



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:48 PM BST

PDB ID : 1H3Z
Title : SOLUTION STRUCTURE OF A PWWP DOMAIN FROM SCHIZOSACCHAROMYCES POMBE
Authors : Slater, L.M.; Allen, M.D.; Bycroft, M.
Deposited on : 2002-09-23

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-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

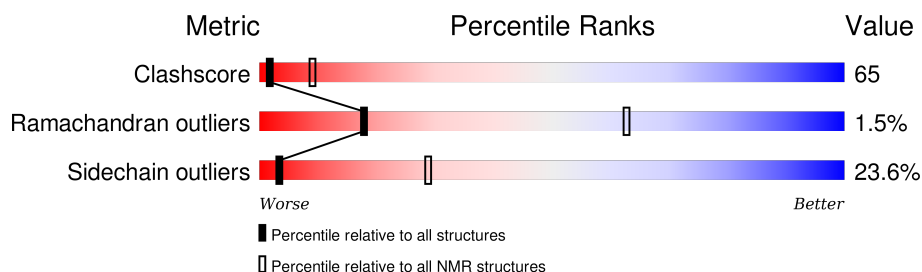
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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	109	 23% 60% 10% 6%

2 Ensemble composition and analysis

This entry contains 23 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:122-A:222 (101)	0.27	7

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 6, 7, 11, 12, 14, 18, 21, 22
2	2, 16, 23
3	8, 15, 19
4	10, 20
Single-model clusters	9; 13; 17

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1731 atoms, of which 877 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HYPOTHETICAL 62.8 KDA PROTEIN C215.07C.

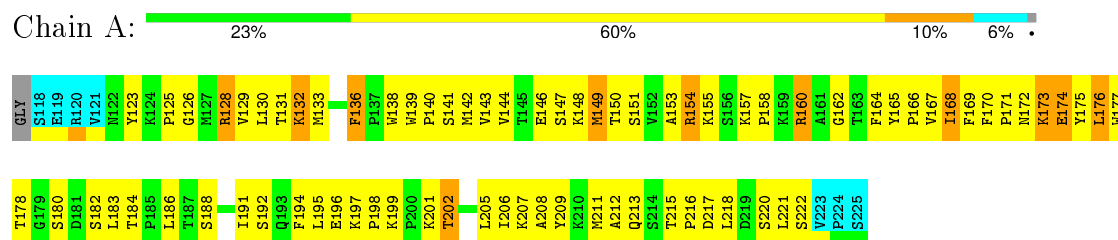
Mol	Chain	Residues	Atoms						Trace
1	A	108	Total	C	H	N	O	S	0
			1731	553	877	139	157	5	

4 Residue-property plots

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: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C

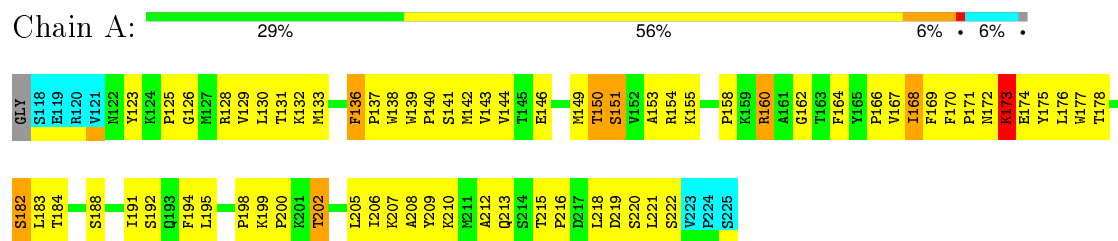


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

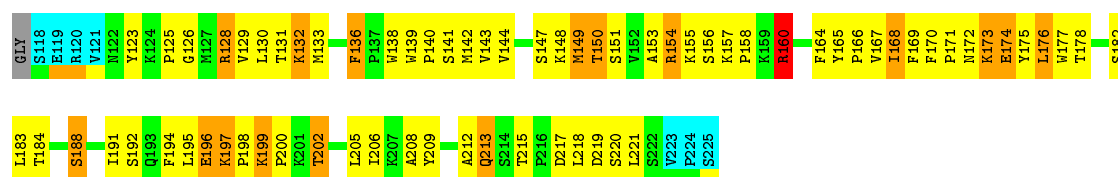
- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



4.2.2 Score per residue for model 2

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C

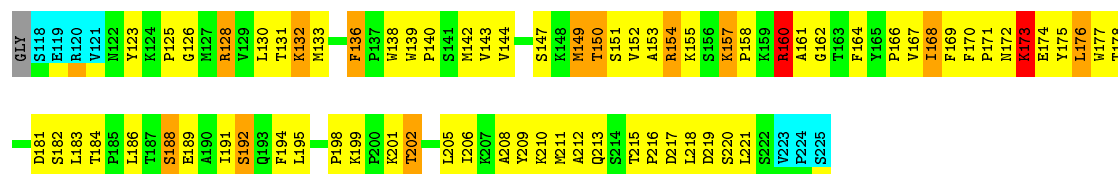




4.2.3 Score per residue for model 3

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C

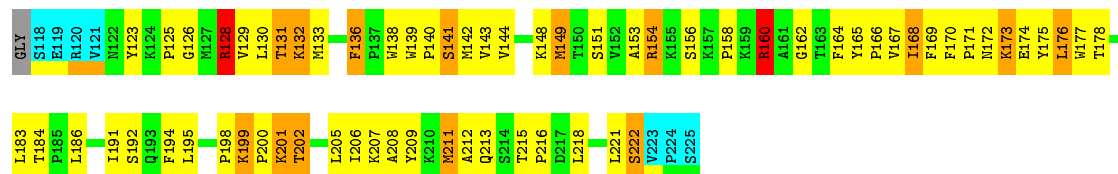
Chain A: 27% 53% 11% 6%



4.2.4 Score per residue for model 4

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C

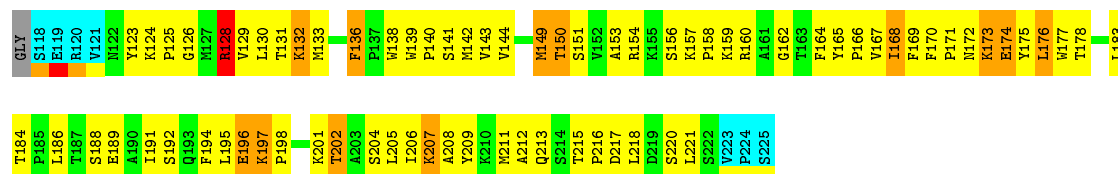
Chain A: 32% 46% 13% 6%



4.2.5 Score per residue for model 5

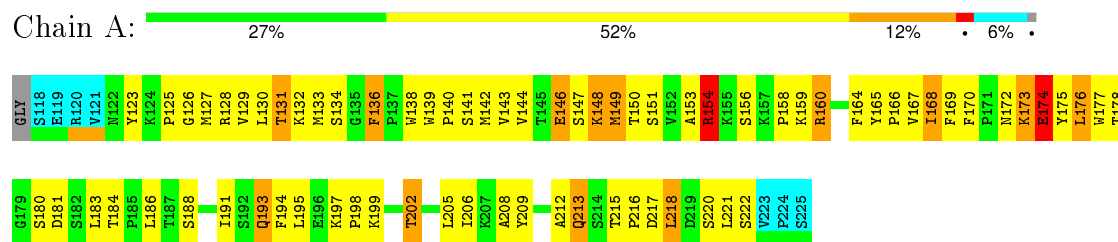
- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C

Chain A: 26% 55% 11% 6%



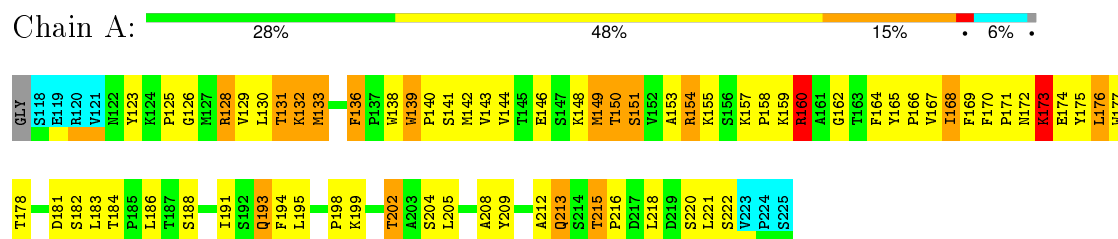
4.2.6 Score per residue for model 6

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



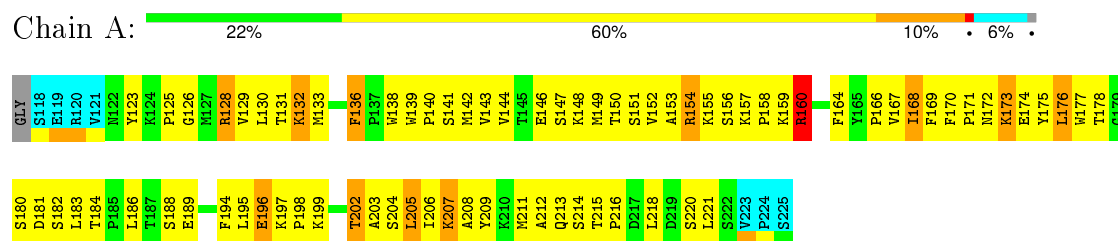
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



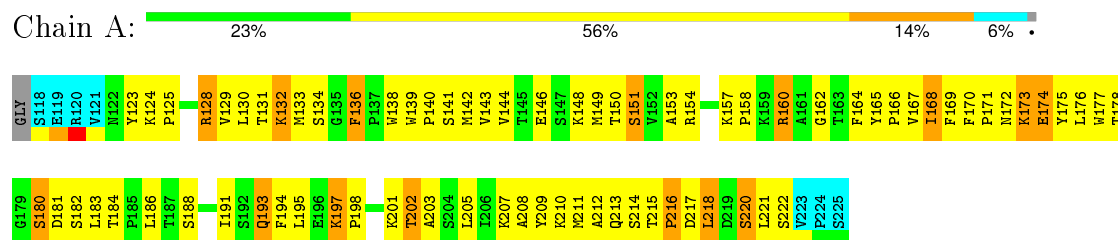
4.2.8 Score per residue for model 8

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



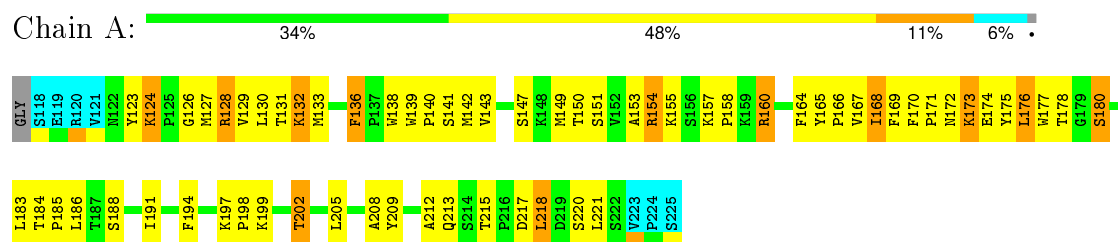
4.2.9 Score per residue for model 9

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



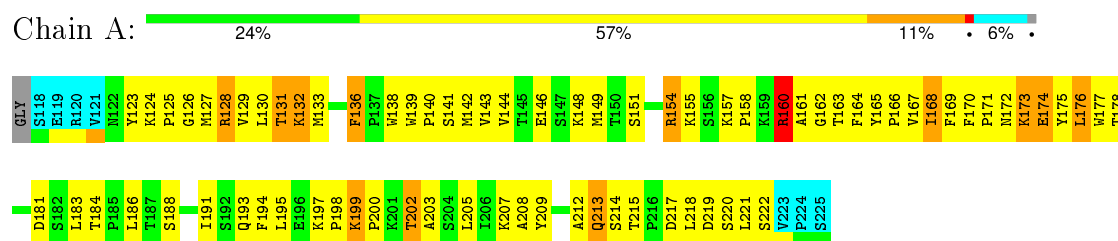
4.2.10 Score per residue for model 10

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



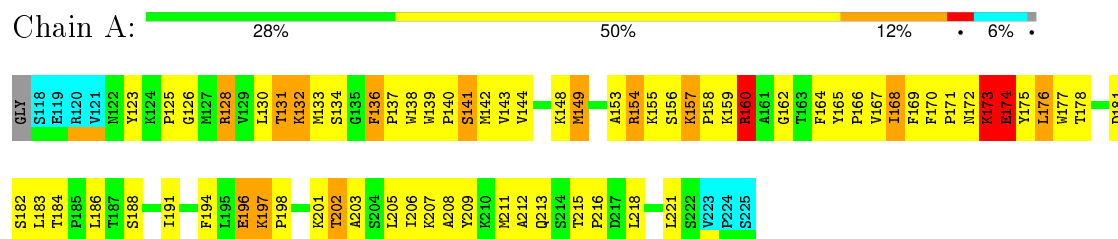
4.2.11 Score per residue for model 11

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



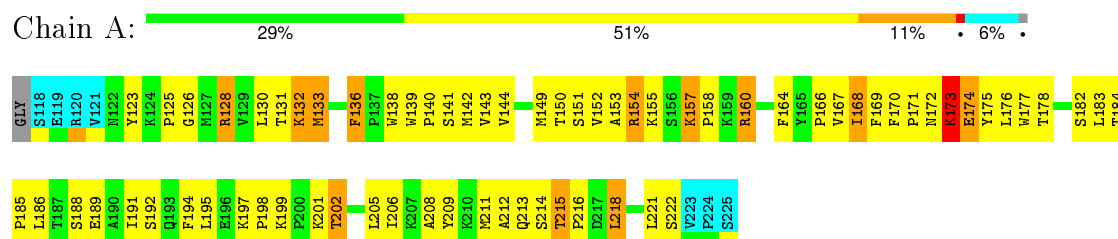
4.2.12 Score per residue for model 12

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



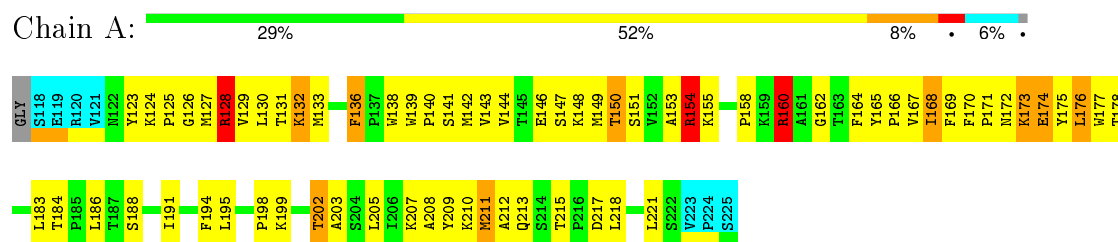
4.2.13 Score per residue for model 13

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



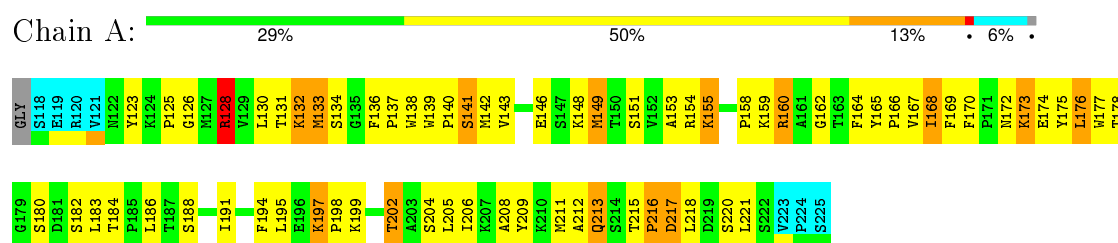
4.2.14 Score per residue for model 14

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



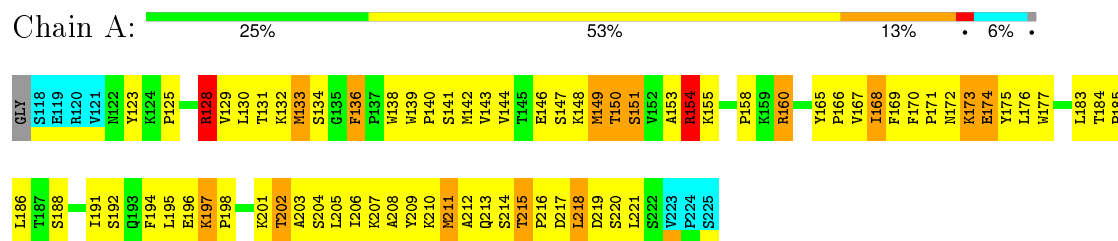
4.2.15 Score per residue for model 15

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



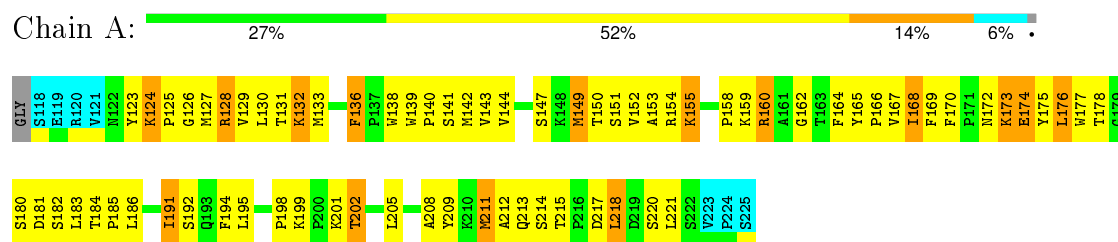
4.2.16 Score per residue for model 16

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



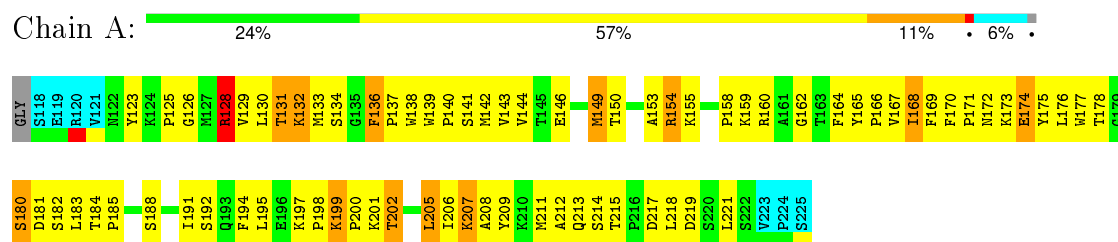
4.2.17 Score per residue for model 17

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



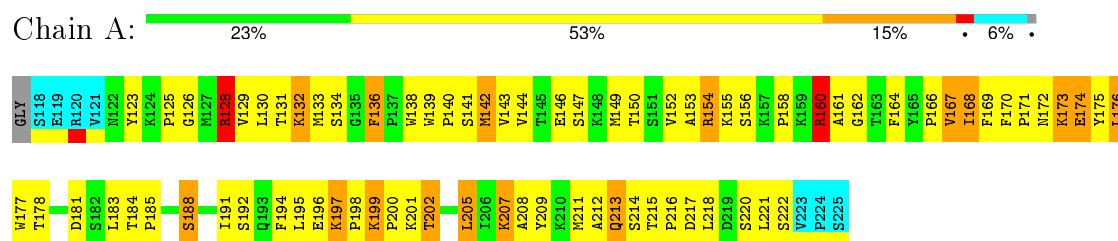
4.2.18 Score per residue for model 18

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



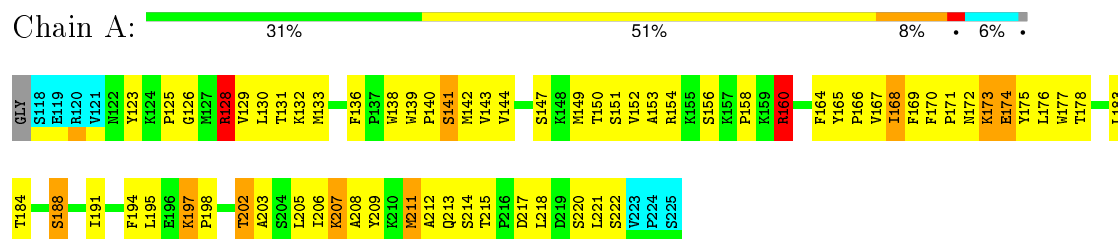
4.2.19 Score per residue for model 19

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



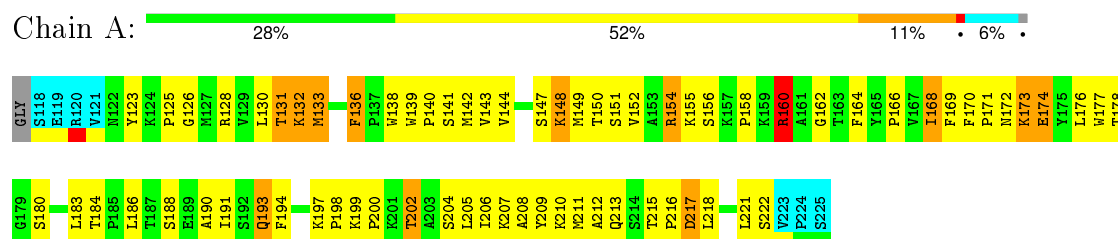
4.2.20 Score per residue for model 20

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



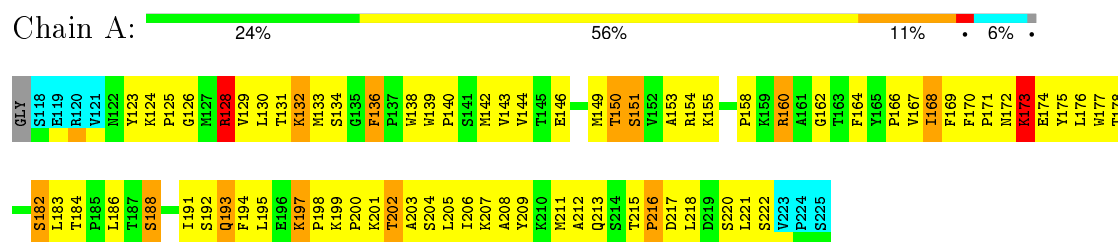
4.2.21 Score per residue for model 21

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



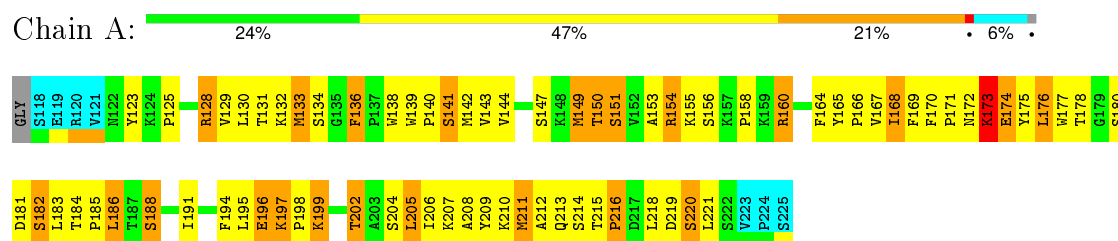
4.2.22 Score per residue for model 22

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



4.2.23 Score per residue for model 23

- Molecule 1: HYPOTHETICAL 62.8 KDA PROTEIN C215.07C



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY SIMULATED ANNEALING*.

Of the 30 calculated structures, 23 were deposited, based on the following criterion: *NO VIOLATION GREATER THAN 0.25Å AND NO VIOLATIONS GREATER THAN 5 DEGREES*.

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

Software name	Classification	Version
X-PLOR 3.8	refinement	
ANSIG 3.3	structure solution	

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)	BMRB entry 5538, BMRB entry 5902
Number of chemical shift lists	2
Total number of shifts	2495
Number of shifts mapped to atoms	1255
Number of unparsed shifts	0
Number of shifts with mapping errors	1240
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.8±0.4
All	All	0	65

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	154	ARG	Sidechain	23
1	A	128	ARG	Sidechain	22
1	A	160	ARG	Sidechain	20

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	800	821	821	105±9
All	All	18400	18883	18883	2426

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 65.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:MET:HE3	1:A:153:ALA:HB1	1.02	1.27	4	10
1:A:215:THR:HG21	1:A:221:LEU:HD13	1.00	1.32	12	23
1:A:131:THR:CG2	1:A:178:THR:HG21	0.96	1.89	12	13
1:A:123:TYR:HB3	1:A:143:VAL:HG21	0.89	1.44	17	21
1:A:215:THR:CG2	1:A:221:LEU:HD13	0.88	1.97	9	19
1:A:131:THR:HG22	1:A:183:LEU:HD21	0.86	1.43	13	11
1:A:131:THR:HG22	1:A:178:THR:HG21	0.86	1.47	18	17
1:A:153:ALA:HB2	1:A:175:TYR:HB2	0.85	1.47	19	15
1:A:149:MET:HE2	1:A:153:ALA:HB1	0.83	1.51	17	4
1:A:202:THR:HG23	1:A:205:LEU:HB3	0.82	1.50	15	23
1:A:178:THR:HG23	1:A:183:LEU:HD11	0.81	1.50	10	21
1:A:186:LEU:HD11	1:A:191:ILE:HG13	0.81	1.52	10	13
1:A:215:THR:HG21	1:A:221:LEU:CD1	0.80	2.05	7	14
1:A:153:ALA:HB2	1:A:175:TYR:CB	0.80	2.07	12	17
1:A:131:THR:HG22	1:A:183:LEU:CD2	0.79	2.08	13	13
1:A:170:PHE:CG	1:A:212:ALA:HB2	0.76	2.14	3	21
1:A:131:THR:CG2	1:A:183:LEU:HD21	0.76	2.10	19	20
1:A:188:SER:HA	1:A:191:ILE:HD12	0.74	1.59	13	12
1:A:149:MET:CE	1:A:153:ALA:HB1	0.74	2.13	8	10
1:A:148:LYS:HD2	1:A:218:LEU:HD11	0.74	1.58	12	4
1:A:131:THR:HG23	1:A:183:LEU:HD21	0.74	1.58	21	8
1:A:191:ILE:HG23	1:A:213:GLN:CG	0.73	2.14	17	1
1:A:168:ILE:C	1:A:168:ILE:HD13	0.72	2.05	8	9
1:A:168:ILE:HD13	1:A:168:ILE:C	0.72	2.05	19	14
1:A:130:LEU:HD22	1:A:138:TRP:C	0.72	2.05	4	21
1:A:178:THR:HG23	1:A:183:LEU:CD1	0.71	2.15	10	20
1:A:170:PHE:CD2	1:A:212:ALA:HB2	0.70	2.21	16	20
1:A:191:ILE:HG23	1:A:213:GLN:HG2	0.70	1.63	17	1
1:A:205:LEU:O	1:A:208:ALA:HB3	0.70	1.85	1	21
1:A:160:ARG:HD3	1:A:164:PHE:CZ	0.70	2.21	8	5
1:A:168:ILE:HD11	1:A:173:LYS:HA	0.69	1.63	8	18
1:A:194:PHE:CD2	1:A:209:TYR:CD2	0.69	2.81	21	11
1:A:194:PHE:CD1	1:A:209:TYR:CG	0.69	2.81	4	10
1:A:194:PHE:CE1	1:A:209:TYR:CD2	0.68	2.81	4	7
1:A:140:PRO:HG2	1:A:208:ALA:HB1	0.68	1.65	12	19
1:A:194:PHE:CD2	1:A:209:TYR:CG	0.68	2.82	8	12
1:A:160:ARG:CD	1:A:164:PHE:CE1	0.67	2.76	20	3
1:A:130:LEU:HG	1:A:186:LEU:HD13	0.67	1.67	8	4
1:A:144:VAL:HG22	1:A:166:PRO:O	0.67	1.88	2	20
1:A:130:LEU:HD13	1:A:138:TRP:CB	0.67	2.19	11	14
1:A:148:LYS:CD	1:A:218:LEU:HD11	0.66	2.20	12	1
1:A:194:PHE:CE1	1:A:205:LEU:HD23	0.66	2.25	10	11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:LEU:HD11	1:A:191:ILE:CG1	0.66	2.20	4	5
1:A:131:THR:HG23	1:A:178:THR:HG21	0.66	1.67	4	1
1:A:130:LEU:HD21	1:A:209:TYR:OH	0.65	1.91	18	5
1:A:139:TRP:CD2	1:A:205:LEU:HD12	0.64	2.27	6	19
1:A:194:PHE:CE1	1:A:205:LEU:CD2	0.64	2.81	14	12
1:A:169:PHE:CZ	1:A:176:LEU:HD22	0.64	2.27	9	23
1:A:160:ARG:CG	1:A:164:PHE:CZ	0.64	2.81	18	8
1:A:149:MET:HE3	1:A:153:ALA:CB	0.64	2.20	18	5
1:A:194:PHE:CE2	1:A:209:TYR:HB2	0.63	2.28	17	13
1:A:160:ARG:NE	1:A:164:PHE:CE1	0.63	2.67	20	1
1:A:194:PHE:CE2	1:A:205:LEU:CD2	0.63	2.81	18	10
1:A:160:ARG:CD	1:A:164:PHE:CZ	0.63	2.81	2	8
1:A:170:PHE:CD2	1:A:212:ALA:CB	0.62	2.82	4	16
1:A:130:LEU:HD13	1:A:138:TRP:HB3	0.62	1.69	11	14
1:A:144:VAL:HG11	1:A:168:ILE:HB	0.62	1.71	14	4
1:A:194:PHE:CE1	1:A:209:TYR:HB2	0.62	2.30	15	10
1:A:130:LEU:HD23	1:A:139:TRP:C	0.62	2.14	16	21
1:A:158:PRO:CD	1:A:177:TRP:CB	0.62	2.77	10	13
1:A:150:THR:HG23	1:A:152:VAL:H	0.62	1.55	20	2
1:A:160:ARG:HD3	1:A:164:PHE:CE1	0.61	2.30	8	2
1:A:160:ARG:CG	1:A:164:PHE:CE1	0.61	2.84	20	5
1:A:130:LEU:HD23	1:A:139:TRP:O	0.60	1.96	11	22
1:A:149:MET:CG	1:A:153:ALA:CB	0.60	2.80	15	1
1:A:169:PHE:CE1	1:A:176:LEU:HD22	0.60	2.31	21	22
1:A:191:ILE:HG23	1:A:213:GLN:CD	0.60	2.17	17	1
1:A:215:THR:HG23	1:A:220:SER:HB3	0.60	1.72	10	1
1:A:194:PHE:CD1	1:A:209:TYR:CB	0.60	2.85	16	10
1:A:131:THR:CG2	1:A:183:LEU:CD2	0.59	2.80	2	17
1:A:194:PHE:CE2	1:A:205:LEU:HD23	0.59	2.32	6	6
1:A:204:SER:O	1:A:207:LYS:HG2	0.59	1.97	5	1
1:A:173:LYS:O	1:A:175:TYR:CE1	0.59	2.55	8	1
1:A:170:PHE:O	1:A:208:ALA:HB1	0.59	1.98	19	3
1:A:173:LYS:O	1:A:175:TYR:CE2	0.59	2.55	16	10
1:A:158:PRO:HD3	1:A:177:TRP:CG	0.59	2.33	19	15
1:A:148:LYS:HE3	1:A:218:LEU:HD21	0.58	1.75	7	1
1:A:194:PHE:CD2	1:A:209:TYR:CB	0.58	2.86	14	13
1:A:158:PRO:CD	1:A:177:TRP:CG	0.58	2.86	21	10
1:A:153:ALA:CB	1:A:175:TYR:CB	0.58	2.82	19	19
1:A:129:VAL:HG21	1:A:183:LEU:HD22	0.58	1.76	23	6
1:A:171:PRO:HG3	1:A:207:LYS:CG	0.58	2.29	18	3
1:A:191:ILE:O	1:A:213:GLN:NE2	0.58	2.37	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:THR:OG1	1:A:169:PHE:CZ	0.57	2.56	14	9
1:A:173:LYS:CG	1:A:173:LYS:O	0.57	2.52	1	4
1:A:194:PHE:CZ	1:A:198:PRO:HB3	0.57	2.35	2	21
1:A:149:MET:CE	1:A:153:ALA:CB	0.57	2.82	8	1
1:A:194:PHE:CE2	1:A:209:TYR:CD2	0.57	2.91	22	8
1:A:160:ARG:HG3	1:A:164:PHE:CZ	0.57	2.35	13	12
1:A:130:LEU:HD22	1:A:138:TRP:HB3	0.57	1.76	9	10
1:A:170:PHE:O	1:A:208:ALA:CB	0.57	2.53	10	19
1:A:195:LEU:CD1	1:A:213:GLN:OE1	0.56	2.53	17	1
1:A:126:GLY:N	1:A:218:LEU:HD12	0.56	2.15	17	2
1:A:191:ILE:HG22	1:A:213:GLN:CG	0.56	2.31	9	1
1:A:169:PHE:CE1	1:A:176:LEU:HB3	0.56	2.35	9	23
1:A:132:LYS:CE	1:A:138:TRP:CZ2	0.56	2.88	22	1
1:A:131:THR:HG21	1:A:178:THR:HG21	0.56	1.72	12	3
1:A:172:ASN:O	1:A:174:GLU:N	0.56	2.39	22	4
1:A:133:MET:HE3	1:A:136:PHE:CD2	0.56	2.36	15	2
1:A:139:TRP:CH2	1:A:205:LEU:HB2	0.56	2.35	19	23
1:A:160:ARG:O	1:A:160:ARG:CZ	0.56	2.53	8	2
1:A:132:LYS:HE2	1:A:138:TRP:CZ2	0.56	2.35	22	1
1:A:158:PRO:HD3	1:A:177:TRP:CB	0.56	2.31	7	23
1:A:202:THR:HG23	1:A:205:LEU:CB	0.55	2.30	2	11
1:A:165:TYR:CD1	1:A:165:TYR:N	0.55	2.68	11	4
1:A:131:THR:HG23	1:A:183:LEU:CD2	0.55	2.31	12	5
1:A:157:LYS:HG3	1:A:177:TRP:CZ2	0.55	2.37	12	4
1:A:165:TYR:N	1:A:165:TYR:CD1	0.55	2.74	2	9
1:A:162:GLY:O	1:A:164:PHE:CD1	0.55	2.59	19	15
1:A:171:PRO:CG	1:A:207:LYS:CD	0.55	2.85	5	1
1:A:194:PHE:CE2	1:A:209:TYR:CB	0.55	2.89	17	11
1:A:194:PHE:CD1	1:A:209:TYR:CD2	0.55	2.95	16	8
1:A:194:PHE:CE1	1:A:205:LEU:HD21	0.55	2.37	8	5
1:A:133:MET:CE	1:A:176:LEU:HD13	0.55	2.32	8	1
1:A:149:MET:CG	1:A:153:ALA:HB3	0.55	2.32	17	4
1:A:160:ARG:O	1:A:160:ARG:NE	0.55	2.40	8	3
1:A:130:LEU:HB2	1:A:184:THR:CG2	0.55	2.32	14	23
1:A:130:LEU:CB	1:A:184:THR:CG2	0.55	2.85	14	19
1:A:132:LYS:HG3	1:A:138:TRP:CE2	0.55	2.37	3	15
1:A:139:TRP:HB3	1:A:169:PHE:CE2	0.54	2.37	23	5
1:A:194:PHE:CE2	1:A:205:LEU:HD21	0.54	2.36	18	5
1:A:194:PHE:CZ	1:A:209:TYR:CD2	0.54	2.95	4	4
1:A:131:THR:HG23	1:A:141:SER:OG	0.54	2.02	17	4
1:A:160:ARG:CD	1:A:161:ALA:N	0.54	2.70	19	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:ILE:HA	1:A:174:GLU:O	0.54	2.03	1	23
1:A:209:TYR:O	1:A:213:GLN:CB	0.54	2.56	2	8
1:A:186:LEU:HD11	1:A:191:ILE:HG12	0.54	1.80	16	1
1:A:131:THR:CG2	1:A:141:SER:OG	0.54	2.56	17	4
1:A:168:ILE:HG13	1:A:221:LEU:HD21	0.54	1.77	20	5
1:A:194:PHE:CE2	1:A:198:PRO:HA	0.54	2.38	4	10
1:A:126:GLY:HA2	1:A:218:LEU:CB	0.54	2.33	13	16
1:A:128:ARG:CG	1:A:128:ARG:O	0.54	2.56	7	2
1:A:194:PHE:CG	1:A:209:TYR:CD2	0.54	2.96	13	5
1:A:186:LEU:HD21	1:A:191:ILE:HD11	0.54	1.79	21	3
1:A:194:PHE:CD2	1:A:198:PRO:HA	0.53	2.38	18	10
1:A:173:LYS:O	1:A:173:LYS:CD	0.53	2.56	1	1
1:A:194:PHE:CZ	1:A:205:LEU:HD23	0.53	2.38	18	9
1:A:132:LYS:CD	1:A:138:TRP:CZ2	0.53	2.92	20	4
1:A:138:TRP:CZ3	1:A:184:THR:HB	0.53	2.39	20	23
1:A:128:ARG:N	1:A:142:MET:SD	0.53	2.82	23	10
1:A:160:ARG:HG2	1:A:164:PHE:CZ	0.53	2.39	4	4
1:A:148:LYS:HG2	1:A:218:LEU:HD21	0.53	1.81	16	1
1:A:194:PHE:CE1	1:A:198:PRO:HA	0.53	2.39	17	13
1:A:128:ARG:O	1:A:128:ARG:CG	0.53	2.57	23	3
1:A:132:LYS:HD2	1:A:138:TRP:CZ2	0.52	2.39	23	3
1:A:201:LYS:O	1:A:201:LYS:CD	0.52	2.57	9	3
1:A:192:SER:HA	1:A:195:LEU:HD12	0.52	1.81	3	4
1:A:165:TYR:HB2	1:A:183:LEU:CD1	0.52	2.34	20	3
1:A:194:PHE:CD1	1:A:198:PRO:HA	0.52	2.39	10	13
1:A:172:ASN:N	1:A:172:ASN:OD1	0.52	2.41	2	2
1:A:215:THR:HG23	1:A:220:SER:CB	0.52	2.35	10	1
1:A:217:ASP:OD2	1:A:219:ASP:CB	0.52	2.58	11	1
1:A:160:ARG:HG3	1:A:164:PHE:CE1	0.52	2.39	13	8
1:A:132:LYS:CE	1:A:133:MET:O	0.52	2.57	13	6
1:A:149:MET:O	1:A:154:ARG:NH1	0.52	2.43	6	1
1:A:172:ASN:ND2	1:A:172:ASN:N	0.52	2.57	11	1
1:A:173:LYS:O	1:A:173:LYS:CG	0.52	2.55	15	4
1:A:209:TYR:O	1:A:213:GLN:HG3	0.52	2.05	17	1
1:A:144:VAL:CG2	1:A:149:MET:SD	0.52	2.98	23	9
1:A:195:LEU:HD11	1:A:213:GLN:HG3	0.52	1.81	8	10
1:A:203:ALA:O	1:A:207:LYS:CG	0.52	2.57	12	4
1:A:133:MET:HB3	1:A:136:PHE:HB2	0.52	1.82	21	23
1:A:168:ILE:CD1	1:A:168:ILE:C	0.52	2.78	17	13
1:A:123:TYR:OH	1:A:184:THR:HA	0.52	2.05	8	18
1:A:128:ARG:CA	1:A:142:MET:SD	0.52	2.98	13	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:171:PRO:CB	1:A:211:MET:SD	0.52	2.98	3	7
1:A:139:TRP:CD1	1:A:140:PRO:HD2	0.51	2.39	8	23
1:A:194:PHE:CD2	1:A:195:LEU:HD23	0.51	2.40	17	1
1:A:172:ASN:O	1:A:173:LYS:C	0.51	2.49	22	21
1:A:138:TRP:CE3	1:A:184:THR:HG22	0.51	2.40	16	5
1:A:157:LYS:HE3	1:A:177:TRP:CH2	0.51	2.41	7	2
1:A:128:ARG:CG	1:A:142:MET:SD	0.51	2.99	12	2
1:A:149:MET:HG2	1:A:153:ALA:CB	0.51	2.36	15	1
1:A:168:ILE:C	1:A:168:ILE:CD1	0.51	2.79	23	8
1:A:171:PRO:CG	1:A:207:LYS:CG	0.51	2.88	18	1
1:A:146:GLU:O	1:A:154:ARG:NH1	0.51	2.44	6	1
1:A:132:LYS:HB3	1:A:138:TRP:CD2	0.51	2.41	1	8
1:A:130:LEU:CD2	1:A:139:TRP:C	0.51	2.79	2	14
1:A:202:THR:CG2	1:A:205:LEU:CB	0.51	2.88	2	4
1:A:158:PRO:HD2	1:A:177:TRP:CG	0.51	2.41	10	8
1:A:133:MET:HB3	1:A:136:PHE:CB	0.51	2.36	21	5
1:A:149:MET:HE2	1:A:153:ALA:CB	0.51	2.31	8	3
1:A:129:VAL:HG22	1:A:141:SER:O	0.51	2.06	1	7
1:A:132:LYS:HB3	1:A:138:TRP:CE2	0.51	2.41	16	6
1:A:160:ARG:HD2	1:A:164:PHE:CZ	0.51	2.41	20	3
1:A:202:THR:CG2	1:A:205:LEU:HB3	0.50	2.35	16	18
1:A:171:PRO:HG3	1:A:207:LYS:CD	0.50	2.35	5	1
1:A:142:MET:HB3	1:A:168:ILE:CG2	0.50	2.36	14	21
1:A:173:LYS:HD3	1:A:221:LEU:CD2	0.50	2.36	5	1
1:A:130:LEU:CB	1:A:184:THR:HG22	0.50	2.37	8	9
1:A:171:PRO:HB3	1:A:211:MET:CB	0.50	2.37	18	2
1:A:208:ALA:O	1:A:212:ALA:CB	0.50	2.60	12	3
1:A:194:PHE:CE1	1:A:209:TYR:CB	0.50	2.95	9	9
1:A:191:ILE:CG2	1:A:213:GLN:HG2	0.50	2.37	17	1
1:A:204:SER:HA	1:A:207:LYS:HG2	0.50	1.83	5	1
1:A:158:PRO:HB2	1:A:160:ARG:CD	0.50	2.37	12	4
1:A:160:ARG:HD2	1:A:164:PHE:CE1	0.50	2.42	8	3
1:A:209:TYR:O	1:A:213:GLN:HB2	0.49	2.07	1	19
1:A:138:TRP:CZ3	1:A:182:SER:O	0.49	2.65	1	3
1:A:139:TRP:CZ2	1:A:205:LEU:HB2	0.49	2.42	18	6
1:A:129:VAL:CG2	1:A:183:LEU:HD22	0.49	2.37	11	4
1:A:166:PRO:HB3	1:A:177:TRP:CH2	0.49	2.42	9	13
1:A:128:ARG:NE	1:A:216:PRO:O	0.49	2.43	19	2
1:A:205:LEU:O	1:A:208:ALA:CB	0.49	2.60	1	2
1:A:166:PRO:HB3	1:A:177:TRP:CZ2	0.49	2.43	9	5
1:A:205:LEU:O	1:A:208:ALA:N	0.49	2.46	7	12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:MET:HG3	1:A:153:ALA:HB3	0.49	1.85	8	2
1:A:195:LEU:HD11	1:A:213:GLN:OE1	0.49	2.07	17	1
1:A:173:LYS:NZ	1:A:222:SER:O	0.49	2.44	4	1
1:A:138:TRP:CE3	1:A:184:THR:CG2	0.49	2.96	16	3
1:A:153:ALA:CB	1:A:175:TYR:HB2	0.49	2.35	17	12
1:A:174:GLU:O	1:A:175:TYR:CD1	0.49	2.66	1	1
1:A:194:PHE:CE1	1:A:206:ILE:HA	0.48	2.43	2	9
1:A:132:LYS:HE2	1:A:133:MET:N	0.48	2.22	18	4
1:A:158:PRO:CD	1:A:177:TRP:HB3	0.48	2.38	18	7
1:A:131:THR:CG2	1:A:178:THR:CG2	0.48	2.80	12	1
1:A:171:PRO:CG	1:A:207:LYS:HG3	0.48	2.38	18	1
1:A:167:VAL:O	1:A:175:TYR:HA	0.48	2.08	8	22
1:A:193:GLN:HG2	1:A:194:PHE:N	0.48	2.24	21	2
1:A:149:MET:HG3	1:A:153:ALA:CB	0.48	2.38	15	3
1:A:149:MET:HB3	1:A:153:ALA:CB	0.48	2.39	23	4
1:A:165:TYR:CE2	1:A:180:SER:HB2	0.48	2.44	17	1
1:A:158:PRO:HB2	1:A:160:ARG:NE	0.48	2.24	2	2
1:A:160:ARG:HG2	1:A:164:PHE:CE1	0.48	2.44	22	3
1:A:132:LYS:HE3	1:A:133:MET:N	0.48	2.24	17	2
1:A:150:THR:HG23	1:A:152:VAL:HB	0.48	1.85	8	4
1:A:139:TRP:CB	1:A:169:PHE:CE2	0.48	2.96	23	1
1:A:153:ALA:HB2	1:A:175:TYR:CD2	0.48	2.43	9	2
1:A:171:PRO:HG3	1:A:207:LYS:HG3	0.48	1.84	18	1
1:A:129:VAL:O	1:A:141:SER:O	0.48	2.32	5	7
1:A:130:LEU:HD11	1:A:209:TYR:OH	0.48	2.08	7	3
1:A:168:ILE:CD1	1:A:173:LYS:HA	0.48	2.38	19	13
1:A:168:ILE:HD13	1:A:168:ILE:O	0.48	2.07	10	3
1:A:191:ILE:CG2	1:A:213:GLN:CG	0.47	2.92	9	2
1:A:174:GLU:C	1:A:175:TYR:CG	0.47	2.87	1	1
1:A:148:LYS:HG3	1:A:218:LEU:HD21	0.47	1.86	9	2
1:A:173:LYS:CD	1:A:222:SER:O	0.47	2.62	21	1
1:A:191:ILE:HG22	1:A:192:SER:N	0.47	2.23	17	1
1:A:170:PHE:CB	1:A:212:ALA:HB2	0.47	2.40	5	3
1:A:158:PRO:O	1:A:160:ARG:NH2	0.47	2.43	8	1
1:A:158:PRO:HB2	1:A:160:ARG:HG3	0.47	1.86	8	2
1:A:129:VAL:CA	1:A:186:LEU:HB3	0.47	2.39	10	4
1:A:133:MET:CE	1:A:136:PHE:CD2	0.47	2.97	15	1
1:A:140:PRO:CG	1:A:208:ALA:HB1	0.47	2.38	1	5
1:A:191:ILE:HG23	1:A:209:TYR:HD1	0.47	1.70	1	1
1:A:149:MET:O	1:A:150:THR:O	0.47	2.33	7	4
1:A:194:PHE:C	1:A:194:PHE:CD1	0.47	2.88	9	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:THR:OG1	1:A:151:SER:N	0.47	2.48	14	8
1:A:192:SER:OG	1:A:213:GLN:NE2	0.47	2.48	22	1
1:A:142:MET:HE1	1:A:217:ASP:HA	0.47	1.86	3	1
1:A:160:ARG:NE	1:A:164:PHE:CD1	0.47	2.83	20	1
1:A:149:MET:SD	1:A:177:TRP:CZ2	0.47	3.08	19	4
1:A:140:PRO:HD3	1:A:209:TYR:CE2	0.47	2.45	18	2
1:A:173:LYS:HD3	1:A:221:LEU:HD21	0.47	1.85	5	1
1:A:173:LYS:O	1:A:174:GLU:O	0.47	2.33	23	1
1:A:169:PHE:HB2	1:A:174:GLU:CB	0.47	2.40	12	1
1:A:186:LEU:HD21	1:A:191:ILE:HG12	0.47	1.87	23	1
1:A:213:GLN:OE1	1:A:213:GLN:O	0.47	2.33	1	3
1:A:171:PRO:HG3	1:A:207:LYS:CB	0.47	2.39	12	5
1:A:131:THR:OG1	1:A:141:SER:OG	0.47	2.32	12	3
1:A:216:PRO:HG2	1:A:220:SER:CB	0.47	2.40	22	2
1:A:172:ASN:C	1:A:173:LYS:CD	0.47	2.83	23	1
1:A:176:LEU:HG	1:A:177:TRP:N	0.46	2.26	8	16
1:A:173:LYS:HE3	1:A:221:LEU:CD2	0.46	2.40	11	2
1:A:142:MET:SD	1:A:218:LEU:N	0.46	2.89	2	1
1:A:195:LEU:HD11	1:A:213:GLN:HG2	0.46	1.87	1	4
1:A:126:GLY:O	1:A:142:MET:SD	0.46	2.74	19	6
1:A:171:PRO:O	1:A:211:MET:SD	0.46	2.74	22	1
1:A:142:MET:CE	1:A:217:ASP:HA	0.46	2.40	3	1
1:A:173:LYS:O	1:A:173:LYS:HG2	0.46	2.10	1	2
1:A:149:MET:HB3	1:A:153:ALA:HB3	0.46	1.85	14	4
1:A:157:LYS:CG	1:A:158:PRO:HD2	0.46	2.41	5	2
1:A:126:GLY:HA2	1:A:218:LEU:HD12	0.46	1.85	6	1
1:A:125:PRO:HA	1:A:143:VAL:O	0.46	2.11	7	22
1:A:219:ASP:N	1:A:219:ASP:OD1	0.46	2.46	2	1
1:A:173:LYS:CD	1:A:221:LEU:CD2	0.46	2.92	5	1
1:A:146:GLU:OE2	1:A:146:GLU:O	0.46	2.34	11	1
1:A:165:TYR:CE2	1:A:180:SER:HB3	0.46	2.45	9	1
1:A:216:PRO:HD2	1:A:220:SER:CB	0.46	2.41	8	6
1:A:171:PRO:O	1:A:172:ASN:HB2	0.46	2.11	21	14
1:A:194:PHE:CZ	1:A:206:ILE:HA	0.46	2.46	23	12
1:A:178:THR:CG2	1:A:183:LEU:HD11	0.46	2.37	19	3
1:A:217:ASP:OD1	1:A:217:ASP:N	0.46	2.48	14	4
1:A:194:PHE:CE2	1:A:206:ILE:HA	0.46	2.46	22	7
1:A:139:TRP:CE2	1:A:205:LEU:HD12	0.46	2.46	6	2
1:A:148:LYS:HD2	1:A:218:LEU:CD2	0.46	2.41	6	1
1:A:173:LYS:CE	1:A:222:SER:O	0.46	2.64	20	1
1:A:213:GLN:OE1	1:A:213:GLN:HA	0.46	2.11	23	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:ASP:N	1:A:181:ASP:OD1	0.46	2.48	6	1
1:A:204:SER:O	1:A:207:LYS:CG	0.46	2.64	5	1
1:A:173:LYS:O	1:A:175:TYR:CZ	0.46	2.69	23	3
1:A:186:LEU:CD2	1:A:191:ILE:HD11	0.46	2.41	17	1
1:A:195:LEU:HG	1:A:213:GLN:OE1	0.46	2.11	17	1
1:A:168:ILE:O	1:A:168:ILE:HD13	0.45	2.10	20	3
1:A:197:LYS:O	1:A:197:LYS:CG	0.45	2.64	20	1
1:A:132:LYS:CE	1:A:133:MET:N	0.45	2.79	17	1
1:A:209:TYR:HB3	1:A:213:GLN:NE2	0.45	2.26	17	1
1:A:146:GLU:HA	1:A:149:MET:CB	0.45	2.41	15	1
1:A:133:MET:SD	1:A:176:LEU:HD13	0.45	2.51	15	1
1:A:168:ILE:HD12	1:A:170:PHE:CZ	0.45	2.47	1	1
1:A:126:GLY:O	1:A:217:ASP:OD1	0.45	2.34	22	1
1:A:173:LYS:HG2	1:A:175:TYR:OH	0.45	2.11	2	2
1:A:144:VAL:CG2	1:A:166:PRO:O	0.45	2.62	6	4
1:A:215:THR:CG2	1:A:221:LEU:CD1	0.45	2.89	7	1
1:A:168:ILE:CD1	1:A:221:LEU:HD21	0.45	2.41	6	1
1:A:171:PRO:HB2	1:A:211:MET:SD	0.45	2.51	12	2
1:A:213:GLN:OE1	1:A:213:GLN:CA	0.45	2.64	22	2
1:A:149:MET:SD	1:A:166:PRO:HB2	0.45	2.52	21	9
1:A:173:LYS:HG2	1:A:173:LYS:O	0.45	2.12	17	4
1:A:137:PRO:HG3	1:A:200:PRO:CD	0.45	2.42	18	1
1:A:129:VAL:CG2	1:A:183:LEU:CD2	0.45	2.94	5	2
1:A:173:LYS:NZ	1:A:175:TYR:OH	0.45	2.48	2	1
1:A:211:MET:SD	1:A:211:MET:O	0.45	2.74	14	2
1:A:191:ILE:HG22	1:A:213:GLN:HG3	0.45	1.88	9	3
1:A:149:MET:HE3	1:A:166:PRO:CB	0.45	2.42	11	1
1:A:193:GLN:CG	1:A:194:PHE:N	0.45	2.79	22	5
1:A:213:GLN:HA	1:A:213:GLN:OE1	0.45	2.11	3	2
1:A:160:ARG:CD	1:A:160:ARG:N	0.45	2.80	20	1
1:A:194:PHE:CZ	1:A:198:PRO:CB	0.45	3.00	2	5
1:A:123:TYR:OH	1:A:184:THR:CA	0.45	2.64	8	2
1:A:128:ARG:HG3	1:A:186:LEU:O	0.44	2.12	23	6
1:A:168:ILE:HG13	1:A:173:LYS:HG3	0.44	1.89	14	1
1:A:131:THR:OG1	1:A:141:SER:CB	0.44	2.66	4	2
1:A:124:LYS:CG	1:A:127:MET:HG3	0.44	2.42	10	3
1:A:172:ASN:N	1:A:172:ASN:ND2	0.44	2.63	5	1
1:A:133:MET:SD	1:A:176:LEU:CD1	0.44	3.05	15	2
1:A:173:LYS:HE2	1:A:221:LEU:CD2	0.44	2.43	21	1
1:A:194:PHE:CD1	1:A:194:PHE:C	0.44	2.90	4	3
1:A:131:THR:HB	1:A:169:PHE:CZ	0.44	2.47	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:LYS:CD	1:A:221:LEU:HG	0.44	2.42	4	1
1:A:158:PRO:HB2	1:A:160:ARG:CG	0.44	2.42	8	2
1:A:195:LEU:CD1	1:A:213:GLN:HG3	0.44	2.43	8	2
1:A:203:ALA:O	1:A:207:LYS:HG2	0.44	2.13	22	1
1:A:129:VAL:HG21	1:A:183:LEU:CD2	0.44	2.41	23	1
1:A:168:ILE:HD13	1:A:169:PHE:N	0.44	2.27	21	1
1:A:194:PHE:O	1:A:197:LYS:C	0.44	2.55	19	10
1:A:171:PRO:O	1:A:172:ASN:CB	0.44	2.65	11	2
1:A:171:PRO:HB3	1:A:211:MET:SD	0.44	2.52	5	3
1:A:160:ARG:HG3	1:A:161:ALA:N	0.44	2.26	11	1
1:A:141:SER:HA	1:A:168:ILE:O	0.44	2.12	23	12
1:A:130:LEU:HD22	1:A:138:TRP:CB	0.44	2.41	4	4
1:A:128:ARG:O	1:A:128:ARG:HG3	0.44	2.13	13	3
1:A:131:THR:HG21	1:A:167:VAL:HG21	0.44	1.88	13	2
1:A:140:PRO:HB2	1:A:212:ALA:CB	0.44	2.43	4	1
1:A:141:SER:HB2	1:A:167:VAL:CG2	0.44	2.43	2	1
1:A:149:MET:HE1	1:A:177:TRP:CE2	0.44	2.48	1	2
1:A:149:MET:HE2	1:A:175:TYR:HB3	0.44	1.89	11	1
1:A:191:ILE:CG2	1:A:213:GLN:HB2	0.44	2.43	16	5
1:A:124:LYS:CG	1:A:127:MET:SD	0.44	3.06	17	1
1:A:173:LYS:CG	1:A:175:TYR:OH	0.44	2.66	9	1
1:A:126:GLY:O	1:A:217:ASP:CG	0.44	2.56	21	1
1:A:160:ARG:NE	1:A:164:PHE:CE2	0.43	2.86	6	1
1:A:173:LYS:HD3	1:A:222:SER:O	0.43	2.12	21	1
1:A:196:GLU:CG	1:A:197:LYS:N	0.43	2.81	8	5
1:A:128:ARG:CG	1:A:186:LEU:O	0.43	2.66	15	1
1:A:142:MET:O	1:A:167:VAL:HA	0.43	2.14	11	3
1:A:160:ARG:HD2	1:A:161:ALA:N	0.43	2.28	19	1
1:A:213:GLN:O	1:A:213:GLN:OE1	0.43	2.36	22	1
1:A:180:SER:HA	1:A:183:LEU:HB2	0.43	1.90	10	1
1:A:213:GLN:CA	1:A:213:GLN:OE1	0.43	2.65	3	1
1:A:199:LYS:HA	1:A:200:PRO:C	0.43	2.33	2	8
1:A:144:VAL:HG21	1:A:149:MET:SD	0.43	2.54	23	6
1:A:168:ILE:CG1	1:A:173:LYS:HG3	0.43	2.43	5	1
1:A:201:LYS:CD	1:A:201:LYS:O	0.43	2.67	13	1
1:A:146:GLU:O	1:A:146:GLU:OE1	0.43	2.37	22	1
1:A:165:TYR:HB2	1:A:183:LEU:HD11	0.43	1.89	20	1
1:A:132:LYS:HD2	1:A:138:TRP:CE2	0.43	2.49	1	2
1:A:124:LYS:HG2	1:A:127:MET:SD	0.43	2.53	17	2
1:A:195:LEU:CG	1:A:213:GLN:OE1	0.43	2.66	17	1
1:A:123:TYR:CD1	1:A:129:VAL:HG11	0.43	2.49	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:ARG:O	1:A:128:ARG:HG2	0.42	2.14	5	3
1:A:146:GLU:CG	1:A:154:ARG:HD2	0.42	2.44	8	3
1:A:170:PHE:HE1	1:A:221:LEU:HD11	0.42	1.73	17	1
1:A:168:ILE:HD12	1:A:221:LEU:HD21	0.42	1.91	6	1
1:A:126:GLY:CA	1:A:218:LEU:HB2	0.42	2.44	10	1
1:A:201:LYS:O	1:A:201:LYS:HD2	0.42	2.13	9	1
1:A:139:TRP:CZ2	1:A:205:LEU:CA	0.42	3.02	20	2
1:A:158:PRO:HG2	1:A:160:ARG:NH2	0.42	2.28	20	1
1:A:186:LEU:CD1	1:A:191:ILE:HG13	0.42	2.43	12	1
1:A:129:VAL:HA	1:A:186:LEU:HB3	0.42	1.91	10	1
1:A:168:ILE:HG13	1:A:221:LEU:CD2	0.42	2.44	1	4
1:A:171:PRO:HG3	1:A:207:LYS:HB3	0.42	1.92	23	2
1:A:216:PRO:O	1:A:217:ASP:OD1	0.42	2.38	15	1
1:A:132:LYS:HD3	1:A:138:TRP:CZ2	0.42	2.49	20	1
1:A:191:ILE:O	1:A:195:LEU:HG	0.42	2.14	2	4
1:A:142:MET:SD	1:A:217:ASP:C	0.42	2.98	2	1
1:A:144:VAL:CG2	1:A:149:MET:CG	0.42	2.98	18	1
1:A:195:LEU:CD1	1:A:213:GLN:HG2	0.42	2.45	18	1
1:A:126:GLY:HA2	1:A:218:LEU:HB2	0.42	1.91	5	2
1:A:164:PHE:N	1:A:164:PHE:CD1	0.42	2.86	23	1
1:A:197:LYS:CG	1:A:197:LYS:O	0.42	2.68	9	1
1:A:172:ASN:O	1:A:173:LYS:HG2	0.42	2.14	22	12
1:A:130:LEU:HD23	1:A:130:LEU:HA	0.42	1.67	15	6
1:A:149:MET:HA	1:A:175:TYR:CE2	0.42	2.49	8	1
1:A:124:LYS:HG3	1:A:127:MET:CG	0.42	2.44	17	1
1:A:170:PHE:HB3	1:A:208:ALA:O	0.42	2.14	17	1
1:A:207:LYS:O	1:A:211:MET:HB2	0.42	2.15	16	3
1:A:137:PRO:O	1:A:138:TRP:C	0.42	2.58	15	3
1:A:173:LYS:O	1:A:173:LYS:HG3	0.42	2.14	12	1
1:A:153:ALA:CB	1:A:175:TYR:HB3	0.42	2.43	12	1
1:A:157:LYS:HA	1:A:177:TRP:CD1	0.42	2.49	13	1
1:A:213:GLN:OE1	1:A:213:GLN:C	0.42	2.58	8	1
1:A:198:PRO:O	1:A:199:LYS:HD3	0.42	2.15	23	1
1:A:130:LEU:HA	1:A:130:LEU:HD23	0.42	1.68	3	3
1:A:194:PHE:CE1	1:A:209:TYR:CG	0.42	3.07	4	1
1:A:178:THR:OG1	1:A:182:SER:OG	0.42	2.38	12	1
1:A:149:MET:HG2	1:A:153:ALA:HB3	0.42	1.90	15	1
1:A:184:THR:OG1	1:A:185:PRO:HD2	0.41	2.15	13	2
1:A:149:MET:HE1	1:A:166:PRO:CB	0.41	2.45	17	2
1:A:126:GLY:C	1:A:142:MET:SD	0.41	2.98	19	1
1:A:173:LYS:CE	1:A:221:LEU:HG	0.41	2.45	21	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:MET:CE	1:A:169:PHE:CZ	0.41	3.04	8	1
1:A:194:PHE:CE1	1:A:198:PRO:CB	0.41	3.03	8	1
1:A:221:LEU:HD12	1:A:221:LEU:HA	0.41	1.76	10	1
1:A:160:ARG:HD3	1:A:160:ARG:N	0.41	2.30	20	1
1:A:131:THR:OG1	1:A:141:SER:HB2	0.41	2.15	4	1
1:A:158:PRO:CG	1:A:177:TRP:HB3	0.41	2.46	14	1
1:A:171:PRO:HB3	1:A:211:MET:HB2	0.41	1.93	23	1
1:A:130:LEU:HB2	1:A:184:THR:HG23	0.41	1.91	16	2
1:A:216:PRO:O	1:A:217:ASP:CG	0.41	2.59	5	1
1:A:160:ARG:CD	1:A:160:ARG:H	0.41	2.29	20	1
1:A:133:MET:HE1	1:A:176:LEU:HD13	0.41	1.91	8	1
1:A:127:MET:O	1:A:142:MET:CG	0.41	2.68	6	1
1:A:149:MET:HE1	1:A:153:ALA:HB1	0.41	1.92	14	1
1:A:165:TYR:O	1:A:167:VAL:HG13	0.41	2.15	10	1
1:A:158:PRO:HD3	1:A:177:TRP:HB2	0.41	1.91	3	2
1:A:132:LYS:HB3	1:A:138:TRP:CG	0.41	2.51	5	1
1:A:203:ALA:O	1:A:207:LYS:HG3	0.41	2.16	14	3
1:A:126:GLY:CA	1:A:218:LEU:HB3	0.41	2.45	13	1
1:A:152:VAL:O	1:A:155:LYS:HG2	0.41	2.16	17	1
1:A:166:PRO:HB3	1:A:177:TRP:CZ3	0.41	2.51	15	2
1:A:128:ARG:HG3	1:A:186:LEU:HD23	0.41	1.92	23	1
1:A:155:LYS:O	1:A:155:LYS:HG3	0.41	2.15	15	1
1:A:158:PRO:HB2	1:A:160:ARG:HD3	0.41	1.91	20	1
1:A:132:LYS:O	1:A:132:LYS:HG3	0.41	2.16	2	1
1:A:126:GLY:CA	1:A:218:LEU:HD12	0.41	2.46	6	1
1:A:128:ARG:HG3	1:A:142:MET:SD	0.41	2.56	12	2
1:A:146:GLU:OE2	1:A:157:LYS:HD2	0.41	2.16	9	1
1:A:217:ASP:OD2	1:A:219:ASP:HB2	0.41	2.16	11	1
1:A:169:PHE:HB2	1:A:174:GLU:HB2	0.41	1.92	16	1
1:A:164:PHE:CD1	1:A:164:PHE:N	0.41	2.88	6	2
1:A:146:GLU:HG3	1:A:154:ARG:CG	0.41	2.46	7	1
1:A:131:THR:HG1	1:A:141:SER:CB	0.41	2.28	4	1
1:A:124:LYS:HG3	1:A:127:MET:HG3	0.41	1.92	17	1
1:A:216:PRO:HG2	1:A:220:SER:HB2	0.40	1.91	22	1
1:A:214:SER:O	1:A:216:PRO:HD3	0.40	2.16	9	1
1:A:150:THR:CG2	1:A:152:VAL:HB	0.40	2.46	3	1
1:A:202:THR:O	1:A:206:ILE:HG13	0.40	2.16	2	2
1:A:173:LYS:HD3	1:A:175:TYR:OH	0.40	2.16	1	1
1:A:127:MET:C	1:A:142:MET:HG3	0.40	2.37	17	1
1:A:172:ASN:C	1:A:173:LYS:HD2	0.40	2.37	23	1
1:A:217:ASP:C	1:A:217:ASP:OD1	0.40	2.60	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:VAL:CG2	1:A:141:SER:O	0.40	2.69	1	1
1:A:172:ASN:O	1:A:173:LYS:CG	0.40	2.70	23	1
1:A:203:ALA:HB1	1:A:207:LYS:HE3	0.40	1.91	16	1
1:A:126:GLY:HA2	1:A:142:MET:SD	0.40	2.56	20	1
1:A:217:ASP:OD1	1:A:217:ASP:C	0.40	2.60	20	1
1:A:209:TYR:O	1:A:213:GLN:HB3	0.40	2.17	2	1
1:A:132:LYS:HE3	1:A:136:PHE:O	0.40	2.17	4	1
1:A:169:PHE:CE1	1:A:176:LEU:CB	0.40	3.05	8	1
1:A:203:ALA:O	1:A:207:LYS:HB3	0.40	2.17	8	1
1:A:190:ALA:O	1:A:193:GLN:HG2	0.40	2.16	21	1
1:A:131:THR:OG1	1:A:141:SER:HB3	0.40	2.17	21	1
1:A:139:TRP:CE3	1:A:205:LEU:HD12	0.40	2.50	6	1
1:A:127:MET:O	1:A:142:MET:HG3	0.40	2.17	14	1
1:A:146:GLU:OE2	1:A:154:ARG:NE	0.40	2.54	19	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	101/109 (93%)	93±2 (92±2%)	7±2 (7±2%)	2±1 (2±1%)	18	63
All	All	2323/2507 (93%)	2129 (92%)	158 (7%)	36 (2%)	18	63

All 4 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	150	THR	13
1	A	216	PRO	11
1	A	173	LYS	7
1	A	174	GLU	5

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	91/98 (93%)	70±4 (76±4%)	21±4 (24±4%)	3	29
All	All	2093/2254 (93%)	1599 (76%)	494 (24%)	3	29

All 54 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	168	ILE	23
1	A	202	THR	23
1	A	173	LYS	22
1	A	136	PHE	21
1	A	132	LYS	18
1	A	151	SER	18
1	A	155	LYS	18
1	A	199	LYS	15
1	A	188	SER	15
1	A	176	LEU	15
1	A	160	ARG	15
1	A	197	LYS	14
1	A	154	ARG	13
1	A	128	ARG	12
1	A	149	MET	12
1	A	147	SER	12
1	A	174	GLU	12
1	A	182	SER	12
1	A	220	SER	11
1	A	156	SER	10
1	A	181	ASP	9
1	A	211	MET	9
1	A	222	SER	9
1	A	134	SER	9
1	A	214	SER	9
1	A	159	LYS	8
1	A	218	LEU	8
1	A	201	LYS	8
1	A	180	SER	8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	131	THR	7
1	A	192	SER	7
1	A	204	SER	7
1	A	196	GLU	7
1	A	210	LYS	7
1	A	207	LYS	6
1	A	213	GLN	6
1	A	193	GLN	6
1	A	124	LYS	6
1	A	133	MET	6
1	A	141	SER	5
1	A	217	ASP	5
1	A	219	ASP	5
1	A	205	LEU	4
1	A	189	GLU	4
1	A	215	THR	3
1	A	146	GLU	3
1	A	157	LYS	3
1	A	148	LYS	3
1	A	139	TRP	1
1	A	163	THR	1
1	A	191	ILE	1
1	A	142	MET	1
1	A	167	VAL	1
1	A	186	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5538

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	1255
Number of shifts mapped to atoms	1255
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	107	0.68 ± 0.13	Should be applied
$^{13}\text{C}_\beta$	99	0.39 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	107	0.33 ± 0.09	None needed (< 0.5 ppm)
^{15}N	97	0.07 ± 0.28	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 83%, i.e. 1048 atoms were assigned a chemical shift out of a possible 1264. 13 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	481/485 (99%)	192/192 (100%)	198/202 (98%)	91/91 (100%)
Sidechain	508/666 (76%)	374/400 (94%)	130/241 (54%)	4/25 (16%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	59/113 (52%)	56/59 (95%)	0/51 (0%)	3/3 (100%)
Overall	1048/1264 (83%)	622/651 (96%)	328/494 (66%)	98/119 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1117 atoms were assigned a chemical shift out of a possible 1349. 15 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	513/518 (99%)	204/205 (100%)	212/216 (98%)	97/97 (100%)
Sidechain	545/718 (76%)	400/431 (93%)	141/259 (54%)	4/28 (14%)
Aromatic	59/113 (52%)	56/59 (95%)	0/51 (0%)	3/3 (100%)
Overall	1117/1349 (83%)	660/695 (95%)	353/526 (67%)	104/128 (81%)

7.1.4 Statistically unusual chemical shifts ⓘ

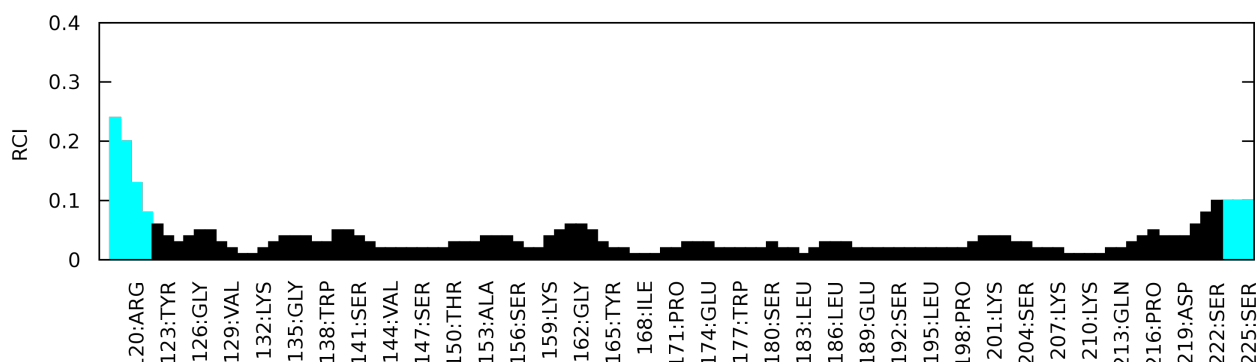
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	132	LYS	HG2	-1.16	2.67 – 0.07	-9.7
1	A	157	LYS	HG3	-0.80	2.76 – -0.04	-7.7
1	A	166	PRO	HB3	-0.39	3.81 – 0.21	-6.7
1	A	198	PRO	HA	2.40	6.05 – 2.75	-6.1
1	A	132	LYS	HG3	-0.23	2.76 – -0.04	-5.7
1	A	140	PRO	HG3	0.04	3.56 – 0.26	-5.7
1	A	157	LYS	HA	2.01	6.46 – 2.06	-5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: BMRB entry 5902

Chemical shift list name: *assigned_chem_shift_list_1*

7.2.1 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	1240
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1240
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

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

- Chain not found in structure. All 1240 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	106	LYS	HB3	1.56	0.02	2
UNMAPPED	65	THR	H	8.222	0.02	1
UNMAPPED	18	LYS	CE	42.155	0.2	1
UNMAPPED	73	LEU	CB	45.737	0.2	1
UNMAPPED	20	TYR	H	7.652	0.02	1
UNMAPPED	71	LYS	HB3	1.875	0.02	1
UNMAPPED	100	GLU	HA	4.013	0.02	1
UNMAPPED	70	PRO	HB3	2.605	0.02	2
UNMAPPED	21	LYS	HD3	1.558	0.02	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	12	SER	C	174.561	0.2	1
UNMAPPED	98	GLU	N	119.555	0.2	1
UNMAPPED	55	TYR	CE2	117.386	0.2	1
UNMAPPED	21	LYS	HA	4.89	0.02	1
UNMAPPED	25	LEU	CG	26.161	0.2	1
UNMAPPED	21	LYS	HG2	1.374	0.02	1
UNMAPPED	83	PHE	HE2	6.385	0.02	1
UNMAPPED	90	LYS	CD	29.011	0.2	1
UNMAPPED	103	PRO	HB3	2.115	0.02	2
UNMAPPED	100	GLU	HG2	2.076	0.02	2
UNMAPPED	25	LEU	CA	53.559	0.2	1
UNMAPPED	25	LEU	HD21	1.052	0.02	2
UNMAPPED	110	TYR	CE2	116.817	0.2	1
UNMAPPED	102	ASN	H	9.201	0.02	1
UNMAPPED	88	LYS	CG	29.03	0.2	1
UNMAPPED	103	PRO	CA	64.531	0.2	1
UNMAPPED	56	GLN	HG3	1.814	0.02	2
UNMAPPED	17	GLN	CB	29.142	0.2	1
UNMAPPED	18	LYS	HE2	2.913	0.02	1
UNMAPPED	88	LYS	CD	24.727	0.2	1
UNMAPPED	67	PHE	HD1	7.116	0.02	1
UNMAPPED	17	GLN	N	120.991	0.2	1
UNMAPPED	95	GLY	HA3	3.95	0.02	2
UNMAPPED	29	LYS	H	9.492	0.02	1
UNMAPPED	88	LYS	CE	42.155	0.2	1
UNMAPPED	31	LYS	HD2	1.547	0.02	1
UNMAPPED	29	LYS	HD2	1.465	0.02	2
UNMAPPED	101	ASN	HA	4.444	0.02	1
UNMAPPED	84	GLY	N	109.334	0.2	1
UNMAPPED	13	ARG	C	176.373	0.2	1
UNMAPPED	64	GLU	N	117.669	0.2	1
UNMAPPED	48	VAL	HG11	0.932	0.02	1
UNMAPPED	98	GLU	CG	37.279	0.2	1
UNMAPPED	14	SER	HB2	3.903	0.02	1
UNMAPPED	27	PHE	HB2	2.686	0.02	2
UNMAPPED	39	ARG	HG2	1.361	0.02	1
UNMAPPED	100	GLU	HB2	1.609	0.02	2
UNMAPPED	87	ASN	H	7.895	0.02	1
UNMAPPED	57	VAL	HB	1.694	0.02	1
UNMAPPED	15	ASN	HD22	6.936	0.02	2
UNMAPPED	25	LEU	HD11	0.867	0.02	2

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	92	PHE	HA	3.421	0.02	1
UNMAPPED	26	VAL	CG2	22.754	0.2	1
UNMAPPED	41	ASP	CA	54.08	0.2	1
UNMAPPED	32	GLY	CA	45.01	0.2	1
UNMAPPED	106	LYS	HD3	1.598	0.02	1
UNMAPPED	21	LYS	HD2	1.558	0.02	1
UNMAPPED	36	TRP	CZ2	113.915	0.2	1
UNMAPPED	16	ARG	CG	26.879	0.2	1
UNMAPPED	41	ASP	HB3	2.614	0.02	2
UNMAPPED	58	PHE	HB2	2.959	0.02	2
UNMAPPED	18	LYS	H	8.269	0.02	1
UNMAPPED	96	LEU	HD22	0.801	0.02	2
UNMAPPED	20	TYR	HB2	2.881	0.02	2
UNMAPPED	35	HIS	HA	3.931	0.02	1
UNMAPPED	31	LYS	HG3	1.423	0.02	1
UNMAPPED	23	GLY	H	9.732	0.02	1
UNMAPPED	17	GLN	HB3	2.09	0.02	2
UNMAPPED	78	GLU	HG2	2.442	0.02	2
UNMAPPED	76	TYR	HB2	2.691	0.02	2
UNMAPPED	110	TYR	HD2	7.12	0.02	1
UNMAPPED	58	PHE	CA	55.789	0.2	1
UNMAPPED	29	LYS	HE2	2.742	0.02	2
UNMAPPED	98	GLU	CA	59.888	0.2	1
UNMAPPED	98	GLU	HB2	2.071	0.02	2
UNMAPPED	24	ASP	N	120.576	0.2	1
UNMAPPED	91	GLY	HA2	4.483	0.02	2
UNMAPPED	26	VAL	H	9.038	0.02	1
UNMAPPED	20	TYR	HE2	6.507	0.02	1
UNMAPPED	79	SER	CB	64.34	0.2	1
UNMAPPED	33	TYR	CB	40.663	0.2	1
UNMAPPED	60	PHE	C	177.327	0.2	1
UNMAPPED	24	ASP	CB	41.086	0.2	1
UNMAPPED	108	SER	HB3	3.872	0.02	1
UNMAPPED	44	PRO	CG	27.237	0.2	1
UNMAPPED	68	LEU	CA	53.655	0.2	1
UNMAPPED	65	THR	C	173.987	0.2	1
UNMAPPED	55	TYR	HB2	2.845	0.02	2
UNMAPPED	104	THR	C	174.723	0.2	1
UNMAPPED	90	LYS	CG	24.424	0.2	1
UNMAPPED	108	SER	CB	63.706	0.2	1
UNMAPPED	59	PHE	CB	38.549	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	105	VAL	CA	62.532	0.2	1
UNMAPPED	43	MET	HG2	1.938	0.02	2
UNMAPPED	80	LYS	HE3	2.892	0.02	1
UNMAPPED	33	TYR	C	172.697	0.2	1
UNMAPPED	19	GLU	C	175.151	0.2	1
UNMAPPED	87	ASN	CA	52.75	0.2	1
UNMAPPED	30	MET	HB2	1.751	0.02	2
UNMAPPED	67	PHE	CD1	130.747	0.2	1
UNMAPPED	34	PRO	HD2	3.92	0.02	2
UNMAPPED	30	MET	H	8.704	0.02	1
UNMAPPED	52	ALA	H	7.939	0.02	1
UNMAPPED	78	GLU	CA	57.879	0.2	1
UNMAPPED	34	PRO	HB2	1.988	0.02	2
UNMAPPED	17	GLN	HE21	7.536	0.02	2
UNMAPPED	92	PHE	CB	39.395	0.2	1
UNMAPPED	63	HIS	HB2	3.33	0.02	2
UNMAPPED	78	GLU	CG	36.741	0.2	1
UNMAPPED	89	ARG	H	8.844	0.02	1
UNMAPPED	97	TRP	H	7.932	0.02	1
UNMAPPED	74	PHE	CZ	129.055	0.2	1
UNMAPPED	94	GLU	N	123.857	0.2	1
UNMAPPED	80	LYS	CB	31.15	0.2	1
UNMAPPED	64	GLU	C	174.104	0.2	1
UNMAPPED	96	LEU	HB3	1.46	0.02	2
UNMAPPED	103	PRO	HG3	1.821	0.02	2
UNMAPPED	51	THR	CG2	21.319	0.2	1
UNMAPPED	86	PRO	CA	63.76	0.2	1
UNMAPPED	94	GLU	HA	4.168	0.02	1
UNMAPPED	46	ALA	CB	18.994	0.2	1
UNMAPPED	30	MET	HA	4.693	0.02	1
UNMAPPED	79	SER	HB2	3.91	0.02	1
UNMAPPED	99	ILE	HD13	0.352	0.02	1
UNMAPPED	105	VAL	HG12	1.099	0.02	2
UNMAPPED	38	ALA	N	129.757	0.2	1
UNMAPPED	58	PHE	HE1	6.856	0.02	1
UNMAPPED	92	PHE	CZ	128.531	0.2	1
UNMAPPED	11	MET	H	8.428	0.02	1
UNMAPPED	97	TRP	CE3	119.384	0.2	1
UNMAPPED	59	PHE	HD2	6.84	0.02	1
UNMAPPED	49	LYS	CE	42.155	0.2	1
UNMAPPED	101	ASN	ND2	116.449	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	97	TRP	CZ2	113.934	0.2	1
UNMAPPED	82	LYS	CB	32.418	0.2	1
UNMAPPED	78	GLU	C	177.394	0.2	1
UNMAPPED	58	PHE	HZ	6.437	0.02	1
UNMAPPED	25	LEU	C	177.65	0.2	1
UNMAPPED	72	ASP	C	173.027	0.2	1
UNMAPPED	84	GLY	H	8.118	0.02	1
UNMAPPED	85	LYS	HE2	3.04	0.02	1
UNMAPPED	86	PRO	HA	4.371	0.02	1
UNMAPPED	66	ALA	HA	4.524	0.02	1
UNMAPPED	67	PHE	N	118.294	0.2	1
UNMAPPED	21	LYS	HE3	3.073	0.02	1
UNMAPPED	38	ALA	HB3	0.767	0.02	1
UNMAPPED	37	PRO	HD2	2.944	0.02	1
UNMAPPED	77	GLU	HG3	2.439	0.02	1
UNMAPPED	85	LYS	HD3	1.72	0.02	2
UNMAPPED	37	PRO	HG3	1.191	0.02	1
UNMAPPED	65	THR	CB	71.739	0.2	1
UNMAPPED	37	PRO	HB3	1.875	0.02	2
UNMAPPED	94	GLU	HB2	2.268	0.02	2
UNMAPPED	105	VAL	HG21	1.225	0.02	2
UNMAPPED	46	ALA	HB2	1.41	0.02	1
UNMAPPED	62	THR	HB	4.035	0.02	1
UNMAPPED	71	LYS	CD	24.597	0.2	1
UNMAPPED	54	LYS	HB2	1.647	0.02	1
UNMAPPED	71	LYS	CA	58.277	0.2	1
UNMAPPED	65	THR	N	112.457	0.2	1
UNMAPPED	18	LYS	HE3	2.913	0.02	1
UNMAPPED	19	GLU	HG3	2.299	0.02	1
UNMAPPED	58	PHE	HD2	6.366	0.02	1
UNMAPPED	67	PHE	CZ	128.383	0.2	1
UNMAPPED	57	VAL	HG13	0.66	0.02	2
UNMAPPED	79	SER	CA	58.289	0.2	1
UNMAPPED	88	LYS	N	119.291	0.2	1
UNMAPPED	73	LEU	HD12	0.557	0.02	2
UNMAPPED	75	PRO	CA	64.216	0.2	1
UNMAPPED	100	GLU	C	177.07	0.2	1
UNMAPPED	80	LYS	HD2	1.47	0.02	1
UNMAPPED	71	LYS	N	116.758	0.2	1
UNMAPPED	51	THR	HA	4.288	0.02	1
UNMAPPED	107	ALA	CA	52.612	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	33	TYR	HB2	3.197	0.02	2
UNMAPPED	74	PHE	CB	41.614	0.2	1
UNMAPPED	104	THR	HG21	1.15	0.02	1
UNMAPPED	83	PHE	CD2	128.553	0.2	1
UNMAPPED	13	ARG	CG	27.0	0.2	1
UNMAPPED	83	PHE	N	112.747	0.2	1
UNMAPPED	87	ASN	HA	4.64	0.02	1
UNMAPPED	81	GLU	H	8.464	0.02	1
UNMAPPED	17	GLN	H	8.383	0.02	1
UNMAPPED	79	SER	HA	4.59	0.02	1
UNMAPPED	59	PHE	CE2	129.7	0.2	1
UNMAPPED	102	ASN	N	117.992	0.2	1
UNMAPPED	83	PHE	HB3	0.655	0.02	2
UNMAPPED	22	CYS	C	175.901	0.2	1
UNMAPPED	91	GLY	CA	45.607	0.2	1
UNMAPPED	89	ARG	HA	4.326	0.02	1
UNMAPPED	11	MET	HA	4.466	0.02	1
UNMAPPED	68	LEU	HD22	0.896	0.02	2
UNMAPPED	29	LYS	CB	34.744	0.2	1
UNMAPPED	62	THR	HG23	1.208	0.02	1
UNMAPPED	92	PHE	HE2	7.565	0.02	1
UNMAPPED	92	PHE	C	177.277	0.2	1
UNMAPPED	40	ILE	H	8.595	0.02	1
UNMAPPED	52	ALA	HB2	1.36	0.02	1
UNMAPPED	16	ARG	HD3	3.275	0.02	1
UNMAPPED	65	THR	HG23	1.035	0.02	1
UNMAPPED	28	ALA	HB3	0.985	0.02	1
UNMAPPED	97	TRP	N	118.923	0.2	1
UNMAPPED	87	ASN	HB3	1.995	0.02	2
UNMAPPED	60	PHE	CA	60.083	0.2	1
UNMAPPED	73	LEU	HD21	0.038	0.02	2
UNMAPPED	42	GLU	N	116.457	0.2	1
UNMAPPED	18	LYS	CD	28.851	0.2	1
UNMAPPED	88	LYS	HG3	1.706	0.02	1
UNMAPPED	58	PHE	CZ	126.446	0.2	1
UNMAPPED	15	ASN	CB	38.655	0.2	1
UNMAPPED	45	GLU	N	121.769	0.2	1
UNMAPPED	42	GLU	HG3	2.369	0.02	1
UNMAPPED	18	LYS	CB	32.841	0.2	1
UNMAPPED	36	TRP	CZ3	119.937	0.2	1
UNMAPPED	33	TYR	CA	55.632	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	98	GLU	HB3	2.38	0.02	2
UNMAPPED	88	LYS	CB	32.101	0.2	1
UNMAPPED	21	LYS	HG3	1.374	0.02	1
UNMAPPED	83	PHE	HE1	6.385	0.02	1
UNMAPPED	68	LEU	CD1	24.486	0.2	2
UNMAPPED	25	LEU	HB2	1.147	0.02	2
UNMAPPED	34	PRO	HB3	2.346	0.02	2
UNMAPPED	82	LYS	HE3	2.664	0.02	2
UNMAPPED	92	PHE	CA	63.151	0.2	1
UNMAPPED	43	MET	HB3	2.744	0.02	2
UNMAPPED	87	ASN	HD22	7.2	0.02	2
UNMAPPED	38	ALA	HB1	0.767	0.02	1
UNMAPPED	15	ASN	ND2	112.493	0.2	1
UNMAPPED	56	GLN	HG2	1.541	0.02	2
UNMAPPED	17	GLN	CA	55.78	0.2	1
UNMAPPED	37	PRO	HB2	1.538	0.02	2
UNMAPPED	35	HIS	H	8.165	0.02	1
UNMAPPED	109	GLY	N	110.277	0.2	1
UNMAPPED	68	LEU	HA	5.0	0.02	1
UNMAPPED	27	PHE	CB	42.566	0.2	1
UNMAPPED	51	THR	CA	61.675	0.2	1
UNMAPPED	24	ASP	H	8.107	0.02	1
UNMAPPED	88	LYS	HB2	1.797	0.02	2
UNMAPPED	99	ILE	CG1	31.182	0.2	1
UNMAPPED	42	GLU	HG2	2.369	0.02	1
UNMAPPED	84	GLY	HA3	4.476	0.02	2
UNMAPPED	27	PHE	N	113.144	0.2	1
UNMAPPED	45	GLU	HG2	2.296	0.02	1
UNMAPPED	18	LYS	HD3	1.636	0.02	1
UNMAPPED	39	ARG	HG3	1.361	0.02	1
UNMAPPED	18	LYS	N	122.938	0.2	1
UNMAPPED	31	LYS	CG	24.694	0.2	1
UNMAPPED	57	VAL	HG23	0.211	0.02	2
UNMAPPED	21	LYS	CB	35.378	0.2	1
UNMAPPED	67	PHE	CE2	130.768	0.2	1
UNMAPPED	32	GLY	HA2	3.667	0.02	2
UNMAPPED	52	ALA	CB	18.994	0.2	1
UNMAPPED	95	GLY	H	8.528	0.02	1
UNMAPPED	82	LYS	HG3	0.771	0.02	2
UNMAPPED	108	SER	N	133.684	0.2	1
UNMAPPED	70	PRO	HG2	2.29	0.02	2

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	44	PRO	HG2	1.392	0.02	2
UNMAPPED	77	GLU	CA	60.191	0.2	1
UNMAPPED	73	LEU	HB2	1.442	0.02	2
UNMAPPED	52	ALA	N	124.197	0.2	1
UNMAPPED	21	LYS	N	119.191	0.2	1
UNMAPPED	20	TYR	N	119.811	0.2	1
UNMAPPED	89	ARG	CG	27.7	0.2	1
UNMAPPED	56	GLN	H	8.623	0.02	1
UNMAPPED	71	LYS	HG3	1.379	0.02	1
UNMAPPED	96	LEU	HD23	0.801	0.02	2
UNMAPPED	16	ARG	HB3	1.793	0.02	2
UNMAPPED	31	LYS	CD	28.795	0.2	1
UNMAPPED	68	LEU	HD11	1.117	0.02	2
UNMAPPED	17	GLN	HB2	2.016	0.02	2
UNMAPPED	76	TYR	HB3	2.764	0.02	2
UNMAPPED	46	ALA	H	8.324	0.02	1
UNMAPPED	12	SER	HB3	3.927	0.02	1
UNMAPPED	88	LYS	HA	4.368	0.02	1
UNMAPPED	29	LYS	HE3	3.044	0.02	2
UNMAPPED	70	PRO	HD2	3.799	0.02	2
UNMAPPED	39	ARG	HA	5.343	0.02	1
UNMAPPED	74	PHE	HE2	7.409	0.02	1
UNMAPPED	83	PHE	HD1	6.448	0.02	1
UNMAPPED	12	SER	CA	58.336	0.2	1
UNMAPPED	16	ARG	HA	4.319	0.02	1
UNMAPPED	53	ASN	HB3	2.837	0.02	1
UNMAPPED	109	GLY	HA2	3.838	0.02	2
UNMAPPED	87	ASN	HD21	4.896	0.02	2
UNMAPPED	82	LYS	H	7.118	0.02	1
UNMAPPED	25	LEU	CD1	25.054	0.2	1
UNMAPPED	75	PRO	HB3	2.666	0.02	2
UNMAPPED	44	PRO	HB2	1.787	0.02	2
UNMAPPED	53	ASN	CA	53.081	0.2	1
UNMAPPED	96	LEU	CA	56.465	0.2	1
UNMAPPED	90	LYS	HE3	3.056	0.02	1
UNMAPPED	80	LYS	CD	29.264	0.2	1
UNMAPPED	97	TRP	NE1	130.578	0.2	1
UNMAPPED	88	LYS	HD3	1.457	0.02	1
UNMAPPED	43	MET	HG3	2.153	0.02	2
UNMAPPED	80	LYS	HE2	2.892	0.02	1
UNMAPPED	99	ILE	HG12	1.0	0.02	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	58	PHE	C	173.684	0.2	1
UNMAPPED	22	CYS	CA	61.759	0.2	1
UNMAPPED	80	LYS	C	177.88	0.2	1
UNMAPPED	69	GLY	HA2	4.082	0.02	2
UNMAPPED	76	TYR	CA	62.321	0.2	1
UNMAPPED	66	ALA	CB	23.222	0.2	1
UNMAPPED	20	TYR	CD1	131.828	0.2	1
UNMAPPED	45	GLU	HG3	2.296	0.02	1
UNMAPPED	34	PRO	HD3	4.045	0.02	2
UNMAPPED	65	THR	HA	5.633	0.02	1
UNMAPPED	41	ASP	HB2	2.2	0.02	2
UNMAPPED	88	LYS	HE3	3.025	0.02	1
UNMAPPED	106	LYS	N	122.914	0.2	1
UNMAPPED	92	PHE	CE2	131.402	0.2	1
UNMAPPED	70	PRO	HG3	2.407	0.02	2
UNMAPPED	45	GLU	HA	4.225	0.02	1
UNMAPPED	26	VAL	HB	2.211	0.02	1
UNMAPPED	57	VAL	N	128.146	0.2	1
UNMAPPED	54	LYS	HG2	1.2	0.02	2
UNMAPPED	25	LEU	HD13	0.867	0.02	2
UNMAPPED	55	TYR	CD2	132.872	0.2	1
UNMAPPED	62	THR	HG21	1.208	0.02	1
UNMAPPED	96	LEU	HB2	1.865	0.02	2
UNMAPPED	59	PHE	HE2	6.859	0.02	1
UNMAPPED	103	PRO	HG2	1.946	0.02	2
UNMAPPED	25	LEU	HG	2.043	0.02	1
UNMAPPED	80	LYS	CE	42.038	0.2	1
UNMAPPED	71	LYS	H	8.613	0.02	1
UNMAPPED	34	PRO	HG3	2.187	0.02	1
UNMAPPED	103	PRO	HD3	3.239	0.02	1
UNMAPPED	34	PRO	HA	4.762	0.02	1
UNMAPPED	79	SER	HB3	3.91	0.02	1
UNMAPPED	59	PHE	C	175.451	0.2	1
UNMAPPED	25	LEU	HA	5.138	0.02	1
UNMAPPED	104	THR	HA	4.327	0.02	1
UNMAPPED	33	TYR	HE1	6.632	0.02	1
UNMAPPED	56	GLN	HA	4.196	0.02	1
UNMAPPED	48	VAL	H	7.727	0.02	1
UNMAPPED	85	LYS	HG2	1.441	0.02	2
UNMAPPED	96	LEU	CD1	26.217	0.2	1
UNMAPPED	56	GLN	CA	55.949	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	40	ILE	HB	2.29	0.02	1
UNMAPPED	73	LEU	CD1	24.225	0.2	2
UNMAPPED	49	LYS	CD	29.1	0.2	1
UNMAPPED	85	LYS	HG3	1.386	0.02	2
UNMAPPED	97	TRP	HB2	3.645	0.02	2
UNMAPPED	42	GLU	H	7.956	0.02	1
UNMAPPED	63	HIS	CB	25.653	0.2	1
UNMAPPED	15	ASN	H	8.472	0.02	1
UNMAPPED	75	PRO	HB2	2.31	0.02	2
UNMAPPED	53	ASN	H	8.38	0.02	1
UNMAPPED	110	TYR	H	7.646	0.02	1
UNMAPPED	80	LYS	N	122.971	0.2	1
UNMAPPED	56	GLN	CB	29.776	0.2	1
UNMAPPED	63	HIS	N	113.977	0.2	1
UNMAPPED	81	GLU	HG2	2.204	0.02	2
UNMAPPED	76	TYR	H	8.528	0.02	1
UNMAPPED	59	PHE	H	8.712	0.02	1
UNMAPPED	109	GLY	C	172.722	0.2	1
UNMAPPED	96	LEU	HD12	0.913	0.02	2
UNMAPPED	96	LEU	HD21	0.801	0.02	2
UNMAPPED	34	PRO	CG	26.879	0.2	1
UNMAPPED	16	ARG	CD	43.197	0.2	1
UNMAPPED	105	VAL	HG22	1.225	0.02	2
UNMAPPED	46	ALA	HB3	1.41	0.02	1
UNMAPPED	54	LYS	CA	55.142	0.2	1
UNMAPPED	63	HIS	HB3	3.704	0.02	2
UNMAPPED	105	VAL	HB	2.434	0.02	1
UNMAPPED	19	GLU	HG2	2.299	0.02	1
UNMAPPED	59	PHE	CD2	129.7	0.2	1
UNMAPPED	26	VAL	N	117.065	0.2	1
UNMAPPED	45	GLU	H	8.584	0.02	1
UNMAPPED	73	LEU	HD13	0.557	0.02	2
UNMAPPED	105	VAL	HA	3.85	0.02	1
UNMAPPED	34	PRO	C	176.761	0.2	1
UNMAPPED	96	LEU	HD13	0.913	0.02	2
UNMAPPED	13	ARG	CB	30.621	0.2	1
UNMAPPED	13	ARG	HD2	3.248	0.02	1
UNMAPPED	90	LYS	HB2	1.936	0.02	2
UNMAPPED	13	ARG	CD	43.197	0.2	1
UNMAPPED	38	ALA	H	9.519	0.02	1
UNMAPPED	96	LEU	CB	41.086	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	19	GLU	CG	35.9	0.2	1
UNMAPPED	106	LYS	CD	28.193	0.2	1
UNMAPPED	93	SER	CA	62.24	0.2	1
UNMAPPED	27	PHE	H	9.511	0.02	1
UNMAPPED	68	LEU	HD21	0.896	0.02	2
UNMAPPED	29	LYS	CE	43.21	0.2	1
UNMAPPED	97	TRP	HZ2	7.467	0.02	1
UNMAPPED	74	PHE	HD1	7.429	0.02	1
UNMAPPED	40	ILE	N	123.258	0.2	1
UNMAPPED	47	ALA	CA	52.83	0.2	1
UNMAPPED	71	LYS	HB2	1.875	0.02	1
UNMAPPED	57	VAL	HG22	0.211	0.02	2
UNMAPPED	101	ASN	C	174.458	0.2	1
UNMAPPED	67	PHE	HA	5.771	0.02	1
UNMAPPED	16	ARG	HD2	3.275	0.02	1
UNMAPPED	23	GLY	C	174.075	0.2	1
UNMAPPED	65	THR	HG22	1.035	0.02	1
UNMAPPED	87	ASN	HB2	2.365	0.02	2
UNMAPPED	13	ARG	HG2	1.667	0.02	1
UNMAPPED	39	ARG	CG	26.868	0.2	1
UNMAPPED	72	ASP	CA	54.262	0.2	1
UNMAPPED	77	GLU	HA	3.554	0.02	1
UNMAPPED	14	SER	CB	63.6	0.2	1
UNMAPPED	87	ASN	ND2	110.906	0.2	1
UNMAPPED	53	ASN	C	173.914	0.2	1
UNMAPPED	26	VAL	HG21	0.479	0.02	2
UNMAPPED	18	LYS	CG	24.368	0.2	1
UNMAPPED	36	TRP	HE1	10.945	0.02	1
UNMAPPED	14	SER	N	115.836	0.2	1
UNMAPPED	31	LYS	HD3	1.547	0.02	1
UNMAPPED	40	ILE	CG2	26.34	0.2	1
UNMAPPED	90	LYS	HE2	3.056	0.02	1
UNMAPPED	45	GLU	CG	36.204	0.2	1
UNMAPPED	45	GLU	HB3	1.999	0.02	1
UNMAPPED	20	TYR	CE2	116.597	0.2	1
UNMAPPED	100	GLU	N	113.401	0.2	1
UNMAPPED	31	LYS	HG2	1.423	0.02	1
UNMAPPED	16	ARG	HG2	1.664	0.02	1
UNMAPPED	39	ARG	C	174.677	0.2	1
UNMAPPED	88	LYS	C	177.094	0.2	1
UNMAPPED	76	TYR	C	176.432	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	104	THR	N	107.505	0.2	1
UNMAPPED	107	ALA	CB	19.1	0.2	1
UNMAPPED	52	ALA	C	177.023	0.2	1
UNMAPPED	92	PHE	HB2	2.509	0.02	2
UNMAPPED	82	LYS	HE2	2.592	0.02	2
UNMAPPED	47	ALA	C	177.65	0.2	1
UNMAPPED	43	MET	HB2	2.621	0.02	2
UNMAPPED	19	GLU	H	8.145	0.02	1
UNMAPPED	70	PRO	CG	27.775	0.2	1
UNMAPPED	100	GLU	HB3	1.814	0.02	2
UNMAPPED	36	TRP	HZ3	7.088	0.02	1
UNMAPPED	81	GLU	C	176.81	0.2	1
UNMAPPED	51	THR	N	113.047	0.2	1
UNMAPPED	101	ASN	H	7.616	0.02	1
UNMAPPED	74	PHE	HE1	7.409	0.02	1
UNMAPPED	82	LYS	HB2	1.004	0.02	2
UNMAPPED	88	LYS	CA	56.488	0.2	1
UNMAPPED	11	MET	HB3	2.107	0.02	2
UNMAPPED	74	PHE	CE1	130.865	0.2	1
UNMAPPED	74	PHE	N	118.332	0.2	1
UNMAPPED	88	LYS	HG2	1.706	0.02	1
UNMAPPED	64	GLU	HB2	1.402	0.02	2
UNMAPPED	86	PRO	HB3	2.385	0.02	2
UNMAPPED	91	GLY	C	174.977	0.2	1
UNMAPPED	84	GLY	HA2	3.866	0.02	2
UNMAPPED	31	LYS	CB	31.784	0.2	1
UNMAPPED	55	TYR	H	8.934	0.02	1
UNMAPPED	12	SER	N	116.455	0.2	1
UNMAPPED	64	GLU	CB	31.361	0.2	1
UNMAPPED	18	LYS	HD2	1.636	0.02	1
UNMAPPED	36	TRP	HB3	3.565	0.02	2
UNMAPPED	68	LEU	HD13	1.117	0.02	2
UNMAPPED	31	LYS	N	123.537	0.2	1
UNMAPPED	90	LYS	HD3	1.74	0.02	1
UNMAPPED	36	TRP	N	126.6	0.2	1
UNMAPPED	70	PRO	HA	4.201	0.02	1
UNMAPPED	73	LEU	HG	1.578	0.02	1
UNMAPPED	49	LYS	H	8.263	0.02	1
UNMAPPED	99	ILE	HA	2.485	0.02	1
UNMAPPED	32	GLY	HA3	4.12	0.02	2
UNMAPPED	52	ALA	CA	52.636	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	20	TYR	CA	58.022	0.2	1
UNMAPPED	66	ALA	CA	50.793	0.2	1
UNMAPPED	50	SER	HA	4.445	0.02	1
UNMAPPED	44	PRO	HG3	1.845	0.02	2
UNMAPPED	69	GLY	CA	43.728	0.2	1
UNMAPPED	48	VAL	HA	4.09	0.02	1
UNMAPPED	11	MET	CB	32.524	0.2	1
UNMAPPED	38	ALA	C	174.274	0.2	1
UNMAPPED	71	LYS	HG2	1.379	0.02	1
UNMAPPED	53	ASN	HB2	2.837	0.02	1
UNMAPPED	16	ARG	HB2	1.885	0.02	2
UNMAPPED	72	ASP	HB3	3.803	0.02	2
UNMAPPED	104	THR	HB	4.47	0.02	1
UNMAPPED	70	PRO	CB	31.89	0.2	1
UNMAPPED	73	LEU	HB3	0.553	0.02	2
UNMAPPED	12	SER	HB2	3.927	0.02	1
UNMAPPED	70	PRO	CD	50.007	0.2	1
UNMAPPED	70	PRO	HD3	4.093	0.02	2
UNMAPPED	110	TYR	HE1	6.843	0.02	1
UNMAPPED	64	GLU	HB3	1.785	0.02	2
UNMAPPED	12	SER	CB	63.706	0.2	1
UNMAPPED	48	VAL	CB	32.207	0.2	1
UNMAPPED	36	TRP	CE3	119.848	0.2	1
UNMAPPED	83	PHE	HD2	6.448	0.02	1
UNMAPPED	85	LYS	C	173.399	0.2	1
UNMAPPED	101	ASN	N	112.775	0.2	1
UNMAPPED	24	ASP	HB2	2.997	0.02	2
UNMAPPED	48	VAL	N	116.981	0.2	1
UNMAPPED	42	GLU	CB	32.418	0.2	1
UNMAPPED	25	LEU	CD2	21.647	0.2	1
UNMAPPED	53	ASN	HD21	6.969	0.02	2
UNMAPPED	101	ASN	CB	40.452	0.2	1
UNMAPPED	44	PRO	CB	32.101	0.2	1
UNMAPPED	68	LEU	CG	27.417	0.2	1
UNMAPPED	75	PRO	HA	4.708	0.02	1
UNMAPPED	60	PHE	HB3	2.565	0.02	1
UNMAPPED	75	PRO	HD2	3.887	0.02	2
UNMAPPED	59	PHE	N	125.687	0.2	1
UNMAPPED	36	TRP	HD1	8.418	0.02	1
UNMAPPED	108	SER	HB2	3.872	0.02	1
UNMAPPED	39	ARG	HB2	1.56	0.02	2

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	44	PRO	HB3	2.153	0.02	2
UNMAPPED	59	PHE	CZ	127.4	0.2	1
UNMAPPED	13	ARG	HA	4.398	0.02	1
UNMAPPED	72	ASP	HB2	2.632	0.02	2
UNMAPPED	93	SER	HA	4.028	0.02	1
UNMAPPED	85	LYS	CE	42.155	0.2	1
UNMAPPED	74	PHE	HA	5.089	0.02	1
UNMAPPED	106	LYS	HE3	2.918	0.02	1
UNMAPPED	53	ASN	N	116.156	0.2	1
UNMAPPED	88	LYS	HE2	3.025	0.02	1
UNMAPPED	97	TRP	HB3	3.315	0.02	2
UNMAPPED	15	ASN	HB2	2.834	0.02	2
UNMAPPED	89	ARG	HG2	1.835	0.02	2
UNMAPPED	31	LYS	HB2	1.79	0.02	2
UNMAPPED	23	GLY	CA	44.562	0.2	1
UNMAPPED	54	LYS	HG3	1.43	0.02	2
UNMAPPED	82	LYS	HD3	1.137	0.02	1
UNMAPPED	66	ALA	HB1	1.29	0.02	1
UNMAPPED	80	LYS	HB3	1.69	0.02	2
UNMAPPED	19	GLU	HB2	1.935	0.02	1
UNMAPPED	53	ASN	CB	38.232	0.2	1
UNMAPPED	13	ARG	H	8.457	0.02	1
UNMAPPED	106	LYS	H	8.076	0.02	1
UNMAPPED	34	PRO	HG2	2.187	0.02	1
UNMAPPED	46	ALA	N	123.879	0.2	1
UNMAPPED	56	GLN	HE22	6.681	0.02	2
UNMAPPED	68	LEU	HD12	1.117	0.02	2
UNMAPPED	38	ALA	CB	23.328	0.2	1
UNMAPPED	43	MET	N	122.243	0.2	1
UNMAPPED	49	LYS	CA	57.184	0.2	1
UNMAPPED	103	PRO	CB	31.467	0.2	1
UNMAPPED	40	ILE	CB	35.299	0.2	1
UNMAPPED	97	TRP	HH2	7.342	0.02	1
UNMAPPED	14	SER	HA	4.463	0.02	1
UNMAPPED	40	ILE	HA	4.082	0.02	1
UNMAPPED	68	LEU	H	8.807	0.02	1
UNMAPPED	82	LYS	CD	29.151	0.2	1
UNMAPPED	63	HIS	CA	54.417	0.2	1
UNMAPPED	33	TYR	CD2	131.913	0.2	1
UNMAPPED	106	LYS	CA	54.847	0.2	1
UNMAPPED	110	TYR	C	180.296	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	109	GLY	CA	45.079	0.2	1
UNMAPPED	40	ILE	HD12	0.814	0.02	1
UNMAPPED	102	ASN	HB2	2.868	0.02	2
UNMAPPED	67	PHE	CB	39.817	0.2	1
UNMAPPED	81	GLU	HG3	2.172	0.02	2
UNMAPPED	67	PHE	HB2	2.696	0.02	2
UNMAPPED	85	LYS	H	7.228	0.02	1
UNMAPPED	34	PRO	CB	31.678	0.2	1
UNMAPPED	98	GLU	C	178.288	0.2	1
UNMAPPED	14	SER	H	8.37	0.02	1
UNMAPPED	98	GLU	HG2	2.69	0.02	2
UNMAPPED	34	PRO	CD	49.591	0.2	1
UNMAPPED	36	TRP	HH2	8.414	0.02	1
UNMAPPED	83	PHE	CE2	128.705	0.2	1
UNMAPPED	61	GLY	N	113.399	0.2	1
UNMAPPED	71	LYS	CB	31.256	0.2	1
UNMAPPED	90	LYS	H	8.914	0.02	1
UNMAPPED	67	PHE	H	8.518	0.02	1
UNMAPPED	105	VAL	HG11	1.099	0.02	2
UNMAPPED	98	GLU	H	8.901	0.02	1
UNMAPPED	83	PHE	CZ	127.531	0.2	1
UNMAPPED	75	PRO	CG	28.327	0.2	1
UNMAPPED	83	PHE	HZ	6.184	0.02	1
UNMAPPED	92	PHE	CD2	129.849	0.2	1
UNMAPPED	85	LYS	CB	31.995	0.2	1
UNMAPPED	13	ARG	HD3	3.248	0.02	1
UNMAPPED	64	GLU	HA	4.382	0.02	1
UNMAPPED	90	LYS	HG3	1.452	0.02	2
UNMAPPED	33	TYR	CE1	117.187	0.2	1
UNMAPPED	36	TRP	CH2	129.286	0.2	1
UNMAPPED	81	GLU	CA	58.657	0.2	1
UNMAPPED	74	PHE	H	8.717	0.02	1
UNMAPPED	106	LYS	HD2	1.598	0.02	1
UNMAPPED	19	GLU	N	121.371	0.2	1
UNMAPPED	29	LYS	HB3	1.068	0.02	2
UNMAPPED	69	GLY	HA3	4.956	0.02	2
UNMAPPED	55	TYR	N	119.243	0.2	1
UNMAPPED	65	THR	HB	3.844	0.02	1
UNMAPPED	105	VAL	CG1	21.524	0.2	2
UNMAPPED	29	LYS	N	127.217	0.2	1
UNMAPPED	75	PRO	HG2	2.293	0.02	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	44	PRO	HA	4.457	0.02	1
UNMAPPED	56	GLN	HB3	1.896	0.02	1
UNMAPPED	31	LYS	H	8.611	0.02	1
UNMAPPED	55	TYR	CB	39.817	0.2	1
UNMAPPED	93	SER	C	178.077	0.2	1
UNMAPPED	99	ILE	C	173.391	0.2	1
UNMAPPED	64	GLU	H	6.786	0.02	1
UNMAPPED	35	HIS	CA	60.588	0.2	1
UNMAPPED	55	TYR	HE1	6.926	0.02	1
UNMAPPED	37	PRO	CD	42.038	0.2	1
UNMAPPED	39	ARG	CB	35.695	0.2	1
UNMAPPED	24	ASP	C	174.873	0.2	1
UNMAPPED	90	LYS	HA	4.255	0.02	1
UNMAPPED	57	VAL	CG1	22.35	0.2	2
UNMAPPED	28	ALA	HB1	0.985	0.02	1
UNMAPPED	93	SER	H	9.063	0.02	1
UNMAPPED	37	PRO	CB	32.101	0.2	1
UNMAPPED	39	ARG	N	118.896	0.2	1
UNMAPPED	67	PHE	HZ	7.253	0.02	1
UNMAPPED	107	ALA	HB1	1.435	0.02	1
UNMAPPED	106	LYS	CG	24.423	0.2	1
UNMAPPED	14	SER	CA	58.473	0.2	1
UNMAPPED	73	LEU	CG	25.397	0.2	1
UNMAPPED	77	GLU	H	9.239	0.02	1
UNMAPPED	85	LYS	HB3	1.842	0.02	2
UNMAPPED	74	PHE	C	173.409	0.2	1
UNMAPPED	49	LYS	HA	4.253	0.02	1
UNMAPPED	85	LYS	N	120.149	0.2	1
UNMAPPED	58	PHE	N	126.952	0.2	1
UNMAPPED	73	LEU	CA	53.376	0.2	1
UNMAPPED	80	LYS	HG2	1.208	0.02	2
UNMAPPED	17	GLN	HG2	2.349	0.02	1
UNMAPPED	105	VAL	N	123.22	0.2	1
UNMAPPED	45	GLU	HB2	1.999	0.02	1
UNMAPPED	11	MET	C	176.243	0.2	1
UNMAPPED	58	PHE	CB	41.297	0.2	1
UNMAPPED	16	ARG	HG3	1.664	0.02	1
UNMAPPED	49	LYS	HD3	1.68	0.02	1
UNMAPPED	25	LEU	N	119.573	0.2	1
UNMAPPED	42	GLU	HB2	1.974	0.02	1
UNMAPPED	25	LEU	HD22	1.052	0.02	2

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	85	LYS	CG	24.811	0.2	1
UNMAPPED	76	TYR	CE2	116.584	0.2	1
UNMAPPED	85	LYS	HA	4.644	0.02	1
UNMAPPED	95	GLY	CA	46.301	0.2	1
UNMAPPED	101	ASN	HD21	6.929	0.02	2
UNMAPPED	96	LEU	CG	25.983	0.2	1
UNMAPPED	92	PHE	HB3	3.129	0.02	2
UNMAPPED	77	GLU	HB2	2.092	0.02	1
UNMAPPED	99	ILE	CA	65.189	0.2	1
UNMAPPED	54	LYS	C	174.76	0.2	1
UNMAPPED	37	PRO	HG2	1.191	0.02	1
UNMAPPED	67	PHE	HD2	7.116	0.02	1
UNMAPPED	51	THR	HB	4.258	0.02	1
UNMAPPED	17	GLN	CG	33.6	0.2	1
UNMAPPED	95	GLY	HA2	3.37	0.02	2
UNMAPPED	64	GLU	HG2	1.99	0.02	1
UNMAPPED	110	TYR	CA	59.095	0.2	1
UNMAPPED	82	LYS	HB3	0.789	0.02	2
UNMAPPED	68	LEU	HG	1.61	0.02	1
UNMAPPED	108	SER	CA	58.273	0.2	1
UNMAPPED	82	LYS	HG2	0.624	0.02	2
UNMAPPED	84	GLY	CA	45.884	0.2	1
UNMAPPED	105	VAL	HG23	1.225	0.02	2
UNMAPPED	95	GLY	N	110.299	0.2	1
UNMAPPED	65	THR	CG2	21.857	0.2	1
UNMAPPED	98	GLU	HG3	3.298	0.02	2
UNMAPPED	73	LEU	C	175.048	0.2	1
UNMAPPED	21	LYS	H	8.87	0.02	1
UNMAPPED	21	LYS	CE	42.155	0.2	1
UNMAPPED	36	TRP	HB2	3.924	0.02	2
UNMAPPED	17	GLN	C	175.44	0.2	1
UNMAPPED	58	PHE	HA	4.732	0.02	1
UNMAPPED	31	LYS	CE	41.988	0.2	1
UNMAPPED	56	GLN	NE2	111.517	0.2	1
UNMAPPED	26	VAL	CG1	17.733	0.2	1
UNMAPPED	41	ASP	N	131.281	0.2	1
UNMAPPED	66	ALA	N	125.094	0.2	1
UNMAPPED	33	TYR	HA	4.935	0.02	1
UNMAPPED	16	ARG	CB	30.516	0.2	1
UNMAPPED	49	LYS	HG2	1.472	0.02	2
UNMAPPED	77	GLU	CG	35.845	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	105	VAL	HG13	1.099	0.02	2
UNMAPPED	67	PHE	CD2	130.747	0.2	1
UNMAPPED	16	ARG	N	120.157	0.2	1
UNMAPPED	79	SER	C	174.491	0.2	1
UNMAPPED	98	GLU	HA	3.419	0.02	1
UNMAPPED	94	GLU	H	9.532	0.02	1
UNMAPPED	13	ARG	HG3	1.667	0.02	1
UNMAPPED	40	ILE	CG1	29.03	0.2	1
UNMAPPED	92	PHE	H	8.415	0.02	1
UNMAPPED	42	GLU	C	175.255	0.2	1
UNMAPPED	74	PHE	HB2	3.039	0.02	2
UNMAPPED	87	ASN	C	174.318	0.2	1
UNMAPPED	11	MET	HB2	2.04	0.02	2
UNMAPPED	104	THR	CG2	21.319	0.2	1
UNMAPPED	41	ASP	HA	5.245	0.02	1
UNMAPPED	83	PHE	C	176.612	0.2	1
UNMAPPED	80	LYS	HB2	1.527	0.02	2
UNMAPPED	90	LYS	HD2	1.74	0.02	1
UNMAPPED	48	VAL	CA	62.4	0.2	1
UNMAPPED	90	LYS	CA	58.651	0.2	1
UNMAPPED	51	THR	H	7.876	0.02	1
UNMAPPED	52	ALA	HA	4.297	0.02	1
UNMAPPED	27	PHE	HA	5.237	0.02	1
UNMAPPED	24	ASP	HB3	2.62	0.02	2
UNMAPPED	47	ALA	HB3	1.41	0.02	1
UNMAPPED	20	TYR	HE1	6.507	0.02	1
UNMAPPED	97	TRP	HE3	7.493	0.02	1
UNMAPPED	66	ALA	HB3	1.29	0.02	1
UNMAPPED	106	LYS	CE	42.038	0.2	1
UNMAPPED	59	PHE	CA	57.024	0.2	1
UNMAPPED	44	PRO	CD	50.593	0.2	1
UNMAPPED	68	LEU	N	123.233	0.2	1
UNMAPPED	54	LYS	HD3	1.55	0.02	1
UNMAPPED	60	PHE	HB2	2.565	0.02	1
UNMAPPED	96	LEU	C	179.292	0.2	1
UNMAPPED	45	GLU	C	176.273	0.2	1
UNMAPPED	102	ASN	HA	5.026	0.02	1
UNMAPPED	58	PHE	HB3	2.427	0.02	2
UNMAPPED	55	TYR	HE2	6.926	0.02	1
UNMAPPED	39	ARG	HB3	1.62	0.02	2
UNMAPPED	56	GLN	HB2	1.896	0.02	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	36	TRP	H	9.21	0.02	1
UNMAPPED	67	PHE	HE1	7.361	0.02	1
UNMAPPED	102	ASN	CB	38.671	0.2	1
UNMAPPED	97	TRP	C	179.546	0.2	1
UNMAPPED	74	PHE	HZ	7.554	0.02	1
UNMAPPED	85	LYS	CD	29.572	0.2	1
UNMAPPED	76	TYR	CE1	116.584	0.2	1
UNMAPPED	78	GLU	CB	30.093	0.2	1
UNMAPPED	100	GLU	CA	57.019	0.2	1
UNMAPPED	18	LYS	HB3	1.645	0.02	1
UNMAPPED	110	TYR	CB	39.295	0.2	1
UNMAPPED	21	LYS	HB3	1.834	0.02	2
UNMAPPED	15	ASN	HB3	2.881	0.02	2
UNMAPPED	89	ARG	HG3	1.893	0.02	2
UNMAPPED	74	PHE	CD1	131.195	0.2	1
UNMAPPED	31	LYS	HB3	1.848	0.02	2
UNMAPPED	57	VAL	CB	33.475	0.2	1
UNMAPPED	17	GLN	NE2	112.493	0.2	1
UNMAPPED	80	LYS	CA	60.356	0.2	1
UNMAPPED	66	ALA	HB2	1.29	0.02	1
UNMAPPED	86	PRO	CD	50.242	0.2	1
UNMAPPED	19	GLU	HB3	1.935	0.02	1
UNMAPPED	73	LEU	CD2	25.983	0.2	2
UNMAPPED	40	ILE	C	174.996	0.2	1
UNMAPPED	61	GLY	C	175.344	0.2	1
UNMAPPED	20	TYR	C	174.042	0.2	1
UNMAPPED	86	PRO	CB	32.428	0.2	1
UNMAPPED	30	MET	HG2	2.21	0.02	2
UNMAPPED	51	THR	HG21	1.02	0.02	1
UNMAPPED	94	GLU	HG2	2.631	0.02	1
UNMAPPED	38	ALA	CA	52.37	0.2	1
UNMAPPED	59	PHE	HD1	6.84	0.02	1
UNMAPPED	74	PHE	CD2	131.195	0.2	1
UNMAPPED	12	SER	H	8.325	0.02	1
UNMAPPED	15	ASN	HA	4.743	0.02	1
UNMAPPED	56	GLN	CG	34.231	0.2	1
UNMAPPED	106	LYS	HG2	1.412	0.02	2
UNMAPPED	40	ILE	HG13	1.146	0.02	1
UNMAPPED	82	LYS	HA	3.915	0.02	1
UNMAPPED	106	LYS	C	176.03	0.2	1
UNMAPPED	82	LYS	CE	41.61	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	61	GLY	HA2	3.071	0.02	2
UNMAPPED	95	GLY	C	174.804	0.2	1
UNMAPPED	92	PHE	HD1	6.137	0.02	1
UNMAPPED	58	PHE	CD2	131.226	0.2	1
UNMAPPED	96	LEU	CD2	21.295	0.2	1
UNMAPPED	76	TYR	CD2	132.961	0.2	1
UNMAPPED	83	PHE	H	7.23	0.02	1
UNMAPPED	102	ASN	C	174.393	0.2	1
UNMAPPED	35	HIS	C	175.832	0.2	1
UNMAPPED	40	ILE	HD13	0.814	0.02	1
UNMAPPED	39	ARG	H	8.845	0.02	1
UNMAPPED	90	LYS	CB	31.89	0.2	1
UNMAPPED	99	ILE	HG23	0.723	0.02	1
UNMAPPED	67	PHE	HB3	2.941	0.02	2
UNMAPPED	109	GLY	HA3	3.969	0.02	2
UNMAPPED	93	SER	N	114.91	0.2	1
UNMAPPED	49	LYS	CB	32.418	0.2	1
UNMAPPED	76	TYR	HD1	6.648	0.02	1
UNMAPPED	13	ARG	N	122.387	0.2	1
UNMAPPED	48	VAL	HG12	0.932	0.02	1
UNMAPPED	61	GLY	CA	46.635	0.2	1
UNMAPPED	54	LYS	CE	42.155	0.2	1
UNMAPPED	89	ARG	CD	42.155	0.2	1
UNMAPPED	100	GLU	H	5.966	0.02	1
UNMAPPED	46	ALA	HB1	1.41	0.02	1
UNMAPPED	26	VAL	HG11	0.308	0.02	2
UNMAPPED	99	ILE	H	7.594	0.02	1
UNMAPPED	18	LYS	HG2	1.23	0.02	1
UNMAPPED	40	ILE	HG21	1.265	0.02	1
UNMAPPED	50	SER	HB3	3.913	0.02	1
UNMAPPED	26	VAL	CB	36.646	0.2	1
UNMAPPED	99	ILE	CB	36.541	0.2	1
UNMAPPED	99	ILE	CD1	15.601	0.2	1
UNMAPPED	62	THR	CG2	23.292	0.2	1
UNMAPPED	110	TYR	HB2	3.102	0.02	2
UNMAPPED	69	GLY	N	108.444	0.2	1
UNMAPPED	76	TYR	CB	39.183	0.2	1
UNMAPPED	103	PRO	HA	4.306	0.02	1
UNMAPPED	109	GLY	H	8.319	0.02	1
UNMAPPED	83	PHE	CA	54.861	0.2	1
UNMAPPED	18	LYS	C	175.394	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	102	ASN	CA	51.455	0.2	1
UNMAPPED	58	PHE	CE1	129.277	0.2	1
UNMAPPED	54	LYS	HE2	2.93	0.02	1
UNMAPPED	15	ASN	C	174.966	0.2	1
UNMAPPED	86	PRO	HB2	1.869	0.02	2
UNMAPPED	29	LYS	CA	53.764	0.2	1
UNMAPPED	103	PRO	HD2	3.239	0.02	1
UNMAPPED	29	LYS	HB2	2.289	0.02	2
UNMAPPED	92	PHE	HE1	7.565	0.02	1
UNMAPPED	49	LYS	N	122.301	0.2	1
UNMAPPED	29	LYS	CG	24.576	0.2	1
UNMAPPED	75	PRO	HG3	2.293	0.02	1
UNMAPPED	52	ALA	HB1	1.36	0.02	1
UNMAPPED	36	TRP	CD1	128.342	0.2	1
UNMAPPED	91	GLY	N	113.995	0.2	1
UNMAPPED	68	LEU	HB2	1.499	0.02	2
UNMAPPED	36	TRP	NE1	129.384	0.2	1
UNMAPPED	37	PRO	CG	26.823	0.2	1
UNMAPPED	60	PHE	N	121.684	0.2	1
UNMAPPED	46	ALA	HA	4.228	0.02	1
UNMAPPED	20	TYR	HD2	6.847	0.02	1
UNMAPPED	57	VAL	C	172.548	0.2	1
UNMAPPED	97	TRP	CD1	125.848	0.2	1
UNMAPPED	72	ASP	HA	5.063	0.02	1
UNMAPPED	63	HIS	HA	3.722	0.02	1
UNMAPPED	55	TYR	CE1	117.386	0.2	1
UNMAPPED	60	PHE	CB	39.817	0.2	1
UNMAPPED	55	TYR	HA	4.467	0.02	1
UNMAPPED	70	PRO	C	178.182	0.2	1
UNMAPPED	73	LEU	N	117.738	0.2	1
UNMAPPED	16	ARG	H	8.224	0.02	1
UNMAPPED	82	LYS	N	116.097	0.2	1
UNMAPPED	85	LYS	HB2	1.736	0.02	2
UNMAPPED	26	VAL	HG23	0.479	0.02	2
UNMAPPED	18	LYS	CA	56.095	0.2	1
UNMAPPED	36	TRP	HE3	8.144	0.02	1
UNMAPPED	33	TYR	N	119.527	0.2	1
UNMAPPED	73	LEU	H	6.983	0.02	1
UNMAPPED	15	ASN	CA	53.188	0.2	1
UNMAPPED	17	GLN	HG3	2.349	0.02	1
UNMAPPED	45	GLU	CA	56.732	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	31	LYS	HA	4.09	0.02	1
UNMAPPED	94	GLU	CB	28.19	0.2	1
UNMAPPED	101	ASN	HB3	0.425	0.02	2
UNMAPPED	32	GLY	N	113.089	0.2	1
UNMAPPED	49	LYS	HD2	1.68	0.02	1
UNMAPPED	30	MET	HB3	1.916	0.02	2
UNMAPPED	42	GLU	HB3	1.974	0.02	1
UNMAPPED	25	LEU	HD23	1.052	0.02	2
UNMAPPED	90	LYS	CE	42.128	0.2	1
UNMAPPED	68	LEU	CD2	26.819	0.2	2
UNMAPPED	106	LYS	CB	33.898	0.2	1
UNMAPPED	103	PRO	CG	30.788	0.2	1
UNMAPPED	79	SER	N	110.918	0.2	1
UNMAPPED	77	GLU	HB3	2.092	0.02	1
UNMAPPED	48	VAL	HG13	0.932	0.02	1
UNMAPPED	22	CYS	HA	3.813	0.02	1
UNMAPPED	59	PHE	HB3	2.474	0.02	1
UNMAPPED	38	ALA	HB2	0.767	0.02	1
UNMAPPED	62	THR	H	7.966	0.02	1
UNMAPPED	36	TRP	HA	5.465	0.02	1
UNMAPPED	49	LYS	HE2	2.999	0.02	2
UNMAPPED	80	LYS	HD3	1.47	0.02	1
UNMAPPED	51	THR	CB	68.779	0.2	1
UNMAPPED	110	TYR	CD2	132.6	0.2	1
UNMAPPED	105	VAL	C	172.386	0.2	1
UNMAPPED	27	PHE	CA	58.556	0.2	1
UNMAPPED	53	ASN	HA	4.514	0.02	1
UNMAPPED	42	GLU	HA	4.618	0.02	1
UNMAPPED	57	VAL	HG21	0.211	0.02	2
UNMAPPED	85	LYS	HE3	3.04	0.02	1
UNMAPPED	59	PHE	HA	4.307	0.02	1
UNMAPPED	11	MET	HG3	2.626	0.02	2
UNMAPPED	21	LYS	CD	23.93	0.2	1
UNMAPPED	98	GLU	CB	30.416	0.2	1
UNMAPPED	67	PHE	CE1	130.768	0.2	1
UNMAPPED	69	GLY	C	172.507	0.2	1
UNMAPPED	84	GLY	C	173.254	0.2	1
UNMAPPED	83	PHE	HA	4.831	0.02	1
UNMAPPED	106	LYS	HE2	2.918	0.02	1
UNMAPPED	36	TRP	CB	33.052	0.2	1
UNMAPPED	99	ILE	HG13	0.019	0.02	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	77	GLU	CB	28.296	0.2	1
UNMAPPED	72	ASP	H	7.74	0.02	1
UNMAPPED	24	ASP	HA	4.624	0.02	1
UNMAPPED	78	GLU	H	8.152	0.02	1
UNMAPPED	16	ARG	CA	56.085	0.2	1
UNMAPPED	71	LYS	HD2	1.462	0.02	1
UNMAPPED	77	GLU	N	117.677	0.2	1
UNMAPPED	102	ASN	HB3	2.512	0.02	2
UNMAPPED	99	ILE	HG22	0.723	0.02	1
UNMAPPED	100	GLU	CG	36.024	0.2	1
UNMAPPED	57	VAL	H	9.095	0.02	1
UNMAPPED	67	PHE	HE2	7.361	0.02	1
UNMAPPED	59	PHE	CE1	129.7	0.2	1
UNMAPPED	92	PHE	N	123.871	0.2	1
UNMAPPED	25	LEU	H	8.571	0.02	1
UNMAPPED	50	SER	C	175.025	0.2	1
UNMAPPED	27	PHE	C	174.954	0.2	1
UNMAPPED	14	SER	C	174.272	0.2	1
UNMAPPED	66	ALA	C	174.208	0.2	1
UNMAPPED	13	ARG	HB2	1.952	0.02	2
UNMAPPED	96	LEU	N	120.727	0.2	1
UNMAPPED	28	ALA	H	9.657	0.02	1
UNMAPPED	36	TRP	HZ2	7.434	0.02	1
UNMAPPED	11	MET	CG	31.842	0.2	1
UNMAPPED	30	MET	CA	53.394	0.2	1
UNMAPPED	60	PHE	HA	4.434	0.02	1
UNMAPPED	50	SER	CA	58.891	0.2	1
UNMAPPED	67	PHE	CA	56.574	0.2	1
UNMAPPED	110	TYR	HE2	6.843	0.02	1
UNMAPPED	11	MET	CA	55.384	0.2	1
UNMAPPED	81	GLU	HA	4.001	0.02	1
UNMAPPED	75	PRO	HD3	4.277	0.02	2
UNMAPPED	44	PRO	CA	62.895	0.2	1
UNMAPPED	47	ALA	HB2	1.41	0.02	1
UNMAPPED	82	LYS	HD2	1.137	0.02	1
UNMAPPED	74	PHE	HB3	3.471	0.02	2
UNMAPPED	75	PRO	C	178.565	0.2	1
UNMAPPED	89	ARG	HD3	3.399	0.02	1
UNMAPPED	82	LYS	C	177.954	0.2	1
UNMAPPED	104	THR	H	7.666	0.02	1
UNMAPPED	54	LYS	HD2	1.55	0.02	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	32	GLY	C	173.601	0.2	1
UNMAPPED	22	CYS	N	118.338	0.2	1
UNMAPPED	73	LEU	HA	5.154	0.02	1
UNMAPPED	28	ALA	CA	49.66	0.2	1
UNMAPPED	20	TYR	CD2	131.828	0.2	1
UNMAPPED	85	LYS	CA	53.591	0.2	1
UNMAPPED	108	SER	C	174.637	0.2	1
UNMAPPED	29	LYS	C	172.547	0.2	1
UNMAPPED	22	CYS	CB	26.182	0.2	1
UNMAPPED	107	ALA	HB2	1.435	0.02	1
UNMAPPED	76	TYR	N	126.012	0.2	1
UNMAPPED	101	ASN	HD22	5.923	0.02	2
UNMAPPED	107	ALA	HB3	1.435	0.02	1
UNMAPPED	97	TRP	HD1	7.344	0.02	1
UNMAPPED	30	MET	N	125.113	0.2	1
UNMAPPED	17	GLN	HA	4.299	0.02	1
UNMAPPED	100	GLU	CB	31.044	0.2	1
UNMAPPED	18	LYS	HB2	1.645	0.02	1
UNMAPPED	110	TYR	HA	4.42	0.02	1
UNMAPPED	92	PHE	CE1	131.402	0.2	1
UNMAPPED	21	LYS	HB2	1.734	0.02	2
UNMAPPED	30	MET	CG	31.541	0.2	1
UNMAPPED	90	LYS	HG2	1.586	0.02	2
UNMAPPED	69	GLY	H	9.47	0.02	1
UNMAPPED	62	THR	HA	4.011	0.02	1
UNMAPPED	26	VAL	HA	5.35	0.02	1
UNMAPPED	57	VAL	CA	60.901	0.2	1
UNMAPPED	65	THR	CA	60.601	0.2	1
UNMAPPED	55	TYR	CD1	132.872	0.2	1
UNMAPPED	86	PRO	CG	27.69	0.2	1
UNMAPPED	59	PHE	HE1	6.859	0.02	1
UNMAPPED	54	LYS	N	117.086	0.2	1
UNMAPPED	55	TYR	C	174.862	0.2	1
UNMAPPED	59	PHE	CD1	129.7	0.2	1
UNMAPPED	33	TYR	HE2	6.632	0.02	1
UNMAPPED	30	MET	HG3	2.295	0.02	2
UNMAPPED	51	THR	HG22	1.02	0.02	1
UNMAPPED	94	GLU	HG3	2.631	0.02	1
UNMAPPED	54	LYS	CG	25.265	0.2	1
UNMAPPED	22	CYS	HB3	2.906	0.02	2
UNMAPPED	43	MET	CB	31.89	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	49	LYS	CG	24.8	0.2	1
UNMAPPED	90	LYS	C	176.913	0.2	1
UNMAPPED	86	PRO	HD3	3.92	0.02	2
UNMAPPED	56	GLN	N	122.009	0.2	1
UNMAPPED	44	PRO	HD3	3.456	0.02	2
UNMAPPED	40	ILE	HG12	1.146	0.02	1
UNMAPPED	86	PRO	HG2	2.053	0.02	2
UNMAPPED	99	ILE	CG2	16.657	0.2	1
UNMAPPED	58	PHE	CD1	131.226	0.2	1
UNMAPPED	76	TYR	CD1	132.961	0.2	1
UNMAPPED	105	VAL	CG2	19.359	0.2	2
UNMAPPED	61	GLY	HA3	5.167	0.02	2
UNMAPPED	49	LYS	C	177.016	0.2	1
UNMAPPED	97	TRP	HA	4.078	0.02	1
UNMAPPED	31	LYS	HE3	2.919	0.02	1
UNMAPPED	89	ARG	CA	55.649	0.2	1
UNMAPPED	97	TRP	CZ3	122.033	0.2	1
UNMAPPED	25	LEU	HB3	1.964	0.02	2
UNMAPPED	78	GLU	HA	4.26	0.02	1
UNMAPPED	88	LYS	H	8.442	0.02	1
UNMAPPED	60	PHE	H	8.597	0.02	1
UNMAPPED	76	TYR	HD2	6.648	0.02	1
UNMAPPED	97	TRP	HZ3	7.246	0.02	1
UNMAPPED	23	GLY	HA2	3.491	0.02	2
UNMAPPED	96	LEU	HG	1.316	0.02	1
UNMAPPED	54	LYS	CD	29.4	0.2	1
UNMAPPED	29	LYS	HG2	1.129	0.02	1
UNMAPPED	89	ARG	N	121.558	0.2	1
UNMAPPED	26	VAL	HG12	0.308	0.02	2
UNMAPPED	88	LYS	HB3	2.06	0.02	2
UNMAPPED	89	ARG	HB3	2.119	0.02	1
UNMAPPED	32	GLY	H	9.053	0.02	1
UNMAPPED	33	TYR	HD1	6.967	0.02	1
UNMAPPED	54	LYS	CB	35.589	0.2	1
UNMAPPED	35	HIS	HB2	1.984	0.02	2
UNMAPPED	57	VAL	HG11	0.66	0.02	2
UNMAPPED	18	LYS	HG3	1.23	0.02	1
UNMAPPED	26	VAL	HG13	0.308	0.02	2
UNMAPPED	30	MET	C	175.625	0.2	1
UNMAPPED	33	TYR	H	8.109	0.02	1
UNMAPPED	26	VAL	CA	59.189	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	57	VAL	HG12	0.66	0.02	2
UNMAPPED	33	TYR	HD2	6.967	0.02	1
UNMAPPED	97	TRP	CA	62.263	0.2	1
UNMAPPED	30	MET	CB	35.589	0.2	1
UNMAPPED	104	THR	HG23	1.15	0.02	1
UNMAPPED	40	ILE	HG22	1.265	0.02	1
UNMAPPED	13	ARG	CA	56.229	0.2	1
UNMAPPED	83	PHE	CB	37.703	0.2	1
UNMAPPED	45	GLU	CB	29.881	0.2	1
UNMAPPED	58	PHE	H	9.075	0.02	1
UNMAPPED	58	PHE	CE2	129.277	0.2	1
UNMAPPED	54	LYS	HE3	2.93	0.02	1
UNMAPPED	79	SER	H	7.547	0.02	1
UNMAPPED	50	SER	HB2	3.913	0.02	1
UNMAPPED	106	LYS	HB2	1.765	0.02	2
UNMAPPED	80	LYS	HG3	1.339	0.02	2
UNMAPPED	49	LYS	HB3	1.824	0.02	2
UNMAPPED	40	ILE	CA	59.768	0.2	1
UNMAPPED	47	ALA	N	120.239	0.2	1
UNMAPPED	76	TYR	HE1	6.542	0.02	1
UNMAPPED	108	SER	H	8.266	0.02	1
UNMAPPED	27	PHE	HB3	2.864	0.02	2
UNMAPPED	65	THR	HG21	1.035	0.02	1
UNMAPPED	47	ALA	CB	19.206	0.2	1
UNMAPPED	53	ASN	ND2	111.863	0.2	1
UNMAPPED	72	ASP	N	118.043	0.2	1
UNMAPPED	73	LEU	HD23	0.038	0.02	2
UNMAPPED	99	ILE	HD12	0.352	0.02	1
UNMAPPED	44	PRO	C	176.758	0.2	1
UNMAPPED	99	ILE	N	117.367	0.2	1
UNMAPPED	72	ASP	CB	43.517	0.2	1
UNMAPPED	110	TYR	HB3	2.894	0.02	2
UNMAPPED	107	ALA	N	122.019	0.2	1
UNMAPPED	106	LYS	HG3	1.254	0.02	2
UNMAPPED	15	ASN	N	120.113	0.2	1
UNMAPPED	76	TYR	HA	4.313	0.02	1
UNMAPPED	26	VAL	HG22	0.479	0.02	2
UNMAPPED	70	PRO	HB2	2.275	0.02	2
UNMAPPED	25	LEU	HD12	0.867	0.02	2
UNMAPPED	20	TYR	CE1	116.597	0.2	1
UNMAPPED	15	ASN	HD21	7.629	0.02	2

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	33	TYR	HB3	2.917	0.02	2
UNMAPPED	57	VAL	HA	4.571	0.02	1
UNMAPPED	28	ALA	C	177.169	0.2	1
UNMAPPED	105	VAL	CB	31.15	0.2	1
UNMAPPED	94	GLU	CA	60.611	0.2	1
UNMAPPED	101	ASN	HB2	1.705	0.02	2
UNMAPPED	103	PRO	HB2	2.313	0.02	2
UNMAPPED	51	THR	C	173.925	0.2	1
UNMAPPED	100	GLU	HG3	2.305	0.02	2
UNMAPPED	25	LEU	CB	41.297	0.2	1
UNMAPPED	68	LEU	C	175.72	0.2	1
UNMAPPED	59	PHE	HZ	6.742	0.02	1
UNMAPPED	110	TYR	CE1	116.817	0.2	1
UNMAPPED	78	GLU	HB3	2.112	0.02	1
UNMAPPED	81	GLU	HB2	1.901	0.02	1
UNMAPPED	96	LEU	HA	3.918	0.02	1
UNMAPPED	92	PHE	HZ	7.649	0.02	1
UNMAPPED	90	LYS	HB3	1.993	0.02	2
UNMAPPED	59	PHE	HB2	2.474	0.02	1
UNMAPPED	96	LEU	H	8.327	0.02	1
UNMAPPED	49	LYS	HE3	3.041	0.02	2
UNMAPPED	83	PHE	CD1	128.553	0.2	1
UNMAPPED	74	PHE	CE2	130.865	0.2	1
UNMAPPED	74	PHE	CA	54.693	0.2	1
UNMAPPED	110	TYR	CD1	132.6	0.2	1
UNMAPPED	94	GLU	CG	37.279	0.2	1
UNMAPPED	71	LYS	HA	4.149	0.02	1
UNMAPPED	29	LYS	HD3	-0.007	0.02	2
UNMAPPED	64	GLU	CG	36.204	0.2	1
UNMAPPED	21	LYS	CA	53.776	0.2	1
UNMAPPED	85	LYS	HD2	1.884	0.02	2
UNMAPPED	14	SER	HB3	3.903	0.02	1
UNMAPPED	107	ALA	H	8.344	0.02	1
UNMAPPED	28	ALA	HA	5.564	0.02	1
UNMAPPED	31	LYS	CA	58.383	0.2	1
UNMAPPED	11	MET	HG2	2.557	0.02	2
UNMAPPED	19	GLU	CB	30.727	0.2	1
UNMAPPED	64	GLU	CA	55.178	0.2	1
UNMAPPED	21	LYS	CG	24.225	0.2	1
UNMAPPED	81	GLU	CG	36.204	0.2	1
UNMAPPED	97	TRP	CH2	126.517	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	22	CYS	H	8.387	0.02	1
UNMAPPED	36	TRP	CA	55.784	0.2	1
UNMAPPED	41	ASP	CB	42.988	0.2	1
UNMAPPED	64	GLU	HG3	1.99	0.02	1
UNMAPPED	102	ASN	ND2	109.629	0.2	1
UNMAPPED	107	ALA	HA	4.275	0.02	1
UNMAPPED	48	VAL	HB	2.12	0.02	1
UNMAPPED	99	ILE	HB	0.789	0.02	1
UNMAPPED	62	THR	CB	67.934	0.2	1
UNMAPPED	20	TYR	CB	41.086	0.2	1
UNMAPPED	71	LYS	HD3	1.462	0.02	1
UNMAPPED	103	PRO	CD	42.976	0.2	1
UNMAPPED	63	HIS	C	173.583	0.2	1
UNMAPPED	20	TYR	HB3	2.092	0.02	2
UNMAPPED	19	GLU	CA	55.683	0.2	1
UNMAPPED	50	SER	CB	63.283	0.2	1
UNMAPPED	99	ILE	HD11	0.352	0.02	1
UNMAPPED	110	TYR	HD1	7.12	0.02	1
UNMAPPED	62	THR	N	111.54	0.2	1
UNMAPPED	50	SER	N	114.172	0.2	1
UNMAPPED	47	ALA	HA	4.248	0.02	1
UNMAPPED	70	PRO	CA	65.062	0.2	1
UNMAPPED	21	LYS	C	175.622	0.2	1
UNMAPPED	13	ARG	HB3	1.826	0.02	2
UNMAPPED	54	LYS	HA	4.535	0.02	1
UNMAPPED	31	LYS	C	177.727	0.2	1
UNMAPPED	11	MET	N	119.359	0.2	1
UNMAPPED	20	TYR	HA	4.595	0.02	1
UNMAPPED	91	GLY	HA3	3.895	0.02	2
UNMAPPED	43	MET	H	8.821	0.02	1
UNMAPPED	37	PRO	C	175.046	0.2	1
UNMAPPED	108	SER	HA	4.463	0.02	1
UNMAPPED	42	GLU	CG	35.486	0.2	1
UNMAPPED	107	ALA	C	177.55	0.2	1
UNMAPPED	26	VAL	C	175.456	0.2	1
UNMAPPED	24	ASP	CA	55.57	0.2	1
UNMAPPED	101	ASN	CA	54.32	0.2	1
UNMAPPED	47	ALA	HB1	1.41	0.02	1
UNMAPPED	29	LYS	HA	4.652	0.02	1
UNMAPPED	55	TYR	HB3	2.674	0.02	2
UNMAPPED	42	GLU	CA	56.009	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	97	TRP	HE1	10.293	0.02	1
UNMAPPED	102	ASN	HD21	8.035	0.02	2
UNMAPPED	53	ASN	HD22	7.562	0.02	2
UNMAPPED	67	PHE	C	175.752	0.2	1
UNMAPPED	89	ARG	HD2	3.399	0.02	1
UNMAPPED	28	ALA	N	123.821	0.2	1
UNMAPPED	93	SER	HB3	4.292	0.02	1
UNMAPPED	83	PHE	CE1	128.705	0.2	1
UNMAPPED	93	SER	CB	52.607	0.2	1
UNMAPPED	87	ASN	CB	40.98	0.2	1
UNMAPPED	28	ALA	CB	23.539	0.2	1
UNMAPPED	104	THR	HG22	1.15	0.02	1
UNMAPPED	62	THR	HG22	1.208	0.02	1
UNMAPPED	87	ASN	N	118.11	0.2	1
UNMAPPED	99	ILE	HG21	0.723	0.02	1
UNMAPPED	17	GLN	HE22	6.906	0.02	2
UNMAPPED	74	PHE	HD2	7.429	0.02	1
UNMAPPED	63	HIS	H	7.838	0.02	1
UNMAPPED	78	GLU	N	114.295	0.2	1
UNMAPPED	23	GLY	N	115.587	0.2	1
UNMAPPED	54	LYS	H	7.688	0.02	1
UNMAPPED	29	LYS	CD	27.741	0.2	1
UNMAPPED	49	LYS	HG3	1.425	0.02	2
UNMAPPED	56	GLN	C	174.247	0.2	1
UNMAPPED	89	ARG	C	177.388	0.2	1
UNMAPPED	80	LYS	CG	23.9	0.2	1
UNMAPPED	40	ILE	CD1	18.4	0.2	1
UNMAPPED	55	TYR	HD2	7.194	0.02	1
UNMAPPED	46	ALA	CA	52.881	0.2	1
UNMAPPED	68	LEU	CB	47.534	0.2	1
UNMAPPED	76	TYR	HE2	6.542	0.02	1
UNMAPPED	92	PHE	HD2	6.137	0.02	1
UNMAPPED	16	ARG	C	175.96	0.2	1
UNMAPPED	58	PHE	HE2	6.856	0.02	1
UNMAPPED	43	MET	CG	32.311	0.2	1
UNMAPPED	51	THR	HG23	1.02	0.02	1
UNMAPPED	37	PRO	HA	4.07	0.02	1
UNMAPPED	56	GLN	HE21	7.614	0.02	2
UNMAPPED	102	ASN	HD22	7.071	0.02	2
UNMAPPED	22	CYS	HB2	2.801	0.02	2
UNMAPPED	43	MET	CA	52.878	0.2	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	18	LYS	HA	4.189	0.02	1
UNMAPPED	86	PRO	HD2	3.619	0.02	2
UNMAPPED	94	GLU	C	178.797	0.2	1
UNMAPPED	82	LYS	CA	57.688	0.2	1
UNMAPPED	43	MET	HA	4.841	0.02	1
UNMAPPED	41	ASP	C	176.207	0.2	1
UNMAPPED	44	PRO	HD2	3.25	0.02	2
UNMAPPED	86	PRO	HG3	2.051	0.02	2
UNMAPPED	48	VAL	CG1	20.87	0.2	1
UNMAPPED	82	LYS	CG	24.1	0.2	1
UNMAPPED	106	LYS	HA	4.089	0.02	1
UNMAPPED	88	LYS	HD2	1.457	0.02	1
UNMAPPED	33	TYR	CD1	131.913	0.2	1
UNMAPPED	80	LYS	HA	3.84	0.02	1
UNMAPPED	62	THR	CA	61.97	0.2	1
UNMAPPED	47	ALA	H	8.136	0.02	1
UNMAPPED	21	LYS	HE2	3.073	0.02	1
UNMAPPED	40	ILE	HD11	0.814	0.02	1
UNMAPPED	37	PRO	HD3	2.944	0.02	1
UNMAPPED	31	LYS	HE2	2.919	0.02	1
UNMAPPED	34	PRO	CA	61.882	0.2	1
UNMAPPED	68	LEU	HB3	1.894	0.02	2
UNMAPPED	46	ALA	C	177.568	0.2	1
UNMAPPED	20	TYR	HD1	6.847	0.02	1
UNMAPPED	78	GLU	HG3	2.33	0.02	2
UNMAPPED	94	GLU	HB3	2.139	0.02	2
UNMAPPED	23	GLY	HA3	4.459	0.02	2
UNMAPPED	91	GLY	H	9.021	0.02	1
UNMAPPED	19	GLU	HA	4.358	0.02	1
UNMAPPED	71	LYS	CG	19.155	0.2	1
UNMAPPED	54	LYS	HB3	1.647	0.02	1
UNMAPPED	29	LYS	HG3	1.129	0.02	1
UNMAPPED	89	ARG	CB	29.353	0.2	1
UNMAPPED	48	VAL	C	176.226	0.2	1
UNMAPPED	89	ARG	HB2	2.119	0.02	1
UNMAPPED	58	PHE	HD1	6.366	0.02	1
UNMAPPED	80	LYS	H	7.651	0.02	1
UNMAPPED	35	HIS	HB3	2.397	0.02	2
UNMAPPED	43	MET	C	174.084	0.2	1
UNMAPPED	105	VAL	H	7.312	0.02	1
UNMAPPED	40	ILE	HG23	1.265	0.02	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	75	PRO	CB	32.524	0.2	1
UNMAPPED	96	LEU	HD11	0.913	0.02	2
UNMAPPED	49	LYS	HB2	1.871	0.02	2
UNMAPPED	36	TRP	C	174.593	0.2	1
UNMAPPED	92	PHE	CD1	129.849	0.2	1
UNMAPPED	97	TRP	CB	28.085	0.2	1
UNMAPPED	81	GLU	HB3	1.901	0.02	1
UNMAPPED	75	PRO	CD	50.476	0.2	1
UNMAPPED	78	GLU	HB2	2.112	0.02	1
UNMAPPED	81	GLU	N	119.502	0.2	1
UNMAPPED	62	THR	C	175.838	0.2	1
UNMAPPED	83	PHE	HB2	2.44	0.02	2
UNMAPPED	33	TYR	CE2	117.187	0.2	1
UNMAPPED	77	GLU	HG2	2.439	0.02	1
UNMAPPED	81	GLU	CB	28.507	0.2	1
UNMAPPED	12	SER	HA	4.476	0.02	1
UNMAPPED	68	LEU	HD23	0.896	0.02	2
UNMAPPED	50	SER	H	8.19	0.02	1
UNMAPPED	55	TYR	HD1	7.194	0.02	1
UNMAPPED	90	LYS	N	126.946	0.2	1
UNMAPPED	104	THR	CA	60.896	0.2	1
UNMAPPED	93	SER	HB2	4.292	0.02	1
UNMAPPED	55	TYR	CA	57.393	0.2	1
UNMAPPED	77	GLU	C	179.322	0.2	1
UNMAPPED	57	VAL	CG2	22.936	0.2	2
UNMAPPED	35	HIS	CB	29.987	0.2	1
UNMAPPED	52	ALA	HB3	1.36	0.02	1
UNMAPPED	103	PRO	C	177.396	0.2	1
UNMAPPED	104	THR	CB	68.251	0.2	1
UNMAPPED	28	ALA	HB2	0.985	0.02	1
UNMAPPED	71	LYS	C	176.479	0.2	1
UNMAPPED	35	HIS	N	118.609	0.2	1
UNMAPPED	73	LEU	HD11	0.557	0.02	2
UNMAPPED	37	PRO	CA	62.703	0.2	1
UNMAPPED	39	ARG	CA	53.348	0.2	1
UNMAPPED	110	TYR	N	124.142	0.2	1
UNMAPPED	73	LEU	HD22	0.038	0.02	2
UNMAPPED	86	PRO	C	175.645	0.2	1
UNMAPPED	38	ALA	HA	5.039	0.02	1
UNMAPPED	61	GLY	H	10.347	0.02	1
UNMAPPED	41	ASP	H	9.054	0.02	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	66	ALA	H	8.979	0.02	1

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	100	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	92	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	100	0.00 \pm 0.00	None needed (< 0.5 ppm)
^{15}N	93	0.00 \pm 0.00	None needed (< 0.5 ppm)

7.2.3 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 1264. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/485 (0%)	0/192 (0%)	0/202 (0%)	0/91 (0%)
Sidechain	0/666 (0%)	0/400 (0%)	0/241 (0%)	0/25 (0%)
Aromatic	0/113 (0%)	0/59 (0%)	0/51 (0%)	0/3 (0%)
Overall	0/1264 (0%)	0/651 (0%)	0/494 (0%)	0/119 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1349. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/518 (0%)	0/205 (0%)	0/216 (0%)	0/97 (0%)
Sidechain	0/718 (0%)	0/431 (0%)	0/259 (0%)	0/28 (0%)
Aromatic	0/113 (0%)	0/59 (0%)	0/51 (0%)	0/3 (0%)
Overall	0/1349 (0%)	0/695 (0%)	0/526 (0%)	0/128 (0%)

7.2.4 Statistically unusual chemical shifts [i](#)

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

Mol	Chain	Res	Type	Atom	Shift, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
???	UNMAPPED	37	PRO	CD	42.04	55.31 – 45.41	-8.4
???	UNMAPPED	93	SER	CB	52.61	71.24 – 56.34	-7.5
???	UNMAPPED	103	PRO	CD	42.98	55.31 – 45.41	-7.5
???	UNMAPPED	101	ASN	HB3	0.42	4.41 – 1.11	-7.1
???	UNMAPPED	29	LYS	HD3	-0.01	2.75 – 0.45	-7.0
???	UNMAPPED	40	ILE	CG2	26.34	24.63 – 10.43	6.2
???	UNMAPPED	83	PHE	HB3	0.66	4.85 – 1.05	-6.0
???	UNMAPPED	87	ASN	HD21	4.90	9.74 – 4.94	-5.1
???	UNMAPPED	71	LYS	CG	19.16	30.67 – 19.17	-5.0

7.2.5 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.