Full wwPDB NMR Structure Validation Report (i)

Sep 19, 2016 – 05:54 PM EDT

PDB ID	:	5LAO
Title	:	S-nitrosylated 3D NMR structure of the cytoplasmic rhodanese domain of the inner membrane protein YgaP from Escherichia coli
Authors	:	Eichmann, C.; Tzitzilonis, C.; Nakamura, T.; Maslennikov, I.; Kwiatkowski, W.; Choe, S.; Lipton, S.A.; Guntert, P.; Riek, R.
Deposited on	:	2016-06-14

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

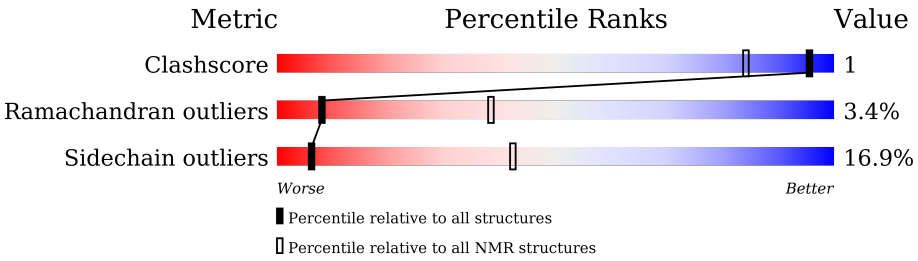
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027939
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	108	78% 12% 10%

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 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:2-A:64, A:70-A:103 (97)	0.41	14

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1659 atoms, of which 835 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Inner membrane protein YgaP.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	108	1659	519	835	147	157	1	0

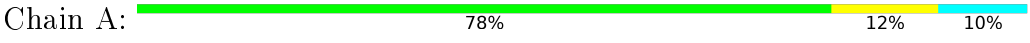
4 Residue-property plots (i)

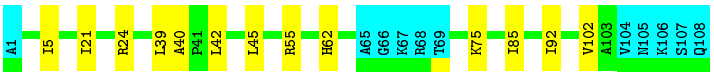
4.1 Average score per residue in the NMR ensemble

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: Inner membrane protein YgaP

Chain A:





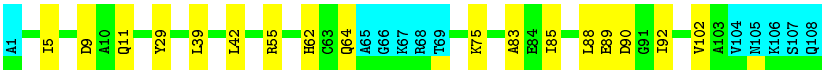
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Inner membrane protein YgaP

Chain A:



4.2.2 Score per residue for model 2

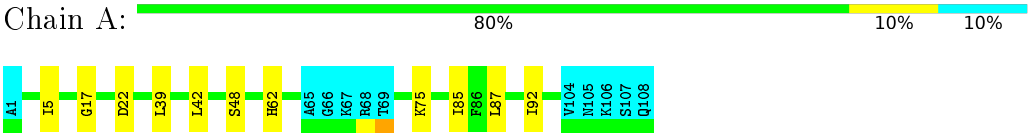
• Molecule 1: Inner membrane protein YgaP

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Inner membrane protein YgaP

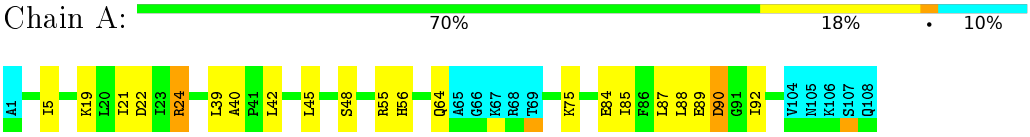
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Inner membrane protein YgaP

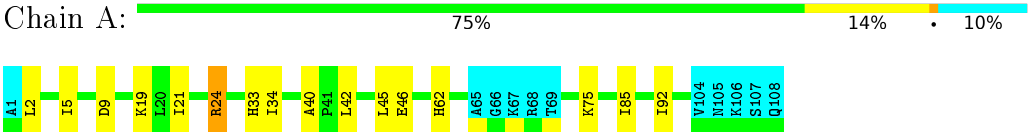
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Inner membrane protein YgaP

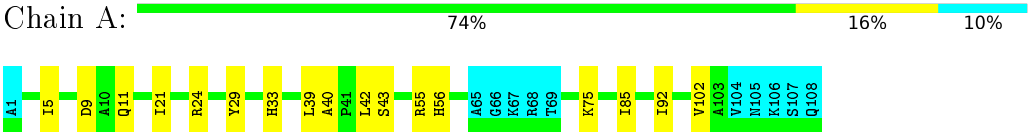
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Inner membrane protein YgaP

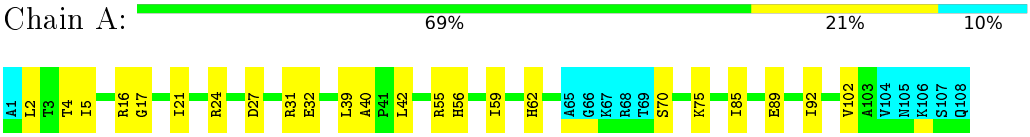
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Inner membrane protein YgaP

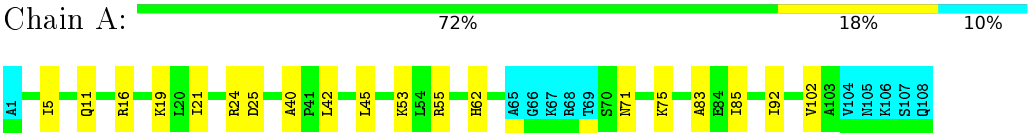
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Inner membrane protein YgaP

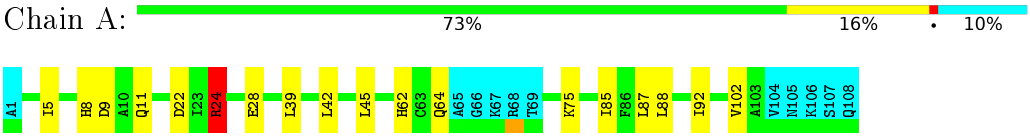
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Inner membrane protein YgaP

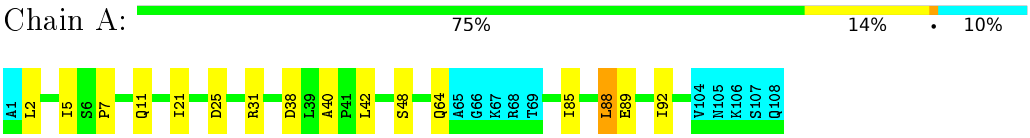
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Inner membrane protein YgaP

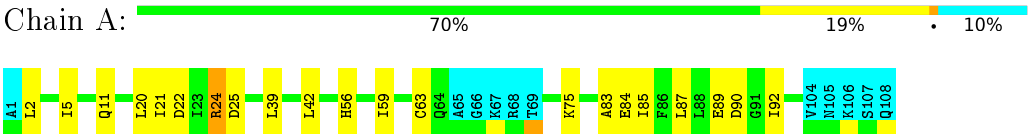
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Inner membrane protein YgaP

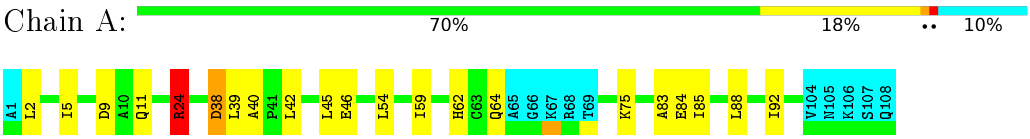
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Inner membrane protein YgaP

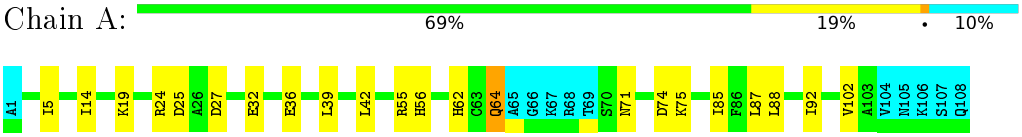
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Inner membrane protein YgaP

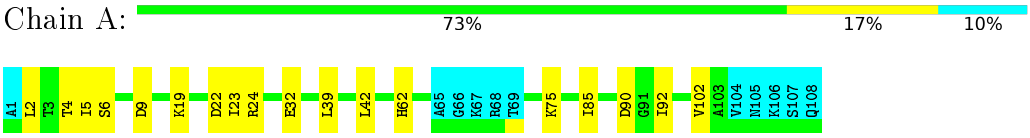
Chain A:



4.2.14 Score per residue for model 14 (medoid)

• Molecule 1: Inner membrane protein YgaP

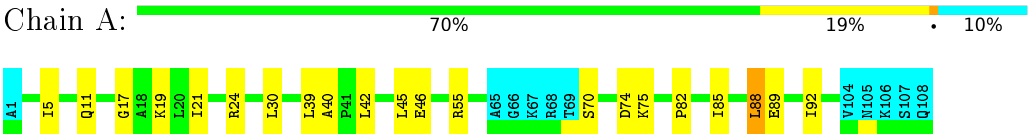
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Inner membrane protein YgaP

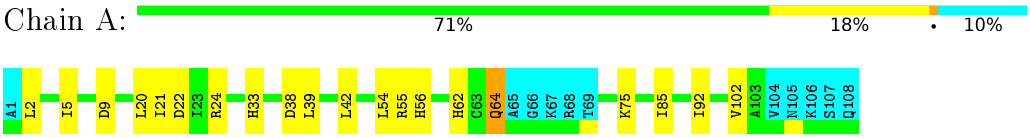
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Inner membrane protein YgaP

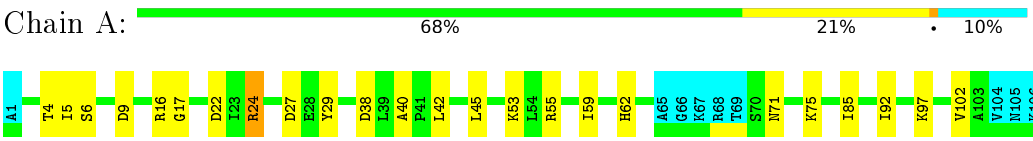
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Inner membrane protein YgaP

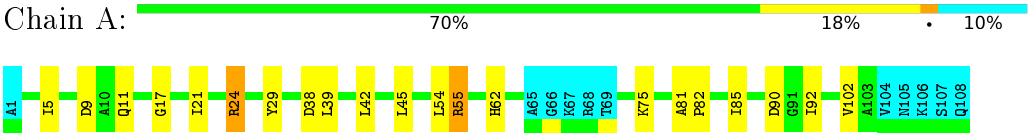
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Inner membrane protein YgaP

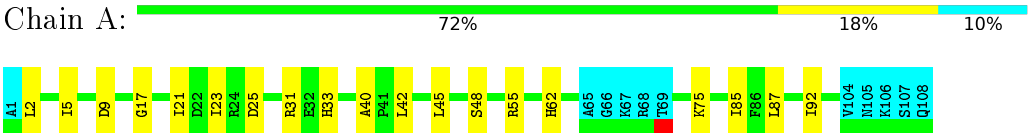
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Inner membrane protein YgaP

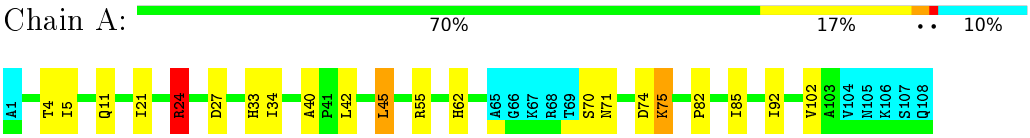
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Inner membrane protein YgaP

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *energy minimization*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *STRUCTURES WITH THE LEAST RESTRAINT VIOLATIONS*.

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

Software name	Classification	Version
OPAL	refinement	3.97

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)	5lao_cs.cif
Number of chemical shift lists	1
Total number of shifts	964
Number of shifts mapped to atoms	0
Number of unparsed shifts	964
Number of shifts with mapping errors	0
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

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.52±0.01	0±0/759 (0.0±0.0%)	1.00±0.03	0±1/1033 (0.0±0.1%)
All	All	0.52	0/15180 (0.0%)	1.00	7/20660 (0.0%)

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	0.7±0.6
All	All	0	14

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	24	ARG	CD-NE-CZ	6.83	133.16	123.60	20	2
1	A	16	ARG	NE-CZ-NH2	-5.80	117.40	120.30	7	1
1	A	55	ARG	NE-CZ-NH2	-5.58	117.51	120.30	7	1
1	A	90	ASP	CB-CG-OD2	5.43	123.18	118.30	1	1
1	A	24	ARG	NE-CZ-NH2	-5.31	117.64	120.30	20	1
1	A	24	ARG	NE-CZ-NH1	5.25	122.93	120.30	16	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	24	ARG	Sidechain	5
1	A	31	ARG	Sidechain	4

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	16	ARG	Sidechain	2
1	A	55	ARG	Sidechain	2
1	A	29	TYR	Sidechain	1

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	744	748	748	2±2
All	All	14880	14960	14960	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:40:ALA:HB1	1:A:45:LEU:HD11	0.68	1.65	5	2
1:A:40:ALA:HB1	1:A:45:LEU:HD21	0.66	1.67	12	5
1:A:21:ILE:HG23	1:A:40:ALA:HB3	0.58	1.74	19	9
1:A:38:ASP:HB3	1:A:54:LEU:HD21	0.58	1.76	18	1
1:A:38:ASP:CB	1:A:54:LEU:HD21	0.54	2.32	18	3
1:A:40:ALA:HB1	1:A:45:LEU:CD1	0.53	2.34	15	1
1:A:33:HIS:CG	1:A:34:ILE:H	0.51	2.24	5	2
1:A:21:ILE:HD11	1:A:54:LEU:HD22	0.51	1.82	16	2
1:A:40:ALA:HB1	1:A:45:LEU:CD2	0.49	2.37	12	1
1:A:7:PRO:HA	1:A:88:LEU:HD11	0.47	1.84	10	1
1:A:38:ASP:HB2	1:A:54:LEU:HD21	0.46	1.86	16	1
1:A:2:LEU:HD12	1:A:2:LEU:H	0.46	1.71	10	1
1:A:81:ALA:HB1	1:A:82:PRO:HA	0.45	1.89	18	1
1:A:75:LYS:H	1:A:75:LYS:CD	0.45	2.25	20	1
1:A:89:GLU:HG3	1:A:90:ASP:H	0.42	1.74	4	1
1:A:20:LEU:C	1:A:21:ILE:HD12	0.42	2.35	16	2
1:A:21:ILE:CD1	1:A:54:LEU:HD22	0.41	2.45	16	1
1:A:88:LEU:HD13	1:A:89:GLU:N	0.40	2.31	15	1
1:A:14:ILE:HG21	1:A:36:GLU:HB3	0.40	1.94	13	1
1:A:88:LEU:HD13	1:A:89:GLU:H	0.40	1.75	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:HIS:CG	1:A:34:ILE:N	0.40	2.89	5	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/108 (90%)	81±3 (84±3%)	13±3 (13±3%)	3±1 (3±1%)	8	38
All	All	1940/2160 (90%)	1621 (84%)	253 (13%)	66 (3%)	8	38

All 14 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	39	LEU	14
1	A	24	ARG	13
1	A	17	GLY	6
1	A	55	ARG	6
1	A	2	LEU	6
1	A	64	GLN	5
1	A	83	ALA	5
1	A	82	PRO	2
1	A	89	GLU	2
1	A	23	ILE	2
1	A	90	ASP	2
1	A	31	ARG	1
1	A	71	ASN	1
1	A	40	ALA	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	77/85 (91%)	64±3 (83±3%)	13±3 (17±3%)	6 42
All	All	1540/1700 (91%)	1279 (83%)	261 (17%)	6 42

All 42 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	5	ILE	20
1	A	92	ILE	20
1	A	42	LEU	20
1	A	85	ILE	20
1	A	75	LYS	19
1	A	62	HIS	15
1	A	102	VAL	11
1	A	9	ASP	10
1	A	11	GLN	10
1	A	88	LEU	7
1	A	22	ASP	7
1	A	56	HIS	7
1	A	25	ASP	6
1	A	19	LYS	6
1	A	24	ARG	6
1	A	59	ILE	5
1	A	55	ARG	5
1	A	45	LEU	5
1	A	74	ASP	4
1	A	4	THR	4
1	A	29	TYR	4
1	A	84	GLU	4
1	A	48	SER	4
1	A	27	ASP	4
1	A	64	GLN	4
1	A	70	SER	3
1	A	32	GLU	3
1	A	38	ASP	3
1	A	46	GLU	3
1	A	33	HIS	3
1	A	90	ASP	3
1	A	71	ASN	3
1	A	89	GLU	2
1	A	6	SER	2
1	A	53	LYS	2
1	A	97	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	43	SER	1
1	A	8	HIS	1
1	A	87	LEU	1
1	A	2	LEU	1
1	A	28	GLU	1
1	A	30	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

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

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: 5lao_cs.cif

Chemical shift list name: *Rhoda_SNOC_shifted_chemshifts.txt*

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	964
Number of shifts mapped to atoms	0
Number of unparsed shifts	964
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Entity instance (chain) must be specified. All 964 occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	21	ILE	H	9.314	0.000	?
2	?	21	ILE	CA	59.589	0.000	?
3	?	21	ILE	HA	4.638	0.004	?
4	?	21	ILE	CB	39.463	0.000	?
5	?	93	ASP	H	9.105	0.005	?
6	?	93	ASP	CA	57.166	0.000	?
7	?	93	ASP	HA	4.488	0.004	?
8	?	93	ASP	CB	38.764	0.000	?
9	?	93	ASP	HB2	3.025	0.000	?
10	?	93	ASP	HB3	2.676	0.004	?
11	?	60	ILE	H	9.016	0.005	?
12	?	60	ILE	CA	57.896	0.071	?
13	?	60	ILE	HA	4.976	0.001	?
14	?	60	ILE	CB	39.696	0.000	?
15	?	103	ALA	H	8.958	0.003	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	?	103	ALA	CA	49.945	0.000	?
17	?	103	ALA	HA	4.526	0.000	?
18	?	103	ALA	CB	18.732	0.000	?
19	?	103	ALA	HB1	0.646	0.001	?
20	?	103	ALA	HB2	0.646	0.001	?
21	?	103	ALA	HB3	0.646	0.001	?
22	?	62	HIS	H	9.258	0.000	?
23	?	62	HIS	CA	53.672	0.000	?
24	?	62	HIS	HA	5.800	0.000	?
25	?	62	HIS	CB	35.673	0.000	?
26	?	62	HIS	HB2	3.172	0.000	?
27	?	62	HIS	HB3	2.725	0.000	?
28	?	38	ASP	H	8.969	0.000	?
29	?	38	ASP	CA	52.614	0.000	?
30	?	38	ASP	HA	4.845	0.004	?
31	?	38	ASP	CB	44.402	0.009	?
32	?	38	ASP	HB2	2.395	0.000	?
33	?	38	ASP	HB3	2.331	0.004	?
34	?	61	PHE	H	8.942	0.000	?
35	?	61	PHE	CA	56.467	0.000	?
36	?	61	PHE	HA	5.779	0.000	?
37	?	61	PHE	CB	42.731	0.033	?
38	?	61	PHE	HB2	2.844	0.003	?
39	?	61	PHE	HB3	2.749	0.000	?
40	?	61	PHE	CE1	129.971	0.000	?
41	?	20	LEU	H	8.765	0.000	?
42	?	20	LEU	CA	52.740	0.000	?
43	?	20	LEU	HA	5.110	0.000	?
44	?	20	LEU	CB	43.772	0.117	?
45	?	20	LEU	HB2	1.648	0.000	?
46	?	20	LEU	HB3	0.992	0.004	?
47	?	20	LEU	CG	22.925	0.000	?
48	?	20	LEU	CD2	26.419	0.000	?
49	?	52	ALA	H	8.590	0.000	?
50	?	52	ALA	CA	55.070	0.000	?
51	?	52	ALA	HA	3.871	0.000	?
52	?	52	ALA	CB	17.800	0.000	?
53	?	52	ALA	HB1	1.409	0.000	?
54	?	52	ALA	HB2	1.409	0.000	?
55	?	52	ALA	HB3	1.409	0.000	?
56	?	83	ALA	H	8.500	0.000	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	?	83	ALA	CA	52.973	0.000	?
58	?	83	ALA	HA	4.132	0.004	?
59	?	83	ALA	CB	19.198	0.000	?
60	?	83	ALA	HB1	1.350	0.000	?
61	?	83	ALA	HB2	1.350	0.000	?
62	?	83	ALA	HB3	1.350	0.000	?
63	?	22	ASP	H	8.661	0.000	?
64	?	22	ASP	CA	51.435	0.000	?
65	?	22	ASP	HA	3.839	0.007	?
66	?	22	ASP	CB	42.188	0.114	?
67	?	22	ASP	HB2	2.751	0.000	?
68	?	22	ASP	HB3	2.460	0.000	?
69	?	40	ALA	H	8.672	0.006	?
70	?	40	ALA	CA	48.784	0.000	?
71	?	40	ALA	HA	4.440	0.001	?
72	?	40	ALA	CB	18.222	0.099	?
73	?	40	ALA	HB1	0.999	0.002	?
74	?	40	ALA	HB2	0.999	0.002	?
75	?	40	ALA	HB3	0.999	0.002	?
76	?	59	ILE	H	8.706	0.005	?
77	?	59	ILE	CA	58.869	0.000	?
78	?	59	ILE	HA	4.530	0.005	?
79	?	59	ILE	CB	42.491	0.000	?
80	?	59	ILE	HD11	-0.068	0.001	?
81	?	59	ILE	HD12	-0.068	0.001	?
82	?	59	ILE	HD13	-0.068	0.001	?
83	?	59	ILE	CD1	16.635	0.000	?
84	?	14	ILE	H	8.747	0.000	?
85	?	14	ILE	CA	64.387	0.000	?
86	?	14	ILE	HA	3.911	0.000	?
87	?	14	ILE	CB	38.115	0.000	?
88	?	14	ILE	CD1	15.005	0.000	?
89	?	26	ALA	H	8.752	0.001	?
90	?	26	ALA	CA	55.303	0.000	?
91	?	26	ALA	HA	3.929	0.000	?
92	?	26	ALA	CB	18.033	0.000	?
93	?	26	ALA	HB1	1.364	0.007	?
94	?	26	ALA	HB2	1.364	0.007	?
95	?	26	ALA	HB3	1.364	0.007	?
96	?	50	LEU	H	8.604	0.002	?
97	?	50	LEU	CA	51.985	0.000	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	?	50	LEU	HA	4.239	0.000	?
99	?	50	LEU	CB	42.702	0.043	?
100	?	50	LEU	HB2	1.641	0.000	?
101	?	50	LEU	HB3	1.240	0.000	?
102	?	50	LEU	HG	1.549	0.004	?
103	?	96	LYS	H	8.649	0.002	?
104	?	96	LYS	CA	59.091	0.000	?
105	?	96	LYS	HA	4.084	0.003	?
106	?	96	LYS	CB	31.623	0.000	?
107	?	96	LYS	HB2	1.902	0.005	?
108	?	46	GLU	H	8.548	0.000	?
109	?	46	GLU	CA	58.797	0.000	?
110	?	46	GLU	HA	3.810	0.000	?
111	?	46	GLU	CB	29.913	0.000	?
112	?	46	GLU	HB2	2.022	0.000	?
113	?	46	GLU	HB3	1.939	0.000	?
114	?	36	GLU	H	8.598	0.000	?
115	?	36	GLU	CA	57.861	0.000	?
116	?	36	GLU	HA	4.081	0.000	?
117	?	36	GLU	CB	28.282	0.000	?
118	?	36	GLU	HB2	2.158	0.000	?
119	?	36	GLU	HB3	1.923	0.000	?
120	?	36	GLU	CG	36.435	0.000	?
121	?	36	GLU	HG2	2.435	0.000	?
122	?	36	GLU	HG3	2.273	0.005	?
123	?	27	ASP	H	8.699	0.000	?
124	?	27	ASP	CA	56.700	0.000	?
125	?	27	ASP	HA	4.311	0.000	?
126	?	27	ASP	CB	39.463	0.000	?
127	?	27	ASP	HB2	2.664	0.000	?
128	?	27	ASP	HB3	2.598	0.005	?
129	?	66	GLY	H	8.879	0.156	?
130	?	66	GLY	CA	44.934	0.000	?
131	?	48	SER	H	8.598	0.000	?
132	?	48	SER	CA	57.956	0.000	?
133	?	48	SER	HA	4.641	0.004	?
134	?	48	SER	CB	64.387	0.000	?
135	?	43	SER	H	8.506	0.001	?
136	?	43	SER	CA	60.660	0.000	?
137	?	43	SER	HA	4.136	0.000	?
138	?	43	SER	CB	61.387	0.010	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	?	53	LYS	H	8.342	0.004	?
140	?	53	LYS	CA	57.399	0.000	?
141	?	53	LYS	HA	4.152	0.004	?
142	?	53	LYS	HB2	1.850	0.000	?
143	?	53	LYS	HB3	1.744	0.005	?
144	?	74	ASP	H	8.349	0.000	?
145	?	74	ASP	CA	56.700	0.000	?
146	?	74	ASP	HA	4.220	0.005	?
147	?	74	ASP	CB	39.463	0.000	?
148	?	74	ASP	HB2	2.625	0.000	?
149	?	74	ASP	HB3	2.533	0.004	?
150	?	99	GLY	H	7.891	0.003	?
151	?	99	GLY	CA	44.246	0.000	?
152	?	17	GLY	H	7.762	0.000	?
153	?	17	GLY	CA	44.732	0.040	?
154	?	49	GLY	H	7.843	0.000	?
155	?	49	GLY	CA	43.892	0.002	?
156	?	102	VAL	H	7.994	0.001	?
157	?	102	VAL	CA	59.003	0.060	?
158	?	102	VAL	HA	4.593	0.006	?
159	?	102	VAL	CB	35.503	0.000	?
160	?	11	GLN	H	8.343	0.003	?
161	?	11	GLN	CA	59.728	0.000	?
162	?	11	GLN	HA	3.990	0.002	?
163	?	11	GLN	CB	28.282	0.000	?
164	?	11	GLN	HB2	2.112	0.000	?
165	?	11	GLN	HB3	2.002	0.000	?
166	?	11	GLN	CG	34.093	0.092	?
167	?	33	HIS	H	8.286	0.000	?
168	?	33	HIS	CA	53.766	0.000	?
169	?	33	HIS	HA	4.593	0.006	?
170	?	33	HIS	CB	30.146	0.000	?
171	?	33	HIS	HB2	3.007	0.000	?
172	?	33	HIS	HB3	2.733	0.000	?
173	?	58	GLN	H	8.349	0.000	?
174	?	58	GLN	CA	54.910	0.000	?
175	?	58	GLN	HA	5.433	0.000	?
176	?	58	GLN	HB2	2.155	0.004	?
177	?	58	GLN	HB3	1.739	0.004	?
178	?	58	GLN	CG	34.338	0.000	?
179	?	58	GLN	HG2	2.500	0.006	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	?	58	GLN	HG3	2.369	0.000	?
181	?	104	VAL	H	8.243	0.000	?
182	?	104	VAL	CA	59.495	0.000	?
183	?	104	VAL	HA	4.557	0.003	?
184	?	104	VAL	CB	33.884	0.000	?
185	?	30	LEU	H	8.252	0.003	?
186	?	30	LEU	CA	56.700	0.000	?
187	?	30	LEU	HA	3.914	0.002	?
188	?	30	LEU	CB	41.241	0.039	?
189	?	30	LEU	HB2	1.798	0.000	?
190	?	30	LEU	HB3	1.653	0.000	?
191	?	30	LEU	CG	26.652	0.000	?
192	?	79	ILE	H	8.152	0.000	?
193	?	79	ILE	CA	63.921	0.000	?
194	?	79	ILE	HA	3.787	0.000	?
195	?	79	ILE	CB	38.310	0.037	?
196	?	79	ILE	HD11	0.571	0.003	?
197	?	79	ILE	HD12	0.571	0.003	?
198	?	79	ILE	HD13	0.571	0.003	?
199	?	79	ILE	CD1	13.840	0.000	?
200	?	3	THR	H	7.947	0.000	?
201	?	3	THR	CA	61.391	0.000	?
202	?	3	THR	HA	4.465	0.004	?
203	?	3	THR	CB	69.745	0.000	?
204	?	71	ASN	H	7.887	0.000	?
205	?	71	ASN	CA	54.596	0.000	?
206	?	71	ASN	HA	4.179	0.004	?
207	?	71	ASN	CB	38.391	0.000	?
208	?	23	ILE	H	7.832	0.003	?
209	?	23	ILE	CA	59.728	0.000	?
210	?	23	ILE	HA	5.262	0.000	?
211	?	23	ILE	CB	37.327	0.000	?
212	?	54	LEU	H	7.793	0.000	?
213	?	54	LEU	CA	53.439	0.000	?
214	?	54	LEU	HA	4.292	0.000	?
215	?	54	LEU	CB	41.047	0.203	?
216	?	54	LEU	HB2	1.704	0.000	?
217	?	54	LEU	HB3	1.541	0.000	?
218	?	80	ALA	H	7.842	0.000	?
219	?	80	ALA	CA	51.110	0.000	?
220	?	80	ALA	HA	4.443	0.000	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	?	80	ALA	CB	19.681	0.053	?
222	?	80	ALA	HB1	1.506	0.002	?
223	?	80	ALA	HB2	1.506	0.002	?
224	?	80	ALA	HB3	1.506	0.002	?
225	?	76	LEU	H	8.090	0.002	?
226	?	76	LEU	CA	57.166	0.000	?
227	?	76	LEU	HA	3.581	0.001	?
228	?	76	LEU	CB	39.696	0.000	?
229	?	76	LEU	HB2	1.547	0.000	?
230	?	76	LEU	HB3	0.707	0.001	?
231	?	76	LEU	CG	25.720	0.000	?
232	?	76	LEU	HG	1.349	0.000	?
233	?	76	LEU	HD11	0.282	0.001	?
234	?	76	LEU	HD12	0.282	0.001	?
235	?	76	LEU	HD13	0.282	0.001	?
236	?	76	LEU	HD21	-0.194	0.000	?
237	?	76	LEU	HD22	-0.194	0.000	?
238	?	76	LEU	HD23	-0.194	0.000	?
239	?	76	LEU	CD1	25.021	0.000	?
240	?	76	LEU	CD2	20.362	0.000	?
241	?	77	ALA	H	8.042	0.004	?
242	?	77	ALA	CA	54.604	0.000	?
243	?	77	ALA	HA	3.978	0.005	?
244	?	77	ALA	CB	17.353	0.000	?
245	?	77	ALA	HB1	1.424	0.000	?
246	?	77	ALA	HB2	1.424	0.000	?
247	?	77	ALA	HB3	1.424	0.000	?
248	?	2	LEU	H	7.890	0.000	?
249	?	2	LEU	CA	53.827	0.000	?
250	?	2	LEU	HA	4.474	0.004	?
251	?	2	LEU	CB	42.229	0.000	?
252	?	2	LEU	HD11	0.790	0.003	?
253	?	2	LEU	HD12	0.790	0.003	?
254	?	2	LEU	HD13	0.790	0.003	?
255	?	2	LEU	CD1	22.925	0.000	?
256	?	45	LEU	H	8.040	0.000	?
257	?	45	LEU	CA	57.127	0.104	?
258	?	45	LEU	HA	3.822	0.001	?
259	?	45	LEU	CB	41.094	0.000	?
260	?	45	LEU	HB2	1.994	0.000	?
261	?	45	LEU	HB3	1.171	0.000	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	?	84	GLU	H	8.148	0.000	?
263	?	84	GLU	CA	55.937	0.000	?
264	?	84	GLU	HA	4.214	0.000	?
265	?	84	GLU	CB	30.213	0.000	?
266	?	84	GLU	HB2	2.130	0.005	?
267	?	84	GLU	HB3	1.966	0.005	?
268	?	84	GLU	CG	36.202	0.000	?
269	?	92	ILE	H	8.242	0.003	?
270	?	92	ILE	CA	63.222	0.000	?
271	?	92	ILE	HA	3.870	0.000	?
272	?	92	ILE	CB	38.065	0.000	?
273	?	37	ALA	H	8.144	0.000	?
274	?	37	ALA	CA	51.808	0.001	?
275	?	37	ALA	HA	4.464	0.000	?
276	?	37	ALA	CB	20.595	0.000	?
277	?	37	ALA	HB1	1.575	0.000	?
278	?	37	ALA	HB2	1.575	0.000	?
279	?	37	ALA	HB3	1.575	0.000	?
280	?	1	ALA	H	8.144	0.003	?
281	?	1	ALA	CA	51.808	0.104	?
282	?	1	ALA	HA	4.245	0.002	?
283	?	1	ALA	CB	18.643	0.000	?
284	?	1	ALA	HB1	1.327	0.000	?
285	?	1	ALA	HB2	1.327	0.000	?
286	?	1	ALA	HB3	1.327	0.000	?
287	?	105	ASN	H	8.145	0.001	?
288	?	105	ASN	CA	53.200	0.000	?
289	?	105	ASN	HA	4.726	0.000	?
290	?	105	ASN	CB	38.764	0.000	?
291	?	88	LEU	H	8.248	0.003	?
292	?	88	LEU	CA	54.331	0.000	?
293	?	88	LEU	HA	4.444	0.000	?
294	?	88	LEU	CB	42.957	0.000	?
295	?	88	LEU	HB2	2.019	0.000	?
296	?	88	LEU	HB3	0.992	0.000	?
297	?	88	LEU	CG	25.254	0.000	?
298	?	24	ARG	H	8.172	0.000	?
299	?	24	ARG	CA	55.943	0.000	?
300	?	24	ARG	HA	4.192	0.005	?
301	?	24	ARG	CB	30.612	0.000	?
302	?	24	ARG	HB2	2.152	0.000	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	?	24	ARG	HB3	1.955	0.000	?
304	?	24	ARG	CG	26.399	0.079	?
305	?	24	ARG	HG2	1.887	0.003	?
306	?	24	ARG	HG3	1.803	0.000	?
307	?	18	ALA	H	7.989	0.000	?
308	?	18	ALA	CA	52.270	0.000	?
309	?	15	ALA	H	7.776	0.006	?
310	?	15	ALA	CA	54.138	0.000	?
311	?	15	ALA	HA	4.169	0.004	?
312	?	15	ALA	CB	17.040	0.000	?
313	?	15	ALA	HB1	1.510	0.006	?
314	?	15	ALA	HB2	1.510	0.006	?
315	?	15	ALA	HB3	1.510	0.006	?
316	?	97	LYS	H	8.233	0.000	?
317	?	97	LYS	CA	58.797	0.000	?
318	?	97	LYS	HA	4.032	0.001	?
319	?	97	LYS	CB	31.776	0.000	?
320	?	97	LYS	HB2	1.945	0.002	?
321	?	85	ILE	H	7.892	0.006	?
322	?	85	ILE	CA	58.564	0.000	?
323	?	85	ILE	HA	5.257	0.000	?
324	?	85	ILE	CB	40.162	0.000	?
325	?	9	ASP	H	7.633	0.000	?
326	?	9	ASP	CA	56.465	0.005	?
327	?	9	ASP	HA	4.339	0.000	?
328	?	9	ASP	CB	39.230	0.000	?
329	?	9	ASP	HB2	2.846	0.001	?
330	?	9	ASP	HB3	2.478	0.000	?
331	?	57	GLU	H	7.690	0.000	?
332	?	57	GLU	CA	58.871	0.000	?
333	?	57	GLU	HA	4.014	0.004	?
334	?	57	GLU	CB	29.447	0.000	?
335	?	57	GLU	HB2	2.029	0.001	?
336	?	57	GLU	HB3	1.874	0.010	?
337	?	57	GLU	CG	36.289	0.113	?
338	?	19	LYS	H	7.638	0.000	?
339	?	19	LYS	CA	52.274	0.000	?
340	?	19	LYS	HA	4.284	0.000	?
341	?	19	LYS	CB	32.856	0.000	?
342	?	19	LYS	HB2	1.597	0.004	?
343	?	19	LYS	HB3	1.411	0.003	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	?	19	LYS	CG	23.362	0.093	?
345	?	19	LYS	HG2	1.256	0.002	?
346	?	19	LYS	CD	27.101	0.000	?
347	?	13	LEU	H	7.577	0.003	?
348	?	13	LEU	CA	57.399	0.000	?
349	?	13	LEU	HA	3.869	0.000	?
350	?	13	LEU	CB	41.085	0.036	?
351	?	13	LEU	HB2	1.504	0.000	?
352	?	13	LEU	HB3	1.095	0.000	?
353	?	13	LEU	CG	26.372	0.114	?
354	?	29	TYR	H	7.537	0.003	?
355	?	29	TYR	HA	4.088	0.000	?
356	?	29	TYR	CB	38.997	0.000	?
357	?	98	ALA	H	7.484	0.000	?
358	?	98	ALA	CA	51.576	0.000	?
359	?	98	ALA	HA	4.250	0.000	?
360	?	98	ALA	CB	17.744	0.000	?
361	?	32	GLU	H	7.535	0.000	?
362	?	32	GLU	CA	55.769	0.000	?
363	?	32	GLU	HA	4.888	0.006	?
364	?	32	GLU	CB	31.698	0.000	?
365	?	32	GLU	HB2	2.042	0.004	?
366	?	32	GLU	HB3	1.957	0.004	?
367	?	32	GLU	CG	35.614	0.000	?
368	?	47	GLN	H	7.439	0.000	?
369	?	47	GLN	CA	57.399	0.000	?
370	?	47	GLN	HA	4.292	0.000	?
371	?	47	GLN	CB	29.447	0.000	?
372	?	47	GLN	HB2	2.148	0.000	?
373	?	47	GLN	HB3	2.106	0.000	?
374	?	47	GLN	CG	33.407	0.000	?
375	?	16	ARG	H	7.267	0.002	?
376	?	16	ARG	CA	55.536	0.000	?
377	?	16	ARG	HA	4.386	0.001	?
378	?	16	ARG	CB	29.990	0.140	?
379	?	16	ARG	HB2	2.151	0.005	?
380	?	16	ARG	HB3	1.815	0.005	?
381	?	72	ASN	H	7.280	0.000	?
382	?	72	ASN	CA	52.507	0.000	?
383	?	72	ASN	HA	5.128	0.000	?
384	?	72	ASN	CB	39.013	0.085	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	?	72	ASN	HB2	2.666	0.001	?
386	?	72	ASN	HB3	2.457	0.000	?
387	?	70	SER	H	7.385	0.012	?
388	?	70	SER	CA	61.391	0.000	?
389	?	70	SER	HA	4.010	0.005	?
390	?	70	SER	CB	65.442	0.034	?
391	?	70	SER	HB2	4.004	0.004	?
392	?	70	SER	HB3	3.937	0.008	?
393	?	55	ARG	H	6.978	0.003	?
394	?	55	ARG	CA	56.949	0.000	?
395	?	31	ARG	H	7.133	0.000	?
396	?	31	ARG	CA	59.030	0.000	?
397	?	31	ARG	HA	4.095	0.005	?
398	?	31	ARG	CB	30.347	0.051	?
399	?	31	ARG	HB2	1.946	0.005	?
400	?	31	ARG	CG	27.583	0.000	?
401	?	31	ARG	HG2	1.841	0.004	?
402	?	31	ARG	HG3	1.612	0.004	?
403	?	31	ARG	CD	42.957	0.000	?
404	?	31	ARG	HD2	3.251	0.001	?
405	?	12	GLU	H	7.234	0.000	?
406	?	12	GLU	CA	58.797	0.000	?
407	?	12	GLU	HA	4.033	0.000	?
408	?	12	GLU	CB	28.748	0.000	?
409	?	12	GLU	HB2	2.059	0.005	?
410	?	12	GLU	HB3	1.994	0.005	?
411	?	12	GLU	CG	34.106	0.000	?
412	?	12	GLU	HG2	2.342	0.000	?
413	?	12	GLU	HG3	2.229	0.000	?
414	?	78	ALA	H	7.379	0.000	?
415	?	78	ALA	CA	54.049	0.000	?
416	?	78	ALA	HA	4.152	0.004	?
417	?	78	ALA	CB	17.520	0.000	?
418	?	28	GLU	H	7.433	0.004	?
419	?	28	GLU	CA	58.328	0.050	?
420	?	28	GLU	HA	4.081	0.000	?
421	?	28	GLU	CB	28.981	0.000	?
422	?	28	GLU	HB2	2.326	0.000	?
423	?	28	GLU	HB3	2.183	0.000	?
424	?	28	GLU	CG	36.435	0.000	?
425	?	56	HIS	H	7.289	0.000	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
426	?	56	HIS	CA	54.879	0.099	?
427	?	56	HIS	HA	4.599	0.004	?
428	?	56	HIS	CB	32.941	0.000	?
429	?	56	HIS	HB2	3.033	0.000	?
430	?	56	HIS	HB3	2.861	0.000	?
431	?	81	ALA	H	7.231	0.002	?
432	?	81	ALA	CA	51.809	0.000	?
433	?	81	ALA	HA	4.438	0.004	?
434	?	81	ALA	CB	16.868	0.000	?
435	?	81	ALA	HB1	1.443	0.006	?
436	?	81	ALA	HB2	1.443	0.006	?
437	?	81	ALA	HB3	1.443	0.006	?
438	?	44	VAL	H	7.182	0.001	?
439	?	44	VAL	CA	64.924	0.000	?
440	?	44	VAL	HA	3.827	0.000	?
441	?	44	VAL	CB	31.310	0.000	?
442	?	73	ALA	H	7.224	0.003	?
443	?	73	ALA	CA	56.467	0.000	?
444	?	73	ALA	HA	3.736	0.000	?
445	?	73	ALA	HB1	1.468	0.000	?
446	?	73	ALA	HB2	1.468	0.000	?
447	?	73	ALA	HB3	1.468	0.000	?
448	?	73	ALA	CB	18.732	0.000	?
449	?	100	LEU	H	6.971	0.000	?
450	?	100	LEU	CA	52.748	0.023	?
451	?	100	LEU	HA	4.278	0.002	?
452	?	100	LEU	CB	36.657	0.028	?
453	?	100	LEU	HB2	0.294	0.000	?
454	?	25	ASP	H	7.690	0.000	?
455	?	25	ASP	CA	53.870	0.000	?
456	?	25	ASP	HA	4.610	0.005	?
457	?	25	ASP	CB	41.559	0.000	?
458	?	4	THR	H	8.516	0.003	?
459	?	4	THR	CA	61.595	0.000	?
460	?	4	THR	HA	5.255	0.005	?
461	?	4	THR	CB	69.027	0.000	?
462	?	8	HIS	H	8.111	0.002	?
463	?	8	HIS	HA	4.052	0.000	?
464	?	8	HIS	CB	28.737	0.037	?
465	?	8	HIS	HB2	3.026	0.004	?
466	?	8	HIS	HB3	2.967	0.004	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
467	?	75	LYS	H	7.638	0.000	?
468	?	75	LYS	CA	58.128	0.084	?
469	?	75	LYS	HA	4.039	0.001	?
470	?	75	LYS	CB	31.660	0.000	?
471	?	75	LYS	HB2	1.807	0.001	?
472	?	75	LYS	HB3	1.654	0.004	?
473	?	75	LYS	CG	24.089	0.000	?
474	?	75	LYS	HG2	1.447	0.004	?
475	?	75	LYS	HG3	1.346	0.001	?
476	?	75	LYS	CD	28.748	0.000	?
477	?	75	LYS	HE2	2.922	0.001	?
478	?	34	ILE	H	9.971	0.000	?
479	?	34	ILE	CA	60.194	0.000	?
480	?	34	ILE	HA	3.964	0.001	?
481	?	34	ILE	CB	38.298	0.000	?
482	?	34	ILE	CD1	10.993	0.000	?
483	?	42	LEU	H	8.298	0.009	?
484	?	42	LEU	CA	58.098	0.000	?
485	?	42	LEU	HA	3.880	0.000	?
486	?	42	LEU	CB	41.301	0.103	?
487	?	42	LEU	HB2	1.880	0.001	?
488	?	42	LEU	HB3	1.408	0.000	?
489	?	42	LEU	CG	25.953	0.000	?
490	?	86	PHE	H	9.005	0.006	?
491	?	86	PHE	CA	54.509	0.000	?
492	?	86	PHE	HA	5.384	0.000	?
493	?	86	PHE	CB	42.860	0.050	?
494	?	86	PHE	CD1	131.705	0.000	?
495	?	95	TRP	H	7.897	0.000	?
496	?	95	TRP	CA	61.126	0.000	?
497	?	69	THR	H	10.170	0.008	?
498	?	69	THR	CA	63.455	0.000	?
499	?	69	THR	HA	3.731	0.002	?
500	?	69	THR	CB	66.484	0.000	?
501	?	87	LEU	H	8.804	0.002	?
502	?	87	LEU	CA	52.042	0.000	?
503	?	87	LEU	HA	5.312	0.000	?
504	?	87	LEU	CB	42.712	0.052	?
505	?	87	LEU	HB2	1.831	0.003	?
506	?	87	LEU	HB3	1.458	0.000	?
507	?	87	LEU	CG	26.419	0.000	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
508	?	10	ALA	H	8.818	0.007	?
509	?	10	ALA	CA	54.331	0.000	?
510	?	10	ALA	HA	3.757	0.000	?
511	?	10	ALA	HB1	1.506	0.006	?
512	?	10	ALA	HB2	1.506	0.006	?
513	?	10	ALA	HB3	1.506	0.006	?
514	?	10	ALA	CB	17.549	0.000	?
515	?	18	ALA	CB	18.933	0.101	?
516	?	95	TRP	CB	28.981	0.000	?
517	?	55	ARG	CB	29.214	0.000	?
518	?	39	LEU	CA	54.138	0.000	?
519	?	39	LEU	H	8.180	0.000	?
520	?	65	ALA	CA	50.877	0.000	?
521	?	67	LYS	CA	58.400	0.000	?
522	?	67	LYS	H	8.201	0.000	?
523	?	91	GLY	CA	46.263	0.000	?
524	?	91	GLY	H	7.693	0.002	?
525	?	2	LEU	HB2	1.544	0.004	?
526	?	2	LEU	HB3	1.436	0.004	?
527	?	2	LEU	CG	26.419	0.000	?
528	?	2	LEU	HG	1.583	0.004	?
529	?	2	LEU	HD21	0.712	0.002	?
530	?	2	LEU	HD22	0.712	0.002	?
531	?	2	LEU	HD23	0.712	0.002	?
532	?	2	LEU	CD2	22.925	0.000	?
533	?	3	THR	HB	4.098	0.000	?
534	?	3	THR	HG21	1.285	0.000	?
535	?	3	THR	HG22	1.285	0.000	?
536	?	3	THR	HG23	1.285	0.000	?
537	?	3	THR	CG2	21.294	0.000	?
538	?	4	THR	HB	4.134	0.003	?
539	?	4	THR	HG21	1.209	0.004	?
540	?	4	THR	HG22	1.209	0.004	?
541	?	4	THR	HG23	1.209	0.004	?
542	?	4	THR	CG2	21.049	0.000	?
543	?	11	GLN	HG2	2.354	0.003	?
544	?	11	GLN	HG3	2.220	0.000	?
545	?	11	GLN	HE21	7.485	0.000	?
546	?	11	GLN	HE22	6.524	0.003	?
547	?	13	LEU	HG	1.400	0.001	?
548	?	13	LEU	HD11	0.354	0.001	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
549	?	13	LEU	HD12	0.354	0.001	?
550	?	13	LEU	HD13	0.354	0.001	?
551	?	13	LEU	HD21	0.085	0.001	?
552	?	13	LEU	HD22	0.085	0.001	?
553	?	13	LEU	HD23	0.085	0.001	?
554	?	13	LEU	CD1	22.426	0.098	?
555	?	13	LEU	CD2	24.089	0.000	?
556	?	14	ILE	HB	1.795	0.004	?
557	?	14	ILE	HG21	0.884	0.000	?
558	?	14	ILE	HG22	0.884	0.000	?
559	?	14	ILE	HG23	0.884	0.000	?
560	?	14	ILE	CG2	16.402	0.000	?
561	?	14	ILE	CG1	28.282	0.000	?
562	?	14	ILE	HG12	1.572	0.000	?
563	?	14	ILE	HD11	0.747	0.004	?
564	?	14	ILE	HD12	0.747	0.004	?
565	?	14	ILE	HD13	0.747	0.004	?
566	?	16	ARG	CG	27.117	0.000	?
567	?	16	ARG	HG2	1.807	0.005	?
568	?	16	ARG	HG3	1.680	0.005	?
569	?	16	ARG	CD	42.648	0.000	?
570	?	16	ARG	HD2	3.164	0.004	?
571	?	16	ARG	HD3	3.119	0.006	?
572	?	17	GLY	HA2	4.492	0.005	?
573	?	18	ALA	HA	4.227	0.004	?
574	?	18	ALA	HB1	0.883	0.001	?
575	?	18	ALA	HB2	0.883	0.001	?
576	?	18	ALA	HB3	0.883	0.001	?
577	?	19	LYS	HD2	1.543	0.004	?
578	?	19	LYS	CE	41.220	0.000	?
579	?	19	LYS	HE2	2.803	0.004	?
580	?	19	LYS	HE3	2.663	0.005	?
581	?	20	LEU	HG	0.622	0.002	?
582	?	20	LEU	HD11	1.281	0.006	?
583	?	20	LEU	HD12	1.281	0.006	?
584	?	20	LEU	HD13	1.281	0.006	?
585	?	20	LEU	HD21	0.365	0.000	?
586	?	20	LEU	HD22	0.365	0.000	?
587	?	20	LEU	HD23	0.365	0.000	?
588	?	20	LEU	CD1	26.419	0.000	?
589	?	21	ILE	HB	1.611	0.002	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
590	?	21	ILE	HG21	0.826	0.000	?
591	?	21	ILE	HG22	0.826	0.000	?
592	?	21	ILE	HG23	0.826	0.000	?
593	?	21	ILE	CG2	18.033	0.000	?
594	?	21	ILE	CG1	26.885	0.000	?
595	?	21	ILE	HG12	1.240	0.000	?
596	?	21	ILE	HG13	0.796	0.002	?
597	?	21	ILE	HD11	0.652	0.003	?
598	?	21	ILE	HD12	0.652	0.003	?
599	?	21	ILE	HD13	0.652	0.003	?
600	?	21	ILE	CD1	13.823	0.076	?
601	?	23	ILE	HB	2.096	0.000	?
602	?	23	ILE	HG21	1.002	0.001	?
603	?	23	ILE	HG22	1.002	0.001	?
604	?	23	ILE	HG23	1.002	0.001	?
605	?	23	ILE	CG2	18.039	0.067	?
606	?	23	ILE	CG1	27.094	4.822	?
607	?	23	ILE	HG12	1.152	0.019	?
608	?	23	ILE	HG13	1.108	0.005	?
609	?	23	ILE	HD11	0.647	0.000	?
610	?	23	ILE	HD12	0.647	0.000	?
611	?	23	ILE	HD13	0.647	0.000	?
612	?	23	ILE	CD1	14.772	0.000	?
613	?	24	ARG	HE	9.063	0.000	?
614	?	25	ASP	HB2	2.880	0.000	?
615	?	25	ASP	HB3	2.664	0.000	?
616	?	28	GLU	HG2	2.218	0.004	?
617	?	29	TYR	HB2	2.926	0.002	?
618	?	29	TYR	HB3	2.780	0.000	?
619	?	30	LEU	HG	1.762	0.000	?
620	?	30	LEU	HD11	0.899	0.001	?
621	?	30	LEU	HD12	0.899	0.001	?
622	?	30	LEU	HD13	0.899	0.001	?
623	?	30	LEU	HD21	0.862	0.004	?
624	?	30	LEU	HD22	0.862	0.004	?
625	?	30	LEU	HD23	0.862	0.004	?
626	?	30	LEU	CD1	23.304	0.000	?
627	?	30	LEU	CD2	23.344	0.105	?
628	?	32	GLU	HG2	1.916	0.006	?
629	?	32	GLU	HG3	1.842	0.004	?
630	?	34	ILE	HB	1.156	0.003	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
631	?	34	ILE	HG21	0.135	0.001	?
632	?	34	ILE	HG22	0.135	0.001	?
633	?	34	ILE	HG23	0.135	0.001	?
634	?	34	ILE	CG2	16.402	0.000	?
635	?	34	ILE	CG1	27.816	0.000	?
636	?	34	ILE	HG12	0.949	0.000	?
637	?	34	ILE	HG13	-0.561	0.000	?
638	?	39	LEU	HA	4.342	0.000	?
639	?	39	LEU	CB	41.553	0.021	?
640	?	39	LEU	HB2	1.123	0.000	?
641	?	39	LEU	CG	26.652	0.000	?
642	?	39	LEU	HG	1.026	0.000	?
643	?	39	LEU	HD11	0.483	0.005	?
644	?	39	LEU	HD12	0.483	0.005	?
645	?	39	LEU	HD13	0.483	0.005	?
646	?	39	LEU	HD21	0.424	0.000	?
647	?	39	LEU	HD22	0.424	0.000	?
648	?	39	LEU	HD23	0.424	0.000	?
649	?	39	LEU	CD1	21.061	0.000	?
650	?	39	LEU	CD2	25.254	0.000	?
651	?	42	LEU	HG	1.643	0.001	?
652	?	42	LEU	HD11	0.752	0.004	?
653	?	42	LEU	HD12	0.752	0.004	?
654	?	42	LEU	HD13	0.752	0.004	?
655	?	42	LEU	HD21	0.697	0.001	?
656	?	42	LEU	HD22	0.697	0.001	?
657	?	42	LEU	HD23	0.697	0.001	?
658	?	42	LEU	CD1	25.720	0.000	?
659	?	42	LEU	CD2	22.226	0.000	?
660	?	43	SER	HB2	3.874	0.000	?
661	?	43	SER	HB3	3.804	0.001	?
662	?	44	VAL	HB	2.181	0.000	?
663	?	44	VAL	HG11	0.963	0.000	?
664	?	44	VAL	HG12	0.963	0.000	?
665	?	44	VAL	HG13	0.963	0.000	?
666	?	44	VAL	HG21	0.901	0.000	?
667	?	44	VAL	HG22	0.901	0.000	?
668	?	44	VAL	HG23	0.901	0.000	?
669	?	44	VAL	CG1	21.760	0.000	?
670	?	44	VAL	CG2	19.897	0.000	?
671	?	45	LEU	CG	25.254	0.000	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
672	?	45	LEU	HG	1.601	0.000	?
673	?	45	LEU	HD11	0.767	0.002	?
674	?	45	LEU	HD12	0.767	0.002	?
675	?	45	LEU	HD13	0.767	0.002	?
676	?	45	LEU	CD1	25.720	0.000	?
677	?	46	GLU	CG	36.901	0.000	?
678	?	46	GLU	HG2	2.337	0.000	?
679	?	46	GLU	HG3	1.959	0.000	?
680	?	47	GLN	HG2	2.487	0.004	?
681	?	47	GLN	HG3	2.358	0.006	?
682	?	48	SER	HB2	3.913	0.000	?
683	?	48	SER	HB3	3.785	0.000	?
684	?	50	LEU	CG	27.101	0.000	?
685	?	50	LEU	HD11	0.842	0.000	?
686	?	50	LEU	HD12	0.842	0.000	?
687	?	50	LEU	HD13	0.842	0.000	?
688	?	50	LEU	HD21	0.695	0.005	?
689	?	50	LEU	HD22	0.695	0.005	?
690	?	50	LEU	HD23	0.695	0.005	?
691	?	50	LEU	CD1	24.788	0.000	?
692	?	50	LEU	CD2	24.075	0.000	?
693	?	53	LYS	CG	24.075	0.000	?
694	?	53	LYS	HG2	1.423	0.000	?
695	?	53	LYS	HG3	1.295	0.000	?
696	?	53	LYS	CD	28.554	0.087	?
697	?	53	LYS	HD2	1.641	0.005	?
698	?	53	LYS	CE	41.220	0.000	?
699	?	53	LYS	HE2	2.917	0.004	?
700	?	54	LEU	CG	26.885	0.000	?
701	?	54	LEU	HG	1.443	0.000	?
702	?	54	LEU	HD11	0.738	0.000	?
703	?	54	LEU	HD12	0.738	0.000	?
704	?	54	LEU	HD13	0.738	0.000	?
705	?	54	LEU	HD21	0.689	0.004	?
706	?	54	LEU	HD22	0.689	0.004	?
707	?	54	LEU	HD23	0.689	0.004	?
708	?	54	LEU	CD1	24.788	0.000	?
709	?	54	LEU	CD2	24.788	0.000	?
710	?	55	ARG	HA	3.984	0.000	?
711	?	55	ARG	HB2	1.761	0.006	?
712	?	55	ARG	HB3	1.692	0.005	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
713	?	55	ARG	CG	27.350	0.000	?
714	?	55	ARG	HG2	1.660	0.006	?
715	?	55	ARG	HG3	1.460	0.004	?
716	?	55	ARG	CD	43.190	0.000	?
717	?	55	ARG	HD2	3.189	0.005	?
718	?	55	ARG	HD3	3.120	0.005	?
719	?	57	GLU	HG2	2.208	0.042	?
720	?	59	ILE	HB	1.217	0.004	?
721	?	59	ILE	HG21	0.795	0.001	?
722	?	59	ILE	HG22	0.795	0.001	?
723	?	59	ILE	HG23	0.795	0.001	?
724	?	59	ILE	CG2	14.275	0.095	?
725	?	59	ILE	CG1	27.117	0.000	?
726	?	59	ILE	HG12	1.391	0.004	?
727	?	60	ILE	HB	1.651	0.000	?
728	?	60	ILE	HG21	0.629	0.000	?
729	?	60	ILE	HG22	0.629	0.000	?
730	?	60	ILE	HG23	0.629	0.000	?
731	?	60	ILE	CG2	17.577	0.000	?
732	?	60	ILE	CG1	26.186	0.000	?
733	?	60	ILE	HG12	1.427	0.007	?
734	?	60	ILE	HG13	0.672	0.000	?
735	?	60	ILE	HD11	0.614	0.005	?
736	?	60	ILE	HD12	0.614	0.005	?
737	?	60	ILE	HD13	0.614	0.005	?
738	?	60	ILE	CD1	15.238	0.000	?
739	?	61	PHE	HD1	7.088	0.001	?
740	?	61	PHE	HD2	7.088	0.001	?
741	?	61	PHE	HE1	6.983	0.005	?
742	?	61	PHE	HE2	6.983	0.005	?
743	?	61	PHE	CD1	131.938	0.000	?
744	?	61	PHE	CZ	127.708	0.098	?
745	?	61	PHE	HZ	6.890	0.003	?
746	?	65	ALA	HA	5.044	0.000	?
747	?	65	ALA	HB1	1.448	0.000	?
748	?	65	ALA	HB2	1.448	0.000	?
749	?	65	ALA	HB3	1.448	0.000	?
750	?	65	ALA	CB	19.896	0.000	?
751	?	66	GLY	HA2	4.488	0.005	?
752	?	67	LYS	HA	4.182	0.000	?
753	?	67	LYS	CE	40.861	0.000	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
754	?	67	LYS	HE2	2.618	0.003	?
755	?	69	THR	HB	4.170	0.000	?
756	?	69	THR	HG21	1.058	0.000	?
757	?	69	THR	HG22	1.058	0.000	?
758	?	69	THR	HG23	1.058	0.000	?
759	?	69	THR	CG2	23.391	0.000	?
760	?	71	ASN	HB2	2.832	0.004	?
761	?	71	ASN	HB3	2.780	0.004	?
762	?	72	ASN	HD21	8.045	0.002	?
763	?	75	LYS	HD2	1.629	0.001	?
764	?	75	LYS	CE	40.912	0.126	?
765	?	78	ALA	HB1	1.464	0.005	?
766	?	78	ALA	HB2	1.464	0.005	?
767	?	78	ALA	HB3	1.464	0.005	?
768	?	79	ILE	HB	1.807	0.000	?
769	?	79	ILE	HG21	0.896	0.000	?
770	?	79	ILE	HG22	0.896	0.000	?
771	?	79	ILE	HG23	0.896	0.000	?
772	?	79	ILE	CG2	17.520	0.000	?
773	?	79	ILE	CG1	28.968	0.053	?
774	?	79	ILE	HG12	1.791	0.007	?
775	?	79	ILE	HG13	1.041	0.004	?
776	?	85	ILE	HB	1.703	0.002	?
777	?	85	ILE	HG21	0.894	0.004	?
778	?	85	ILE	HG22	0.894	0.004	?
779	?	85	ILE	HG23	0.894	0.004	?
780	?	85	ILE	CG2	19.224	0.090	?
781	?	85	ILE	CG1	26.151	0.046	?
782	?	85	ILE	HG12	1.445	0.004	?
783	?	85	ILE	HD11	0.794	0.004	?
784	?	85	ILE	HD12	0.794	0.004	?
785	?	85	ILE	HD13	0.794	0.004	?
786	?	85	ILE	CD1	15.471	0.000	?
787	?	84	GLU	HG2	2.190	0.004	?
788	?	84	GLU	HG3	2.164	0.004	?
789	?	86	PHE	HB2	2.856	0.008	?
790	?	86	PHE	HB3	2.620	0.004	?
791	?	86	PHE	HD1	6.932	0.001	?
792	?	86	PHE	HD2	6.932	0.001	?
793	?	86	PHE	HE1	7.013	0.000	?
794	?	86	PHE	HE2	7.013	0.000	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
795	?	86	PHE	CE1	129.467	0.000	?
796	?	86	PHE	CZ	128.962	0.000	?
797	?	86	PHE	HZ	7.147	0.004	?
798	?	87	LEU	HG	1.611	0.000	?
799	?	87	LEU	HD11	0.846	0.000	?
800	?	87	LEU	HD12	0.846	0.000	?
801	?	87	LEU	HD13	0.846	0.000	?
802	?	87	LEU	HD21	0.790	0.000	?
803	?	87	LEU	HD22	0.790	0.000	?
804	?	87	LEU	HD23	0.790	0.000	?
805	?	87	LEU	CD1	23.623	0.000	?
806	?	87	LEU	CD2	24.788	0.000	?
807	?	88	LEU	HG	1.609	0.000	?
808	?	88	LEU	HD11	0.842	0.000	?
809	?	88	LEU	HD12	0.842	0.000	?
810	?	88	LEU	HD13	0.842	0.000	?
811	?	88	LEU	HD21	0.525	0.000	?
812	?	88	LEU	HD22	0.525	0.000	?
813	?	88	LEU	HD23	0.525	0.000	?
814	?	88	LEU	CD1	23.856	0.000	?
815	?	88	LEU	CD2	26.092	0.000	?
816	?	91	GLY	HA2	3.734	0.000	?
817	?	92	ILE	HB	1.549	0.000	?
818	?	92	ILE	HG21	1.196	0.000	?
819	?	92	ILE	HG22	1.196	0.000	?
820	?	92	ILE	HG23	1.196	0.000	?
821	?	92	ILE	CG2	16.635	0.000	?
822	?	92	ILE	CG1	29.447	0.000	?
823	?	92	ILE	HG12	1.264	0.001	?
824	?	92	ILE	HG13	1.139	0.007	?
825	?	92	ILE	HD11	0.758	0.004	?
826	?	92	ILE	HD12	0.758	0.004	?
827	?	92	ILE	HD13	0.758	0.004	?
828	?	92	ILE	CD1	14.330	0.062	?
829	?	95	TRP	HA	3.791	0.007	?
830	?	95	TRP	HB2	2.910	0.001	?
831	?	95	TRP	HB3	2.909	0.000	?
832	?	95	TRP	CD1	126.115	0.000	?
833	?	95	TRP	HD1	6.412	0.000	?
834	?	95	TRP	HE3	7.038	0.003	?
835	?	95	TRP	CZ2	115.633	0.000	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
836	?	95	TRP	HE1	10.467	0.008	?
837	?	95	TRP	HZ3	6.727	0.003	?
838	?	95	TRP	HZ2	7.435	0.001	?
839	?	95	TRP	HH2	6.854	0.000	?
840	?	96	LYS	HG2	1.758	0.001	?
841	?	96	LYS	HG3	1.500	0.005	?
842	?	98	ALA	HB1	1.267	0.000	?
843	?	98	ALA	HB2	1.267	0.000	?
844	?	98	ALA	HB3	1.267	0.000	?
845	?	99	GLY	HA2	3.988	0.006	?
846	?	100	LEU	CG	25.953	0.000	?
847	?	100	LEU	HG	0.684	0.000	?
848	?	100	LEU	HD11	0.261	0.033	?
849	?	100	LEU	HD12	0.261	0.033	?
850	?	100	LEU	HD13	0.261	0.033	?
851	?	100	LEU	CD1	21.294	0.000	?
852	?	100	LEU	CD2	23.608	0.068	?
853	?	102	VAL	HB	1.811	0.000	?
854	?	102	VAL	HG11	0.786	0.000	?
855	?	102	VAL	HG12	0.786	0.000	?
856	?	102	VAL	HG13	0.786	0.000	?
857	?	102	VAL	HG21	0.786	0.000	?
858	?	102	VAL	HG22	0.786	0.000	?
859	?	102	VAL	HG23	0.786	0.000	?
860	?	102	VAL	CG1	18.033	0.000	?
861	?	104	VAL	HB	2.047	0.000	?
862	?	104	VAL	HG11	0.930	0.001	?
863	?	104	VAL	HG12	0.930	0.001	?
864	?	104	VAL	HG13	0.930	0.001	?
865	?	104	VAL	HG21	0.866	0.004	?
866	?	104	VAL	HG22	0.866	0.004	?
867	?	104	VAL	HG23	0.866	0.004	?
868	?	104	VAL	CG1	20.828	0.000	?
869	?	104	VAL	CG2	19.380	0.096	?
870	?	105	ASN	HB2	2.913	0.001	?
871	?	105	ASN	HB3	2.705	0.000	?
872	?	49	GLY	HA2	4.231	0.000	?
873	?	68	ARG	H	9.080	0.000	?
874	?	5	ILE	H	8.917	0.006	?
875	?	94	GLY	H	8.060	0.000	?
876	?	94	GLY	HA2	3.883	0.004	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
877	?	5	ILE	HA	4.974	0.000	?
878	?	7	PRO	HD2	3.945	0.006	?
879	?	51	PRO	HA	4.333	0.000	?
880	?	51	PRO	HB2	2.405	0.000	?
881	?	51	PRO	HB3	1.704	0.000	?
882	?	51	PRO	HG2	2.003	0.004	?
883	?	82	PRO	HD2	3.492	0.004	?
884	?	82	PRO	HD3	3.400	0.004	?
885	?	82	PRO	HB2	2.468	0.005	?
886	?	82	PRO	HG2	1.907	0.004	?
887	?	82	PRO	HG3	1.664	0.006	?
888	?	5	ILE	HB	1.822	0.005	?
889	?	5	ILE	HG12	1.578	0.006	?
890	?	5	ILE	HG21	0.843	0.001	?
891	?	5	ILE	HG22	0.843	0.001	?
892	?	5	ILE	HG23	0.843	0.001	?
893	?	5	ILE	HD11	0.338	0.000	?
894	?	5	ILE	HD12	0.338	0.000	?
895	?	5	ILE	HD13	0.338	0.000	?
896	?	63	CYS	H	8.139	0.004	?
897	?	63	CYS	HA	5.032	0.006	?
898	?	101	PRO	HA	4.475	0.000	?
899	?	107	SER	HA	4.766	0.012	?
900	?	107	SER	CA	56.717	0.000	?
901	?	107	SER	HB2	4.314	0.005	?
902	?	107	SER	HB3	4.056	0.011	?
903	?	107	SER	CB	62.579	0.000	?
904	?	35	PRO	HG2	2.006	0.003	?
905	?	35	PRO	CG	26.235	0.000	?
906	?	51	PRO	CG	26.879	0.019	?
907	?	51	PRO	HD2	4.068	0.000	?
908	?	51	PRO	HD3	3.345	0.000	?
909	?	51	PRO	CD	50.178	0.000	?
910	?	51	PRO	CA	62.291	0.000	?
911	?	82	PRO	HA	4.675	0.008	?
912	?	82	PRO	CA	62.903	0.000	?
913	?	82	PRO	HB3	1.985	0.004	?
914	?	82	PRO	CB	32.259	2.246	?
915	?	82	PRO	CG	23.571	0.000	?
916	?	82	PRO	CD	49.013	0.000	?
917	?	35	PRO	HD3	3.781	0.006	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
918	?	35	PRO	CD	51.110	0.000	?
919	?	35	PRO	HD2	3.961	0.000	?
920	?	35	PRO	HA	4.184	0.000	?
921	?	35	PRO	CA	66.018	0.000	?
922	?	35	PRO	HB2	2.113	0.004	?
923	?	35	PRO	HB3	1.498	0.000	?
924	?	35	PRO	HG3	1.923	0.007	?
925	?	101	PRO	CA	63.455	0.000	?
926	?	101	PRO	HD2	3.674	0.000	?
927	?	101	PRO	HD3	3.532	0.000	?
928	?	101	PRO	CD	50.178	0.000	?
929	?	101	PRO	HG2	2.147	0.004	?
930	?	101	PRO	CG	27.100	0.068	?
931	?	101	PRO	HG3	1.995	0.006	?
932	?	101	PRO	HB3	1.863	0.005	?
933	?	101	PRO	HB2	2.312	0.004	?
934	?	101	PRO	CB	32.184	1.358	?
935	?	41	PRO	HD2	3.431	0.000	?
936	?	41	PRO	CD	49.712	0.000	?
937	?	41	PRO	HD3	3.288	0.000	?
938	?	41	PRO	HA	4.114	0.000	?
939	?	41	PRO	CA	61.592	0.000	?
940	?	41	PRO	HG2	2.210	0.000	?
941	?	41	PRO	CG	26.885	0.000	?
942	?	41	PRO	HG3	2.047	0.000	?
943	?	41	PRO	HB3	1.638	0.000	?
944	?	41	PRO	HB2	2.399	0.001	?
945	?	5	ILE	CA	58.098	0.000	?
946	?	5	ILE	HG13	1.158	0.006	?
947	?	7	PRO	HG2	2.110	0.005	?
948	?	7	PRO	CG	27.097	0.074	?
949	?	7	PRO	HB3	1.962	0.000	?
950	?	7	PRO	HG3	1.651	0.002	?
951	?	7	PRO	HB2	2.308	0.000	?
952	?	7	PRO	HA	3.997	0.004	?
953	?	7	PRO	CA	65.552	0.000	?
954	?	7	PRO	HD3	3.779	0.005	?
955	?	7	PRO	CD	51.110	0.000	?
956	?	5	ILE	CB	42.520	0.077	?
957	?	5	ILE	CG1	28.515	0.000	?
958	?	5	ILE	CG2	17.334	0.000	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
959	?	5	ILE	CD1	14.306	0.000	?
960	?	63	CYS	CA	56.131	0.000	?
961	?	63	CYS	HB2	3.524	0.006	?
962	?	63	CYS	HB3	2.531	0.005	?
963	?	63	CYS	CB	28.109	0.000	?
964	?	94	GLY	CA	44.750	0.000	?

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

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 1168. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/473 (0%)	0/188 (0%)	0/194 (0%)	0/91 (0%)
Sidechain	0/629 (0%)	0/366 (0%)	0/240 (0%)	0/23 (0%)
Aromatic	0/66 (0%)	0/36 (0%)	0/25 (0%)	0/5 (0%)
Overall	0/1168 (0%)	0/590 (0%)	0/459 (0%)	0/119 (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 1301. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/528 (0%)	0/210 (0%)	0/216 (0%)	0/102 (0%)
Sidechain	0/707 (0%)	0/412 (0%)	0/265 (0%)	0/30 (0%)
Aromatic	0/66 (0%)	0/36 (0%)	0/25 (0%)	0/5 (0%)
Overall	0/1301 (0%)	0/658 (0%)	0/506 (0%)	0/137 (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 (Rhoda_SNOC_shifte
RCI is only applicable to proteins.