



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 01:04 AM BST

PDB ID : 2LCW  
Title : solution structure of FUS/TLS RRM domain  
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Deposited on : 2011-05-10

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

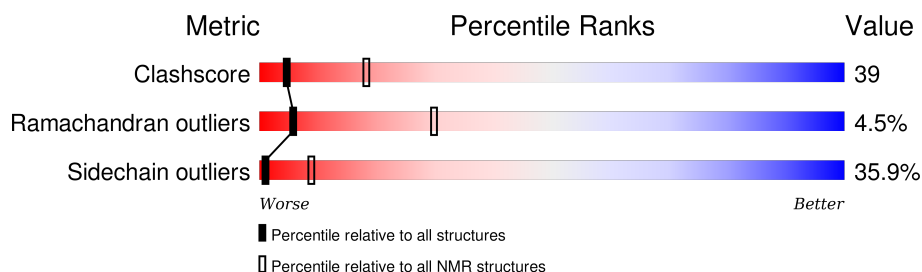
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	116	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:284-A:325, A:335-A:368 (76)	0.33	17

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. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1626 atoms, of which 799 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RNA-binding protein FUS.

Mol	Chain	Residues	Atoms						Trace
1	A	108	Total	C	H	N	O	S	0
			1626	513	799	146	167	1	

There are 8 discrepancies between the modelled and reference sequences:

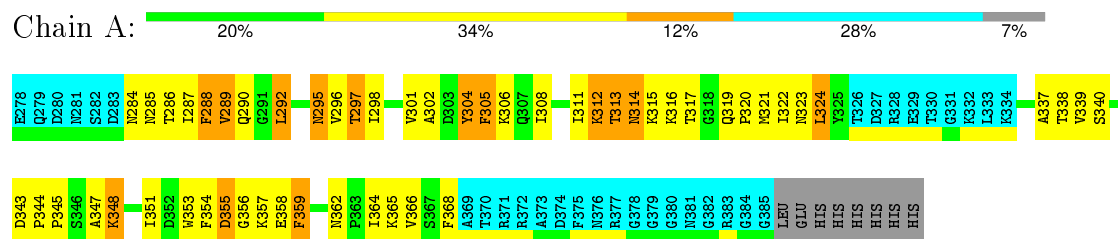
Chain	Residue	Modelled	Actual	Comment	Reference
A	386	LEU	-	EXPRESSION TAG	UNP P35637
A	387	GLU	-	EXPRESSION TAG	UNP P35637
A	388	HIS	-	EXPRESSION TAG	UNP P35637
A	389	HIS	-	EXPRESSION TAG	UNP P35637
A	390	HIS	-	EXPRESSION TAG	UNP P35637
A	391	HIS	-	EXPRESSION TAG	UNP P35637
A	392	HIS	-	EXPRESSION TAG	UNP P35637
A	393	HIS	-	EXPRESSION TAG	UNP P35637

## 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: RNA-binding protein FUS

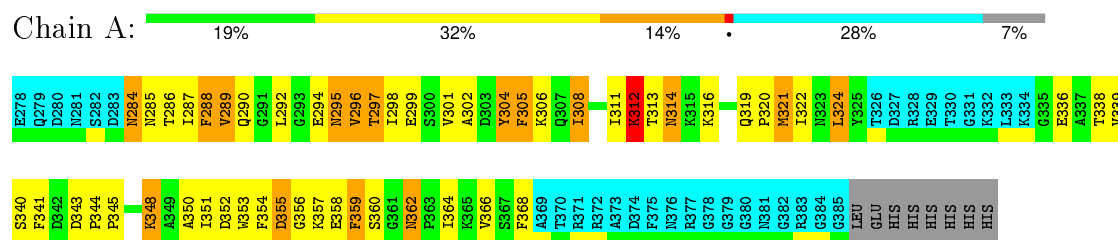


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

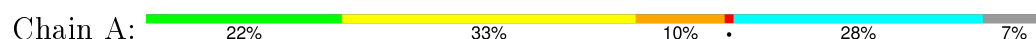
#### 4.2.1 Score per residue for model 1

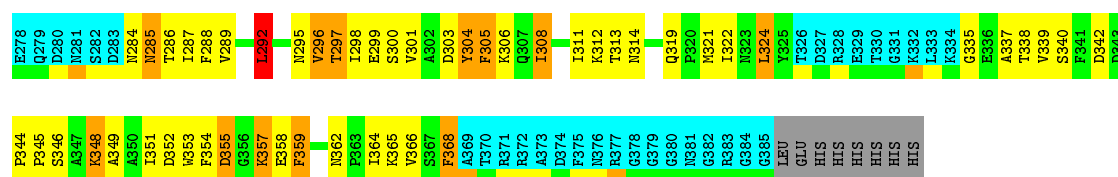
- Molecule 1: RNA-binding protein FUS



#### 4.2.2 Score per residue for model 2

- Molecule 1: RNA-binding protein FUS





### 4.2.3 Score per residue for model 3

- Molecule 1: RNA-binding protein FUS

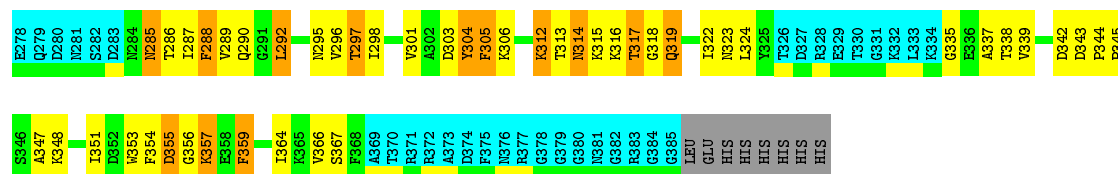
Chain A: 22% 31% 13% 28% 7%



### 4.2.4 Score per residue for model 4

- Molecule 1: RNA-binding protein FUS

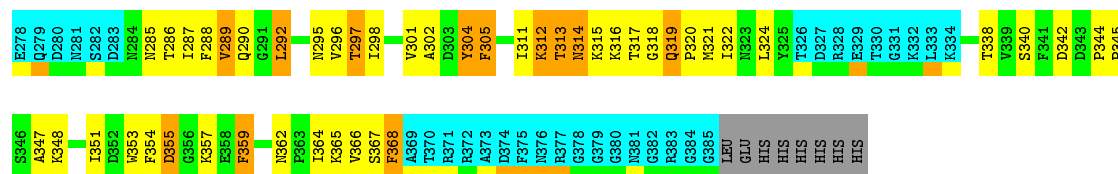
Chain A: 25% 29% 11% 28% 7%



### 4.2.5 Score per residue for model 5

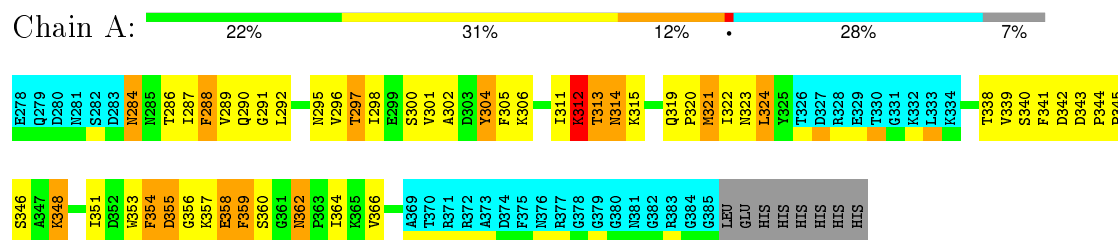
- Molecule 1: RNA-binding protein FUS

Chain A: 25% 30% 10% 28% 7%



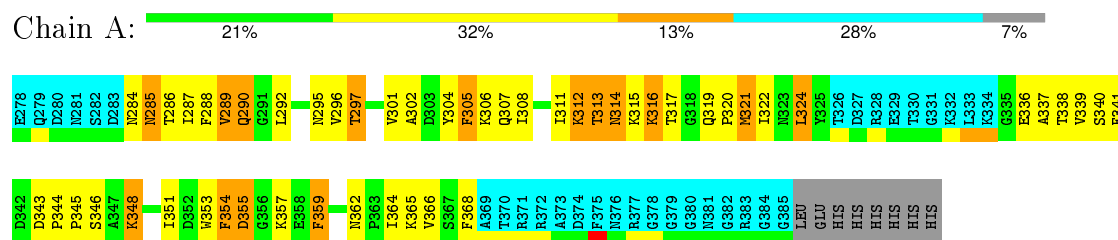
### 4.2.6 Score per residue for model 6

- Molecule 1: RNA-binding protein FUS



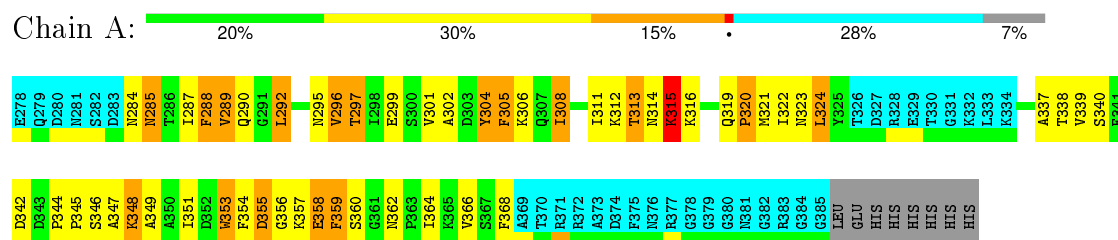
#### 4.2.7 Score per residue for model 7

- Molecule 1: RNA-binding protein FUS



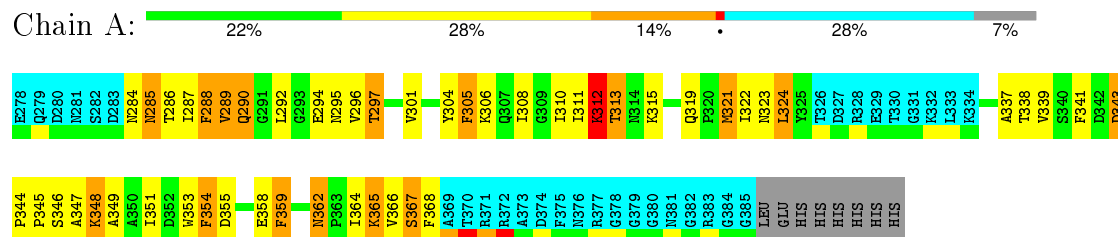
#### 4.2.8 Score per residue for model 8

- Molecule 1: RNA-binding protein FUS



#### 4.2.9 Score per residue for model 9

- Molecule 1: RNA-binding protein FUS

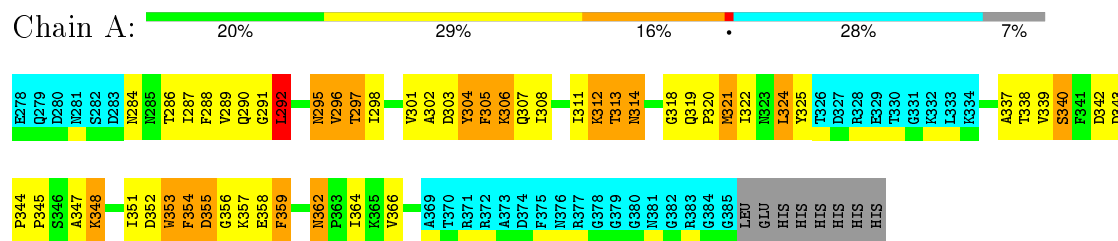






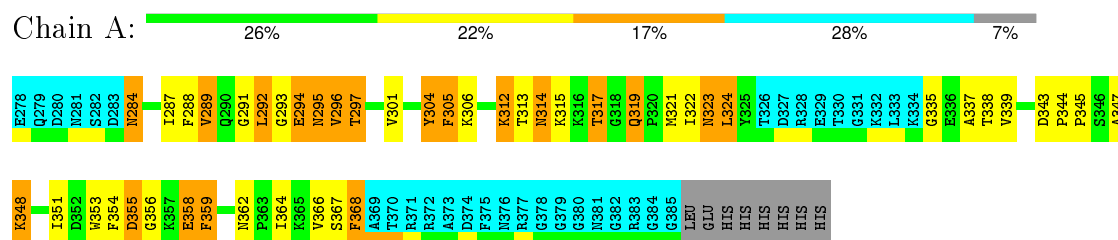
## 4.2.14 Score per residue for model 14

- Molecule 1: RNA-binding protein FUS



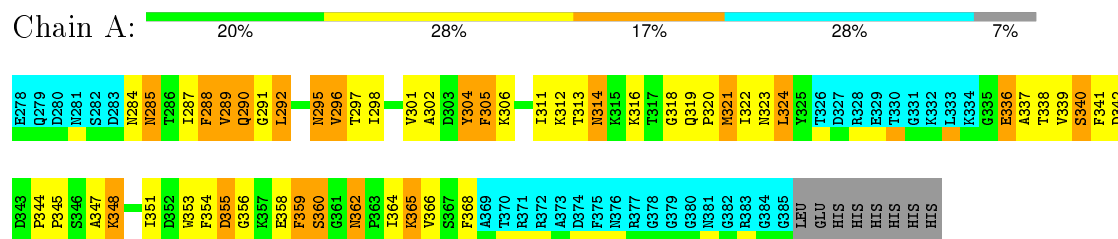
## 4.2.15 Score per residue for model 15

- Molecule 1: RNA-binding protein FUS



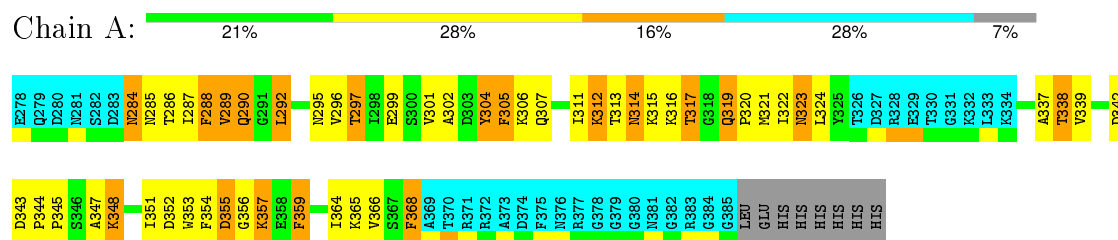
## 4.2.16 Score per residue for model 16

- Molecule 1: RNA-binding protein FUS



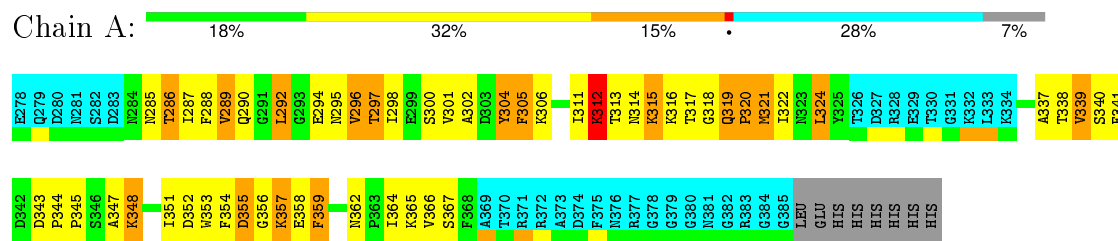
## 4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: RNA-binding protein FUS



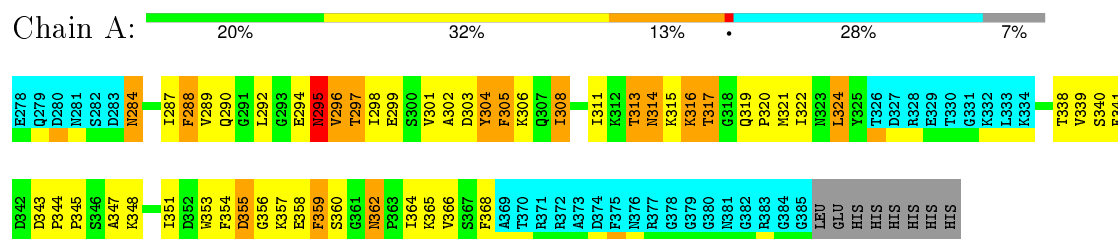
### 4.2.18 Score per residue for model 18

- Molecule 1: RNA-binding protein FUS



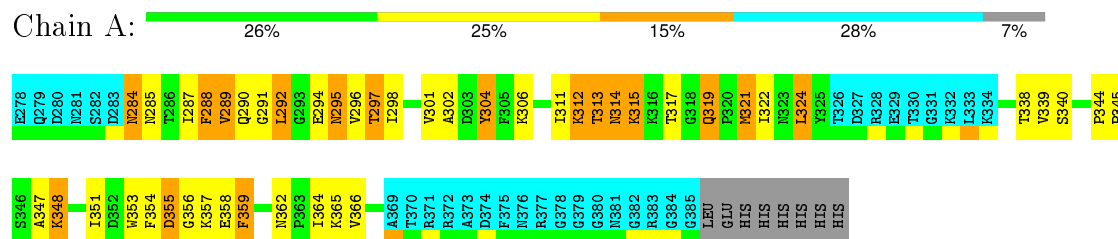
### 4.2.19 Score per residue for model 19

- Molecule 1: RNA-binding protein FUS



### 4.2.20 Score per residue for model 20

- Molecule 1: RNA-binding protein FUS



## 5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy and the least restraint violations*.

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

Software name	Classification	Version
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2lcw_cs.str
Number of chemical shift lists	1
Total number of shifts	1220
Number of shifts mapped to atoms	0
Number of unparsed shifts	43
Number of shifts with mapping errors	1177
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	587	575	575	46±7
All	All	11740	11500	11500	910

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:296:VAL:HG22	1:A:324:LEU:HD23	1.05	1.24	10	1
1:A:296:VAL:HG12	1:A:324:LEU:HD23	0.91	1.35	3	1
1:A:287:ILE:HD12	1:A:366:VAL:HG13	0.84	1.48	7	12
1:A:297:THR:O	1:A:301:VAL:HG23	0.80	1.76	9	20
1:A:311:ILE:HG23	1:A:340:SER:O	0.79	1.78	16	12
1:A:289:VAL:HG13	1:A:366:VAL:HG22	0.79	1.54	13	8
1:A:316:LYS:HD3	1:A:317:THR:HG23	0.79	1.53	7	1
1:A:348:LYS:HA	1:A:351:ILE:HD12	0.78	1.56	3	20
1:A:292:LEU:HD12	1:A:295:ASN:ND2	0.78	1.94	12	1
1:A:305:PHE:CD2	1:A:339:VAL:HG21	0.78	2.14	18	2
1:A:296:VAL:HG12	1:A:324:LEU:HD22	0.75	1.56	6	2
1:A:292:LEU:HD21	1:A:359:PHE:CE2	0.75	2.16	13	1
1:A:301:VAL:HG11	1:A:339:VAL:CG2	0.75	2.12	1	9
1:A:285:ASN:O	1:A:347:ALA:HB2	0.75	1.82	18	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:298:ILE:HD11	1:A:324:LEU:HD11	0.75	1.56	3	4
1:A:296:VAL:O	1:A:324:LEU:HD13	0.75	1.82	4	3
1:A:287:ILE:HD12	1:A:366:VAL:CG1	0.74	2.12	5	10
1:A:291:GLY:C	1:A:292:LEU:HD13	0.74	2.02	3	2
1:A:291:GLY:O	1:A:364:ILE:HG22	0.73	1.83	10	6
1:A:287:ILE:HD11	1:A:305:PHE:CE2	0.73	2.18	2	3
1:A:322:ILE:HG23	1:A:338:THR:O	0.73	1.83	4	10
1:A:314:ASN:ND2	1:A:317:THR:OG1	0.72	2.23	12	2
1:A:292:LEU:HD21	1:A:336:GLU:HA	0.72	1.59	3	1
1:A:292:LEU:HD12	1:A:296:VAL:HG22	0.72	1.60	6	3
1:A:298:ILE:CD1	1:A:324:LEU:HD11	0.72	2.15	1	4
1:A:305:PHE:O	1:A:311:ILE:HD11	0.70	1.85	17	4
1:A:324:LEU:HD23	1:A:337:ALA:CB	0.70	2.16	18	4
1:A:292:LEU:HD22	1:A:359:PHE:CD2	0.70	2.20	15	3
1:A:358:GLU:HA	1:A:362:ASN:O	0.69	1.87	10	15
1:A:296:VAL:O	1:A:296:VAL:HG12	0.69	1.85	19	2
1:A:288:PHE:CE1	1:A:338:THR:HG22	0.68	2.23	16	6
1:A:287:ILE:HD12	1:A:366:VAL:HG11	0.68	1.64	18	2
1:A:351:ILE:HD13	1:A:368:PHE:CE1	0.68	2.24	9	1
1:A:289:VAL:CG1	1:A:364:ILE:HD12	0.67	2.20	9	3
1:A:322:ILE:HG12	1:A:339:VAL:HG23	0.67	1.66	18	1
1:A:288:PHE:CD1	1:A:338:THR:HG22	0.66	2.26	10	9
1:A:316:LYS:CD	1:A:317:THR:HG23	0.66	2.19	7	1
1:A:305:PHE:HB3	1:A:311:ILE:HD11	0.66	1.67	3	3
1:A:323:ASN:O	1:A:337:ALA:HB1	0.66	1.90	11	8
1:A:351:ILE:HG23	1:A:366:VAL:O	0.66	1.90	13	1
1:A:287:ILE:CG2	1:A:347:ALA:HB1	0.65	2.21	5	6
1:A:296:VAL:CG1	1:A:324:LEU:HD22	0.65	2.22	6	3
1:A:292:LEU:N	1:A:292:LEU:CD2	0.65	2.60	14	2
1:A:322:ILE:HG12	1:A:339:VAL:HG22	0.64	1.69	9	9
1:A:354:PHE:HB3	1:A:364:ILE:HD11	0.63	1.69	15	1
1:A:314:ASN:HD21	1:A:317:THR:HG23	0.62	1.54	3	2
1:A:296:VAL:CG1	1:A:337:ALA:HB2	0.61	2.25	3	2
1:A:301:VAL:HG11	1:A:339:VAL:HG21	0.61	1.72	10	3
1:A:354:PHE:O	1:A:356:GLY:N	0.61	2.34	12	10
1:A:292:LEU:HD12	1:A:359:PHE:CD2	0.61	2.30	3	3
1:A:354:PHE:HB2	1:A:366:VAL:HG21	0.61	1.72	8	10
1:A:292:LEU:HD13	1:A:292:LEU:N	0.61	2.10	16	3
1:A:353:TRP:CD1	1:A:353:TRP:C	0.61	2.74	12	8
1:A:296:VAL:HG13	1:A:324:LEU:HD22	0.60	1.72	18	1
1:A:302:ALA:HA	1:A:311:ILE:HD13	0.60	1.73	6	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:298:ILE:HD12	1:A:298:ILE:N	0.60	2.11	19	1
1:A:298:ILE:HD13	1:A:324:LEU:HD21	0.60	1.73	13	1
1:A:288:PHE:O	1:A:288:PHE:CD1	0.60	2.55	4	3
1:A:314:ASN:OD1	1:A:317:THR:OG1	0.60	2.19	13	1
1:A:353:TRP:C	1:A:353:TRP:CD1	0.60	2.76	14	12
1:A:296:VAL:HG22	1:A:324:LEU:HD13	0.60	1.74	12	1
1:A:359:PHE:CD1	1:A:364:ILE:HG21	0.59	2.33	8	2
1:A:296:VAL:HG13	1:A:296:VAL:O	0.59	1.97	1	7
1:A:288:PHE:CZ	1:A:338:THR:HG21	0.59	2.32	3	5
1:A:313:THR:HA	1:A:320:PRO:HA	0.59	1.74	19	8
1:A:289:VAL:HG13	1:A:366:VAL:CG2	0.59	2.26	13	2
1:A:298:ILE:HG23	1:A:322:ILE:HD12	0.59	1.74	10	6
1:A:296:VAL:O	1:A:296:VAL:HG13	0.59	1.98	14	2
1:A:313:THR:HG23	1:A:319:GLN:C	0.58	2.18	15	4
1:A:324:LEU:HD23	1:A:337:ALA:HB1	0.58	1.74	17	5
1:A:298:ILE:HG23	1:A:322:ILE:HB	0.58	1.75	4	3
1:A:314:ASN:OD1	1:A:321:MET:CG	0.58	2.52	6	7
1:A:301:VAL:HG11	1:A:339:VAL:HG22	0.58	1.74	2	4
1:A:358:GLU:CA	1:A:362:ASN:O	0.57	2.51	10	12
1:A:298:ILE:HD12	1:A:324:LEU:HD21	0.57	1.75	19	1
1:A:292:LEU:CB	1:A:296:VAL:HG22	0.57	2.29	7	1
1:A:351:ILE:HD13	1:A:368:PHE:CD2	0.57	2.35	5	1
1:A:296:VAL:CG2	1:A:337:ALA:HB2	0.57	2.30	8	2
1:A:287:ILE:HD11	1:A:305:PHE:CZ	0.57	2.35	5	3
1:A:288:PHE:CD2	1:A:338:THR:HG22	0.57	2.35	5	1
1:A:292:LEU:HD12	1:A:295:ASN:HD21	0.56	1.61	12	1
1:A:292:LEU:HD22	1:A:292:LEU:N	0.56	2.15	3	2
1:A:353:TRP:CD1	1:A:354:PHE:CD1	0.56	2.93	3	5
1:A:324:LEU:HD12	1:A:324:LEU:N	0.56	2.15	16	2
1:A:359:PHE:HD2	1:A:364:ILE:HG21	0.56	1.60	6	3
1:A:354:PHE:O	1:A:355:ASP:C	0.56	2.44	1	19
1:A:292:LEU:HD22	1:A:296:VAL:CB	0.56	2.30	13	1
1:A:292:LEU:HD22	1:A:292:LEU:H	0.56	1.61	3	1
1:A:351:ILE:HD11	1:A:368:PHE:CD1	0.56	2.36	15	1
1:A:359:PHE:N	1:A:362:ASN:O	0.56	2.38	3	15
1:A:305:PHE:CZ	1:A:354:PHE:CE2	0.56	2.94	8	6
1:A:292:LEU:N	1:A:292:LEU:HD12	0.56	2.16	19	1
1:A:292:LEU:H	1:A:292:LEU:HD22	0.56	1.61	16	1
1:A:359:PHE:HB2	1:A:364:ILE:HD13	0.56	1.76	18	1
1:A:296:VAL:O	1:A:297:THR:HG23	0.56	2.01	12	3
1:A:308:ILE:HG23	1:A:341:PHE:CE2	0.55	2.36	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:296:VAL:HG22	1:A:324:LEU:HD22	0.55	1.77	14	1
1:A:292:LEU:HD22	1:A:335:GLY:O	0.55	2.00	2	2
1:A:284:ASN:OD1	1:A:368:PHE:CD1	0.55	2.59	7	1
1:A:351:ILE:CD1	1:A:368:PHE:CE1	0.55	2.89	7	4
1:A:324:LEU:HD23	1:A:324:LEU:N	0.55	2.17	2	2
1:A:302:ALA:HB1	1:A:320:PRO:HG2	0.55	1.77	1	5
1:A:292:LEU:HD22	1:A:296:VAL:HB	0.55	1.78	13	1
1:A:311:ILE:HD13	1:A:339:VAL:CG1	0.55	2.31	19	1
1:A:344:PRO:N	1:A:345:PRO:HD2	0.54	2.17	4	20
1:A:304:TYR:CE1	1:A:359:PHE:CZ	0.54	2.95	16	12
1:A:314:ASN:ND2	1:A:319:GLN:O	0.54	2.41	15	2
1:A:301:VAL:O	1:A:305:PHE:HB2	0.54	2.01	12	15
1:A:289:VAL:HG13	1:A:364:ILE:HD12	0.54	1.79	9	2
1:A:302:ALA:HA	1:A:311:ILE:HD12	0.54	1.78	14	2
1:A:288:PHE:HD1	1:A:338:THR:HG22	0.54	1.63	12	1
1:A:354:PHE:CB	1:A:366:VAL:HG21	0.54	2.33	8	5
1:A:351:ILE:O	1:A:355:ASP:CB	0.54	2.56	11	8
1:A:291:GLY:C	1:A:292:LEU:HD23	0.54	2.23	15	1
1:A:353:TRP:CE3	1:A:354:PHE:CZ	0.53	2.96	2	6
1:A:304:TYR:CZ	1:A:305:PHE:CD1	0.53	2.97	15	4
1:A:353:TRP:CZ3	1:A:354:PHE:CZ	0.53	2.96	8	5
1:A:312:LYS:O	1:A:321:MET:N	0.53	2.41	18	8
1:A:304:TYR:CZ	1:A:305:PHE:CE1	0.53	2.97	2	3
1:A:305:PHE:CZ	1:A:354:PHE:CD2	0.53	2.95	11	3
1:A:305:PHE:CE1	1:A:354:PHE:CE2	0.53	2.97	1	10
1:A:308:ILE:HG21	1:A:354:PHE:CE2	0.53	2.39	11	1
1:A:304:TYR:CE2	1:A:359:PHE:CZ	0.53	2.97	20	2
1:A:305:PHE:CE1	1:A:354:PHE:CZ	0.53	2.96	12	2
1:A:301:VAL:CG1	1:A:339:VAL:HG21	0.53	2.34	13	5
1:A:315:LYS:HD2	1:A:315:LYS:N	0.53	2.19	11	1
1:A:292:LEU:N	1:A:292:LEU:HD23	0.52	2.19	20	1
1:A:314:ASN:OD1	1:A:318:GLY:N	0.52	2.42	18	1
1:A:288:PHE:CE1	1:A:338:THR:HG21	0.52	2.40	3	3
1:A:351:ILE:O	1:A:355:ASP:HB3	0.52	2.04	9	9
1:A:353:TRP:CD1	1:A:354:PHE:CD2	0.52	2.97	9	1
1:A:304:TYR:CZ	1:A:359:PHE:CE2	0.52	2.98	17	2
1:A:289:VAL:HG12	1:A:364:ILE:HB	0.52	1.80	13	2
1:A:295:ASN:O	1:A:296:VAL:C	0.52	2.48	2	4
1:A:288:PHE:CE2	1:A:367:SER:CB	0.52	2.93	9	1
1:A:314:ASN:O	1:A:318:GLY:N	0.52	2.40	11	8
1:A:301:VAL:HB	1:A:322:ILE:HD13	0.52	1.81	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:ILE:HD11	1:A:349:ALA:O	0.52	2.05	9	3
1:A:287:ILE:HG23	1:A:347:ALA:HB1	0.52	1.81	15	3
1:A:292:LEU:CD1	1:A:296:VAL:HG13	0.52	2.35	6	1
1:A:296:VAL:CG2	1:A:324:LEU:HD23	0.51	2.16	10	1
1:A:298:ILE:HG21	1:A:319:GLN:HE22	0.51	1.65	19	1
1:A:296:VAL:HG12	1:A:296:VAL:O	0.51	2.04	18	1
1:A:304:TYR:CE1	1:A:305:PHE:CD2	0.51	2.98	6	2
1:A:295:ASN:CG	1:A:295:ASN:O	0.51	2.47	20	1
1:A:305:PHE:CE1	1:A:354:PHE:CE1	0.51	2.98	9	1
1:A:304:TYR:CE1	1:A:305:PHE:CD1	0.51	2.99	2	3
1:A:321:MET:O	1:A:340:SER:OG	0.50	2.29	18	2
1:A:298:ILE:N	1:A:298:ILE:CD1	0.50	2.74	19	1
1:A:314:ASN:HB3	1:A:317:THR:OG1	0.50	2.06	11	1
1:A:288:PHE:HD2	1:A:338:THR:HG22	0.50	1.65	5	1
1:A:311:ILE:HD13	1:A:339:VAL:HG13	0.50	1.83	19	1
1:A:292:LEU:HD23	1:A:295:ASN:HD21	0.50	1.66	19	1
1:A:304:TYR:CE1	1:A:359:PHE:CE2	0.50	2.99	2	4
1:A:289:VAL:HA	1:A:365:LYS:O	0.50	2.07	16	1
1:A:290:GLN:O	1:A:364:ILE:HA	0.50	2.06	6	5
1:A:292:LEU:HD22	1:A:359:PHE:HD2	0.49	1.66	18	1
1:A:311:ILE:HB	1:A:320:PRO:HB3	0.49	1.84	19	6
1:A:304:TYR:CE2	1:A:305:PHE:CE1	0.49	3.01	11	1
1:A:292:LEU:HD12	1:A:359:PHE:HD2	0.49	1.66	3	2
1:A:359:PHE:CD2	1:A:364:ILE:HG21	0.49	2.43	1	6
1:A:287:ILE:CD1	1:A:305:PHE:CZ	0.49	2.96	19	7
1:A:284:ASN:O	1:A:285:ASN:ND2	0.49	2.45	2	1
1:A:313:THR:HA	1:A:320:PRO:CA	0.49	2.36	19	1
1:A:301:VAL:HG22	1:A:359:PHE:HZ	0.49	1.68	14	2
1:A:284:ASN:ND2	1:A:368:PHE:CD1	0.49	2.80	17	2
1:A:314:ASN:ND2	1:A:317:THR:HG23	0.49	2.21	3	1
1:A:285:ASN:HA	1:A:347:ALA:HB2	0.48	1.84	4	2
1:A:296:VAL:HG22	1:A:324:LEU:CD2	0.48	2.38	15	1
1:A:288:PHE:CD2	1:A:290:GLN:OE1	0.48	2.66	4	3
1:A:314:ASN:OD1	1:A:316:LYS:HB2	0.48	2.08	19	1
1:A:348:LYS:C	1:A:348:LYS:CD	0.48	2.82	16	3
1:A:288:PHE:CE1	1:A:338:THR:CG2	0.48	2.96	14	9
1:A:351:ILE:O	1:A:355:ASP:HB2	0.48	2.07	2	7
1:A:287:ILE:HD13	1:A:341:PHE:HE2	0.48	1.67	6	1
1:A:319:GLN:HG2	1:A:320:PRO:N	0.48	2.22	18	2
1:A:296:VAL:HG23	1:A:337:ALA:HB2	0.48	1.86	8	1
1:A:287:ILE:HG12	1:A:339:VAL:HG12	0.48	1.86	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:317:THR:HG22	1:A:319:GLN:H	0.47	1.68	10	2
1:A:288:PHE:CE2	1:A:290:GLN:CG	0.47	2.97	13	1
1:A:317:THR:HG21	1:A:319:GLN:HG2	0.47	1.86	19	1
1:A:296:VAL:O	1:A:296:VAL:CG1	0.47	2.56	19	1
1:A:339:VAL:CG1	1:A:341:PHE:CE1	0.47	2.97	7	1
1:A:288:PHE:CZ	1:A:338:THR:CG2	0.47	2.98	15	4
1:A:343:ASP:N	1:A:343:ASP:OD1	0.47	2.48	9	1
1:A:289:VAL:CG2	1:A:339:VAL:HG23	0.47	2.40	1	2
1:A:314:ASN:OD1	1:A:319:GLN:O	0.47	2.32	17	1
1:A:298:ILE:HD13	1:A:324:LEU:HD11	0.47	1.87	18	1
1:A:289:VAL:HG22	1:A:366:VAL:HG22	0.47	1.85	11	1
1:A:285:ASN:ND2	1:A:341:PHE:CB	0.47	2.78	16	1
1:A:347:ALA:HB3	1:A:368:PHE:CE1	0.47	2.44	3	2
1:A:351:ILE:HD13	1:A:368:PHE:CD1	0.47	2.45	9	1
1:A:323:ASN:O	1:A:324:LEU:HD23	0.47	2.10	4	1
1:A:301:VAL:O	1:A:305:PHE:CB	0.47	2.63	10	3
1:A:308:ILE:HD13	1:A:350:ALA:HA	0.47	1.87	1	1
1:A:304:TYR:CZ	1:A:359:PHE:CZ	0.46	3.02	11	1
1:A:314:ASN:OD1	1:A:316:LYS:N	0.46	2.49	10	1
1:A:292:LEU:CD2	1:A:359:PHE:CE1	0.46	2.98	8	1
1:A:312:LYS:HB2	1:A:340:SER:CB	0.46	2.40	1	1
1:A:312:LYS:CE	1:A:341:PHE:O	0.46	2.64	9	1
1:A:292:LEU:CD2	1:A:359:PHE:CD2	0.46	2.98	10	2
1:A:322:ILE:HG12	1:A:339:VAL:HG13	0.46	1.86	4	1
1:A:290:GLN:CD	1:A:290:GLN:N	0.46	2.68	4	1
1:A:301:VAL:HG22	1:A:359:PHE:CZ	0.46	2.45	13	4
1:A:288:PHE:CD1	1:A:288:PHE:O	0.46	2.69	18	1
1:A:317:THR:OG1	1:A:319:GLN:HG3	0.46	2.11	20	2
1:A:295:ASN:C	1:A:295:ASN:ND2	0.46	2.68	15	1
1:A:359:PHE:HD1	1:A:364:ILE:HG21	0.46	1.68	8	2
1:A:313:THR:CA	1:A:320:PRO:HA	0.46	2.40	19	2
1:A:356:GLY:HA2	1:A:364:ILE:O	0.46	2.11	6	2
1:A:353:TRP:CZ2	1:A:354:PHE:CE1	0.45	3.04	8	1
1:A:319:GLN:NE2	1:A:320:PRO:O	0.45	2.50	19	1
1:A:298:ILE:CD1	1:A:324:LEU:HD21	0.45	2.41	19	1
1:A:305:PHE:CE1	1:A:354:PHE:CD2	0.45	3.04	11	1
1:A:311:ILE:CG2	1:A:320:PRO:CB	0.45	2.94	14	3
1:A:292:LEU:CD2	1:A:359:PHE:CD1	0.45	2.98	8	1
1:A:351:ILE:CD1	1:A:368:PHE:CE2	0.45	2.99	16	1
1:A:296:VAL:CG2	1:A:337:ALA:CB	0.45	2.95	2	1
1:A:287:ILE:HD13	1:A:341:PHE:CE2	0.45	2.47	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:354:PHE:HB3	1:A:357:LYS:HG2	0.45	1.89	17	3
1:A:324:LEU:N	1:A:324:LEU:HD12	0.45	2.27	3	1
1:A:284:ASN:ND2	1:A:368:PHE:CE1	0.45	2.84	2	1
1:A:292:LEU:CD1	1:A:359:PHE:CE2	0.45	3.00	7	1
1:A:314:ASN:O	1:A:315:LYS:CB	0.44	2.65	8	1
1:A:313:THR:HG23	1:A:319:GLN:CA	0.44	2.42	17	1
1:A:287:ILE:CD1	1:A:305:PHE:CE2	0.44	3.00	10	1
1:A:324:LEU:HB3	1:A:337:ALA:HB2	0.44	1.88	2	1
1:A:285:ASN:N	1:A:285:ASN:ND2	0.44	2.63	12	1
1:A:292:LEU:N	1:A:292:LEU:HD22	0.44	2.25	14	1
1:A:314:ASN:OD1	1:A:317:THR:N	0.44	2.44	10	1
1:A:351:ILE:HD12	1:A:368:PHE:CE1	0.44	2.47	7	1
1:A:292:LEU:HG	1:A:296:VAL:HG22	0.44	1.89	7	1
1:A:323:ASN:O	1:A:337:ALA:CB	0.44	2.66	8	3
1:A:292:LEU:HD13	1:A:295:ASN:ND2	0.44	2.28	11	1
1:A:296:VAL:CG1	1:A:324:LEU:CB	0.44	2.96	6	2
1:A:288:PHE:CG	1:A:290:GLN:OE1	0.44	2.70	4	1
1:A:296:VAL:HG13	1:A:324:LEU:CB	0.44	2.43	18	1
1:A:351:ILE:CD1	1:A:368:PHE:CD1	0.44	3.00	15	1
1:A:314:ASN:HB2	1:A:321:MET:CG	0.44	2.43	5	2
1:A:298:ILE:HD12	1:A:322:ILE:O	0.44	2.12	16	1
1:A:288:PHE:CD1	1:A:338:THR:CG2	0.44	3.00	7	1
1:A:353:TRP:CD1	1:A:357:LYS:HG3	0.44	2.47	11	1
1:A:302:ALA:O	1:A:306:LYS:HB3	0.44	2.13	14	1
1:A:294:GLU:O	1:A:294:GLU:HG3	0.43	2.13	3	1
1:A:296:VAL:CG2	1:A:337:ALA:HB3	0.43	2.43	2	1
1:A:354:PHE:CD2	1:A:357:LYS:HD3	0.43	2.48	12	1
1:A:324:LEU:HD23	1:A:337:ALA:HB2	0.43	1.86	18	1
1:A:296:VAL:O	1:A:297:THR:CG2	0.43	2.67	16	1
1:A:288:PHE:CE2	1:A:367:SER:HB2	0.43	2.49	9	1
1:A:284:ASN:OD1	1:A:368:PHE:CZ	0.43	2.71	3	1
1:A:314:ASN:OD1	1:A:321:MET:HG3	0.43	2.13	6	1
1:A:292:LEU:HD22	1:A:359:PHE:CE2	0.43	2.48	5	1
1:A:292:LEU:CD2	1:A:292:LEU:N	0.43	2.82	12	1
1:A:314:ASN:OD1	1:A:321:MET:CB	0.43	2.67	1	1
1:A:295:ASN:ND2	1:A:296:VAL:N	0.43	2.67	16	1
1:A:296:VAL:CG1	1:A:324:LEU:HD23	0.43	2.26	3	1
1:A:288:PHE:CE2	1:A:367:SER:HB3	0.43	2.48	9	1
1:A:292:LEU:N	1:A:292:LEU:CD1	0.42	2.82	19	1
1:A:304:TYR:OH	1:A:364:ILE:HD13	0.42	2.13	1	1
1:A:354:PHE:HB2	1:A:366:VAL:CG2	0.42	2.43	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:359:PHE:HB2	1:A:364:ILE:CG2	0.42	2.44	9	1
1:A:290:GLN:NE2	1:A:336:GLU:HB2	0.42	2.29	16	1
1:A:292:LEU:HD12	1:A:296:VAL:HG13	0.42	1.90	6	1
1:A:314:ASN:O	1:A:316:LYS:N	0.42	2.52	11	1
1:A:298:ILE:CD1	1:A:322:ILE:O	0.42	2.66	1	1
1:A:314:ASN:OD1	1:A:314:ASN:N	0.42	2.53	6	1
1:A:289:VAL:O	1:A:290:GLN:NE2	0.42	2.52	19	2
1:A:296:VAL:HG22	1:A:324:LEU:HB3	0.42	1.92	8	1
1:A:285:ASN:HD22	1:A:347:ALA:HB2	0.42	1.74	16	1
1:A:314:ASN:ND2	1:A:317:THR:N	0.42	2.66	20	2
1:A:286:THR:OG1	1:A:340:SER:HA	0.42	2.14	18	1
1:A:314:ASN:C	1:A:316:LYS:N	0.42	2.73	11	1
1:A:292:LEU:CD1	1:A:359:PHE:CD2	0.42	3.03	2	1
1:A:289:VAL:HG21	1:A:305:PHE:CE2	0.42	2.50	11	1
1:A:295:ASN:O	1:A:297:THR:N	0.42	2.52	16	2
1:A:284:ASN:ND2	1:A:284:ASN:N	0.42	2.68	6	2
1:A:313:THR:OG1	1:A:319:GLN:N	0.42	2.53	19	1
1:A:351:ILE:HD13	1:A:368:PHE:CZ	0.42	2.50	16	1
1:A:292:LEU:HD23	1:A:296:VAL:CG2	0.42	2.45	3	1
1:A:317:THR:HG21	1:A:319:GLN:CD	0.42	2.35	10	1
1:A:311:ILE:CG2	1:A:320:PRO:HB3	0.42	2.45	18	2
1:A:287:ILE:CD1	1:A:366:VAL:HG13	0.42	2.35	7	1
1:A:288:PHE:CE1	1:A:290:GLN:OE1	0.42	2.72	9	1
1:A:317:THR:CG2	1:A:319:GLN:CG	0.41	2.98	19	1
1:A:339:VAL:HG12	1:A:341:PHE:CE1	0.41	2.49	7	1
1:A:339:VAL:HG12	1:A:341:PHE:CZ	0.41	2.50	7	1
1:A:290:GLN:O	1:A:365:LYS:N	0.41	2.53	9	1
1:A:351:ILE:O	1:A:355:ASP:CG	0.41	2.58	19	1
1:A:348:LYS:C	1:A:348:LYS:HD3	0.41	2.36	10	1
1:A:301:VAL:HG11	1:A:339:VAL:HG23	0.41	1.92	12	1
1:A:339:VAL:CG1	1:A:341:PHE:CZ	0.41	3.03	7	2
1:A:339:VAL:HG11	1:A:341:PHE:CZ	0.41	2.50	12	1
1:A:301:VAL:CG1	1:A:339:VAL:CG2	0.41	2.98	13	2
1:A:306:LYS:O	1:A:306:LYS:CG	0.41	2.68	11	1
1:A:344:PRO:N	1:A:345:PRO:CD	0.41	2.84	7	2
1:A:343:ASP:OD1	1:A:346:SER:CB	0.41	2.68	9	1
1:A:314:ASN:ND2	1:A:321:MET:HG2	0.41	2.30	2	1
1:A:314:ASN:ND2	1:A:317:THR:H	0.41	2.13	5	1
1:A:351:ILE:HG23	1:A:355:ASP:HB2	0.41	1.91	8	1
1:A:312:LYS:O	1:A:321:MET:HB2	0.41	2.16	12	1
1:A:315:LYS:CD	1:A:315:LYS:N	0.41	2.84	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:311:ILE:O	1:A:313:THR:N	0.41	2.53	9	1
1:A:312:LYS:HB3	1:A:340:SER:CB	0.41	2.46	6	1
1:A:296:VAL:HG13	1:A:324:LEU:CD2	0.41	2.45	18	1
1:A:311:ILE:CB	1:A:320:PRO:HB3	0.41	2.45	3	2
1:A:296:VAL:CG1	1:A:296:VAL:O	0.41	2.68	2	2
1:A:353:TRP:CE2	1:A:354:PHE:CE1	0.41	3.09	8	1
1:A:348:LYS:CD	1:A:348:LYS:C	0.41	2.88	13	2
1:A:289:VAL:CG1	1:A:366:VAL:HG22	0.41	2.36	13	1
1:A:291:GLY:O	1:A:364:ILE:CG2	0.41	2.66	14	1
1:A:313:THR:HG22	1:A:318:GLY:C	0.41	2.36	3	1
1:A:314:ASN:ND2	1:A:317:THR:CB	0.41	2.84	15	1
1:A:284:ASN:O	1:A:285:ASN:CB	0.41	2.68	2	1
1:A:341:PHE:CD2	1:A:347:ALA:HA	0.41	2.51	9	1
1:A:288:PHE:C	1:A:288:PHE:CD1	0.41	2.93	9	1
1:A:312:LYS:N	1:A:340:SER:O	0.41	2.53	6	1
1:A:296:VAL:HG23	1:A:324:LEU:HB3	0.41	1.92	12	1
1:A:297:THR:O	1:A:301:VAL:CG2	0.41	2.69	18	1
1:A:290:GLN:NE2	1:A:336:GLU:CB	0.41	2.84	16	1
1:A:323:ASN:O	1:A:337:ALA:CA	0.41	2.69	9	2
1:A:295:ASN:ND2	1:A:359:PHE:CD1	0.41	2.89	1	1
1:A:296:VAL:HG12	1:A:324:LEU:HB3	0.41	1.93	7	1
1:A:292:LEU:HD12	1:A:296:VAL:CG2	0.41	2.39	6	1
1:A:292:LEU:HD22	1:A:335:GLY:C	0.40	2.35	4	1
1:A:312:LYS:CG	1:A:341:PHE:O	0.40	2.69	13	1
1:A:311:ILE:HG22	1:A:320:PRO:CB	0.40	2.46	14	1
1:A:287:ILE:HD13	1:A:305:PHE:CE2	0.40	2.51	10	1
1:A:285:ASN:OD1	1:A:344:PRO:CD	0.40	2.69	7	1
1:A:292:LEU:HB3	1:A:295:ASN:ND2	0.40	2.31	20	1
1:A:287:ILE:CD1	1:A:366:VAL:CG1	0.40	2.99	7	1
1:A:302:ALA:HB1	1:A:320:PRO:CG	0.40	2.46	19	1
1:A:288:PHE:O	1:A:288:PHE:CG	0.40	2.75	13	2
1:A:296:VAL:HG13	1:A:324:LEU:HB3	0.40	1.93	18	1
1:A:306:LYS:CD	1:A:306:LYS:O	0.40	2.69	11	1
1:A:292:LEU:HD13	1:A:364:ILE:HG22	0.40	1.93	2	1
1:A:292:LEU:CG	1:A:296:VAL:HG22	0.40	2.46	7	1
1:A:296:VAL:CG2	1:A:324:LEU:CB	0.40	3.00	9	1
1:A:323:ASN:O	1:A:337:ALA:HA	0.40	2.16	9	1
1:A:313:THR:OG1	1:A:314:ASN:N	0.40	2.55	19	1
1:A:288:PHE:CZ	1:A:325:TYR:OH	0.40	2.73	14	1
1:A:312:LYS:O	1:A:321:MET:CB	0.40	2.70	15	1
1:A:314:ASN:CG	1:A:317:THR:OG1	0.40	2.59	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:353:TRP:CD1	1:A:357:LYS:HD2	0.40	2.51	2	1
1:A:302:ALA:O	1:A:306:LYS:CG	0.40	2.69	7	1
1:A:302:ALA:CA	1:A:311:ILE:HD13	0.40	2.44	6	1
1:A:304:TYR:OH	1:A:359:PHE:CE1	0.40	2.71	19	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	76/116 (66%)	61±2 (80±2%)	12±2 (16±3%)	3±1 (5±2%)	6	30
All	All	1520/2320 (66%)	1215 (80%)	236 (16%)	69 (5%)	6	30

All 13 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	355	ASP	18
1	A	312	LYS	15
1	A	296	VAL	9
1	A	292	LEU	6
1	A	284	ASN	5
1	A	320	PRO	4
1	A	315	LYS	3
1	A	354	PHE	2
1	A	295	ASN	2
1	A	285	ASN	2
1	A	343	ASP	1
1	A	360	SER	1
1	A	293	GLY	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	64/95 (67%)	41±3 (64±5%)	23±3 (36±5%)	1	9
All	All	1280/1900 (67%)	820 (64%)	460 (36%)	1	9

All 49 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	304	TYR	20
1	A	359	PHE	20
1	A	295	ASN	19
1	A	319	GLN	19
1	A	297	THR	18
1	A	306	LYS	18
1	A	313	THR	18
1	A	305	PHE	17
1	A	289	VAL	16
1	A	348	LYS	16
1	A	314	ASN	16
1	A	324	LEU	16
1	A	357	LYS	14
1	A	315	LYS	14
1	A	288	PHE	12
1	A	343	ASP	11
1	A	312	LYS	11
1	A	292	LEU	11
1	A	290	GLN	10
1	A	316	LYS	10
1	A	365	LYS	10
1	A	284	ASN	10
1	A	321	MET	10
1	A	285	ASN	10
1	A	342	ASP	8
1	A	308	ILE	7
1	A	352	ASP	7
1	A	360	SER	7
1	A	362	ASN	7
1	A	368	PHE	7
1	A	303	ASP	6
1	A	367	SER	6
1	A	346	SER	6

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Mol	Chain	Res	Type	Models (Total)
1	A	336	GLU	6
1	A	307	GLN	5
1	A	358	GLU	5
1	A	294	GLU	5
1	A	299	GLU	5
1	A	317	THR	5
1	A	323	ASN	4
1	A	300	SER	4
1	A	354	PHE	3
1	A	340	SER	3
1	A	353	TRP	3
1	A	286	THR	1
1	A	341	PHE	1
1	A	338	THR	1
1	A	339	VAL	1
1	A	310	ILE	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 7 Chemical shift validation

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

### 7.1 Chemical shift list 1

File name: 2lcw\_cs.str

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	1220
Number of shifts mapped to atoms	0
Number of unparsed shifts	43
Number of shifts with mapping errors	1177
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- Entity instance (chain) must be specified. All 43 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
105	?	10	ILE	HG13	1.188	?	2
147	?	13	GLN	HG3	1.644	?	2
241	?	21	ILE	HG13	1.162	?	2
255	?	22	GLU	HG3	2.259	?	2
285	?	25	ALA	HB1	1.464	?	1
335	?	29	LYS	HG3	1.267	?	2
349	?	30	GLN	HG3	2.313	?	2
365	?	31	ILE	HG13	1.175	?	2
389	?	33	ILE	HG13	1.282	?	2
407	?	34	ILE	HG13	0.522	?	2
424	?	35	LYS	HE3	3.043	?	2
462	?	38	LYS	HG3	1.482	?	2
476	?	39	LYS	HG3	1.412	?	2
518	?	43	PRO	HD3	3.674	?	2
520	?	43	PRO	HG3	1.941	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
534	?	44	MET	HG3	2.287	?	2
549	?	45	ILE	HG13	1.013	?	2
633	?	52	GLU	HG3	2.262	?	2
665	?	55	LYS	HG3	1.441	?	2
696	?	57	LYS	HD3	1.597	?	2
698	?	57	LYS	HE3	2.966	?	2
700	?	57	LYS	HG3	1.446	?	2
717	?	59	GLU	HG3	2.148	?	2
724	?	60	ALA	HB1	0.972	?	1
795	?	67	PRO	HD3	3.912	?	2
797	?	67	PRO	HG3	1.843	?	2
807	?	68	PRO	HD3	3.505	?	2
809	?	68	PRO	HG3	2.018	?	2
823	?	70	ALA	HB1	1.608	?	1
839	?	71	LYS	HE3	3.101	?	2
847	?	72	ALA	HB1	1.410	?	1
856	?	73	ALA	HB1	1.658	?	1
873	?	74	ILE	HG13	0.351	?	2
943	?	80	LYS	HD3	1.545	?	2
945	?	80	LYS	HE3	2.451	?	2
947	?	80	LYS	HG3	1.261	?	2
958	?	81	GLU	HG3	1.812	?	2
1006	?	86	PRO	HD3	3.802	?	2
1008	?	86	PRO	HG3	2.025	?	2
1022	?	87	ILE	HG13	1.375	?	2
1040	?	88	LYS	HG3	1.452	?	2
1081	?	92	ALA	HB1	1.265	?	1
1125	?	96	ALA	HB1	1.283	?	1

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

- Residue not found in structure. All 1177 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	92	ALA	N	124.386	-1.0	1
A	104	ASN	CA	53.209	-1.0	1
A	102	GLY	C	176.286	-1.0	1
A	92	ALA	CA	52.098	-1.0	1
A	24	VAL	C	173.016	-1.0	1
A	15	LEU	HD12	-0.157	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	37	ASN	N	124.092	-1.0	1
A	49	THR	CG2	21.868	-1.0	1
A	7	ASN	HB2	2.502	-1.0	2
A	63	SER	HA	5.261	-1.0	1
A	40	THR	HA	4.465	-1.0	1
A	9	THR	C	177.117	-1.0	1
A	38	LYS	CE	42.118	-1.0	1
A	54	GLY	H	8.423	-1.0	1
A	72	ALA	CA	54.715	-1.0	1
A	19	VAL	HG22	0.796	-1.0	2
A	87	ILE	HD13	0.79	-1.0	1
A	93	THR	N	116.073	-1.0	1
A	62	VAL	HG13	0.3	-1.0	2
A	20	THR	CG2	21.783	-1.0	1
A	33	ILE	HG23	0.885	-1.0	1
A	55	LYS	HB2	1.666	-1.0	2
A	45	ILE	HG22	0.726	-1.0	1
A	76	TRP	C	173.272	-1.0	1
A	50	ASP	HB3	3.057	-1.0	2
A	56	LEU	H	8.768	-1.0	1
A	42	GLN	HB2	1.821	-1.0	2
A	104	ASN	HB3	2.798	-1.0	2
A	33	ILE	CG1	28.001	-1.0	1
A	42	GLN	HG2	2.38	-1.0	2
A	30	GLN	HG2	2.427	-1.0	2
A	24	VAL	HG12	0.853	-1.0	2
A	17	GLU	CG	36.21	-1.0	1
A	81	GLU	CB	32.042	-1.0	1
A	24	VAL	HB	2.202	-1.0	1
A	24	VAL	CA	67.254	-1.0	1
A	91	PHE	CA	61.155	-1.0	1
A	51	ARG	CA	58.562	-1.0	1
A	100	ARG	CA	56.492	-1.0	1
A	53	THR	C	173.851	-1.0	1
A	19	VAL	CA	61.877	-1.0	1
A	19	VAL	HB	1.997	-1.0	1
A	44	MET	C	176.474	-1.0	1
A	39	LYS	CA	58.319	-1.0	1
A	15	LEU	N	117.824	-1.0	1
A	18	ASN	HD22	6.988	-1.0	2
A	2	GLN	HG2	2.311	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	23	SER	H	8.236	-1.0	1
A	48	TYR	CB	39.199	-1.0	1
A	31	ILE	HG23	0.862	-1.0	1
A	91	PHE	HB2	2.834	-1.0	2
A	72	ALA	HB2	1.41	-1.0	1
A	96	ALA	HB3	1.283	-1.0	1
A	6	ASP	N	119.436	-1.0	1
A	76	TRP	CA	59.462	-1.0	1
A	77	PHE	N	112.019	-1.0	1
A	48	TYR	N	121.842	-1.0	1
A	42	GLN	N	118.894	-1.0	1
A	83	SER	HB3	3.996	-1.0	2
A	106	ARG	N	120.341	-1.0	1
A	96	ALA	HB2	1.283	-1.0	1
A	104	ASN	N	118.527	-1.0	1
A	6	ASP	HA	4.695	-1.0	1
A	97	ASP	N	118.483	-1.0	1
A	1	GLU	HB2	1.935	-1.0	2
A	13	GLN	CD	181.893	-1.0	1
A	83	SER	HB2	3.439	-1.0	2
A	104	ASN	CB	38.879	-1.0	1
A	46	ASN	CB	40.47	-1.0	1
A	79	GLY	H	8.615	-1.0	1
A	15	LEU	HD11	-0.157	-1.0	2
A	28	PHE	C	173.082	-1.0	1
A	14	GLY	C	175.436	-1.0	1
A	27	TYR	C	172.908	-1.0	1
A	86	PRO	CG	27.698	-1.0	1
A	10	ILE	HG23	0.822	-1.0	1
A	61	THR	CG2	22.522	-1.0	1
A	46	ASN	N	124.735	-1.0	1
A	83	SER	CB	62.519	-1.0	1
A	35	LYS	CB	33.664	-1.0	1
A	103	GLY	HA3	3.952	-1.0	2
A	16	GLY	N	105.063	-1.0	1
A	101	GLY	CA	45.38	-1.0	1
A	94	ARG	HG2	1.631	-1.0	2
A	99	ASN	C	175.348	-1.0	1
A	97	ASP	HA	4.498	-1.0	1
A	9	THR	HG22	1.157	-1.0	1
A	93	THR	CG2	21.582	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	55	LYS	HD2	1.694	-1.0	2
A	38	LYS	N	127.969	-1.0	1
A	44	MET	HB2	1.672	-1.0	2
A	68	PRO	HB2	1.862	-1.0	2
A	67	PRO	HA	4.45	-1.0	1
A	4	ASN	HA	4.637	-1.0	1
A	40	THR	HB	4.412	-1.0	1
A	57	LYS	HE2	3.015	-1.0	2
A	12	VAL	CG1	22.228	-1.0	2
A	62	VAL	H	8.071	-1.0	1
A	44	MET	H	8.874	-1.0	1
A	30	GLN	C	173.79	-1.0	1
A	74	ILE	HD12	-0.202	-1.0	1
A	64	PHE	C	174.605	-1.0	1
A	33	ILE	HD13	0.916	-1.0	1
A	51	ARG	HB3	1.894	-1.0	2
A	1	GLU	CG	36.159	-1.0	1
A	56	LEU	CG	27.515	-1.0	1
A	76	TRP	CH2	124.42	-1.0	1
A	2	GLN	CB	29.639	-1.0	1
A	19	VAL	HA	4.152	-1.0	1
A	59	GLU	HA	5.521	-1.0	1
A	15	LEU	HB2	1.174	-1.0	2
A	19	VAL	HG11	0.821	-1.0	2
A	2	GLN	N	121.692	-1.0	1
A	93	THR	CB	69.708	-1.0	1
A	45	ILE	HA	4.802	-1.0	1
A	4	ASN	H	8.528	-1.0	1
A	29	LYS	CA	58.28	-1.0	1
A	102	GLY	CA	45.338	-1.0	1
A	98	PHE	HD2	7.178	-1.0	3
A	42	GLN	CB	29.23	-1.0	1
A	81	GLU	CG	36.346	-1.0	1
A	56	LEU	CD2	23.962	-1.0	2
A	19	VAL	CG1	22.736	-1.0	2
A	65	ASP	HA	4.435	-1.0	1
A	53	THR	HA	4.436	-1.0	1
A	17	GLU	HB3	2.045	-1.0	2
A	87	ILE	HG12	1.531	-1.0	2
A	24	VAL	HG21	0.833	-1.0	2
A	49	THR	N	116.554	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	87	ILE	C	174.495	-1.0	1
A	18	ASN	N	116.66	-1.0	1
A	30	GLN	HA	4.135	-1.0	1
A	105	GLY	HA3	3.951	-1.0	2
A	67	PRO	HG2	2.377	-1.0	2
A	21	ILE	HG22	0.933	-1.0	1
A	20	THR	CB	72.948	-1.0	1
A	30	GLN	CA	57.546	-1.0	1
A	2	GLN	HE22	6.888	-1.0	2
A	101	GLY	HA3	3.959	-1.0	2
A	58	GLY	H	8.334	-1.0	1
A	99	ASN	HB2	2.635	-1.0	2
A	75	ASP	N	117.867	-1.0	1
A	43	PRO	HA	4.595	-1.0	1
A	12	VAL	H	8.94	-1.0	1
A	94	ARG	CG	27.128	-1.0	1
A	33	ILE	CA	61.641	-1.0	1
A	80	LYS	HD2	1.43	-1.0	2
A	88	LYS	HE2	2.982	-1.0	2
A	105	GLY	H	8.477	-1.0	1
A	64	PHE	CD2	131.385	-1.0	3
A	90	SER	HB3	4.097	-1.0	2
A	100	ARG	CB	30.519	-1.0	1
A	91	PHE	CE1	129.653	-1.0	3
A	89	VAL	C	177.16	-1.0	1
A	71	LYS	N	116.308	-1.0	1
A	60	ALA	HB2	0.972	-1.0	1
A	106	ARG	CB	30.629	-1.0	1
A	34	ILE	HB	1.673	-1.0	1
A	36	THR	CB	70.809	-1.0	1
A	70	ALA	HB2	1.608	-1.0	1
A	60	ALA	HB3	0.972	-1.0	1
A	21	ILE	HG12	1.664	-1.0	2
A	33	ILE	CG2	17.709	-1.0	1
A	36	THR	N	118.312	-1.0	1
A	85	ASN	ND2	114.688	-1.0	1
A	4	ASN	CA	53.861	-1.0	1
A	35	LYS	HG2	1.399	-1.0	2
A	88	LYS	H	8.353	-1.0	1
A	54	GLY	N	111.295	-1.0	1
A	78	ASP	CB	41.886	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	31	ILE	CB	40.334	-1.0	1
A	99	ASN	HA	4.609	-1.0	1
A	62	VAL	HG22	0.008	-1.0	2
A	26	ASP	HB2	2.63	-1.0	2
A	12	VAL	HB	1.641	-1.0	1
A	95	ARG	HB2	1.683	-1.0	2
A	53	THR	H	8.087	-1.0	1
A	107	GLY	H	8.522	-1.0	1
A	12	VAL	HG12	0.863	-1.0	2
A	9	THR	HA	5.557	-1.0	1
A	98	PHE	C	174.878	-1.0	1
A	64	PHE	CA	58.204	-1.0	1
A	40	THR	HG21	1.14	-1.0	1
A	46	ASN	ND2	111.542	-1.0	1
A	108	GLY	HA3	3.963	-1.0	2
A	89	VAL	CA	61.361	-1.0	1
A	89	VAL	HG21	0.984	-1.0	2
A	3	ASP	CA	54.062	-1.0	1
A	57	LYS	HG2	1.43	-1.0	2
A	21	ILE	CG2	17.289	-1.0	1
A	27	TYR	CE2	119.161	-1.0	3
A	68	PRO	CB	30.997	-1.0	1
A	37	ASN	C	174.235	-1.0	1
A	56	LEU	HD11	1.001	-1.0	2
A	28	PHE	CE2	130.528	-1.0	3
A	34	ILE	CG1	28.699	-1.0	1
A	47	LEU	HD23	0.619	-1.0	2
A	89	VAL	HG11	1.104	-1.0	2
A	65	ASP	H	8.512	-1.0	1
A	94	ARG	H	8.493	-1.0	1
A	59	GLU	HB2	1.852	-1.0	2
A	17	GLU	HG2	2.287	-1.0	2
A	48	TYR	H	7.666	-1.0	1
A	88	LYS	HD2	1.694	-1.0	2
A	89	VAL	N	125.661	-1.0	1
A	75	ASP	H	7.937	-1.0	1
A	86	PRO	HB3	2.17	-1.0	2
A	76	TRP	NE1	128.097	-1.0	1
A	34	ILE	HG12	1.644	-1.0	2
A	15	LEU	HD13	-0.157	-1.0	2
A	89	VAL	HG13	1.104	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	76	TRP	HA	4.356	-1.0	1
A	56	LEU	HD12	1.001	-1.0	2
A	7	ASN	HB3	2.995	-1.0	2
A	52	GLU	C	172.201	-1.0	1
A	20	THR	HG21	1.268	-1.0	1
A	62	VAL	C	175.994	-1.0	1
A	38	LYS	CD	28.686	-1.0	1
A	69	SER	HB2	3.05	-1.0	2
A	25	ALA	N	123.198	-1.0	1
A	51	ARG	N	127.794	-1.0	1
A	100	ARG	HD2	3.163	-1.0	2
A	19	VAL	HG21	0.796	-1.0	2
A	99	ASN	CG	173.452	-1.0	1
A	53	THR	HG22	1.227	-1.0	1
A	70	ALA	C	172.686	-1.0	1
A	25	ALA	CB	17.738	-1.0	1
A	58	GLY	C	177.876	-1.0	1
A	55	LYS	HB3	1.85	-1.0	2
A	1	GLU	HA	4.352	-1.0	1
A	50	ASP	HB2	2.458	-1.0	2
A	21	ILE	HA	3.518	-1.0	1
A	35	LYS	H	8.68	-1.0	1
A	10	ILE	CD1	13.885	-1.0	1
A	24	VAL	HG13	0.853	-1.0	2
A	26	ASP	H	8.312	-1.0	1
A	51	ARG	CG	27.052	-1.0	1
A	59	GLU	CG	36.449	-1.0	1
A	51	ARG	CD	43.278	-1.0	1
A	73	ALA	HA	4.279	-1.0	1
A	32	GLY	H	7.344	-1.0	1
A	38	LYS	HA	4.004	-1.0	1
A	51	ARG	CB	30.167	-1.0	1
A	40	THR	CA	61.26	-1.0	1
A	16	GLY	HA2	3.791	-1.0	2
A	56	LEU	HG	1.803	-1.0	1
A	36	THR	C	176.394	-1.0	1
A	93	THR	HA	4.208	-1.0	1
A	90	SER	HA	4.71	-1.0	1
A	78	ASP	C	172.542	-1.0	1
A	87	ILE	CA	59.491	-1.0	1
A	59	GLU	CA	53.025	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	25	ALA	HB3	1.464	-1.0	1
A	13	GLN	C	175.631	-1.0	1
A	62	VAL	CB	34.685	-1.0	1
A	34	ILE	HG21	0.808	-1.0	1
A	7	ASN	HD22	7.1	-1.0	2
A	48	TYR	CA	57.894	-1.0	1
A	86	PRO	HA	4.667	-1.0	1
A	87	ILE	HD11	0.79	-1.0	1
A	77	PHE	C	173.747	-1.0	1
A	19	VAL	H	6.855	-1.0	1
A	2	GLN	NE2	112.707	-1.0	1
A	41	GLY	C	176.727	-1.0	1
A	43	PRO	HB3	2.222	-1.0	2
A	100	ARG	CG	27.253	-1.0	1
A	44	MET	CA	55.419	-1.0	1
A	103	GLY	CA	45.346	-1.0	1
A	39	LYS	HA	4.258	-1.0	1
A	15	LEU	C	174.111	-1.0	1
A	4	ASN	HB3	2.202	-1.0	2
A	34	ILE	HD13	0.747	-1.0	1
A	80	LYS	HA	4.462	-1.0	1
A	56	LEU	HB2	1.529	-1.0	2
A	85	ASN	CG	173.345	-1.0	1
A	40	THR	C	174.021	-1.0	1
A	87	ILE	CB	41.671	-1.0	1
A	10	ILE	HG22	0.822	-1.0	1
A	74	ILE	C	172.435	-1.0	1
A	61	THR	HG21	1.461	-1.0	1
A	89	VAL	HB	1.95	-1.0	1
A	89	VAL	HG12	1.104	-1.0	2
A	63	SER	C	177.943	-1.0	1
A	73	ALA	CA	55.379	-1.0	1
A	20	THR	H	7.328	-1.0	1
A	9	THR	HG23	1.157	-1.0	1
A	102	GLY	N	108.692	-1.0	1
A	56	LEU	HB3	1.89	-1.0	2
A	28	PHE	HE2	6.88	-1.0	3
A	2	GLN	C	175.248	-1.0	1
A	92	ALA	HB3	1.265	-1.0	1
A	44	MET	HB3	2.026	-1.0	2
A	27	TYR	HE2	6.21	-1.0	3

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	5	SER	HA	4.163	-1.0	1
A	25	ALA	HA	3.899	-1.0	1
A	39	LYS	N	117.413	-1.0	1
A	97	ASP	C	174.302	-1.0	1
A	1	GLU	CB	30.392	-1.0	1
A	83	SER	N	125.136	-1.0	1
A	88	LYS	HA	5.192	-1.0	1
A	23	SER	N	115.921	-1.0	1
A	74	ILE	HD11	-0.202	-1.0	1
A	27	TYR	HB2	2.805	-1.0	2
A	51	ARG	C	173.101	-1.0	1
A	18	ASN	HD21	7.639	-1.0	2
A	36	THR	H	8.456	-1.0	1
A	63	SER	HB3	3.669	-1.0	2
A	63	SER	H	7.695	-1.0	1
A	2	GLN	HB2	1.97	-1.0	2
A	88	LYS	HB2	1.539	-1.0	2
A	15	LEU	HB3	1.157	-1.0	2
A	67	PRO	HB3	2.218	-1.0	2
A	21	ILE	HD13	0.948	-1.0	1
A	13	GLN	H	8.747	-1.0	1
A	71	LYS	CB	32.442	-1.0	1
A	73	ALA	HB2	1.658	-1.0	1
A	24	VAL	CG2	22.833	-1.0	2
A	31	ILE	H	7.809	-1.0	1
A	74	ILE	HG23	0.859	-1.0	1
A	49	THR	CA	60.693	-1.0	1
A	55	LYS	CE	42.156	-1.0	1
A	30	GLN	HE22	6.793	-1.0	2
A	91	PHE	H	8.919	-1.0	1
A	34	ILE	C	174.663	-1.0	1
A	31	ILE	HD12	0.345	-1.0	1
A	54	GLY	C	176.747	-1.0	1
A	21	ILE	HG21	0.933	-1.0	1
A	23	SER	HB3	4.075	-1.0	2
A	33	ILE	N	117.784	-1.0	1
A	95	ARG	HD2	3.089	-1.0	2
A	14	GLY	CA	45.43	-1.0	1
A	107	GLY	CA	45.441	-1.0	1
A	86	PRO	HG2	2.176	-1.0	2
A	35	LYS	HB2	1.211	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	65	ASP	N	119.943	-1.0	1
A	5	SER	C	176.37	-1.0	1
A	33	ILE	CB	38.659	-1.0	1
A	76	TRP	HE1	9.783	-1.0	1
A	11	PHE	HD1	7.114	-1.0	3
A	31	ILE	HG12	1.368	-1.0	2
A	31	ILE	CG1	29.685	-1.0	1
A	7	ASN	CA	53.158	-1.0	1
A	76	TRP	HB2	2.544	-1.0	2
A	4	ASN	HD21	7.594	-1.0	2
A	31	ILE	CG2	19.32	-1.0	1
A	74	ILE	HG21	0.859	-1.0	1
A	91	PHE	HD1	7.324	-1.0	3
A	61	THR	CB	71.224	-1.0	1
A	78	ASP	HB3	3.206	-1.0	2
A	36	THR	CA	61.34	-1.0	1
A	75	ASP	C	172.054	-1.0	1
A	48	TYR	HB3	3.169	-1.0	2
A	54	GLY	CA	45.703	-1.0	1
A	57	LYS	N	118.264	-1.0	1
A	44	MET	HG2	2.384	-1.0	2
A	76	TRP	N	117.313	-1.0	1
A	82	PHE	HD1	6.219	-1.0	3
A	25	ALA	H	8.695	-1.0	1
A	45	ILE	H	7.73	-1.0	1
A	91	PHE	HE1	7.177	-1.0	3
A	86	PRO	HD2	3.934	-1.0	2
A	56	LEU	C	172.534	-1.0	1
A	5	SER	CA	60.846	-1.0	1
A	35	LYS	HA	4.084	-1.0	1
A	41	GLY	CA	45.73	-1.0	1
A	26	ASP	HB3	2.759	-1.0	2
A	8	ASN	HB3	3.541	-1.0	2
A	79	GLY	N	115.548	-1.0	1
A	64	PHE	HA	4.854	-1.0	1
A	88	LYS	CG	24.412	-1.0	1
A	26	ASP	CB	41.052	-1.0	1
A	36	THR	HG22	0.88	-1.0	1
A	3	ASP	N	121.801	-1.0	1
A	93	THR	C	176.032	-1.0	1
A	11	PHE	CA	55.362	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	77	PHE	CD1	132.09	-1.0	3
A	89	VAL	HG22	0.984	-1.0	2
A	56	LEU	HD21	0.837	-1.0	2
A	42	GLN	HE21	7.593	-1.0	2
A	13	GLN	HA	4.779	-1.0	1
A	21	ILE	CG1	28.974	-1.0	1
A	73	ALA	HB3	1.658	-1.0	1
A	13	GLN	N	122.289	-1.0	1
A	87	ILE	HG21	0.731	-1.0	1
A	10	ILE	HD11	0.249	-1.0	1
A	32	GLY	N	107.416	-1.0	1
A	83	SER	C	175.543	-1.0	1
A	22	GLU	CA	60.613	-1.0	1
A	60	ALA	H	8.93	-1.0	1
A	46	ASN	H	8.384	-1.0	1
A	73	ALA	C	171.039	-1.0	1
A	87	ILE	N	117.27	-1.0	1
A	19	VAL	N	118.323	-1.0	1
A	27	TYR	CB	39.932	-1.0	1
A	11	PHE	HA	5.42	-1.0	1
A	94	ARG	HB3	1.807	-1.0	2
A	10	ILE	H	8.77	-1.0	1
A	86	PRO	HB2	1.873	-1.0	2
A	71	LYS	H	7.159	-1.0	1
A	19	VAL	CB	32.513	-1.0	1
A	27	TYR	N	119.224	-1.0	1
A	37	ASN	CB	38.927	-1.0	1
A	80	LYS	C	175.853	-1.0	1
A	99	ASN	CB	38.727	-1.0	1
A	76	TRP	CZ2	114.228	-1.0	1
A	20	THR	HG22	1.268	-1.0	1
A	12	VAL	CG2	21.742	-1.0	2
A	93	THR	CA	62.255	-1.0	1
A	82	PHE	CE1	131.178	-1.0	3
A	99	ASN	N	120.016	-1.0	1
A	53	THR	HG23	1.227	-1.0	1
A	11	PHE	C	177.066	-1.0	1
A	34	ILE	CD1	13.831	-1.0	1
A	33	ILE	HG21	0.885	-1.0	1
A	100	ARG	HG2	1.697	-1.0	2
A	29	LYS	HB3	2.164	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	78	ASP	N	118.408	-1.0	1
A	38	LYS	HD2	1.686	-1.0	2
A	66	ASP	H	8.323	-1.0	1
A	88	LYS	CB	35.049	-1.0	1
A	21	ILE	HB	1.864	-1.0	1
A	87	ILE	HB	1.805	-1.0	1
A	105	GLY	N	109.166	-1.0	1
A	8	ASN	HD22	7.299	-1.0	2
A	56	LEU	HD13	1.001	-1.0	2
A	17	GLU	CA	57.281	-1.0	1
A	57	LYS	HD2	1.678	-1.0	2
A	106	ARG	CD	43.281	-1.0	1
A	4	ASN	C	174.415	-1.0	1
A	82	PHE	N	127.08	-1.0	1
A	40	THR	N	105.547	-1.0	1
A	82	PHE	CB	41.994	-1.0	1
A	40	THR	CB	70.997	-1.0	1
A	16	GLY	HA3	4.095	-1.0	2
A	85	ASN	H	7.762	-1.0	1
A	100	ARG	HB2	1.751	-1.0	2
A	39	LYS	CG	25.167	-1.0	1
A	15	LEU	CB	42.433	-1.0	1
A	25	ALA	HB2	1.464	-1.0	1
A	42	GLN	C	177.178	-1.0	1
A	62	VAL	CA	61.426	-1.0	1
A	30	GLN	NE2	111.886	-1.0	1
A	56	LEU	CB	41.654	-1.0	1
A	63	SER	N	121.689	-1.0	1
A	3	ASP	C	174.336	-1.0	1
A	6	ASP	CB	40.935	-1.0	1
A	100	ARG	C	173.627	-1.0	1
A	27	TYR	HA	4.2	-1.0	1
A	79	GLY	CA	46.072	-1.0	1
A	44	MET	N	124.162	-1.0	1
A	63	SER	CB	64.427	-1.0	1
A	85	ASN	HD21	7.368	-1.0	2
A	1	GLU	HG2	2.298	-1.0	2
A	35	LYS	N	130.372	-1.0	1
A	81	GLU	H	8.201	-1.0	1
A	52	GLU	HG2	2.304	-1.0	2
A	86	PRO	CA	62.71	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	106	ARG	C	173.491	-1.0	1
A	44	MET	CB	30.555	-1.0	1
A	13	GLN	CB	34.132	-1.0	1
A	44	MET	HA	4.432	-1.0	1
A	69	SER	N	114.544	-1.0	1
A	93	THR	H	8.312	-1.0	1
A	82	PHE	HB3	2.877	-1.0	2
A	4	ASN	HB2	1.933	-1.0	2
A	34	ILE	HD12	0.747	-1.0	1
A	21	ILE	C	173.198	-1.0	1
A	91	PHE	N	120.115	-1.0	1
A	96	ALA	HA	4.209	-1.0	1
A	83	SER	CA	58.371	-1.0	1
A	36	THR	CG2	21.433	-1.0	1
A	10	ILE	HG21	0.822	-1.0	1
A	73	ALA	N	120.524	-1.0	1
A	91	PHE	CB	39.503	-1.0	1
A	108	GLY	C	176.199	-1.0	1
A	41	GLY	HA2	3.686	-1.0	2
A	89	VAL	HA	4.963	-1.0	1
A	15	LEU	CD1	21.734	-1.0	2
A	3	ASP	HA	4.568	-1.0	1
A	45	ILE	CD1	14.377	-1.0	1
A	13	GLN	HG2	2.002	-1.0	2
A	24	VAL	H	7.973	-1.0	1
A	102	GLY	H	8.281	-1.0	1
A	35	LYS	CA	57.473	-1.0	1
A	103	GLY	H	8.364	-1.0	1
A	52	GLU	HB3	2.147	-1.0	2
A	33	ILE	H	8.173	-1.0	1
A	48	TYR	CD1	132.507	-1.0	3
A	77	PHE	HZ	6.836	-1.0	1
A	92	ALA	HB2	1.265	-1.0	1
A	23	SER	CA	61.239	-1.0	1
A	41	GLY	HA3	4.183	-1.0	2
A	67	PRO	HD2	4.251	-1.0	2
A	87	ILE	CD1	15.114	-1.0	1
A	98	PHE	H	7.99	-1.0	1
A	30	GLN	HB2	2.028	-1.0	2
A	28	PHE	HB3	3.419	-1.0	2
A	82	PHE	C	175.349	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	54	GLY	HA2	3.757	-1.0	2
A	44	MET	HE3	2.066	-1.0	1
A	27	TYR	HB3	3.083	-1.0	2
A	74	ILE	HA	3.414	-1.0	1
A	34	ILE	N	131.781	-1.0	1
A	2	GLN	HB3	2.049	-1.0	2
A	95	ARG	HG2	1.571	-1.0	2
A	94	ARG	C	174.426	-1.0	1
A	73	ALA	CB	19.131	-1.0	1
A	8	ASN	N	119.436	-1.0	1
A	38	LYS	HE2	3.037	-1.0	2
A	21	ILE	HD12	0.948	-1.0	1
A	66	ASP	HB2	2.737	-1.0	2
A	47	LEU	N	122.487	-1.0	1
A	48	TYR	C	173.649	-1.0	1
A	43	PRO	CA	62.822	-1.0	1
A	24	VAL	CG1	24.328	-1.0	2
A	42	GLN	CD	182.295	-1.0	1
A	81	GLU	CA	55.924	-1.0	1
A	74	ILE	HG22	0.859	-1.0	1
A	66	ASP	HA	5.399	-1.0	1
A	45	ILE	CG1	27.923	-1.0	1
A	43	PRO	CG	27.44	-1.0	1
A	61	THR	C	176.172	-1.0	1
A	100	ARG	HA	4.273	-1.0	1
A	95	ARG	CG	27.074	-1.0	1
A	12	VAL	CB	34.8	-1.0	1
A	96	ALA	H	8.402	-1.0	1
A	18	ASN	CB	38.485	-1.0	1
A	101	GLY	H	8.413	-1.0	1
A	22	GLU	HB2	1.983	-1.0	2
A	12	VAL	N	127.993	-1.0	1
A	30	GLN	CG	34.376	-1.0	1
A	106	ARG	HD2	3.163	-1.0	2
A	39	LYS	HE2	3.011	-1.0	2
A	93	THR	HG23	1.151	-1.0	1
A	75	ASP	CB	40.531	-1.0	1
A	35	LYS	HB3	1.47	-1.0	2
A	36	THR	HA	4.415	-1.0	1
A	74	ILE	H	7.574	-1.0	1
A	7	ASN	N	119.696	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	43	PRO	HG2	2.009	-1.0	2
A	102	GLY	HA3	3.958	-1.0	2
A	81	GLU	HA	4.698	-1.0	1
A	11	PHE	CD1	131.67	-1.0	3
A	55	LYS	CA	55.842	-1.0	1
A	15	LEU	HD23	0.294	-1.0	2
A	7	ASN	CB	38.859	-1.0	1
A	90	SER	CA	56.936	-1.0	1
A	27	TYR	H	7.533	-1.0	1
A	55	LYS	CG	25.111	-1.0	1
A	28	PHE	H	7.974	-1.0	1
A	51	ARG	HA	4.045	-1.0	1
A	61	THR	CA	59.625	-1.0	1
A	33	ILE	C	173.301	-1.0	1
A	29	LYS	HE2	3.022	-1.0	2
A	99	ASN	H	8.336	-1.0	1
A	35	LYS	C	175.376	-1.0	1
A	75	ASP	HA	4.311	-1.0	1
A	52	GLU	HA	4.278	-1.0	1
A	62	VAL	CG2	20.84	-1.0	2
A	74	ILE	CB	38.743	-1.0	1
A	4	ASN	CG	173.005	-1.0	1
A	29	LYS	H	8.325	-1.0	1
A	5	SER	N	117.091	-1.0	1
A	103	GLY	N	108.844	-1.0	1
A	52	GLU	CA	58.524	-1.0	1
A	14	GLY	HA2	3.742	-1.0	2
A	74	ILE	CA	65.844	-1.0	1
A	84	GLY	C	177.188	-1.0	1
A	13	GLN	NE2	113.45	-1.0	1
A	85	ASN	N	119.051	-1.0	1
A	8	ASN	HB2	2.45	-1.0	2
A	30	GLN	H	7.518	-1.0	1
A	66	ASP	N	116.125	-1.0	1
A	99	ASN	HD21	7.586	-1.0	2
A	104	ASN	H	8.438	-1.0	1
A	84	GLY	HA3	4.164	-1.0	2
A	90	SER	HB2	3.978	-1.0	2
A	101	GLY	N	109.586	-1.0	1
A	13	GLN	HE22	7.011	-1.0	2
A	33	ILE	HA	4.089	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	89	VAL	HG23	0.984	-1.0	2
A	32	GLY	CA	44.994	-1.0	1
A	29	LYS	HA	4.917	-1.0	1
A	22	GLU	N	118.154	-1.0	1
A	82	PHE	H	9.162	-1.0	1
A	40	THR	H	7.422	-1.0	1
A	68	PRO	CD	50.624	-1.0	1
A	86	PRO	C	173.474	-1.0	1
A	98	PHE	HA	4.49	-1.0	1
A	8	ASN	ND2	113.442	-1.0	1
A	22	GLU	CB	28.791	-1.0	1
A	99	ASN	HD22	6.894	-1.0	2
A	15	LEU	H	8.442	-1.0	1
A	47	LEU	HD21	0.619	-1.0	2
A	45	ILE	HD13	0.876	-1.0	1
A	47	LEU	HD13	0.768	-1.0	2
A	69	SER	CB	62.773	-1.0	1
A	62	VAL	HA	4.244	-1.0	1
A	85	ASN	CA	50.471	-1.0	1
A	6	ASP	H	8.218	-1.0	1
A	38	LYS	C	172.702	-1.0	1
A	12	VAL	HG21	0.683	-1.0	2
A	1	GLU	HB3	2.075	-1.0	2
A	76	TRP	HZ3	7.022	-1.0	1
A	53	THR	CG2	21.143	-1.0	1
A	49	THR	HG23	1.04	-1.0	1
A	20	THR	HG23	1.268	-1.0	1
A	18	ASN	C	175.9	-1.0	1
A	38	LYS	CB	32.167	-1.0	1
A	80	LYS	CB	32.426	-1.0	1
A	72	ALA	CB	17.82	-1.0	1
A	57	LYS	C	173.648	-1.0	1
A	45	ILE	HG21	0.726	-1.0	1
A	71	LYS	C	172.333	-1.0	1
A	59	GLU	N	116.119	-1.0	1
A	29	LYS	HB2	2.048	-1.0	2
A	7	ASN	ND2	109.876	-1.0	1
A	17	GLU	N	113.781	-1.0	1
A	29	LYS	HG2	1.767	-1.0	2
A	57	LYS	HB3	1.883	-1.0	2
A	24	VAL	N	124.867	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	21	ILE	CA	65.772	-1.0	1
A	24	VAL	HG11	0.853	-1.0	2
A	17	GLU	CB	30.436	-1.0	1
A	17	GLU	HA	4.119	-1.0	1
A	68	PRO	C	171.345	-1.0	1
A	24	VAL	CB	31.533	-1.0	1
A	39	LYS	CB	32.797	-1.0	1
A	100	ARG	N	121.374	-1.0	1
A	56	LEU	HA	4.356	-1.0	1
A	106	ARG	H	8.244	-1.0	1
A	77	PHE	HD1	7.561	-1.0	3
A	100	ARG	HB3	1.883	-1.0	2
A	39	LYS	CD	28.903	-1.0	1
A	104	ASN	C	174.547	-1.0	1
A	3	ASP	HB3	2.706	-1.0	2
A	78	ASP	HA	4.464	-1.0	1
A	60	ALA	C	173.923	-1.0	1
A	39	LYS	HB3	1.952	-1.0	2
A	34	ILE	HG23	0.808	-1.0	1
A	85	ASN	C	178.02	-1.0	1
A	6	ASP	CA	53.094	-1.0	1
A	77	PHE	CA	59.921	-1.0	1
A	78	ASP	HB2	2.77	-1.0	2
A	44	MET	CE	17.045	-1.0	1
A	13	GLN	CG	35.472	-1.0	1
A	104	ASN	CG	173.294	-1.0	1
A	13	GLN	CA	54.11	-1.0	1
A	10	ILE	CG2	19.066	-1.0	1
A	61	THR	HB	4.112	-1.0	1
A	34	ILE	HD11	0.747	-1.0	1
A	53	THR	CB	71.197	-1.0	1
A	22	GLU	HA	3.986	-1.0	1
A	46	ASN	CA	51.561	-1.0	1
A	37	ASN	HB2	2.557	-1.0	2
A	35	LYS	CG	24.881	-1.0	1
A	61	THR	HA	5.743	-1.0	1
A	34	ILE	CB	37.995	-1.0	1
A	87	ILE	CG2	18.736	-1.0	1
A	28	PHE	CD2	132.251	-1.0	3
A	38	LYS	HB3	1.87	-1.0	2
A	94	ARG	HB2	1.695	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	11	PHE	HB3	2.825	-1.0	2
A	27	TYR	CD2	132.545	-1.0	3
A	61	THR	HG23	1.461	-1.0	1
A	18	ASN	H	8.407	-1.0	1
A	16	GLY	CA	44.094	-1.0	1
A	67	PRO	CA	66.924	-1.0	1
A	44	MET	HE2	2.066	-1.0	1
A	59	GLU	H	7.202	-1.0	1
A	90	SER	N	119.538	-1.0	1
A	6	ASP	HB3	2.749	-1.0	2
A	22	GLU	HB3	2.083	-1.0	2
A	6	ASP	C	175.048	-1.0	1
A	2	GLN	CD	182.095	-1.0	1
A	87	ILE	CG1	24.92	-1.0	1
A	72	ALA	HA	4.166	-1.0	1
A	80	LYS	HB3	2.302	-1.0	2
A	46	ASN	HD22	6.654	-1.0	2
A	47	LEU	HB3	1.702	-1.0	2
A	52	GLU	CB	30.278	-1.0	1
A	74	ILE	N	119.875	-1.0	1
A	7	ASN	H	7.734	-1.0	1
A	71	LYS	CE	42.484	-1.0	1
A	30	GLN	HB3	2.112	-1.0	2
A	82	PHE	HB2	2.181	-1.0	2
A	28	PHE	HB2	2.772	-1.0	2
A	54	GLY	HA3	4.187	-1.0	2
A	32	GLY	C	180.182	-1.0	1
A	10	ILE	HA	5.165	-1.0	1
A	55	LYS	N	119.673	-1.0	1
A	19	VAL	HG12	0.821	-1.0	2
A	2	GLN	CA	55.996	-1.0	1
A	77	PHE	HA	4.648	-1.0	1
A	72	ALA	C	170.53	-1.0	1
A	45	ILE	HB	1.46	-1.0	1
A	67	PRO	CG	28.312	-1.0	1
A	47	LEU	HB2	1.397	-1.0	2
A	88	LYS	HB3	1.824	-1.0	2
A	90	SER	C	176.533	-1.0	1
A	42	GLN	CA	53.581	-1.0	1
A	66	ASP	HB3	2.815	-1.0	2
A	7	ASN	HA	4.628	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	29	LYS	CB	31.291	-1.0	1
A	43	PRO	CB	32.696	-1.0	1
A	49	THR	HA	4.806	-1.0	1
A	42	GLN	CG	33.392	-1.0	1
A	87	ILE	HG23	0.731	-1.0	1
A	40	THR	CG2	21.241	-1.0	1
A	56	LEU	CD1	26.357	-1.0	2
A	18	ASN	CG	172.618	-1.0	1
A	53	THR	HB	4.334	-1.0	1
A	76	TRP	CD1	126.817	-1.0	1
A	85	ASN	HD22	7.035	-1.0	2
A	32	GLY	HA2	3.901	-1.0	2
A	84	GLY	HA2	3.605	-1.0	2
A	30	GLN	CB	29.898	-1.0	1
A	69	SER	HA	4.036	-1.0	1
A	9	THR	N	118.65	-1.0	1
A	84	GLY	N	103.581	-1.0	1
A	68	PRO	HA	4.419	-1.0	1
A	60	ALA	N	123.607	-1.0	1
A	20	THR	CA	58.698	-1.0	1
A	30	GLN	CD	182.286	-1.0	1
A	88	LYS	HG2	1.492	-1.0	2
A	19	VAL	C	177.655	-1.0	1
A	2	GLN	HE21	7.671	-1.0	2
A	77	PHE	CB	40.73	-1.0	1
A	77	PHE	CE1	131.749	-1.0	3
A	29	LYS	N	118.82	-1.0	1
A	55	LYS	CB	33.821	-1.0	1
A	75	ASP	HB3	2.739	-1.0	2
A	47	LEU	HG	1.5	-1.0	1
A	50	ASP	H	8.939	-1.0	1
A	22	GLU	H	8.814	-1.0	1
A	29	LYS	CG	24.017	-1.0	1
A	15	LEU	HD22	0.294	-1.0	2
A	53	THR	N	107.065	-1.0	1
A	47	LEU	HA	4.715	-1.0	1
A	69	SER	H	8.004	-1.0	1
A	4	ASN	ND2	115.469	-1.0	1
A	55	LYS	C	173.854	-1.0	1
A	55	LYS	CD	28.913	-1.0	1
A	95	ARG	CD	43.358	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	34	ILE	HA	3.787	-1.0	1
A	47	LEU	HD12	0.768	-1.0	2
A	31	ILE	HG21	0.862	-1.0	1
A	66	ASP	C	175.936	-1.0	1
A	18	ASN	HB3	2.91	-1.0	2
A	23	SER	C	172.447	-1.0	1
A	37	ASN	ND2	113.836	-1.0	1
A	7	ASN	C	176.539	-1.0	1
A	72	ALA	H	7.924	-1.0	1
A	97	ASP	H	8.206	-1.0	1
A	9	THR	CB	71.225	-1.0	1
A	20	THR	C	175.266	-1.0	1
A	83	SER	H	9.193	-1.0	1
A	47	LEU	H	8.594	-1.0	1
A	62	VAL	HG21	0.008	-1.0	2
A	77	PHE	HE1	6.986	-1.0	3
A	51	ARG	HD2	3.207	-1.0	2
A	28	PHE	CB	40.003	-1.0	1
A	14	GLY	HA3	4.536	-1.0	2
A	68	PRO	HG2	2.131	-1.0	2
A	33	ILE	HG12	1.693	-1.0	2
A	106	ARG	HA	4.351	-1.0	1
A	49	THR	H	8.965	-1.0	1
A	45	ILE	CG2	16.571	-1.0	1
A	12	VAL	HG11	0.863	-1.0	2
A	53	THR	CA	61.944	-1.0	1
A	48	TYR	HA	4.767	-1.0	1
A	40	THR	HG22	1.14	-1.0	1
A	71	LYS	CD	28.731	-1.0	1
A	88	LYS	CD	28.839	-1.0	1
A	17	GLU	H	8.134	-1.0	1
A	3	ASP	CB	41.071	-1.0	1
A	58	GLY	N	108.514	-1.0	1
A	9	THR	CA	62.314	-1.0	1
A	37	ASN	HD22	7.208	-1.0	2
A	68	PRO	CA	66.235	-1.0	1
A	13	GLN	HE21	7.958	-1.0	2
A	57	LYS	HA	4.288	-1.0	1
A	56	LEU	HD23	0.837	-1.0	2
A	39	LYS	H	8.314	-1.0	1
A	68	PRO	CG	28.298	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	95	ARG	CB	30.966	-1.0	1
A	10	ILE	HD13	0.249	-1.0	1
A	57	LYS	CB	34.062	-1.0	1
A	34	ILE	CG2	16.628	-1.0	1
A	31	ILE	HD13	0.345	-1.0	1
A	16	GLY	C	177.771	-1.0	1
A	45	ILE	HD12	0.876	-1.0	1
A	59	GLU	C	173.86	-1.0	1
A	69	SER	CA	61.837	-1.0	1
A	39	LYS	HG2	1.527	-1.0	2
A	18	ASN	CA	52.478	-1.0	1
A	91	PHE	HB3	3.082	-1.0	2
A	31	ILE	C	175.599	-1.0	1
A	48	TYR	CE1	118.217	-1.0	3
A	28	PHE	N	112.595	-1.0	1
A	105	GLY	C	176.074	-1.0	1
A	12	VAL	HG22	0.683	-1.0	2
A	45	ILE	CB	42.226	-1.0	1
A	38	LYS	CG	24.941	-1.0	1
A	76	TRP	HZ2	7.335	-1.0	1
A	22	GLU	C	171.799	-1.0	1
A	73	ALA	H	8.104	-1.0	1
A	71	LYS	HE2	3.132	-1.0	2
A	57	LYS	CA	56.264	-1.0	1
A	49	THR	HG22	1.04	-1.0	1
A	15	LEU	HG	1.116	-1.0	1
A	45	ILE	N	126.237	-1.0	1
A	38	LYS	CA	58.458	-1.0	1
A	62	VAL	HG11	0.3	-1.0	2
A	25	ALA	CA	55.695	-1.0	1
A	53	THR	HG21	1.227	-1.0	1
A	15	LEU	HA	3.706	-1.0	1
A	5	SER	H	8.47	-1.0	1
A	64	PHE	H	9.025	-1.0	1
A	94	ARG	CA	56.055	-1.0	1
A	23	SER	HB2	4.009	-1.0	2
A	55	LYS	HE2	2.998	-1.0	2
A	13	GLN	HB3	2.124	-1.0	2
A	95	ARG	HB3	1.806	-1.0	2
A	38	LYS	HG2	1.562	-1.0	2
A	71	LYS	HA	3.775	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	71	LYS	HD2	1.892	-1.0	2
A	30	GLN	N	116.232	-1.0	1
A	59	GLU	HB3	1.991	-1.0	2
A	69	SER	HB3	3.895	-1.0	2
A	93	THR	HG22	1.151	-1.0	1
A	80	LYS	CA	55.15	-1.0	1
A	80	LYS	N	120.271	-1.0	1
A	59	GLU	CB	34.304	-1.0	1
A	22	GLU	HG2	2.476	-1.0	2
A	89	VAL	CB	34.77	-1.0	1
A	94	ARG	CB	30.911	-1.0	1
A	43	PRO	HD2	3.846	-1.0	2
A	81	GLU	HG2	2.206	-1.0	2
A	93	THR	HB	4.07	-1.0	1
A	11	PHE	H	9.548	-1.0	1
A	7	ASN	HD21	7.434	-1.0	2
A	39	LYS	CE	42.117	-1.0	1
A	67	PRO	HB2	2.197	-1.0	2
A	17	GLU	C	173.937	-1.0	1
A	25	ALA	C	171.061	-1.0	1
A	80	LYS	H	8.013	-1.0	1
A	34	ILE	HG22	0.808	-1.0	1
A	94	ARG	N	124.359	-1.0	1
A	91	PHE	HA	4.673	-1.0	1
A	28	PHE	HA	4.33	-1.0	1
A	85	ASN	CB	41.117	-1.0	1
A	70	ALA	H	7.383	-1.0	1
A	37	ASN	HA	4.53	-1.0	1
A	82	PHE	HE1	6.952	-1.0	3
A	47	LEU	CD1	25.846	-1.0	2
A	75	ASP	HB2	2.63	-1.0	2
A	104	ASN	ND2	112.397	-1.0	1
A	87	ILE	HA	5.146	-1.0	1
A	1	GLU	C	174.257	-1.0	1
A	10	ILE	CG1	26.332	-1.0	1
A	89	VAL	CG2	24.305	-1.0	2
A	37	ASN	HB3	3.274	-1.0	2
A	35	LYS	CD	29.774	-1.0	1
A	98	PHE	CA	58.16	-1.0	1
A	9	THR	H	8.428	-1.0	1
A	71	LYS	HG2	1.591	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	48	TYR	HE1	6.848	-1.0	3
A	11	PHE	HB2	2.689	-1.0	2
A	61	THR	HG22	1.461	-1.0	1
A	64	PHE	HB3	3.456	-1.0	2
A	104	ASN	HD22	6.94	-1.0	2
A	44	MET	HE1	2.066	-1.0	1
A	36	THR	HB	3.731	-1.0	1
A	26	ASP	HA	4.323	-1.0	1
A	6	ASP	HB2	2.627	-1.0	2
A	52	GLU	H	8.561	-1.0	1
A	70	ALA	N	122.649	-1.0	1
A	94	ARG	HD2	3.09	-1.0	2
A	82	PHE	HA	4.496	-1.0	1
A	65	ASP	CB	42.034	-1.0	1
A	88	LYS	N	122.271	-1.0	1
A	55	LYS	HG2	1.423	-1.0	2
A	46	ASN	HD21	6.964	-1.0	2
A	108	GLY	CA	45.344	-1.0	1
A	79	GLY	C	175.68	-1.0	1
A	19	VAL	CG2	21.302	-1.0	2
A	33	ILE	HD11	0.916	-1.0	1
A	1	GLU	CA	56.516	-1.0	1
A	76	TRP	H	8.475	-1.0	1
A	10	ILE	HG12	1.289	-1.0	2
A	89	VAL	H	9.414	-1.0	1
A	82	PHE	CD1	132.136	-1.0	3
A	10	ILE	HB	1.844	-1.0	1
A	94	ARG	HA	4.337	-1.0	1
A	67	PRO	CB	29.83	-1.0	1
A	19	VAL	HG13	0.821	-1.0	2
A	62	VAL	HB	1.354	-1.0	1
A	71	LYS	CG	25.067	-1.0	1
A	107	GLY	C	175.834	-1.0	1
A	67	PRO	CD	51.216	-1.0	1
A	8	ASN	CB	38.495	-1.0	1
A	71	LYS	HB2	1.997	-1.0	2
A	60	ALA	CA	50.943	-1.0	1
A	71	LYS	CA	59.002	-1.0	1
A	74	ILE	CD1	13.335	-1.0	1
A	47	LEU	CB	42.277	-1.0	1
A	29	LYS	CE	42.181	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	49	THR	HB	3.856	-1.0	1
A	58	GLY	HA3	4.23	-1.0	2
A	24	VAL	HG23	0.833	-1.0	2
A	49	THR	CB	71.437	-1.0	1
A	106	ARG	CG	27.108	-1.0	1
A	106	ARG	HB2	1.736	-1.0	2
A	95	ARG	CA	56.142	-1.0	1
A	30	GLN	HE21	7.632	-1.0	2
A	20	THR	N	111.636	-1.0	1
A	31	ILE	HD11	0.345	-1.0	1
A	106	ARG	HB3	1.893	-1.0	2
A	3	ASP	H	8.436	-1.0	1
A	14	GLY	N	109.212	-1.0	1
A	5	SER	HB2	3.897	-1.0	2
A	96	ALA	CB	19.193	-1.0	1
A	65	ASP	HB3	2.609	-1.0	2
A	57	LYS	CE	41.52	-1.0	1
A	90	SER	H	8.945	-1.0	1
A	76	TRP	CE3	120.915	-1.0	1
A	93	THR	HG21	1.151	-1.0	1
A	96	ALA	N	125.127	-1.0	1
A	31	ILE	HB	1.844	-1.0	1
A	65	ASP	CA	57.442	-1.0	1
A	10	ILE	CB	39.88	-1.0	1
A	108	GLY	H	8.331	-1.0	1
A	98	PHE	CB	39.303	-1.0	1
A	4	ASN	HD22	6.995	-1.0	2
A	95	ARG	N	122.515	-1.0	1
A	15	LEU	HD21	0.294	-1.0	2
A	70	ALA	CB	17.864	-1.0	1
A	74	ILE	HG12	1.441	-1.0	2
A	58	GLY	HA2	3.774	-1.0	2
A	77	PHE	HB3	3.462	-1.0	2
A	21	ILE	H	9.074	-1.0	1
A	76	TRP	HD1	5.24	-1.0	1
A	10	ILE	N	118.556	-1.0	1
A	57	LYS	CD	28.992	-1.0	1
A	47	LEU	HD11	0.768	-1.0	2
A	18	ASN	HB2	2.733	-1.0	2
A	103	GLY	C	175.798	-1.0	1
A	31	ILE	N	116.489	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	85	ASN	HA	5.334	-1.0	1
A	37	ASN	H	8.794	-1.0	1
A	5	SER	CB	63.136	-1.0	1
A	41	GLY	N	111.631	-1.0	1
A	61	THR	H	8.452	-1.0	1
A	78	ASP	H	7.978	-1.0	1
A	104	ASN	HD21	7.599	-1.0	2
A	36	THR	HG21	0.88	-1.0	1
A	18	ASN	ND2	113.323	-1.0	1
A	95	ARG	H	8.343	-1.0	1
A	20	THR	HB	4.691	-1.0	1
A	80	LYS	CG	26.439	-1.0	1
A	88	LYS	C	174.393	-1.0	1
A	11	PHE	N	123.798	-1.0	1
A	81	GLU	HB3	1.888	-1.0	2
A	26	ASP	CA	57.323	-1.0	1
A	37	ASN	HD21	7.653	-1.0	2
A	60	ALA	HA	5.607	-1.0	1
A	11	PHE	CB	41.868	-1.0	1
A	85	ASN	HB3	2.915	-1.0	2
A	42	GLN	HE22	6.983	-1.0	2
A	55	LYS	HA	4.353	-1.0	1
A	79	GLY	HA2	3.887	-1.0	2
A	98	PHE	HB2	3.022	-1.0	2
A	77	PHE	CZ	128.357	-1.0	1
A	10	ILE	HD12	0.249	-1.0	1
A	98	PHE	N	120.321	-1.0	1
A	87	ILE	H	8.469	-1.0	1
A	8	ASN	C	175.327	-1.0	1
A	92	ALA	CB	19.406	-1.0	1
A	95	ARG	HA	4.228	-1.0	1
A	45	ILE	HD11	0.876	-1.0	1
A	107	GLY	N	109.856	-1.0	1
A	28	PHE	CA	61.784	-1.0	1
A	38	LYS	H	8.962	-1.0	1
A	27	TYR	HD2	5.836	-1.0	3
A	27	TYR	CA	61.016	-1.0	1
A	37	ASN	CG	173.207	-1.0	1
A	28	PHE	HD2	7.419	-1.0	3
A	12	VAL	HG23	0.683	-1.0	2
A	45	ILE	CA	59.216	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	101	GLY	C	175.739	-1.0	1
A	37	ASN	CA	53.064	-1.0	1
A	46	ASN	C	176.836	-1.0	1
A	19	VAL	HG23	0.796	-1.0	2
A	99	ASN	CA	53.313	-1.0	1
A	49	THR	HG21	1.04	-1.0	1
A	105	GLY	CA	45.602	-1.0	1
A	33	ILE	CD1	12.292	-1.0	1
A	62	VAL	HG12	0.3	-1.0	2
A	72	ALA	N	119.806	-1.0	1
A	33	ILE	HG22	0.885	-1.0	1
A	45	ILE	HG23	0.726	-1.0	1
A	31	ILE	CD1	12.038	-1.0	1
A	99	ASN	HB3	2.775	-1.0	2
A	84	GLY	H	8.446	-1.0	1
A	42	GLN	HB3	2.19	-1.0	2
A	23	SER	HA	4.384	-1.0	1
A	78	ASP	CA	58.69	-1.0	1
A	13	GLN	HB2	1.762	-1.0	2
A	32	GLY	HA3	4.082	-1.0	2
A	24	VAL	HA	3.748	-1.0	1
A	96	ALA	C	173.226	-1.0	1
A	8	ASN	HD21	8.016	-1.0	2
A	28	PHE	HZ	6.98	-1.0	1
A	82	PHE	CA	56.716	-1.0	1
A	76	TRP	HE3	7.4	-1.0	1
A	9	THR	CG2	21.208	-1.0	1
A	15	LEU	CG	26.412	-1.0	1
A	95	ARG	C	174.306	-1.0	1
A	62	VAL	N	120.2	-1.0	1
A	83	SER	HA	3.803	-1.0	1
A	29	LYS	C	173.682	-1.0	1
A	15	LEU	CA	55.718	-1.0	1
A	31	ILE	HG22	0.862	-1.0	1
A	72	ALA	HB3	1.41	-1.0	1
A	35	LYS	HE2	3.109	-1.0	2
A	31	ILE	CA	58.221	-1.0	1
A	76	TRP	CB	30.777	-1.0	1
A	80	LYS	CD	28.067	-1.0	1
A	92	ALA	HA	4.356	-1.0	1
A	76	TRP	HB3	3.096	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	63	SER	CA	57.662	-1.0	1
A	48	TYR	HB2	2.814	-1.0	2
A	87	ILE	HG22	0.731	-1.0	1
A	34	ILE	H	8.687	-1.0	1
A	65	ASP	C	174.396	-1.0	1
A	44	MET	CG	32.736	-1.0	1
A	47	LEU	CD2	23.808	-1.0	2
A	8	ASN	H	8.35	-1.0	1
A	42	GLN	NE2	113.062	-1.0	1
A	98	PHE	HB3	3.091	-1.0	2
A	56	LEU	N	122.426	-1.0	1
A	66	ASP	CB	42.919	-1.0	1
A	69	SER	C	176.535	-1.0	1
A	56	LEU	CA	56.255	-1.0	1
A	55	LYS	H	7.767	-1.0	1
A	86	PRO	CD	50.873	-1.0	1
A	46	ASN	HB3	2.564	-1.0	2
A	46	ASN	CG	173.942	-1.0	1
A	50	ASP	C	173.38	-1.0	1
A	35	LYS	CE	41.836	-1.0	1
A	59	GLU	HG2	2.221	-1.0	2
A	97	ASP	CB	40.907	-1.0	1
A	86	PRO	CB	31.87	-1.0	1
A	57	LYS	CG	25.25	-1.0	1
A	12	VAL	HA	4.958	-1.0	1
A	92	ALA	C	172.984	-1.0	1
A	64	PHE	HB2	2.798	-1.0	2
A	15	LEU	CD2	26.404	-1.0	2
A	74	ILE	CG2	17.009	-1.0	1
A	9	THR	HG21	1.157	-1.0	1
A	35	LYS	HD2	1.627	-1.0	2
A	47	LEU	C	174.19	-1.0	1
A	90	SER	CB	66.47	-1.0	1
A	12	VAL	HG13	0.863	-1.0	2
A	68	PRO	HD2	3.743	-1.0	2
A	108	GLY	N	108.889	-1.0	1
A	87	ILE	HD12	0.79	-1.0	1
A	68	PRO	HB3	2.401	-1.0	2
A	88	LYS	CA	54.138	-1.0	1
A	97	ASP	CA	54.091	-1.0	1
A	57	LYS	H	8.012	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	40	THR	HG23	1.14	-1.0	1
A	52	GLU	N	117.542	-1.0	1
A	36	THR	HG23	0.88	-1.0	1
A	23	SER	CB	62.838	-1.0	1
A	45	ILE	HG12	1.437	-1.0	2
A	21	ILE	N	122.147	-1.0	1
A	74	ILE	HD13	-0.202	-1.0	1
A	26	ASP	C	173.108	-1.0	1
A	33	ILE	HD12	0.916	-1.0	1
A	74	ILE	HB	1.72	-1.0	1
A	99	ASN	ND2	112.559	-1.0	1
A	49	THR	C	176.654	-1.0	1
A	21	ILE	CB	37.583	-1.0	1
A	80	LYS	HB2	2.078	-1.0	2
A	106	ARG	HG2	1.597	-1.0	2
A	88	LYS	CE	42.088	-1.0	1
A	77	PHE	H	8.488	-1.0	1
A	34	ILE	CA	61.37	-1.0	1
A	2	GLN	CG	33.799	-1.0	1
A	21	ILE	HD11	0.948	-1.0	1
A	52	GLU	CG	36.661	-1.0	1
A	47	LEU	CG	26.779	-1.0	1
A	8	ASN	CA	53.204	-1.0	1
A	71	LYS	HB3	2.166	-1.0	2
A	60	ALA	CB	24.059	-1.0	1
A	81	GLU	N	115.765	-1.0	1
A	10	ILE	C	176.837	-1.0	1
A	80	LYS	HG2	1.504	-1.0	2
A	47	LEU	CA	53.332	-1.0	1
A	29	LYS	CD	29.955	-1.0	1
A	43	PRO	CD	50.512	-1.0	1
A	64	PHE	CB	41.976	-1.0	1
A	17	GLU	HB2	2.012	-1.0	2
A	29	LYS	HD2	1.73	-1.0	2
A	24	VAL	HG22	0.833	-1.0	2
A	39	LYS	C	172.261	-1.0	1
A	45	ILE	C	176.415	-1.0	1
A	104	ASN	HA	4.718	-1.0	1
A	41	GLY	H	8.644	-1.0	1
A	43	PRO	C	172.629	-1.0	1
A	21	ILE	HG23	0.933	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	12	VAL	CA	59.835	-1.0	1
A	76	TRP	HH2	7.14	-1.0	1
A	100	ARG	H	8.181	-1.0	1
A	16	GLY	H	8.006	-1.0	1
A	64	PHE	N	122.64	-1.0	1
A	5	SER	HB3	4.167	-1.0	2
A	2	GLN	HA	4.266	-1.0	1
A	65	ASP	HB2	2.42	-1.0	2
A	8	ASN	HA	4.868	-1.0	1
A	94	ARG	CD	43.357	-1.0	1
A	58	GLY	CA	46.364	-1.0	1
A	21	ILE	CD1	12.95	-1.0	1
A	89	VAL	CG1	22.372	-1.0	2
A	75	ASP	CA	57.161	-1.0	1
A	31	ILE	HA	4.239	-1.0	1
A	56	LEU	HD22	0.837	-1.0	2
A	7	ASN	CG	173.792	-1.0	1
A	81	GLU	C	173.263	-1.0	1
A	50	ASP	N	123.826	-1.0	1
A	92	ALA	H	8.563	-1.0	1
A	51	ARG	H	8.958	-1.0	1
A	70	ALA	CA	55.036	-1.0	1
A	10	ILE	CA	59.298	-1.0	1
A	64	PHE	HD2	7.042	-1.0	3
A	106	ARG	CA	56.227	-1.0	1
A	61	THR	N	108.384	-1.0	1
A	2	GLN	H	8.621	-1.0	1
A	80	LYS	HE2	2.667	-1.0	2
A	70	ALA	HB3	1.608	-1.0	1
A	79	GLY	HA3	4.263	-1.0	2
A	50	ASP	HA	4.624	-1.0	1
A	57	LYS	HB2	1.541	-1.0	2
A	62	VAL	CG1	19.94	-1.0	2
A	12	VAL	C	176.965	-1.0	1
A	4	ASN	CB	38.534	-1.0	1
A	91	PHE	C	173.349	-1.0	1
A	42	GLN	H	7.662	-1.0	1
A	51	ARG	HG2	1.678	-1.0	2
A	84	GLY	CA	45.052	-1.0	1
A	4	ASN	N	120.292	-1.0	1
A	62	VAL	HG23	0.008	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	70	ALA	HA	3.593	-1.0	1
A	46	ASN	HA	4.941	-1.0	1
A	74	ILE	CG1	29.428	-1.0	1
A	66	ASP	CA	50.793	-1.0	1
A	26	ASP	N	115.503	-1.0	1
A	9	THR	HB	4.119	-1.0	1
A	97	ASP	HB3	2.586	-1.0	2
A	20	THR	HA	4.719	-1.0	1
A	50	ASP	CB	42.867	-1.0	1
A	81	GLU	HB2	1.565	-1.0	2
A	18	ASN	HA	4.941	-1.0	1
A	14	GLY	H	8.236	-1.0	1
A	43	PRO	HB2	1.569	-1.0	2
A	96	ALA	CA	52.77	-1.0	1
A	42	GLN	HA	4.669	-1.0	1
A	33	ILE	HB	1.824	-1.0	1
A	48	TYR	HD1	7.165	-1.0	3
A	107	GLY	HA3	3.955	-1.0	2
A	50	ASP	CA	54.088	-1.0	1
A	22	GLU	CG	37.142	-1.0	1
A	80	LYS	CE	42.494	-1.0	1
A	47	LEU	HD22	0.619	-1.0	2
A	39	LYS	HD2	1.706	-1.0	2

### 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
$^{13}\text{C}_\alpha$	108	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	94	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	107	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{15}\text{N}$	103	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)

### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 901. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/372 (0%)	0/148 (0%)	0/152 (0%)	0/72 (0%)
Sidechain	0/447 (0%)	0/261 (0%)	0/170 (0%)	0/16 (0%)
Aromatic	0/82 (0%)	0/44 (0%)	0/37 (0%)	0/1 (0%)
Overall	0/901 (0%)	0/453 (0%)	0/359 (0%)	0/89 (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 1278. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/532 (0%)	0/212 (0%)	0/216 (0%)	0/104 (0%)
Sidechain	0/655 (0%)	0/383 (0%)	0/235 (0%)	0/37 (0%)
Aromatic	0/91 (0%)	0/49 (0%)	0/41 (0%)	0/1 (0%)
Overall	0/1278 (0%)	0/644 (0%)	0/492 (0%)	0/142 (0%)

#### 7.1.4 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, ppm	Expected range, ppm	Z-score
1	A	76	TRP	HD1	5.24	8.95 – 5.35	-5.3

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned\_chem\_shift\_list\_1). RCI is only applicable to proteins.