



Full wwPDB NMR Structure Validation Report ⓘ

May 2, 2017 – 01:04 PM EDT

PDB ID : 5L7B
Title : Solution structure of the human SNF5/INI1 domain
Authors : Allen, M.D.; Zinzalla, G.; Bycroft, M.
Deposited on : 2016-06-02

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 ⓘ symbol.

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 : rb-20029077
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

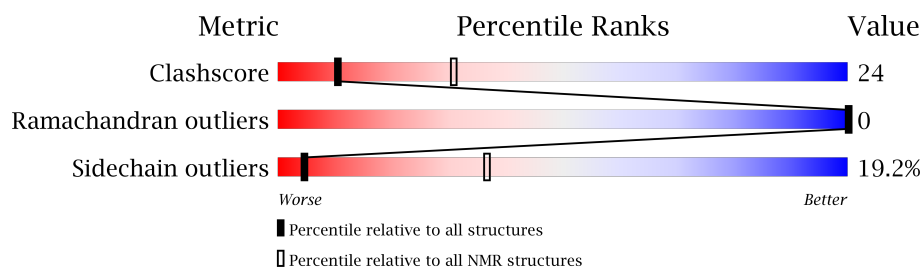
1 Overall quality at a glance

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	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 ≥ 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	78	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:185-A:248 (64)	0.15	6

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1205 atoms, of which 597 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	76	1205	383	597	95	125	5	0

There are 3 discrepancies between the modelled and reference sequences:

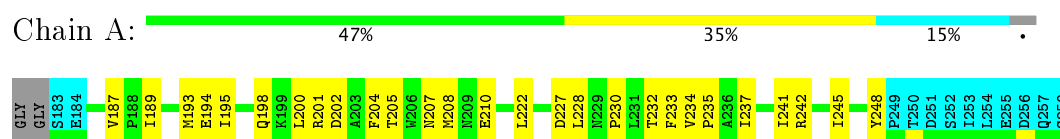
Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLY	-	expression tag	UNP Q12824
A	182	GLY	-	expression tag	UNP Q12824
A	183	SER	-	expression tag	UNP Q12824

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: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

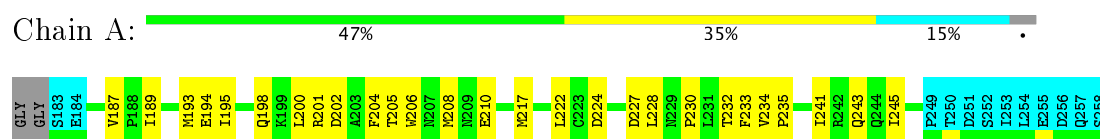


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

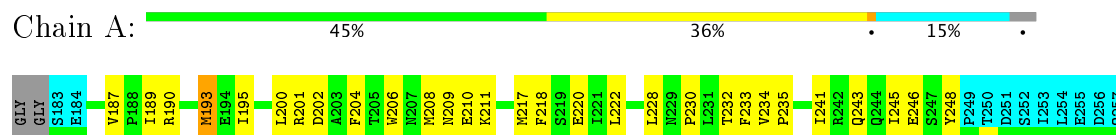
4.2.1 Score per residue for model 1

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



4.2.2 Score per residue for model 2

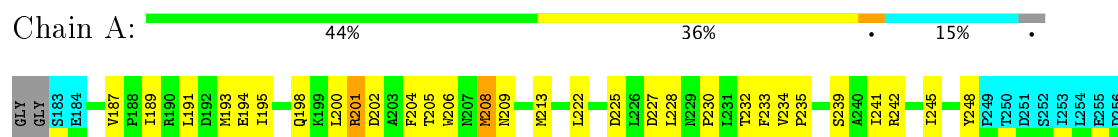
- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



S258

4.2.3 Score per residue for model 3

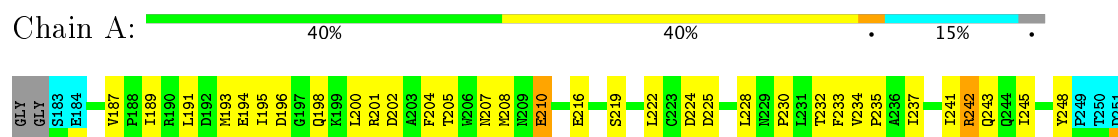
- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



Q257
S258

4.2.4 Score per residue for model 4

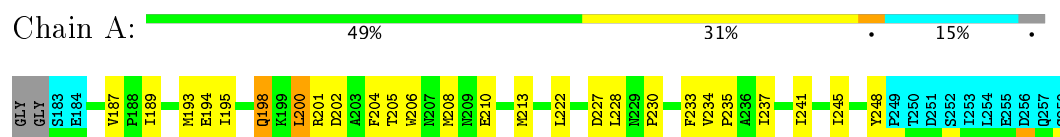
- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



S252
L253
L254
E255
D256
Q257
S258

4.2.5 Score per residue for model 5

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1





4.2.7 Score per residue for model 7

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

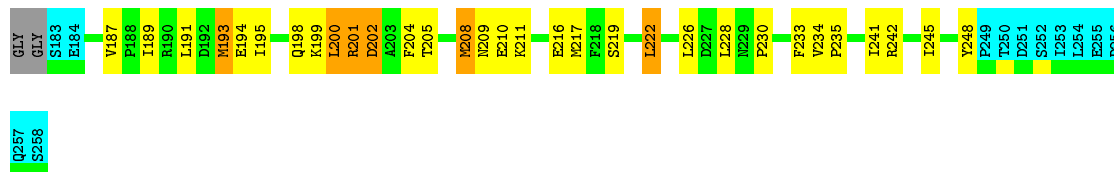
Chain A: 44% 35% 15%



4.2.8 Score per residue for model 8

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

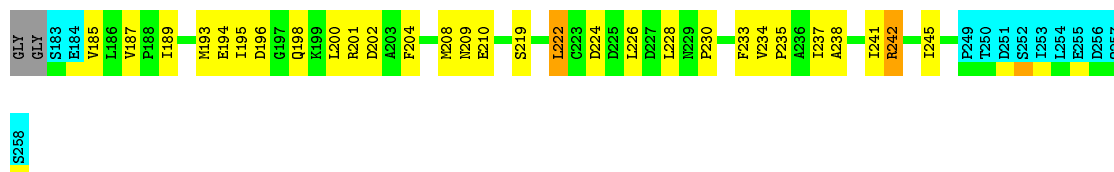
Chain A: 42% 32% 8% 15%



4.2.9 Score per residue for model 9

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

Chain A: 45% 35% 15%



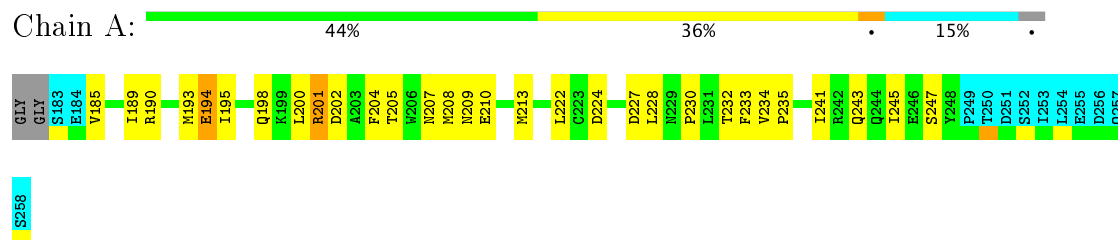
4.2.10 Score per residue for model 10

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

Chain A: 45% 35% 15%

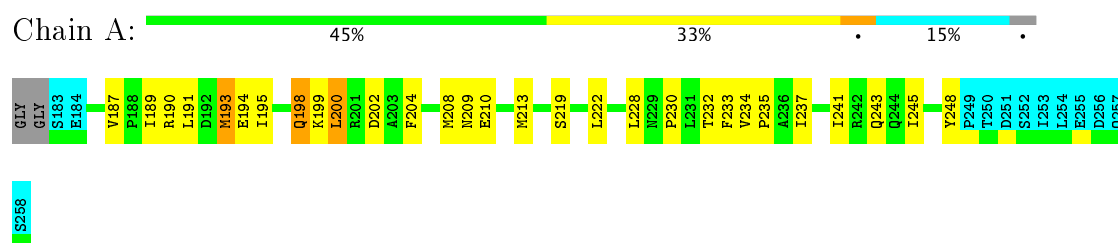
4.2.14 Score per residue for model 14

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



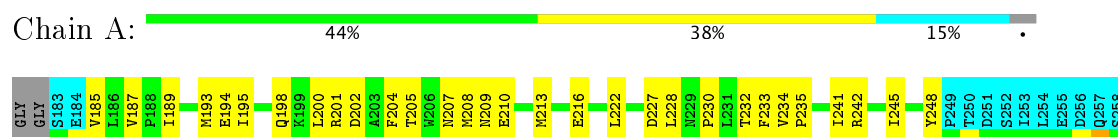
4.2.15 Score per residue for model 15

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



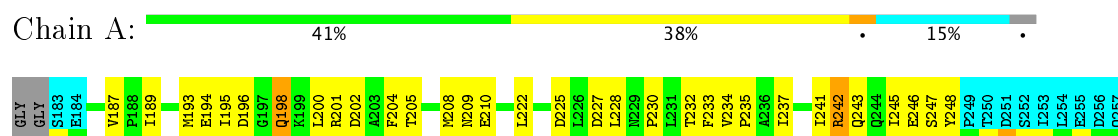
4.2.16 Score per residue for model 16

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



4.2.17 Score per residue for model 17

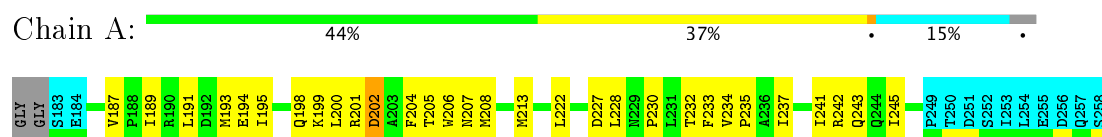
- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



S258

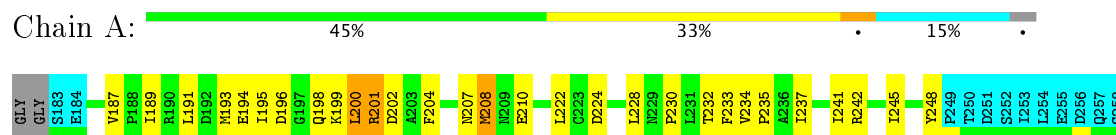
4.2.18 Score per residue for model 18

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



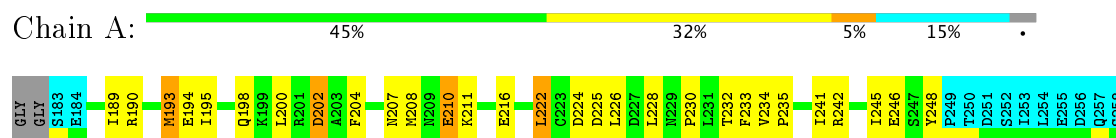
4.2.19 Score per residue for model 19

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



4.2.20 Score per residue for model 20

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle 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
CNS	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)	5l7b_cs.cif
Number of chemical shift lists	1
Total number of shifts	918
Number of shifts mapped to atoms	0
Number of unparsed shifts	918
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 ⓘ

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	516	516	516	24±4
All	All	10320	10320	10320	488

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:LEU:HD11	1:A:204:PHE:CE2	0.83	2.09	18	1
1:A:189:ILE:HG21	1:A:204:PHE:CE2	0.82	2.09	7	8
1:A:200:LEU:HD23	1:A:228:LEU:HD11	0.81	1.53	2	5
1:A:193:MET:HG3	1:A:200:LEU:HD12	0.79	1.53	8	4
1:A:189:ILE:HG21	1:A:204:PHE:CE1	0.78	2.13	15	12
1:A:193:MET:CG	1:A:200:LEU:HD12	0.77	2.09	8	1
1:A:195:ILE:HD13	1:A:233:PHE:CE1	0.77	2.15	7	1
1:A:228:LEU:HD22	1:A:233:PHE:CZ	0.76	2.15	16	13
1:A:242:ARG:HA	1:A:245:ILE:HD12	0.75	1.57	16	5
1:A:195:ILE:HG21	1:A:232:THR:OG1	0.73	1.83	3	14
1:A:241:ILE:HG22	1:A:245:ILE:HD11	0.72	1.62	14	18
1:A:228:LEU:HD22	1:A:233:PHE:CE1	0.71	2.20	15	8
1:A:200:LEU:HD23	1:A:228:LEU:CD1	0.70	2.15	20	3
1:A:193:MET:HG2	1:A:200:LEU:HD12	0.70	1.62	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:230:PRO:HA	1:A:234:VAL:HG23	0.69	1.64	4	20
1:A:228:LEU:HD22	1:A:233:PHE:CE2	0.66	2.26	17	5
1:A:200:LEU:HD12	1:A:201:ARG:N	0.65	2.06	18	15
1:A:194:GLU:C	1:A:195:ILE:HD12	0.65	2.12	7	1
1:A:195:ILE:HD13	1:A:233:PHE:CZ	0.65	2.26	7	1
1:A:230:PRO:CA	1:A:234:VAL:HG23	0.64	2.23	2	20
1:A:200:LEU:HD13	1:A:200:LEU:C	0.63	2.14	15	3
1:A:200:LEU:HD13	1:A:200:LEU:O	0.61	1.96	8	3
1:A:194:GLU:HA	1:A:198:GLN:O	0.60	1.97	9	19
1:A:195:ILE:HD12	1:A:233:PHE:CD2	0.60	2.31	12	1
1:A:208:MET:HG2	1:A:245:ILE:HG23	0.59	1.73	20	11
1:A:200:LEU:HD22	1:A:201:ARG:N	0.59	2.11	8	2
1:A:208:MET:CG	1:A:245:ILE:HG23	0.58	2.29	2	2
1:A:200:LEU:C	1:A:200:LEU:HD13	0.57	2.19	20	2
1:A:191:LEU:CD1	1:A:204:PHE:CE2	0.56	2.87	18	2
1:A:241:ILE:O	1:A:245:ILE:HG13	0.56	2.01	18	18
1:A:195:ILE:CG1	1:A:233:PHE:CZ	0.56	2.88	2	18
1:A:195:ILE:HD12	1:A:233:PHE:CG	0.55	2.36	12	1
1:A:202:ASP:CG	1:A:222:LEU:HD21	0.55	2.22	20	1
1:A:187:VAL:HG13	1:A:248:TYR:CD1	0.54	2.38	7	5
1:A:191:LEU:HD13	1:A:202:ASP:CB	0.54	2.32	18	1
1:A:241:ILE:HG22	1:A:245:ILE:CD1	0.54	2.31	14	13
1:A:187:VAL:HG13	1:A:248:TYR:CG	0.54	2.38	16	9
1:A:191:LEU:HD21	1:A:204:PHE:CE2	0.53	2.39	18	1
1:A:206:TRP:CD1	1:A:245:ILE:HD13	0.52	2.39	3	5
1:A:202:ASP:OD2	1:A:226:LEU:HD11	0.52	2.05	8	1
1:A:200:LEU:O	1:A:200:LEU:HD13	0.52	2.05	7	2
1:A:222:LEU:HD23	1:A:226:LEU:HD12	0.52	1.81	8	1
1:A:189:ILE:CG2	1:A:204:PHE:CE1	0.52	2.92	15	11
1:A:189:ILE:HG21	1:A:204:PHE:CZ	0.52	2.39	18	2
1:A:191:LEU:HD11	1:A:204:PHE:CD2	0.52	2.40	18	1
1:A:228:LEU:HB3	1:A:233:PHE:CD2	0.51	2.41	7	9
1:A:228:LEU:HB3	1:A:233:PHE:CD1	0.51	2.40	15	11
1:A:187:VAL:CG2	1:A:208:MET:CG	0.50	2.89	7	10
1:A:200:LEU:HD22	1:A:228:LEU:HD13	0.50	1.82	3	5
1:A:189:ILE:CG2	1:A:204:PHE:CE2	0.50	2.93	14	6
1:A:191:LEU:HD21	1:A:204:PHE:CZ	0.49	2.43	18	1
1:A:189:ILE:HG21	1:A:204:PHE:HE2	0.49	1.68	3	4
1:A:241:ILE:O	1:A:245:ILE:HG12	0.48	2.08	5	2
1:A:200:LEU:HD12	1:A:200:LEU:C	0.48	2.28	5	4
1:A:185:VAL:HG11	1:A:208:MET:SD	0.48	2.48	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:200:LEU:HD22	1:A:233:PHE:CD1	0.48	2.43	14	6
1:A:208:MET:HG2	1:A:245:ILE:CG2	0.47	2.39	2	3
1:A:234:VAL:HB	1:A:235:PRO:HD3	0.47	1.87	19	2
1:A:191:LEU:CD1	1:A:204:PHE:CE1	0.47	2.98	3	3
1:A:195:ILE:HG12	1:A:233:PHE:CZ	0.47	2.45	20	7
1:A:198:GLN:NE2	1:A:228:LEU:HD23	0.47	2.25	7	3
1:A:202:ASP:OD1	1:A:226:LEU:HD11	0.47	2.10	20	1
1:A:198:GLN:OE1	1:A:228:LEU:HD23	0.47	2.09	18	2
1:A:206:TRP:CD1	1:A:245:ILE:CD1	0.46	2.98	18	5
1:A:200:LEU:C	1:A:200:LEU:HD12	0.46	2.31	6	6
1:A:200:LEU:HD22	1:A:233:PHE:CD2	0.46	2.45	13	5
1:A:189:ILE:HG21	1:A:204:PHE:HE1	0.46	1.68	1	3
1:A:200:LEU:CD2	1:A:233:PHE:CD1	0.45	2.99	4	3
1:A:200:LEU:CD2	1:A:233:PHE:CD2	0.45	3.00	16	4
1:A:200:LEU:CD2	1:A:233:PHE:CE2	0.44	3.01	1	3
1:A:210:GLU:N	1:A:210:GLU:OE1	0.44	2.51	5	1
1:A:233:PHE:O	1:A:237:ILE:HG13	0.44	2.13	19	12
1:A:195:ILE:HG21	1:A:232:THR:CB	0.44	2.42	15	1
1:A:195:ILE:CG1	1:A:233:PHE:CE2	0.44	3.01	8	2
1:A:230:PRO:O	1:A:234:VAL:HG23	0.44	2.13	18	11
1:A:217:MET:HG3	1:A:218:PHE:N	0.43	2.28	2	1
1:A:191:LEU:HD12	1:A:204:PHE:CE1	0.43	2.48	3	2
1:A:187:VAL:HG13	1:A:248:TYR:CD2	0.43	2.49	3	1
1:A:234:VAL:HB	1:A:235:PRO:CD	0.43	2.43	10	18
1:A:198:GLN:NE2	1:A:228:LEU:CD2	0.43	2.81	8	4
1:A:210:GLU:OE2	1:A:210:GLU:N	0.43	2.52	9	4
1:A:191:LEU:HD13	1:A:237:ILE:HG23	0.43	1.91	15	1
1:A:198:GLN:CD	1:A:228:LEU:HD23	0.42	2.35	18	1
1:A:191:LEU:HD13	1:A:202:ASP:HB3	0.42	1.92	18	1
1:A:230:PRO:O	1:A:234:VAL:HB	0.42	2.14	8	3
1:A:195:ILE:HG12	1:A:233:PHE:CE2	0.41	2.50	8	2
1:A:234:VAL:N	1:A:235:PRO:HD2	0.41	2.31	20	1
1:A:187:VAL:CG1	1:A:248:TYR:CG	0.41	3.04	12	1
1:A:195:ILE:N	1:A:195:ILE:HD12	0.41	2.30	7	1
1:A:191:LEU:CD1	1:A:237:ILE:HG23	0.41	2.44	15	1
1:A:202:ASP:OD2	1:A:222:LEU:HD21	0.41	2.15	20	1
1:A:220:GLU:OE1	1:A:234:VAL:HG21	0.41	2.15	2	1
1:A:219:SER:OG	1:A:238:ALA:HB2	0.41	2.16	9	1
1:A:200:LEU:CD2	1:A:233:PHE:CE1	0.41	3.04	4	1
1:A:191:LEU:HD12	1:A:204:PHE:CE2	0.41	2.51	13	2
1:A:189:ILE:CB	1:A:204:PHE:CE1	0.41	3.04	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:239:SER:HA	1:A:242:ARG:HG2	0.41	1.92	3	2
1:A:241:ILE:CG2	1:A:245:ILE:HD11	0.41	2.42	14	1
1:A:187:VAL:CG2	1:A:208:MET:HG2	0.40	2.46	9	2
1:A:222:LEU:HD23	1:A:226:LEU:CD1	0.40	2.46	9	1
1:A:210:GLU:OE1	1:A:210:GLU:N	0.40	2.54	4	1
1:A:189:ILE:HG22	1:A:191:LEU:CD2	0.40	2.47	8	1
1:A:228:LEU:HD13	1:A:233:PHE:CD2	0.40	2.51	19	1
1:A:195:ILE:CD1	1:A:195:ILE:N	0.40	2.85	7	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	64/78 (82%)	61±1 (95±1%)	3±1 (5±1%)	0±0 (0±0%)	100	100
All	All	1280/1560 (82%)	1213 (95%)	67 (5%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	59/71 (83%)	48±2 (81±4%)	11±2 (19±4%)	5	37
All	All	1180/1420 (83%)	954 (81%)	226 (19%)	5	37

All 27 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	193	MET	20
1	A	222	LEU	19
1	A	202	ASP	18
1	A	205	THR	13
1	A	210	GLU	12
1	A	227	ASP	11
1	A	207	ASN	11
1	A	243	GLN	10
1	A	242	ARG	9
1	A	209	ASN	9
1	A	224	ASP	8
1	A	225	ASP	8
1	A	199	LYS	8
1	A	211	LYS	7
1	A	190	ARG	7
1	A	201	ARG	6
1	A	213	MET	6
1	A	208	MET	5
1	A	198	GLN	5
1	A	200	LEU	5
1	A	216	GLU	5
1	A	196	ASP	5
1	A	246	GLU	5
1	A	247	SER	4
1	A	194	GLU	4
1	A	217	MET	3
1	A	219	SER	3

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: 5l7b_cs.cif

Chemical shift list name: *snf5.bmr.b.data*

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	918
Number of shifts mapped to atoms	0
Number of unparsed shifts	918
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 918 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	183	SER	N	115.880	0.10	1
2	?	183	SER	H	8.361	0.01	1
3	?	183	SER	CA	58.240	0.10	1
4	?	183	SER	HA	4.383	0.01	1
5	?	183	SER	C	173.490	0.10	1
6	?	183	SER	CB	63.620	0.10	1
7	?	183	SER	HB2	3.770	0.01	2
8	?	183	SER	HB3	3.770	0.01	2
9	?	184	GLU	N	122.450	0.10	1
10	?	184	GLU	H	8.433	0.01	1
11	?	184	GLU	CA	56.370	0.10	1
12	?	184	GLU	HA	4.214	0.01	1
13	?	184	GLU	C	175.020	0.10	1
14	?	184	GLU	CB	30.080	0.10	1
15	?	184	GLU	HB2	1.783	0.01	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	?	184	GLU	HB3	1.836	0.01	2
17	?	184	GLU	HG2	2.064	0.01	2
18	?	184	GLU	HG3	2.135	0.01	2
19	?	185	VAL	N	123.980	0.10	1
20	?	185	VAL	H	8.021	0.01	1
21	?	185	VAL	CA	62.440	0.10	1
22	?	185	VAL	HA	3.992	0.01	1
23	?	185	VAL	C	173.010	0.10	1
24	?	185	VAL	CB	32.910	0.10	1
25	?	185	VAL	HB	1.841	0.01	1
26	?	185	VAL	CG1	21.270	0.10	1
27	?	185	VAL	HG11	0.801	0.01	2
28	?	185	VAL	HG12	0.801	0.01	2
29	?	185	VAL	HG13	0.801	0.01	2
30	?	185	VAL	CG2	20.490	0.10	1
31	?	185	VAL	HG21	0.839	0.01	2
32	?	185	VAL	HG22	0.839	0.01	2
33	?	185	VAL	HG23	0.839	0.01	2
34	?	186	LEU	N	125.730	0.10	1
35	?	186	LEU	H	8.153	0.01	1
36	?	186	LEU	CA	53.080	0.10	1
37	?	186	LEU	HA	4.849	0.01	1
38	?	186	LEU	C	175.770	0.10	1
39	?	186	LEU	CB	42.040	0.10	1
40	?	186	LEU	HB2	0.937	0.01	1
41	?	186	LEU	HB3	1.672	0.01	1
42	?	186	LEU	HG	1.426	0.01	1
43	?	186	LEU	CD1	24.920	0.10	1
44	?	186	LEU	HD11	0.748	0.01	2
45	?	186	LEU	HD12	0.748	0.01	2
46	?	186	LEU	HD13	0.748	0.01	2
47	?	186	LEU	CD2	22.550	0.10	1
48	?	186	LEU	HD21	0.582	0.01	2
49	?	186	LEU	HD22	0.582	0.01	2
50	?	186	LEU	HD23	0.582	0.01	2
51	?	187	VAL	N	123.990	0.10	1
52	?	187	VAL	H	9.086	0.01	1
53	?	187	VAL	CA	58.760	0.10	1
54	?	187	VAL	HA	4.106	0.01	1
55	?	187	VAL	C	173.030	0.10	1
56	?	187	VAL	CB	34.380	0.10	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	?	187	VAL	HB	1.879	0.01	1
58	?	187	VAL	HG11	0.528	0.01	2
59	?	187	VAL	HG12	0.528	0.01	2
60	?	187	VAL	HG13	0.528	0.01	2
61	?	187	VAL	CG2	20.460	0.10	1
62	?	187	VAL	HG21	0.654	0.01	2
63	?	187	VAL	HG22	0.654	0.01	2
64	?	187	VAL	HG23	0.654	0.01	2
65	?	188	PRO	CA	62.810	0.10	1
66	?	188	PRO	HA	4.396	0.01	1
67	?	188	PRO	C	174.410	0.10	1
68	?	188	PRO	CB	31.640	0.10	1
69	?	188	PRO	HB2	2.068	0.01	2
70	?	188	PRO	HB3	1.750	0.01	2
71	?	188	PRO	HG2	2.106	0.01	2
72	?	188	PRO	HG3	1.877	0.01	2
73	?	188	PRO	CD	50.740	0.10	1
74	?	188	PRO	HD2	3.717	0.01	2
75	?	188	PRO	HD3	3.427	0.01	2
76	?	189	ILE	N	123.950	0.10	1
77	?	189	ILE	H	8.639	0.01	1
78	?	189	ILE	CA	57.430	0.10	1
79	?	189	ILE	HA	4.206	0.01	1
80	?	189	ILE	C	174.880	0.10	1
81	?	189	ILE	CB	36.830	0.10	1
82	?	189	ILE	HB	0.879	0.01	1
83	?	189	ILE	HG12	1.430	0.01	2
84	?	189	ILE	HG13	0.877	0.01	2
85	?	189	ILE	CG2	17.690	0.10	1
86	?	189	ILE	HG21	0.278	0.01	2
87	?	189	ILE	HG22	0.278	0.01	2
88	?	189	ILE	HG23	0.278	0.01	2
89	?	189	ILE	CD1	10.390	0.10	1
90	?	189	ILE	HD11	0.423	0.01	2
91	?	189	ILE	HD12	0.423	0.01	2
92	?	189	ILE	HD13	0.423	0.01	2
93	?	190	ARG	N	126.150	0.10	1
94	?	190	ARG	H	8.963	0.01	1
95	?	190	ARG	CA	54.820	0.10	1
96	?	190	ARG	HA	4.690	0.01	1
97	?	190	ARG	C	174.830	0.10	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	?	190	ARG	CB	32.100	0.10	1
99	?	190	ARG	HB2	1.672	0.01	2
100	?	190	ARG	HB3	1.576	0.01	2
101	?	190	ARG	HG2	1.468	0.01	2
102	?	190	ARG	HG3	1.385	0.01	2
103	?	190	ARG	CD	43.090	0.10	1
104	?	190	ARG	HD2	3.084	0.01	2
105	?	190	ARG	HD3	3.084	0.01	2
106	?	190	ARG	HE	7.235	0.01	1
107	?	191	LEU	N	124.310	0.10	1
108	?	191	LEU	H	8.833	0.01	1
109	?	191	LEU	CA	52.860	0.10	1
110	?	191	LEU	HA	4.707	0.01	1
111	?	191	LEU	C	175.110	0.10	1
112	?	191	LEU	CB	43.940	0.10	1
113	?	191	LEU	HB2	1.159	0.01	1
114	?	191	LEU	HB3	1.676	0.01	1
115	?	191	LEU	HG	1.479	0.01	1
116	?	191	LEU	HD11	0.958	0.01	2
117	?	191	LEU	HD12	0.958	0.01	2
118	?	191	LEU	HD13	0.958	0.01	2
119	?	191	LEU	HD21	0.736	0.01	2
120	?	191	LEU	HD22	0.736	0.01	2
121	?	191	LEU	HD23	0.736	0.01	2
122	?	192	ASP	N	123.710	0.10	1
123	?	192	ASP	H	8.805	0.01	1
124	?	192	ASP	CA	54.050	0.10	1
125	?	192	ASP	HA	5.110	0.01	1
126	?	192	ASP	C	173.590	0.10	1
127	?	192	ASP	CB	40.660	0.10	1
128	?	192	ASP	HB2	2.657	0.01	1
129	?	192	ASP	HB3	2.468	0.01	1
130	?	193	MET	N	120.490	0.10	1
131	?	193	MET	H	8.960	0.01	1
132	?	193	MET	CA	54.680	0.10	1
133	?	193	MET	HA	4.273	0.01	1
134	?	193	MET	C	173.510	0.10	1
135	?	193	MET	CB	37.440	0.10	1
136	?	193	MET	HB2	1.893	0.01	2
137	?	193	MET	HB3	2.154	0.01	2
138	?	193	MET	HG2	2.357	0.01	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	?	193	MET	HG3	2.490	0.01	2
140	?	193	MET	CE	17.220	0.10	1
141	?	193	MET	HE1	1.897	0.01	2
142	?	193	MET	HE2	1.897	0.01	2
143	?	193	MET	HE3	1.897	0.01	2
144	?	194	GLU	N	122.880	0.10	1
145	?	194	GLU	H	8.510	0.01	1
146	?	194	GLU	CA	55.650	0.10	1
147	?	194	GLU	HA	5.177	0.01	1
148	?	194	GLU	C	174.000	0.10	1
149	?	194	GLU	CB	31.940	0.10	1
150	?	194	GLU	HB2	1.805	0.01	2
151	?	194	GLU	HB3	1.805	0.01	2
152	?	194	GLU	HG2	1.768	0.01	2
153	?	194	GLU	HG3	1.768	0.01	2
154	?	195	ILE	N	124.840	0.10	1
155	?	195	ILE	H	8.499	0.01	1
156	?	195	ILE	CA	61.020	0.10	1
157	?	195	ILE	HA	4.075	0.01	1
158	?	195	ILE	C	175.420	0.10	1
159	?	195	ILE	CB	39.740	0.10	1
160	?	195	ILE	HB	1.209	0.01	1
161	?	195	ILE	CG1	26.320	0.10	1
162	?	195	ILE	HG12	0.627	0.01	2
163	?	195	ILE	HG13	0.818	0.01	2
164	?	195	ILE	CG2	16.690	0.10	1
165	?	195	ILE	HG21	0.494	0.01	2
166	?	195	ILE	HG22	0.494	0.01	2
167	?	195	ILE	HG23	0.494	0.01	2
168	?	195	ILE	CD1	12.130	0.10	1
169	?	195	ILE	HD11	-0.167	0.01	2
170	?	195	ILE	HD12	-0.167	0.01	2
171	?	195	ILE	HD13	-0.167	0.01	2
172	?	196	ASP	N	129.330	0.10	1
173	?	196	ASP	H	9.400	0.01	1
174	?	196	ASP	CA	55.270	0.10	1
175	?	196	ASP	HA	4.222	0.01	1
176	?	196	ASP	C	175.010	0.10	1
177	?	196	ASP	CB	39.680	0.10	1
178	?	196	ASP	HB2	2.553	0.01	2
179	?	196	ASP	HB3	2.923	0.01	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	?	197	GLY	N	103.460	0.10	1
181	?	197	GLY	H	8.679	0.01	1
182	?	197	GLY	CA	45.340	0.10	1
183	?	197	GLY	HA2	3.982	0.01	2
184	?	197	GLY	HA3	3.714	0.01	2
185	?	197	GLY	C	173.160	0.10	1
186	?	198	GLN	N	120.480	0.10	1
187	?	198	GLN	H	7.968	0.01	1
188	?	198	GLN	CA	54.620	0.10	1
189	?	198	GLN	HA	4.567	0.01	1
190	?	198	GLN	C	173.540	0.10	1
191	?	198	GLN	CB	30.630	0.10	1
192	?	198	GLN	HB2	2.288	0.01	2
193	?	198	GLN	HB3	2.087	0.01	2
194	?	198	GLN	HG2	2.252	0.01	2
195	?	198	GLN	HG3	2.252	0.01	2
196	?	198	GLN	NE2	113.880	0.10	1
197	?	198	GLN	HE21	6.967	0.01	1
198	?	198	GLN	HE22	7.608	0.01	1
199	?	199	LYS	N	124.060	0.10	1
200	?	199	LYS	H	8.560	0.01	1
201	?	199	LYS	CA	55.710	0.10	1
202	?	199	LYS	HA	4.891	0.01	1
203	?	199	LYS	C	174.470	0.10	1
204	?	199	LYS	CB	34.890	0.10	1
205	?	199	LYS	HB2	1.679	0.01	2
206	?	199	LYS	HB3	1.643	0.01	2
207	?	199	LYS	HG2	1.222	0.01	2
208	?	199	LYS	HG3	1.312	0.01	2
209	?	199	LYS	HD2	1.556	0.01	2
210	?	199	LYS	HD3	1.556	0.01	2
211	?	199	LYS	HE2	2.842	0.01	2
212	?	199	LYS	HE3	2.842	0.01	2
213	?	200	LEU	N	124.240	0.10	1
214	?	200	LEU	H	8.651	0.01	1
215	?	200	LEU	CA	54.520	0.10	1
216	?	200	LEU	HA	4.434	0.01	1
217	?	200	LEU	C	173.050	0.10	1
218	?	200	LEU	CB	44.950	0.10	1
219	?	200	LEU	HB2	1.669	0.01	1
220	?	200	LEU	HB3	1.171	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	?	200	LEU	HG	1.272	0.01	1
222	?	200	LEU	HD11	0.777	0.01	2
223	?	200	LEU	HD12	0.777	0.01	2
224	?	200	LEU	HD13	0.777	0.01	2
225	?	200	LEU	HD21	0.744	0.01	2
226	?	200	LEU	HD22	0.744	0.01	2
227	?	200	LEU	HD23	0.744	0.01	2
228	?	201	ARG	N	127.940	0.10	1
229	?	201	ARG	H	8.619	0.01	1
230	?	201	ARG	CA	54.650	0.10	1
231	?	201	ARG	HA	5.188	0.01	1
232	?	201	ARG	C	173.790	0.10	1
233	?	201	ARG	CB	31.940	0.10	1
234	?	201	ARG	HB2	1.716	0.01	2
235	?	201	ARG	HB3	1.644	0.01	2
236	?	201	ARG	HG2	1.563	0.01	2
237	?	201	ARG	HG3	1.519	0.01	2
238	?	201	ARG	CD	43.230	0.10	1
239	?	201	ARG	HD2	3.093	0.01	2
240	?	201	ARG	HD3	3.093	0.01	2
241	?	201	ARG	HE	7.136	0.01	1
242	?	202	ASP	N	123.110	0.10	1
243	?	202	ASP	H	8.662	0.01	1
244	?	202	ASP	CA	53.280	0.10	1
245	?	202	ASP	HA	4.797	0.01	1
246	?	202	ASP	C	172.870	0.10	1
247	?	202	ASP	CB	44.680	0.10	1
248	?	202	ASP	HB2	2.342	0.01	1
249	?	202	ASP	HB3	2.533	0.01	1
250	?	203	ALA	N	123.810	0.10	1
251	?	203	ALA	H	9.060	0.01	1
252	?	203	ALA	CA	51.570	0.10	1
253	?	203	ALA	HA	5.093	0.01	1
254	?	203	ALA	C	174.650	0.10	1
255	?	203	ALA	CB	21.470	0.10	1
256	?	203	ALA	HB1	1.299	0.01	2
257	?	203	ALA	HB2	1.299	0.01	2
258	?	203	ALA	HB3	1.299	0.01	2
259	?	204	PHE	N	118.340	0.10	1
260	?	204	PHE	H	8.337	0.01	1
261	?	204	PHE	CA	56.100	0.10	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	?	204	PHE	HA	4.920	0.01	1
263	?	204	PHE	C	172.910	0.10	1
264	?	204	PHE	CB	39.530	0.10	1
265	?	204	PHE	HB2	3.435	0.01	1
266	?	204	PHE	HB3	3.090	0.01	1
267	?	204	PHE	HD1	6.937	0.01	3
268	?	204	PHE	HD2	6.937	0.01	3
269	?	204	PHE	HE1	6.913	0.01	3
270	?	204	PHE	HE2	6.913	0.01	3
271	?	204	PHE	HZ	6.847	0.01	1
272	?	205	THR	N	112.460	0.10	1
273	?	205	THR	H	8.586	0.01	1
274	?	205	THR	CA	60.540	0.10	1
275	?	205	THR	HA	4.937	0.01	1
276	?	205	THR	C	172.310	0.10	1
277	?	205	THR	CB	71.100	0.10	1
278	?	205	THR	HB	3.780	0.01	1
279	?	205	THR	CG2	22.430	0.10	1
280	?	205	THR	HG21	0.925	0.01	2
281	?	205	THR	HG22	0.925	0.01	2
282	?	205	THR	HG23	0.925	0.01	2
283	?	206	TRP	N	125.340	0.10	1
284	?	206	TRP	H	9.208	0.01	1
285	?	206	TRP	CA	55.710	0.10	1
286	?	206	TRP	HA	4.370	0.01	1
287	?	206	TRP	C	173.330	0.10	1
288	?	206	TRP	CB	31.890	0.10	1
289	?	206	TRP	HB2	2.906	0.01	1
290	?	206	TRP	HB3	2.719	0.01	1
291	?	206	TRP	HD1	6.650	0.01	1
292	?	206	TRP	HE1	10.322	0.01	1
293	?	206	TRP	HE3	6.929	0.01	1
294	?	206	TRP	HZ2	7.304	0.01	1
295	?	206	TRP	HZ3	6.222	0.01	1
296	?	206	TRP	HH2	6.600	0.01	1
297	?	207	ASN	N	125.740	0.10	1
298	?	207	ASN	H	7.681	0.01	1
299	?	207	ASN	CA	51.300	0.10	1
300	?	207	ASN	HA	4.795	0.01	1
301	?	207	ASN	C	175.100	0.10	1
302	?	207	ASN	CB	38.040	0.10	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	?	207	ASN	HB2	2.346	0.01	2
304	?	207	ASN	HB3	2.577	0.01	2
305	?	207	ASN	ND2	111.780	0.10	1
306	?	207	ASN	HD21	6.917	0.01	1
307	?	207	ASN	HD22	7.550	0.01	1
308	?	208	MET	N	123.880	0.10	1
309	?	208	MET	H	8.908	0.01	1
310	?	208	MET	CA	56.480	0.10	1
311	?	208	MET	HA	4.388	0.01	1
312	?	208	MET	C	176.580	0.10	1
313	?	208	MET	CB	31.400	0.10	1
314	?	208	MET	HB2	2.114	0.01	1
315	?	208	MET	HB3	1.984	0.01	1
316	?	208	MET	HG2	2.547	0.01	2
317	?	208	MET	HG3	2.454	0.01	2
318	?	208	MET	CE	16.190	0.10	1
319	?	208	MET	HE1	2.031	0.01	2
320	?	208	MET	HE2	2.031	0.01	2
321	?	208	MET	HE3	2.031	0.01	2
322	?	209	ASN	N	115.660	0.10	1
323	?	209	ASN	H	8.275	0.01	1
324	?	209	ASN	CA	52.770	0.10	1
325	?	209	ASN	HA	4.712	0.01	1
326	?	209	ASN	C	174.230	0.10	1
327	?	209	ASN	CB	38.460	0.10	1
328	?	209	ASN	HB2	2.606	0.01	2
329	?	209	ASN	HB3	2.821	0.01	2
330	?	209	ASN	ND2	112.430	0.10	1
331	?	209	ASN	HD21	6.860	0.01	1
332	?	209	ASN	HD22	7.664	0.01	1
333	?	210	GLU	N	121.680	0.10	1
334	?	210	GLU	H	7.403	0.01	1
335	?	210	GLU	CA	56.610	0.10	1
336	?	210	GLU	HA	3.928	0.01	1
337	?	210	GLU	C	176.060	0.10	1
338	?	210	GLU	CB	29.710	0.10	1
339	?	210	GLU	HB2	1.807	0.01	1
340	?	210	GLU	HB3	1.864	0.01	1
341	?	210	GLU	HG2	2.038	0.01	2
342	?	210	GLU	HG3	2.038	0.01	2
343	?	211	LYS	N	125.000	0.10	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	?	211	LYS	H	8.613	0.01	1
345	?	211	LYS	CA	56.170	0.10	1
346	?	211	LYS	HA	4.414	0.01	1
347	?	211	LYS	C	175.990	0.10	1
348	?	211	LYS	CB	33.710	0.10	1
349	?	211	LYS	HB2	1.826	0.01	2
350	?	211	LYS	HB3	1.627	0.01	2
351	?	211	LYS	HG2	1.365	0.01	2
352	?	211	LYS	HG3	1.533	0.01	2
353	?	211	LYS	HD2	1.537	0.01	2
354	?	211	LYS	HD3	1.594	0.01	2
355	?	211	LYS	HE2	2.914	0.01	2
356	?	211	LYS	HE3	2.914	0.01	2
357	?	212	LEU	N	120.920	0.10	1
358	?	212	LEU	H	8.377	0.01	1
359	?	212	LEU	CA	56.130	0.10	1
360	?	212	LEU	HA	4.357	0.01	1
361	?	212	LEU	C	176.360	0.10	1
362	?	212	LEU	CB	42.890	0.10	1
363	?	212	LEU	HB2	1.512	0.01	1
364	?	212	LEU	HB3	1.659	0.01	1
365	?	212	LEU	HG	1.528	0.01	1
366	?	212	LEU	HD11	0.838	0.01	2
367	?	212	LEU	HD12	0.838	0.01	2
368	?	212	LEU	HD13	0.838	0.01	2
369	?	212	LEU	HD21	0.778	0.01	2
370	?	212	LEU	HD22	0.778	0.01	2
371	?	212	LEU	HD23	0.778	0.01	2
372	?	213	MET	N	119.790	0.10	1
373	?	213	MET	H	8.461	0.01	1
374	?	213	MET	CA	54.850	0.10	1
375	?	213	MET	HA	4.758	0.01	1
376	?	213	MET	C	174.760	0.10	1
377	?	213	MET	CB	33.060	0.10	1
378	?	213	MET	HB2	1.932	0.01	2
379	?	213	MET	HB3	1.863	0.01	2
380	?	213	MET	HG2	2.540	0.01	2
381	?	213	MET	HG3	2.427	0.01	2
382	?	213	MET	CE	16.140	0.10	1
383	?	213	MET	HE1	2.026	0.01	2
384	?	213	MET	HE2	2.026	0.01	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	?	213	MET	HE3	2.026	0.01	2
386	?	214	THR	N	115.680	0.10	1
387	?	214	THR	H	7.732	0.01	1
388	?	214	THR	CA	59.400	0.10	1
389	?	214	THR	HA	4.966	0.01	1
390	?	214	THR	C	173.590	0.10	1
391	?	214	THR	CB	69.330	0.10	1
392	?	214	THR	HB	4.704	0.01	1
393	?	214	THR	CG2	22.020	0.10	1
394	?	214	THR	HG1	6.042	0.01	1
395	?	214	THR	HG21	1.379	0.01	2
396	?	214	THR	HG22	1.379	0.01	2
397	?	214	THR	HG23	1.379	0.01	2
398	?	215	PRO	CA	66.050	0.10	1
399	?	215	PRO	HA	4.052	0.01	1
400	?	215	PRO	C	177.800	0.10	1
401	?	215	PRO	CB	31.950	0.10	1
402	?	215	PRO	HB2	1.675	0.01	2
403	?	215	PRO	HB3	1.889	0.01	2
404	?	215	PRO	HG2	1.137	0.01	2
405	?	215	PRO	HG3	1.757	0.01	2
406	?	215	PRO	HD2	4.051	0.01	2
407	?	215	PRO	HD3	3.802	0.01	2
408	?	216	GLU	N	119.730	0.10	1
409	?	216	GLU	H	9.106	0.01	1
410	?	216	GLU	CA	62.700	0.10	1
411	?	216	GLU	HA	3.697	0.01	1
412	?	216	GLU	C	177.050	0.10	1
413	?	216	GLU	CB	28.030	0.10	1
414	?	216	GLU	HB2	2.047	0.01	2
415	?	216	GLU	HB3	1.834	0.01	2
416	?	216	GLU	HG2	2.560	0.01	2
417	?	216	GLU	HG3	2.560	0.01	2
418	?	217	MET	N	120.730	0.10	1
419	?	217	MET	H	7.992	0.01	1
420	?	217	MET	CA	59.100	0.10	1
421	?	217	MET	HA	4.066	0.01	1
422	?	217	MET	C	178.310	0.10	1
423	?	217	MET	CB	34.500	0.10	1
424	?	217	MET	HB2	2.217	0.01	2
425	?	217	MET	HB3	2.300	0.01	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
426	?	217	MET	HG2	2.590	0.01	2
427	?	217	MET	HG3	2.590	0.01	2
428	?	217	MET	CE	16.870	0.10	1
429	?	217	MET	HE1	2.166	0.01	2
430	?	217	MET	HE2	2.166	0.01	2
431	?	217	MET	HE3	2.166	0.01	2
432	?	218	PHE	N	119.240	0.10	1
433	?	218	PHE	H	8.441	0.01	1
434	?	218	PHE	CA	61.530	0.10	1
435	?	218	PHE	HA	4.064	0.01	1
436	?	218	PHE	C	176.610	0.10	1
437	?	218	PHE	CB	40.000	0.10	1
438	?	218	PHE	HB2	3.149	0.01	1
439	?	218	PHE	HB3	3.370	0.01	1
440	?	218	PHE	HD1	6.973	0.01	3
441	?	218	PHE	HD2	6.973	0.01	3
442	?	218	PHE	HE1	6.737	0.01	3
443	?	218	PHE	HE2	6.737	0.01	3
444	?	218	PHE	HZ	6.468	0.01	1
445	?	219	SER	N	114.820	0.10	1
446	?	219	SER	H	8.162	0.01	1
447	?	219	SER	CA	62.700	0.10	1
448	?	219	SER	HA	3.845	0.01	1
449	?	219	SER	C	174.820	0.10	1
450	?	219	SER	CB	63.780	0.10	1
451	?	219	SER	HB2	3.790	0.01	2
452	?	219	SER	HB3	4.254	0.01	2
453	?	220	GLU	N	122.400	0.10	1
454	?	220	GLU	H	8.038	0.01	1
455	?	220	GLU	CA	59.980	0.10	1
456	?	220	GLU	HA	3.628	0.01	1
457	?	220	GLU	C	178.210	0.10	1
458	?	220	GLU	CB	29.480	0.10	1
459	?	220	GLU	HB2	1.969	0.01	1
460	?	220	GLU	HB3	2.150	0.01	1
461	?	220	GLU	HG2	2.426	0.01	2
462	?	220	GLU	HG3	2.426	0.01	2
463	?	221	ILE	N	121.000	0.10	1
464	?	221	ILE	H	7.301	0.01	1
465	?	221	ILE	CA	64.910	0.10	1
466	?	221	ILE	HA	3.570	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
467	?	221	ILE	C	177.220	0.10	1
468	?	221	ILE	CB	37.800	0.10	1
469	?	221	ILE	HB	1.618	0.01	1
470	?	221	ILE	CG1	27.440	0.10	1
471	?	221	ILE	HG12	0.951	0.01	2
472	?	221	ILE	HG13	0.951	0.01	2
473	?	221	ILE	CG2	16.830	0.10	1
474	?	221	ILE	HG21	0.667	0.01	2
475	?	221	ILE	HG22	0.667	0.01	2
476	?	221	ILE	HG23	0.667	0.01	2
477	?	221	ILE	CD1	13.480	0.10	1
478	?	221	ILE	HD11	0.760	0.01	2
479	?	221	ILE	HD12	0.760	0.01	2
480	?	221	ILE	HD13	0.760	0.01	2
481	?	222	LEU	N	120.550	0.10	1
482	?	222	LEU	H	7.659	0.01	1
483	?	222	LEU	CA	57.930	0.10	1
484	?	222	LEU	HA	3.773	0.01	1
485	?	222	LEU	C	178.300	0.10	1
486	?	222	LEU	CB	41.940	0.10	1
487	?	222	LEU	HB2	1.306	0.01	1
488	?	222	LEU	HB3	1.109	0.01	1
489	?	222	LEU	HG	1.202	0.01	1
490	?	222	LEU	CD1	24.530	0.10	1
491	?	222	LEU	HD11	0.576	0.01	2
492	?	222	LEU	HD12	0.576	0.01	2
493	?	222	LEU	HD13	0.576	0.01	2
494	?	222	LEU	CD2	24.820	0.10	1
495	?	222	LEU	HD21	0.570	0.01	2
496	?	222	LEU	HD22	0.570	0.01	2
497	?	222	LEU	HD23	0.570	0.01	2
498	?	223	CYS	N	113.560	0.10	1
499	?	223	CYS	H	8.002	0.01	1
500	?	223	CYS	CA	64.570	0.10	1
501	?	223	CYS	HA	3.657	0.01	1
502	?	223	CYS	C	176.220	0.10	1
503	?	223	CYS	CB	25.880	0.10	1
504	?	223	CYS	HB2	2.705	0.01	1
505	?	223	CYS	HB3	2.927	0.01	1
506	?	223	CYS	HG	2.656	0.01	1
507	?	224	ASP	N	119.120	0.10	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
508	?	224	ASP	H	7.485	0.01	1
509	?	224	ASP	CA	56.850	0.10	1
510	?	224	ASP	HA	4.410	0.01	1
511	?	224	ASP	C	177.800	0.10	1
512	?	224	ASP	CB	40.860	0.10	1
513	?	224	ASP	HB2	2.667	0.01	2
514	?	224	ASP	HB3	2.667	0.01	2
515	?	225	ASP	N	119.760	0.10	1
516	?	225	ASP	H	8.188	0.01	1
517	?	225	ASP	CA	57.230	0.10	1
518	?	225	ASP	HA	4.233	0.01	1
519	?	225	ASP	C	177.520	0.10	1
520	?	225	ASP	CB	40.690	0.10	1
521	?	225	ASP	HB2	2.629	0.01	2
522	?	225	ASP	HB3	2.493	0.01	2
523	?	226	LEU	N	115.940	0.10	1
524	?	226	LEU	H	7.848	0.01	1
525	?	226	LEU	CA	54.240	0.10	1
526	?	226	LEU	HA	4.230	0.01	1
527	?	226	LEU	C	174.920	0.10	1
528	?	226	LEU	CB	42.200	0.10	1
529	?	226	LEU	HB2	1.404	0.01	2
530	?	226	LEU	HB3	1.368	0.01	2
531	?	226	LEU	HG	1.574	0.01	1
532	?	226	LEU	CD1	25.690	0.10	1
533	?	226	LEU	HD11	0.696	0.01	2
534	?	226	LEU	HD12	0.696	0.01	2
535	?	226	LEU	HD13	0.696	0.01	2
536	?	226	LEU	CD2	21.980	0.10	1
537	?	226	LEU	HD21	0.710	0.01	2
538	?	226	LEU	HD22	0.710	0.01	2
539	?	226	LEU	HD23	0.710	0.01	2
540	?	227	ASP	N	118.880	0.10	1
541	?	227	ASP	H	7.557	0.01	1
542	?	227	ASP	CA	55.160	0.10	1
543	?	227	ASP	HA	4.253	0.01	1
544	?	227	ASP	C	174.060	0.10	1
545	?	227	ASP	CB	38.940	0.10	1
546	?	227	ASP	HB2	2.481	0.01	2
547	?	227	ASP	HB3	2.917	0.01	2
548	?	228	LEU	N	117.460	0.10	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
549	?	228	LEU	H	8.085	0.01	1
550	?	228	LEU	CA	52.540	0.10	1
551	?	228	LEU	HA	4.272	0.01	1
552	?	228	LEU	C	176.400	0.10	1
553	?	228	LEU	CB	43.530	0.10	1
554	?	228	LEU	HB2	0.626	0.01	1
555	?	228	LEU	HB3	1.115	0.01	1
556	?	228	LEU	CG	27.830	0.10	1
557	?	228	LEU	HG	1.119	0.01	1
558	?	228	LEU	CD1	25.540	0.10	1
559	?	228	LEU	HD11	0.104	0.01	2
560	?	228	LEU	HD12	0.104	0.01	2
561	?	228	LEU	HD13	0.104	0.01	2
562	?	228	LEU	CD2	21.310	0.10	1
563	?	228	LEU	HD21	0.110	0.01	2
564	?	228	LEU	HD22	0.110	0.01	2
565	?	228	LEU	HD23	0.110	0.01	2
566	?	229	ASN	N	120.110	0.10	1
567	?	229	ASN	H	8.430	0.01	1
568	?	229	ASN	CA	50.950	0.10	1
569	?	229	ASN	HA	4.706	0.01	1
570	?	229	ASN	C	173.830	0.10	1
571	?	229	ASN	CB	38.560	0.10	1
572	?	229	ASN	HB2	2.973	0.01	2
573	?	229	ASN	HB3	3.295	0.01	2
574	?	229	ASN	ND2	112.190	0.10	1
575	?	229	ASN	HD21	7.033	0.01	1
576	?	229	ASN	HD22	7.892	0.01	1
577	?	230	PRO	CA	64.550	0.10	1
578	?	230	PRO	HA	4.653	0.01	1
579	?	230	PRO	C	178.710	0.10	1
580	?	230	PRO	CB	32.350	0.10	1
581	?	230	PRO	HB2	2.252	0.01	2
582	?	230	PRO	HB3	1.979	0.01	2
583	?	230	PRO	CD	50.830	0.10	1
584	?	230	PRO	HG2	2.007	0.01	2
585	?	230	PRO	HG3	2.007	0.01	2
586	?	230	PRO	HD2	4.268	0.01	2
587	?	230	PRO	HD3	3.947	0.01	2
588	?	231	LEU	N	116.640	0.10	1
589	?	231	LEU	H	7.634	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
590	?	231	LEU	CA	57.450	0.10	1
591	?	231	LEU	HA	3.983	0.01	1
592	?	231	LEU	C	177.880	0.10	1
593	?	231	LEU	CB	41.400	0.10	1
594	?	231	LEU	HB2	1.484	0.01	2
595	?	231	LEU	HB3	1.742	0.01	2
596	?	231	LEU	HG	1.633	0.01	1
597	?	231	LEU	CD1	24.650	0.10	1
598	?	231	LEU	HD11	0.909	0.01	2
599	?	231	LEU	HD12	0.909	0.01	2
600	?	231	LEU	HD13	0.909	0.01	2
601	?	231	LEU	CD2	22.970	0.10	1
602	?	231	LEU	HD21	0.832	0.01	2
603	?	231	LEU	HD22	0.832	0.01	2
604	?	231	LEU	HD23	0.832	0.01	2
605	?	232	THR	N	105.090	0.10	1
606	?	232	THR	H	6.944	0.01	1
607	?	232	THR	CA	61.490	0.10	1
608	?	232	THR	HA	4.144	0.01	1
609	?	232	THR	C	176.400	0.10	1
610	?	232	THR	CB	68.440	0.10	1
611	?	232	THR	HB	3.853	0.01	1
612	?	232	THR	HG1	5.243	0.01	1
613	?	232	THR	HG21	0.922	0.01	2
614	?	232	THR	HG22	0.922	0.01	2
615	?	232	THR	HG23	0.922	0.01	2
616	?	233	PHE	N	119.260	0.10	1
617	?	233	PHE	H	8.435	0.01	1
618	?	233	PHE	CA	63.100	0.10	1
619	?	233	PHE	HA	4.116	0.01	1
620	?	233	PHE	C	176.870	0.10	1
621	?	233	PHE	CB	40.760	0.10	1
622	?	233	PHE	HB2	2.703	0.01	1
623	?	233	PHE	HB3	3.075	0.01	1
624	?	233	PHE	HZ	7.193	0.01	1
625	?	233	PHE	HD1	7.310	0.01	2
626	?	233	PHE	HD2	7.310	0.01	2
627	?	233	PHE	HE1	7.197	0.01	2
628	?	233	PHE	HE2	7.197	0.01	2
629	?	234	VAL	N	118.520	0.10	1
630	?	234	VAL	H	8.240	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
631	?	234	VAL	CA	69.380	0.10	1
632	?	234	VAL	HA	3.755	0.01	1
633	?	234	VAL	C	174.210	0.10	1
634	?	234	VAL	CB	27.980	0.10	1
635	?	234	VAL	HB	2.506	0.01	1
636	?	234	VAL	CG1	20.340	0.10	1
637	?	234	VAL	HG11	0.906	0.01	2
638	?	234	VAL	HG12	0.906	0.01	2
639	?	234	VAL	HG13	0.906	0.01	2
640	?	234	VAL	CG2	25.180	0.10	1
641	?	234	VAL	HG21	1.003	0.01	2
642	?	234	VAL	HG22	1.003	0.01	2
643	?	234	VAL	HG23	1.003	0.01	2
644	?	235	PRO	CA	64.970	0.10	1
645	?	235	PRO	HA	4.302	0.01	1
646	?	235	PRO	C	178.990	0.10	1
647	?	235	PRO	CB	30.350	0.10	1
648	?	235	PRO	HB2	1.780	0.01	2
649	?	235	PRO	HB3	2.157	0.01	2
650	?	235	PRO	HG2	1.913	0.01	2
651	?	235	PRO	HG3	1.944	0.01	2
652	?	235	PRO	CD	49.150	0.10	1
653	?	235	PRO	HD2	3.405	0.01	2
654	?	235	PRO	HD3	3.481	0.01	2
655	?	236	ALA	N	118.820	0.10	1
656	?	236	ALA	H	6.536	0.01	1
657	?	236	ALA	CA	54.870	0.10	1
658	?	236	ALA	HA	4.049	0.01	1
659	?	236	ALA	C	179.780	0.10	1
660	?	236	ALA	CB	19.380	0.10	1
661	?	236	ALA	HB1	1.295	0.01	2
662	?	236	ALA	HB2	1.295	0.01	2
663	?	236	ALA	HB3	1.295	0.01	2
664	?	237	ILE	N	120.950	0.10	1
665	?	237	ILE	H	8.945	0.01	1
666	?	237	ILE	CA	65.850	0.10	1
667	?	237	ILE	HA	3.473	0.01	1
668	?	237	ILE	C	176.710	0.10	1
669	?	237	ILE	CB	38.170	0.10	1
670	?	237	ILE	HB	1.874	0.01	1
671	?	237	ILE	CG1	28.910	0.10	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
672	?	237	ILE	HG12	2.002	0.01	2
673	?	237	ILE	HG13	0.787	0.01	2
674	?	237	ILE	CG2	18.650	0.10	1
675	?	237	ILE	HG21	0.929	0.01	2
676	?	237	ILE	HG22	0.929	0.01	2
677	?	237	ILE	HG23	0.929	0.01	2
678	?	237	ILE	CD1	15.270	0.10	1
679	?	237	ILE	HD11	0.735	0.01	2
680	?	237	ILE	HD12	0.735	0.01	2
681	?	237	ILE	HD13	0.735	0.01	2
682	?	238	ALA	N	121.490	0.10	1
683	?	238	ALA	H	8.398	0.01	1
684	?	238	ALA	CA	56.020	0.10	1
685	?	238	ALA	HA	3.558	0.01	1
686	?	238	ALA	C	178.670	0.10	1
687	?	238	ALA	CB	17.940	0.10	1
688	?	238	ALA	HB1	1.269	0.01	2
689	?	238	ALA	HB2	1.269	0.01	2
690	?	238	ALA	HB3	1.269	0.01	2
691	?	239	SER	N	109.950	0.10	1
692	?	239	SER	H	7.724	0.01	1
693	?	239	SER	CA	61.280	0.10	1
694	?	239	SER	HA	4.063	0.01	1
695	?	239	SER	C	175.760	0.10	1
696	?	239	SER	CB	62.820	0.10	1
697	?	239	SER	HB2	3.821	0.01	2
698	?	239	SER	HB3	3.887	0.01	2
699	?	240	ALA	N	124.880	0.10	1
700	?	240	ALA	H	7.539	0.01	1
701	?	240	ALA	CA	55.150	0.10	1
702	?	240	ALA	HA	4.114	0.01	1
703	?	240	ALA	C	179.510	0.10	1
704	?	240	ALA	CB	18.080	0.10	1
705	?	240	ALA	HB1	1.371	0.01	2
706	?	240	ALA	HB2	1.371	0.01	2
707	?	240	ALA	HB3	1.371	0.01	2
708	?	241	ILE	N	117.550	0.10	1
709	?	241	ILE	H	8.337	0.01	1
710	?	241	ILE	CA	65.970	0.10	1
711	?	241	ILE	HA	3.205	0.01	1
712	?	241	ILE	C	176.620	0.10	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
713	?	241	ILE	CB	38.280	0.10	1
714	?	241	ILE	HB	1.499	0.01	1
715	?	241	ILE	HG12	1.901	0.01	2
716	?	241	ILE	HG13	0.608	0.01	2
717	?	241	ILE	CG2	15.720	0.10	1
718	?	241	ILE	HG21	-0.262	0.01	2
719	?	241	ILE	HG22	-0.262	0.01	2
720	?	241	ILE	HG23	-0.262	0.01	2
721	?	241	ILE	CD1	14.840	0.10	1
722	?	241	ILE	HD11	0.683	0.01	2
723	?	241	ILE	HD12	0.683	0.01	2
724	?	241	ILE	HD13	0.683	0.01	2
725	?	242	ARG	N	116.540	0.10	1
726	?	242	ARG	H	7.958	0.01	1
727	?	242	ARG	CA	60.830	0.10	1
728	?	242	ARG	HA	3.560	0.01	1
729	?	242	ARG	C	177.840	0.10	1
730	?	242	ARG	CB	29.460	0.10	1
731	?	242	ARG	HB2	1.679	0.01	2
732	?	242	ARG	HB3	1.679	0.01	2
733	?	242	ARG	HG2	1.675	0.01	2
734	?	242	ARG	HG3	1.675	0.01	2
735	?	242	ARG	HD2	3.106	0.01	2
736	?	242	ARG	HD3	3.106	0.01	2
737	?	242	ARG	HE	7.337	0.01	1
738	?	243	GLN	N	117.210	0.10	1
739	?	243	GLN	H	8.251	0.01	1
740	?	243	GLN	CA	58.800	0.10	1
741	?	243	GLN	HA	3.948	0.01	1
742	?	243	GLN	C	178.140	0.10	1
743	?	243	GLN	CB	28.480	0.10	1
744	?	243	GLN	HB2	2.087	0.01	2
745	?	243	GLN	HB3	2.087	0.01	2
746	?	243	GLN	HG2	2.436	0.01	2
747	?	243	GLN	HG3	2.276	0.01	2
748	?	243	GLN	NE2	111.580	0.10	1
749	?	243	GLN	HE21	6.725	0.01	1
750	?	243	GLN	HE22	7.321	0.01	1
751	?	244	GLN	N	118.130	0.10	1
752	?	244	GLN	H	7.673	0.01	1
753	?	244	GLN	CA	59.050	0.10	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
754	?	244	GLN	HA	4.026	0.01	1
755	?	244	GLN	C	177.990	0.10	1
756	?	244	GLN	CB	29.240	0.10	1
757	?	244	GLN	HB2	2.088	0.01	1
758	?	244	GLN	HB3	1.859	0.01	1
759	?	244	GLN	HG2	2.608	0.01	2
760	?	244	GLN	HG3	2.272	0.01	2
761	?	244	GLN	HE21	7.137	0.01	1
762	?	244	GLN	HE22	7.187	0.01	1
763	?	245	ILE	N	117.410	0.10	1
764	?	245	ILE	H	8.109	0.01	1
765	?	245	ILE	CA	64.990	0.10	1
766	?	245	ILE	HA	3.896	0.01	1
767	?	245	ILE	C	177.440	0.10	1
768	?	245	ILE	CB	38.130	0.10	1
769	?	245	ILE	HB	1.844	0.01	1
770	?	245	ILE	HG12	1.309	0.01	2
771	?	245	ILE	HG13	0.862	0.01	2
772	?	245	ILE	CG2	17.190	0.10	1
773	?	245	ILE	HG21	0.710	0.01	2
774	?	245	ILE	HG22	0.710	0.01	2
775	?	245	ILE	HG23	0.710	0.01	2
776	?	245	ILE	CD1	13.620	0.10	1
777	?	245	ILE	HD11	0.135	0.01	2
778	?	245	ILE	HD12	0.135	0.01	2
779	?	245	ILE	HD13	0.135	0.01	2
780	?	246	GLU	N	119.110	0.10	1
781	?	246	GLU	H	7.806	0.01	1
782	?	246	GLU	CA	58.370	0.10	1
783	?	246	GLU	HA	4.016	0.01	1
784	?	246	GLU	C	176.760	0.10	1
785	?	246	GLU	CB	29.410	0.10	1
786	?	246	GLU	HB2	2.004	0.01	2
787	?	246	GLU	HB3	2.004	0.01	2
788	?	246	GLU	HG2	2.232	0.01	2
789	?	246	GLU	HG3	2.330	0.01	2
790	?	247	SER	N	111.570	0.10	1
791	?	247	SER	H	7.596	0.01	1
792	?	247	SER	CA	58.670	0.10	1
793	?	247	SER	HA	4.351	0.01	1
794	?	247	SER	C	173.010	0.10	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
795	?	247	SER	CB	63.850	0.10	1
796	?	247	SER	HB2	3.818	0.01	2
797	?	247	SER	HB3	3.842	0.01	2
798	?	248	TYR	N	125.450	0.10	1
799	?	248	TYR	H	7.527	0.01	1
800	?	248	TYR	CA	57.600	0.10	1
801	?	248	TYR	HA	4.607	0.01	1
802	?	248	TYR	C	173.320	0.10	1
803	?	248	TYR	CB	38.390	0.10	1
804	?	248	TYR	HB2	2.956	0.01	1
805	?	248	TYR	HB3	3.097	0.01	1
806	?	248	TYR	HD1	7.100	0.01	3
807	?	248	TYR	HD2	7.100	0.01	3
808	?	248	TYR	HE1	6.744	0.01	3
809	?	248	TYR	HE2	6.744	0.01	3
810	?	249	PRO	CA	63.230	0.10	1
811	?	249	PRO	HA	4.386	0.01	1
812	?	249	PRO	C	176.100	0.10	1
813	?	249	PRO	CB	31.340	0.10	1
814	?	249	PRO	HB2	1.815	0.01	2
815	?	249	PRO	HB3	2.095	0.01	2
816	?	249	PRO	HG2	1.814	0.01	2
817	?	249	PRO	HG3	1.814	0.01	2
818	?	249	PRO	CD	50.400	0.10	1
819	?	249	PRO	HD2	3.681	0.01	1
820	?	249	PRO	HD3	2.909	0.01	1
821	?	250	THR	N	113.830	0.10	1
822	?	250	THR	H	8.120	0.01	1
823	?	250	THR	CA	61.810	0.10	1
824	?	250	THR	HA	4.253	0.01	1
825	?	250	THR	C	173.990	0.10	1
826	?	250	THR	CB	69.690	0.10	1
827	?	250	THR	HB	4.241	0.01	1
828	?	250	THR	CG2	21.590	0.10	1
829	?	250	THR	HG21	1.207	0.01	2
830	?	250	THR	HG22	1.207	0.01	2
831	?	250	THR	HG23	1.207	0.01	2
832	?	251	ASP	N	121.790	0.10	1
833	?	251	ASP	H	8.288	0.01	1
834	?	251	ASP	CA	54.410	0.10	1
835	?	251	ASP	HA	4.540	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
836	?	251	ASP	C	175.590	0.10	1
837	?	251	ASP	CB	40.970	0.10	1
838	?	251	ASP	HB2	2.559	0.01	2
839	?	251	ASP	HB3	2.612	0.01	2
840	?	252	SER	N	115.790	0.10	1
841	?	252	SER	H	8.142	0.01	1
842	?	252	SER	CA	58.410	0.10	1
843	?	252	SER	HA	4.333	0.01	1
844	?	252	SER	C	173.560	0.10	1
845	?	252	SER	CB	63.720	0.10	1
846	?	252	SER	HB2	3.726	0.01	2
847	?	252	SER	HB3	3.726	0.01	2
848	?	253	ILE	N	122.240	0.10	1
849	?	253	ILE	H	8.026	0.01	1
850	?	253	ILE	CA	61.210	0.10	1
851	?	253	ILE	HA	4.091	0.01	1
852	?	253	ILE	C	175.390	0.10	1
853	?	253	ILE	CB	38.420	0.10	1
854	?	253	ILE	HB	1.812	0.01	1
855	?	253	ILE	HG12	1.377	0.01	2
856	?	253	ILE	HG13	1.102	0.01	2
857	?	253	ILE	CG2	17.340	0.10	1
858	?	253	ILE	HG21	0.804	0.01	2
859	?	253	ILE	HG22	0.804	0.01	2
860	?	253	ILE	HG23	0.804	0.01	2
861	?	253	ILE	CD1	12.770	0.10	1
862	?	253	ILE	HD11	0.782	0.01	2
863	?	253	ILE	HD12	0.782	0.01	2
864	?	253	ILE	HD13	0.782	0.01	2
865	?	254	LEU	N	126.050	0.10	1
866	?	254	LEU	H	8.214	0.01	1
867	?	254	LEU	CA	54.900	0.10	1
868	?	254	LEU	HA	4.278	0.01	1
869	?	254	LEU	C	176.510	0.10	1
870	?	254	LEU	CB	42.110	0.10	1
871	?	254	LEU	HB2	1.546	0.01	2
872	?	254	LEU	HB3	1.491	0.01	2
873	?	254	LEU	HG	1.545	0.01	1
874	?	254	LEU	HD11	0.835	0.01	2
875	?	254	LEU	HD12	0.835	0.01	2
876	?	254	LEU	HD13	0.835	0.01	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
877	?	254	LEU	HD21	0.776	0.01	2
878	?	254	LEU	HD22	0.776	0.01	2
879	?	254	LEU	HD23	0.776	0.01	2
880	?	255	GLU	N	121.850	0.10	1
881	?	255	GLU	H	8.313	0.01	1
882	?	255	GLU	CA	56.460	0.10	1
883	?	255	GLU	HA	4.177	0.01	1
884	?	255	GLU	C	175.380	0.10	1
885	?	255	GLU	CB	30.330	0.10	1
886	?	255	GLU	HB2	1.841	0.01	2
887	?	255	GLU	HB3	1.943	0.01	2
888	?	255	GLU	HG2	2.146	0.01	2
889	?	255	GLU	HG3	2.181	0.01	2
890	?	256	ASP	N	121.260	0.10	1
891	?	256	ASP	H	8.320	0.01	1
892	?	256	ASP	CA	54.400	0.10	1
893	?	256	ASP	HA	4.486	0.01	1
894	?	256	ASP	C	175.370	0.10	1
895	?	256	ASP	CB	41.000	0.10	1
896	?	256	ASP	HB2	2.545	0.01	2
897	?	256	ASP	HB3	2.625	0.01	2
898	?	257	GLN	N	121.200	0.10	1
899	?	257	GLN	H	8.294	0.01	1
900	?	257	GLN	CA	55.500	0.10	1
901	?	257	GLN	HA	4.327	0.01	1
902	?	257	GLN	C	174.520	0.10	1
903	?	257	GLN	CB	29.360	0.10	1
904	?	257	GLN	HB2	2.129	0.01	2
905	?	257	GLN	HB3	1.874	0.01	2
906	?	257	GLN	HG2	2.281	0.01	2
907	?	257	GLN	HG3	2.281	0.01	2
908	?	257	GLN	NE2	112.950	0.10	1
909	?	257	GLN	HE21	6.883	0.01	1
910	?	257	GLN	HE22	7.425	0.01	1
911	?	258	SER	N	122.900	0.10	1
912	?	258	SER	H	8.011	0.01	1
913	?	258	SER	CA	60.150	0.10	1
914	?	258	SER	HA	4.143	0.01	1
915	?	258	SER	C	177.920	0.10	1
916	?	258	SER	CB	64.660	0.10	1
917	?	258	SER	HB2	3.769	0.01	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
918	?	258	SER	HB3	3.769	0.01	2

7.1.2 Chemical shift referencing [i](#)

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

7.1.3 Completeness of resonance assignments [i](#)

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 808. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/312 (0%)	0/124 (0%)	0/128 (0%)	0/60 (0%)
Sidechain	0/449 (0%)	0/262 (0%)	0/170 (0%)	0/17 (0%)
Aromatic	0/47 (0%)	0/25 (0%)	0/21 (0%)	0/1 (0%)
Overall	0/808 (0%)	0/411 (0%)	0/319 (0%)	0/78 (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 938. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/370 (0%)	0/147 (0%)	0/152 (0%)	0/71 (0%)
Sidechain	0/521 (0%)	0/304 (0%)	0/199 (0%)	0/18 (0%)
Aromatic	0/47 (0%)	0/25 (0%)	0/21 (0%)	0/1 (0%)
Overall	0/938 (0%)	0/476 (0%)	0/372 (0%)	0/90 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (snf5.bmr.b.data). RCI is only applicable to proteins.