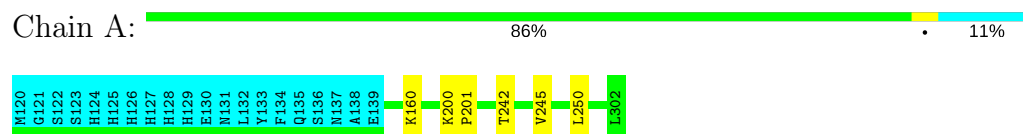
### 4.2.10 Score per residue for model 10

- Molecule 1: Fatty acid synthase subunit alpha



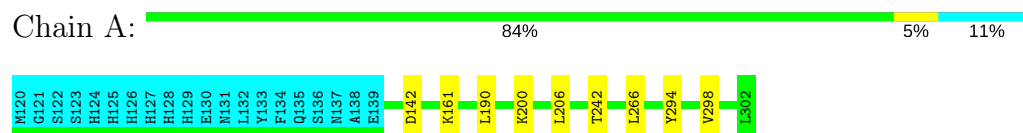
### 4.2.11 Score per residue for model 11

- Molecule 1: Fatty acid synthase subunit alpha



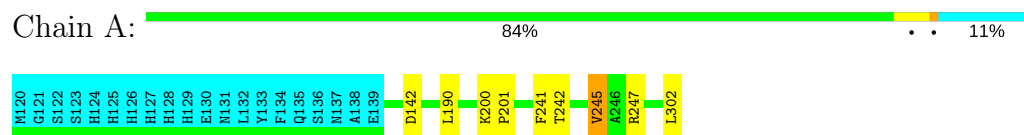
### 4.2.12 Score per residue for model 12

- Molecule 1: Fatty acid synthase subunit alpha



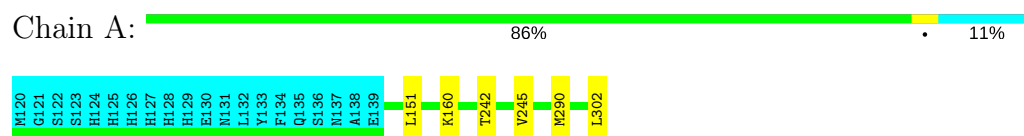
### 4.2.13 Score per residue for model 13

- Molecule 1: Fatty acid synthase subunit alpha



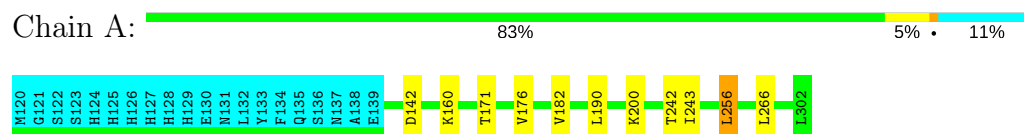
### 4.2.14 Score per residue for model 14

- Molecule 1: Fatty acid synthase subunit alpha



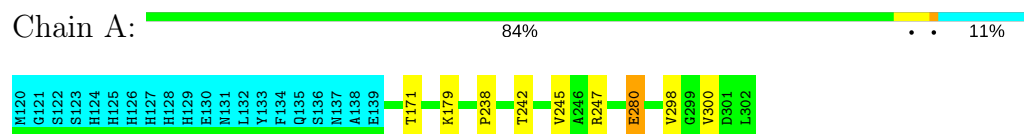
### 4.2.15 Score per residue for model 15

- Molecule 1: Fatty acid synthase subunit alpha



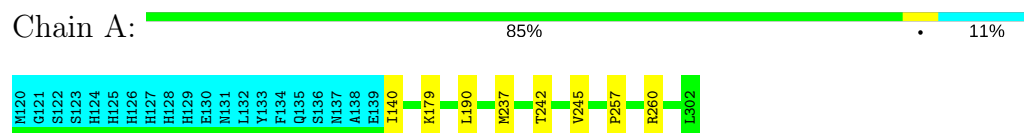
### 4.2.16 Score per residue for model 16

- Molecule 1: Fatty acid synthase subunit alpha



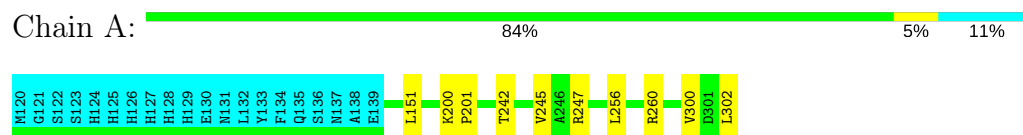
### 4.2.17 Score per residue for model 17

- Molecule 1: Fatty acid synthase subunit alpha



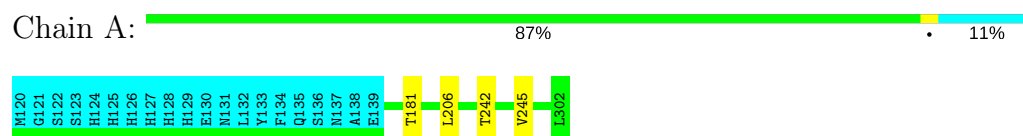
#### 4.2.18 Score per residue for model 18

- Molecule 1: Fatty acid synthase subunit alpha



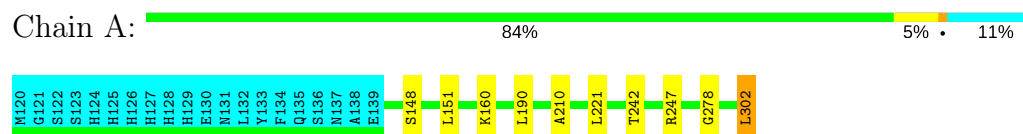
#### 4.2.19 Score per residue for model 19

- Molecule 1: Fatty acid synthase subunit alpha



#### 4.2.20 Score per residue for model 20

- Molecule 1: Fatty acid synthase subunit alpha



## 5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CYANA	refinement	
AMBER	refinement	

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)	2ml8_cs.str
Number of chemical shift lists	1
Total number of shifts	2075
Number of shifts mapped to atoms	2075
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

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

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1223	1266	1266	2±1
All	All	24460	25320	25320	39

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:221:LEU:HD12	1:A:221:LEU:H	0.51	1.64	20	1
1:A:148:SER:HA	1:A:210:ALA:HB1	0.50	1.82	20	1
1:A:302:LEU:HD22	1:A:302:LEU:N	0.50	2.22	18	2
1:A:151:LEU:HD13	1:A:151:LEU:C	0.49	2.28	20	5
1:A:200:LYS:N	1:A:201:PRO:CD	0.47	2.78	11	7
1:A:302:LEU:N	1:A:302:LEU:HD22	0.47	2.25	13	2
1:A:257:PRO:HD2	1:A:260:ARG:CZ	0.47	2.39	17	1
1:A:294:TYR:CE1	1:A:298:VAL:HG11	0.46	2.46	12	2
1:A:140:ILE:HG21	1:A:260:ARG:CZ	0.46	2.41	17	1
1:A:151:LEU:C	1:A:151:LEU:HD13	0.45	2.31	18	2
1:A:260:ARG:HH12	1:A:300:VAL:HG21	0.44	1.71	18	1
1:A:241:PHE:CE2	1:A:245:VAL:HG23	0.44	2.48	13	1
1:A:260:ARG:NH1	1:A:300:VAL:HG21	0.43	2.26	18	1
1:A:302:LEU:N	1:A:302:LEU:CD2	0.43	2.82	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:206:LEU:N	1:A:206:LEU:HD12	0.43	2.28	12	1
1:A:206:LEU:HD12	1:A:206:LEU:N	0.42	2.28	1	2
1:A:256:LEU:H	1:A:256:LEU:HD22	0.41	1.75	15	1
1:A:206:LEU:N	1:A:206:LEU:CD1	0.41	2.84	12	1
1:A:238:PRO:HG2	1:A:280:GLU:HG2	0.41	1.93	16	1
1:A:140:ILE:CG2	1:A:260:ARG:HD3	0.41	2.46	3	1
1:A:298:VAL:HG13	1:A:300:VAL:HG13	0.40	1.92	16	1
1:A:266:LEU:HD12	1:A:266:LEU:C	0.40	2.37	12	1
1:A:152:HIS:CE1	1:A:168:MET:SD	0.40	3.14	1	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	162/183 (89%)	150±2 (93±1%)	11±1 (7±1%)	0±0 (0±0%)	48	82
All	All	3240/3660 (89%)	3009 (93%)	222 (7%)	9 (0%)	48	82

All 3 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	142	ASP	5
1	A	250	LEU	3
1	A	278	GLY	1

### 6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	135/153 (88%)	130±2 (97±2%)	5±2 (3±2%)	46	88
All	All	2700/3060 (88%)	2608 (97%)	92 (3%)	46	88

All 23 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	242	THR	20
1	A	190	LEU	12
1	A	245	VAL	11
1	A	160	LYS	8
1	A	171	THR	7
1	A	247	ARG	6
1	A	200	LYS	4
1	A	181	THR	4
1	A	237	MET	2
1	A	179	LYS	2
1	A	161	LYS	2
1	A	266	LEU	2
1	A	256	LEU	2
1	A	280	GLU	1
1	A	221	LEU	1
1	A	176	VAL	1
1	A	224	GLN	1
1	A	302	LEU	1
1	A	236	LYS	1
1	A	290	MET	1
1	A	243	ILE	1
1	A	182	VAL	1
1	A	150	LEU	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [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 94% for the well-defined parts and 84% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2ml8\_cs.str

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	2075
Number of shifts mapped to atoms	2075
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	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
$^{13}\text{C}_\alpha$	165	$0.10 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	151	$0.52 \pm 0.07$	Should be applied
$^{13}\text{C}'$	155	$0.61 \pm 0.12$	Should be applied
$^{15}\text{N}$	156	$-0.94 \pm 0.31$	Should be applied

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 1803 atoms were assigned a chemical shift out of a possible 1920. 33 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	787/799 (98%)	317/318 (100%)	316/326 (97%)	154/155 (99%)
Sidechain	935/1034 (90%)	573/604 (95%)	350/393 (89%)	12/37 (32%)

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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	81/87 (93%)	43/47 (91%)	37/37 (100%)	1/3 (33%)
Overall	1803/1920 (94%)	933/969 (96%)	703/756 (93%)	167/195 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1821 atoms were assigned a chemical shift out of a possible 2169. 33 out of 34 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	797/899 (89%)	321/358 (90%)	320/366 (87%)	156/175 (89%)
Sidechain	943/1124 (84%)	578/659 (88%)	353/425 (83%)	12/40 (30%)
Aromatic	81/146 (55%)	43/80 (54%)	37/57 (65%)	1/9 (11%)
Overall	1821/2169 (84%)	942/1097 (86%)	710/848 (84%)	169/224 (75%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	253	ARG	HG3	-0.67	3.00 – 0.10	-7.6
1	A	284	LYS	HG3	-0.14	2.76 – -0.04	-5.4

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

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

Random coil index (RCI) for chain A:

