



Full wwPDB NMR Structure Validation Report ⓘ

Feb 22, 2017 – 12:46 AM EST

PDB ID : 2NBJ
Title : DNA-archeal MC1 protein complex structure by NMR
Authors : Paquet, F.; Loth, K.; Landon, C.
Deposited on : 2016-02-25

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
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-20028442
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

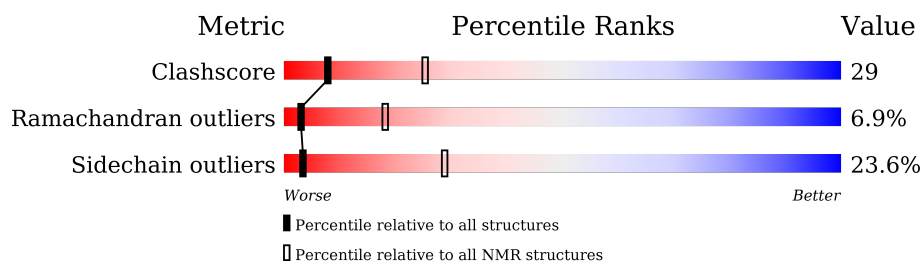
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


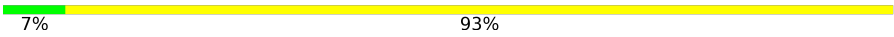
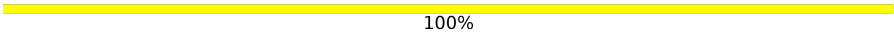
The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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	93	 67% 20% 9% . .
2	B	15	 7% 93%
3	C	15	 100%

2 Ensemble composition and analysis ⓘ

This entry contains 12 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:3-A:92 (90)	0.19	10

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 and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 5, 7, 8, 9, 10, 12
2	3, 6, 11
Single-model clusters	4

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2487 atoms, of which 1122 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Chromosomal protein MC1.

Mol	Chain	Residues	Atoms						Trace
1	A	93	Total	C	H	N	O	S	0
			1534	472	781	147	133	1	

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms						Trace
2	B	15	Total	C	H	N	O	P	0
			466	144	166	63	79	14	

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*T)-3').

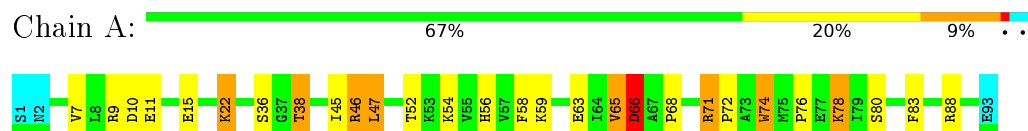
Mol	Chain	Residues	Atoms						Trace
3	C	15	Total	C	H	N	O	P	0
			487	150	175	48	99	15	

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.

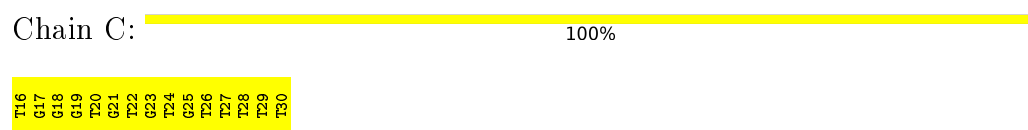
- Molecule 1: Chromosomal protein MC1



- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*A)-3')



- Molecule 3: DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*TP*T)-3')



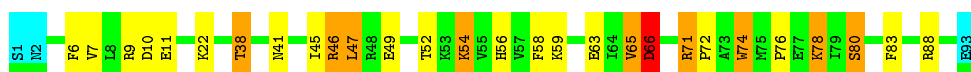
4.2 Scores per residue for each member of the ensemble

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

4.2.1 Score per residue for model 1

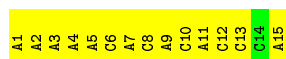
- Molecule 1: Chromosomal protein MC1





- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*CP*A)-3')

Chain B: 7% 93%



- Molecule 3: DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*TP*T)-3')

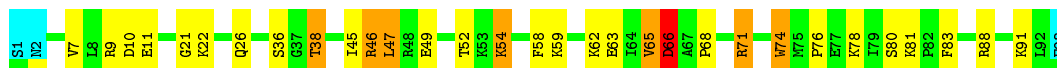
Chain C: 7% 93%



4.2.2 Score per residue for model 2

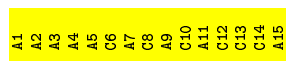
- Molecule 1: Chromosomal protein MC1

Chain A: 63% 25% 8%



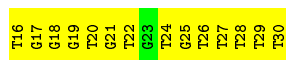
- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*CP*A)-3')

Chain B: 100%



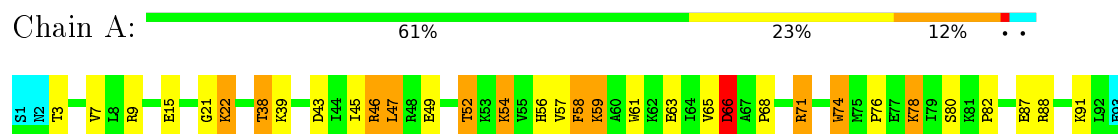
- Molecule 3: DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*TP*T)-3')

Chain C: 7% 93%

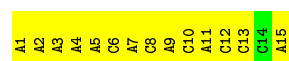


4.2.3 Score per residue for model 3

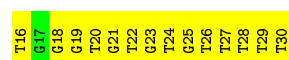
- Molecule 1: Chromosomal protein MC1



- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*A)-3')

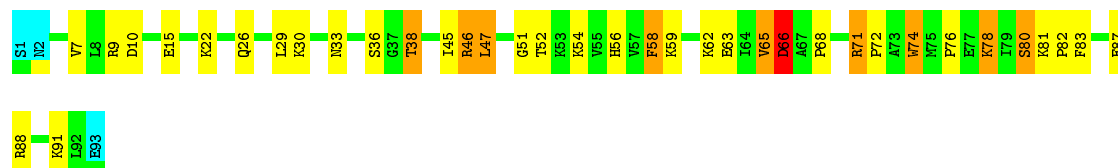


- Molecule 3: DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*TP*T)-3')

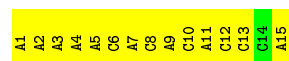


4.2.4 Score per residue for model 4

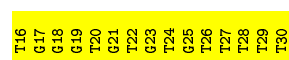
- Molecule 1: Chromosomal protein MC1



- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*A)-3')

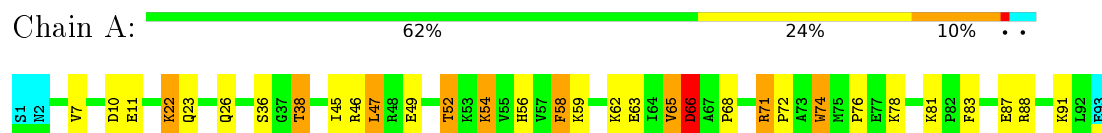


- Molecule 3: DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*TP*T)-3')



4.2.5 Score per residue for model 5

- Molecule 1: Chromosomal protein MC1



- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*CP*A)-3')

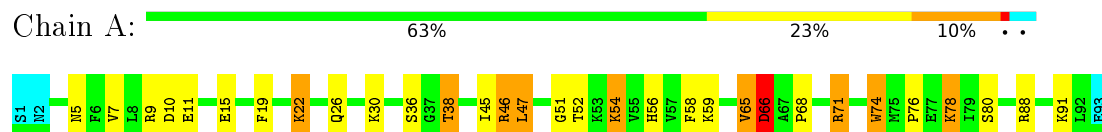


- Molecule 3: DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*TP*T)-3')



4.2.6 Score per residue for model 6

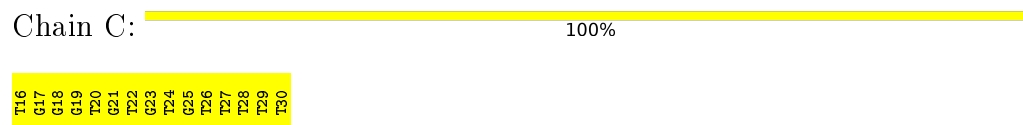
- Molecule 1: Chromosomal protein MC1



- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*CP*A)-3')

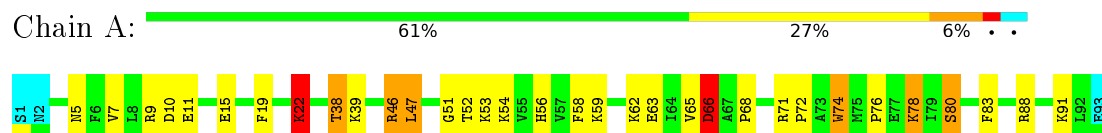


- Molecule 3: DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*TP*T)-3')



4.2.7 Score per residue for model 7

- Molecule 1: Chromosomal protein MC1



- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*CP*A)-3')

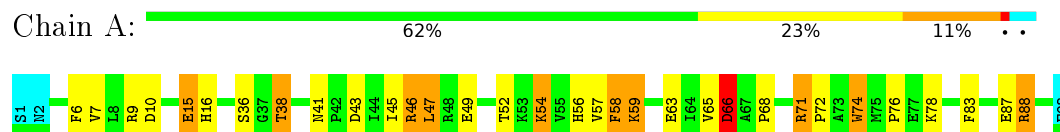


- Molecule 3: DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*TP*T)-3')



4.2.8 Score per residue for model 8

- Molecule 1: Chromosomal protein MC1



- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*CP*A)-3')



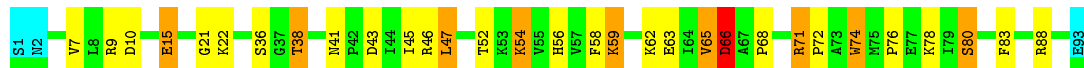
- Molecule 3: DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*TP*T)-3')



4.2.9 Score per residue for model 9

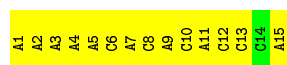
- Molecule 1: Chromosomal protein MC1

Chain A: 



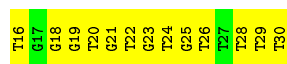
- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*A)-3')

Chain B: 



- Molecule 3: DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*TP*T)-3')

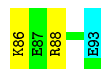
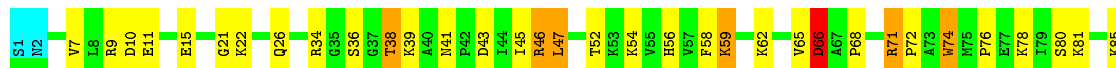
Chain C: 




4.2.10 Score per residue for model 10 (medoid)

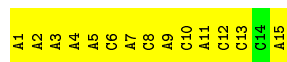
- Molecule 1: Chromosomal protein MC1

Chain A: 



- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*A)-3')

Chain B: 



- Molecule 3: DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*TP*T)-3')

Chain C: 

T16
G17
G18
G19
T20
G21
T22
G23
G25
T26
T27
T28
T29
T30

4.2.11 Score per residue for model 11

- Molecule 1: Chromosomal protein MC1

Chain A: 69% 19% 8% ..

S1
S2
V7
E15
K22
Q23
S36
G37
T38
T44
T45
R46
L47
G51
T52
H56
V57
F58
K59
A60
W61
V65
D66
A67
P68
R71
I74
K75
P76
E77
K78
I79
S80
K81
P82
R88
E93

- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*CP*A)-3')

Chain B: 7% 93%

A1
A2
A3
A4
A5
C6
A7
C8
A9
C10
A11
C12
C13
C14
A15

- Molecule 3: DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*TP*T)-3')

Chain C: 100%

T16
G17
G18
G19
T20
G21
T22
G23
G25
T26
T27
T28
T29
T30

4.2.12 Score per residue for model 12

- Molecule 1: Chromosomal protein MC1

Chain A: 62% 25% 9% ..

S1
S2
F6
V7
L8
R9
D10
E11
E15
K22
Q23
A32
S36
G37
T38
T45
R46
L47
R48
E49
R50
G51
T52
K53
H56
V57
F58
K59
A60
V65
D66
A67
P68
R71
I74
K75
P76
E77
K78
I79
S80
E87
R88
E93

- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*CP*AP*CP*AP*CP*AP*CP*CP*CP*A)-3')

Chain B: 7% 93%

A1
A2
A3
A4
A5
C6
A7
C8
A9
C10
A11
C12
C13
C14
A15

- Molecule 3: DNA (5'-D(P*TP*GP*GP*GP*TP*GP*TP*GP*TP*GP*TP*TP*TP*T)-3')

Chain C: 100%

T16
G17
G18
G19
T20
G21
T22
G23
T24
G25
T26
T27
T28
T29
T30

5 Refinement protocol and experimental data overview

Of the 200 calculated structures, 12 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
HADDOCK	structure solution	
HADDOCK	refinement	
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)	2nbj_cs.cif
Number of chemical shift lists	1
Total number of shifts	714
Number of shifts mapped to atoms	0
Number of unparsed shifts	714
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	729	762	760	16±3
2	B	300	166	167	34±4
3	C	312	175	175	33±3
All	All	16092	13236	13224	855

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:24:DT:H2''	3:C:25:DG:H5''	1.03	1.30	9	12
2:B:10:DC:H2''	2:B:11:DA:H4'	0.98	1.32	5	10
2:B:4:DA:H2''	2:B:5:DA:C8	0.92	1.99	4	12
2:B:10:DC:C2'	2:B:11:DA:H4'	0.91	1.95	1	12
3:C:22:DT:H2''	3:C:23:DG:H5'	0.85	1.46	6	4
2:B:4:DA:H4'	3:C:30:DT:H4'	0.84	1.48	9	10
2:B:1:DA:H2''	2:B:2:DA:H5''	0.84	1.50	1	12
2:B:5:DA:H2'	2:B:6:DC:C6	0.82	2.09	6	12
3:C:21:DG:H2'	3:C:22:DT:C6	0.82	2.10	7	10
2:B:8:DC:H2''	2:B:9:DA:N7	0.82	1.90	4	12
2:B:5:DA:H2'	2:B:6:DC:C5	0.81	2.11	2	12
3:C:29:DT:H3'	3:C:30:DT:H71	0.76	1.55	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:29:DT:C2'	3:C:30:DT:H5'	0.76	2.11	1	12
3:C:28:DT:O2	3:C:29:DT:H1'	0.74	1.82	4	12
1:A:65:VAL:O	1:A:66:ASP:HB2	0.74	1.82	1	12
2:B:3:DA:H2''	2:B:4:DA:OP2	0.74	1.80	2	11
3:C:19:DG:H4'	3:C:20:DT:OP1	0.73	1.83	12	12
3:C:28:DT:H2''	3:C:29:DT:C6	0.71	2.19	2	12
2:B:2:DA:H2''	2:B:3:DA:OP2	0.71	1.85	5	10
2:B:4:DA:C2'	2:B:5:DA:C8	0.71	2.73	12	12
3:C:21:DG:H2'	3:C:22:DT:H71	0.71	1.62	2	7
2:B:1:DA:H2''	2:B:2:DA:C5'	0.70	2.17	3	3
2:B:12:DC:H2''	2:B:13:DC:H5'	0.70	1.62	12	3
1:A:54:LYS:HE3	2:B:4:DA:H3'	0.70	1.64	2	6
2:B:4:DA:H2''	2:B:5:DA:H8	0.69	1.48	3	12
1:A:71:ARG:HG3	3:C:18:DG:H4'	0.68	1.63	6	8
3:C:25:DG:H2''	3:C:26:DT:O4'	0.68	1.88	3	12
2:B:12:DC:H2'	2:B:13:DC:C5	0.67	2.22	9	12
3:C:16:DT:C6	3:C:16:DT:H5''	0.67	2.24	8	5
2:B:10:DC:H2'	2:B:11:DA:H4'	0.67	1.66	1	2
3:C:19:DG:H2''	3:C:20:DT:C5'	0.67	2.20	8	4
2:B:6:DC:H2''	2:B:7:DA:N7	0.66	2.06	9	11
2:B:3:DA:H2''	2:B:4:DA:C8	0.65	2.26	1	12
3:C:16:DT:H5''	3:C:16:DT:H6	0.65	1.52	12	6
1:A:22:LYS:HD2	3:C:22:DT:H5'	0.65	1.67	1	5
3:C:16:DT:H5''	3:C:16:DT:C6	0.65	2.27	1	6
1:A:74:TRP:CZ2	3:C:16:DT:H2'	0.64	2.27	7	12
3:C:16:DT:H6	3:C:16:DT:H5''	0.64	1.53	3	5
3:C:19:DG:H2''	3:C:20:DT:H5''	0.64	1.69	12	2
2:B:11:DA:H2'	2:B:12:DC:C6	0.64	2.28	2	11
1:A:22:LYS:NZ	3:C:22:DT:H3'	0.63	2.09	12	1
3:C:21:DG:H5''	3:C:22:DT:H71	0.62	1.69	12	4
2:B:10:DC:H2'	2:B:11:DA:C4'	0.62	2.25	1	7
1:A:91:LYS:HE2	2:B:4:DA:H5'	0.62	1.71	6	1
1:A:47:LEU:O	1:A:56:HIS:HB2	0.61	1.95	9	10
3:C:19:DG:H2''	3:C:20:DT:O5'	0.61	1.94	6	10
2:B:4:DA:C4'	3:C:30:DT:H4'	0.61	2.24	9	5
2:B:1:DA:C2'	2:B:2:DA:H5''	0.60	2.25	1	5
3:C:18:DG:H5''	3:C:18:DG:C8	0.60	2.31	8	4
3:C:18:DG:H2''	3:C:19:DG:H5'	0.60	1.73	12	1
2:B:10:DC:C2'	2:B:11:DA:C4'	0.59	2.80	9	11
2:B:9:DA:H8	2:B:9:DA:O5'	0.59	1.80	2	8
3:C:28:DT:H2''	3:C:29:DT:O4'	0.59	1.96	12	12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:22:DT:H2''	3:C:23:DG:C8	0.59	2.32	12	4
2:B:10:DC:C3'	2:B:11:DA:H4'	0.58	2.28	6	2
2:B:3:DA:H2	3:C:29:DT:O2	0.58	1.81	5	12
1:A:22:LYS:HE3	3:C:22:DT:H5'	0.58	1.73	11	2
3:C:24:DT:C2'	3:C:25:DG:H5''	0.58	2.27	7	4
3:C:18:DG:C8	3:C:18:DG:H5''	0.57	2.34	2	5
3:C:28:DT:H2''	3:C:29:DT:H6	0.57	1.59	5	12
1:A:9:ARG:HB3	1:A:46:ARG:O	0.57	2.00	2	9
3:C:18:DG:C2'	3:C:19:DG:H5'	0.57	2.30	12	1
1:A:54:LYS:HD3	2:B:4:DA:H5''	0.56	1.77	7	2
1:A:26:GLN:HB2	3:C:21:DG:H5'	0.56	1.78	10	1
1:A:91:LYS:HG2	2:B:4:DA:H5'	0.56	1.76	7	5
2:B:12:DC:H2'	2:B:13:DC:C6	0.56	2.35	12	2
3:C:18:DG:C5'	3:C:18:DG:C8	0.56	2.88	8	5
3:C:16:DT:H5'	3:C:17:DG:C8	0.55	2.35	8	4
2:B:3:DA:H2''	2:B:4:DA:H8	0.55	1.62	1	11
3:C:18:DG:H2'	3:C:19:DG:O4'	0.55	2.02	12	2
2:B:9:DA:H5''	2:B:9:DA:C8	0.55	2.37	12	1
2:B:3:DA:C2'	2:B:4:DA:C8	0.55	2.90	8	12
2:B:9:DA:C5'	2:B:9:DA:C8	0.55	2.89	12	2
2:B:10:DC:O3'	2:B:11:DA:H4'	0.55	2.02	6	1
1:A:74:TRP:CD1	2:B:15:DA:H2	0.55	2.19	7	12
2:B:6:DC:H2''	2:B:7:DA:C8	0.55	2.37	11	4
3:C:29:DT:H2'	3:C:30:DT:H5'	0.55	1.79	2	5
1:A:63:GLU:HG3	1:A:83:PHE:CE1	0.55	2.37	4	7
3:C:17:DG:H1'	3:C:18:DG:N7	0.55	2.17	12	3
3:C:18:DG:C5'	3:C:18:DG:H8	0.54	2.15	3	7
2:B:7:DA:H2''	2:B:8:DC:O4'	0.54	2.02	3	2
2:B:4:DA:C2	3:C:28:DT:O2	0.54	2.61	5	12
2:B:5:DA:C2'	2:B:6:DC:C6	0.54	2.90	3	5
3:C:20:DT:H1'	3:C:21:DG:C8	0.54	2.36	11	1
1:A:47:LEU:N	1:A:47:LEU:HD23	0.54	2.18	3	4
3:C:26:DT:H2''	3:C:27:DT:C6	0.54	2.37	11	8
3:C:20:DT:H4'	3:C:21:DG:H5'	0.54	1.80	11	1
3:C:18:DG:H8	3:C:18:DG:C5'	0.53	2.15	5	4
3:C:21:DG:H5''	3:C:21:DG:C8	0.53	2.37	12	2
1:A:22:LYS:CE	3:C:22:DT:H3'	0.53	2.34	3	2
3:C:18:DG:C8	3:C:18:DG:C5'	0.53	2.92	2	6
2:B:8:DC:H2''	2:B:9:DA:C8	0.53	2.39	7	2
1:A:54:LYS:CE	2:B:4:DA:H3'	0.52	2.33	3	3
3:C:25:DG:C2'	3:C:26:DT:C6	0.52	2.92	6	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LYS:HD2	3:C:22:DT:H3'	0.52	1.81	4	2
2:B:10:DC:H2''	2:B:11:DA:C4'	0.52	2.22	5	2
1:A:54:LYS:CD	2:B:4:DA:H3'	0.52	2.35	4	1
3:C:28:DT:C2'	3:C:29:DT:C6	0.52	2.93	2	7
3:C:21:DG:H2'	3:C:22:DT:H6	0.52	1.59	7	6
1:A:86:LYS:HE3	3:C:29:DT:H5'	0.52	1.80	10	1
1:A:54:LYS:NZ	2:B:4:DA:H3'	0.52	2.19	6	4
2:B:4:DA:H2'	2:B:5:DA:C8	0.51	2.40	12	1
3:C:18:DG:H8	3:C:18:DG:H5''	0.51	1.64	5	1
3:C:25:DG:H2''	3:C:26:DT:C6	0.51	2.40	6	1
1:A:47:LEU:HD23	1:A:47:LEU:N	0.51	2.21	2	8
2:B:10:DC:O2	2:B:11:DA:H1'	0.51	2.05	4	5
2:B:5:DA:OP2	2:B:5:DA:H8	0.50	1.89	8	2
2:B:6:DC:H6	2:B:6:DC:O5'	0.50	1.90	5	1
2:B:11:DA:C3'	2:B:12:DC:H5''	0.50	2.37	5	1
2:B:4:DA:H2	3:C:28:DT:O2	0.50	1.90	10	8
2:B:1:DA:C2	2:B:2:DA:C2	0.50	2.99	12	6
1:A:62:LYS:HA	1:A:81:LYS:O	0.50	2.07	5	4
2:B:10:DC:H2'	2:B:11:DA:O4'	0.50	2.07	9	4
2:B:9:DA:C8	2:B:9:DA:C5'	0.50	2.94	5	1
1:A:72:PRO:HD3	3:C:17:DG:H4'	0.49	1.82	5	4
1:A:66:ASP:HB3	1:A:78:LYS:HA	0.49	1.83	4	7
2:B:4:DA:H2	3:C:28:DT:C2	0.49	2.24	8	6
3:C:20:DT:O3'	3:C:21:DG:H8	0.49	1.91	2	3
3:C:27:DT:H2'	3:C:28:DT:C6	0.49	2.43	12	8
2:B:9:DA:H2'	2:B:10:DC:O4'	0.49	2.07	4	3
2:B:1:DA:C3'	2:B:2:DA:H5''	0.49	2.37	7	1
2:B:9:DA:C8	2:B:9:DA:O5'	0.49	2.66	10	2
2:B:5:DA:H5'	3:C:30:DT:H5''	0.49	1.85	7	1
1:A:63:GLU:O	1:A:80:SER:HA	0.48	2.08	1	4
1:A:57:VAL:HG12	1:A:88:ARG:O	0.48	2.09	8	1
2:B:6:DC:O5'	2:B:6:DC:H6	0.48	1.92	4	1
1:A:5:ASN:HB3	1:A:19:PHE:O	0.48	2.08	6	2
3:C:17:DG:H1'	3:C:18:DG:C8	0.48	2.44	8	3
1:A:22:LYS:HZ1	3:C:22:DT:H3'	0.48	1.69	12	1
1:A:22:LYS:HE3	3:C:22:DT:H3'	0.47	1.85	7	2
1:A:49:GLU:HB2	1:A:56:HIS:CE1	0.47	2.44	12	1
3:C:21:DG:H2'	3:C:22:DT:C7	0.47	2.37	2	1
1:A:6:PHE:CE2	1:A:49:GLU:HG3	0.47	2.44	1	1
1:A:23:GLN:HG2	3:C:21:DG:H5'	0.47	1.86	12	1
2:B:9:DA:C5	2:B:10:DC:C5	0.47	3.03	6	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:4:DA:H2''	2:B:5:DA:O5'	0.47	2.09	12	1
2:B:10:DC:C2	2:B:11:DA:H1'	0.46	2.45	7	1
1:A:22:LYS:HE2	3:C:22:DT:H5'	0.46	1.87	7	1
3:C:27:DT:H6	3:C:27:DT:O5'	0.46	1.92	6	3
1:A:23:GLN:OE1	1:A:23:GLN:HA	0.46	2.10	5	1
3:C:20:DT:H1'	3:C:21:DG:N7	0.46	2.25	11	1
2:B:4:DA:H2''	2:B:5:DA:O4'	0.46	2.11	3	3
1:A:3:THR:HG23	1:A:21:GLY:O	0.45	2.11	3	1
1:A:43:ASP:O	1:A:59:LYS:HA	0.45	2.10	8	2
2:B:9:DA:C8	2:B:9:DA:H5''	0.45	2.46	5	1
1:A:54:LYS:HE2	2:B:4:DA:H3'	0.45	1.88	7	1
1:A:30:LYS:O	1:A:33:ASN:HB2	0.45	2.11	4	1
2:B:13:DC:C6	2:B:14:DC:N4	0.45	2.84	7	1
1:A:23:GLN:HA	1:A:23:GLN:OE1	0.45	2.10	11	1
1:A:32:ALA:HB2	1:A:60:ALA:HB1	0.45	1.87	12	1
1:A:33:ASN:HA	1:A:62:LYS:CE	0.45	2.41	4	1
1:A:21:GLY:O	1:A:22:LYS:HG3	0.45	2.11	9	3
1:A:71:ARG:CD	3:C:18:DG:H4'	0.45	2.42	1	3
1:A:9:ARG:HA	1:A:15:GLU:HA	0.45	1.89	8	4
1:A:43:ASP:O	1:A:59:LYS:HG3	0.45	2.12	10	2
1:A:85:LYS:HD3	1:A:85:LYS:C	0.44	2.32	10	1
3:C:20:DT:O3'	3:C:21:DG:C8	0.44	2.71	2	2
3:C:26:DT:H2''	3:C:27:DT:C5	0.44	2.46	6	3
1:A:58:PHE:HA	1:A:87:GLU:HB2	0.44	1.90	4	5
1:A:71:ARG:CG	3:C:18:DG:H4'	0.44	2.37	6	2
1:A:74:TRP:CH2	3:C:16:DT:H2'	0.43	2.49	4	4
2:B:3:DA:C5	2:B:4:DA:C6	0.43	3.06	4	6
3:C:18:DG:O5'	3:C:18:DG:H8	0.43	1.95	4	2
1:A:61:TRP:O	1:A:82:PRO:HA	0.43	2.13	3	2
1:A:6:PHE:CE1	1:A:49:GLU:HG3	0.43	2.48	8	2
1:A:72:PRO:HB2	1:A:74:TRP:CZ3	0.43	2.49	9	2
3:C:25:DG:H2''	3:C:26:DT:O5'	0.43	2.14	1	1
2:B:3:DA:C5	2:B:4:DA:C5	0.43	3.07	12	1
1:A:65:VAL:O	1:A:66:ASP:CB	0.43	2.67	8	3
3:C:22:DT:H2''	3:C:23:DG:C5'	0.42	2.40	3	1
1:A:52:THR:HB	1:A:54:LYS:HD3	0.42	1.91	5	1
3:C:17:DG:H2''	3:C:18:DG:N7	0.42	2.30	8	1
2:B:6:DC:H4'	3:C:28:DT:H4'	0.42	1.90	1	1
1:A:52:THR:HB	1:A:54:LYS:CD	0.42	2.44	3	1
3:C:16:DT:C5'	3:C:17:DG:C8	0.42	3.03	6	1
2:B:12:DC:C2'	2:B:13:DC:H5'	0.42	2.45	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:6:DC:H5''	2:B:6:DC:H6	0.42	1.74	7	1
1:A:62:LYS:HE2	1:A:80:SER:O	0.42	2.15	9	1
2:B:6:DC:H5''	2:B:6:DC:C6	0.41	2.50	7	1
1:A:29:LEU:CD1	1:A:82:PRO:HG2	0.41	2.45	4	1
2:B:9:DA:O5'	2:B:9:DA:H8	0.41	1.98	7	1
3:C:22:DT:C2'	3:C:23:DG:C8	0.41	3.03	12	1
1:A:72:PRO:HB2	1:A:74:TRP:CE3	0.41	2.50	1	1
2:B:14:DC:N4	3:C:17:DG:C6	0.41	2.88	2	1
3:C:16:DT:O5'	3:C:17:DG:C8	0.41	2.74	11	1
1:A:33:ASN:HA	1:A:62:LYS:HE3	0.41	1.93	4	1
3:C:27:DT:O5'	3:C:27:DT:H6	0.41	1.99	7	1
3:C:19:DG:C2'	3:C:20:DT:O5'	0.41	2.68	4	2
1:A:26:GLN:O	1:A:30:LYS:HE2	0.41	2.16	6	1
1:A:39:LYS:HA	1:A:62:LYS:O	0.41	2.16	7	1
2:B:3:DA:C4	2:B:4:DA:C5	0.41	3.09	7	1
2:B:4:DA:C2	3:C:28:DT:C2	0.41	3.09	9	1
3:C:21:DG:C2'	3:C:22:DT:C6	0.40	3.03	2	1
2:B:3:DA:C6	2:B:4:DA:C6	0.40	3.10	12	1
1:A:71:ARG:HD2	3:C:18:DG:H4'	0.40	1.93	5	1
3:C:21:DG:H2'	3:C:22:DT:C5	0.40	2.50	7	1
3:C:28:DT:H1'	3:C:29:DT:C1'	0.40	2.47	9	1
2:B:2:DA:C2'	2:B:3:DA:OP2	0.40	2.68	2	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	90/93 (97%)	67±1 (75±1%)	17±1 (18±1%)	6±1 (7±1%)	3	18
All	All	1080/1116 (97%)	807 (75%)	198 (18%)	75 (7%)	3	18

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	66	ASP	12
1	A	38	THR	12
1	A	76	PRO	12
1	A	68	PRO	11
1	A	10	ASP	10
1	A	51	GLY	5
1	A	22	LYS	5
1	A	41	ASN	4
1	A	39	LYS	2
1	A	53	LYS	1
1	A	16	HIS	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	76/79 (96%)	58±1 (76±2%)	18±1 (24±2%)	3	29
All	All	912/948 (96%)	697 (76%)	215 (24%)	3	29

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	74	TRP	12
1	A	7	VAL	12
1	A	47	LEU	12
1	A	46	ARG	12
1	A	38	THR	12
1	A	88	ARG	12
1	A	59	LYS	12
1	A	78	LYS	12
1	A	71	ARG	12
1	A	58	PHE	12
1	A	66	ASP	11
1	A	52	THR	11
1	A	45	ILE	11
1	A	80	SER	9
1	A	36	SER	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	54	LYS	8
1	A	11	GLU	7
1	A	15	GLU	7
1	A	65	VAL	7
1	A	22	LYS	4
1	A	26	GLN	3
1	A	49	GLU	3
1	A	34	ARG	1
1	A	57	VAL	1
1	A	53	LYS	1
1	A	8	LEU	1
1	A	44	ILE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: 2nbj_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	714
Number of shifts mapped to atoms	0
Number of unparsed shifts	714
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 714 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	.	2	ASN	HA	4.928	0.04	1
2	.	2	ASN	HB2	2.806	0.04	1
3	.	2	ASN	HB3	2.902	0.04	1
4	.	2	ASN	HD21	7.679	0.04	1
5	.	2	ASN	HD22	7.037	0.04	1
6	.	2	ASN	ND2	114.914	0.20	1
7	.	3	THR	H	8.358	0.04	1
8	.	3	THR	HA	4.064	0.04	1
9	.	3	THR	HB	4.064	0.04	1
10	.	3	THR	HG21	1.195	0.04	1
11	.	3	THR	HG22	1.195	0.04	1
12	.	3	THR	HG23	1.195	0.04	1
13	.	3	THR	N	117.937	0.20	1
14	.	4	ARG	H	8.245	0.04	1
15	.	4	ARG	HA	4.467	0.04	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	.	4	ARG	HB2	1.712	0.04	1
17	.	4	ARG	HB3	1.908	0.04	1
18	.	4	ARG	HG2	1.681	0.04	1
19	.	4	ARG	HG3	1.681	0.04	1
20	.	4	ARG	HD2	3.179	0.04	1
21	.	4	ARG	HD3	3.323	0.04	1
22	.	4	ARG	HE	7.531	0.04	1
23	.	4	ARG	N	127.966	0.20	1
24	.	4	ARG	NE	86.59	0.20	1
25	.	5	ASN	H	8.375	0.04	1
26	.	5	ASN	HA	4.964	0.04	1
27	.	5	ASN	HB2	2.217	0.04	1
28	.	5	ASN	HB3	2.598	0.04	1
29	.	5	ASN	HD21	7.237	0.04	1
30	.	5	ASN	HD22	6.764	0.04	1
31	.	5	ASN	N	119.572	0.20	1
32	.	5	ASN	ND2	114.403	0.20	1
33	.	6	PHE	H	9.047	0.04	1
34	.	6	PHE	HA	5.273	0.04	1
35	.	6	PHE	HB2	2.803	0.04	1
36	.	6	PHE	HB3	3.100	0.04	1
37	.	6	PHE	HD1	7.114	0.04	3
38	.	6	PHE	HD2	7.114	0.04	3
39	.	6	PHE	HE1	7.441	0.04	3
40	.	6	PHE	HE2	7.441	0.04	3
41	.	6	PHE	HZ	6.569	0.04	1
42	.	6	PHE	N	123.046	0.20	1
43	.	7	VAL	H	9.429	0.04	1
44	.	7	VAL	HA	5.105	0.04	1
45	.	7	VAL	HB	2.031	0.04	1
46	.	7	VAL	HG11	1.032	0.04	1
47	.	7	VAL	HG12	1.032	0.04	1
48	.	7	VAL	HG13	1.032	0.04	1
49	.	7	VAL	HG21	1.020	0.04	1
50	.	7	VAL	HG22	1.020	0.04	1
51	.	7	VAL	HG23	1.020	0.04	1
52	.	7	VAL	N	122.034	0.20	1
53	.	8	LEU	H	8.601	0.04	1
54	.	8	LEU	HA	5.061	0.04	1
55	.	8	LEU	HB2	1.839	0.04	1
56	.	8	LEU	HB3	2.033	0.04	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	.	8	LEU	HG	1.619	0.04	1
58	.	8	LEU	HD11	0.949	0.04	1
59	.	8	LEU	HD12	0.949	0.04	1
60	.	8	LEU	HD13	0.949	0.04	1
61	.	8	LEU	HD21	1.021	0.04	1
62	.	8	LEU	HD22	1.021	0.04	1
63	.	8	LEU	HD23	1.021	0.04	1
64	.	8	LEU	N	128.886	0.20	1
65	.	9	ARG	H	8.885	0.04	1
66	.	9	ARG	HA	5.343	0.04	1
67	.	9	ARG	HB2	1.699	0.04	1
68	.	9	ARG	HB3	1.833	0.04	1
69	.	9	ARG	HD2	3.021	0.04	1
70	.	9	ARG	HD3	3.170	0.04	1
71	.	9	ARG	HE	8.182	0.04	1
72	.	9	ARG	N	127.680	0.20	1
73	.	9	ARG	NE	87.76	0.20	1
74	.	10	ASP	H	8.922	0.04	1
75	.	10	ASP	HA	5.036	0.04	1
76	.	10	ASP	HB2	2.945	0.04	1
77	.	10	ASP	HB3	3.448	0.04	1
78	.	10	ASP	N	127.047	0.20	1
79	.	11	GLU	H	9.212	0.04	1
80	.	11	GLU	HA	3.956	0.04	1
81	.	11	GLU	HB2	2.133	0.04	1
82	.	11	GLU	HB3	2.133	0.04	1
83	.	11	GLU	HG2	2.371	0.04	1
84	.	11	GLU	HG3	2.371	0.04	1
85	.	11	GLU	N	121.454	0.20	1
86	.	12	ASP	H	8.070	0.04	1
87	.	12	ASP	HA	4.759	0.04	1
88	.	12	ASP	HB2	2.815	0.04	1
89	.	12	ASP	HB3	2.815	0.04	1
90	.	12	ASP	N	118.948	0.20	1
91	.	13	GLY	H	8.071	0.04	1
92	.	13	GLY	HA2	3.447	0.04	1
93	.	13	GLY	HA3	4.314	0.04	1
94	.	13	GLY	N	109.962	0.20	1
95	.	14	ASN	H	8.416	0.04	1
96	.	14	ASN	HA	4.647	0.04	1
97	.	14	ASN	HB2	2.673	0.04	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	.	14	ASN	HB3	3.187	0.04	1
99	.	14	ASN	HD22	7.192	0.04	1
100	.	14	ASN	N	121.547	0.20	1
101	.	14	ASN	ND2	119.188	0.20	1
102	.	15	GLU	H	8.566	0.04	1
103	.	15	GLU	HA	5.381	0.04	1
104	.	15	GLU	HB2	1.910	0.04	1
105	.	15	GLU	HB3	1.910	0.04	1
106	.	15	GLU	HG2	2.564	0.04	1
107	.	15	GLU	HG3	2.564	0.04	1
108	.	15	GLU	N	123.920	0.20	1
109	.	16	HIS	H	8.966	0.04	1
110	.	16	HIS	HA	4.886	0.04	1
111	.	16	HIS	HB2	3.060	0.04	1
112	.	16	HIS	HB3	3.466	0.04	1
113	.	16	HIS	HD2	6.985	0.04	1
114	.	16	HIS	HE1	8.507	0.04	1
115	.	16	HIS	N	121.736	0.20	1
116	.	17	GLY	H	8.418	0.04	1
117	.	17	GLY	HA2	3.847	0.04	1
118	.	17	GLY	HA3	4.090	0.04	1
119	.	17	GLY	N	111.919	0.20	1
120	.	18	VAL	H	7.560	0.04	1
121	.	18	VAL	HA	4.819	0.04	1
122	.	18	VAL	HB	1.830	0.04	1
123	.	18	VAL	HG11	0.810	0.04	1
124	.	18	VAL	HG12	0.810	0.04	1
125	.	18	VAL	HG13	0.810	0.04	1
126	.	18	VAL	HG21	0.895	0.04	1
127	.	18	VAL	HG22	0.895	0.04	1
128	.	18	VAL	HG23	0.895	0.04	1
129	.	18	VAL	N	119.397	0.20	1
130	.	19	PHE	H	9.550	0.04	1
131	.	19	PHE	HA	4.954	0.04	1
132	.	19	PHE	HB2	2.623	0.04	1
133	.	19	PHE	HB3	3.100	0.04	1
134	.	19	PHE	HD1	7.202	0.04	3
135	.	19	PHE	HD2	7.202	0.04	3
136	.	19	PHE	HE1	7.163	0.04	3
137	.	19	PHE	HE2	7.163	0.04	3
138	.	19	PHE	N	128.079	0.20	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	.	20	THR	H	8.779	0.04	1
140	.	20	THR	HA	5.785	0.04	1
141	.	20	THR	HB	4.300	0.04	1
142	.	20	THR	HG21	1.247	0.04	1
143	.	20	THR	HG22	1.247	0.04	1
144	.	20	THR	HG23	1.247	0.04	1
145	.	20	THR	N	114.987	0.20	1
146	.	21	GLY	H	8.550	0.04	1
147	.	21	GLY	HA2	4.092	0.04	1
148	.	21	GLY	HA3	3.861	0.04	1
149	.	21	GLY	N	107.270	0.20	1
150	.	22	LYS	H	8.958	0.04	1
151	.	22	LYS	HA	4.466	0.04	1
152	.	22	LYS	HB2	2.185	0.04	1
153	.	22	LYS	HB3	2.185	0.04	1
154	.	22	LYS	HG2	1.636	0.04	1
155	.	22	LYS	HD2	2.025	0.04	1
156	.	22	LYS	HD3	2.025	0.04	1
157	.	22	LYS	HE2	3.308	0.04	1
158	.	23	GLN	H	7.588	0.04	1
159	.	23	GLN	HA	4.804	0.04	1
160	.	23	GLN	HB2	2.700	0.04	1
161	.	23	GLN	HB3	2.700	0.04	1
162	.	23	GLN	HG2	2.474	0.04	1
163	.	23	GLN	HG3	2.474	0.04	1
164	.	23	GLN	HE21	7.736	0.04	1
165	.	23	GLN	HE22	6.955	0.04	1
166	.	23	GLN	N	116.057	0.20	1
167	.	23	GLN	NE2	112.607	0.20	1
168	.	24	PRO	HA	2.882	0.04	1
169	.	24	PRO	HB2	0.134	0.04	1
170	.	24	PRO	HD2	4.468	0.04	1
171	.	24	PRO	HD3	4.003	0.04	1
172	.	25	ARG	H	8.357	0.04	1
173	.	25	ARG	HA	3.413	0.04	1
174	.	25	ARG	HE	7.322	0.04	1
175	.	25	ARG	HH11	10.070	0.04	2
176	.	25	ARG	HH12	10.070	0.04	2
177	.	25	ARG	HH21	10.099	0.04	2
178	.	25	ARG	HH22	10.099	0.04	2
179	.	25	ARG	N	117.937	0.20	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	.	25	ARG	NE	85.88	0.20	1
181	.	26	GLN	H	7.091	0.04	1
182	.	26	GLN	HA	3.869	0.04	1
183	.	26	GLN	HB2	2.159	0.04	1
184	.	26	GLN	HB3	2.250	0.04	1
185	.	26	GLN	HG2	2.478	0.04	1
186	.	26	GLN	HG3	2.478	0.04	1
187	.	26	GLN	HE21	7.730	0.04	1
188	.	26	GLN	HE22	7.152	0.04	1
189	.	26	GLN	N	117.027	0.20	1
190	.	26	GLN	NE2	113.894	0.20	1
191	.	27	ALA	H	6.568	0.04	1
192	.	27	ALA	HA	3.992	0.04	1
193	.	27	ALA	HB1	0.870	0.04	1
194	.	27	ALA	HB2	0.870	0.04	1
195	.	27	ALA	HB3	0.870	0.04	1
196	.	27	ALA	N	122.097	0.20	1
197	.	28	ALA	H	7.825	0.04	1
198	.	28	ALA	HA	3.194	0.04	1
199	.	28	ALA	HB1	0.135	0.04	1
200	.	28	ALA	HB2	0.135	0.04	1
201	.	28	ALA	HB3	0.135	0.04	1
202	.	28	ALA	N	122.187	0.20	1
203	.	29	LEU	H	7.806	0.04	1
204	.	29	LEU	HA	3.502	0.04	1
205	.	29	LEU	HB2	1.679	0.04	1
206	.	29	LEU	HB3	1.486	0.04	1
207	.	29	LEU	HD11	0.784	0.04	1
208	.	29	LEU	HD12	0.784	0.04	1
209	.	29	LEU	HD13	0.784	0.04	1
210	.	29	LEU	HD21	0.565	0.04	1
211	.	29	LEU	HD22	0.565	0.04	1
212	.	29	LEU	HD23	0.565	0.04	1
213	.	29	LEU	N	120.000	0.20	1
214	.	30	LYS	H	6.659	0.04	1
215	.	30	LYS	HA	4.143	0.04	1
216	.	30	LYS	HB2	2.119	0.04	1
217	.	30	LYS	HB3	2.119	0.04	1
218	.	30	LYS	HG2	1.895	0.04	1
219	.	30	LYS	HG3	1.827	0.04	1
220	.	30	LYS	HD2	1.667	0.04	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	.	30	LYS	HD3	1.667	0.04	1
222	.	30	LYS	HE2	3.184	0.04	1
223	.	30	LYS	HE3	3.184	0.04	1
224	.	30	LYS	N	118.739	0.20	1
225	.	31	ALA	H	7.266	0.04	1
226	.	31	ALA	HA	3.402	0.04	1
227	.	31	ALA	HB1	0.559	0.04	1
228	.	31	ALA	HB2	0.559	0.04	1
229	.	31	ALA	HB3	0.559	0.04	1
230	.	31	ALA	N	124.461	0.20	1
231	.	32	ALA	H	8.814	0.04	1
232	.	32	ALA	HA	3.840	0.04	1
233	.	32	ALA	HB1	1.323	0.04	1
234	.	32	ALA	HB2	1.323	0.04	1
235	.	32	ALA	HB3	1.323	0.04	1
236	.	32	ALA	N	124.503	0.20	1
237	.	33	ASN	H	7.534	0.04	1
238	.	33	ASN	HA	4.446	0.04	1
239	.	33	ASN	HB2	2.900	0.04	1
240	.	33	ASN	HB3	2.900	0.04	1
241	.	33	ASN	HD21	7.728	0.04	1
242	.	33	ASN	HD22	7.157	0.04	1
243	.	33	ASN	N	115.977	0.20	1
244	.	34	ARG	H	7.324	0.04	1
245	.	34	ARG	HA	4.524	0.04	1
246	.	34	ARG	HB2	1.912	0.04	1
247	.	34	ARG	HB3	2.268	0.04	1
248	.	34	ARG	HG2	1.933	0.04	1
249	.	34	ARG	HG3	1.863	0.04	1
250	.	34	ARG	HD2	3.381	0.04	1
251	.	34	ARG	HD3	3.381	0.04	1
252	.	34	ARG	HE	7.526	0.04	1
253	.	34	ARG	N	117.057	0.20	1
254	.	34	ARG	NE	86.59	0.20	1
255	.	35	GLY	H	7.355	0.04	1
256	.	35	GLY	HA2	4.118	0.04	1
257	.	35	GLY	HA3	4.524	0.04	1
258	.	35	GLY	N	109.987	0.20	1
259	.	36	SER	H	8.762	0.04	1
260	.	36	SER	HA	4.825	0.04	1
261	.	36	SER	HB2	4.007	0.04	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	.	36	SER	HB3	4.007	0.04	1
263	.	36	SER	N	114.987	0.20	1
264	.	37	GLY	H	8.952	0.04	1
265	.	37	GLY	HA2	4.315	0.04	1
266	.	37	GLY	HA3	4.315	0.04	1
267	.	37	GLY	N	113.499	0.20	1
268	.	38	THR	H	7.813	0.04	1
269	.	38	THR	HA	5.137	0.04	1
270	.	38	THR	HB	4.645	0.04	1
271	.	38	THR	HG21	1.385	0.04	1
272	.	38	THR	HG22	1.385	0.04	1
273	.	38	THR	HG23	1.385	0.04	1
274	.	38	THR	N	116.086	0.20	1
275	.	39	LYS	H	8.919	0.04	1
276	.	39	LYS	HA	2.109	0.04	1
277	.	39	LYS	HB2	1.410	0.04	1
278	.	39	LYS	HB3	1.465	0.04	1
279	.	39	LYS	HG2	0.555	0.04	1
280	.	39	LYS	HG3	0.879	0.04	1
281	.	40	ALA	H	7.836	0.04	1
282	.	40	ALA	HA	4.002	0.04	1
283	.	40	ALA	HB1	1.285	0.04	1
284	.	40	ALA	HB2	1.285	0.04	1
285	.	40	ALA	HB3	1.285	0.04	1
286	.	40	ALA	N	117.998	0.20	1
287	.	41	ASN	H	7.461	0.04	1
288	.	41	ASN	HA	5.070	0.04	1
289	.	41	ASN	HB2	2.471	0.04	1
290	.	41	ASN	HB3	2.808	0.04	1
291	.	41	ASN	HD21	7.583	0.04	1
292	.	41	ASN	HD22	6.814	0.04	1
293	.	41	ASN	N	117.136	0.20	1
294	.	41	ASN	ND2	114.580	0.20	1
295	.	42	PRO	HA	4.820	0.04	1
296	.	42	PRO	HB2	2.266	0.04	1
297	.	42	PRO	HG2	1.827	0.04	1
298	.	42	PRO	HD2	3.556	0.04	1
299	.	42	PRO	HD3	3.241	0.04	1
300	.	43	ASP	H	9.415	0.04	1
301	.	43	ASP	HA	4.919	0.04	1
302	.	43	ASP	HB2	2.699	0.04	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	.	43	ASP	HB3	2.699	0.04	1
304	.	43	ASP	N	122.572	0.20	1
305	.	44	ILE	H	8.544	0.04	1
306	.	44	ILE	HA	5.114	0.04	1
307	.	44	ILE	HB	2.005	0.04	1
308	.	44	ILE	HG12	1.470	0.04	1
309	.	44	ILE	HG13	1.558	0.04	1
310	.	44	ILE	HG21	0.830	0.04	1
311	.	44	ILE	HG22	0.830	0.04	1
312	.	44	ILE	HG23	0.830	0.04	1
313	.	44	ILE	HD11	0.859	0.04	1
314	.	44	ILE	HD12	0.859	0.04	1
315	.	44	ILE	HD13	0.859	0.04	1
316	.	44	ILE	N	123.424	0.20	1
317	.	45	ILE	H	9.336	0.04	1
318	.	45	ILE	HA	5.109	0.04	1
319	.	45	ILE	HG12	1.323	0.04	1
320	.	45	ILE	HG13	1.685	0.04	1
321	.	45	ILE	HG21	0.798	0.04	1
322	.	45	ILE	HG22	0.798	0.04	1
323	.	45	ILE	HG23	0.798	0.04	1
324	.	45	ILE	HD11	0.533	0.04	1
325	.	45	ILE	HD12	0.533	0.04	1
326	.	45	ILE	HD13	0.533	0.04	1
327	.	45	ILE	N	125.768	0.20	1
328	.	46	ARG	H	8.394	0.04	1
329	.	46	ARG	HA	5.003	0.04	1
330	.	46	ARG	HB2	1.674	0.04	1
331	.	46	ARG	HB3	2.439	0.04	1
332	.	46	ARG	HG2	1.401	0.04	1
333	.	46	ARG	HG3	1.495	0.04	1
334	.	46	ARG	HD2	3.078	0.04	1
335	.	46	ARG	HD3	3.078	0.04	1
336	.	46	ARG	HE	8.181	0.04	1
337	.	46	ARG	N	125.355	0.20	1
338	.	46	ARG	NE	87.76	0.20	1
339	.	47	LEU	H	9.313	0.04	1
340	.	47	LEU	HA	5.409	0.04	1
341	.	47	LEU	HB2	1.580	0.04	1
342	.	47	LEU	HB3	1.876	0.04	1
343	.	47	LEU	HG	0.507	0.04	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	.	47	LEU	HD11	0.616	0.04	1
345	.	47	LEU	HD12	0.616	0.04	1
346	.	47	LEU	HD13	0.616	0.04	1
347	.	47	LEU	HD21	0.510	0.04	1
348	.	47	LEU	HD22	0.510	0.04	1
349	.	47	LEU	HD23	0.510	0.04	1
350	.	47	LEU	N	125.101	0.20	1
351	.	48	ARG	H	9.739	0.04	1
352	.	48	ARG	HA	5.446	0.04	1
353	.	48	ARG	HB2	1.491	0.04	1
354	.	48	ARG	HB3	2.044	0.04	1
355	.	48	ARG	HG2	1.614	0.04	1
356	.	48	ARG	HG3	1.727	0.04	1
357	.	48	ARG	HD2	2.709	0.04	1
358	.	48	ARG	HD3	3.324	0.04	1
359	.	48	ARG	HE	7.954	0.04	1
360	.	48	ARG	N	128.858	0.20	1
361	.	48	ARG	NE	87.76	0.20	1
362	.	49	GLU	H	9.107	0.04	1
363	.	49	GLU	HA	4.292	0.04	1
364	.	49	GLU	HB2	1.982	0.04	1
365	.	49	GLU	HB3	1.943	0.04	1
366	.	49	GLU	HG2	2.343	0.04	1
367	.	49	GLU	HG3	2.343	0.04	1
368	.	50	ARG	H	8.666	0.04	1
369	.	50	ARG	HA	4.023	0.04	1
370	.	50	ARG	HB2	1.613	0.04	1
371	.	50	ARG	HB3	1.736	0.04	1
372	.	50	ARG	HG2	1.915	0.04	1
373	.	50	ARG	HG3	1.915	0.04	1
374	.	50	ARG	HD2	3.182	0.04	1
375	.	50	ARG	HD3	3.182	0.04	1
376	.	50	ARG	HE	7.572	0.04	1
377	.	50	ARG	N	133.146	0.20	1
378	.	51	GLY	H	8.092	0.04	1
379	.	51	GLY	HA2	3.837	0.04	1
380	.	51	GLY	HA3	4.336	0.04	1
381	.	51	GLY	N	111.776	0.20	1
382	.	52	THR	H	8.091	0.04	1
383	.	52	THR	HA	5.089	0.04	1
384	.	52	THR	HB	4.462	0.04	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	.	52	THR	HG1	5.621	0.04	1
386	.	52	THR	HG21	1.166	0.04	1
387	.	52	THR	HG22	1.166	0.04	1
388	.	52	THR	HG23	1.166	0.04	1
389	.	52	THR	N	111.776	0.20	1
390	.	53	LYS	H	8.942	0.04	1
391	.	53	LYS	HA	4.784	0.04	1
392	.	53	LYS	HB2	1.831	0.04	1
393	.	53	LYS	HB3	1.831	0.04	1
394	.	53	LYS	HG2	1.485	0.04	1
395	.	53	LYS	HG3	1.485	0.04	1
396	.	53	LYS	N	121.711	0.20	1
397	.	54	LYS	H	8.161	0.04	1
398	.	54	LYS	HA	4.586	0.04	1
399	.	54	LYS	HB2	1.441	0.04	1
400	.	54	LYS	HB3	1.979	0.04	1
401	.	54	LYS	HG2	1.441	0.04	1
402	.	54	LYS	HG3	1.650	0.04	1
403	.	54	LYS	HD2	1.199	0.04	1
404	.	54	LYS	HD3	1.199	0.04	1
405	.	54	LYS	HE2	2.974	0.04	1
406	.	54	LYS	HE3	2.974	0.04	1
407	.	54	LYS	N	120.936	0.20	1
408	.	55	VAL	H	8.975	0.04	1
409	.	55	VAL	HA	4.466	0.04	1
410	.	55	VAL	HB	2.051	0.04	1
411	.	55	VAL	HG11	0.808	0.04	1
412	.	55	VAL	HG12	0.808	0.04	1
413	.	55	VAL	HG13	0.808	0.04	1
414	.	55	VAL	HG21	0.808	0.04	1
415	.	55	VAL	HG22	0.808	0.04	1
416	.	55	VAL	HG23	0.808	0.04	1
417	.	55	VAL	N	124.820	0.20	1
418	.	56	HIS	H	9.437	0.04	1
419	.	56	HIS	HA	4.466	0.04	1
420	.	56	HIS	HB2	2.905	0.04	1
421	.	56	HIS	HB3	3.416	0.04	1
422	.	56	HIS	HD2	7.441	0.04	1
423	.	56	HIS	HE1	8.013	0.04	1
424	.	56	HIS	N	130.251	0.20	1
425	.	57	VAL	H	8.793	0.04	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
426	.	57	VAL	HA	5.123	0.04	1
427	.	57	VAL	HB	1.971	0.04	1
428	.	57	VAL	HG11	0.821	0.04	1
429	.	57	VAL	HG12	0.821	0.04	1
430	.	57	VAL	HG13	0.821	0.04	1
431	.	57	VAL	HG21	0.821	0.04	1
432	.	57	VAL	HG22	0.821	0.04	1
433	.	57	VAL	HG23	0.821	0.04	1
434	.	57	VAL	N	127.151	0.20	1
435	.	58	PHE	H	9.552	0.04	1
436	.	58	PHE	HA	5.349	0.04	1
437	.	58	PHE	HB2	2.601	0.04	1
438	.	58	PHE	HB3	3.067	0.04	1
439	.	58	PHE	HD1	6.975	0.04	3
440	.	58	PHE	HD2	6.975	0.04	3
441	.	58	PHE	HE1	7.362	0.04	3
442	.	58	PHE	HE2	7.362	0.04	3
443	.	58	PHE	HZ	7.108	0.04	1
444	.	58	PHE	N	126.817	0.20	1
445	.	59	LYS	H	9.296	0.04	1
446	.	59	LYS	HA	5.377	0.04	1
447	.	59	LYS	HB2	2.238	0.04	1
448	.	59	LYS	HB3	2.134	0.04	1
449	.	59	LYS	N	122.262	0.20	1
450	.	60	ALA	H	9.593	0.04	1
451	.	60	ALA	HA	5.583	0.04	1
452	.	60	ALA	HB1	1.325	0.04	1
453	.	60	ALA	HB2	1.325	0.04	1
454	.	60	ALA	HB3	1.325	0.04	1
455	.	60	ALA	N	127.589	0.20	1
456	.	61	TRP	H	9.100	0.04	1
457	.	61	TRP	HA	5.413	0.04	1
458	.	61	TRP	HB2	2.414	0.04	1
459	.	61	TRP	HB3	3.343	0.04	1
460	.	61	TRP	HD1	6.759	0.04	1
461	.	61	TRP	HE1	10.975	0.04	1
462	.	61	TRP	HE3	7.096	0.04	1
463	.	61	TRP	HZ2	7.269	0.04	1
464	.	61	TRP	HZ3	6.759	0.04	1
465	.	61	TRP	HH2	7.059	0.04	1
466	.	61	TRP	N	122.483	0.20	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
467	.	61	TRP	NE1	135.213	0.20	1
468	.	62	LYS	H	7.586	0.04	1
469	.	62	LYS	HA	5.515	0.04	1
470	.	62	LYS	HB2	1.830	0.04	1
471	.	62	LYS	HB3	1.830	0.04	1
472	.	62	LYS	N	116.057	0.20	1
473	.	63	GLU	H	8.947	0.04	1
474	.	63	GLU	HA	4.798	0.04	1
475	.	63	GLU	HB2	2.440	0.04	1
476	.	63	GLU	HB3	2.246	0.04	1
477	.	63	GLU	HG2	2.388	0.04	1
478	.	63	GLU	HG3	2.388	0.04	1
479	.	63	GLU	N	121.399	0.20	1
480	.	64	ILE	H	8.611	0.04	1
481	.	64	ILE	HA	4.795	0.04	1
482	.	64	ILE	HB	1.887	0.04	1
483	.	64	ILE	HG12	1.333	0.04	1
484	.	64	ILE	HG13	1.594	0.04	1
485	.	64	ILE	HG21	0.845	0.04	1
486	.	64	ILE	HG22	0.845	0.04	1
487	.	64	ILE	HG23	0.845	0.04	1
488	.	64	ILE	HD11	0.845	0.04	1
489	.	64	ILE	HD12	0.845	0.04	1
490	.	64	ILE	HD13	0.845	0.04	1
491	.	64	ILE	N	124.661	0.20	1
492	.	65	VAL	H	9.365	0.04	1
493	.	65	VAL	HA	4.841	0.04	1
494	.	65	VAL	HB	2.395	0.04	1
495	.	65	VAL	HG11	0.863	0.04	1
496	.	65	VAL	HG12	0.863	0.04	1
497	.	65	VAL	HG13	0.863	0.04	1
498	.	65	VAL	HG21	1.092	0.04	1
499	.	65	VAL	HG22	1.092	0.04	1
500	.	65	VAL	HG23	1.092	0.04	1
501	.	65	VAL	N	125.146	0.20	1
502	.	66	ASP	H	8.316	0.04	1
503	.	66	ASP	HB2	2.513	0.04	1
504	.	66	ASP	HB3	2.725	0.04	1
505	.	66	ASP	N	121.691	0.20	1
506	.	67	ALA	H	8.302	0.04	1
507	.	67	ALA	HA	4.220	0.04	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
508	.	67	ALA	HB1	1.315	0.04	1
509	.	67	ALA	HB2	1.315	0.04	1
510	.	67	ALA	HB3	1.315	0.04	1
511	.	67	ALA	N	127.040	0.20	1
512	.	68	PRO	HA	4.434	0.04	1
513	.	68	PRO	HB2	2.569	0.04	1
514	.	68	PRO	HB3	2.520	0.04	1
515	.	69	LYS	H	8.481	0.04	1
516	.	69	LYS	HA	3.921	0.04	1
517	.	69	LYS	HB2	1.795	0.04	1
518	.	69	LYS	HB3	1.795	0.04	1
519	.	69	LYS	HG2	1.504	0.04	1
520	.	69	LYS	HG3	1.504	0.04	1
521	.	69	LYS	HD2	2.379	0.04	1
522	.	69	LYS	HD3	2.379	0.04	1
523	.	69	LYS	N	122.731	0.20	1
524	.	70	ASN	H	8.193	0.04	1
525	.	70	ASN	HA	4.674	0.04	1
526	.	70	ASN	HB2	2.777	0.04	1
527	.	70	ASN	HB3	2.777	0.04	1
528	.	70	ASN	HD21	7.640	0.04	1
529	.	70	ASN	HD22	6.911	0.04	1
530	.	70	ASN	N	117.994	0.20	1
531	.	70	ASN	ND2	114.390	0.20	1
532	.	71	ARG	H	7.402	0.04	1
533	.	71	ARG	HA	4.366	0.04	1
534	.	71	ARG	HB2	1.578	0.04	1
535	.	71	ARG	HB3	1.733	0.04	1
536	.	71	ARG	HG2	1.209	0.04	1
537	.	71	ARG	HG3	1.397	0.04	1
538	.	71	ARG	HD2	2.543	0.04	1
539	.	71	ARG	HD3	2.960	0.04	1
540	.	71	ARG	HE	6.711	0.04	1
541	.	71	ARG	HH11	7.438	0.04	1
542	.	71	ARG	HH12	7.438	0.04	1
543	.	71	ARG	N	121.354	0.20	1
544	.	71	ARG	NE	87.91	0.20	1
545	.	72	PRO	HA	4.086	0.04	1
546	.	72	PRO	HB2	0.068	0.04	1
547	.	72	PRO	HB3	1.579	0.04	1
548	.	72	PRO	HD2	3.246	0.04	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
549	.	72	PRO	HD3	2.925	0.04	1
550	.	73	ALA	H	8.512	0.04	1
551	.	73	ALA	HA	3.902	0.04	1
552	.	73	ALA	HB1	1.393	0.04	1
553	.	73	ALA	HB2	1.393	0.04	1
554	.	73	ALA	HB3	1.393	0.04	1
555	.	73	ALA	N	123.915	0.20	1
556	.	74	TRP	H	6.419	0.04	1
557	.	74	TRP	HA	4.396	0.04	1
558	.	74	TRP	HB2	3.022	0.04	1
559	.	74	TRP	HB3	3.461	0.04	1
560	.	74	TRP	HD1	6.845	0.04	1
561	.	74	TRP	HE1	10.278	0.04	1
562	.	74	TRP	HE3	6.815	0.04	1
563	.	74	TRP	HZ2	7.169	0.04	1
564	.	74	TRP	HZ3	7.097	0.04	1
565	.	74	TRP	HH2	6.677	0.04	1
566	.	74	TRP	N	111.494	0.20	1
567	.	74	TRP	NE1	133.346	0.20	1
568	.	75	MET	H	7.060	0.04	1
569	.	75	MET	HA	4.433	0.04	1
570	.	75	MET	HB2	1.731	0.04	1
571	.	75	MET	HB3	1.877	0.04	1
572	.	75	MET	HG2	2.438	0.04	1
573	.	75	MET	HG3	2.438	0.04	1
574	.	75	MET	HE1	1.945	0.04	1
575	.	75	MET	HE2	1.945	0.04	1
576	.	75	MET	HE3	1.945	0.04	1
577	.	75	MET	N	126.637	0.20	1
578	.	76	PRO	HA	4.564	0.04	1
579	.	76	PRO	HB2	2.468	0.04	1
580	.	76	PRO	HB3	2.379	0.04	1
581	.	76	PRO	HD2	3.990	0.04	1
582	.	76	PRO	HD3	3.990	0.04	1
583	.	77	GLU	H	8.139	0.04	1
584	.	77	GLU	HA	3.694	0.04	1
585	.	77	GLU	HB2	2.020	0.04	1
586	.	77	GLU	HB3	2.020	0.04	1
587	.	77	GLU	HG2	2.280	0.04	1
588	.	77	GLU	HG3	2.278	0.04	1
589	.	77	GLU	N	115.293	0.20	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
590	.	78	LYS	H	7.455	0.04	1
591	.	78	LYS	HA	5.097	0.04	1
592	.	78	LYS	HB2	1.886	0.04	1
593	.	78	LYS	HB3	2.137	0.04	1
594	.	78	LYS	HG2	1.483	0.04	1
595	.	78	LYS	HG3	1.533	0.04	1
596	.	78	LYS	HE2	2.928	0.04	1
597	.	78	LYS	HE3	2.928	0.04	1
598	.	78	LYS	N	119.573	0.20	1
599	.	79	ILE	H	8.973	0.04	1
600	.	79	ILE	HA	4.689	0.04	1
601	.	79	ILE	HB	1.887	0.04	1
602	.	79	ILE	HG12	1.401	0.04	1
603	.	79	ILE	HG13	1.685	0.04	1
604	.	79	ILE	HG21	1.400	0.04	1
605	.	79	ILE	HG22	1.400	0.04	1
606	.	79	ILE	HG23	1.400	0.04	1
607	.	79	ILE	HD11	0.885	0.04	1
608	.	79	ILE	HD12	0.885	0.04	1
609	.	79	ILE	HD13	0.885	0.04	1
610	.	79	ILE	N	118.026	0.20	1
611	.	80	SER	H	8.550	0.04	1
612	.	80	SER	HA	5.092	0.04	1
613	.	80	SER	HB2	3.771	0.04	1
614	.	80	SER	HB3	3.832	0.04	1
615	.	80	SER	N	118.300	0.20	1
616	.	81	LYS	H	9.197	0.04	1
617	.	81	LYS	HA	4.800	0.04	1
618	.	81	LYS	HB2	1.664	0.04	1
619	.	81	LYS	HB3	1.867	0.04	1
620	.	81	LYS	HD2	1.396	0.04	1
621	.	81	LYS	HD3	1.396	0.04	1
622	.	81	LYS	N	130.542	0.20	1
623	.	82	PRO	HA	4.995	0.04	1
624	.	82	PRO	HB2	1.925	0.04	1
625	.	82	PRO	HB3	1.925	0.04	1
626	.	82	PRO	HD2	3.757	0.04	1
627	.	82	PRO	HD3	3.756	0.04	1
628	.	83	PHE	H	8.717	0.04	1
629	.	83	PHE	HA	4.037	0.04	1
630	.	83	PHE	HB2	0.234	0.04	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
631	.	83	PHE	HB3	1.378	0.04	1
632	.	83	PHE	HD1	7.057	0.04	1
633	.	83	PHE	HD2	7.057	0.04	1
634	.	83	PHE	HE1	7.224	0.04	1
635	.	83	PHE	HE2	7.224	0.04	1
636	.	83	PHE	HZ	7.223	0.04	1
637	.	83	PHE	N	120.486	0.20	1
638	.	84	VAL	H	7.577	0.04	1
639	.	84	VAL	HA	5.415	0.04	1
640	.	84	VAL	HB	2.119	0.04	1
641	.	84	VAL	HG11	0.508	0.04	1
642	.	84	VAL	HG12	0.508	0.04	1
643	.	84	VAL	HG13	0.508	0.04	1
644	.	84	VAL	HG21	0.561	0.04	1
645	.	84	VAL	HG22	0.561	0.04	1
646	.	84	VAL	HG23	0.561	0.04	1
647	.	84	VAL	N	109.347	0.20	1
648	.	85	LYS	H	9.019	0.04	1
649	.	85	LYS	HA	4.806	0.04	1
650	.	85	LYS	HB2	2.119	0.04	1
651	.	85	LYS	HB3	2.119	0.04	1
652	.	85	LYS	HG2	1.575	0.04	1
653	.	85	LYS	HG3	1.575	0.04	1
654	.	86	LYS	H	9.356	0.04	1
655	.	86	LYS	HA	3.849	0.04	1
656	.	86	LYS	HG2	1.391	0.04	1
657	.	86	LYS	HG3	1.391	0.04	1
658	.	87	GLU	H	9.304	0.04	1
659	.	87	GLU	HA	4.591	0.04	1
660	.	87	GLU	HB2	1.726	0.04	1
661	.	87	GLU	HB3	1.986	0.04	1
662	.	87	GLU	N	129.114	0.20	1
663	.	88	ARG	H	7.431	0.04	1
664	.	88	ARG	HA	4.475	0.04	1
665	.	88	ARG	HG2	1.050	0.04	1
666	.	88	ARG	HG3	1.050	0.04	1
667	.	88	ARG	HD2	3.167	0.04	1
668	.	88	ARG	HD3	3.283	0.04	1
669	.	88	ARG	HE	8.189	0.04	1
670	.	88	ARG	N	112.267	0.20	1
671	.	88	ARG	NE	87.76	0.20	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
672	.	89	ILE	H	8.310	0.04	1
673	.	89	ILE	HA	4.851	0.04	1
674	.	89	ILE	HB	2.976	0.04	1
675	.	89	ILE	HG12	2.406	0.04	1
676	.	89	ILE	HG13	2.406	0.04	1
677	.	89	ILE	HG21	0.595	0.04	1
678	.	89	ILE	HG22	0.595	0.04	1
679	.	89	ILE	HG23	0.595	0.04	1
680	.	89	ILE	HD11	0.968	0.04	1
681	.	89	ILE	HD12	0.968	0.04	1
682	.	89	ILE	HD13	0.968	0.04	1
683	.	89	ILE	N	121.691	0.20	1
684	.	90	GLU	H	9.549	0.04	1
685	.	90	GLU	HA	4.586	0.04	1
686	.	90	GLU	HB2	1.831	0.04	1
687	.	90	GLU	HB3	2.038	0.04	1
688	.	90	GLU	HG2	2.267	0.04	1
689	.	90	GLU	HG3	2.256	0.04	1
690	.	90	GLU	N	128.079	0.20	1
691	.	91	LYS	H	8.600	0.04	1
692	.	91	LYS	HA	5.084	0.04	1
693	.	91	LYS	HB2	1.727	0.04	1
694	.	91	LYS	HB3	1.800	0.04	1
695	.	91	LYS	N	122.698	0.20	1
696	.	92	LEU	H	8.787	0.04	1
697	.	92	LEU	HA	4.449	0.04	1
698	.	92	LEU	HB2	1.536	0.04	1
699	.	92	LEU	HB3	1.690	0.04	1
700	.	92	LEU	HG	1.328	0.04	1
701	.	92	LEU	HD11	0.809	0.04	1
702	.	92	LEU	HD12	0.809	0.04	1
703	.	92	LEU	HD13	0.809	0.04	1
704	.	92	LEU	HD21	0.809	0.04	1
705	.	92	LEU	HD22	0.809	0.04	1
706	.	92	LEU	HD23	0.809	0.04	1
707	.	92	LEU	N	126.698	0.20	1
708	.	93	GLU	H	8.015	0.04	1
709	.	93	GLU	HA	4.088	0.04	1
710	.	93	GLU	HB2	1.906	0.04	1
711	.	93	GLU	HB3	2.053	0.04	1
712	.	93	GLU	HG2	2.268	0.04	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
713	.	93	GLU	HG3	2.268	0.04	1
714	.	93	GLU	N	126.883	0.20	1

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 1794. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/438 (0%)	0/174 (0%)	0/180 (0%)	0/84 (0%)
Sidechain	0/692 (0%)	0/411 (0%)	0/234 (0%)	0/47 (0%)
Aromatic	0/76 (0%)	0/40 (0%)	0/30 (0%)	0/6 (0%)
Overall	0/1794 (0%)	0/973 (0%)	0/648 (0%)	0/173 (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 1826. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/453 (0%)	0/180 (0%)	0/186 (0%)	0/87 (0%)
Sidechain	0/709 (0%)	0/421 (0%)	0/240 (0%)	0/48 (0%)
Aromatic	0/76 (0%)	0/40 (0%)	0/30 (0%)	0/6 (0%)
Overall	0/1826 (0%)	0/989 (0%)	0/660 (0%)	0/177 (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 (assigned_chem_shift_list_1). RCI is only applicable to proteins.