



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 03:09 AM UTC

PDB ID : 2LAN / pdb_00002lan
BMRB ID : 16862
Title : NMR structure of Ca²⁺-bound CaBP1 N-domain with RDC
Authors : Ames, J.
Deposited on : 2011-03-16

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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

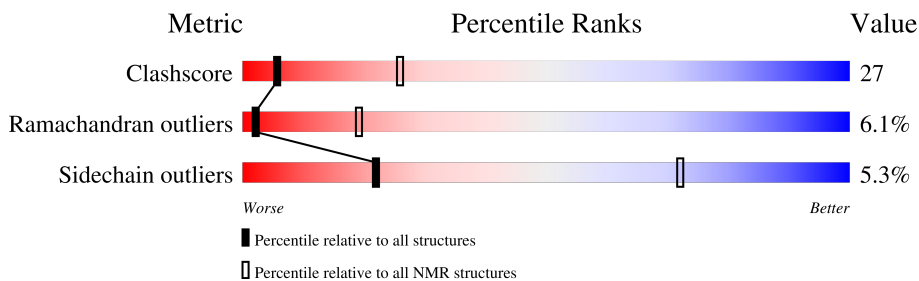
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 66%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	167	

2 Ensemble composition and analysis

This entry contains 15 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:20-A:88 (69)	1.12	14

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 6 single-model clusters were found.

Cluster number	Models
1	1, 10, 14, 15
2	4, 5, 7
3	3, 11
Single-model clusters	2; 6; 8; 9; 12; 13

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1177 atoms, of which 574 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calcium-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	74	1176	374	574	100	120	8	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9NZU7
A	2	GLY	-	expression tag	UNP Q9NZU7
A	3	ASN	-	expression tag	UNP Q9NZU7
A	4	CYS	-	expression tag	UNP Q9NZU7
A	5	VAL	-	expression tag	UNP Q9NZU7
A	6	LYS	-	expression tag	UNP Q9NZU7
A	7	TYR	-	expression tag	UNP Q9NZU7
A	8	PRO	-	expression tag	UNP Q9NZU7
A	9	LEU	-	expression tag	UNP Q9NZU7
A	10	ARG	-	expression tag	UNP Q9NZU7
A	11	ASN	-	expression tag	UNP Q9NZU7
A	12	LEU	-	expression tag	UNP Q9NZU7
A	13	SER	-	expression tag	UNP Q9NZU7
A	14	ARG	-	expression tag	UNP Q9NZU7
A	15	LYS	-	expression tag	UNP Q9NZU7

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Ca
			1	1

K90
L91
LEU
ALA
GLY
THR
ALA
ASP
MET
MET
GLY
GLY
VAL
LYS
GLY
LEU
LEU
ASP
ASP
ALA
PHE
ARG
GLU
PHE
ASP
THR
ASN
GLY
ASP
GLY
GLU
ILE
SER
THR
SER
GLU
LEU
ARG
GLU
GLU
ALA
MET
MET
LYS
LEU
LEU
GLY
HIS
HIS
GLN
VAL
GLY
HIS
HIS
ARG
ASP
ILE
GLU
GLU
ILE
ILE
ARG
ASP
VAL
ASP

LEU
ASN
GLY
ASP
GLY
ARG
VAL
PHE
ASP
GLU
GLU
PHE
VAL
ARG
MET
MET
SER
ARG

4.2.12 Score per residue for model 12

- Molecule 1: Calcium-binding protein 1

Chain A: 23% 16% .. 56%

MET
GLY
ASN
CYS
VAL
LYS
TYR
PRO
LEU
LEU
ARG
ASN
ALA
ASP
SER
ARG
GLY
LYS
VAL
ASP
ASP
S18
L19
E25
A30
R31
R32
E33
F34
D35
K36
D37
K38
D39
G40
N43
C44
R45
R46
L47
C50
M51
T59
L63
Q68
Q69
L70
N71
M72
N73
L74
D79
F80
D81
V84

M87
G88
P89
K90
L91
LEU
ALA
THR
THR
ALA
VAL
ASP
MET
ILE
GLY
VAL
LYS
GLY
ARG
GLY
LEU
ARG
ASP
ASP
MET
SER
MET
SER
ARG

ARG
ASP
VAL
ASP
LEU
ASN
GLY
ASP
PHE
GLY
VAL
VAL
ARG
GLY
MET
MET
SER
ARG

4.2.13 Score per residue for model 13

- Molecule 1: Calcium-binding protein 1

Chain A: 25% 15% .. 56%

MET
GLY
ASN
CYS
VAL
LYS
TYR
PRO
LEU
LEU
ARG
ASN
ALA
ASP
SER
ARG
GLY
LYS
VAL
ASP
ASP
S18
L19
R20
P21
E22
E23
I24
E25
A30
D35
K36
D37
K38
D39
G40
Y41
N43
C44
R45
N49
C50
M51
M54
G55
Y56
N71
M72
N73
G75
D79
F80
D81
D82
F83

P89
K90
L91
LEU
ALA
THR
ALA
ASP
MET
ILE
GLY
VAL
LYS
GLY
LEU
LEU
ARG
ARG
ASP
ALA
PHE
ARG
GLU
PHE
ASP
THR
ASN
GLY
GLY
GLU
GLU
ILE
SER
THR
SER
GLU
LEU
SER
SER
GLY
HIS
GLN
VAL
GLY
HIS
HIS
ARG
ASP
ILE
GLU
GLU
ILE
ILE
ARG
ASP
VAL

ASP
LEU
ASN
GLY
ASP
PHE
GLY
PHE
VAL
VAL
ASP
MET
MET
SER
ARG

4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Calcium-binding protein 1

Chain A: 20% 17% .. 56%

MET
GLY
ASN
CYS
VAL
LYS
TYR
PRO
LEU
LEU
ARG
ASN
ALA
ASP
SER
ARG
GLY
LYS
VAL
ASP
ASP
S18
L19
R20
P21
E25
R28
F31
D35
K36
D37
G40
Y41
N43
C44
R45
D46
Y56
M61
E62
E65
L66
S67
Q68
Q69
I70
N71
L74
G75
G76
H77
V79
D79
F80

D81
D82
F83
V84
E85
L86
M87
G88
P89
K90
L91
LEU
ALA
THR
THR
ALA
ASP
MET
ILE
GLY
VAL
LYS
LEU
ARG
ASP
PHE
PHE
ASP
THR
ASN
GLY
GLY
GLU
GLU
ILE
SER
THR
SER
GLU
LEU
SER
SER
GLY
HIS
GLN
VAL
GLY
HIS
HIS
ARG
ASP

ILE
GLU
GLU
ILE
ILE
ARG
ASP
VAL
ASP
LEU
ASN
GLY
ASP
GLY
ARG
VAL
ASP
PHE
GLU
GLU
PHE
VAL
ARG
MET
MET
SER
ARG

4.2.15 Score per residue for model 15

- Molecule 1: Calcium-binding protein 1

Chain A:  25% 14% 56%

MET
GLY
ASN
CYS
VAL
LYS
TYR
PRO
LEU
ARG
ASN
ASN
LEU
SER
ARG
LYS
ASP
ARG
S18
I19
E23
G40
Y41
I42
M43
L47
G48
N49
C50
Y56
M57
P58
M61
E62
L63
I64
E65
Q68
G69
I70
L74
G75
G76
H77
I78
D79
F80
D81
D82
F83
L86
M87
G88

P89
K90
L91
ALA
LEU
THR
ALA
ASP
MET
ILE
ILE
VAL
VAL
LYS
GLU
LEU
LEU
ASP
ASP
ALA
PHE
ARG
GLU
PHE
ASP
THR
ASN
GLY
ASP
GLY
GLU
GLU
ILE
SER
THR
SER
GLU
LEU
ARG
GLU
ALA
MET
ARG
LYS
LEU
GLY
HIS
GLN
VAL
GLY
HIS
ARG
ASP
ILE
GLU
GLU
ILE
ILE
ASP
VAL

ASP
LEU
ASN
GLY
ASP
ARG
VAL
ASP
PHE
GLU
GLU
PHE
VAL
ARG
MET
MET
SER
ARG

5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.23
X-PLOR NIH	refinement	2.23

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1354
Number of shifts mapped to atoms	668
Number of unparsed shifts	0
Number of shifts with mapping errors	686
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	66%

6 Model quality i

6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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 i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	564	528	527	30±6
All	All	8475	7920	7908	447

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:GLY:O	1:A:77:HIS:N	0.76	2.18	15	1
1:A:43:ASN:HD22	1:A:43:ASN:H	0.68	1.30	15	4
1:A:72:MET:O	1:A:74:LEU:N	0.67	2.27	8	2
1:A:43:ASN:HD22	1:A:43:ASN:N	0.66	1.89	7	5
1:A:56:TYR:O	1:A:56:TYR:CG	0.65	2.48	4	5
1:A:47:LEU:C	1:A:47:LEU:HD23	0.64	2.18	12	1
1:A:70:ILE:O	1:A:74:LEU:N	0.63	2.31	15	1
1:A:43:ASN:H	1:A:43:ASN:ND2	0.63	1.91	15	3
1:A:43:ASN:HD21	1:A:45:ARG:NE	0.62	1.92	10	2
1:A:43:ASN:ND2	1:A:45:ARG:NE	0.62	2.47	10	2
1:A:38:LYS:C	1:A:40:GLY:H	0.61	2.03	3	5
1:A:68:GLN:O	1:A:71:ASN:N	0.60	2.34	12	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:PHE:CD2	1:A:50:CYS:SG	0.60	2.95	11	5
1:A:34:PHE:CG	1:A:50:CYS:SG	0.60	2.94	7	1
1:A:43:ASN:ND2	1:A:43:ASN:N	0.60	2.46	1	3
1:A:28:ARG:NH1	1:A:32:ARG:NH2	0.60	2.50	7	1
1:A:83:PHE:CE1	1:A:87:MET:SD	0.59	2.95	6	2
1:A:30:ALA:HB2	1:A:54:MET:HE1	0.59	1.74	13	1
1:A:40:GLY:O	1:A:41:TYR:CG	0.59	2.56	14	5
1:A:43:ASN:C	1:A:45:ARG:H	0.59	2.06	2	11
1:A:37:ASP:OD1	1:A:38:LYS:N	0.58	2.36	3	4
1:A:34:PHE:CE2	1:A:50:CYS:SG	0.58	2.95	4	4
1:A:57:MET:SD	1:A:57:MET:N	0.58	2.75	15	1
1:A:23:GLU:N	1:A:23:GLU:OE1	0.58	2.37	15	1
1:A:43:ASN:N	1:A:43:ASN:ND2	0.58	2.50	4	2
1:A:35:ASP:OD2	1:A:38:LYS:N	0.58	2.37	7	2
1:A:28:ARG:HH12	1:A:32:ARG:NE	0.58	1.96	7	1
1:A:28:ARG:HH12	1:A:32:ARG:NH2	0.57	1.96	7	1
1:A:50:CYS:SG	1:A:51:MET:N	0.57	2.78	13	4
1:A:43:ASN:CG	1:A:44:CYS:N	0.57	2.62	6	2
1:A:28:ARG:HH12	1:A:32:ARG:CZ	0.57	2.13	7	1
1:A:82:ASP:OD1	1:A:86:LEU:HD13	0.57	1.99	9	1
1:A:63:LEU:N	1:A:63:LEU:HD23	0.56	2.16	7	1
1:A:40:GLY:O	1:A:41:TYR:CD1	0.56	2.58	9	3
1:A:62:GLU:OE1	1:A:63:LEU:N	0.56	2.39	7	1
1:A:39:ASP:OD1	1:A:39:ASP:N	0.56	2.35	12	4
1:A:83:PHE:CZ	1:A:87:MET:SD	0.55	3.00	6	1
1:A:54:MET:SD	1:A:87:MET:SD	0.55	3.04	5	1
1:A:51:MET:SD	1:A:87:MET:SD	0.55	3.04	8	1
1:A:35:ASP:OD1	1:A:36:LYS:N	0.55	2.38	12	2
1:A:86:LEU:O	1:A:86:LEU:HD13	0.55	2.01	15	4
1:A:35:ASP:CG	1:A:36:LYS:N	0.55	2.64	12	2
1:A:71:ASN:O	1:A:75:GLY:N	0.55	2.39	8	2
1:A:22:GLU:N	1:A:22:GLU:OE1	0.55	2.40	13	1
1:A:30:ALA:O	1:A:34:PHE:CE2	0.55	2.60	12	1
1:A:49:ASN:OD1	1:A:52:ARG:NH2	0.55	2.39	3	1
1:A:43:ASN:ND2	1:A:76:GLY:O	0.55	2.40	6	1
1:A:74:LEU:O	1:A:74:LEU:HD23	0.55	2.02	7	1
1:A:40:GLY:O	1:A:41:TYR:CD2	0.55	2.60	1	5
1:A:38:LYS:C	1:A:40:GLY:N	0.54	2.64	3	5
1:A:35:ASP:CG	1:A:36:LYS:H	0.54	2.09	12	1
1:A:66:LEU:O	1:A:69:GLN:N	0.54	2.40	14	3
1:A:54:MET:O	1:A:55:GLY:C	0.54	2.51	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ARG:NH1	1:A:32:ARG:CZ	0.54	2.69	7	1
1:A:43:ASN:ND2	1:A:43:ASN:H	0.54	2.00	11	1
1:A:43:ASN:OD1	1:A:43:ASN:N	0.54	2.41	12	3
1:A:87:MET:O	1:A:88:GLY:C	0.54	2.51	11	4
1:A:74:LEU:H	1:A:74:LEU:HD23	0.54	1.63	9	1
1:A:66:LEU:N	1:A:66:LEU:CD2	0.53	2.71	4	2
1:A:27:LEU:HD11	1:A:87:MET:SD	0.53	2.44	5	1
1:A:85:GLU:N	1:A:85:GLU:OE1	0.53	2.42	5	1
1:A:79:ASP:OD1	1:A:80:PHE:N	0.53	2.42	7	2
1:A:81:ASP:OD1	1:A:82:ASP:N	0.53	2.42	15	1
1:A:66:LEU:N	1:A:66:LEU:HD22	0.53	2.18	4	1
1:A:60:GLU:O	1:A:64:ILE:HD13	0.53	2.04	5	1
1:A:76:GLY:O	1:A:77:HIS:CG	0.53	2.62	10	3
1:A:43:ASN:ND2	1:A:76:GLY:C	0.52	2.67	6	1
1:A:32:ARG:C	1:A:34:PHE:N	0.52	2.66	12	2
1:A:43:ASN:OD1	1:A:44:CYS:N	0.52	2.43	6	1
1:A:74:LEU:HD22	1:A:74:LEU:N	0.52	2.18	4	2
1:A:47:LEU:O	1:A:47:LEU:HD13	0.52	2.05	2	1
1:A:56:TYR:CD2	1:A:56:TYR:O	0.52	2.63	13	3
1:A:77:HIS:N	1:A:77:HIS:ND1	0.52	2.57	6	2
1:A:44:CYS:SG	1:A:71:ASN:OD1	0.52	2.67	9	4
1:A:36:LYS:O	1:A:37:ASP:CB	0.52	2.58	11	4
1:A:62:GLU:N	1:A:62:GLU:OE1	0.52	2.43	11	1
1:A:44:CYS:CB	1:A:71:ASN:HD21	0.52	2.18	13	1
1:A:51:MET:C	1:A:51:MET:SD	0.52	2.93	2	1
1:A:74:LEU:N	1:A:74:LEU:CD2	0.52	2.72	4	2
1:A:79:ASP:C	1:A:81:ASP:N	0.51	2.68	6	13
1:A:43:ASN:HD21	1:A:45:ARG:CZ	0.51	2.19	5	2
1:A:63:LEU:CD2	1:A:63:LEU:H	0.51	2.19	7	1
1:A:23:GLU:O	1:A:26:GLU:N	0.51	2.43	5	1
1:A:46:ASP:O	1:A:50:CYS:SG	0.51	2.69	1	2
1:A:56:TYR:O	1:A:57:MET:C	0.51	2.53	8	1
1:A:79:ASP:OD1	1:A:79:ASP:N	0.51	2.40	11	1
1:A:46:ASP:N	1:A:46:ASP:OD1	0.51	2.43	2	1
1:A:69:GLN:O	1:A:73:ASN:N	0.51	2.44	12	1
1:A:27:LEU:N	1:A:27:LEU:CD2	0.50	2.74	8	3
1:A:40:GLY:C	1:A:41:TYR:CG	0.50	2.89	9	2
1:A:47:LEU:HD23	1:A:47:LEU:O	0.50	2.06	1	2
1:A:37:ASP:N	1:A:37:ASP:OD1	0.50	2.41	13	4
1:A:35:ASP:OD1	1:A:37:ASP:OD1	0.50	2.30	2	3
1:A:47:LEU:O	1:A:50:CYS:SG	0.50	2.67	9	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:LEU:O	1:A:75:GLY:C	0.50	2.55	15	2
1:A:70:ILE:O	1:A:74:LEU:O	0.50	2.30	15	1
1:A:87:MET:C	1:A:87:MET:SD	0.49	2.95	10	1
1:A:68:GLN:O	1:A:69:GLN:C	0.49	2.55	12	4
1:A:38:LYS:O	1:A:40:GLY:N	0.49	2.45	3	5
1:A:56:TYR:CD2	1:A:57:MET:N	0.49	2.79	2	1
1:A:27:LEU:N	1:A:27:LEU:HD22	0.49	2.21	8	3
1:A:57:MET:SD	1:A:57:MET:O	0.49	2.70	11	1
1:A:80:PHE:O	1:A:84:VAL:HG23	0.49	2.08	12	4
1:A:37:ASP:OD1	1:A:37:ASP:N	0.49	2.46	9	1
1:A:45:ARG:CG	1:A:46:ASP:N	0.49	2.75	14	1
1:A:83:PHE:C	1:A:83:PHE:CD1	0.49	2.91	14	1
1:A:69:GLN:HE21	1:A:73:ASN:ND2	0.49	2.05	9	1
1:A:74:LEU:CD2	1:A:74:LEU:N	0.49	2.76	10	1
1:A:35:ASP:OD1	1:A:38:LYS:N	0.49	2.46	1	1
1:A:43:ASN:C	1:A:45:ARG:N	0.49	2.71	14	7
1:A:57:MET:N	1:A:58:PRO:CD	0.48	2.76	9	3
1:A:59:THR:OG1	1:A:62:GLU:CD	0.48	2.56	11	1
1:A:47:LEU:HD23	1:A:47:LEU:C	0.48	2.33	1	1
1:A:61:MET:O	1:A:65:GLU:N	0.48	2.45	15	4
1:A:74:LEU:N	1:A:74:LEU:HD22	0.48	2.23	10	1
1:A:20:ARG:CB	1:A:21:PRO:CD	0.48	2.92	1	2
1:A:28:ARG:NH1	1:A:32:ARG:NE	0.48	2.61	7	1
1:A:79:ASP:O	1:A:81:ASP:N	0.48	2.46	6	6
1:A:55:GLY:C	1:A:57:MET:H	0.48	2.15	9	2
1:A:35:ASP:OD2	1:A:39:ASP:CA	0.48	2.62	3	1
1:A:43:ASN:CG	1:A:44:CYS:H	0.48	2.17	6	1
1:A:51:MET:O	1:A:56:TYR:N	0.48	2.45	13	1
1:A:36:LYS:C	1:A:37:ASP:CG	0.48	2.78	11	6
1:A:87:MET:O	1:A:88:GLY:O	0.48	2.32	7	4
1:A:55:GLY:C	1:A:57:MET:N	0.48	2.72	7	3
1:A:63:LEU:HD23	1:A:63:LEU:H	0.48	1.69	7	1
1:A:32:ARG:O	1:A:34:PHE:N	0.47	2.47	12	2
1:A:43:ASN:HD22	1:A:76:GLY:C	0.47	2.16	6	1
1:A:43:ASN:H	1:A:43:ASN:HD22	0.47	1.52	11	1
1:A:74:LEU:HD12	1:A:74:LEU:N	0.47	2.23	14	1
1:A:71:ASN:O	1:A:75:GLY:CA	0.47	2.62	10	2
1:A:43:ASN:CG	1:A:45:ARG:HE	0.47	2.17	10	1
1:A:47:LEU:C	1:A:47:LEU:CD2	0.47	2.88	12	1
1:A:54:MET:O	1:A:56:TYR:N	0.47	2.48	4	1
1:A:43:ASN:O	1:A:45:ARG:N	0.47	2.46	6	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:MET:SD	1:A:57:MET:C	0.47	2.98	11	1
1:A:63:LEU:N	1:A:63:LEU:CD2	0.47	2.78	7	2
1:A:51:MET:SD	1:A:52:ARG:N	0.47	2.88	2	1
1:A:56:TYR:CD1	1:A:56:TYR:N	0.47	2.82	10	2
1:A:56:TYR:C	1:A:56:TYR:CD1	0.46	2.91	4	1
1:A:54:MET:O	1:A:55:GLY:O	0.46	2.32	8	1
1:A:25:GLU:OE1	1:A:28:ARG:CZ	0.46	2.62	14	1
1:A:74:LEU:O	1:A:75:GLY:O	0.46	2.34	15	1
1:A:20:ARG:N	1:A:21:PRO:HD2	0.46	2.25	14	2
1:A:35:ASP:O	1:A:37:ASP:N	0.46	2.48	10	1
1:A:35:ASP:O	1:A:37:ASP:OD2	0.46	2.34	12	1
1:A:59:THR:O	1:A:62:GLU:N	0.46	2.48	4	2
1:A:66:LEU:O	1:A:67:SER:C	0.46	2.59	10	3
1:A:72:MET:SD	1:A:72:MET:N	0.46	2.89	1	1
1:A:61:MET:O	1:A:65:GLU:CB	0.46	2.64	15	4
1:A:73:ASN:O	1:A:74:LEU:C	0.46	2.59	6	2
1:A:35:ASP:OD2	1:A:37:ASP:OD1	0.46	2.34	4	1
1:A:56:TYR:O	1:A:58:PRO:N	0.46	2.49	8	1
1:A:64:ILE:O	1:A:68:GLN:CG	0.46	2.63	15	1
1:A:35:ASP:OD2	1:A:39:ASP:OD1	0.45	2.33	12	1
1:A:35:ASP:OD2	1:A:39:ASP:C	0.45	2.58	11	3
1:A:57:MET:O	1:A:62:GLU:OE1	0.45	2.34	4	1
1:A:50:CYS:O	1:A:53:THR:HG22	0.45	2.10	10	1
1:A:74:LEU:H	1:A:74:LEU:CD2	0.45	2.21	9	1
1:A:66:LEU:CD1	1:A:66:LEU:C	0.45	2.90	8	1
1:A:71:ASN:O	1:A:75:GLY:C	0.45	2.60	14	1
1:A:35:ASP:CG	1:A:37:ASP:OD1	0.45	2.59	8	1
1:A:69:GLN:CD	1:A:69:GLN:C	0.45	2.84	9	1
1:A:62:GLU:CD	1:A:62:GLU:C	0.45	2.84	7	2
1:A:79:ASP:O	1:A:82:ASP:N	0.45	2.50	6	1
1:A:66:LEU:C	1:A:66:LEU:HD13	0.45	2.37	8	1
1:A:39:ASP:CG	1:A:41:TYR:O	0.44	2.60	10	1
1:A:26:GLU:OE1	1:A:26:GLU:C	0.44	2.60	6	1
1:A:72:MET:O	1:A:73:ASN:C	0.44	2.58	2	2
1:A:32:ARG:C	1:A:34:PHE:H	0.44	2.20	12	1
1:A:71:ASN:O	1:A:75:GLY:O	0.44	2.36	14	1
1:A:25:GLU:CD	1:A:25:GLU:C	0.44	2.85	6	3
1:A:55:GLY:O	1:A:56:TYR:C	0.44	2.61	6	1
1:A:35:ASP:O	1:A:37:ASP:OD1	0.44	2.36	7	2
1:A:39:ASP:OD1	1:A:41:TYR:O	0.44	2.36	9	2
1:A:79:ASP:O	1:A:80:PHE:C	0.44	2.60	5	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:C	1:A:68:GLN:N	0.44	2.72	8	1
1:A:40:GLY:O	1:A:79:ASP:OD1	0.44	2.36	3	1
1:A:27:LEU:CD2	1:A:87:MET:SD	0.44	3.06	11	1
1:A:35:ASP:OD1	1:A:35:ASP:C	0.43	2.59	9	2
1:A:87:MET:O	1:A:87:MET:SD	0.43	2.76	9	1
1:A:41:TYR:CD1	1:A:79:ASP:CG	0.43	2.96	10	1
1:A:22:GLU:O	1:A:26:GLU:OE1	0.43	2.35	11	1
1:A:74:LEU:C	1:A:74:LEU:HD23	0.43	2.37	15	1
1:A:37:ASP:OD2	1:A:39:ASP:OD2	0.43	2.36	6	1
1:A:74:LEU:HD23	1:A:74:LEU:C	0.43	2.38	7	1
1:A:47:LEU:CD2	1:A:70:ILE:CD1	0.43	2.96	15	1
1:A:79:ASP:OD1	1:A:81:ASP:OD2	0.43	2.37	15	1
1:A:60:GLU:OE1	1:A:60:GLU:N	0.43	2.44	6	1
1:A:73:ASN:C	1:A:74:LEU:HD22	0.43	2.37	10	1
1:A:51:MET:SD	1:A:63:LEU:CD1	0.43	3.07	12	1
1:A:54:MET:SD	1:A:54:MET:O	0.43	2.76	3	1
1:A:85:GLU:CD	1:A:85:GLU:C	0.43	2.87	4	2
1:A:60:GLU:O	1:A:63:LEU:CD2	0.43	2.66	7	1
1:A:82:ASP:OD1	1:A:82:ASP:C	0.43	2.61	1	2
1:A:24:ILE:O	1:A:25:GLU:C	0.43	2.61	4	1
1:A:22:GLU:CD	1:A:22:GLU:C	0.43	2.86	10	1
1:A:41:TYR:CD1	1:A:79:ASP:OD1	0.43	2.71	13	1
1:A:65:GLU:O	1:A:69:GLN:OE1	0.43	2.36	4	1
1:A:34:PHE:O	1:A:35:ASP:C	0.43	2.61	12	1
1:A:37:ASP:CG	1:A:39:ASP:OD1	0.43	2.62	7	1
1:A:45:ARG:HG3	1:A:46:ASP:N	0.43	2.29	14	1
1:A:59:THR:O	1:A:60:GLU:C	0.42	2.62	4	1
1:A:65:GLU:O	1:A:69:GLN:CB	0.42	2.67	9	1
1:A:39:ASP:OD2	1:A:41:TYR:O	0.42	2.37	10	1
1:A:64:ILE:O	1:A:65:GLU:C	0.42	2.62	6	1
1:A:22:GLU:CD	1:A:22:GLU:O	0.42	2.62	10	1
1:A:62:GLU:OE1	1:A:62:GLU:CA	0.42	2.67	11	1
1:A:41:TYR:OH	1:A:77:HIS:CG	0.42	2.73	2	1
1:A:49:ASN:C	1:A:49:ASN:HD22	0.42	2.20	15	1
1:A:36:LYS:O	1:A:37:ASP:C	0.42	2.63	6	1
1:A:34:PHE:O	1:A:46:ASP:OD2	0.42	2.37	5	1
1:A:35:ASP:OD2	1:A:39:ASP:CG	0.42	2.63	12	1
1:A:65:GLU:CD	1:A:65:GLU:C	0.42	2.87	1	1
1:A:82:ASP:OD1	1:A:82:ASP:O	0.42	2.38	1	1
1:A:86:LEU:CD1	1:A:86:LEU:N	0.42	2.82	4	1
1:A:50:CYS:SG	1:A:83:PHE:CE1	0.42	3.13	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ASP:O	1:A:85:GLU:CD	0.42	2.62	2	1
1:A:20:ARG:O	1:A:23:GLU:N	0.42	2.49	7	1
1:A:46:ASP:OD1	1:A:46:ASP:N	0.41	2.51	11	1
1:A:62:GLU:C	1:A:62:GLU:OE1	0.41	2.63	14	1
1:A:31:PHE:CD1	1:A:31:PHE:C	0.41	2.97	14	2
1:A:37:ASP:OD1	1:A:39:ASP:OD1	0.41	2.38	8	1
1:A:76:GLY:O	1:A:77:HIS:CD2	0.41	2.74	8	1
1:A:74:LEU:C	1:A:74:LEU:HD13	0.41	2.40	12	2
1:A:44:CYS:SG	1:A:71:ASN:ND2	0.41	2.92	13	1
1:A:74:LEU:C	1:A:74:LEU:CD1	0.41	2.93	5	2
1:A:73:ASN:OD1	1:A:73:ASN:C	0.41	2.63	13	1
1:A:27:LEU:HD22	1:A:87:MET:SD	0.41	2.56	11	1
1:A:35:ASP:OD2	1:A:40:GLY:N	0.41	2.54	3	1
1:A:63:LEU:O	1:A:67:SER:OG	0.41	2.37	4	1
1:A:57:MET:N	1:A:58:PRO:HD3	0.41	2.31	7	1
1:A:26:GLU:CD	1:A:26:GLU:O	0.41	2.64	8	1
1:A:59:THR:C	1:A:61:MET:N	0.41	2.78	5	2
1:A:50:CYS:SG	1:A:83:PHE:CZ	0.41	3.14	15	1
1:A:86:LEU:N	1:A:86:LEU:HD12	0.41	2.31	4	1
1:A:36:LYS:O	1:A:45:ARG:NH2	0.41	2.53	9	1
1:A:79:ASP:OD1	1:A:82:ASP:CB	0.40	2.69	9	2
1:A:21:PRO:O	1:A:25:GLU:CG	0.40	2.69	13	1
1:A:65:GLU:OE2	1:A:65:GLU:O	0.40	2.39	15	1
1:A:41:TYR:C	1:A:42:ILE:HG23	0.40	2.40	2	1
1:A:25:GLU:OE1	1:A:28:ARG:NH2	0.40	2.55	14	1
1:A:23:GLU:O	1:A:24:ILE:C	0.40	2.62	5	1
1:A:32:ARG:O	1:A:35:ASP:OD1	0.40	2.40	7	1
1:A:66:LEU:C	1:A:68:GLN:H	0.40	2.25	8	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	69/167 (41%)	55±2 (80±3%)	10±2 (14±3%)	4±1 (6±2%)	2 19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1035/2505 (41%)	827 (80%)	145 (14%)	63 (6%)	2 19

All 17 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	37	ASP	8
1	A	88	GLY	7
1	A	44	CYS	6
1	A	73	ASN	5
1	A	75	GLY	5
1	A	55	GLY	4
1	A	59	THR	4
1	A	20	ARG	3
1	A	39	ASP	3
1	A	54	MET	3
1	A	80	PHE	3
1	A	74	LEU	3
1	A	76	GLY	3
1	A	33	GLU	2
1	A	58	PRO	2
1	A	56	TYR	1
1	A	57	MET	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	62/148 (42%)	59±1 (95±1%)	3±1 (5±1%)	22 72
All	All	930/2220 (42%)	881 (95%)	49 (5%)	22 72

All 25 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	59	THR	7
1	A	43	ASN	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	37	ASP	4
1	A	86	LEU	4
1	A	53	THR	3
1	A	74	LEU	3
1	A	85	GLU	2
1	A	44	CYS	2
1	A	56	TYR	2
1	A	77	HIS	2
1	A	72	MET	1
1	A	78	VAL	1
1	A	47	LEU	1
1	A	41	TYR	1
1	A	64	ILE	1
1	A	38	LYS	1
1	A	36	LYS	1
1	A	66	LEU	1
1	A	35	ASP	1
1	A	62	GLU	1
1	A	79	ASP	1
1	A	39	ASP	1
1	A	49	ASN	1
1	A	67	SER	1
1	A	57	MET	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 i

The completeness of assignment taking into account all chemical shift lists is 66% for the well-defined parts and 65% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping i

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	1354
Number of shifts mapped to atoms	668
Number of unparsed shifts	0
Number of shifts with mapping errors	686
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 686 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	15	LYS	HA	4.313	0.04	1
1	A	15	LYS	HB2	1.87	0.04	2
1	A	15	LYS	HB3	1.8	0.04	2
1	A	15	LYS	C	176.111	0.2	1
1	A	15	LYS	CA	56.722	0.2	1
1	A	15	LYS	CB	32.883	0.2	1
1	A	16	ASP	H	8.219	0.04	1
1	A	16	ASP	HA	4.612	0.04	1
1	A	16	ASP	HB2	2.657	0.04	2
1	A	16	ASP	HB3	2.735	0.04	2
1	A	16	ASP	C	175.635	0.2	1
1	A	16	ASP	CA	54.049	0.2	1
1	A	16	ASP	CB	41.19	0.2	1
1	A	16	ASP	N	119.878	0.2	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	ARG	H	8.01	0.04	1
1	A	17	ARG	HA	4.405	0.04	1
1	A	17	ARG	HB2	1.94	0.04	2
1	A	17	ARG	C	174.866	0.2	1
1	A	17	ARG	CA	55.474	0.2	1
1	A	17	ARG	CB	30.781	0.2	1
1	A	17	ARG	N	119.816	0.2	1
1	A	18	SER	H	8.03	0.04	1
1	A	92	LEU	H	7.837	0.04	1
1	A	92	LEU	HA	4.199	0.04	1
1	A	92	LEU	HB2	1.652	0.04	2
1	A	92	LEU	HB3	1.51	0.04	2
1	A	92	LEU	HD11	0.754	0.04	1
1	A	92	LEU	HD12	0.754	0.04	1
1	A	92	LEU	HD13	0.754	0.04	1
1	A	92	LEU	HD21	0.748	0.04	1
1	A	92	LEU	HD22	0.748	0.04	1
1	A	92	LEU	HD23	0.748	0.04	1
1	A	92	LEU	HG	1.668	0.04	1
1	A	92	LEU	C	177.405	0.2	1
1	A	92	LEU	CA	55.906	0.2	1
1	A	92	LEU	CB	41.937	0.2	1
1	A	92	LEU	CD1	25.27	0.2	1
1	A	92	LEU	CD2	22.99	0.2	1
1	A	92	LEU	N	117.988	0.2	1
1	A	93	ALA	H	7.429	0.04	1
1	A	93	ALA	HA	4.282	0.04	1
1	A	93	ALA	HB1	1.515	0.04	1
1	A	93	ALA	HB2	1.515	0.04	1
1	A	93	ALA	HB3	1.515	0.04	1
1	A	93	ALA	C	177.4	0.2	1
1	A	93	ALA	CA	53.285	0.2	1
1	A	93	ALA	CB	19.251	0.2	1
1	A	93	ALA	N	121.849	0.2	1
1	A	94	GLU	H	8.127	0.04	1
1	A	94	GLU	HA	4.423	0.04	1
1	A	94	GLU	HB2	2.162	0.04	2
1	A	94	GLU	C	176.9	0.2	1
1	A	94	GLU	CA	57.1	0.2	1
1	A	94	GLU	CB	30.15	0.2	1
1	A	94	GLU	N	118.932	0.2	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	95	THR	H	7.93	0.04	1
1	A	95	THR	HA	4.417	0.04	1
1	A	95	THR	HB	4.352	0.04	1
1	A	95	THR	HG21	1.28	0.04	1
1	A	95	THR	HG22	1.28	0.04	1
1	A	95	THR	HG23	1.28	0.04	1
1	A	95	THR	C	174.663	0.2	1
1	A	95	THR	CA	61.848	0.2	1
1	A	95	THR	CB	70.11	0.2	1
1	A	95	THR	CG2	21.83	0.2	1
1	A	95	THR	N	113.151	0.2	1
1	A	96	ALA	H	8.216	0.04	1
1	A	96	ALA	HA	4.305	0.04	1
1	A	96	ALA	HB1	1.444	0.04	1
1	A	96	ALA	HB2	1.444	0.04	1
1	A	96	ALA	HB3	1.444	0.04	1
1	A	96	ALA	C	177.477	0.2	1
1	A	96	ALA	CA	53.206	0.2	1
1	A	96	ALA	CB	19.436	0.2	1
1	A	96	ALA	N	125.432	0.2	1
1	A	97	ASP	H	8.211	0.04	1
1	A	97	ASP	C	176.233	0.2	1
1	A	97	ASP	CA	54.743	0.2	1
1	A	97	ASP	CB	41.246	0.2	1
1	A	97	ASP	N	118.477	0.2	1
1	A	98	MET	H	8.106	0.04	1
1	A	98	MET	HA	4.495	0.04	1
1	A	98	MET	HB2	2.099	0.04	2
1	A	98	MET	C	176.197	0.2	1
1	A	98	MET	CA	55.984	0.2	1
1	A	98	MET	CB	33.021	0.2	1
1	A	98	MET	N	119.877	0.2	1
1	A	99	ILE	H	8.045	0.04	1
1	A	99	ILE	HA	4.164	0.04	1
1	A	99	ILE	HB	1.912	0.04	1
1	A	99	ILE	HD11	0.878	0.04	1
1	A	99	ILE	HD12	0.878	0.04	1
1	A	99	ILE	HD13	0.878	0.04	1
1	A	99	ILE	HG12	1.583	0.04	2
1	A	99	ILE	HG13	1.264	0.04	2
1	A	99	ILE	HG21	0.985	0.04	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	ILE	HG22	0.985	0.04	1
1	A	99	ILE	HG23	0.985	0.04	1
1	A	99	ILE	C	175.982	0.2	1
1	A	99	ILE	CA	61.7	0.2	1
1	A	99	ILE	CB	38.572	0.2	1
1	A	99	ILE	CD1	13.33	0.2	1
1	A	99	ILE	CG1	27.64	0.2	1
1	A	99	ILE	CG2	17.8	0.2	1
1	A	99	ILE	N	121.235	0.2	1
1	A	100	GLY	H	8.467	0.04	1
1	A	100	GLY	HA2	4.262	0.04	2
1	A	100	GLY	HA3	4.039	0.04	2
1	A	100	GLY	C	174.458	0.2	1
1	A	100	GLY	CA	45.249	0.2	1
1	A	100	GLY	N	112.837	0.2	1
1	A	101	VAL	H	8.18	0.04	1
1	A	101	VAL	HA	3.944	0.04	1
1	A	101	VAL	HB	2.209	0.04	1
1	A	101	VAL	HG11	1.082	0.04	1
1	A	101	VAL	HG12	1.082	0.04	1
1	A	101	VAL	HG13	1.082	0.04	1
1	A	101	VAL	HG21	1.151	0.04	1
1	A	101	VAL	HG22	1.151	0.04	1
1	A	101	VAL	HG23	1.151	0.04	1
1	A	101	VAL	C	177.29	0.2	1
1	A	101	VAL	CA	65.721	0.2	1
1	A	101	VAL	CB	32.001	0.2	1
1	A	101	VAL	CG1	21.15	0.2	1
1	A	101	VAL	CG2	22.03	0.2	1
1	A	101	VAL	N	119.763	0.2	1
1	A	102	LYS	H	8.371	0.04	1
1	A	102	LYS	HA	4.018	0.04	1
1	A	102	LYS	HB2	1.902	0.04	2
1	A	102	LYS	C	178.292	0.2	1
1	A	102	LYS	CA	59.78	0.2	1
1	A	102	LYS	CB	32.459	0.2	1
1	A	102	LYS	N	121.994	0.2	1
1	A	103	GLU	H	8.311	0.04	1
1	A	103	GLU	HA	4.243	0.04	1
1	A	103	GLU	HB2	2.354	0.04	2
1	A	103	GLU	HB3	2.096	0.04	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	GLU	C	179.983	0.2	1
1	A	103	GLU	CA	59.947	0.2	1
1	A	103	GLU	CB	29.194	0.2	1
1	A	103	GLU	N	119.064	0.2	1
1	A	104	LEU	H	8.314	0.04	1
1	A	104	LEU	HA	4.34	0.04	1
1	A	104	LEU	HB2	2.257	0.04	2
1	A	104	LEU	HB3	1.685	0.04	2
1	A	104	LEU	C	179.074	0.2	1
1	A	104	LEU	CA	58.346	0.2	1
1	A	104	LEU	CB	42.35	0.2	1
1	A	104	LEU	N	121.269	0.2	1
1	A	105	ARG	H	8.702	0.04	1
1	A	105	ARG	HA	4.029	0.04	1
1	A	105	ARG	HB2	2.706	0.04	2
1	A	105	ARG	HB3	1.902	0.04	2
1	A	105	ARG	C	178.887	0.2	1
1	A	105	ARG	CA	59.688	0.2	1
1	A	105	ARG	CB	29.392	0.2	1
1	A	105	ARG	N	120.637	0.2	1
1	A	106	ASP	H	8.085	0.04	1
1	A	106	ASP	HA	4.444	0.04	1
1	A	106	ASP	HB2	2.808	0.04	2
1	A	106	ASP	HB3	2.736	0.04	2
1	A	106	ASP	C	178.65	0.2	1
1	A	106	ASP	CA	57.486	0.2	1
1	A	106	ASP	CB	40.15	0.2	1
1	A	106	ASP	N	120.04	0.2	1
1	A	107	ALA	H	7.962	0.04	1
1	A	107	ALA	HA	4.127	0.04	1
1	A	107	ALA	HB1	1.669	0.04	1
1	A	107	ALA	HB2	1.669	0.04	1
1	A	107	ALA	HB3	1.669	0.04	1
1	A	107	ALA	C	178.387	0.2	1
1	A	107	ALA	CA	54.965	0.2	1
1	A	107	ALA	CB	18.229	0.2	1
1	A	107	ALA	N	122.925	0.2	1
1	A	108	PHE	H	8.392	0.04	1
1	A	108	PHE	HA	3.089	0.04	1
1	A	108	PHE	HB2	3.174	0.04	2
1	A	108	PHE	HB3	2.91	0.04	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	108	PHE	HD1	6.595	0.04	3
1	A	108	PHE	HD2	6.595	0.04	3
1	A	108	PHE	HE1	7.06	0.04	3
1	A	108	PHE	HE2	7.06	0.04	3
1	A	108	PHE	HZ	7.386	0.04	1
1	A	108	PHE	C	176.894	0.2	1
1	A	108	PHE	CA	61.3	0.2	1
1	A	108	PHE	CB	39.52	0.2	1
1	A	108	PHE	N	118.738	0.2	1
1	A	109	ARG	H	7.748	0.04	1
1	A	109	ARG	HA	3.984	0.04	1
1	A	109	ARG	HB2	2.01	0.04	2
1	A	109	ARG	C	178.317	0.2	1
1	A	109	ARG	CA	58.87	0.2	1
1	A	109	ARG	CB	30.081	0.2	1
1	A	109	ARG	N	115.762	0.2	1
1	A	110	GLU	H	7.437	0.04	1
1	A	110	GLU	HA	3.964	0.04	1
1	A	110	GLU	HB2	2.038	0.04	2
1	A	110	GLU	C	178.128	0.2	1
1	A	110	GLU	CA	58.373	0.2	1
1	A	110	GLU	CB	29.297	0.2	1
1	A	110	GLU	N	117.304	0.2	1
1	A	111	PHE	H	7.577	0.04	1
1	A	111	PHE	HA	4.518	0.04	1
1	A	111	PHE	HB2	2.817	0.04	2
1	A	111	PHE	C	176.554	0.2	1
1	A	111	PHE	CA	58.031	0.2	1
1	A	111	PHE	CB	39.258	0.2	1
1	A	111	PHE	N	116.764	0.2	1
1	A	112	ASP	H	7.519	0.04	1
1	A	112	ASP	HA	4.565	0.04	1
1	A	112	ASP	HB2	1.805	0.04	2
1	A	112	ASP	HB3	2.655	0.04	2
1	A	112	ASP	C	176.98	0.2	1
1	A	112	ASP	CA	52.316	0.2	1
1	A	112	ASP	CB	39.066	0.2	1
1	A	112	ASP	N	118.644	0.2	1
1	A	113	THR	H	7.909	0.04	1
1	A	113	THR	HA	4.016	0.04	1
1	A	113	THR	HB	4.246	0.04	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	113	THR	HG21	1.321	0.04	1
1	A	113	THR	HG22	1.321	0.04	1
1	A	113	THR	HG23	1.321	0.04	1
1	A	113	THR	C	176.393	0.2	1
1	A	113	THR	CA	65.145	0.2	1
1	A	113	THR	CB	68.837	0.2	1
1	A	113	THR	CG2	22.56	0.2	1
1	A	113	THR	N	118.287	0.2	1
1	A	114	ASN	H	8.077	0.04	1
1	A	114	ASN	HA	4.873	0.04	1
1	A	114	ASN	HB2	3.336	0.04	2
1	A	114	ASN	HB3	2.916	0.04	2
1	A	114	ASN	C	176.65	0.2	1
1	A	114	ASN	CA	51.994	0.2	1
1	A	114	ASN	CB	37.379	0.2	1
1	A	114	ASN	N	115.932	0.2	1
1	A	115	GLY	H	7.699	0.04	1
1	A	115	GLY	HA2	3.865	0.04	2
1	A	115	GLY	HA3	3.865	0.04	2
1	A	115	GLY	C	174.8	0.2	1
1	A	115	GLY	CA	47.476	0.2	1
1	A	115	GLY	N	109.332	0.2	1
1	A	116	ASP	H	8.023	0.04	1
1	A	116	ASP	HA	4.571	0.04	1
1	A	116	ASP	HB2	2.471	0.04	2
1	A	116	ASP	HB3	3.164	0.04	2
1	A	116	ASP	C	177.569	0.2	1
1	A	116	ASP	CA	53.37	0.2	1
1	A	116	ASP	CB	40.43	0.2	1
1	A	116	ASP	N	118.9	0.2	1
1	A	117	GLY	H	10.37	0.04	1
1	A	117	GLY	HA2	4.327	0.04	2
1	A	117	GLY	HA3	3.648	0.04	2
1	A	117	GLY	C	173.2	0.2	1
1	A	117	GLY	CA	45.638	0.2	1
1	A	117	GLY	N	112.57	0.2	1
1	A	118	GLU	H	7.912	0.04	1
1	A	118	GLU	HA	4.92	0.04	1
1	A	118	GLU	HB2	1.792	0.04	2
1	A	118	GLU	HB3	1.873	0.04	2
1	A	118	GLU	C	174.368	0.2	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	118	GLU	CA	54.009	0.2	1
1	A	118	GLU	CB	33.717	0.2	1
1	A	118	GLU	N	117.446	0.2	1
1	A	119	ILE	H	9.396	0.04	1
1	A	119	ILE	HA	4.955	0.04	1
1	A	119	ILE	HB	2.06	0.04	1
1	A	119	ILE	HD11	0.311	0.04	1
1	A	119	ILE	HD12	0.311	0.04	1
1	A	119	ILE	HD13	0.311	0.04	1
1	A	119	ILE	HG12	0.933	0.04	2
1	A	119	ILE	HG13	0.439	0.04	2
1	A	119	ILE	HG21	0.932	0.04	1
1	A	119	ILE	HG22	0.932	0.04	1
1	A	119	ILE	HG23	0.932	0.04	1
1	A	119	ILE	C	175.569	0.2	1
1	A	119	ILE	CA	59.779	0.2	1
1	A	119	ILE	CB	37.986	0.2	1
1	A	119	ILE	CD1	14.52	0.2	1
1	A	119	ILE	CG2	18.66	0.2	1
1	A	119	ILE	N	126.916	0.2	1
1	A	120	SER	H	9.274	0.04	1
1	A	120	SER	HA	4.88	0.04	1
1	A	120	SER	HB2	4.499	0.04	2
1	A	120	SER	HB3	4.063	0.04	2
1	A	120	SER	C	175.616	0.2	1
1	A	120	SER	CA	56.953	0.2	1
1	A	120	SER	CB	65.788	0.2	1
1	A	120	SER	N	124.347	0.2	1
1	A	121	THR	H	8.793	0.04	1
1	A	121	THR	HA	3.843	0.04	1
1	A	121	THR	HB	4.229	0.04	1
1	A	121	THR	HG21	1.267	0.04	1
1	A	121	THR	HG22	1.267	0.04	1
1	A	121	THR	HG23	1.267	0.04	1
1	A	121	THR	CA	66.94	0.2	1
1	A	121	THR	CB	67.965	0.2	1
1	A	121	THR	CG2	22.85	0.2	1
1	A	121	THR	N	114.11	0.2	1
1	A	122	SER	HA	4.242	0.04	1
1	A	122	SER	HB2	3.936	0.04	2
1	A	122	SER	HB3	3.936	0.04	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	122	SER	C	177.216	0.2	1
1	A	122	SER	CA	62.34	0.2	1
1	A	122	SER	CB	62.34	0.2	1
1	A	123	GLU	H	7.752	0.04	1
1	A	123	GLU	HA	4.231	0.04	1
1	A	123	GLU	HB2	2.445	0.04	2
1	A	123	GLU	HB3	2.344	0.04	2
1	A	123	GLU	C	180.458	0.2	1
1	A	123	GLU	CA	58.708	0.2	1
1	A	123	GLU	CB	29.512	0.2	1
1	A	123	GLU	N	123.363	0.2	1
1	A	124	LEU	H	8.815	0.04	1
1	A	124	LEU	HA	3.988	0.04	1
1	A	124	LEU	HB2	2.006	0.04	2
1	A	124	LEU	HB3	1.526	0.04	2
1	A	124	LEU	HD11	0.981	0.04	1
1	A	124	LEU	HD12	0.981	0.04	1
1	A	124	LEU	HD13	0.981	0.04	1
1	A	124	LEU	HD21	0.968	0.04	1
1	A	124	LEU	HD22	0.968	0.04	1
1	A	124	LEU	HD23	0.968	0.04	1
1	A	124	LEU	HG	1.658	0.04	1
1	A	124	LEU	C	177.807	0.2	1
1	A	124	LEU	CA	57.972	0.2	1
1	A	124	LEU	CB	41.353	0.2	1
1	A	124	LEU	CD1	23.28	0.2	1
1	A	124	LEU	CD2	26.62	0.2	1
1	A	124	LEU	N	122.468	0.2	1
1	A	125	ARG	H	8.34	0.04	1
1	A	125	ARG	HA	3.696	0.04	1
1	A	125	ARG	HB2	2.061	0.04	2
1	A	125	ARG	HB3	1.949	0.04	2
1	A	125	ARG	C	178.343	0.2	1
1	A	125	ARG	CA	60.485	0.2	1
1	A	125	ARG	CB	30.323	0.2	1
1	A	125	ARG	N	119.165	0.2	1
1	A	126	GLU	H	7.675	0.04	1
1	A	126	GLU	HA	4.179	0.04	1
1	A	126	GLU	HB2	1.726	0.04	2
1	A	126	GLU	HB3	1.635	0.04	2
1	A	126	GLU	C	178.776	0.2	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	126	GLU	CA	58.707	0.2	1
1	A	126	GLU	CB	29.607	0.2	1
1	A	126	GLU	N	117.125	0.2	1
1	A	127	ALA	H	7.9	0.04	1
1	A	127	ALA	HA	3.87	0.04	1
1	A	127	ALA	HB1	0.797	0.04	1
1	A	127	ALA	HB2	0.797	0.04	1
1	A	127	ALA	HB3	0.797	0.04	1
1	A	127	ALA	C	180.006	0.2	1
1	A	127	ALA	CA	54.967	0.2	1
1	A	127	ALA	CB	17.785	0.2	1
1	A	127	ALA	N	121.671	0.2	1
1	A	128	MET	H	8.353	0.04	1
1	A	128	MET	HA	4.211	0.04	1
1	A	128	MET	HB2	2.122	0.04	2
1	A	128	MET	C	178.16	0.2	1
1	A	128	MET	CA	57.67	0.2	1
1	A	128	MET	CB	31.93	0.2	1
1	A	128	MET	N	115.083	0.2	1
1	A	129	ARG	H	7.904	0.04	1
1	A	129	ARG	HA	3.747	0.04	1
1	A	129	ARG	HB2	2.06	0.04	2
1	A	129	ARG	CA	59.32	0.2	1
1	A	129	ARG	CB	29.812	0.2	1
1	A	129	ARG	N	119.493	0.2	1
1	A	130	LYS	HA	4.073	0.04	1
1	A	130	LYS	HB2	1.962	0.04	2
1	A	130	LYS	C	178.421	0.2	1
1	A	130	LYS	CA	59.13	0.2	1
1	A	130	LYS	CB	32.67	0.2	1
1	A	131	LEU	H	8.059	0.04	1
1	A	131	LEU	HA	4.246	0.04	1
1	A	131	LEU	HB2	1.798	0.04	2
1	A	131	LEU	HB3	1.543	0.04	2
1	A	131	LEU	HD11	0.897	0.04	1
1	A	131	LEU	HD12	0.897	0.04	1
1	A	131	LEU	HD13	0.897	0.04	1
1	A	131	LEU	HD21	0.965	0.04	1
1	A	131	LEU	HD22	0.965	0.04	1
1	A	131	LEU	HD23	0.965	0.04	1
1	A	131	LEU	C	178.363	0.2	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	131	LEU	CA	57.177	0.2	1
1	A	131	LEU	CB	43.352	0.2	1
1	A	131	LEU	CD1	25.09	0.2	1
1	A	131	LEU	CD2	23.73	0.2	1
1	A	131	LEU	N	118.2	0.2	1
1	A	132	LEU	H	8.292	0.04	1
1	A	132	LEU	HA	4.416	0.04	1
1	A	132	LEU	HB2	1.744	0.04	2
1	A	132	LEU	HB3	1.401	0.04	2
1	A	132	LEU	HD11	0.811	0.04	1
1	A	132	LEU	HD12	0.811	0.04	1
1	A	132	LEU	HD13	0.811	0.04	1
1	A	132	LEU	C	178.404	0.2	1
1	A	132	LEU	CA	55.369	0.2	1
1	A	132	LEU	CB	42.9	0.2	1
1	A	132	LEU	CD1	25.81	0.2	1
1	A	132	LEU	N	115.873	0.2	1
1	A	133	GLY	H	7.672	0.04	1
1	A	133	GLY	HA2	4.162	0.04	2
1	A	133	GLY	HA3	3.875	0.04	2
1	A	133	GLY	CA	46.107	0.2	1
1	A	133	GLY	N	107.097	0.2	1
1	A	135	GLN	HA	4.326	0.04	1
1	A	135	GLN	HB2	2.096	0.04	2
1	A	135	GLN	HB3	1.982	0.04	2
1	A	135	GLN	C	175.917	0.2	1
1	A	135	GLN	CA	56.39	0.2	1
1	A	135	GLN	CB	29.39	0.2	1
1	A	136	VAL	H	7.878	0.04	1
1	A	136	VAL	HA	4.25	0.04	1
1	A	136	VAL	HB	2.089	0.04	1
1	A	136	VAL	HG11	0.967	0.04	1
1	A	136	VAL	HG12	0.967	0.04	1
1	A	136	VAL	HG13	0.967	0.04	1
1	A	136	VAL	HG21	0.926	0.04	1
1	A	136	VAL	HG22	0.926	0.04	1
1	A	136	VAL	HG23	0.926	0.04	1
1	A	136	VAL	C	175.832	0.2	1
1	A	136	VAL	CA	61.833	0.2	1
1	A	136	VAL	CB	33.037	0.2	1
1	A	136	VAL	CG1	21.78	0.2	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	136	VAL	CG2	20.99	0.2	1
1	A	136	VAL	N	119.53	0.2	1
1	A	137	GLY	H	8.736	0.04	1
1	A	137	GLY	HA2	4.043	0.04	2
1	A	137	GLY	HA3	4.043	0.04	2
1	A	137	GLY	CA	45.086	0.2	1
1	A	137	GLY	N	112.04	0.2	1
1	A	141	ILE	HA	3.765	0.04	1
1	A	141	ILE	HB	2.058	0.04	1
1	A	141	ILE	HD11	0.782	0.04	1
1	A	141	ILE	HD12	0.782	0.04	1
1	A	141	ILE	HD13	0.782	0.04	1
1	A	141	ILE	HG12	1.505	0.04	2
1	A	141	ILE	HG13	1.318	0.04	2
1	A	141	ILE	HG21	0.962	0.04	1
1	A	141	ILE	HG22	0.962	0.04	1
1	A	141	ILE	HG23	0.962	0.04	1
1	A	141	ILE	C	176.974	0.2	1
1	A	141	ILE	CA	63.18	0.2	1
1	A	141	ILE	CB	36.74	0.2	1
1	A	141	ILE	CD1	12.41	0.2	1
1	A	141	ILE	CG2	18.24	0.2	1
1	A	142	GLU	H	8.067	0.04	1
1	A	142	GLU	HA	3.955	0.04	1
1	A	142	GLU	HB2	2.104	0.04	2
1	A	142	GLU	C	179.211	0.2	1
1	A	142	GLU	CA	59.384	0.2	1
1	A	142	GLU	CB	29.116	0.2	1
1	A	142	GLU	N	118.989	0.2	1
1	A	143	GLU	H	7.633	0.04	1
1	A	143	GLU	HA	4.045	0.04	1
1	A	143	GLU	HB2	2.157	0.04	2
1	A	143	GLU	C	178.455	0.2	1
1	A	143	GLU	CA	59.228	0.2	1
1	A	143	GLU	CB	29.628	0.2	1
1	A	143	GLU	N	117.954	0.2	1
1	A	144	ILE	H	7.598	0.04	1
1	A	144	ILE	HA	3.805	0.04	1
1	A	144	ILE	HB	1.972	0.04	1
1	A	144	ILE	HD11	0.802	0.04	1
1	A	144	ILE	HD12	0.802	0.04	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	144	ILE	HD13	0.802	0.04	1
1	A	144	ILE	HG12	1.819	0.04	2
1	A	144	ILE	HG13	1.086	0.04	2
1	A	144	ILE	HG21	0.902	0.04	1
1	A	144	ILE	HG22	0.902	0.04	1
1	A	144	ILE	HG23	0.902	0.04	1
1	A	144	ILE	C	178.092	0.2	1
1	A	144	ILE	CA	64.947	0.2	1
1	A	144	ILE	CB	38.457	0.2	1
1	A	144	ILE	CD1	13.7	0.2	1
1	A	144	ILE	CG1	28.91	0.2	1
1	A	144	ILE	CG2	17.44	0.2	1
1	A	144	ILE	N	119.581	0.2	1
1	A	145	ILE	H	8.035	0.04	1
1	A	145	ILE	HA	3.7	0.04	1
1	A	145	ILE	HB	1.995	0.04	1
1	A	145	ILE	HD11	0.744	0.04	1
1	A	145	ILE	HD12	0.744	0.04	1
1	A	145	ILE	HD13	0.744	0.04	1
1	A	145	ILE	HG12	1.575	0.04	2
1	A	145	ILE	HG13	1.21	0.04	2
1	A	145	ILE	HG21	0.905	0.04	1
1	A	145	ILE	HG22	0.905	0.04	1
1	A	145	ILE	HG23	0.905	0.04	1
1	A	145	ILE	C	177.184	0.2	1
1	A	145	ILE	CA	64.377	0.2	1
1	A	145	ILE	CB	37.478	0.2	1
1	A	145	ILE	CD1	13.06	0.2	1
1	A	145	ILE	CG2	17.37	0.2	1
1	A	145	ILE	N	116.702	0.2	1
1	A	146	ARG	H	7.554	0.04	1
1	A	146	ARG	HA	4.091	0.04	1
1	A	146	ARG	C	177.768	0.2	1
1	A	146	ARG	CA	59.241	0.2	1
1	A	146	ARG	CB	30.132	0.2	1
1	A	146	ARG	N	118.923	0.2	1
1	A	147	ASP	H	7.653	0.04	1
1	A	147	ASP	HA	4.58	0.04	1
1	A	147	ASP	HB2	2.782	0.04	2
1	A	147	ASP	C	177.272	0.2	1
1	A	147	ASP	CA	55.858	0.2	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	ASP	CB	41.799	0.2	1
1	A	147	ASP	N	116.963	0.2	1
1	A	148	VAL	H	7.725	0.04	1
1	A	148	VAL	HA	4.134	0.04	1
1	A	148	VAL	HB	2.182	0.04	1
1	A	148	VAL	HG11	1.002	0.04	1
1	A	148	VAL	HG12	1.002	0.04	1
1	A	148	VAL	HG13	1.002	0.04	1
1	A	148	VAL	C	176.607	0.2	1
1	A	148	VAL	CA	63.064	0.2	1
1	A	148	VAL	CB	32.842	0.2	1
1	A	148	VAL	CG1	21.76	0.2	1
1	A	148	VAL	N	113.98	0.2	1
1	A	149	ASP	H	7.964	0.04	1
1	A	149	ASP	HA	4.737	0.04	1
1	A	149	ASP	HB2	2.271	0.04	2
1	A	149	ASP	HB3	2.979	0.04	2
1	A	149	ASP	C	176.889	0.2	1
1	A	149	ASP	CA	52.729	0.2	1
1	A	149	ASP	CB	39.201	0.2	1
1	A	149	ASP	N	119.37	0.2	1
1	A	150	LEU	H	7.857	0.04	1
1	A	150	LEU	HA	4.127	0.04	1
1	A	150	LEU	HB2	1.882	0.04	2
1	A	150	LEU	HB3	1.664	0.04	2
1	A	150	LEU	HD11	1.013	0.04	1
1	A	150	LEU	HD12	1.013	0.04	1
1	A	150	LEU	HD13	1.013	0.04	1
1	A	150	LEU	HD21	0.909	0.04	1
1	A	150	LEU	HD22	0.909	0.04	1
1	A	150	LEU	HD23	0.909	0.04	1
1	A	150	LEU	C	178.431	0.2	1
1	A	150	LEU	CA	57.443	0.2	1
1	A	150	LEU	CB	42.547	0.2	1
1	A	150	LEU	CD1	25.35	0.2	1
1	A	150	LEU	CD2	22.76	0.2	1
1	A	150	LEU	N	126.597	0.2	1
1	A	151	ASN	H	8.015	0.04	1
1	A	151	ASN	HA	4.856	0.04	1
1	A	151	ASN	HB2	3.347	0.04	2
1	A	151	ASN	HB3	2.928	0.04	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	151	ASN	C	176.665	0.2	1
1	A	151	ASN	CA	51.684	0.2	1
1	A	151	ASN	CB	37.338	0.2	1
1	A	151	ASN	N	112.525	0.2	1
1	A	152	GLY	H	7.623	0.04	1
1	A	152	GLY	HA2	3.865	0.04	2
1	A	152	GLY	HA3	3.865	0.04	2
1	A	152	GLY	C	174.818	0.2	1
1	A	152	GLY	CA	47.652	0.2	1
1	A	152	GLY	N	108.895	0.2	1
1	A	153	ASP	H	8.025	0.04	1
1	A	153	ASP	HA	4.569	0.04	1
1	A	153	ASP	HB2	2.471	0.04	2
1	A	153	ASP	HB3	3.138	0.04	2
1	A	153	ASP	C	177.77	0.2	1
1	A	153	ASP	CA	53.422	0.2	1
1	A	153	ASP	CB	40.612	0.2	1
1	A	153	ASP	N	118.899	0.2	1
1	A	154	GLY	H	10.378	0.04	1
1	A	154	GLY	HA2	4.17	0.04	2
1	A	154	GLY	HA3	3.539	0.04	2
1	A	154	GLY	C	173.426	0.2	1
1	A	154	GLY	CA	45.831	0.2	1
1	A	154	GLY	N	112.922	0.2	1
1	A	155	ARG	H	8.05	0.04	1
1	A	155	ARG	HA	4.915	0.04	1
1	A	155	ARG	HB2	1.623	0.04	2
1	A	155	ARG	C	174.5	0.2	1
1	A	155	ARG	CA	53.847	0.2	1
1	A	155	ARG	CB	33.02	0.2	1
1	A	155	ARG	N	118.172	0.2	1
1	A	156	VAL	H	9.407	0.04	1
1	A	156	VAL	HA	5.107	0.04	1
1	A	156	VAL	HB	2.268	0.04	1
1	A	156	VAL	HG11	1.202	0.04	1
1	A	156	VAL	HG12	1.202	0.04	1
1	A	156	VAL	HG13	1.202	0.04	1
1	A	156	VAL	HG21	0.85	0.04	1
1	A	156	VAL	HG22	0.85	0.04	1
1	A	156	VAL	HG23	0.85	0.04	1
1	A	156	VAL	C	175.615	0.2	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	156	VAL	CA	61.303	0.2	1
1	A	156	VAL	CB	32.915	0.2	1
1	A	156	VAL	CG1	21.55	0.2	1
1	A	156	VAL	CG2	21.73	0.2	1
1	A	156	VAL	N	126.397	0.2	1
1	A	157	ASP	H	8.805	0.04	1
1	A	157	ASP	HA	5.174	0.04	1
1	A	157	ASP	HB2	2.797	0.04	2
1	A	157	ASP	HB3	3.32	0.04	2
1	A	157	ASP	C	176.218	0.2	1
1	A	157	ASP	CA	52.653	0.2	1
1	A	157	ASP	CB	41.905	0.2	1
1	A	157	ASP	N	127.907	0.2	1
1	A	158	PHE	H	8.836	0.04	1
1	A	158	PHE	HA	3.73	0.04	1
1	A	158	PHE	HB2	2.718	0.04	2
1	A	158	PHE	HB3	2.501	0.04	2
1	A	158	PHE	HD1	6.679	0.04	3
1	A	158	PHE	HD2	6.679	0.04	3
1	A	158	PHE	HE1	7.086	0.04	3
1	A	158	PHE	HE2	7.086	0.04	3
1	A	158	PHE	HZ	7.115	0.04	1
1	A	158	PHE	C	176.547	0.2	1
1	A	158	PHE	CA	62.579	0.2	1
1	A	158	PHE	CB	38.636	0.2	1
1	A	158	PHE	N	118.693	0.2	1
1	A	159	GLU	H	8.159	0.04	1
1	A	159	GLU	HA	3.76	0.04	1
1	A	159	GLU	HB2	2.184	0.04	2
1	A	159	GLU	C	180.429	0.2	1
1	A	159	GLU	CA	60.258	0.2	1
1	A	159	GLU	CB	28.882	0.2	1
1	A	159	GLU	N	117.881	0.2	1
1	A	160	GLU	H	8.583	0.04	1
1	A	160	GLU	HA	4.042	0.04	1
1	A	160	GLU	C	179.544	0.2	1
1	A	160	GLU	CA	58.867	0.2	1
1	A	160	GLU	CB	29.685	0.2	1
1	A	160	GLU	N	120.813	0.2	1
1	A	161	PHE	H	8.835	0.04	1
1	A	161	PHE	HA	4.035	0.04	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	161	PHE	HB2	3.124	0.04	2
1	A	161	PHE	HD1	6.936	0.04	3
1	A	161	PHE	HD2	6.936	0.04	3
1	A	161	PHE	HE1	7.159	0.04	3
1	A	161	PHE	HE2	7.159	0.04	3
1	A	161	PHE	HZ	7.05	0.04	1
1	A	161	PHE	C	176.432	0.2	1
1	A	161	PHE	CA	61.384	0.2	1
1	A	161	PHE	CB	39.65	0.2	1
1	A	161	PHE	N	123.389	0.2	1
1	A	162	VAL	H	8.474	0.04	1
1	A	162	VAL	HA	3.034	0.04	1
1	A	162	VAL	HB	3.033	0.04	1
1	A	162	VAL	HG11	0.69	0.04	1
1	A	162	VAL	HG12	0.69	0.04	1
1	A	162	VAL	HG13	0.69	0.04	1
1	A	162	VAL	HG21	0.385	0.04	1
1	A	162	VAL	HG22	0.385	0.04	1
1	A	162	VAL	HG23	0.385	0.04	1
1	A	162	VAL	C	179.125	0.2	1
1	A	162	VAL	CA	66.924	0.2	1
1	A	162	VAL	CB	31.415	0.2	1
1	A	162	VAL	CG1	21.34	0.2	1
1	A	162	VAL	CG2	23.4	0.2	1
1	A	162	VAL	N	119.378	0.2	1
1	A	163	ARG	H	7.513	0.04	1
1	A	163	ARG	HA	3.974	0.04	1
1	A	163	ARG	HB2	1.864	0.04	2
1	A	163	ARG	C	178.602	0.2	1
1	A	163	ARG	CA	59.25	0.2	1
1	A	163	ARG	CB	29.451	0.2	1
1	A	163	ARG	N	119.505	0.2	1
1	A	164	MET	H	7.735	0.04	1
1	A	164	MET	HA	4.015	0.04	1
1	A	164	MET	C	177.036	0.2	1
1	A	164	MET	CA	58.674	0.2	1
1	A	164	MET	CB	32.734	0.2	1
1	A	164	MET	N	119.076	0.2	1
1	A	165	MET	H	7.482	0.04	1
1	A	165	MET	HA	4.418	0.04	1
1	A	165	MET	C	176.607	0.2	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	165	MET	CA	54.799	0.2	1
1	A	165	MET	CB	32.119	0.2	1
1	A	165	MET	N	114.128	0.2	1
1	A	166	SER	H	7.53	0.04	1
1	A	166	SER	HA	4.59	0.04	1
1	A	166	SER	HB2	3.889	0.04	2
1	A	166	SER	C	173.167	0.2	1
1	A	166	SER	CA	58.521	0.2	1
1	A	166	SER	CB	64.174	0.2	1
1	A	166	SER	N	114.238	0.2	1
1	A	167	ARG	H	7.462	0.04	1
1	A	167	ARG	HA	4.181	0.04	1
1	A	167	ARG	HB2	1.783	0.04	2
1	A	167	ARG	CA	57.959	0.2	1
1	A	167	ARG	CB	31.435	0.2	1
1	A	167	ARG	N	127.118	0.2	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	147	-0.36 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	134	0.02 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	138	-0.40 ± 0.15	None needed (< 0.5 ppm)
^{15}N	139	0.66 ± 0.15	Should be applied

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 66%, i.e. 625 atoms were assigned a chemical shift out of a possible 948. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	332/347 (96%)	137/142 (96%)	130/138 (94%)	65/67 (97%)
Sidechain	269/536 (50%)	178/342 (52%)	91/171 (53%)	0/23 (0%)
Aromatic	24/65 (37%)	24/32 (75%)	0/32 (0%)	0/1 (0%)
Overall	625/948 (66%)	339/516 (66%)	221/341 (65%)	65/91 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure.

The overall completeness is 65%, i.e. 669 atoms were assigned a chemical shift out of a possible 1022. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	355/370 (96%)	146/151 (97%)	140/148 (95%)	69/71 (97%)
Sidechain	290/587 (49%)	192/376 (51%)	98/187 (52%)	0/24 (0%)
Aromatic	24/65 (37%)	24/32 (75%)	0/32 (0%)	0/1 (0%)
Overall	669/1022 (65%)	362/559 (65%)	238/367 (65%)	69/96 (72%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

