



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 11:34 PM BST

PDB ID : 2JXY  
Title : Solution structure of the hemopexin-like domain of MMP12  
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Deposited on : 2007-12-01

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

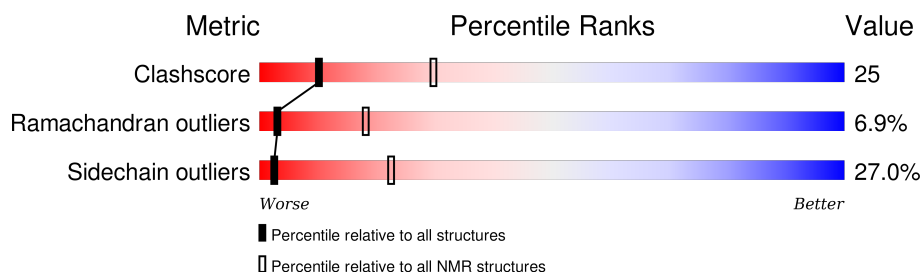
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 79%.

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	194	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:281-A:470 (190)	0.70	1

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

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

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

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3243 atoms, of which 1595 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

Mol	Chain	Residues	Atoms						Trace
1	A	194	Total	C	H	N	O	S	0
			3242	1089	1595	267	286	5	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	MET	-	EXPRESSION TAG	UNP P39900

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

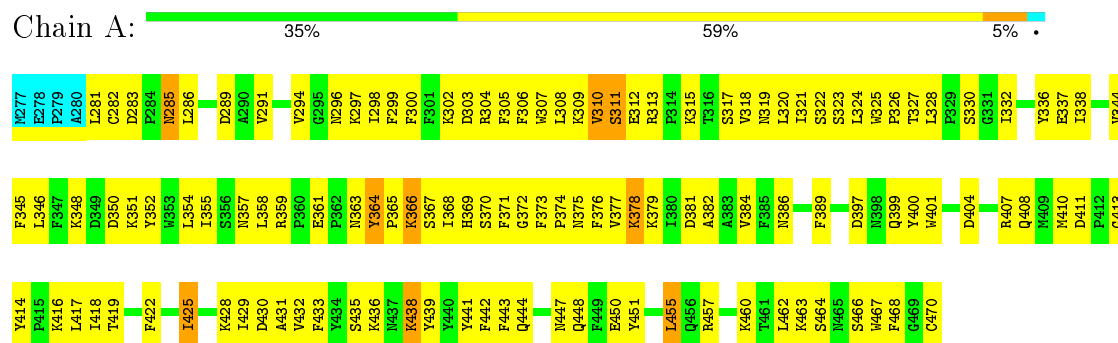
Mol	Chain	Residues	Atoms	
2	A	1	Total	Ca
			1	1

## 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: Macrophage metalloelastase

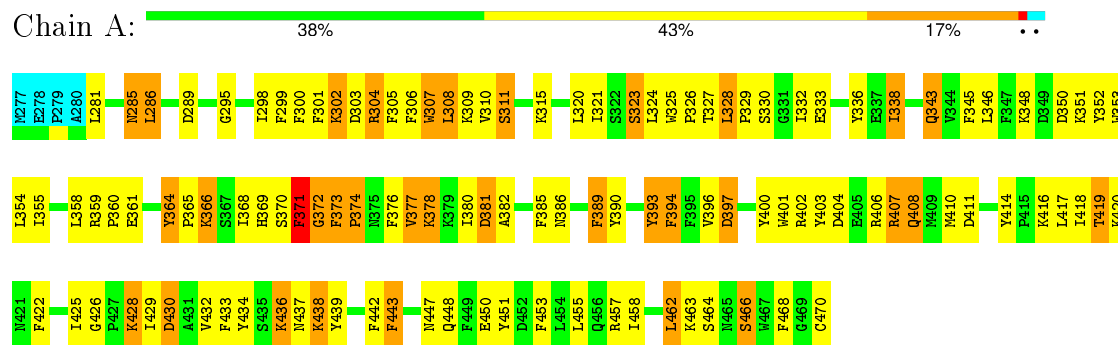


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Macrophage metalloelastase



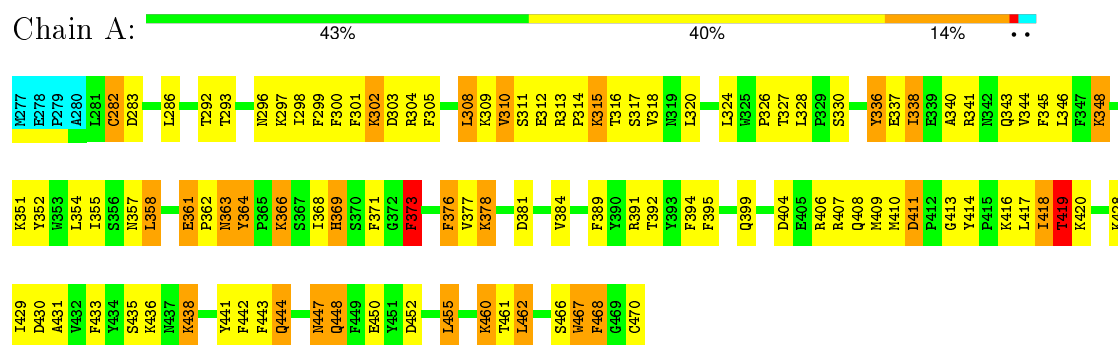
### 4.2.2 Score per residue for model 2

#### • Molecule 1: Macrophage metalloelastase



### 4.2.3 Score per residue for model 3

#### • Molecule 1: Macrophage metalloelastase



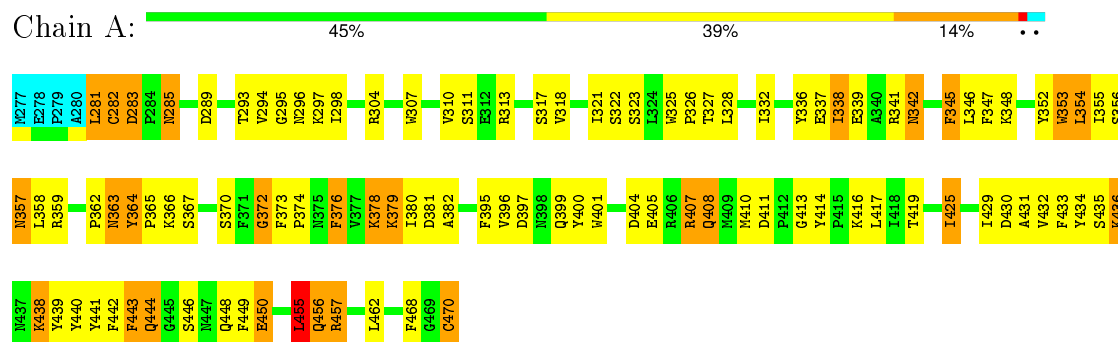
### 4.2.4 Score per residue for model 4

#### • Molecule 1: Macrophage metalloelastase



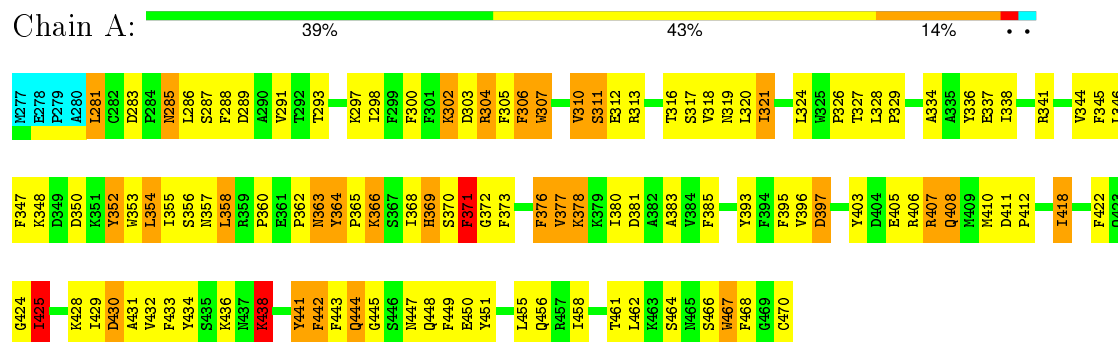
### 4.2.5 Score per residue for model 5

- Molecule 1: Macrophage metalloelastase



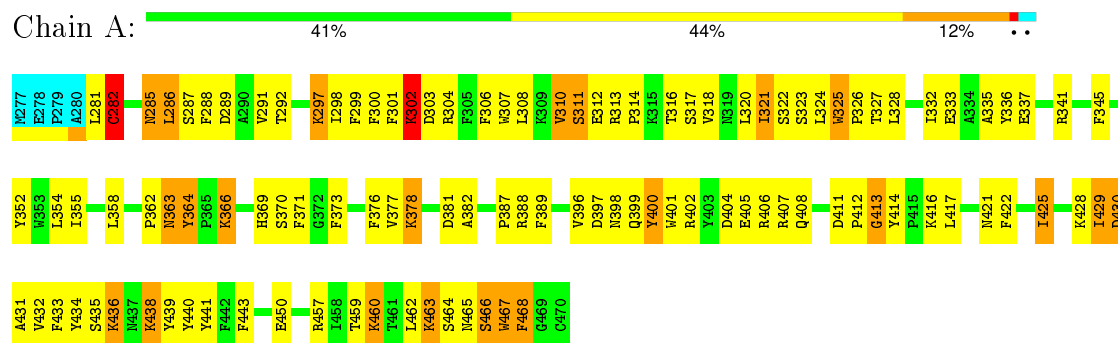
### 4.2.6 Score per residue for model 6

- Molecule 1: Macrophage metalloelastase



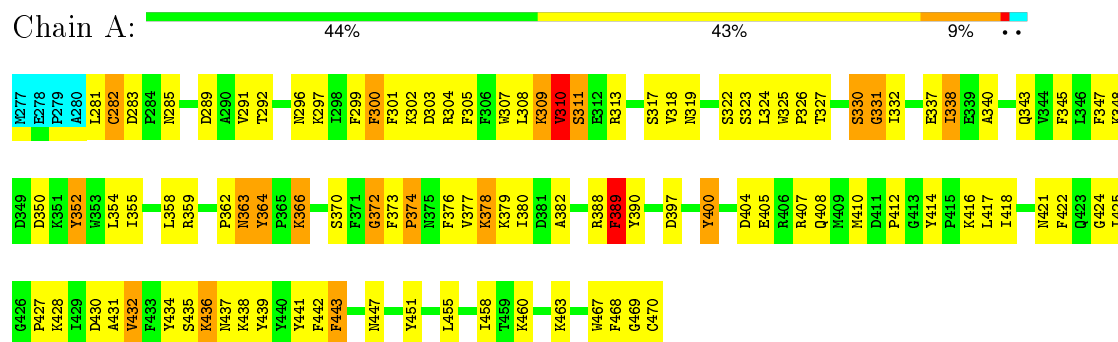
### 4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase



### 4.2.8 Score per residue for model 8

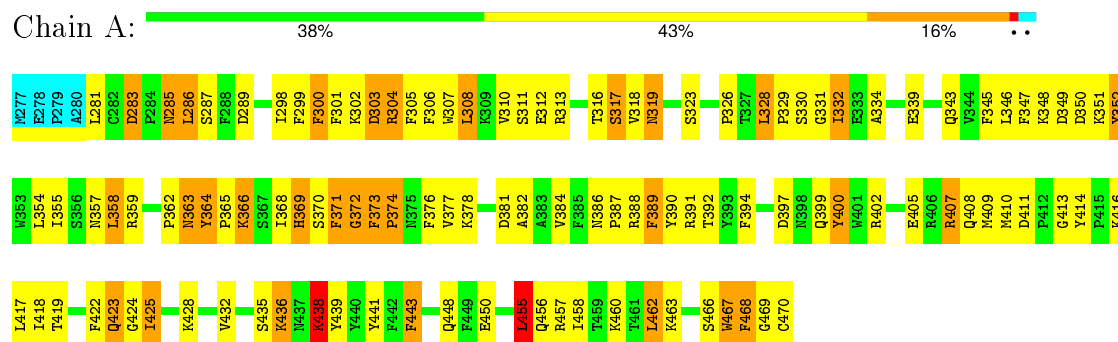
- Molecule 1: Macrophage metalloelastase





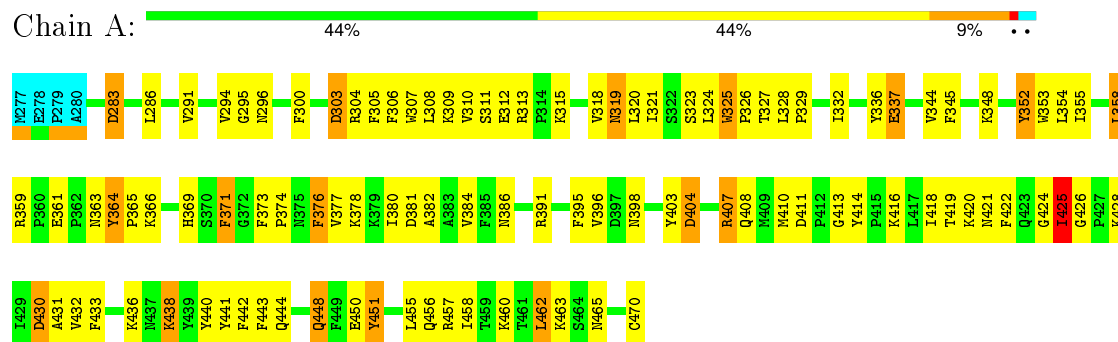
### 4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase



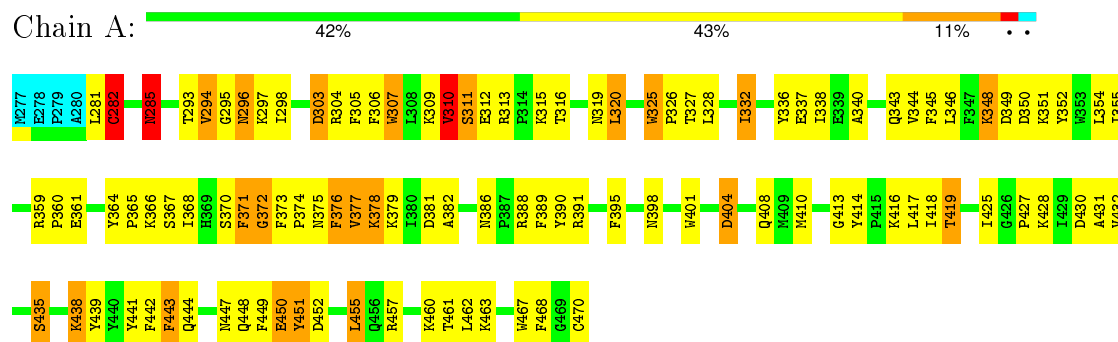
### 4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase



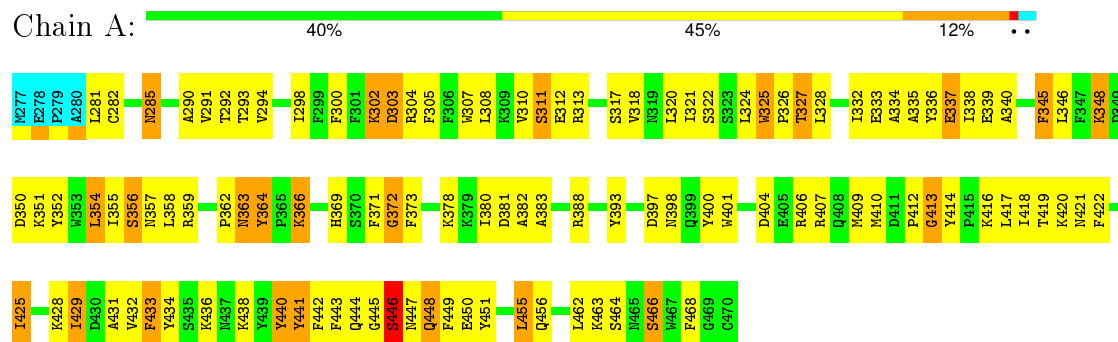
## 4.2.14 Score per residue for model 14

- Molecule 1: Macrophage metalloelastase



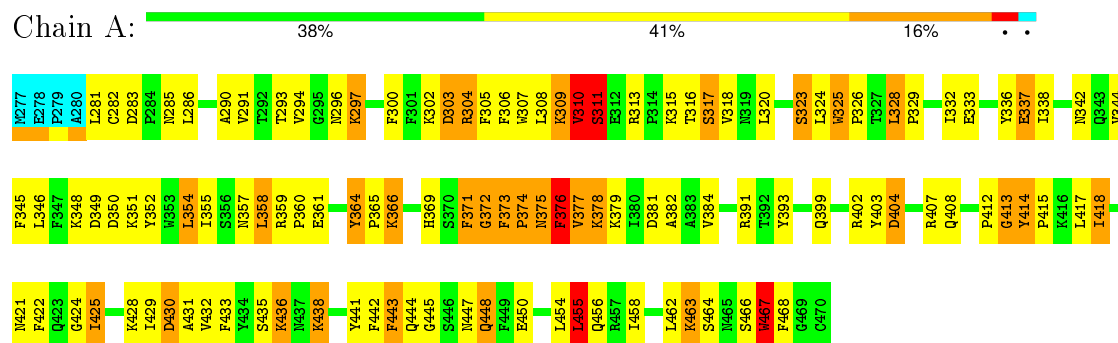
## 4.2.15 Score per residue for model 15

- Molecule 1: Macrophage metalloelastase



## 4.2.16 Score per residue for model 16

- Molecule 1: Macrophage metalloelastase



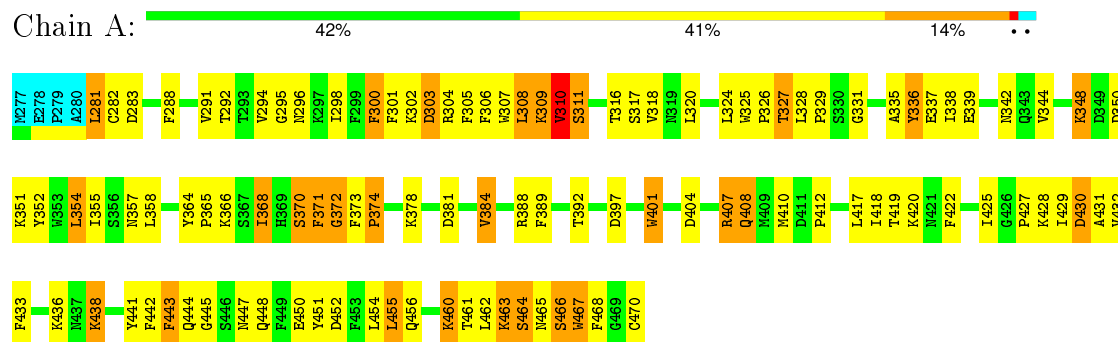
## 4.2.17 Score per residue for model 17

- Molecule 1: Macrophage metalloelastase



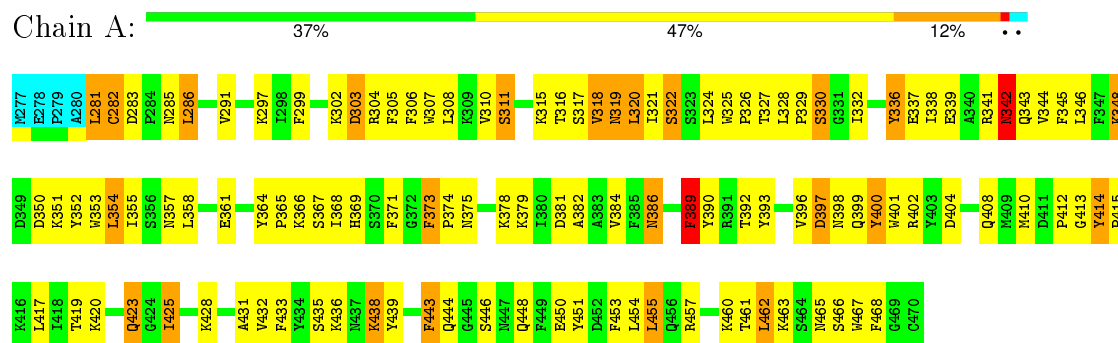
## 4.2.18 Score per residue for model 18

- Molecule 1: Macrophage metalloelastase



## 4.2.19 Score per residue for model 19

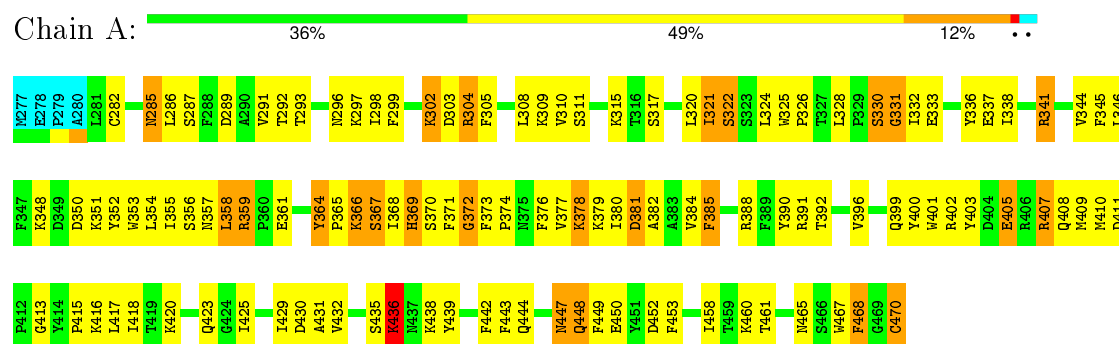
- Molecule 1: Macrophage metalloelastase



#### 4.2.20 Score per residue for model 20

- Molecule 1: Macrophage metalloelastase

Chain A:



## 5 Refinement protocol and experimental data overview

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

Of the 1600 calculated structures, 20 were deposited, based on the following criterion: *lowest target function*.

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

Software name	Classification	Version
DYANA	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)	BMRB entry 7414, BMRB entry 15578
Number of chemical shift lists	2
Total number of shifts	5866
Number of shifts mapped to atoms	4253
Number of unparsed shifts	0
Number of shifts with mapping errors	1613
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts ⓘ

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	1618	1568	1565	80±15
All	All	32380	31360	31324	1602

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:281:LEU:HD11	1:A:307:TRP:CZ3	1.00	1.91	17	1
1:A:328:LEU:HD21	1:A:355:ILE:HD11	0.94	1.40	10	3
1:A:346:LEU:HD23	1:A:355:ILE:HD13	0.92	1.37	2	2
1:A:291:VAL:HG21	1:A:442:PHE:CZ	0.91	2.01	15	1
1:A:298:ILE:HD13	1:A:300:PHE:CZ	0.90	2.01	13	1
1:A:432:VAL:HG21	1:A:442:PHE:CE1	0.88	2.02	8	3
1:A:368:ILE:HD12	1:A:377:VAL:HG13	0.88	1.45	2	1
1:A:286:LEU:HD11	1:A:307:TRP:CZ2	0.88	2.04	16	2
1:A:336:TYR:OH	1:A:338:ILE:HD11	0.87	1.69	10	1
1:A:327:THR:O	1:A:328:LEU:HD22	0.87	1.70	6	13
1:A:334:ALA:HB1	1:A:383:ALA:HB2	0.86	1.46	15	1
1:A:281:LEU:HD11	1:A:316:THR:OG1	0.85	1.71	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:450:GLU:O	1:A:458:ILE:HG23	0.84	1.72	1	3
1:A:382:ALA:HB1	1:A:432:VAL:HG12	0.84	1.50	1	5
1:A:354:LEU:HD23	1:A:364:TYR:CE2	0.83	2.08	18	3
1:A:350:ASP:O	1:A:368:ILE:HG23	0.82	1.74	13	1
1:A:338:ILE:HD12	1:A:345:PHE:CE1	0.82	2.10	10	2
1:A:291:VAL:HG22	1:A:431:ALA:HB1	0.81	1.50	4	5
1:A:291:VAL:HG21	1:A:442:PHE:CE1	0.81	2.11	15	1
1:A:291:VAL:HG21	1:A:300:PHE:CE2	0.80	2.11	16	1
1:A:424:GLY:CA	1:A:458:ILE:HD11	0.80	2.06	12	2
1:A:337:GLU:OE1	1:A:344:VAL:HG22	0.80	1.75	19	1
1:A:462:LEU:HD11	1:A:466:SER:CB	0.79	2.07	15	3
1:A:364:TYR:N	1:A:365:PRO:CD	0.79	2.46	12	3
1:A:328:LEU:HD13	1:A:329:PRO:HD2	0.79	1.54	10	6
1:A:290:ALA:HB2	1:A:333:GLU:O	0.78	1.77	15	2
1:A:429:ILE:HD11	1:A:440:TYR:OH	0.78	1.77	15	1
1:A:336:TYR:CZ	1:A:338:ILE:HD11	0.77	2.14	10	1
1:A:347:PHE:CZ	1:A:380:ILE:HD12	0.77	2.15	5	1
1:A:288:PHE:CE2	1:A:300:PHE:CD1	0.77	2.72	4	2
1:A:281:LEU:HD13	1:A:316:THR:OG1	0.77	1.80	17	1
1:A:396:VAL:HG22	1:A:397:ASP:OD1	0.76	1.79	19	1
1:A:298:ILE:HD12	1:A:310:VAL:HG23	0.76	1.58	20	1
1:A:462:LEU:HD12	1:A:466:SER:CB	0.74	2.10	13	7
1:A:449:PHE:CE1	1:A:461:THR:HG22	0.74	2.16	14	1
1:A:462:LEU:HD12	1:A:466:SER:HB3	0.74	1.57	1	7
1:A:347:PHE:CE1	1:A:380:ILE:HD12	0.74	2.18	5	1
1:A:299:PHE:CD1	1:A:308:LEU:HD23	0.73	2.18	9	1
1:A:432:VAL:HG23	1:A:441:TYR:O	0.73	1.82	16	2
1:A:425:ILE:HD13	1:A:425:ILE:N	0.72	2.00	10	3
1:A:425:ILE:N	1:A:425:ILE:HD13	0.72	1.99	6	1
1:A:425:ILE:HG21	1:A:442:PHE:CD2	0.72	2.20	16	2
1:A:281:LEU:HD21	1:A:307:TRP:CD1	0.72	2.20	5	1
1:A:354:LEU:HD12	1:A:355:ILE:N	0.72	1.98	8	5
1:A:346:LEU:HD23	1:A:355:ILE:CD1	0.71	2.16	2	1
1:A:334:ALA:HB1	1:A:383:ALA:CB	0.71	2.15	15	2
1:A:297:LYS:HA	1:A:310:VAL:HG11	0.71	1.62	5	3
1:A:345:PHE:C	1:A:346:LEU:HD23	0.71	2.05	10	1
1:A:354:LEU:C	1:A:354:LEU:HD12	0.71	2.05	18	2
1:A:345:PHE:C	1:A:346:LEU:HD22	0.70	2.06	2	8
1:A:384:VAL:HG11	1:A:432:VAL:HG12	0.70	1.62	18	1
1:A:425:ILE:CG2	1:A:429:ILE:HD13	0.70	2.17	5	1
1:A:428:LYS:C	1:A:429:ILE:HD12	0.70	2.07	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:298:ILE:O	1:A:298:ILE:HD12	0.69	1.86	13	1
1:A:353:TRP:NE1	1:A:364:TYR:CE1	0.69	2.60	12	1
1:A:396:VAL:HG12	1:A:397:ASP:OD2	0.69	1.88	6	1
1:A:281:LEU:HD13	1:A:468:PHE:CE2	0.69	2.23	1	1
1:A:418:ILE:HG22	1:A:425:ILE:HD11	0.69	1.63	14	2
1:A:346:LEU:N	1:A:346:LEU:HD23	0.69	2.03	10	1
1:A:354:LEU:HD12	1:A:354:LEU:C	0.68	2.08	19	1
1:A:297:LYS:HA	1:A:310:VAL:HG21	0.68	1.65	20	4
1:A:304:ARG:O	1:A:320:LEU:HD12	0.68	1.89	20	1
1:A:382:ALA:HB1	1:A:432:VAL:HG22	0.68	1.64	14	3
1:A:424:GLY:HA3	1:A:458:ILE:HD11	0.68	1.64	12	3
1:A:429:ILE:HD11	1:A:442:PHE:HB3	0.68	1.66	3	3
1:A:281:LEU:HD22	1:A:468:PHE:HB3	0.67	1.65	15	1
1:A:432:VAL:CG2	1:A:442:PHE:CE1	0.67	2.77	1	2
1:A:461:THR:O	1:A:461:THR:HG22	0.67	1.89	6	1
1:A:364:TYR:CD1	1:A:364:TYR:C	0.67	2.67	12	1
1:A:354:LEU:HD13	1:A:354:LEU:C	0.67	2.09	17	1
1:A:346:LEU:CD2	1:A:355:ILE:HD13	0.67	2.18	2	1
1:A:432:VAL:HG21	1:A:442:PHE:CZ	0.67	2.24	8	2
1:A:357:ASN:O	1:A:358:LEU:HD23	0.67	1.88	4	5
1:A:418:ILE:HD13	1:A:427:PRO:O	0.67	1.90	18	2
1:A:281:LEU:HD23	1:A:307:TRP:CH2	0.66	2.25	19	2
1:A:327:THR:C	1:A:328:LEU:HD22	0.66	2.09	9	6
1:A:328:LEU:HD11	1:A:346:LEU:HD11	0.66	1.66	10	1
1:A:354:LEU:HD23	1:A:354:LEU:O	0.66	1.90	13	2
1:A:462:LEU:HD11	1:A:466:SER:HB3	0.66	1.67	15	1
1:A:399:GLN:O	1:A:418:ILE:HD11	0.65	1.91	20	5
1:A:338:ILE:HD11	1:A:385:PHE:HB3	0.65	1.66	20	1
1:A:281:LEU:HD13	1:A:468:PHE:CD2	0.65	2.26	1	1
1:A:421:ASN:ND2	1:A:422:PHE:CZ	0.65	2.65	15	1
1:A:281:LEU:CD2	1:A:468:PHE:CD1	0.65	2.79	11	1
1:A:299:PHE:CE2	1:A:308:LEU:HD23	0.65	2.26	8	2
1:A:433:PHE:CE1	1:A:443:PHE:CZ	0.65	2.85	7	1
1:A:443:PHE:CE2	1:A:448:GLN:NE2	0.64	2.65	2	3
1:A:373:PHE:CD2	1:A:373:PHE:O	0.64	2.50	20	2
1:A:328:LEU:HD11	1:A:355:ILE:HD11	0.64	1.66	14	2
1:A:299:PHE:CD2	1:A:308:LEU:HD21	0.64	2.27	3	1
1:A:291:VAL:HG23	1:A:299:PHE:O	0.64	1.93	7	1
1:A:382:ALA:HB2	1:A:431:ALA:HA	0.64	1.69	16	5
1:A:432:VAL:HG13	1:A:441:TYR:O	0.64	1.93	12	1
1:A:327:THR:HG23	1:A:327:THR:O	0.64	1.93	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:310:VAL:HG13	1:A:311:SER:N	0.64	2.08	16	1
1:A:384:VAL:CG2	1:A:432:VAL:HG13	0.63	2.23	10	2
1:A:449:PHE:CE2	1:A:461:THR:CG2	0.63	2.81	20	1
1:A:336:TYR:CE2	1:A:338:ILE:HD11	0.63	2.28	2	1
1:A:443:PHE:CE1	1:A:448:GLN:CG	0.63	2.81	15	2
1:A:281:LEU:CD2	1:A:468:PHE:CE1	0.63	2.82	11	1
1:A:355:ILE:N	1:A:355:ILE:HD12	0.63	2.09	11	4
1:A:336:TYR:CZ	1:A:345:PHE:CB	0.63	2.81	9	2
1:A:336:TYR:CE1	1:A:345:PHE:CB	0.63	2.81	2	3
1:A:369:HIS:NE2	1:A:373:PHE:CD1	0.63	2.66	16	1
1:A:369:HIS:CE1	1:A:373:PHE:CD2	0.63	2.87	16	1
1:A:384:VAL:O	1:A:392:THR:HG23	0.63	1.93	20	6
1:A:338:ILE:HD12	1:A:345:PHE:CD1	0.63	2.28	10	1
1:A:443:PHE:CD2	1:A:448:GLN:NE2	0.62	2.67	2	1
1:A:369:HIS:CE1	1:A:373:PHE:CG	0.62	2.87	16	1
1:A:291:VAL:HG22	1:A:431:ALA:CB	0.62	2.23	20	1
1:A:307:TRP:CD1	1:A:317:SER:O	0.62	2.52	18	1
1:A:328:LEU:HD21	1:A:360:PRO:HG3	0.62	1.71	9	1
1:A:298:ILE:H	1:A:310:VAL:HG11	0.62	1.55	15	4
1:A:364:TYR:N	1:A:365:PRO:HD2	0.62	2.10	12	1
1:A:332:ILE:HG23	1:A:347:PHE:O	0.62	1.94	5	1
1:A:425:ILE:HG21	1:A:442:PHE:CG	0.62	2.30	17	1
1:A:281:LEU:HD22	1:A:468:PHE:CD1	0.62	2.29	11	1
1:A:316:THR:CG2	1:A:468:PHE:CD1	0.62	2.82	6	1
1:A:400:TYR:O	1:A:400:TYR:CD1	0.61	2.53	20	1
1:A:425:ILE:HG22	1:A:429:ILE:HD13	0.61	1.71	5	1
1:A:422:PHE:O	1:A:425:ILE:HD11	0.61	1.95	6	2
1:A:338:ILE:O	1:A:338:ILE:HG23	0.61	1.95	4	7
1:A:448:GLN:NE2	1:A:462:LEU:HD21	0.61	2.09	13	1
1:A:298:ILE:HD13	1:A:300:PHE:CE2	0.61	2.31	13	1
1:A:338:ILE:HG23	1:A:338:ILE:O	0.61	1.95	13	1
1:A:434:TYR:CD2	1:A:434:TYR:O	0.61	2.53	6	2
1:A:325:TRP:HB3	1:A:328:LEU:HD23	0.61	1.72	9	8
1:A:329:PRO:O	1:A:332:ILE:HD11	0.61	1.94	12	1
1:A:282:CYS:SG	1:A:470:CYS:CB	0.61	2.89	5	1
1:A:467:TRP:O	1:A:468:PHE:CD1	0.61	2.54	18	1
1:A:395:PHE:CE2	1:A:432:VAL:HG21	0.61	2.30	14	1
1:A:462:LEU:HD11	1:A:466:SER:OG	0.61	1.95	2	2
1:A:316:THR:HG22	1:A:468:PHE:CD1	0.61	2.31	6	1
1:A:291:VAL:HG11	1:A:443:PHE:CE1	0.61	2.31	6	1
1:A:294:VAL:HG23	1:A:297:LYS:HB2	0.61	1.72	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:LEU:HD23	1:A:309:LYS:N	0.61	2.10	20	1
1:A:299:PHE:CE1	1:A:308:LEU:HD23	0.61	2.30	9	1
1:A:429:ILE:HD11	1:A:442:PHE:CD1	0.60	2.31	16	2
1:A:361:GLU:OE2	1:A:364:TYR:CE1	0.60	2.54	3	1
1:A:327:THR:O	1:A:327:THR:HG23	0.60	1.96	12	3
1:A:332:ILE:HG13	1:A:346:LEU:HD12	0.60	1.74	14	1
1:A:368:ILE:HD12	1:A:377:VAL:CG1	0.60	2.25	2	1
1:A:337:GLU:HG2	1:A:344:VAL:HG22	0.60	1.74	6	1
1:A:297:LYS:HA	1:A:310:VAL:HG23	0.60	1.73	19	3
1:A:294:VAL:HG22	1:A:337:GLU:CD	0.60	2.16	17	1
1:A:361:GLU:OE1	1:A:364:TYR:CE1	0.60	2.54	10	1
1:A:332:ILE:HD13	1:A:346:LEU:HD12	0.60	1.72	5	2
1:A:298:ILE:CD1	1:A:310:VAL:HG23	0.60	2.27	20	1
1:A:336:TYR:CZ	1:A:345:PHE:CG	0.60	2.90	2	1
1:A:403:TYR:CE1	1:A:404:ASP:O	0.60	2.55	12	3
1:A:286:LEU:CD1	1:A:307:TRP:CZ2	0.60	2.83	16	1
1:A:347:PHE:CD1	1:A:347:PHE:N	0.59	2.70	10	1
1:A:336:TYR:CD1	1:A:336:TYR:C	0.59	2.75	18	2
1:A:305:PHE:CE1	1:A:320:LEU:HD12	0.59	2.31	4	3
1:A:443:PHE:CZ	1:A:448:GLN:OE1	0.59	2.55	6	2
1:A:400:TYR:CE1	1:A:401:TRP:O	0.59	2.55	5	2
1:A:466:SER:O	1:A:467:TRP:CD1	0.59	2.55	19	2
1:A:372:GLY:O	1:A:373:PHE:C	0.59	2.40	11	10
1:A:336:TYR:C	1:A:336:TYR:CD1	0.59	2.75	3	1
1:A:389:PHE:C	1:A:390:TYR:CG	0.59	2.75	14	4
1:A:293:THR:HG21	1:A:434:TYR:O	0.59	1.97	5	1
1:A:358:LEU:HD23	1:A:359:ARG:HG2	0.59	1.73	17	1
1:A:361:GLU:OE1	1:A:364:TYR:CD1	0.59	2.55	10	1
1:A:281:LEU:O	1:A:468:PHE:CZ	0.59	2.55	5	1
1:A:441:TYR:N	1:A:441:TYR:CD1	0.59	2.68	15	1
1:A:354:LEU:C	1:A:355:ILE:HD12	0.59	2.18	15	3
1:A:296:ASN:O	1:A:310:VAL:HG21	0.59	1.98	8	2
1:A:438:LYS:O	1:A:439:TYR:CD1	0.59	2.55	14	3
1:A:421:ASN:O	1:A:422:PHE:CD1	0.59	2.56	2	2
1:A:306:PHE:CD1	1:A:306:PHE:O	0.59	2.56	7	1
1:A:432:VAL:HG22	1:A:442:PHE:HB3	0.59	1.75	6	1
1:A:395:PHE:CD2	1:A:429:ILE:HG21	0.59	2.33	2	3
1:A:368:ILE:CD1	1:A:377:VAL:HG21	0.59	2.28	9	1
1:A:462:LEU:HD22	1:A:466:SER:HB2	0.58	1.73	10	1
1:A:336:TYR:CG	1:A:336:TYR:O	0.58	2.56	18	8
1:A:443:PHE:CD1	1:A:443:PHE:C	0.58	2.75	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:281:LEU:HD21	1:A:468:PHE:CE1	0.58	2.33	11	1
1:A:425:ILE:HG22	1:A:442:PHE:CZ	0.58	2.33	20	1
1:A:346:LEU:HD22	1:A:346:LEU:N	0.58	2.13	2	2
1:A:377:VAL:HG22	1:A:396:VAL:HG11	0.58	1.76	13	1
1:A:299:PHE:CZ	1:A:308:LEU:HD23	0.58	2.34	13	1
1:A:290:ALA:HB2	1:A:332:ILE:O	0.58	1.97	10	1
1:A:382:ALA:HB3	1:A:432:VAL:HG12	0.58	1.75	4	1
1:A:290:ALA:HB2	1:A:333:GLU:C	0.58	2.19	15	1
1:A:286:LEU:CD2	1:A:288:PHE:CZ	0.58	2.86	10	1
1:A:396:VAL:HG21	1:A:401:TRP:CZ3	0.58	2.33	20	1
1:A:298:ILE:HD11	1:A:309:LYS:O	0.58	1.98	13	1
1:A:421:ASN:OD1	1:A:422:PHE:CE2	0.58	2.57	7	4
1:A:372:GLY:O	1:A:373:PHE:CD2	0.58	2.57	6	1
1:A:294:VAL:O	1:A:294:VAL:HG23	0.58	1.98	18	2
1:A:352:TYR:CD1	1:A:352:TYR:C	0.58	2.77	12	1
1:A:454:LEU:HD23	1:A:455:LEU:CD2	0.58	2.29	16	1
1:A:334:ALA:HB1	1:A:383:ALA:HB3	0.57	1.74	10	2
1:A:357:ASN:C	1:A:358:LEU:HD23	0.57	2.19	2	2
1:A:352:TYR:C	1:A:352:TYR:CD1	0.57	2.76	8	3
1:A:288:PHE:CD2	1:A:300:PHE:CE1	0.57	2.92	18	1
1:A:364:TYR:CD2	1:A:365:PRO:HD3	0.57	2.34	12	1
1:A:352:TYR:CD1	1:A:368:ILE:HG23	0.57	2.34	19	2
1:A:380:ILE:HG23	1:A:395:PHE:O	0.57	1.98	5	1
1:A:373:PHE:CZ	1:A:375:ASN:O	0.57	2.57	17	1
1:A:434:TYR:O	1:A:434:TYR:CG	0.57	2.57	6	2
1:A:401:TRP:CH2	1:A:411:ASP:O	0.57	2.57	9	1
1:A:300:PHE:N	1:A:300:PHE:CD1	0.57	2.73	8	2
1:A:425:ILE:HD13	1:A:425:ILE:H	0.57	1.58	19	4
1:A:307:TRP:CZ3	1:A:468:PHE:CE1	0.57	2.92	7	1
1:A:281:LEU:O	1:A:468:PHE:CE1	0.57	2.57	5	1
1:A:432:VAL:HG21	1:A:442:PHE:CE2	0.57	2.35	5	2
1:A:328:LEU:HD12	1:A:346:LEU:HD12	0.57	1.76	4	1
1:A:343:GLN:NE2	1:A:354:LEU:HD21	0.57	2.15	3	2
1:A:425:ILE:CG2	1:A:442:PHE:CZ	0.57	2.87	6	1
1:A:362:PRO:O	1:A:363:ASN:CB	0.57	2.53	6	9
1:A:309:LYS:HB2	1:A:316:THR:HG22	0.57	1.76	16	1
1:A:292:THR:HG21	1:A:337:GLU:CD	0.57	2.20	3	1
1:A:400:TYR:C	1:A:400:TYR:CD1	0.57	2.78	10	2
1:A:468:PHE:CD1	1:A:468:PHE:C	0.57	2.79	3	2
1:A:316:THR:HG21	1:A:468:PHE:CE2	0.57	2.35	18	1
1:A:332:ILE:HD12	1:A:346:LEU:HB3	0.57	1.75	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:281:LEU:HD22	1:A:468:PHE:CB	0.57	2.30	15	1
1:A:433:PHE:CZ	1:A:441:TYR:CB	0.57	2.88	9	3
1:A:337:GLU:CB	1:A:344:VAL:HA	0.57	2.29	18	1
1:A:330:SER:O	1:A:331:GLY:C	0.56	2.42	8	2
1:A:332:ILE:CG2	1:A:335:ALA:HB2	0.56	2.30	2	1
1:A:309:LYS:HG2	1:A:316:THR:HG22	0.56	1.77	18	1
1:A:281:LEU:HD22	1:A:468:PHE:CE2	0.56	2.34	14	1
1:A:306:PHE:CD2	1:A:319:ASN:O	0.56	2.58	12	2
1:A:384:VAL:HB	1:A:432:VAL:HG23	0.56	1.76	19	2
1:A:467:TRP:O	1:A:468:PHE:CG	0.56	2.58	7	2
1:A:441:TYR:CE1	1:A:450:GLU:CG	0.56	2.88	10	2
1:A:373:PHE:CG	1:A:373:PHE:O	0.56	2.56	20	1
1:A:298:ILE:HG21	1:A:300:PHE:CZ	0.56	2.35	9	1
1:A:301:PHE:CD1	1:A:332:ILE:HD13	0.56	2.35	11	2
1:A:327:THR:HG22	1:A:327:THR:O	0.56	2.00	1	1
1:A:292:THR:HG21	1:A:337:GLU:OE1	0.56	2.00	3	1
1:A:281:LEU:CD2	1:A:307:TRP:CH2	0.56	2.88	19	1
1:A:370:SER:O	1:A:371:PHE:CG	0.56	2.59	1	3
1:A:328:LEU:HD13	1:A:329:PRO:CD	0.56	2.29	16	3
1:A:425:ILE:CD1	1:A:425:ILE:N	0.56	2.68	10	3
1:A:443:PHE:CZ	1:A:448:GLN:CD	0.56	2.78	10	2
1:A:382:ALA:CB	1:A:432:VAL:HG12	0.56	2.31	20	7
1:A:353:TRP:CH2	1:A:365:PRO:HA	0.56	2.35	5	1
1:A:433:PHE:O	1:A:433:PHE:CD1	0.56	2.59	15	2
1:A:371:PHE:CG	1:A:371:PHE:O	0.56	2.58	15	2
1:A:281:LEU:HD11	1:A:307:TRP:CE3	0.56	2.33	17	1
1:A:332:ILE:HG21	1:A:346:LEU:HD12	0.56	1.78	11	3
1:A:369:HIS:CE1	1:A:373:PHE:CD1	0.56	2.94	16	1
1:A:294:VAL:HG22	1:A:337:GLU:OE1	0.56	2.00	15	1
1:A:364:TYR:CD1	1:A:366:LYS:CE	0.56	2.88	4	3
1:A:336:TYR:OH	1:A:345:PHE:CD2	0.56	2.59	9	1
1:A:369:HIS:C	1:A:369:HIS:CD2	0.55	2.79	20	3
1:A:443:PHE:CE2	1:A:448:GLN:CG	0.55	2.89	20	1
1:A:453:PHE:CD1	1:A:453:PHE:O	0.55	2.60	4	2
1:A:288:PHE:CE1	1:A:443:PHE:CZ	0.55	2.93	18	1
1:A:299:PHE:CE2	1:A:308:LEU:HD21	0.55	2.36	11	2
1:A:325:TRP:CH2	1:A:346:LEU:HD21	0.55	2.36	19	1
1:A:336:TYR:O	1:A:336:TYR:CG	0.55	2.60	16	4
1:A:293:THR:HG22	1:A:298:ILE:HG22	0.55	1.78	5	1
1:A:307:TRP:CZ3	1:A:468:PHE:CE2	0.55	2.95	6	1
1:A:443:PHE:C	1:A:443:PHE:CD1	0.55	2.79	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:369:HIS:CE1	1:A:373:PHE:CE2	0.55	2.94	16	1
1:A:299:PHE:CE2	1:A:308:LEU:CD2	0.55	2.90	11	2
1:A:432:VAL:CG2	1:A:442:PHE:CZ	0.55	2.90	1	1
1:A:347:PHE:CD2	1:A:352:TYR:CB	0.55	2.90	10	1
1:A:462:LEU:HD21	1:A:466:SER:OG	0.55	2.00	2	1
1:A:372:GLY:O	1:A:373:PHE:CG	0.55	2.59	6	1
1:A:301:PHE:CD2	1:A:332:ILE:CG1	0.55	2.90	7	1
1:A:288:PHE:CD2	1:A:300:PHE:CD1	0.55	2.95	18	2
1:A:364:TYR:CG	1:A:365:PRO:HD3	0.55	2.37	12	1
1:A:354:LEU:C	1:A:354:LEU:HD13	0.55	2.22	3	2
1:A:286:LEU:HD22	1:A:307:TRP:CZ2	0.55	2.37	2	1
1:A:306:PHE:CD1	1:A:306:PHE:C	0.55	2.79	18	4
1:A:344:VAL:CG1	1:A:346:LEU:CD2	0.55	2.85	14	1
1:A:369:HIS:O	1:A:369:HIS:CD2	0.54	2.60	20	1
1:A:286:LEU:HD11	1:A:307:TRP:CH2	0.54	2.37	7	1
1:A:384:VAL:HG13	1:A:432:VAL:HG13	0.54	1.78	16	2
1:A:344:VAL:HG12	1:A:346:LEU:CD2	0.54	2.32	14	3
1:A:288:PHE:CE2	1:A:443:PHE:CE2	0.54	2.95	9	2
1:A:395:PHE:CD1	1:A:418:ILE:HG23	0.54	2.37	6	1
1:A:389:PHE:O	1:A:390:TYR:CD2	0.54	2.60	1	4
1:A:466:SER:O	1:A:467:TRP:CG	0.54	2.61	6	1
1:A:371:PHE:CD1	1:A:371:PHE:C	0.54	2.81	12	1
1:A:354:LEU:HD12	1:A:355:ILE:H	0.54	1.60	7	2
1:A:368:ILE:N	1:A:368:ILE:HD13	0.54	2.18	18	1
1:A:292:THR:HB	1:A:335:ALA:HB3	0.54	1.78	18	1
1:A:293:THR:HG21	1:A:435:SER:CB	0.54	2.32	9	3
1:A:439:TYR:CD1	1:A:450:GLU:OE2	0.54	2.60	2	3
1:A:355:ILE:CD1	1:A:355:ILE:N	0.54	2.70	1	2
1:A:301:PHE:CE2	1:A:332:ILE:HD13	0.54	2.38	1	1
1:A:441:TYR:CE1	1:A:450:GLU:OE1	0.54	2.61	3	1
1:A:281:LEU:CD2	1:A:307:TRP:CZ2	0.54	2.91	6	1
1:A:289:ASP:O	1:A:431:ALA:HB2	0.54	2.02	6	1
1:A:306:PHE:CD2	1:A:319:ASN:ND2	0.54	2.76	9	1
1:A:312:GLU:O	1:A:313:ARG:C	0.54	2.46	9	2
1:A:291:VAL:CG2	1:A:431:ALA:HB1	0.54	2.32	8	1
1:A:301:PHE:CE1	1:A:332:ILE:HD13	0.54	2.38	8	1
1:A:414:TYR:N	1:A:415:PRO:HD3	0.54	2.18	19	3
1:A:288:PHE:CE2	1:A:300:PHE:CG	0.54	2.96	18	1
1:A:444:GLN:CG	1:A:444:GLN:O	0.54	2.56	4	1
1:A:336:TYR:CZ	1:A:345:PHE:CD2	0.54	2.96	2	1
1:A:352:TYR:CD1	1:A:352:TYR:N	0.53	2.76	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:370:SER:O	1:A:371:PHE:CD2	0.53	2.61	6	2
1:A:374:PRO:O	1:A:375:ASN:CB	0.53	2.57	10	2
1:A:288:PHE:CG	1:A:443:PHE:CD2	0.53	2.96	18	1
1:A:412:PRO:O	1:A:413:GLY:C	0.53	2.46	16	1
1:A:336:TYR:CE1	1:A:345:PHE:HB3	0.53	2.39	9	1
1:A:433:PHE:C	1:A:433:PHE:CD1	0.53	2.81	17	2
1:A:455:LEU:HD23	1:A:455:LEU:N	0.53	2.18	14	1
1:A:429:ILE:CD1	1:A:442:PHE:CD1	0.53	2.91	16	1
1:A:306:PHE:C	1:A:306:PHE:CD1	0.53	2.82	1	2
1:A:306:PHE:C	1:A:307:TRP:CE3	0.53	2.82	18	1
1:A:337:GLU:HG3	1:A:344:VAL:HG22	0.53	1.80	12	1
1:A:298:ILE:HD12	1:A:298:ILE:C	0.53	2.23	13	1
1:A:463:LYS:CD	1:A:463:LYS:N	0.53	2.72	18	1
1:A:443:PHE:CD1	1:A:448:GLN:HG2	0.53	2.38	15	1
1:A:425:ILE:H	1:A:425:ILE:HD13	0.53	1.61	10	1
1:A:364:TYR:CD2	1:A:366:LYS:HD2	0.53	2.38	17	6
1:A:400:TYR:CE2	1:A:416:LYS:HB2	0.53	2.39	20	1
1:A:323:SER:HB3	1:A:324:LEU:HD12	0.53	1.80	16	1
1:A:308:LEU:C	1:A:308:LEU:HD23	0.53	2.24	20	1
1:A:371:PHE:O	1:A:371:PHE:CD2	0.53	2.62	20	1
1:A:308:LEU:C	1:A:308:LEU:HD13	0.52	2.25	9	1
1:A:336:TYR:CD2	1:A:338:ILE:HD11	0.52	2.39	2	1
1:A:286:LEU:CD2	1:A:307:TRP:CZ2	0.52	2.92	2	1
1:A:310:VAL:HG13	1:A:311:SER:H	0.52	1.62	18	2
1:A:298:ILE:HD12	1:A:300:PHE:CZ	0.52	2.39	6	3
1:A:439:TYR:CG	1:A:450:GLU:OE2	0.52	2.63	2	1
1:A:433:PHE:CE2	1:A:441:TYR:HB2	0.52	2.40	17	1
1:A:431:ALA:HB3	1:A:442:PHE:CE2	0.52	2.40	15	1
1:A:364:TYR:CE2	1:A:366:LYS:HD3	0.52	2.40	17	5
1:A:447:ASN:OD1	1:A:449:PHE:CD2	0.52	2.63	2	1
1:A:299:PHE:CZ	1:A:308:LEU:CD2	0.52	2.92	13	1
1:A:288:PHE:CD1	1:A:443:PHE:CD2	0.52	2.98	6	1
1:A:390:TYR:O	1:A:405:GLU:CB	0.52	2.58	20	1
1:A:332:ILE:HD12	1:A:332:ILE:N	0.52	2.19	2	1
1:A:310:VAL:O	1:A:311:SER:C	0.52	2.47	18	5
1:A:305:PHE:CD2	1:A:319:ASN:O	0.52	2.62	8	1
1:A:418:ILE:HD12	1:A:427:PRO:O	0.52	2.05	17	1
1:A:328:LEU:CD1	1:A:346:LEU:HD11	0.52	2.33	10	1
1:A:318:VAL:O	1:A:318:VAL:HG12	0.52	2.03	10	2
1:A:310:VAL:HG22	1:A:311:SER:H	0.52	1.65	17	5
1:A:449:PHE:CE2	1:A:461:THR:HG23	0.52	2.40	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:393:TYR:CD1	1:A:393:TYR:N	0.52	2.76	6	2
1:A:336:TYR:HB2	1:A:383:ALA:HB3	0.52	1.82	4	1
1:A:433:PHE:CE2	1:A:441:TYR:HB3	0.52	2.40	3	1
1:A:338:ILE:HD12	1:A:340:ALA:HB3	0.52	1.82	3	1
1:A:353:TRP:CZ3	1:A:361:GLU:O	0.52	2.63	20	2
1:A:462:LEU:CD2	1:A:467:TRP:CZ2	0.52	2.92	2	1
1:A:336:TYR:CE1	1:A:347:PHE:CE2	0.52	2.98	9	1
1:A:400:TYR:CD1	1:A:400:TYR:C	0.52	2.82	11	5
1:A:421:ASN:ND2	1:A:422:PHE:CE2	0.52	2.78	17	1
1:A:291:VAL:CG2	1:A:300:PHE:CD2	0.52	2.94	16	1
1:A:449:PHE:CD1	1:A:449:PHE:N	0.52	2.78	15	1
1:A:325:TRP:CE3	1:A:328:LEU:HD12	0.51	2.41	10	1
1:A:400:TYR:O	1:A:400:TYR:CG	0.51	2.63	10	2
1:A:462:LEU:CD1	1:A:466:SER:CB	0.51	2.88	2	1
1:A:364:TYR:CD1	1:A:366:LYS:HE3	0.51	2.40	3	10
1:A:433:PHE:CZ	1:A:441:TYR:HB2	0.51	2.39	9	1
1:A:309:LYS:C	1:A:310:VAL:HG12	0.51	2.24	8	1
1:A:281:LEU:HD23	1:A:307:TRP:CZ2	0.51	2.40	6	1
1:A:433:PHE:CZ	1:A:441:TYR:CG	0.51	2.98	3	1
1:A:384:VAL:HG11	1:A:432:VAL:CG1	0.51	2.35	12	1
1:A:337:GLU:CG	1:A:344:VAL:HG22	0.51	2.36	12	2
1:A:281:LEU:HD23	1:A:307:TRP:CZ3	0.51	2.40	19	1
1:A:310:VAL:HG13	1:A:312:GLU:H	0.51	1.66	11	1
1:A:328:LEU:HD11	1:A:346:LEU:CD1	0.51	2.36	16	1
1:A:364:TYR:CD1	1:A:366:LYS:HE2	0.51	2.40	4	3
1:A:281:LEU:O	1:A:282:CYS:CB	0.51	2.59	14	2
1:A:443:PHE:CE1	1:A:448:GLN:HG3	0.51	2.40	15	1
1:A:307:TRP:CZ3	1:A:318:VAL:N	0.51	2.78	15	1
1:A:395:PHE:CE1	1:A:418:ILE:HG23	0.51	2.41	6	1
1:A:364:TYR:CG	1:A:366:LYS:CE	0.51	2.94	1	1
1:A:462:LEU:CG	1:A:466:SER:OG	0.51	2.59	2	1
1:A:400:TYR:CE2	1:A:416:LYS:CB	0.51	2.94	20	1
1:A:348:LYS:O	1:A:349:ASP:C	0.51	2.49	13	1
1:A:443:PHE:CZ	1:A:448:GLN:HG3	0.51	2.40	16	2
1:A:310:VAL:O	1:A:313:ARG:CD	0.51	2.59	13	1
1:A:468:PHE:CD1	1:A:468:PHE:N	0.51	2.74	17	1
1:A:422:PHE:O	1:A:425:ILE:CD1	0.51	2.59	2	6
1:A:354:LEU:HD11	1:A:356:SER:OG	0.51	2.06	10	1
1:A:374:PRO:HG2	1:A:377:VAL:HG13	0.51	1.82	8	1
1:A:286:LEU:CD1	1:A:307:TRP:CH2	0.51	2.93	7	1
1:A:301:PHE:CE2	1:A:332:ILE:HG13	0.51	2.41	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:364:TYR:CE2	1:A:366:LYS:HG3	0.51	2.41	18	1
1:A:364:TYR:CE1	1:A:366:LYS:HE3	0.51	2.41	3	1
1:A:357:ASN:O	1:A:358:LEU:CD2	0.51	2.59	16	5
1:A:338:ILE:O	1:A:338:ILE:CG2	0.51	2.59	5	3
1:A:364:TYR:N	1:A:365:PRO:HD3	0.51	2.21	20	12
1:A:347:PHE:CG	1:A:380:ILE:HD12	0.51	2.41	8	1
1:A:347:PHE:CZ	1:A:380:ILE:CD1	0.50	2.94	5	1
1:A:461:THR:C	1:A:462:LEU:HD13	0.50	2.27	19	1
1:A:355:ILE:HD12	1:A:355:ILE:N	0.50	2.20	10	2
1:A:449:PHE:CZ	1:A:461:THR:HG23	0.50	2.41	20	1
1:A:337:GLU:CD	1:A:344:VAL:HG22	0.50	2.26	19	1
1:A:442:PHE:CZ	1:A:449:PHE:CB	0.50	2.94	20	1
1:A:391:ARG:CG	1:A:392:THR:N	0.50	2.74	20	1
1:A:364:TYR:CD2	1:A:366:LYS:CD	0.50	2.94	9	4
1:A:367:SER:O	1:A:370:SER:CB	0.50	2.59	20	1
1:A:389:PHE:O	1:A:390:TYR:CB	0.50	2.59	14	4
1:A:399:GLN:OE1	1:A:415:PRO:CB	0.50	2.60	20	1
1:A:387:PRO:HG3	1:A:434:TYR:CE2	0.50	2.41	7	1
1:A:394:PHE:CD1	1:A:403:TYR:CD1	0.50	2.99	4	1
1:A:443:PHE:CE1	1:A:448:GLN:HG2	0.50	2.41	2	2
1:A:453:PHE:CD1	1:A:453:PHE:C	0.50	2.84	13	1
1:A:328:LEU:HD11	1:A:355:ILE:HG12	0.50	1.83	12	1
1:A:291:VAL:HG12	1:A:300:PHE:HA	0.50	1.82	15	2
1:A:438:LYS:CG	1:A:438:LYS:O	0.50	2.60	15	3
1:A:338:ILE:HG13	1:A:385:PHE:CD2	0.50	2.42	20	1
1:A:350:ASP:O	1:A:351:LYS:CG	0.50	2.60	15	10
1:A:422:PHE:HB2	1:A:425:ILE:HD11	0.50	1.82	18	1
1:A:370:SER:O	1:A:371:PHE:CB	0.50	2.58	6	2
1:A:352:TYR:HD2	1:A:368:ILE:HG23	0.50	1.66	4	2
1:A:288:PHE:CE2	1:A:443:PHE:CZ	0.50	3.00	9	1
1:A:329:PRO:O	1:A:332:ILE:CD1	0.50	2.60	12	1
1:A:443:PHE:CE2	1:A:448:GLN:HG2	0.50	2.42	20	1
1:A:281:LEU:HD11	1:A:307:TRP:HZ3	0.50	1.58	17	1
1:A:384:VAL:CG1	1:A:432:VAL:HG13	0.50	2.36	16	1
1:A:292:THR:HG21	1:A:337:GLU:OE2	0.50	2.07	3	1
1:A:433:PHE:CE2	1:A:441:TYR:CB	0.50	2.94	3	2
1:A:432:VAL:CG2	1:A:433:PHE:N	0.50	2.75	13	1
1:A:298:ILE:HD12	1:A:310:VAL:HB	0.50	1.84	18	1
1:A:443:PHE:CD1	1:A:464:SER:HA	0.50	2.42	15	1
1:A:377:VAL:CG1	1:A:378:LYS:N	0.49	2.74	6	2
1:A:285:ASN:ND2	1:A:285:ASN:N	0.49	2.58	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:374:PRO:HB3	1:A:401:TRP:CZ2	0.49	2.42	13	1
1:A:429:ILE:CD1	1:A:431:ALA:O	0.49	2.60	7	1
1:A:288:PHE:CE1	1:A:443:PHE:CE2	0.49	3.00	18	1
1:A:422:PHE:CE2	1:A:456:GLN:HG2	0.49	2.43	13	1
1:A:304:ARG:HG2	1:A:305:PHE:CD2	0.49	2.42	11	1
1:A:352:TYR:CZ	1:A:366:LYS:HB2	0.49	2.42	5	2
1:A:298:ILE:CG2	1:A:300:PHE:CZ	0.49	2.95	9	1
1:A:336:TYR:CZ	1:A:345:PHE:HB2	0.49	2.42	9	2
1:A:443:PHE:CD1	1:A:448:GLN:CG	0.49	2.95	15	1
1:A:309:LYS:CB	1:A:316:THR:HG22	0.49	2.37	10	1
1:A:281:LEU:HD11	1:A:307:TRP:CH2	0.49	2.42	11	1
1:A:350:ASP:OD1	1:A:368:ILE:HD11	0.49	2.08	1	1
1:A:310:VAL:HG22	1:A:311:SER:N	0.49	2.23	15	8
1:A:302:LYS:O	1:A:305:PHE:O	0.49	2.30	20	2
1:A:425:ILE:HG22	1:A:442:PHE:CE1	0.49	2.43	20	2
1:A:395:PHE:CD1	1:A:418:ILE:HG12	0.49	2.43	9	1
1:A:352:TYR:N	1:A:352:TYR:CD1	0.49	2.80	5	2
1:A:431:ALA:O	1:A:432:VAL:HG13	0.49	2.08	14	1
1:A:310:VAL:HG13	1:A:311:SER:OG	0.49	2.07	16	1
1:A:374:PRO:CB	1:A:401:TRP:CZ2	0.49	2.96	20	1
1:A:374:PRO:HB2	1:A:401:TRP:CZ2	0.49	2.42	20	1
1:A:294:VAL:HG12	1:A:294:VAL:O	0.49	2.07	9	2
1:A:425:ILE:CG2	1:A:442:PHE:CG	0.49	2.96	17	1
1:A:286:LEU:HD23	1:A:286:LEU:C	0.49	2.27	1	1
1:A:429:ILE:HG12	1:A:442:PHE:CD1	0.49	2.42	13	2
1:A:458:ILE:HG22	1:A:458:ILE:O	0.49	2.07	11	1
1:A:421:ASN:OD1	1:A:422:PHE:CD2	0.49	2.66	7	2
1:A:436:LYS:HG2	1:A:441:TYR:CE1	0.49	2.43	13	1
1:A:345:PHE:CE2	1:A:352:TYR:CE1	0.49	3.01	11	1
1:A:355:ILE:O	1:A:355:ILE:HG22	0.49	2.07	7	1
1:A:462:LEU:CD1	1:A:466:SER:OG	0.49	2.61	2	1
1:A:318:VAL:HG12	1:A:318:VAL:O	0.49	2.08	7	1
1:A:288:PHE:CE2	1:A:300:PHE:CE1	0.49	3.01	4	2
1:A:398:ASN:O	1:A:417:LEU:CD1	0.49	2.61	14	2
1:A:462:LEU:HD11	1:A:466:SER:HB2	0.49	1.83	2	1
1:A:286:LEU:HD13	1:A:287:SER:N	0.49	2.22	9	1
1:A:441:TYR:CZ	1:A:450:GLU:CG	0.49	2.96	5	2
1:A:432:VAL:HG23	1:A:442:PHE:CD1	0.49	2.43	1	1
1:A:422:PHE:CE2	1:A:451:TYR:CD1	0.49	3.01	1	1
1:A:393:TYR:CE2	1:A:400:TYR:OH	0.49	2.58	15	1
1:A:441:TYR:CE1	1:A:450:GLU:HG3	0.48	2.43	14	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:428:LYS:O	1:A:444:GLN:CG	0.48	2.61	9	1
1:A:449:PHE:HB2	1:A:451:TYR:CE1	0.48	2.43	13	1
1:A:387:PRO:O	1:A:390:TYR:CE1	0.48	2.66	11	1
1:A:373:PHE:CZ	1:A:377:VAL:O	0.48	2.66	14	1
1:A:443:PHE:CZ	1:A:448:GLN:CG	0.48	2.96	16	2
1:A:453:PHE:O	1:A:453:PHE:CD1	0.48	2.67	13	2
1:A:441:TYR:CZ	1:A:450:GLU:HG2	0.48	2.43	13	1
1:A:288:PHE:CZ	1:A:443:PHE:CE2	0.48	3.01	18	1
1:A:291:VAL:HG23	1:A:433:PHE:HB3	0.48	1.86	19	1
1:A:367:SER:HB3	1:A:369:HIS:CE1	0.48	2.43	19	1
1:A:431:ALA:O	1:A:432:VAL:CG1	0.48	2.61	14	1
1:A:373:PHE:HA	1:A:377:VAL:HG12	0.48	1.85	1	1
1:A:355:ILE:N	1:A:355:ILE:CD1	0.48	2.77	11	1
1:A:374:PRO:HD2	1:A:377:VAL:HG21	0.48	1.85	12	1
1:A:306:PHE:HB3	1:A:321:ILE:HD11	0.48	1.84	19	1
1:A:373:PHE:CZ	1:A:375:ASN:HA	0.48	2.44	10	2
1:A:338:ILE:HD11	1:A:385:PHE:CB	0.48	2.38	20	1
1:A:371:PHE:CD2	1:A:371:PHE:O	0.48	2.66	11	2
1:A:364:TYR:CE1	1:A:366:LYS:CE	0.48	2.97	4	3
1:A:315:LYS:O	1:A:316:THR:CG2	0.48	2.62	3	1
1:A:443:PHE:CE1	1:A:464:SER:HB2	0.48	2.44	18	1
1:A:433:PHE:CZ	1:A:441:TYR:HB3	0.48	2.43	5	1
1:A:441:TYR:CZ	1:A:450:GLU:OE1	0.48	2.66	17	1
1:A:467:TRP:C	1:A:468:PHE:CD2	0.48	2.87	7	2
1:A:307:TRP:CZ3	1:A:468:PHE:CZ	0.48	3.02	6	2
1:A:303:ASP:O	1:A:305:PHE:N	0.48	2.44	16	2
1:A:336:TYR:O	1:A:336:TYR:CD2	0.48	2.67	5	2
1:A:374:PRO:HG2	1:A:401:TRP:CH2	0.48	2.42	1	1
1:A:449:PHE:CE2	1:A:461:THR:HG21	0.48	2.43	20	1
1:A:412:PRO:O	1:A:414:TYR:N	0.48	2.46	19	1
1:A:421:ASN:OD1	1:A:422:PHE:CZ	0.48	2.67	4	1
1:A:369:HIS:CE1	1:A:373:PHE:CE1	0.48	3.01	16	1
1:A:440:TYR:CD1	1:A:440:TYR:C	0.48	2.84	15	1
1:A:449:PHE:CZ	1:A:461:THR:CG2	0.48	2.96	20	1
1:A:425:ILE:HG21	1:A:442:PHE:CE2	0.48	2.44	6	2
1:A:462:LEU:HD13	1:A:462:LEU:N	0.48	2.24	19	1
1:A:291:VAL:CG2	1:A:300:PHE:CE2	0.48	2.94	16	1
1:A:429:ILE:HD12	1:A:444:GLN:OE1	0.48	2.08	16	1
1:A:344:VAL:HG12	1:A:346:LEU:HD22	0.48	1.86	10	1
1:A:298:ILE:O	1:A:308:LEU:CD2	0.48	2.61	9	1
1:A:297:LYS:CA	1:A:310:VAL:HG11	0.48	2.36	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:281:LEU:HB3	1:A:468:PHE:CZ	0.48	2.44	2	1
1:A:301:PHE:CD1	1:A:301:PHE:N	0.48	2.82	9	2
1:A:374:PRO:O	1:A:376:PHE:N	0.48	2.47	13	1
1:A:336:TYR:CG	1:A:337:GLU:N	0.48	2.81	19	2
1:A:354:LEU:HD22	1:A:354:LEU:O	0.48	2.09	15	1
1:A:327:THR:CG2	1:A:327:THR:O	0.47	2.62	2	3
1:A:422:PHE:HB2	1:A:425:ILE:HD12	0.47	1.86	2	1
1:A:295:GLY:O	1:A:296:ASN:CB	0.47	2.62	9	2
1:A:419:THR:O	1:A:423:GLN:N	0.47	2.47	19	2
1:A:455:LEU:O	1:A:456:GLN:CB	0.47	2.62	5	2
1:A:285:ASN:HD22	1:A:285:ASN:N	0.47	2.07	14	1
1:A:310:VAL:HG13	1:A:312:GLU:N	0.47	2.24	11	1
1:A:281:LEU:CD1	1:A:307:TRP:CZ3	0.47	2.83	17	1
1:A:354:LEU:CD1	1:A:354:LEU:C	0.47	2.81	17	1
1:A:374:PRO:HD2	1:A:377:VAL:HG12	0.47	1.85	16	1
1:A:354:LEU:HD23	1:A:361:GLU:CG	0.47	2.38	16	1
1:A:288:PHE:CD1	1:A:443:PHE:CE2	0.47	3.01	18	1
1:A:338:ILE:CG2	1:A:339:GLU:N	0.47	2.77	18	1
1:A:291:VAL:HG12	1:A:431:ALA:HB1	0.47	1.86	18	1
1:A:440:TYR:HB3	1:A:442:PHE:CE1	0.47	2.43	5	1
1:A:368:ILE:O	1:A:372:GLY:N	0.47	2.47	6	2
1:A:328:LEU:CD1	1:A:346:LEU:HD12	0.47	2.39	4	1
1:A:348:LYS:O	1:A:350:ASP:N	0.47	2.47	10	1
1:A:434:TYR:CD1	1:A:439:TYR:O	0.47	2.67	2	1
1:A:311:SER:O	1:A:312:GLU:C	0.47	2.51	17	4
1:A:288:PHE:CD2	1:A:443:PHE:CE2	0.47	3.03	18	1
1:A:364:TYR:CD1	1:A:365:PRO:N	0.47	2.83	12	1
1:A:352:TYR:CE2	1:A:366:LYS:HB2	0.47	2.45	12	1
1:A:307:TRP:CE2	1:A:318:VAL:HG12	0.47	2.44	5	1
1:A:418:ILE:CG2	1:A:425:ILE:HD11	0.47	2.39	14	2
1:A:346:LEU:N	1:A:346:LEU:CD2	0.47	2.74	10	1
1:A:298:ILE:HD12	1:A:300:PHE:HZ	0.47	1.69	3	1
1:A:407:ARG:O	1:A:408:GLN:CB	0.47	2.62	12	9
1:A:368:ILE:CD1	1:A:377:VAL:HG13	0.47	2.30	2	1
1:A:344:VAL:O	1:A:345:PHE:CD1	0.47	2.68	9	1
1:A:307:TRP:CH2	1:A:318:VAL:HG13	0.47	2.45	8	1
1:A:352:TYR:CD2	1:A:366:LYS:HB3	0.47	2.44	11	1
1:A:307:TRP:NE1	1:A:318:VAL:HG22	0.47	2.24	18	1
1:A:315:LYS:HG2	1:A:468:PHE:CE2	0.47	2.45	3	1
1:A:414:TYR:CE2	1:A:416:LYS:HG3	0.47	2.45	4	11
1:A:301:PHE:CD2	1:A:332:ILE:HB	0.47	2.45	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:316:THR:HG21	1:A:468:PHE:CD1	0.47	2.43	11	3
1:A:305:PHE:CD2	1:A:318:VAL:CG1	0.47	2.98	6	1
1:A:372:GLY:O	1:A:374:PRO:N	0.47	2.47	11	6
1:A:306:PHE:CZ	1:A:319:ASN:HB2	0.47	2.44	10	4
1:A:293:THR:HG21	1:A:435:SER:HB2	0.47	1.86	3	2
1:A:418:ILE:H	1:A:418:ILE:HD12	0.47	1.68	8	2
1:A:352:TYR:CZ	1:A:366:LYS:HB3	0.47	2.45	18	8
1:A:293:THR:HG21	1:A:435:SER:OG	0.47	2.09	9	1
1:A:286:LEU:HD23	1:A:287:SER:H	0.47	1.69	11	1
1:A:459:THR:OG1	1:A:460:LYS:N	0.47	2.47	7	1
1:A:300:PHE:C	1:A:300:PHE:CD1	0.47	2.87	18	1
1:A:347:PHE:CE2	1:A:380:ILE:HB	0.47	2.45	5	1
1:A:448:GLN:O	1:A:462:LEU:CD2	0.47	2.63	5	1
1:A:461:THR:O	1:A:461:THR:CG2	0.47	2.60	6	1
1:A:347:PHE:CE2	1:A:352:TYR:CE1	0.47	3.02	6	1
1:A:343:GLN:NE2	1:A:354:LEU:HD11	0.47	2.25	14	1
1:A:369:HIS:CE1	1:A:373:PHE:CZ	0.47	3.02	16	1
1:A:352:TYR:O	1:A:352:TYR:CG	0.47	2.67	11	1
1:A:460:LYS:HE2	1:A:462:LEU:HD22	0.47	1.86	18	1
1:A:339:GLU:O	1:A:342:ASN:N	0.47	2.48	18	1
1:A:418:ILE:HG22	1:A:425:ILE:CD1	0.47	2.39	14	1
1:A:364:TYR:CD2	1:A:366:LYS:HD3	0.47	2.44	6	2
1:A:434:TYR:CE1	1:A:439:TYR:O	0.47	2.68	2	1
1:A:375:ASN:O	1:A:376:PHE:C	0.47	2.54	13	1
1:A:400:TYR:CE1	1:A:402:ARG:HG3	0.47	2.45	7	1
1:A:341:ARG:O	1:A:342:ASN:CB	0.47	2.63	19	2
1:A:448:GLN:CB	1:A:462:LEU:CD2	0.47	2.92	16	1
1:A:439:TYR:CE1	1:A:452:ASP:HB2	0.47	2.44	10	1
1:A:395:PHE:HE2	1:A:432:VAL:HG21	0.47	1.69	9	2
1:A:300:PHE:O	1:A:307:TRP:CE3	0.47	2.68	8	1
1:A:354:LEU:HD22	1:A:354:LEU:C	0.47	2.30	15	1
1:A:433:PHE:CD1	1:A:433:PHE:N	0.46	2.83	5	3
1:A:301:PHE:CE1	1:A:321:ILE:HG12	0.46	2.45	2	1
1:A:298:ILE:CG2	1:A:300:PHE:CE1	0.46	2.98	9	1
1:A:301:PHE:CD2	1:A:332:ILE:HG12	0.46	2.45	7	1
1:A:292:THR:HB	1:A:335:ALA:HB1	0.46	1.86	7	2
1:A:418:ILE:CD1	1:A:427:PRO:O	0.46	2.63	17	3
1:A:403:TYR:CE2	1:A:405:GLU:OE2	0.46	2.67	6	1
1:A:307:TRP:CE2	1:A:316:THR:CB	0.46	2.98	14	1
1:A:460:LYS:O	1:A:461:THR:HG23	0.46	2.10	3	1
1:A:418:ILE:O	1:A:420:LYS:N	0.46	2.48	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:451:TYR:CE1	1:A:456:GLN:HA	0.46	2.45	6	1
1:A:306:PHE:CE2	1:A:319:ASN:HB3	0.46	2.45	14	1
1:A:301:PHE:CZ	1:A:332:ILE:HD13	0.46	2.45	1	1
1:A:429:ILE:CD1	1:A:444:GLN:OE1	0.46	2.64	16	1
1:A:430:ASP:CB	1:A:443:PHE:O	0.46	2.64	2	5
1:A:433:PHE:CE1	1:A:441:TYR:O	0.46	2.69	9	1
1:A:364:TYR:CD2	1:A:366:LYS:HE3	0.46	2.45	8	3
1:A:461:THR:HG22	1:A:461:THR:O	0.46	2.10	18	1
1:A:436:LYS:HD3	1:A:441:TYR:CE1	0.46	2.46	10	2
1:A:308:LEU:C	1:A:308:LEU:CD2	0.46	2.84	20	1
1:A:433:PHE:N	1:A:433:PHE:CD1	0.46	2.84	1	2
1:A:391:ARG:CZ	1:A:404:ASP:OD1	0.46	2.63	9	1
1:A:288:PHE:CG	1:A:443:PHE:CE2	0.46	3.03	18	1
1:A:307:TRP:CE3	1:A:318:VAL:HB	0.46	2.46	17	1
1:A:448:GLN:CB	1:A:462:LEU:HD21	0.46	2.40	14	1
1:A:432:VAL:HG23	1:A:440:TYR:CD1	0.46	2.44	15	1
1:A:299:PHE:HB3	1:A:301:PHE:CE1	0.46	2.45	3	1
1:A:356:SER:O	1:A:358:LEU:N	0.46	2.49	6	3
1:A:311:SER:OG	1:A:312:GLU:N	0.46	2.49	9	1
1:A:422:PHE:HB3	1:A:451:TYR:CE2	0.46	2.46	8	2
1:A:460:LYS:C	1:A:461:THR:CG2	0.46	2.84	13	1
1:A:388:ARG:O	1:A:390:TYR:CE2	0.46	2.68	11	1
1:A:352:TYR:CZ	1:A:366:LYS:CB	0.46	2.99	18	2
1:A:377:VAL:HG12	1:A:378:LYS:N	0.46	2.24	10	1
1:A:380:ILE:HG22	1:A:381:ASP:N	0.46	2.26	12	3
1:A:432:VAL:HB	1:A:442:PHE:CD1	0.46	2.45	13	3
1:A:382:ALA:HB3	1:A:395:PHE:HD2	0.46	1.70	12	1
1:A:430:ASP:N	1:A:430:ASP:OD1	0.46	2.49	6	2
1:A:455:LEU:CD2	1:A:455:LEU:N	0.46	2.78	14	1
1:A:334:ALA:HB1	1:A:382:ALA:HA	0.46	1.88	4	1
1:A:329:PRO:HG3	1:A:353:TRP:CZ3	0.46	2.46	1	1
1:A:325:TRP:CG	1:A:328:LEU:CB	0.46	2.99	10	1
1:A:302:LYS:O	1:A:304:ARG:N	0.46	2.49	6	3
1:A:299:PHE:HB3	1:A:301:PHE:CZ	0.46	2.46	3	2
1:A:364:TYR:CG	1:A:366:LYS:HE3	0.46	2.46	7	4
1:A:429:ILE:CD1	1:A:442:PHE:CD2	0.46	2.98	20	1
1:A:371:PHE:O	1:A:371:PHE:CG	0.46	2.69	20	1
1:A:445:GLY:O	1:A:447:ASN:ND2	0.46	2.49	16	3
1:A:352:TYR:CD2	1:A:368:ILE:HG23	0.46	2.45	4	1
1:A:393:TYR:C	1:A:394:PHE:CD1	0.46	2.89	1	1
1:A:293:THR:HG21	1:A:435:SER:HB3	0.46	1.87	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:336:TYR:CE1	1:A:345:PHE:CG	0.46	3.04	2	1
1:A:437:ASN:O	1:A:439:TYR:CD2	0.46	2.69	17	2
1:A:293:THR:O	1:A:337:GLU:CG	0.46	2.63	13	1
1:A:419:THR:HG23	1:A:420:LYS:N	0.46	2.26	18	2
1:A:449:PHE:CD1	1:A:461:THR:HG23	0.46	2.46	17	1
1:A:386:ASN:ND2	1:A:393:TYR:CE1	0.46	2.83	17	2
1:A:441:TYR:CD1	1:A:450:GLU:HG3	0.46	2.46	6	1
1:A:293:THR:HG21	1:A:435:SER:HA	0.46	1.86	14	1
1:A:385:PHE:C	1:A:385:PHE:CD1	0.46	2.89	1	1
1:A:447:ASN:OD1	1:A:449:PHE:CE2	0.46	2.69	2	1
1:A:321:ILE:O	1:A:324:LEU:N	0.46	2.47	10	5
1:A:431:ALA:HB3	1:A:443:PHE:HB2	0.46	1.87	3	1
1:A:372:GLY:C	1:A:373:PHE:CD1	0.46	2.89	20	1
1:A:352:TYR:CE1	1:A:366:LYS:HB3	0.46	2.47	9	2
1:A:338:ILE:CG2	1:A:338:ILE:O	0.46	2.64	13	1
1:A:463:LYS:O	1:A:466:SER:N	0.46	2.49	17	1
1:A:397:ASP:OD1	1:A:397:ASP:N	0.46	2.49	19	1
1:A:392:THR:HG22	1:A:393:TYR:H	0.46	1.70	19	1
1:A:318:VAL:O	1:A:318:VAL:HG13	0.46	2.11	15	1
1:A:299:PHE:CD1	1:A:308:LEU:HD21	0.45	2.47	2	1
1:A:432:VAL:HG12	1:A:442:PHE:HD1	0.45	1.71	9	1
1:A:298:ILE:CD1	1:A:300:PHE:CZ	0.45	2.90	13	1
1:A:345:PHE:O	1:A:346:LEU:HD22	0.45	2.11	5	2
1:A:441:TYR:CE2	1:A:450:GLU:HG3	0.45	2.47	5	1
1:A:433:PHE:CE2	1:A:435:SER:HB3	0.45	2.46	19	1
1:A:338:ILE:CD1	1:A:340:ALA:HB3	0.45	2.40	3	1
1:A:321:ILE:HG22	1:A:322:SER:N	0.45	2.27	20	3
1:A:354:LEU:O	1:A:354:LEU:HD13	0.45	2.11	11	1
1:A:387:PRO:HG2	1:A:434:TYR:CZ	0.45	2.47	7	1
1:A:391:ARG:NH1	1:A:404:ASP:OD2	0.45	2.50	14	1
1:A:403:TYR:CD2	1:A:410:MET:HB3	0.45	2.46	4	1
1:A:393:TYR:N	1:A:393:TYR:CD1	0.45	2.84	1	1
1:A:403:TYR:CE2	1:A:410:MET:HB3	0.45	2.45	10	2
1:A:467:TRP:O	1:A:468:PHE:C	0.45	2.55	10	2
1:A:354:LEU:C	1:A:354:LEU:CD1	0.45	2.78	18	2
1:A:281:LEU:HD21	1:A:307:TRP:CE3	0.45	2.46	17	1
1:A:395:PHE:CE2	1:A:432:VAL:HG11	0.45	2.46	17	1
1:A:293:THR:HG22	1:A:433:PHE:CE2	0.45	2.46	6	1
1:A:468:PHE:CD1	1:A:470:CYS:HB2	0.45	2.47	20	2
1:A:307:TRP:CZ3	1:A:318:VAL:HB	0.45	2.47	11	2
1:A:307:TRP:HE1	1:A:318:VAL:HG22	0.45	1.72	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:281:LEU:HA	1:A:286:LEU:HD12	0.45	1.89	17	1
1:A:297:LYS:HG2	1:A:299:PHE:CZ	0.45	2.47	19	1
1:A:291:VAL:HG11	1:A:442:PHE:HZ	0.45	1.71	15	1
1:A:302:LYS:N	1:A:305:PHE:O	0.45	2.49	1	4
1:A:336:TYR:OH	1:A:345:PHE:CG	0.45	2.64	9	1
1:A:436:LYS:HE3	1:A:441:TYR:CE2	0.45	2.46	8	1
1:A:400:TYR:CE2	1:A:418:ILE:HA	0.45	2.46	13	1
1:A:448:GLN:HB3	1:A:462:LEU:HD21	0.45	1.87	11	1
1:A:433:PHE:CE2	1:A:443:PHE:CE1	0.45	3.05	12	1
1:A:373:PHE:CD1	1:A:377:VAL:HG21	0.45	2.46	6	1
1:A:360:PRO:O	1:A:361:GLU:C	0.45	2.54	16	4
1:A:299:PHE:C	1:A:300:PHE:CG	0.45	2.90	11	1
1:A:288:PHE:CD2	1:A:443:PHE:CD1	0.45	3.04	7	1
1:A:301:PHE:O	1:A:302:LYS:C	0.45	2.54	7	1
1:A:414:TYR:N	1:A:415:PRO:CD	0.45	2.79	19	1
1:A:463:LYS:O	1:A:466:SER:CB	0.45	2.65	16	1
1:A:308:LEU:HD21	1:A:313:ARG:CZ	0.45	2.41	16	1
1:A:344:VAL:N	1:A:355:ILE:O	0.45	2.49	3	1
1:A:315:LYS:C	1:A:316:THR:HG23	0.45	2.32	3	1
1:A:418:ILE:O	1:A:419:THR:C	0.45	2.53	14	5
1:A:296:ASN:ND2	1:A:296:ASN:O	0.45	2.50	20	2
1:A:462:LEU:CD2	1:A:466:SER:OG	0.45	2.65	2	1
1:A:307:TRP:CE3	1:A:317:SER:O	0.45	2.69	11	1
1:A:298:ILE:C	1:A:299:PHE:CD1	0.45	2.90	11	2
1:A:327:THR:O	1:A:327:THR:CG2	0.45	2.63	12	1
1:A:294:VAL:O	1:A:296:ASN:N	0.45	2.49	12	2
1:A:393:TYR:CD2	1:A:400:TYR:CE1	0.45	3.05	4	2
1:A:441:TYR:CD2	1:A:448:GLN:OE1	0.45	2.69	16	1
1:A:447:ASN:ND2	1:A:447:ASN:N	0.45	2.64	20	1
1:A:463:LYS:O	1:A:464:SER:C	0.45	2.55	17	2
1:A:433:PHE:O	1:A:441:TYR:N	0.45	2.49	6	1
1:A:418:ILE:O	1:A:421:ASN:N	0.45	2.50	16	1
1:A:286:LEU:HD23	1:A:287:SER:N	0.45	2.27	20	1
1:A:338:ILE:CD1	1:A:385:PHE:CD2	0.45	3.00	6	1
1:A:336:TYR:CE2	1:A:338:ILE:CG1	0.44	3.00	10	1
1:A:328:LEU:HD23	1:A:360:PRO:HB3	0.44	1.90	10	1
1:A:443:PHE:CZ	1:A:448:GLN:NE2	0.44	2.84	9	1
1:A:364:TYR:CZ	1:A:366:LYS:HD3	0.44	2.47	15	2
1:A:425:ILE:O	1:A:444:GLN:NE2	0.44	2.49	12	1
1:A:345:PHE:CE2	1:A:354:LEU:HD13	0.44	2.48	12	1
1:A:432:VAL:HG21	1:A:442:PHE:CD2	0.44	2.47	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:354:LEU:CD1	1:A:354:LEU:N	0.44	2.80	15	1
1:A:448:GLN:HG2	1:A:462:LEU:HD23	0.44	1.88	3	1
1:A:369:HIS:CD2	1:A:369:HIS:C	0.44	2.90	12	2
1:A:344:VAL:C	1:A:345:PHE:CD1	0.44	2.91	9	1
1:A:440:TYR:N	1:A:440:TYR:CD1	0.44	2.84	7	1
1:A:305:PHE:HB3	1:A:307:TRP:CH2	0.44	2.47	18	1
1:A:425:ILE:HD13	1:A:426:GLY:H	0.44	1.73	12	1
1:A:281:LEU:HB2	1:A:468:PHE:CE2	0.44	2.47	5	1
1:A:428:LYS:O	1:A:444:GLN:NE2	0.44	2.50	4	1
1:A:380:ILE:CG2	1:A:381:ASP:N	0.44	2.81	1	1
1:A:306:PHE:CE2	1:A:319:ASN:C	0.44	2.91	2	2
1:A:291:VAL:HG13	1:A:300:PHE:CE1	0.44	2.47	9	1
1:A:384:VAL:HG11	1:A:432:VAL:HG22	0.44	1.88	4	1
1:A:286:LEU:HD11	1:A:307:TRP:CZ3	0.44	2.47	1	1
1:A:373:PHE:CZ	1:A:376:PHE:HA	0.44	2.47	1	1
1:A:368:ILE:O	1:A:371:PHE:CD1	0.44	2.69	20	1
1:A:303:ASP:O	1:A:331:GLY:N	0.44	2.49	11	2
1:A:467:TRP:C	1:A:468:PHE:CG	0.44	2.90	7	2
1:A:356:SER:O	1:A:357:ASN:CB	0.44	2.65	17	2
1:A:320:LEU:H	1:A:320:LEU:HD23	0.44	1.71	19	1
1:A:292:THR:OG1	1:A:335:ALA:CB	0.44	2.66	4	1
1:A:325:TRP:CZ3	1:A:328:LEU:HD12	0.44	2.48	10	1
1:A:384:VAL:HG23	1:A:432:VAL:HG13	0.44	1.88	10	1
1:A:444:GLN:O	1:A:447:ASN:ND2	0.44	2.50	3	3
1:A:448:GLN:O	1:A:462:LEU:HD23	0.44	2.12	11	2
1:A:462:LEU:HD12	1:A:466:SER:OG	0.44	2.12	11	1
1:A:379:LYS:O	1:A:396:VAL:HG23	0.44	2.13	5	1
1:A:447:ASN:HB3	1:A:449:PHE:CD1	0.44	2.47	6	1
1:A:449:PHE:CD1	1:A:461:THR:HG22	0.44	2.47	14	1
1:A:338:ILE:HD12	1:A:385:PHE:CE2	0.44	2.47	6	1
1:A:447:ASN:HB3	1:A:449:PHE:CE1	0.44	2.47	6	1
1:A:286:LEU:HD22	1:A:307:TRP:CZ3	0.44	2.48	19	1
1:A:394:PHE:CD2	1:A:403:TYR:CD1	0.44	3.05	10	1
1:A:391:ARG:NH1	1:A:411:ASP:OD2	0.44	2.51	3	1
1:A:312:GLU:O	1:A:314:PRO:N	0.44	2.51	7	1
1:A:306:PHE:CB	1:A:319:ASN:O	0.44	2.66	6	1
1:A:440:TYR:HB3	1:A:442:PHE:CE2	0.44	2.48	10	1
1:A:453:PHE:C	1:A:455:LEU:N	0.44	2.70	13	2
1:A:283:ASP:O	1:A:285:ASN:ND2	0.44	2.50	9	2
1:A:350:ASP:O	1:A:350:ASP:CG	0.44	2.54	9	2
1:A:300:PHE:CD1	1:A:300:PHE:N	0.44	2.86	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:281:LEU:CB	1:A:468:PHE:CD2	0.44	3.01	5	1
1:A:395:PHE:HE2	1:A:432:VAL:HG11	0.44	1.73	17	1
1:A:301:PHE:CD1	1:A:321:ILE:HD11	0.44	2.47	2	1
1:A:352:TYR:O	1:A:352:TYR:CD2	0.44	2.71	9	1
1:A:449:PHE:CD2	1:A:461:THR:CG2	0.44	3.01	13	1
1:A:306:PHE:CD1	1:A:319:ASN:O	0.44	2.70	19	1
1:A:425:ILE:CG1	1:A:426:GLY:N	0.44	2.81	1	1
1:A:448:GLN:HB3	1:A:462:LEU:CD2	0.44	2.43	16	1
1:A:329:PRO:O	1:A:330:SER:CB	0.43	2.66	19	2
1:A:300:PHE:C	1:A:301:PHE:CD1	0.43	2.91	9	1
1:A:350:ASP:OD1	1:A:369:HIS:ND1	0.43	2.50	11	1
1:A:455:LEU:O	1:A:456:GLN:C	0.43	2.56	15	4
1:A:353:TRP:CD1	1:A:364:TYR:CD1	0.43	3.06	12	1
1:A:425:ILE:CG2	1:A:442:PHE:CE1	0.43	3.01	6	1
1:A:442:PHE:N	1:A:442:PHE:CD1	0.43	2.86	6	1
1:A:348:LYS:O	1:A:351:LYS:O	0.43	2.37	16	11
1:A:305:PHE:CD2	1:A:318:VAL:HG12	0.43	2.48	8	1
1:A:313:ARG:CG	1:A:315:LYS:O	0.43	2.66	12	1
1:A:393:TYR:CB	1:A:401:TRP:O	0.43	2.66	1	1
1:A:440:TYR:CD1	1:A:440:TYR:N	0.43	2.85	10	1
1:A:465:ASN:O	1:A:468:PHE:N	0.43	2.51	18	1
1:A:358:LEU:CG	1:A:358:LEU:O	0.43	2.66	12	1
1:A:310:VAL:CG2	1:A:311:SER:N	0.43	2.81	1	2
1:A:429:ILE:CG1	1:A:442:PHE:CD1	0.43	3.01	16	1
1:A:418:ILE:C	1:A:420:LYS:N	0.43	2.70	1	5
1:A:303:ASP:O	1:A:304:ARG:CB	0.43	2.64	8	1
1:A:299:PHE:N	1:A:299:PHE:CD1	0.43	2.86	11	1
1:A:299:PHE:CD2	1:A:308:LEU:CD2	0.43	3.01	1	2
1:A:419:THR:O	1:A:423:GLN:CA	0.43	2.67	11	1
1:A:283:ASP:O	1:A:465:ASN:ND2	0.43	2.52	12	1
1:A:425:ILE:HG21	1:A:442:PHE:CD1	0.43	2.48	17	1
1:A:438:LYS:O	1:A:438:LYS:CG	0.43	2.67	4	2
1:A:403:TYR:CD1	1:A:403:TYR:C	0.43	2.91	1	1
1:A:291:VAL:CG2	1:A:442:PHE:CZ	0.43	2.90	15	1
1:A:390:TYR:O	1:A:405:GLU:N	0.43	2.50	20	1
1:A:435:SER:O	1:A:436:LYS:CB	0.43	2.66	20	2
1:A:464:SER:O	1:A:465:ASN:C	0.43	2.57	18	1
1:A:295:GLY:CA	1:A:339:GLU:OE1	0.43	2.66	18	1
1:A:292:THR:OG1	1:A:335:ALA:HB1	0.43	2.13	4	1
1:A:291:VAL:HG21	1:A:300:PHE:CZ	0.43	2.46	16	1
1:A:310:VAL:O	1:A:311:SER:O	0.43	2.36	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:384:VAL:CG1	1:A:432:VAL:HG12	0.43	2.41	18	1
1:A:424:GLY:C	1:A:425:ILE:CG2	0.43	2.86	12	1
1:A:300:PHE:O	1:A:306:PHE:CB	0.43	2.67	16	1
1:A:425:ILE:HD11	1:A:451:TYR:CD1	0.43	2.49	15	1
1:A:304:ARG:CD	1:A:304:ARG:N	0.43	2.81	10	1
1:A:294:VAL:HG13	1:A:294:VAL:O	0.43	2.14	13	1
1:A:438:LYS:CE	1:A:438:LYS:HA	0.43	2.43	5	1
1:A:332:ILE:CG2	1:A:334:ALA:O	0.43	2.66	4	1
1:A:309:LYS:CD	1:A:315:LYS:O	0.43	2.67	3	1
1:A:403:TYR:CG	1:A:403:TYR:O	0.43	2.70	20	1
1:A:346:LEU:CD2	1:A:346:LEU:N	0.43	2.81	2	1
1:A:293:THR:CG2	1:A:435:SER:OG	0.43	2.67	9	1
1:A:434:TYR:O	1:A:434:TYR:CD2	0.43	2.71	8	1
1:A:329:PRO:HG3	1:A:353:TRP:CE3	0.43	2.49	13	1
1:A:433:PHE:CE1	1:A:441:TYR:CB	0.43	3.02	18	1
1:A:364:TYR:CG	1:A:365:PRO:CD	0.43	3.02	12	1
1:A:425:ILE:HD12	1:A:442:PHE:CE2	0.43	2.48	14	1
1:A:295:GLY:O	1:A:296:ASN:OD1	0.43	2.37	14	1
1:A:296:ASN:O	1:A:296:ASN:ND2	0.43	2.52	3	1
1:A:442:PHE:CZ	1:A:449:PHE:HB2	0.43	2.49	20	1
1:A:434:TYR:CG	1:A:434:TYR:O	0.43	2.70	13	2
1:A:325:TRP:CE3	1:A:328:LEU:HG	0.43	2.48	15	1
1:A:352:TYR:CE1	1:A:366:LYS:HB2	0.43	2.48	10	1
1:A:321:ILE:O	1:A:322:SER:C	0.43	2.56	5	5
1:A:373:PHE:CZ	1:A:380:ILE:HG12	0.43	2.49	6	1
1:A:374:PRO:CG	1:A:401:TRP:CH2	0.43	3.01	1	1
1:A:430:ASP:N	1:A:443:PHE:O	0.42	2.51	10	1
1:A:362:PRO:O	1:A:363:ASN:CG	0.42	2.58	8	2
1:A:350:ASP:CG	1:A:350:ASP:O	0.42	2.56	6	2
1:A:414:TYR:CZ	1:A:416:LYS:HG3	0.42	2.49	5	1
1:A:292:THR:CG2	1:A:293:THR:N	0.42	2.81	17	1
1:A:306:PHE:CD1	1:A:321:ILE:HG13	0.42	2.49	19	1
1:A:373:PHE:N	1:A:374:PRO:HD3	0.42	2.28	20	3
1:A:412:PRO:O	1:A:413:GLY:O	0.42	2.37	16	4
1:A:467:TRP:O	1:A:469:GLY:N	0.42	2.52	11	1
1:A:338:ILE:O	1:A:341:ARG:N	0.42	2.52	20	1
1:A:401:TRP:CZ2	1:A:412:PRO:HA	0.42	2.49	18	1
1:A:442:PHE:HB2	1:A:449:PHE:CZ	0.42	2.49	5	1
1:A:325:TRP:HB3	1:A:328:LEU:CB	0.42	2.44	10	1
1:A:380:ILE:HA	1:A:396:VAL:HG22	0.42	1.90	20	1
1:A:336:TYR:CE1	1:A:345:PHE:HB2	0.42	2.49	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:384:VAL:CG1	1:A:385:PHE:N	0.42	2.82	13	1
1:A:306:PHE:CZ	1:A:319:ASN:CB	0.42	3.03	12	1
1:A:322:SER:O	1:A:324:LEU:N	0.42	2.53	19	1
1:A:344:VAL:O	1:A:355:ILE:HG22	0.42	2.13	4	1
1:A:438:LYS:HA	1:A:438:LYS:CE	0.42	2.45	16	1
1:A:440:TYR:CD1	1:A:441:TYR:N	0.42	2.87	15	1
1:A:399:GLN:CB	1:A:416:LYS:O	0.42	2.67	20	1
1:A:322:SER:O	1:A:323:SER:C	0.42	2.57	9	2
1:A:383:ALA:HB1	1:A:394:PHE:CE1	0.42	2.48	13	1
1:A:463:LYS:C	1:A:465:ASN:N	0.42	2.72	7	1
1:A:451:TYR:CD2	1:A:458:ILE:HG13	0.42	2.50	17	1
1:A:389:PHE:O	1:A:390:TYR:CG	0.42	2.72	14	2
1:A:298:ILE:C	1:A:298:ILE:HD12	0.42	2.35	4	1
1:A:431:ALA:CB	1:A:442:PHE:CE2	0.42	3.03	15	1
1:A:344:VAL:CG1	1:A:346:LEU:HD21	0.42	2.45	3	2
1:A:354:LEU:HD13	1:A:355:ILE:N	0.42	2.30	3	1
1:A:337:GLU:HB3	1:A:344:VAL:HG12	0.42	1.92	20	1
1:A:338:ILE:O	1:A:340:ALA:N	0.42	2.53	8	4
1:A:424:GLY:HA3	1:A:458:ILE:HD12	0.42	1.91	9	1
1:A:396:VAL:O	1:A:398:ASN:N	0.42	2.53	13	3
1:A:281:LEU:O	1:A:468:PHE:CE2	0.42	2.72	5	1
1:A:307:TRP:CD2	1:A:318:VAL:HB	0.42	2.50	17	1
1:A:437:ASN:O	1:A:438:LYS:C	0.42	2.58	17	1
1:A:354:LEU:O	1:A:360:PRO:CB	0.42	2.67	6	1
1:A:373:PHE:CE2	1:A:380:ILE:HG12	0.42	2.50	6	1
1:A:367:SER:O	1:A:370:SER:N	0.42	2.51	14	1
1:A:373:PHE:CE1	1:A:375:ASN:HA	0.42	2.50	4	1
1:A:337:GLU:CD	1:A:338:ILE:N	0.42	2.72	16	1
1:A:442:PHE:CZ	1:A:449:PHE:HB3	0.42	2.49	20	1
1:A:455:LEU:O	1:A:456:GLN:NE2	0.42	2.53	11	1
1:A:389:PHE:O	1:A:391:ARG:CG	0.42	2.67	11	1
1:A:307:TRP:CE2	1:A:316:THR:OG1	0.42	2.72	14	1
1:A:343:GLN:CG	1:A:355:ILE:O	0.42	2.67	1	1
1:A:329:PRO:CB	1:A:348:LYS:HD3	0.42	2.44	16	1
1:A:443:PHE:CE1	1:A:448:GLN:HB3	0.42	2.50	3	1
1:A:296:ASN:CG	1:A:296:ASN:O	0.42	2.58	3	1
1:A:467:TRP:C	1:A:469:GLY:N	0.42	2.73	11	1
1:A:373:PHE:O	1:A:373:PHE:CD2	0.42	2.73	7	1
1:A:443:PHE:CZ	1:A:464:SER:HB2	0.42	2.49	18	1
1:A:354:LEU:HD12	1:A:354:LEU:O	0.42	2.12	18	1
1:A:425:ILE:CG2	1:A:442:PHE:CD1	0.42	3.03	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:400:TYR:CD1	1:A:401:TRP:N	0.42	2.87	5	1
1:A:443:PHE:CD1	1:A:444:GLN:N	0.42	2.87	5	1
1:A:322:SER:C	1:A:324:LEU:N	0.42	2.70	19	1
1:A:396:VAL:O	1:A:397:ASP:CB	0.42	2.68	1	1
1:A:301:PHE:CZ	1:A:306:PHE:CE1	0.42	3.08	9	1
1:A:348:LYS:N	1:A:351:LYS:O	0.42	2.49	13	1
1:A:448:GLN:HG3	1:A:462:LEU:HD23	0.42	1.91	12	1
1:A:362:PRO:O	1:A:363:ASN:HB2	0.42	2.14	5	2
1:A:436:LYS:HD3	1:A:439:TYR:CD1	0.42	2.50	5	1
1:A:376:PHE:O	1:A:377:VAL:O	0.42	2.38	14	1
1:A:368:ILE:O	1:A:370:SER:N	0.42	2.53	1	1
1:A:354:LEU:HD23	1:A:361:GLU:HG2	0.42	1.90	16	1
1:A:286:LEU:HD22	1:A:288:PHE:CZ	0.42	2.50	10	1
1:A:400:TYR:CG	1:A:400:TYR:O	0.42	2.73	9	3
1:A:332:ILE:HG12	1:A:346:LEU:HD12	0.42	1.90	2	1
1:A:469:GLY:O	1:A:470:CYS:SG	0.42	2.78	8	1
1:A:307:TRP:CD1	1:A:318:VAL:HG22	0.42	2.50	12	1
1:A:455:LEU:HD11	1:A:457:ARG:HB2	0.42	1.91	5	1
1:A:380:ILE:HG22	1:A:381:ASP:H	0.42	1.75	15	1
1:A:399:GLN:O	1:A:418:ILE:CD1	0.41	2.68	10	1
1:A:352:TYR:O	1:A:352:TYR:CD1	0.41	2.73	3	2
1:A:468:PHE:CE1	1:A:470:CYS:HB2	0.41	2.50	20	2
1:A:385:PHE:CG	1:A:386:ASN:N	0.41	2.87	2	1
1:A:422:PHE:CB	1:A:425:ILE:HD11	0.41	2.45	11	1
1:A:300:PHE:CD1	1:A:301:PHE:N	0.41	2.88	18	1
1:A:422:PHE:CE1	1:A:451:TYR:CE2	0.41	3.08	18	1
1:A:433:PHE:CE1	1:A:441:TYR:HB3	0.41	2.50	18	1
1:A:369:HIS:HB2	1:A:373:PHE:CG	0.41	2.50	12	1
1:A:381:ASP:O	1:A:430:ASP:O	0.41	2.38	17	1
1:A:431:ALA:C	1:A:432:VAL:HG13	0.41	2.35	14	1
1:A:285:ASN:O	1:A:285:ASN:CG	0.41	2.58	14	1
1:A:444:GLN:CD	1:A:444:GLN:O	0.41	2.59	15	1
1:A:424:GLY:H	1:A:425:ILE:HD13	0.41	1.75	10	2
1:A:356:SER:N	1:A:359:ARG:O	0.41	2.52	10	1
1:A:377:VAL:O	1:A:378:LYS:CB	0.41	2.68	3	1
1:A:343:GLN:OE1	1:A:345:PHE:CE1	0.41	2.72	8	1
1:A:357:ASN:O	1:A:358:LEU:CG	0.41	2.68	16	1
1:A:374:PRO:O	1:A:375:ASN:CG	0.41	2.58	16	1
1:A:281:LEU:HB3	1:A:468:PHE:CE2	0.41	2.50	16	1
1:A:373:PHE:C	1:A:373:PHE:CD1	0.41	2.92	3	1
1:A:391:ARG:HG2	1:A:392:THR:N	0.41	2.30	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:436:LYS:HG3	1:A:441:TYR:CE1	0.41	2.50	2	1
1:A:321:ILE:C	1:A:323:SER:N	0.41	2.74	2	2
1:A:425:ILE:HG12	1:A:442:PHE:CD2	0.41	2.50	9	1
1:A:296:ASN:OD1	1:A:296:ASN:C	0.41	2.56	14	1
1:A:296:ASN:N	1:A:296:ASN:OD1	0.41	2.53	16	1
1:A:322:SER:O	1:A:325:TRP:O	0.41	2.38	15	1
1:A:349:ASP:O	1:A:378:LYS:O	0.41	2.39	10	1
1:A:351:LYS:CB	1:A:366:LYS:O	0.41	2.69	13	1
1:A:462:LEU:CB	1:A:466:SER:HB3	0.41	2.45	7	1
1:A:358:LEU:HD12	1:A:358:LEU:O	0.41	2.16	12	1
1:A:393:TYR:CE1	1:A:402:ARG:NE	0.41	2.88	16	1
1:A:354:LEU:HD13	1:A:354:LEU:N	0.41	2.31	15	1
1:A:307:TRP:CE3	1:A:307:TRP:HA	0.41	2.51	15	1
1:A:362:PRO:C	1:A:363:ASN:CG	0.41	2.79	8	2
1:A:372:GLY:O	1:A:373:PHE:CD1	0.41	2.73	20	1
1:A:381:ASP:CG	1:A:429:ILE:O	0.41	2.59	4	3
1:A:352:TYR:CE2	1:A:366:LYS:HB3	0.41	2.50	11	1
1:A:368:ILE:C	1:A:370:SER:N	0.41	2.73	18	2
1:A:432:VAL:CG2	1:A:442:PHE:CD2	0.41	3.04	5	1
1:A:364:TYR:CZ	1:A:366:LYS:HE3	0.41	2.49	3	1
1:A:330:SER:O	1:A:332:ILE:N	0.41	2.54	20	1
1:A:442:PHE:HB2	1:A:451:TYR:CE1	0.41	2.50	13	1
1:A:433:PHE:O	1:A:433:PHE:CG	0.41	2.73	18	1
1:A:389:PHE:CD2	1:A:402:ARG:NH1	0.41	2.88	19	1
1:A:432:VAL:HG23	1:A:442:PHE:CE1	0.41	2.48	1	1
1:A:321:ILE:HD12	1:A:330:SER:HB3	0.41	1.93	10	1
1:A:430:ASP:OD1	1:A:430:ASP:N	0.41	2.54	7	1
1:A:305:PHE:CD2	1:A:318:VAL:HB	0.41	2.50	19	1
1:A:354:LEU:CD2	1:A:361:GLU:CG	0.41	2.99	16	1
1:A:445:GLY:O	1:A:447:ASN:CG	0.41	2.59	16	1
1:A:321:ILE:O	1:A:323:SER:N	0.41	2.53	2	1
1:A:332:ILE:CG2	1:A:346:LEU:HD12	0.41	2.45	11	1
1:A:419:THR:O	1:A:423:GLN:CG	0.41	2.69	11	1
1:A:436:LYS:HD3	1:A:441:TYR:CD1	0.41	2.50	7	1
1:A:305:PHE:CB	1:A:307:TRP:CH2	0.41	3.04	18	1
1:A:396:VAL:CG1	1:A:401:TRP:CZ3	0.41	3.03	5	1
1:A:398:ASN:O	1:A:398:ASN:OD1	0.41	2.38	17	1
1:A:352:TYR:CE2	1:A:368:ILE:HG22	0.41	2.51	6	1
1:A:368:ILE:O	1:A:373:PHE:N	0.41	2.54	6	1
1:A:287:SER:O	1:A:302:LYS:CE	0.41	2.68	6	1
1:A:398:ASN:CG	1:A:398:ASN:O	0.41	2.59	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:464:SER:O	1:A:465:ASN:CG	0.41	2.59	10	1
1:A:329:PRO:HG3	1:A:353:TRP:CH2	0.41	2.51	10	1
1:A:306:PHE:CE1	1:A:319:ASN:HB2	0.41	2.51	10	1
1:A:453:PHE:O	1:A:454:LEU:C	0.41	2.59	19	2
1:A:399:GLN:CG	1:A:416:LYS:O	0.41	2.69	20	1
1:A:350:ASP:OD2	1:A:350:ASP:O	0.41	2.39	20	1
1:A:286:LEU:CD2	1:A:307:TRP:CH2	0.41	3.04	2	1
1:A:306:PHE:O	1:A:319:ASN:O	0.41	2.38	9	1
1:A:436:LYS:HE2	1:A:441:TYR:CE1	0.41	2.51	9	1
1:A:424:GLY:HA3	1:A:458:ILE:CD1	0.41	2.46	8	1
1:A:282:CYS:CA	1:A:470:CYS:SG	0.41	3.08	13	1
1:A:349:ASP:O	1:A:350:ASP:CB	0.41	2.68	13	1
1:A:328:LEU:CD1	1:A:329:PRO:HD2	0.41	2.46	11	1
1:A:281:LEU:HB3	1:A:468:PHE:CD2	0.41	2.50	5	1
1:A:393:TYR:CE1	1:A:402:ARG:NH1	0.41	2.89	19	1
1:A:467:TRP:HA	1:A:467:TRP:CE3	0.41	2.50	4	1
1:A:302:LYS:O	1:A:305:PHE:N	0.41	2.54	1	1
1:A:374:PRO:HD2	1:A:377:VAL:CG1	0.41	2.45	16	1
1:A:290:ALA:O	1:A:291:VAL:HG13	0.41	2.15	10	1
1:A:304:ARG:O	1:A:320:LEU:CD1	0.41	2.66	20	1
1:A:395:PHE:CE1	1:A:432:VAL:HG11	0.41	2.50	2	1
1:A:455:LEU:C	1:A:456:GLN:OE1	0.40	2.60	2	1
1:A:464:SER:C	1:A:466:SER:N	0.40	2.74	18	1
1:A:450:GLU:OE1	1:A:451:TYR:O	0.40	2.40	14	1
1:A:324:LEU:O	1:A:325:TRP:C	0.40	2.60	16	1
1:A:420:LYS:O	1:A:421:ASN:C	0.40	2.59	15	1
1:A:465:ASN:O	1:A:470:CYS:C	0.40	2.59	10	2
1:A:286:LEU:CD2	1:A:288:PHE:CE2	0.40	3.05	10	1
1:A:400:TYR:CZ	1:A:416:LYS:HB2	0.40	2.51	20	1
1:A:299:PHE:CZ	1:A:308:LEU:HD11	0.40	2.51	20	1
1:A:368:ILE:HD11	1:A:377:VAL:HG21	0.40	1.93	9	1
1:A:334:ALA:HB3	1:A:347:PHE:HB2	0.40	1.91	11	1
1:A:402:ARG:HB3	1:A:402:ARG:CZ	0.40	2.46	11	1
1:A:455:LEU:O	1:A:456:GLN:CD	0.40	2.59	6	1
1:A:344:VAL:HG12	1:A:346:LEU:HD23	0.40	1.93	14	1
1:A:376:PHE:O	1:A:377:VAL:C	0.40	2.59	16	1
1:A:308:LEU:HD23	1:A:317:SER:CB	0.40	2.46	16	1
1:A:462:LEU:HG	1:A:463:LYS:N	0.40	2.32	15	1
1:A:345:PHE:CE1	1:A:354:LEU:HD13	0.40	2.50	20	1
1:A:419:THR:O	1:A:422:PHE:C	0.40	2.60	13	1
1:A:383:ALA:CB	1:A:394:PHE:CE1	0.40	3.05	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:452:ASP:OD1	1:A:454:LEU:CB	0.40	2.69	18	1
1:A:433:PHE:CG	1:A:434:TYR:N	0.40	2.89	6	1
1:A:432:VAL:HA	1:A:442:PHE:CG	0.40	2.51	15	1
1:A:303:ASP:O	1:A:304:ARG:HB2	0.40	2.15	20	2
1:A:439:TYR:CD2	1:A:452:ASP:OD1	0.40	2.74	20	1
1:A:298:ILE:O	1:A:308:LEU:HD12	0.40	2.15	18	1
1:A:290:ALA:HA	1:A:431:ALA:HB2	0.40	1.93	17	1
1:A:429:ILE:HD11	1:A:442:PHE:CG	0.40	2.51	16	1
1:A:462:LEU:HD12	1:A:466:SER:HB2	0.40	1.92	16	1
1:A:455:LEU:C	1:A:456:GLN:CD	0.40	2.80	16	1
1:A:291:VAL:O	1:A:335:ALA:O	0.40	2.40	15	1
1:A:445:GLY:O	1:A:446:SER:CB	0.40	2.68	15	1
1:A:298:ILE:HD12	1:A:300:PHE:CE2	0.40	2.52	10	1
1:A:300:PHE:CE1	1:A:301:PHE:O	0.40	2.75	18	1
1:A:294:VAL:HG23	1:A:297:LYS:CB	0.40	2.45	14	1
1:A:364:TYR:CD2	1:A:366:LYS:HG2	0.40	2.51	14	1
1:A:369:HIS:C	1:A:371:PHE:N	0.40	2.74	1	1
1:A:432:VAL:HG23	1:A:440:TYR:CE1	0.40	2.51	15	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	189/194 (97%)	138±5 (73±3%)	38±5 (20±3%)	13±3 (7±1%)	3	18
All	All	3780/3880 (97%)	2753 (73%)	767 (20%)	260 (7%)	3	18

All 48 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	326	PRO	20
1	A	378	LYS	16
1	A	413	GLY	15
1	A	455	LEU	14

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Mol	Chain	Res	Type	Models (Total)
1	A	303	ASP	13
1	A	372	GLY	12
1	A	311	SER	12
1	A	436	LYS	11
1	A	373	PHE	10
1	A	282	CYS	10
1	A	285	ASN	9
1	A	376	PHE	9
1	A	310	VAL	9
1	A	374	PRO	8
1	A	371	PHE	8
1	A	425	ILE	7
1	A	438	LYS	6
1	A	363	ASN	6
1	A	467	TRP	6
1	A	377	VAL	5
1	A	295	GLY	4
1	A	332	ILE	4
1	A	321	ILE	3
1	A	419	THR	3
1	A	412	PRO	3
1	A	446	SER	3
1	A	375	ASN	3
1	A	358	LEU	3
1	A	468	PHE	2
1	A	331	GLY	2
1	A	389	PHE	2
1	A	342	ASN	2
1	A	465	ASN	2
1	A	418	ILE	2
1	A	408	GLN	2
1	A	397	ASP	2
1	A	302	LYS	1
1	A	330	SER	1
1	A	312	GLU	1
1	A	350	ASP	1
1	A	294	VAL	1
1	A	314	PRO	1
1	A	430	ASP	1
1	A	349	ASP	1
1	A	432	VAL	1
1	A	456	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	340	ALA	1
1	A	359	ARG	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/178 (98%)	128±5 (73±3%)	47±5 (27±3%)	2	22
All	All	3500/3560 (98%)	2556 (73%)	944 (27%)	2	22

All 139 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	ARG	18
1	A	410	MET	18
1	A	364	TYR	17
1	A	407	ARG	16
1	A	378	LYS	16
1	A	438	LYS	16
1	A	285	ASN	16
1	A	358	LEU	15
1	A	404	ASP	15
1	A	348	LYS	15
1	A	325	TRP	15
1	A	366	LYS	14
1	A	428	LYS	14
1	A	417	LEU	14
1	A	320	LEU	14
1	A	460	LYS	14
1	A	371	PHE	14
1	A	463	LYS	13
1	A	317	SER	13
1	A	359	ARG	13
1	A	381	ASP	13
1	A	470	CYS	13
1	A	302	LYS	13

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Mol	Chain	Res	Type	Models (Total)
1	A	354	LEU	12
1	A	397	ASP	12
1	A	411	ASP	12
1	A	457	ARG	11
1	A	376	PHE	11
1	A	289	ASP	11
1	A	308	LEU	11
1	A	443	PHE	11
1	A	430	ASP	11
1	A	369	HIS	11
1	A	313	ARG	11
1	A	379	LYS	10
1	A	447	ASN	10
1	A	323	SER	10
1	A	283	ASP	10
1	A	408	GLN	10
1	A	337	GLU	10
1	A	388	ARG	9
1	A	448	GLN	9
1	A	286	LEU	9
1	A	389	PHE	9
1	A	339	GLU	9
1	A	315	LYS	9
1	A	425	ILE	9
1	A	455	LEU	9
1	A	282	CYS	9
1	A	436	LYS	9
1	A	370	SER	9
1	A	444	GLN	8
1	A	324	LEU	8
1	A	406	ARG	8
1	A	386	ASN	8
1	A	467	TRP	8
1	A	367	SER	7
1	A	409	MET	7
1	A	450	GLU	7
1	A	399	GLN	7
1	A	400	TYR	7
1	A	303	ASP	7
1	A	435	SER	7
1	A	401	TRP	7
1	A	281	LEU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	309	LYS	7
1	A	405	GLU	7
1	A	466	SER	6
1	A	464	SER	6
1	A	357	ASN	6
1	A	341	ARG	6
1	A	333	GLU	6
1	A	310	VAL	6
1	A	328	LEU	5
1	A	462	LEU	5
1	A	345	PHE	5
1	A	429	ILE	5
1	A	322	SER	5
1	A	312	GLU	5
1	A	330	SER	5
1	A	361	GLU	4
1	A	336	TYR	4
1	A	423	GLN	4
1	A	377	VAL	4
1	A	343	GLN	4
1	A	297	LYS	4
1	A	419	THR	4
1	A	352	TYR	4
1	A	363	ASN	4
1	A	394	PHE	4
1	A	452	ASP	4
1	A	338	ILE	4
1	A	319	ASN	4
1	A	327	THR	4
1	A	311	SER	4
1	A	451	TYR	3
1	A	446	SER	3
1	A	292	THR	3
1	A	307	TRP	3
1	A	349	ASP	3
1	A	356	SER	3
1	A	300	PHE	3
1	A	402	ARG	3
1	A	441	TYR	2
1	A	468	PHE	2
1	A	346	LEU	2
1	A	368	ILE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	418	ILE	2
1	A	375	ASN	2
1	A	353	TRP	2
1	A	296	ASN	2
1	A	391	ARG	2
1	A	414	TYR	2
1	A	421	ASN	2
1	A	306	PHE	2
1	A	342	ASN	2
1	A	440	TYR	2
1	A	293	THR	1
1	A	305	PHE	1
1	A	459	THR	1
1	A	456	GLN	1
1	A	385	PHE	1
1	A	321	ILE	1
1	A	298	ILE	1
1	A	396	VAL	1
1	A	355	ILE	1
1	A	434	TYR	1
1	A	373	PHE	1
1	A	301	PHE	1
1	A	318	VAL	1
1	A	442	PHE	1
1	A	384	VAL	1
1	A	432	VAL	1
1	A	347	PHE	1
1	A	433	PHE	1
1	A	437	ASN	1
1	A	287	SER	1
1	A	350	ASP	1
1	A	393	TYR	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 [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

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

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 78% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 7414

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	2173
Number of shifts mapped to atoms	2173
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	31

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	192	$2.92 \pm 0.14$	Should be applied
$^{13}\text{C}_\beta$	184	$3.19 \pm 0.17$	Should be applied
$^{13}\text{C}'$	176	$3.15 \pm 0.12$	Should be applied
$^{15}\text{N}$	179	$0.21 \pm 0.22$	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 77%, i.e. 1972 atoms were assigned a chemical shift out of a possible 2546. 22 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	909/926 (98%)	367/368 (100%)	364/380 (96%)	178/178 (100%)
Sidechain	992/1250 (79%)	596/746 (80%)	380/438 (87%)	16/66 (24%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	71/370 (19%)	66/196 (34%)	0/167 (0%)	5/7 (71%)
Overall	1972/2546 (77%)	1029/1310 (79%)	744/985 (76%)	199/251 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1991 atoms were assigned a chemical shift out of a possible 2590. 22 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	917/944 (97%)	370/375 (99%)	368/388 (95%)	179/181 (99%)
Sidechain	1003/1276 (79%)	603/762 (79%)	384/448 (86%)	16/66 (24%)
Aromatic	71/370 (19%)	66/196 (34%)	0/167 (0%)	5/7 (71%)
Overall	1991/2590 (77%)	1039/1333 (78%)	752/1003 (75%)	200/254 (79%)

#### 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	359	ARG	CD	23.47	47.57 – 38.77	-22.4
1	A	359	ARG	CG	40.33	33.23 – 21.23	10.9
1	A	392	THR	HG23	-1.21	2.29 – -0.01	-10.2
1	A	392	THR	HG21	-1.21	2.29 – -0.01	-10.2
1	A	392	THR	HG22	-1.21	2.29 – -0.01	-10.2
1	A	369	HIS	HD2	10.35	9.28 – 4.78	7.4
1	A	450	GLU	HG3	0.75	3.31 – 1.21	-7.2
1	A	415	PRO	HB3	-0.47	3.81 – 0.21	-6.9
1	A	410	MET	CG	23.73	38.33 – 25.73	-6.6
1	A	365	PRO	CG	20.18	32.66 – 21.76	-6.4
1	A	365	PRO	HB3	-0.30	3.81 – 0.21	-6.4
1	A	359	ARG	HD2	1.65	4.27 – 1.97	-6.4
1	A	298	ILE	HG21	-0.94	2.13 – -0.57	-6.4
1	A	298	ILE	HG23	-0.94	2.13 – -0.57	-6.4
1	A	298	ILE	HG22	-0.94	2.13 – -0.57	-6.4
1	A	416	LYS	HE3	1.70	3.86 – 1.96	-6.3
1	A	297	LYS	CD	21.56	34.86 – 23.06	-6.3
1	A	359	ARG	HD3	1.54	4.36 – 1.86	-6.3
1	A	359	ARG	HG2	3.19	2.92 – 0.22	6.0
1	A	402	ARG	CG	20.12	33.23 – 21.23	-5.9
1	A	425	ILE	HG23	-0.78	2.13 – -0.57	-5.8
1	A	425	ILE	HG22	-0.78	2.13 – -0.57	-5.8

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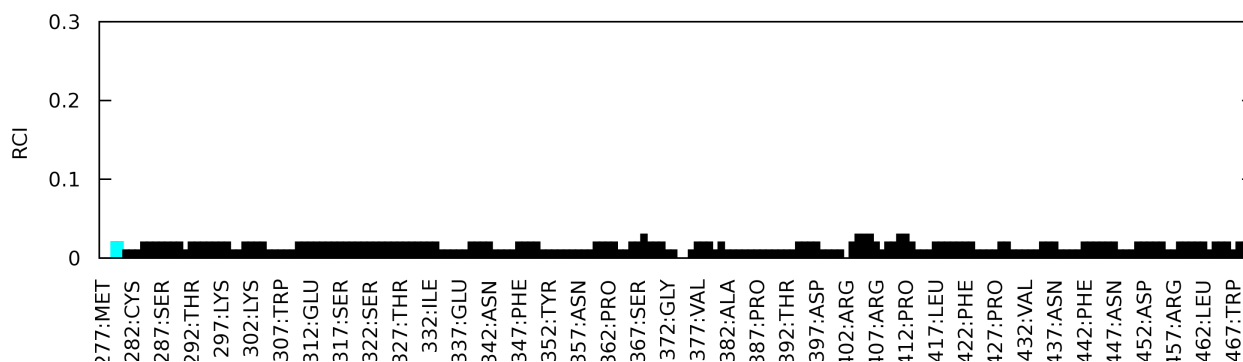
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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	425	ILE	HG21	-0.78	2.13 – -0.57	-5.8
1	A	319	ASN	HB3	0.88	4.41 – 1.11	-5.7
1	A	415	PRO	CG	21.23	32.66 – 21.76	-5.5
1	A	359	ARG	HG3	3.13	3.00 – 0.10	5.5
1	A	427	PRO	CG	21.31	32.66 – 21.76	-5.4
1	A	448	GLN	HG3	0.82	3.75 – 0.85	-5.1
1	A	380	ILE	HD13	-0.79	2.13 – -0.77	-5.1
1	A	380	ILE	HD12	-0.79	2.13 – -0.77	-5.1
1	A	380	ILE	HD11	-0.79	2.13 – -0.77	-5.1

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

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

Random coil index (RCI) for chain A:



## 7.2 Chemical shift list 2

File name: BMRB entry 15578

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

### 7.2.1 Bookkeeping [i](#)

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

Total number of shifts	3693
------------------------	------



Number of shifts mapped to atoms	2080
Number of unparsed shifts	0
Number of shifts with mapping errors	1613
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	19

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

- Residue not found in structure. All 1613 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	152	ARG	CD	40.569	0.3	1
A	126	SER	HB3	3.839	0.02	2
A	68	HIS	HB2	2.02	0.02	2
A	126	SER	C	170.638	0.3	1
A	109	PHE	H	9.128	0.02	1
A	76	ILE	HD12	0.903	0.02	1
A	92	HIS	CB	31.092	0.3	1
A	87	ILE	HG13	0.429	0.02	2
A	84	GLY	H	5.621	0.02	1
A	56	LEU	H	7.552	0.02	1
A	36	VAL	HG22	0.401	0.02	1
A	54	ASP	HA	4.421	0.02	1
A	43	LEU	HB2	2.013	0.02	1
A	37	TRP	NE1	128.128	0.3	1
A	75	GLY	C	171.758	0.3	1
A	78	ALA	HB1	1.003	0.02	1
A	108	LEU	CA	55.908	0.3	1
A	83	PRO	CD	47.677	0.3	1
A	70	PHE	CA	54.14	0.3	1
A	55	ILE	CG1	23.524	0.3	1
A	73	LYS	C	175.036	0.3	1
A	108	LEU	HD11	0.65	0.02	1
A	55	ILE	HG13	1.233	0.02	2
A	151	ILE	HG21	0.759	0.02	1
A	113	VAL	HG22	0.012	0.02	1
A	59	PHE	C	173.396	0.3	1
A	42	PRO	CB	29.517	0.3	1
A	21	MET	CA	50.542	0.3	1
A	110	LEU	HD23	0.691	0.02	1
A	110	LEU	CA	55.112	0.3	1
A	124	HIS	CA	52.444	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	12	TYR	H	8.546	0.02	1
A	156	SER	HA	4.169	0.02	1
A	91	ALA	HB2	0.905	0.02	1
A	38	SER	CA	58.68	0.3	1
A	67	ASP	N	120.204	0.3	1
A	10	ILE	HG23	0.276	0.02	1
A	28	TYR	HA	4.088	0.02	1
A	54	ASP	CB	38.363	0.3	1
A	157	LEU	HD22	0.532	0.02	1
A	30	ILE	CG1	24.43	0.3	1
A	144	PHE	C	171.789	0.3	1
A	125	SER	CA	52.441	0.3	1
A	17	TYR	CB	36.071	0.3	1
A	21	MET	HE2	0.306	0.02	1
A	52	MET	N	119.106	0.3	1
A	16	ASN	HB3	2.796	0.02	2
A	30	ILE	N	113.835	0.3	1
A	43	LEU	H	7.204	0.02	1
A	106	THR	CG2	21.791	0.3	1
A	81	PHE	CA	53.974	0.3	1
A	146	LEU	C	174.323	0.3	1
A	152	ARG	HG2	1.65	0.02	2
A	87	ILE	C	171.613	0.3	1
A	85	SER	CB	61.644	0.3	1
A	18	THR	N	115.752	0.3	1
A	9	TYR	C	171.18	0.3	1
A	120	LEU	H	7.639	0.02	1
A	127	ASP	C	171.04	0.3	1
A	75	GLY	CA	43.631	0.3	1
A	133	PHE	H	7.992	0.02	1
A	134	PRO	CB	24.689	0.3	1
A	120	LEU	HG	1.915	0.02	1
A	30	ILE	HG12	1.547	0.02	2
A	116	ILE	HD13	-0.609	0.02	1
A	103	SER	CA	52.091	0.3	1
A	85	SER	HB2	4.006	0.02	2
A	103	SER	HA	4.026	0.02	1
A	59	PHE	CA	54.085	0.3	1
A	6	ARG	H	7.458	0.02	1
A	100	THR	CA	52.624	0.3	1
A	57	VAL	CA	59.008	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	31	ARG	CB	27.322	0.3	1
A	14	ILE	CD1	10.326	0.3	1
A	73	LYS	HG3	1.194	0.02	2
A	12	TYR	CB	40.428	0.3	1
A	106	THR	HG23	0.203	0.02	1
A	55	ILE	HD11	0.996	0.02	1
A	70	PHE	N	120.039	0.3	1
A	69	ALA	N	123.252	0.3	1
A	111	THR	HG23	1.254	0.02	1
A	39	ASN	HB3	2.802	0.02	2
A	114	HIS	N	117.899	0.3	1
A	89	GLY	H	7.783	0.02	1
A	128	PRO	HG3	1.493	0.02	2
A	112	ALA	CB	14.414	0.3	1
A	32	LYS	CE	38.848	0.3	1
A	87	ILE	CA	59.1	0.3	1
A	13	ARG	HD2	2.89	0.02	1
A	133	PHE	CA	53.846	0.3	1
A	47	LYS	CD	27.337	0.3	1
A	125	SER	HB2	4.26	0.02	2
A	47	LYS	HA	3.314	0.02	1
A	127	ASP	CA	48.143	0.3	1
A	105	GLY	HA2	3.914	0.02	2
A	25	ASP	HB3	2.515	0.02	2
A	83	PRO	HG2	1.861	0.02	1
A	40	VAL	CG1	18.555	0.3	1
A	120	LEU	CB	39.402	0.3	1
A	77	LEU	HD21	0.181	0.02	1
A	152	ARG	CB	27.236	0.3	1
A	21	MET	HB2	2.157	0.02	2
A	18	THR	HB	3.739	0.02	1
A	97	GLU	CA	53.325	0.3	1
A	30	ILE	CA	59.172	0.3	1
A	110	LEU	HD12	0.421	0.02	1
A	69	ALA	C	177.582	0.3	1
A	57	VAL	C	172.353	0.3	1
A	135	THR	HA	4.538	0.02	1
A	131	VAL	HG21	0.934	0.02	1
A	4	VAL	HG12	0.416	0.02	1
A	66	ASP	HA	4.946	0.02	1
A	49	ASN	HD22	7.584	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	5	TRP	CB	25.732	0.3	1
A	75	GLY	N	110.629	0.3	1
A	23	ARG	HA	3.648	0.02	1
A	154	ILE	HA	4.415	0.02	1
A	23	ARG	CG	23.803	0.3	1
A	151	ILE	CG1	28.01	0.3	1
A	141	ILE	HG21	0.923	0.02	1
A	37	TRP	HA	4.688	0.02	1
A	35	GLN	HE22	6.887	0.02	1
A	102	HIS	CB	28.205	0.3	1
A	90	ASP	N	122.517	0.3	1
A	53	ALA	CB	19.466	0.3	1
A	152	ARG	HB2	1.85	0.02	2
A	77	LEU	HG	1.599	0.02	1
A	23	ARG	HG3	0.87	0.02	2
A	10	ILE	HD11	0.014	0.02	1
A	154	ILE	CG2	17.76	0.3	1
A	160	ASP	N	116.396	0.3	1
A	50	THR	HG23	0.996	0.02	1
A	121	GLY	N	106.953	0.3	1
A	67	ASP	C	172.107	0.3	1
A	135	THR	CA	59.162	0.3	1
A	83	PRO	HA	4.258	0.02	1
A	118	HIS	HD2	6.589	0.02	1
A	78	ALA	N	114.363	0.3	1
A	26	VAL	CG1	21.225	0.3	1
A	66	ASP	H	7.949	0.02	1
A	19	PRO	HB3	1.97	0.02	2
A	93	PHE	N	122.387	0.3	1
A	133	PHE	HB3	3.097	0.02	2
A	20	ASP	CG	178.21	0.3	1
A	82	GLY	HA3	4.215	0.02	2
A	102	HIS	C	173.225	0.3	1
A	146	LEU	HD23	0.62	0.02	1
A	137	LYS	HG2	1.13	0.02	1
A	157	LEU	HB3	1.726	0.02	2
A	28	TYR	HB2	3.188	0.02	2
A	105	GLY	C	170.977	0.3	1
A	100	THR	HA	4.807	0.02	1
A	56	LEU	CA	50.569	0.3	1
A	147	SER	HB3	3.777	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	67	ASP	CB	37.206	0.3	1
A	20	ASP	H	8.739	0.02	1
A	26	VAL	HG21	0.784	0.02	1
A	54	ASP	N	121.373	0.3	1
A	146	LEU	HB2	1.368	0.02	1
A	13	ARG	CD	39.796	0.3	1
A	116	ILE	CD1	9.301	0.3	1
A	58	VAL	N	126.808	0.3	1
A	106	THR	C	169.737	0.3	1
A	35	GLN	CG	31.187	0.3	1
A	40	VAL	HG13	0.807	0.02	1
A	83	PRO	HD3	3.49	0.02	2
A	61	ARG	N	118.113	0.3	1
A	26	VAL	HG23	0.784	0.02	1
A	158	TYR	HA	4.004	0.02	1
A	35	GLN	C	175.057	0.3	1
A	95	GLU	HA	4.784	0.02	1
A	128	PRO	HD3	3.625	0.02	2
A	16	ASN	HD22	6.887	0.02	1
A	57	VAL	HG12	0.605	0.02	1
A	55	ILE	CD1	11.616	0.3	1
A	84	GLY	HA3	3.534	0.02	2
A	85	SER	N	114.47	0.3	1
A	29	ALA	HB2	1.386	0.02	1
A	14	ILE	H	9.11	0.02	1
A	37	TRP	N	116.762	0.3	1
A	55	ILE	HG23	0.824	0.02	1
A	81	PHE	H	11.91	0.02	1
A	68	HIS	HA	4.524	0.02	1
A	125	SER	HA	4.709	0.02	1
A	76	ILE	HB	2.011	0.02	1
A	153	GLY	H	8.269	0.02	1
A	76	ILE	CB	35.314	0.3	1
A	152	ARG	HA	3.991	0.02	1
A	40	VAL	HG11	0.807	0.02	1
A	40	VAL	N	105.538	0.3	1
A	84	GLY	N	106.878	0.3	1
A	90	ASP	CA	53.741	0.3	1
A	150	ASP	HB3	2.722	0.02	2
A	22	ASN	HD22	6.879	0.02	1
A	116	ILE	HG23	0.064	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	54	ASP	HB2	2.869	0.02	1
A	72	GLY	N	110.15	0.3	1
A	117	GLY	C	174.779	0.3	1
A	97	GLU	HB2	1.678	0.02	1
A	58	VAL	CB	34.171	0.3	1
A	18	THR	HG23	1.301	0.02	1
A	22	ASN	CA	50.426	0.3	1
A	121	GLY	CA	41.547	0.3	1
A	61	ARG	HB2	1.545	0.02	1
A	36	VAL	H	7.579	0.02	1
A	122	LEU	CB	39.562	0.3	1
A	85	SER	C	173.297	0.3	1
A	142	ASN	CA	52.678	0.3	1
A	144	PHE	HB3	2.772	0.02	2
A	9	TYR	H	6.867	0.02	1
A	48	ILE	H	8.683	0.02	1
A	143	THR	HG23	0.999	0.02	1
A	70	PHE	CB	36.0	0.3	1
A	133	PHE	C	174.562	0.3	1
A	140	ASP	HB3	2.627	0.02	2
A	99	TRP	HB2	2.477	0.02	2
A	137	LYS	CA	52.617	0.3	1
A	12	TYR	HA	5.741	0.02	1
A	33	ALA	HA	3.827	0.02	1
A	151	ILE	HG22	0.759	0.02	1
A	146	LEU	CD2	24.082	0.3	1
A	113	VAL	HG21	0.012	0.02	1
A	42	PRO	CA	60.612	0.3	1
A	104	GLY	H	9.473	0.02	1
A	129	LYS	CE	39.711	0.3	1
A	21	MET	HA	4.477	0.02	1
A	77	LEU	CA	52.773	0.3	1
A	48	ILE	HG21	0.653	0.02	1
A	119	SER	HB2	3.401	0.02	1
A	10	ILE	CG2	14.085	0.3	1
A	77	LEU	HD12	-0.036	0.02	1
A	154	ILE	HD13	0.757	0.02	1
A	122	LEU	HB3	1.084	0.02	2
A	101	THR	HG21	0.434	0.02	1
A	54	ASP	CA	55.075	0.3	1
A	79	HIS	HA	4.757	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	70	PHE	HA	4.829	0.02	1
A	132	MET	HE2	0.364	0.02	1
A	137	LYS	HD2	1.491	0.02	1
A	80	ALA	N	122.807	0.3	1
A	73	LYS	CE	39.307	0.3	1
A	101	THR	H	7.908	0.02	1
A	144	PHE	HA	4.01	0.02	1
A	10	ILE	HA	4.04	0.02	1
A	81	PHE	CB	38.59	0.3	1
A	68	HIS	CB	27.631	0.3	1
A	117	GLY	CA	45.442	0.3	1
A	108	LEU	HD23	-0.33	0.02	1
A	129	LYS	H	8.151	0.02	1
A	37	TRP	C	177.917	0.3	1
A	69	ALA	HB2	1.189	0.02	1
A	85	SER	CA	55.943	0.3	1
A	63	ALA	CA	50.239	0.3	1
A	96	ASP	HA	4.149	0.02	1
A	87	ILE	CG1	25.333	0.3	1
A	97	GLU	N	130.48	0.3	1
A	44	LYS	C	173.352	0.3	1
A	26	VAL	CA	64.009	0.3	1
A	153	GLY	HA2	3.868	0.02	2
A	145	ARG	N	126.185	0.3	1
A	118	HIS	N	119.129	0.3	1
A	122	LEU	H	8.289	0.02	1
A	69	ALA	HB3	1.189	0.02	1
A	110	LEU	HB3	1.448	0.02	2
A	29	ALA	C	176.604	0.3	1
A	40	VAL	CA	57.522	0.3	1
A	123	GLY	HA2	4.316	0.02	2
A	131	VAL	HG13	1.121	0.02	1
A	83	PRO	C	171.928	0.3	1
A	68	HIS	C	169.937	0.3	1
A	65	GLY	N	108.634	0.3	1
A	157	LEU	CD1	22.689	0.3	1
A	148	ALA	CA	52.787	0.3	1
A	70	PHE	H	7.92	0.02	1
A	79	HIS	CA	51.16	0.3	1
A	22	ASN	HA	4.537	0.02	1
A	78	ALA	HA	4.778	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	89	GLY	N	119.477	0.3	1
A	40	VAL	HG22	1.051	0.02	1
A	36	VAL	N	116.949	0.3	1
A	151	ILE	HD11	0.648	0.02	1
A	116	ILE	H	8.806	0.02	1
A	73	LYS	HA	3.469	0.02	1
A	142	ASN	N	118.248	0.3	1
A	43	LEU	HD13	0.594	0.02	1
A	107	ASN	HD21	7.93	0.02	1
A	93	PHE	CB	38.434	0.3	1
A	17	TYR	HA	3.981	0.02	1
A	137	LYS	N	129.709	0.3	1
A	107	ASN	N	125.523	0.3	1
A	35	GLN	NE2	112.879	0.3	1
A	104	GLY	HA2	4.005	0.02	2
A	28	TYR	C	173.49	0.3	1
A	131	VAL	H	11.387	0.02	1
A	46	SER	C	168.253	0.3	1
A	68	HIS	H	7.446	0.02	1
A	39	ASN	CA	52.229	0.3	1
A	129	LYS	CB	29.213	0.3	1
A	14	ILE	HG23	-0.016	0.02	1
A	59	PHE	HA	5.275	0.02	1
A	130	ALA	N	123.681	0.3	1
A	89	GLY	HA2	4.071	0.02	2
A	93	PHE	HA	4.186	0.02	1
A	169	ASN	HB3	2.56	0.02	2
A	47	LYS	C	173.735	0.3	1
A	148	ALA	C	177.381	0.3	1
A	79	HIS	C	168.551	0.3	1
A	34	PHE	N	113.9	0.3	1
A	117	GLY	N	108.98	0.3	1
A	132	MET	CB	24.407	0.3	1
A	145	ARG	CA	51.352	0.3	1
A	60	ALA	CA	48.363	0.3	1
A	143	THR	CG2	18.57	0.3	1
A	72	GLY	C	170.435	0.3	1
A	58	VAL	HG23	0.791	0.02	1
A	125	SER	H	6.729	0.02	1
A	146	LEU	CG	28.996	0.3	1
A	151	ILE	HG13	0.796	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	120	LEU	CD2	19.032	0.3	1
A	117	GLY	HA3	2.234	0.02	2
A	23	ARG	CB	26.961	0.3	1
A	155	GLN	HE22	7.649	0.02	1
A	76	ILE	N	129.153	0.3	1
A	122	LEU	HD13	0.611	0.02	1
A	64	HIS	H	7.794	0.02	1
A	87	ILE	HG21	0.359	0.02	1
A	14	ILE	CG2	13.861	0.3	1
A	24	GLU	HB2	1.874	0.02	1
A	89	GLY	CA	43.776	0.3	1
A	13	ARG	HB2	1.496	0.02	1
A	113	VAL	CA	65.574	0.3	1
A	146	LEU	H	8.071	0.02	1
A	139	VAL	CA	56.548	0.3	1
A	154	ILE	HG12	1.471	0.02	2
A	122	LEU	N	120.575	0.3	1
A	149	ASP	HB3	2.395	0.02	2
A	113	VAL	H	8.248	0.02	1
A	91	ALA	HB1	0.905	0.02	1
A	131	VAL	CG2	17.863	0.3	1
A	12	TYR	HB2	2.861	0.02	2
A	136	TYR	HB2	2.64	0.02	2
A	36	VAL	CG1	20.036	0.3	1
A	25	ASP	HB2	2.757	0.02	2
A	29	ALA	HA	3.799	0.02	1
A	77	LEU	HB2	1.317	0.02	1
A	107	ASN	CA	52.769	0.3	1
A	107	ASN	HB2	3.046	0.02	2
A	128	PRO	HG2	1.609	0.02	2
A	57	VAL	H	8.712	0.02	1
A	120	LEU	HD11	0.206	0.02	1
A	91	ALA	HA	4.6	0.02	1
A	148	ALA	N	123.484	0.3	1
A	137	LYS	HB3	1.545	0.02	2
A	78	ALA	CA	48.606	0.3	1
A	141	ILE	CG2	14.761	0.3	1
A	109	PHE	N	119.852	0.3	1
A	31	ARG	C	177.059	0.3	1
A	26	VAL	HG11	0.875	0.02	1
A	61	ARG	C	173.16	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	32	LYS	HG2	1.481	0.02	2
A	33	ALA	CB	16.021	0.3	1
A	139	VAL	HG12	0.729	0.02	1
A	118	HIS	C	178.098	0.3	1
A	13	ARG	CA	51.743	0.3	1
A	35	GLN	CB	25.719	0.3	1
A	19	PRO	HG2	1.8	0.02	2
A	36	VAL	C	175.451	0.3	1
A	11	THR	HG22	0.968	0.02	1
A	116	ILE	HG21	0.064	0.02	1
A	150	ASP	N	118.753	0.3	1
A	148	ALA	HB3	1.348	0.02	1
A	77	LEU	H	8.452	0.02	1
A	27	ASP	H	8.3	0.02	1
A	130	ALA	H	8.124	0.02	1
A	154	ILE	C	175.368	0.3	1
A	11	THR	CA	55.86	0.3	1
A	80	ALA	HB3	1.156	0.02	1
A	36	VAL	HG12	1.014	0.02	1
A	20	ASP	HB2	2.582	0.02	2
A	43	LEU	HD23	0.54	0.02	1
A	71	ASP	CA	50.975	0.3	1
A	168	PRO	CB	29.196	0.3	1
A	149	ASP	CA	55.509	0.3	1
A	108	LEU	CD2	19.105	0.3	1
A	156	SER	CA	58.902	0.3	1
A	76	ILE	CA	59.727	0.3	1
A	138	TYR	C	172.175	0.3	1
A	53	ALA	HB1	0.836	0.02	1
A	22	ASN	HD21	7.551	0.02	1
A	98	PHE	HA	4.688	0.02	1
A	46	SER	N	116.544	0.3	1
A	129	LYS	HA	4.002	0.02	1
A	41	THR	HG21	1.379	0.02	1
A	122	LEU	HD23	0.584	0.02	1
A	88	GLY	C	171.663	0.3	1
A	156	SER	CB	59.864	0.3	1
A	27	ASP	C	176.864	0.3	1
A	108	LEU	HB3	1.403	0.02	2
A	143	THR	CB	66.707	0.3	1
A	130	ALA	HB3	1.691	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	110	LEU	H	8.738	0.02	1
A	142	ASN	CB	35.677	0.3	1
A	92	HIS	N	121.186	0.3	1
A	110	LEU	CD2	22.983	0.3	1
A	32	LYS	C	175.953	0.3	1
A	15	ASN	HB3	2.411	0.02	2
A	33	ALA	H	7.948	0.02	1
A	79	HIS	H	9.104	0.02	1
A	159	GLY	N	109.424	0.3	1
A	150	ASP	H	7.384	0.02	1
A	41	THR	C	169.788	0.3	1
A	32	LYS	CG	21.55	0.3	1
A	35	GLN	H	8.04	0.02	1
A	59	PHE	HB2	2.981	0.02	2
A	11	THR	C	171.799	0.3	1
A	21	MET	CG	29.118	0.3	1
A	14	ILE	HD13	0.878	0.02	1
A	143	THR	HG22	0.999	0.02	1
A	30	ILE	HG22	0.64	0.02	1
A	77	LEU	CB	41.185	0.3	1
A	141	ILE	C	174.349	0.3	1
A	140	ASP	CA	52.171	0.3	1
A	27	ASP	CB	37.356	0.3	1
A	130	ALA	CB	17.019	0.3	1
A	157	LEU	HD23	0.532	0.02	1
A	37	TRP	HB3	2.961	0.02	2
A	129	LYS	HG3	1.254	0.02	2
A	24	GLU	HA	4.023	0.02	1
A	33	ALA	HB1	0.986	0.02	1
A	25	ASP	CB	37.939	0.3	1
A	21	MET	C	172.078	0.3	1
A	142	ASN	HD22	7.904	0.02	1
A	17	TYR	N	114.955	0.3	1
A	52	MET	CB	29.079	0.3	1
A	118	HIS	HA	4.677	0.02	1
A	34	PHE	CB	35.926	0.3	1
A	159	GLY	HA3	3.777	0.02	2
A	116	ILE	HG13	0.184	0.02	2
A	154	ILE	N	123.062	0.3	1
A	88	GLY	CA	43.885	0.3	1
A	103	SER	H	6.877	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	144	PHE	CA	57.134	0.3	1
A	119	SER	H	8.593	0.02	1
A	95	GLU	C	173.234	0.3	1
A	65	GLY	H	7.675	0.02	1
A	90	ASP	HA	4.085	0.02	1
A	28	TYR	H	8.09	0.02	1
A	156	SER	H	8.084	0.02	1
A	145	ARG	HB3	1.309	0.02	2
A	105	GLY	H	7.801	0.02	1
A	16	ASN	H	7.718	0.02	1
A	143	THR	H	7.545	0.02	1
A	143	THR	HG21	0.999	0.02	1
A	134	PRO	N	139.453	0.3	1
A	9	TYR	CA	53.836	0.3	1
A	35	GLN	HA	4.101	0.02	1
A	43	LEU	CD1	20.207	0.3	1
A	148	ALA	CB	14.997	0.3	1
A	86	GLY	C	172.254	0.3	1
A	79	HIS	CB	28.092	0.3	1
A	141	ILE	CA	61.865	0.3	1
A	24	GLU	CA	56.726	0.3	1
A	98	PHE	C	174.583	0.3	1
A	58	VAL	CG1	18.293	0.3	1
A	40	VAL	HG21	1.051	0.02	1
A	96	ASP	N	122.597	0.3	1
A	68	HIS	HB3	2.471	0.02	2
A	31	ARG	N	119.589	0.3	1
A	158	TYR	H	7.608	0.02	1
A	31	ARG	HG2	1.65	0.02	2
A	43	LEU	HG	1.571	0.02	1
A	92	HIS	CA	48.022	0.3	1
A	58	VAL	HB	1.601	0.02	1
A	12	TYR	N	117.274	0.3	1
A	36	VAL	HG23	0.401	0.02	1
A	31	ARG	HB2	1.958	0.02	2
A	108	LEU	CB	38.199	0.3	1
A	69	ALA	CB	15.391	0.3	1
A	155	GLN	HG2	2.961	0.02	2
A	56	LEU	HG	1.519	0.02	1
A	108	LEU	HD12	0.65	0.02	1
A	112	ALA	N	123.596	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	146	LEU	HD22	0.62	0.02	1
A	106	THR	HB	2.355	0.02	1
A	55	ILE	HG12	1.379	0.02	2
A	154	ILE	HG23	1.455	0.02	1
A	121	GLY	H	8.146	0.02	1
A	122	LEU	HG	1.25	0.02	1
A	124	HIS	CB	26.77	0.3	1
A	104	GLY	HA3	3.714	0.02	2
A	99	TRP	C	172.106	0.3	1
A	129	LYS	CA	53.46	0.3	1
A	126	SER	CA	55.809	0.3	1
A	147	SER	N	117.994	0.3	1
A	56	LEU	HA	4.965	0.02	1
A	10	ILE	HG22	0.276	0.02	1
A	33	ALA	N	123.489	0.3	1
A	17	TYR	CA	55.977	0.3	1
A	120	LEU	N	113.75	0.3	1
A	156	SER	HB2	3.916	0.02	1
A	21	MET	HE3	0.306	0.02	1
A	16	ASN	HB2	2.939	0.02	2
A	124	HIS	HB2	2.951	0.02	2
A	24	GLU	C	176.605	0.3	1
A	88	GLY	N	106.059	0.3	1
A	73	LYS	CA	55.642	0.3	1
A	52	MET	HG2	1.829	0.02	1
A	92	HIS	HE1	9.175	0.02	1
A	72	GLY	HA2	4.328	0.02	2
A	152	ARG	HG3	1.496	0.02	2
A	128	PRO	CD	47.953	0.3	1
A	73	LYS	HE2	2.444	0.02	1
A	5	TRP	N	122.976	0.3	1
A	120	LEU	CD1	22.0	0.3	1
A	143	THR	HB	4.232	0.02	1
A	58	VAL	H	8.713	0.02	1
A	88	GLY	HA3	2.959	0.02	2
A	92	HIS	HD2	6.899	0.02	1
A	158	TYR	HB2	3.097	0.02	1
A	61	ARG	H	8.738	0.02	1
A	30	ILE	HG13	0.966	0.02	2
A	134	PRO	HA	3.745	0.02	1
A	116	ILE	HD12	-0.609	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	49	ASN	C	172.268	0.3	1
A	57	VAL	HG23	0.852	0.02	1
A	11	THR	H	9.097	0.02	1
A	99	TRP	CA	50.853	0.3	1
A	69	ALA	H	7.94	0.02	1
A	56	LEU	HD21	1.012	0.02	1
A	37	TRP	H	6.641	0.02	1
A	115	ALA	CA	53.084	0.3	1
A	156	SER	N	117.418	0.3	1
A	39	ASN	N	114.792	0.3	1
A	128	PRO	CB	29.1	0.3	1
A	17	TYR	C	172.355	0.3	1
A	157	LEU	HD11	0.629	0.02	1
A	23	ARG	HD3	2.47	0.02	2
A	73	LYS	HG2	1.468	0.02	2
A	131	VAL	CG1	20.531	0.3	1
A	144	PHE	N	123.197	0.3	1
A	56	LEU	N	129.919	0.3	1
A	52	MET	HA	4.36	0.02	1
A	36	VAL	CG2	18.987	0.3	1
A	107	ASN	ND2	111.286	0.3	1
A	20	ASP	CA	53.31	0.3	1
A	60	ALA	HB1	0.816	0.02	1
A	55	ILE	HD12	0.996	0.02	1
A	56	LEU	HD13	0.785	0.02	1
A	112	ALA	CA	52.335	0.3	1
A	142	ASN	HA	4.443	0.02	1
A	120	LEU	HD12	0.206	0.02	1
A	113	VAL	CG2	20.408	0.3	1
A	47	LYS	CG	22.99	0.3	1
A	141	ILE	CG1	24.352	0.3	1
A	70	PHE	HB2	4.168	0.02	2
A	126	SER	N	120.056	0.3	1
A	135	THR	H	7.884	0.02	1
A	105	GLY	HA3	3.829	0.02	2
A	137	LYS	HA	3.9	0.02	1
A	57	VAL	CG2	17.393	0.3	1
A	13	ARG	CB	32.535	0.3	1
A	94	ASP	N	120.718	0.3	1
A	152	ARG	CA	56.494	0.3	1
A	25	ASP	N	119.843	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	97	GLU	CB	28.562	0.3	1
A	113	VAL	HG13	0.587	0.02	1
A	110	LEU	HD11	0.421	0.02	1
A	73	LYS	N	124.041	0.3	1
A	56	LEU	C	172.963	0.3	1
A	16	ASN	ND2	114.847	0.3	1
A	61	ARG	CB	31.059	0.3	1
A	107	ASN	H	8.498	0.02	1
A	153	GLY	CA	44.637	0.3	1
A	15	ASN	ND2	112.162	0.3	1
A	143	THR	HA	4.281	0.02	1
A	11	THR	CB	69.955	0.3	1
A	38	SER	H	8.963	0.02	1
A	4	VAL	HG11	0.416	0.02	1
A	36	VAL	HB	1.972	0.02	1
A	138	TYR	N	123.949	0.3	1
A	31	ARG	HD2	3.178	0.02	1
A	30	ILE	HD12	0.18	0.02	1
A	71	ASP	CB	38.918	0.3	1
A	20	ASP	C	173.123	0.3	1
A	139	VAL	HA	3.789	0.02	1
A	168	PRO	CA	60.173	0.3	1
A	169	ASN	CB	35.859	0.3	1
A	99	TRP	HE3	7.123	0.02	1
A	127	ASP	HB3	2.316	0.02	2
A	21	MET	HG2	2.208	0.02	2
A	154	ILE	HB	2.053	0.02	1
A	30	ILE	C	174.488	0.3	1
A	35	GLN	HE21	7.533	0.02	1
A	99	TRP	N	116.741	0.3	1
A	110	LEU	HA	3.035	0.02	1
A	76	ILE	HG23	1.164	0.02	1
A	58	VAL	CA	58.098	0.3	1
A	51	GLY	CA	41.364	0.3	1
A	154	ILE	CG1	27.868	0.3	1
A	96	ASP	CB	37.657	0.3	1
A	113	VAL	HG12	0.587	0.02	1
A	118	HIS	H	7.123	0.02	1
A	50	THR	HG22	0.996	0.02	1
A	42	PRO	HG2	1.505	0.02	1
A	104	GLY	CA	42.184	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	119	SER	C	173.05	0.3	1
A	135	THR	CB	69.073	0.3	1
A	64	HIS	CA	54.639	0.3	1
A	14	ILE	HG13	0.661	0.02	2
A	19	PRO	HB2	2.129	0.02	2
A	22	ASN	HB3	2.641	0.02	2
A	82	GLY	HA2	4.34	0.02	2
A	108	LEU	N	131.606	0.3	1
A	49	ASN	CG	176.922	0.3	1
A	139	VAL	H	5.727	0.02	1
A	5	TRP	HE1	9.288	0.02	1
A	148	ALA	H	8.77	0.02	1
A	123	GLY	H	8.271	0.02	1
A	30	ILE	HG21	0.64	0.02	1
A	87	ILE	HD13	0.324	0.02	1
A	140	ASP	CB	39.22	0.3	1
A	124	HIS	N	115.595	0.3	1
A	109	PHE	HA	3.795	0.02	1
A	111	THR	H	7.283	0.02	1
A	18	THR	H	8.09	0.02	1
A	147	SER	HB2	4.099	0.02	2
A	67	ASP	CA	52.652	0.3	1
A	63	ALA	H	9.118	0.02	1
A	33	ALA	HB2	0.986	0.02	1
A	25	ASP	CA	54.232	0.3	1
A	14	ILE	N	127.164	0.3	1
A	26	VAL	H	7.683	0.02	1
A	137	LYS	H	7.841	0.02	1
A	52	MET	CA	52.309	0.3	1
A	153	GLY	N	106.9	0.3	1
A	81	PHE	N	131.38	0.3	1
A	128	PRO	HD2	3.932	0.02	2
A	77	LEU	CD2	18.824	0.3	1
A	15	ASN	HA	4.207	0.02	1
A	56	LEU	CD1	21.751	0.3	1
A	57	VAL	HG13	0.605	0.02	1
A	84	GLY	HA2	4.04	0.02	2
A	19	PRO	CD	47.924	0.3	1
A	76	ILE	CD1	9.716	0.3	1
A	29	ALA	HB1	1.386	0.02	1
A	132	MET	HA	4.497	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	116	ILE	C	174.612	0.3	1
A	151	ILE	H	7.888	0.02	1
A	96	ASP	H	8.161	0.02	1
A	118	HIS	CB	25.289	0.3	1
A	18	THR	C	170.997	0.3	1
A	63	ALA	HB3	1.37	0.02	1
A	48	ILE	CG1	23.295	0.3	1
A	67	ASP	H	7.98	0.02	1
A	13	ARG	HA	4.694	0.02	1
A	44	LYS	CA	51.438	0.3	1
A	137	LYS	HB2	1.472	0.02	2
A	26	VAL	C	174.401	0.3	1
A	51	GLY	HA2	4.306	0.02	2
A	24	GLU	CB	25.74	0.3	1
A	150	ASP	HB2	2.976	0.02	2
A	58	VAL	CG2	17.999	0.3	1
A	79	HIS	HD2	6.472	0.02	1
A	116	ILE	HG22	0.064	0.02	1
A	48	ILE	HG13	0.815	0.02	2
A	141	ILE	HD11	0.598	0.02	1
A	127	ASP	HA	4.62	0.02	1
A	100	THR	N	126.21	0.3	1
A	18	THR	HG22	1.301	0.02	1
A	22	ASN	CB	35.26	0.3	1
A	107	ASN	HA	4.715	0.02	1
A	55	ILE	CA	58.738	0.3	1
A	97	GLU	HA	4.349	0.02	1
A	144	PHE	HB2	2.962	0.02	2
A	147	SER	H	8.822	0.02	1
A	94	ASP	C	173.832	0.3	1
A	122	LEU	C	174.906	0.3	1
A	135	THR	HG21	1.13	0.02	1
A	61	ARG	HA	5.156	0.02	1
A	30	ILE	HA	3.429	0.02	1
A	82	GLY	CA	41.621	0.3	1
A	69	ALA	CA	50.835	0.3	1
A	96	ASP	HB3	2.588	0.02	2
A	30	ILE	HD13	0.18	0.02	1
A	111	THR	CG2	19.492	0.3	1
A	80	ALA	H	8.589	0.02	1
A	32	LYS	CD	25.0	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	116	ILE	CG2	16.179	0.3	1
A	146	LEU	CB	40.376	0.3	1
A	137	LYS	CB	31.697	0.3	1
A	50	THR	N	111.621	0.3	1
A	101	THR	N	122.666	0.3	1
A	151	ILE	HG23	0.759	0.02	1
A	43	LEU	CG	26.192	0.3	1
A	86	GLY	HA3	3.627	0.02	2
A	129	LYS	CD	26.216	0.3	1
A	102	HIS	HB2	3.136	0.02	2
A	48	ILE	HG22	0.653	0.02	1
A	4	VAL	HB	1.215	0.02	1
A	87	ILE	HA	4.13	0.02	1
A	67	ASP	HB2	2.952	0.02	1
A	10	ILE	CG1	25.467	0.3	1
A	77	LEU	HD13	-0.036	0.02	1
A	154	ILE	HD12	0.757	0.02	1
A	141	ILE	HA	3.703	0.02	1
A	109	PHE	C	172.747	0.3	1
A	46	SER	HA	4.522	0.02	1
A	114	HIS	H	6.874	0.02	1
A	132	MET	HE3	0.364	0.02	1
A	81	PHE	C	172.848	0.3	1
A	41	THR	HA	5.168	0.02	1
A	64	HIS	HA	4.702	0.02	1
A	123	GLY	N	109.69	0.3	1
A	84	GLY	C	168.95	0.3	1
A	10	ILE	HG12	0.654	0.02	2
A	4	VAL	CG1	24.761	0.3	1
A	10	ILE	HB	1.25	0.02	1
A	145	ARG	CB	30.566	0.3	1
A	120	LEU	HD22	0.732	0.02	1
A	75	GLY	HA3	3.305	0.02	2
A	92	HIS	HA	5.695	0.02	1
A	118	HIS	HB3	2.353	0.02	2
A	132	MET	N	115.3	0.3	1
A	93	PHE	C	170.893	0.3	1
A	42	PRO	C	172.744	0.3	1
A	59	PHE	H	8.296	0.02	1
A	69	ALA	HB1	1.189	0.02	1
A	151	ILE	HD13	0.648	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	138	TYR	HB2	2.923	0.02	2
A	113	VAL	C	175.735	0.3	1
A	109	PHE	HD1	6.555	0.02	3
A	48	ILE	C	172.186	0.3	1
A	120	LEU	HA	4.224	0.02	1
A	110	LEU	HB2	1.682	0.02	2
A	144	PHE	H	7.162	0.02	1
A	60	ALA	H	9.049	0.02	1
A	123	GLY	HA3	3.511	0.02	2
A	34	PHE	C	175.936	0.3	1
A	58	VAL	HG11	0.626	0.02	1
A	106	THR	H	9.101	0.02	1
A	76	ILE	HD13	0.903	0.02	1
A	74	GLY	N	121.103	0.3	1
A	99	TRP	CB	23.024	0.3	1
A	152	ARG	CG	24.38	0.3	1
A	66	ASP	C	170.985	0.3	1
A	50	THR	H	7.384	0.02	1
A	100	THR	HG23	0.939	0.02	1
A	103	SER	HB2	3.078	0.02	1
A	11	THR	HB	3.977	0.02	1
A	87	ILE	H	8.938	0.02	1
A	155	GLN	C	177.321	0.3	1
A	11	THR	CG2	19.124	0.3	1
A	55	ILE	N	124.32	0.3	1
A	106	THR	HG21	0.203	0.02	1
A	122	LEU	HD12	0.611	0.02	1
A	43	LEU	HD12	0.594	0.02	1
A	157	LEU	CA	53.831	0.3	1
A	60	ALA	HB2	0.816	0.02	1
A	82	GLY	N	105.239	0.3	1
A	111	THR	HG21	1.254	0.02	1
A	90	ASP	H	8.265	0.02	1
A	93	PHE	CA	54.121	0.3	1
A	40	VAL	C	171.526	0.3	1
A	83	PRO	CA	61.327	0.3	1
A	45	PHE	CA	52.812	0.3	1
A	32	LYS	N	118.961	0.3	1
A	160	ASP	H	7.879	0.02	1
A	113	VAL	CG1	21.065	0.3	1
A	147	SER	HA	4.418	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	112	ALA	HB3	0.953	0.02	1
A	141	ILE	CB	34.827	0.3	1
A	61	ARG	HG2	1.294	0.02	1
A	117	GLY	H	7.604	0.02	1
A	136	TYR	CA	56.066	0.3	1
A	39	ASN	CB	36.206	0.3	1
A	50	THR	C	169.819	0.3	1
A	14	ILE	HG22	-0.016	0.02	1
A	57	VAL	CG1	18.025	0.3	1
A	48	ILE	CA	56.182	0.3	1
A	15	ASN	C	171.058	0.3	1
A	71	ASP	HB2	3.009	0.02	2
A	58	VAL	C	171.925	0.3	1
A	89	GLY	HA3	3.665	0.02	2
A	77	LEU	HD23	0.181	0.02	1
A	48	ILE	HD11	0.541	0.02	1
A	39	ASN	HD22	6.917	0.02	1
A	79	HIS	HB2	3.219	0.02	2
A	97	GLU	CG	32.661	0.3	1
A	123	GLY	CA	40.113	0.3	1
A	35	GLN	N	118.904	0.3	1
A	160	ASP	HB2	2.615	0.02	2
A	115	ALA	HB1	1.06	0.02	1
A	61	ARG	CA	51.021	0.3	1
A	132	MET	CA	50.715	0.3	1
A	13	ARG	C	171.433	0.3	1
A	60	ALA	CB	20.011	0.3	1
A	99	TRP	H	7.319	0.02	1
A	107	ASN	HD22	6.255	0.02	1
A	50	THR	CB	68.127	0.3	1
A	36	VAL	CA	63.266	0.3	1
A	17	TYR	H	8.537	0.02	1
A	139	VAL	HB	1.754	0.02	1
A	23	ARG	CD	40.427	0.3	1
A	168	PRO	CD	46.964	0.3	1
A	151	ILE	HG12	1.67	0.02	2
A	117	GLY	HA2	3.768	0.02	2
A	95	GLU	HB2	1.986	0.02	2
A	47	LYS	HD2	1.65	0.02	1
A	23	ARG	CA	57.689	0.3	1
A	44	LYS	HG2	1.297	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	100	THR	HG21	0.939	0.02	1
A	95	GLU	HG3	2.097	0.02	2
A	14	ILE	CG1	25.155	0.3	1
A	136	TYR	C	171.319	0.3	1
A	134	PRO	C	171.414	0.3	1
A	77	LEU	HA	4.374	0.02	1
A	15	ASN	HD22	7.021	0.02	1
A	4	VAL	CA	59.78	0.3	1
A	105	GLY	N	108.27	0.3	1
A	72	GLY	CA	40.898	0.3	1
A	15	ASN	CA	53.577	0.3	1
A	17	TYR	HB3	2.482	0.02	2
A	31	ARG	CG	24.141	0.3	1
A	50	THR	HG21	0.996	0.02	1
A	154	ILE	HG13	1.457	0.02	2
A	48	ILE	CD1	9.75	0.3	1
A	143	THR	N	109.5	0.3	1
A	149	ASP	HB2	2.719	0.02	2
A	157	LEU	N	118.102	0.3	1
A	44	LYS	H	8.119	0.02	1
A	12	TYR	HB3	2.23	0.02	2
A	136	TYR	HB3	2.17	0.02	2
A	6	ARG	CB	27.705	0.3	1
A	83	PRO	N	133.221	0.3	1
A	49	ASN	CB	37.074	0.3	1
A	31	ARG	HB3	1.882	0.02	2
A	46	SER	HB2	3.422	0.02	2
A	136	TYR	N	127.452	0.3	1
A	159	GLY	CA	41.313	0.3	1
A	65	GLY	C	172.207	0.3	1
A	77	LEU	N	127.756	0.3	1
A	56	LEU	CG	24.39	0.3	1
A	155	GLN	HA	4.189	0.02	1
A	56	LEU	HB3	1.328	0.02	2
A	27	ASP	N	118.287	0.3	1
A	32	LYS	HG3	1.408	0.02	2
A	82	GLY	H	8.163	0.02	1
A	139	VAL	HG13	0.729	0.02	1
A	6	ARG	HA	4.423	0.02	1
A	74	GLY	C	171.413	0.3	1
A	141	ILE	HG12	1.051	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	120	LEU	CG	23.209	0.3	1
A	155	GLN	HB3	2.197	0.02	2
A	35	GLN	CA	55.576	0.3	1
A	33	ALA	C	175.821	0.3	1
A	157	LEU	HA	4.036	0.02	1
A	19	PRO	HG3	1.716	0.02	2
A	11	THR	HG23	0.968	0.02	1
A	154	ILE	CB	35.774	0.3	1
A	144	PHE	CB	36.701	0.3	1
A	58	VAL	HA	4.856	0.02	1
A	77	LEU	CD1	21.201	0.3	1
A	56	LEU	CD2	21.216	0.3	1
A	141	ILE	H	7.777	0.02	1
A	157	LEU	CB	40.492	0.3	1
A	46	SER	H	7.975	0.02	1
A	36	VAL	HG11	1.014	0.02	1
A	20	ASP	HB3	2.403	0.02	2
A	35	GLN	HG2	2.446	0.02	2
A	51	GLY	H	8.207	0.02	1
A	19	PRO	C	174.321	0.3	1
A	151	ILE	HB	1.62	0.02	1
A	108	LEU	CD1	24.797	0.3	1
A	118	HIS	CA	54.974	0.3	1
A	158	TYR	CA	56.804	0.3	1
A	14	ILE	HG12	1.609	0.02	2
A	5	TRP	C	172.235	0.3	1
A	90	ASP	C	170.711	0.3	1
A	92	HIS	H	9.018	0.02	1
A	145	ARG	HG2	1.36	0.02	2
A	44	LYS	CB	38.3	0.3	1
A	146	LEU	HG	1.32	0.02	1
A	147	SER	CB	63.168	0.3	1
A	53	ALA	HB2	0.836	0.02	1
A	65	GLY	CA	42.867	0.3	1
A	4	VAL	N	110.21	0.3	1
A	79	HIS	N	113.788	0.3	1
A	15	ASN	N	128.561	0.3	1
A	56	LEU	HD11	0.785	0.02	1
A	122	LEU	HD22	0.584	0.02	1
A	52	MET	HB2	2.406	0.02	1
A	22	ASN	HB2	2.728	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	142	ASN	C	173.703	0.3	1
A	18	THR	HG21	1.301	0.02	1
A	128	PRO	HB3	1.385	0.02	2
A	143	THR	CA	58.367	0.3	1
A	130	ALA	HB2	1.691	0.02	1
A	101	THR	C	171.412	0.3	1
A	80	ALA	HA	4.134	0.02	1
A	92	HIS	HB3	2.356	0.02	2
A	135	THR	HG22	1.13	0.02	1
A	30	ILE	HB	2.035	0.02	1
A	137	LYS	C	170.759	0.3	1
A	114	HIS	HA	4.244	0.02	1
A	83	PRO	HB2	2.123	0.02	2
A	53	ALA	H	7.904	0.02	1
A	38	SER	HB3	4.073	0.02	2
A	152	ARG	H	8.484	0.02	1
A	69	ALA	HA	4.511	0.02	1
A	116	ILE	CG1	26.482	0.3	1
A	137	LYS	CG	21.203	0.3	1
A	77	LEU	C	173.288	0.3	1
A	139	VAL	HG23	0.675	0.02	1
A	42	PRO	CG	24.247	0.3	1
A	47	LYS	N	127.558	0.3	1
A	122	LEU	HA	4.398	0.02	1
A	14	ILE	HD12	0.878	0.02	1
A	114	HIS	CA	56.08	0.3	1
A	64	HIS	HB2	4.095	0.02	2
A	99	TRP	HB3	1.777	0.02	2
A	124	HIS	HA	4.953	0.02	1
A	154	ILE	H	8.587	0.02	1
A	4	VAL	HA	4.392	0.02	1
A	27	ASP	CA	55.161	0.3	1
A	6	ARG	HB2	1.837	0.02	1
A	154	ILE	HD11	0.757	0.02	1
A	141	ILE	HB	1.768	0.02	1
A	130	ALA	CA	48.997	0.3	1
A	85	SER	H	8.293	0.02	1
A	65	GLY	HA2	3.713	0.02	2
A	76	ILE	HG12	1.628	0.02	2
A	152	ARG	HD2	3.124	0.02	1
A	131	VAL	N	130.727	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	4	VAL	CG2	24.152	0.3	1
A	68	HIS	HD2	6.444	0.02	1
A	141	ILE	CD1	10.725	0.3	1
A	159	GLY	HA2	4.208	0.02	2
A	16	ASN	HA	4.58	0.02	1
A	115	ALA	HA	4.017	0.02	1
A	126	SER	H	8.764	0.02	1
A	60	ALA	N	125.759	0.3	1
A	122	LEU	CD2	20.325	0.3	1
A	94	ASP	H	7.912	0.02	1
A	155	GLN	NE2	117.198	0.3	1
A	145	ARG	HB2	1.542	0.02	2
A	31	ARG	H	8.2	0.02	1
A	109	PHE	HD2	6.836	0.02	3
A	116	ILE	HA	3.432	0.02	1
A	95	GLU	N	120.958	0.3	1
A	73	LYS	H	8.668	0.02	1
A	86	GLY	CA	44.259	0.3	1
A	131	VAL	HG11	1.121	0.02	1
A	71	ASP	HA	4.825	0.02	1
A	151	ILE	CA	63.079	0.3	1
A	169	ASN	HA	4.775	0.02	1
A	129	LYS	N	116.552	0.3	1
A	146	LEU	HD11	1.166	0.02	1
A	112	ALA	H	9.132	0.02	1
A	35	GLN	HB2	2.158	0.02	1
A	130	ALA	C	176.866	0.3	1
A	134	PRO	HB2	1.924	0.02	1
A	27	ASP	HB3	2.585	0.02	2
A	142	ASN	HB2	2.819	0.02	2
A	122	LEU	CG	23.564	0.3	1
A	76	ILE	H	10.567	0.02	1
A	22	ASN	C	174.513	0.3	1
A	78	ALA	HB3	1.003	0.02	1
A	45	PHE	CB	39.011	0.3	1
A	49	ASN	N	119.411	0.3	1
A	155	GLN	HG3	2.913	0.02	2
A	108	LEU	HD13	0.65	0.02	1
A	115	ALA	H	8.639	0.02	1
A	39	ASN	C	174.066	0.3	1
A	106	THR	HA	3.581	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	98	PHE	CA	53.991	0.3	1
A	154	ILE	HG22	1.455	0.02	1
A	145	ARG	HD3	2.931	0.02	2
A	110	LEU	HD21	0.691	0.02	1
A	88	GLY	H	7.576	0.02	1
A	110	LEU	CG	23.361	0.3	1
A	126	SER	CB	61.315	0.3	1
A	91	ALA	CA	48.137	0.3	1
A	48	ILE	CB	37.688	0.3	1
A	10	ILE	HG21	0.276	0.02	1
A	124	HIS	C	172.617	0.3	1
A	101	THR	HA	4.544	0.02	1
A	92	HIS	C	169.965	0.3	1
A	48	ILE	HD12	0.541	0.02	1
A	39	ASN	HD21	7.524	0.02	1
A	5	TRP	H	7.929	0.02	1
A	13	ARG	N	118.851	0.3	1
A	99	TRP	NE1	126.897	0.3	1
A	97	GLU	CD	180.485	0.3	1
A	124	HIS	HB3	2.803	0.02	2
A	115	ALA	HB2	1.06	0.02	1
A	121	GLY	HA2	4.063	0.02	2
A	73	LYS	HD2	1.522	0.02	1
A	100	THR	CG2	17.802	0.3	1
A	45	PHE	HB2	2.402	0.02	2
A	108	LEU	H	8.41	0.02	1
A	66	ASP	HB2	2.786	0.02	2
A	72	GLY	HA3	4.169	0.02	2
A	102	HIS	H	7.498	0.02	1
A	11	THR	N	117.229	0.3	1
A	146	LEU	CA	51.999	0.3	1
A	74	GLY	HA2	4.111	0.02	2
A	71	ASP	N	116.247	0.3	1
A	88	GLY	HA2	3.665	0.02	2
A	169	ASN	N	119.792	0.3	1
A	100	THR	HG22	0.939	0.02	1
A	116	ILE	HD11	-0.609	0.02	1
A	122	LEU	HD11	0.611	0.02	1
A	151	ILE	N	118.9	0.3	1
A	32	LYS	HD2	0.861	0.02	2
A	48	ILE	HB	1.81	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	57	VAL	HG22	0.852	0.02	1
A	87	ILE	HG23	0.359	0.02	1
A	103	SER	C	173.13	0.3	1
A	140	ASP	HA	4.139	0.02	1
A	45	PHE	H	8.109	0.02	1
A	42	PRO	HD2	2.88	0.02	1
A	56	LEU	HD22	1.012	0.02	1
A	91	ALA	C	171.694	0.3	1
A	15	ASN	CB	38.873	0.3	1
A	115	ALA	CB	15.398	0.3	1
A	113	VAL	HG11	0.587	0.02	1
A	111	THR	HB	4.223	0.02	1
A	16	ASN	CG	175.137	0.3	1
A	95	GLU	H	8.007	0.02	1
A	100	THR	C	172.185	0.3	1
A	157	LEU	HD21	0.532	0.02	1
A	157	LEU	HD12	0.629	0.02	1
A	91	ALA	HB3	0.905	0.02	1
A	55	ILE	CG2	12.079	0.3	1
A	120	LEU	C	175.22	0.3	1
A	20	ASP	CB	39.097	0.3	1
A	129	LYS	HB2	1.689	0.02	1
A	55	ILE	HD13	0.996	0.02	1
A	49	ASN	CA	50.628	0.3	1
A	56	LEU	HD12	0.785	0.02	1
A	108	LEU	HG	0.968	0.02	1
A	62	GLY	CA	43.728	0.3	1
A	14	ILE	HA	4.217	0.02	1
A	78	ALA	C	173.574	0.3	1
A	120	LEU	HD13	0.206	0.02	1
A	73	LYS	CB	29.28	0.3	1
A	21	MET	N	113.047	0.3	1
A	86	GLY	N	112.395	0.3	1
A	70	PHE	HB3	3.105	0.02	2
A	9	TYR	HB3	2.608	0.02	2
A	140	ASP	N	119.172	0.3	1
A	79	HIS	HE1	8.032	0.02	1
A	38	SER	N	117.922	0.3	1
A	32	LYS	HA	3.802	0.02	1
A	101	THR	HG22	0.434	0.02	1
A	109	PHE	HE1	7.171	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	112	ALA	HA	3.989	0.02	1
A	44	LYS	HA	4.335	0.02	1
A	146	LEU	CD1	28.215	0.3	1
A	14	ILE	CB	33.524	0.3	1
A	40	VAL	HA	4.684	0.02	1
A	109	PHE	HB2	3.315	0.02	2
A	131	VAL	CB	28.285	0.3	1
A	148	ALA	HB1	1.348	0.02	1
A	154	ILE	CA	58.219	0.3	1
A	108	LEU	HD22	-0.33	0.02	1
A	131	VAL	HG23	0.934	0.02	1
A	71	ASP	C	174.565	0.3	1
A	80	ALA	HB1	1.156	0.02	1
A	152	ARG	C	177.87	0.3	1
A	30	ILE	HD11	0.18	0.02	1
A	15	ASN	H	9.604	0.02	1
A	145	ARG	CD	40.602	0.3	1
A	169	ASN	CA	48.443	0.3	1
A	148	ALA	HA	3.957	0.02	1
A	95	GLU	CB	26.431	0.3	1
A	127	ASP	HB2	2.911	0.02	2
A	132	MET	H	7.541	0.02	1
A	103	SER	N	115.418	0.3	1
A	141	ILE	HG23	0.923	0.02	1
A	51	GLY	HA3	3.998	0.02	2
A	129	LYS	HD3	1.562	0.02	2
A	135	THR	CG2	19.149	0.3	1
A	24	GLU	N	116.093	0.3	1
A	12	TYR	C	169.021	0.3	1
A	41	THR	HG23	1.379	0.02	1
A	122	LEU	HD21	0.584	0.02	1
A	57	VAL	N	125.516	0.3	1
A	76	ILE	HG22	1.164	0.02	1
A	128	PRO	CG	24.21	0.3	1
A	10	ILE	HD13	0.014	0.02	1
A	135	THR	C	170.456	0.3	1
A	96	ASP	CA	51.205	0.3	1
A	23	ARG	H	8.902	0.02	1
A	130	ALA	HB1	1.691	0.02	1
A	45	PHE	HA	5.582	0.02	1
A	98	PHE	HB2	2.451	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	62	GLY	N	108.004	0.3	1
A	25	ASP	HA	4.555	0.02	1
A	137	LYS	CD	26.187	0.3	1
A	146	LEU	HD21	0.62	0.02	1
A	72	GLY	H	8.792	0.02	1
A	61	ARG	HD2	3.165	0.02	1
A	87	ILE	N	134.118	0.3	1
A	140	ASP	C	176.195	0.3	1
A	76	ILE	CG2	15.732	0.3	1
A	14	ILE	HD11	0.878	0.02	1
A	159	GLY	H	8.299	0.02	1
A	87	ILE	HD12	0.324	0.02	1
A	127	ASP	N	126.571	0.3	1
A	23	ARG	HB3	1.234	0.02	2
A	147	SER	CA	54.845	0.3	1
A	62	GLY	HA3	3.657	0.02	2
A	119	SER	CA	60.246	0.3	1
A	19	PRO	HD3	3.488	0.02	2
A	33	ALA	HB3	0.986	0.02	1
A	47	LYS	HB3	0.994	0.02	2
A	32	LYS	H	8.462	0.02	1
A	102	HIS	HA	4.712	0.02	1
A	145	ARG	HA	3.872	0.02	1
A	132	MET	HB3	1.692	0.02	2
A	19	PRO	CG	24.249	0.3	1
A	55	ILE	HG21	0.824	0.02	1
A	116	ILE	HB	1.284	0.02	1
A	116	ILE	CB	34.496	0.3	1
A	63	ALA	HB2	1.37	0.02	1
A	48	ILE	CG2	14.284	0.3	1
A	47	LYS	HG2	0.799	0.02	1
A	32	LYS	HB2	1.439	0.02	1
A	23	ARG	N	125.97	0.3	1
A	146	LEU	HD12	1.166	0.02	1
A	93	PHE	H	8.971	0.02	1
A	48	ILE	HG12	0.989	0.02	2
A	60	ALA	HA	4.754	0.02	1
A	160	ASP	CA	48.436	0.3	1
A	115	ALA	N	120.337	0.3	1
A	126	SER	HB2	4.093	0.02	2
A	145	ARG	H	7.112	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	43	LEU	HA	4.334	0.02	1
A	30	ILE	CG2	15.987	0.3	1
A	55	ILE	CB	37.326	0.3	1
A	87	ILE	HG12	0.875	0.02	2
A	125	SER	C	172.66	0.3	1
A	18	THR	CA	55.892	0.3	1
A	20	ASP	N	121.788	0.3	1
A	128	PRO	HB2	1.713	0.02	2
A	96	ASP	HB2	2.702	0.02	2
A	32	LYS	CB	27.967	0.3	1
A	129	LYS	C	174.023	0.3	1
A	49	ASN	H	8.727	0.02	1
A	157	LEU	C	175.397	0.3	1
A	113	VAL	HG23	0.012	0.02	1
A	42	PRO	HB2	1.559	0.02	1
A	21	MET	CB	36.413	0.3	1
A	110	LEU	HD22	0.691	0.02	1
A	110	LEU	CB	40.146	0.3	1
A	142	ASN	H	8.452	0.02	1
A	86	GLY	HA2	3.894	0.02	2
A	129	LYS	CG	21.943	0.3	1
A	102	HIS	HB3	2.697	0.02	2
A	77	LEU	CG	23.227	0.3	1
A	48	ILE	HG23	0.653	0.02	1
A	133	PHE	N	128.151	0.3	1
A	87	ILE	HB	1.37	0.02	1
A	45	PHE	C	173.785	0.3	1
A	119	SER	N	122.583	0.3	1
A	41	THR	CG2	21.848	0.3	1
A	55	ILE	C	170.451	0.3	1
A	125	SER	CB	62.609	0.3	1
A	94	ASP	CA	55.648	0.3	1
A	21	MET	HE1	0.306	0.02	1
A	41	THR	HB	3.983	0.02	1
A	29	ALA	CB	15.638	0.3	1
A	73	LYS	CG	21.871	0.3	1
A	142	ASN	HD21	6.956	0.02	1
A	10	ILE	HG13	0.1	0.02	2
A	138	TYR	CB	35.556	0.3	1
A	136	TYR	H	8.973	0.02	1
A	75	GLY	HA2	3.92	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	118	HIS	HB2	3.627	0.02	2
A	39	ASN	HA	4.557	0.02	1
A	10	ILE	C	172.521	0.3	1
A	111	THR	CA	63.87	0.3	1
A	15	ASN	HD21	7.946	0.02	1
A	118	HIS	HE1	8.373	0.02	1
A	13	ARG	HG2	1.462	0.02	1
A	141	ILE	N	124.692	0.3	1
A	141	ILE	HD12	0.598	0.02	1
A	25	ASP	H	7.409	0.02	1
A	39	ASN	ND2	111.562	0.3	1
A	138	TYR	HB3	2.605	0.02	2
A	37	TRP	CA	55.625	0.3	1
A	63	ALA	C	174.207	0.3	1
A	52	MET	H	8.181	0.02	1
A	113	VAL	CB	28.258	0.3	1
A	103	SER	CB	60.76	0.3	1
A	85	SER	HB3	3.835	0.02	2
A	55	ILE	H	8.785	0.02	1
A	57	VAL	HG21	0.852	0.02	1
A	84	GLY	CA	41.277	0.3	1
A	80	ALA	C	177.15	0.3	1
A	115	ALA	C	176.179	0.3	1
A	28	TYR	CB	35.942	0.3	1
A	155	GLN	CG	32.087	0.3	1
A	57	VAL	CB	29.83	0.3	1
A	155	GLN	CB	23.892	0.3	1
A	51	GLY	N	109.896	0.3	1
A	16	ASN	CB	35.78	0.3	1
A	11	THR	HA	5.24	0.02	1
A	108	LEU	C	173.484	0.3	1
A	21	MET	H	6.811	0.02	1
A	136	TYR	HA	4.567	0.02	1
A	104	GLY	N	115.132	0.3	1
A	106	THR	HG22	0.203	0.02	1
A	43	LEU	HD11	0.594	0.02	1
A	49	ASN	ND2	109.786	0.3	1
A	114	HIS	HB2	3.788	0.02	2
A	4	VAL	C	172.708	0.3	1
A	60	ALA	HB3	0.816	0.02	1
A	64	HIS	N	124.847	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	111	THR	HG22	1.254	0.02	1
A	39	ASN	HB2	2.905	0.02	2
A	6	ARG	N	115.526	0.3	1
A	108	LEU	CG	25.05	0.3	1
A	83	PRO	CB	28.9	0.3	1
A	38	SER	C	173.046	0.3	1
A	27	ASP	HA	4.249	0.02	1
A	112	ALA	HB2	0.953	0.02	1
A	29	ALA	H	7.984	0.02	1
A	42	PRO	N	128.123	0.3	1
A	47	LYS	CE	40.16	0.3	1
A	130	ALA	HA	4.459	0.02	1
A	125	SER	HB3	3.362	0.02	2
A	26	VAL	HG12	0.875	0.02	1
A	136	TYR	CB	36.108	0.3	1
A	127	ASP	CB	39.163	0.3	1
A	135	THR	N	116.478	0.3	1
A	14	ILE	HG21	-0.016	0.02	1
A	23	ARG	HD2	2.55	0.02	2
A	71	ASP	HB3	2.476	0.02	2
A	77	LEU	HD22	0.181	0.02	1
A	21	MET	HB3	1.273	0.02	2
A	14	ILE	CA	58.6	0.3	1
A	80	ALA	CA	47.825	0.3	1
A	40	VAL	HB	2.576	0.02	1
A	153	GLY	C	174.279	0.3	1
A	30	ILE	CB	32.607	0.3	1
A	110	LEU	HD13	0.421	0.02	1
A	160	ASP	HB3	2.529	0.02	2
A	6	ARG	C	177.138	0.3	1
A	108	LEU	HD21	-0.33	0.02	1
A	111	THR	N	112.535	0.3	1
A	63	ALA	N	134.082	0.3	1
A	58	VAL	HG21	0.791	0.02	1
A	4	VAL	HG13	0.416	0.02	1
A	49	ASN	HD21	6.672	0.02	1
A	50	THR	CA	57.521	0.3	1
A	36	VAL	CB	28.204	0.3	1
A	26	VAL	N	123.993	0.3	1
A	57	VAL	HA	5.07	0.02	1
A	155	GLN	H	8.652	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	168	PRO	CG	24.288	0.3	1
A	145	ARG	CG	22.997	0.3	1
A	99	TRP	HE1	10.109	0.02	1
A	95	GLU	HB3	1.85	0.02	2
A	137	LYS	HE2	2.801	0.02	1
A	131	VAL	HA	4.291	0.02	1
A	15	ASN	HB2	2.999	0.02	2
A	31	ARG	HG3	1.492	0.02	2
A	123	GLY	C	170.905	0.3	1
A	157	LEU	H	6.749	0.02	1
A	102	HIS	CA	50.934	0.3	1
A	95	GLU	HG2	2.208	0.02	2
A	44	LYS	N	122.655	0.3	1
A	26	VAL	HG13	0.875	0.02	1
A	150	ASP	CB	41.541	0.3	1
A	152	ARG	HB3	1.792	0.02	2
A	5	TRP	HA	4.982	0.02	1
A	4	VAL	CB	38.285	0.3	1
A	23	ARG	HG2	0.917	0.02	2
A	104	GLY	C	170.841	0.3	1
A	17	TYR	HB2	2.721	0.02	2
A	31	ARG	CD	41.111	0.3	1
A	14	ILE	C	172.315	0.3	1
A	127	ASP	H	8.848	0.02	1
A	49	ASN	HB2	2.778	0.02	1
A	151	ILE	CD1	10.325	0.3	1
A	106	THR	CA	59.841	0.3	1
A	6	ARG	CA	51.629	0.3	1
A	10	ILE	CD1	10.099	0.3	1
A	75	GLY	H	8.417	0.02	1
A	30	ILE	H	7.983	0.02	1
A	157	LEU	HB2	1.777	0.02	2
A	137	LYS	CE	39.436	0.3	1
A	34	PHE	H	7.649	0.02	1
A	97	GLU	HG2	2.505	0.02	1
A	46	SER	HB3	3.314	0.02	2
A	87	ILE	HD11	0.324	0.02	1
A	47	LYS	CB	30.468	0.3	1
A	43	LEU	N	111.126	0.3	1
A	56	LEU	HB2	1.566	0.02	2
A	119	SER	CB	60.549	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	52	MET	C	172.201	0.3	1
A	108	LEU	HA	4.315	0.02	1
A	13	ARG	CG	26.116	0.3	1
A	155	GLN	HB2	2.097	0.02	2
A	40	VAL	HG12	0.807	0.02	1
A	83	PRO	HD2	3.673	0.02	2
A	29	ALA	N	121.412	0.3	1
A	28	TYR	HB3	2.985	0.02	2
A	26	VAL	HA	3.402	0.02	1
A	90	ASP	HB2	2.888	0.02	1
A	25	ASP	C	176.396	0.3	1
A	16	ASN	HD21	7.821	0.02	1
A	57	VAL	HG11	0.605	0.02	1
A	31	ARG	HA	4.002	0.02	1
A	128	PRO	N	136.982	0.3	1
A	19	PRO	CB	28.839	0.3	1
A	29	ALA	HB3	1.386	0.02	1
A	121	GLY	C	171.493	0.3	1
A	4	VAL	H	8.229	0.02	1
A	35	GLN	HG3	2.33	0.02	2
A	151	ILE	CG2	14.021	0.3	1
A	43	LEU	HD21	0.54	0.02	1
A	55	ILE	HG22	0.824	0.02	1
A	158	TYR	CB	38.603	0.3	1
A	63	ALA	HB1	1.37	0.02	1
A	76	ILE	HA	3.823	0.02	1
A	94	ASP	HA	4.086	0.02	1
A	145	ARG	HG3	1.29	0.02	2
A	102	HIS	N	120.547	0.3	1
A	149	ASP	C	175.908	0.3	1
A	41	THR	CB	69.444	0.3	1
A	53	ALA	HB3	0.836	0.02	1
A	138	TYR	HA	3.647	0.02	1
A	67	ASP	HA	4.321	0.02	1
A	28	TYR	N	119.607	0.3	1
A	141	ILE	HD13	0.598	0.02	1
A	139	VAL	N	124.19	0.3	1
A	71	ASP	H	8.218	0.02	1
A	155	GLN	N	123.4	0.3	1
A	23	ARG	HB2	1.345	0.02	2
A	169	ASN	H	8.381	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	114	HIS	C	172.67	0.3	1
A	16	ASN	N	113.007	0.3	1
A	114	HIS	HB3	2.982	0.02	2
A	151	ILE	C	174.834	0.3	1
A	10	ILE	H	8.194	0.02	1
A	122	LEU	CA	52.311	0.3	1
A	47	LYS	H	8.057	0.02	1
A	124	HIS	H	8.353	0.02	1
A	49	ASN	HA	4.74	0.02	1
A	54	ASP	C	174.181	0.3	1
A	82	GLY	C	168.147	0.3	1
A	106	THR	N	124.763	0.3	1
A	92	HIS	HB2	3.048	0.02	2
A	135	THR	HG23	1.13	0.02	1
A	74	GLY	H	10.689	0.02	1
A	83	PRO	HB3	1.711	0.02	2
A	140	ASP	HB2	2.912	0.02	2
A	38	SER	HB2	4.258	0.02	2
A	133	PHE	HB2	3.537	0.02	2
A	45	PHE	N	119.696	0.3	1
A	32	LYS	CA	55.402	0.3	1
A	30	ILE	CD1	5.65	0.3	1
A	139	VAL	HG22	0.675	0.02	1
A	56	LEU	CB	40.78	0.3	1
A	37	TRP	HE1	10.027	0.02	1
A	43	LEU	CA	56.586	0.3	1
A	64	HIS	HB3	3.377	0.02	2
A	109	PHE	CA	58.876	0.3	1
A	155	GLN	HE21	8.256	0.02	1
A	143	THR	C	171.121	0.3	1
A	122	LEU	HB2	1.402	0.02	2
A	16	ASN	C	167.039	0.3	1
A	48	ILE	N	123.812	0.3	1
A	65	GLY	HA3	3.991	0.02	2
A	113	VAL	HA	3.083	0.02	1
A	138	TYR	H	8.5	0.02	1
A	97	GLU	C	173.785	0.3	1
A	132	MET	HE1	0.364	0.02	1
A	76	ILE	HG13	1.295	0.02	2
A	29	ALA	CA	52.892	0.3	1
A	87	ILE	CD1	11.492	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	98	PHE	H	8.983	0.02	1
A	73	LYS	CD	26.27	0.3	1
A	150	ASP	HA	4.697	0.02	1
A	86	GLY	H	8.902	0.02	1
A	139	VAL	CG2	16.492	0.3	1
A	68	HIS	CA	51.106	0.3	1
A	19	PRO	HD2	3.653	0.02	2
A	140	ASP	H	7.794	0.02	1
A	55	ILE	HB	1.759	0.02	1
A	111	THR	CB	65.404	0.3	1
A	41	THR	H	7.459	0.02	1
A	91	ALA	H	8.581	0.02	1
A	128	PRO	CA	60.153	0.3	1
A	122	LEU	CD1	22.163	0.3	1
A	63	ALA	CB	15.032	0.3	1
A	87	ILE	CG2	13.428	0.3	1
A	169	ASN	HB2	2.724	0.02	2
A	37	TRP	CB	27.639	0.3	1
A	26	VAL	CB	28.581	0.3	1
A	100	THR	H	8.338	0.02	1
A	153	GLY	HA3	3.705	0.02	2
A	149	ASP	N	117.544	0.3	1
A	10	ILE	CB	37.489	0.3	1
A	9	TYR	HA	4.715	0.02	1
A	32	LYS	HD3	0.827	0.02	2
A	40	VAL	CB	29.799	0.3	1
A	131	VAL	HG12	1.121	0.02	1
A	58	VAL	HG13	0.626	0.02	1
A	76	ILE	HD11	0.903	0.02	1
A	151	ILE	CB	35.565	0.3	1
A	52	MET	CG	32.012	0.3	1
A	43	LEU	C	173.45	0.3	1
A	157	LEU	CD2	21.097	0.3	1
A	28	TYR	CA	58.942	0.3	1
A	79	HIS	HB3	3.023	0.02	2
A	66	ASP	N	126.858	0.3	1
A	24	GLU	CG	33.519	0.3	1
A	46	SER	CA	53.971	0.3	1
A	40	VAL	HG23	1.051	0.02	1
A	155	GLN	CA	55.862	0.3	1
A	105	GLY	CA	43.136	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	16	ASN	CA	49.167	0.3	1
A	5	TRP	NE1	125.655	0.3	1
A	27	ASP	HB2	2.717	0.02	2
A	142	ASN	HB3	2.682	0.02	2
A	157	LEU	CG	24.413	0.3	1
A	24	GLU	H	9.022	0.02	1
A	36	VAL	HG21	0.401	0.02	1
A	34	PHE	CA	61.08	0.3	1
A	13	ARG	H	8.291	0.02	1
A	78	ALA	HB2	1.003	0.02	1
A	83	PRO	CG	24.248	0.3	1
A	128	PRO	C	175.042	0.3	1
A	133	PHE	HA	4.854	0.02	1
A	112	ALA	HB1	0.953	0.02	1
A	98	PHE	CB	36.429	0.3	1
A	60	ALA	C	172.015	0.3	1
A	154	ILE	HG21	1.455	0.02	1
A	120	LEU	HB2	1.264	0.02	1
A	145	ARG	HD2	3.032	0.02	2
A	93	PHE	HB2	2.053	0.02	1
A	62	GLY	C	173.05	0.3	1
A	101	THR	HG23	0.434	0.02	1
A	91	ALA	CB	18.087	0.3	1
A	38	SER	CB	60.893	0.3	1
A	99	TRP	HA	4.309	0.02	1
A	101	THR	HB	4.262	0.02	1
A	48	ILE	HD13	0.541	0.02	1
A	80	ALA	CB	16.133	0.3	1
A	132	MET	C	174.389	0.3	1
A	115	ALA	HB3	1.06	0.02	1
A	121	GLY	HA3	3.312	0.02	2
A	61	ARG	CG	25.953	0.3	1
A	68	HIS	N	119.701	0.3	1
A	45	PHE	HB3	2.104	0.02	2
A	78	ALA	H	7.398	0.02	1
A	40	VAL	H	7.025	0.02	1
A	66	ASP	HB3	2.936	0.02	2
A	149	ASP	HA	4.222	0.02	1
A	58	VAL	HG22	0.791	0.02	1
A	19	PRO	N	139.641	0.3	1
A	57	VAL	HB	2.064	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	23	ARG	C	175.219	0.3	1
A	74	GLY	HA3	3.382	0.02	2
A	24	GLU	HG2	2.201	0.02	1
A	131	VAL	HB	2.381	0.02	1
A	158	TYR	N	112.416	0.3	1
A	134	PRO	CA	60.989	0.3	1
A	9	TYR	N	119.899	0.3	1
A	107	ASN	C	173.528	0.3	1
A	41	THR	N	109.982	0.3	1
A	48	ILE	HA	4.504	0.02	1
A	87	ILE	HG22	0.359	0.02	1
A	59	PHE	CB	38.106	0.3	1
A	150	ASP	CA	54.95	0.3	1
A	131	VAL	C	176.244	0.3	1
A	139	VAL	CB	32.316	0.3	1
A	56	LEU	HD23	1.012	0.02	1
A	111	THR	HA	4.021	0.02	1
A	31	ARG	CA	57.446	0.3	1
A	36	VAL	HA	3.538	0.02	1
A	151	ILE	HD12	0.648	0.02	1
A	54	ASP	H	7.962	0.02	1
A	63	ALA	HA	4.239	0.02	1
A	157	LEU	HD13	0.629	0.02	1
A	12	TYR	CA	52.174	0.3	1
A	106	THR	CB	65.705	0.3	1
A	154	ILE	CD1	12.083	0.3	1
A	34	PHE	HA	3.633	0.02	1
A	107	ASN	CB	38.909	0.3	1
A	107	ASN	HB3	3.006	0.02	2
A	14	ILE	HB	1.614	0.02	1
A	126	SER	HA	4.657	0.02	1
A	87	ILE	CB	35.347	0.3	1
A	50	THR	CG2	17.974	0.3	1
A	47	LYS	CA	52.434	0.3	1
A	112	ALA	C	175.911	0.3	1
A	78	ALA	CB	19.999	0.3	1
A	119	SER	HA	4.165	0.02	1
A	9	TYR	HB2	2.748	0.02	2
A	151	ILE	HA	3.539	0.02	1
A	33	ALA	CA	52.703	0.3	1
A	139	VAL	HG11	0.729	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	40	VAL	CG2	15.979	0.3	1
A	53	ALA	HA	4.422	0.02	1
A	120	LEU	CA	52.096	0.3	1
A	47	LYS	HE2	2.939	0.02	1
A	157	LEU	HG	1.657	0.02	1
A	150	ASP	C	175.04	0.3	1
A	18	THR	HA	4.702	0.02	1
A	97	GLU	H	9.391	0.02	1
A	109	PHE	HB3	3.035	0.02	2
A	131	VAL	CA	61.992	0.3	1
A	11	THR	HG21	0.968	0.02	1
A	147	SER	C	172.27	0.3	1
A	148	ALA	HB2	1.348	0.02	1
A	26	VAL	HB	2.478	0.02	1
A	39	ASN	H	8.012	0.02	1
A	160	ASP	HA	4.555	0.02	1
A	135	THR	HB	3.959	0.02	1
A	131	VAL	HG22	0.934	0.02	1
A	19	PRO	CA	60.248	0.3	1
A	80	ALA	HB2	1.156	0.02	1
A	36	VAL	HG13	1.014	0.02	1
A	19	PRO	HA	4.256	0.02	1
A	145	ARG	C	171.975	0.3	1
A	43	LEU	HD22	0.54	0.02	1
A	5	TRP	CA	52.628	0.3	1
A	149	ASP	CB	41.001	0.3	1
A	89	GLY	C	169.466	0.3	1
A	22	ASN	H	8.82	0.02	1
A	139	VAL	C	169.317	0.3	1
A	10	ILE	N	128.394	0.3	1
A	116	ILE	N	115.625	0.3	1
A	21	MET	HG3	1.955	0.02	2
A	41	THR	CA	57.105	0.3	1
A	146	LEU	HA	3.882	0.02	1
A	141	ILE	HG22	0.923	0.02	1
A	120	LEU	HD21	0.732	0.02	1
A	129	LYS	HD2	2.465	0.02	2
A	53	ALA	CA	46.873	0.3	1
A	62	GLY	H	9.407	0.02	1
A	41	THR	HG22	1.379	0.02	1
A	110	LEU	HG	0.92	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	76	ILE	HG21	1.164	0.02	1
A	38	SER	HA	4.199	0.02	1
A	10	ILE	HD12	0.014	0.02	1
A	128	PRO	HA	2.464	0.02	1
A	108	LEU	HB2	1.657	0.02	2
A	156	SER	C	172.161	0.3	1
A	51	GLY	C	170.557	0.3	1
A	110	LEU	CD1	20.856	0.3	1
A	9	TYR	CB	35.46	0.3	1
A	26	VAL	CG2	18.584	0.3	1
A	120	LEU	HD23	0.732	0.02	1
A	58	VAL	HG12	0.626	0.02	1
A	114	HIS	CB	26.379	0.3	1
A	64	HIS	C	173.48	0.3	1
A	74	GLY	CA	40.107	0.3	1
A	59	PHE	HB3	2.857	0.02	2
A	139	VAL	HG21	0.675	0.02	1
A	76	ILE	CG1	25.325	0.3	1
A	98	PHE	N	119.21	0.3	1
A	77	LEU	HD11	-0.036	0.02	1
A	30	ILE	HG23	0.64	0.02	1
A	109	PHE	CB	34.896	0.3	1
A	110	LEU	N	117.948	0.3	1
A	96	ASP	C	176.687	0.3	1
A	73	LYS	HB2	1.502	0.02	1
A	100	THR	HB	4.432	0.02	1
A	133	PHE	CB	37.639	0.3	1
A	62	GLY	HA2	3.851	0.02	2
A	91	ALA	N	119.865	0.3	1
A	37	TRP	HB2	3.059	0.02	2
A	129	LYS	HG2	1.384	0.02	2
A	113	VAL	HB	1.602	0.02	1
A	26	VAL	HG22	0.784	0.02	1
A	152	ARG	N	119.13	0.3	1
A	66	ASP	CA	59.227	0.3	1
A	47	LYS	HB2	1.355	0.02	2
A	125	SER	N	113.754	0.3	1
A	146	LEU	HD13	1.166	0.02	1
A	20	ASP	HA	3.987	0.02	1
A	149	ASP	H	8.18	0.02	1
A	53	ALA	C	173.643	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	139	VAL	CG1	18.263	0.3	1
A	116	ILE	HG12	0.943	0.02	2
A	132	MET	HB2	2.565	0.02	2
A	55	ILE	HA	4.072	0.02	1
A	70	PHE	C	173.477	0.3	1
A	22	ASN	ND2	113.938	0.3	1
A	76	ILE	C	174.175	0.3	1
A	138	TYR	CA	58.346	0.3	1
A	34	PHE	HB2	2.477	0.02	1
A	110	LEU	C	176.089	0.3	1
A	146	LEU	N	121.116	0.3	1
A	10	ILE	CA	56.317	0.3	1
A	111	THR	C	173.916	0.3	1
A	116	ILE	CA	60.522	0.3	1
A	129	LYS	HE2	2.882	0.02	1
A	113	VAL	N	118.495	0.3	1
A	59	PHE	N	125.471	0.3	1
A	90	ASP	CB	36.867	0.3	1
A	53	ALA	N	126.941	0.3	1
A	85	SER	HA	4.349	0.02	1
A	46	SER	CB	63.031	0.3	1
A	22	ASN	N	118.643	0.3	1
A	160	ASP	CB	36.504	0.3	1
A	142	ASN	ND2	115.129	0.3	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
$^{13}\text{C}_\alpha$	344	$2.59 \pm 0.09$	Should be applied
$^{13}\text{C}_\beta$	313	$2.79 \pm 0.18$	Should be applied
$^{13}\text{C}'$	338	$3.09 \pm 0.07$	Should be applied
$^{15}\text{N}$	342	$0.22 \pm 0.41$	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 74%, i.e. 1874 atoms were assigned a chemical shift out of a possible 2546. 22 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.



	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	909/926 (98%)	362/368 (98%)	371/380 (98%)	176/178 (99%)
Sidechain	955/1250 (76%)	569/746 (76%)	370/438 (84%)	16/66 (24%)
Aromatic	10/370 (3%)	5/196 (3%)	0/167 (0%)	5/7 (71%)
Overall	1874/2546 (74%)	936/1310 (71%)	741/985 (75%)	197/251 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 1893 atoms were assigned a chemical shift out of a possible 2590. 22 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	917/944 (97%)	365/375 (97%)	375/388 (97%)	177/181 (98%)
Sidechain	966/1276 (76%)	576/762 (76%)	374/448 (83%)	16/66 (24%)
Aromatic	10/370 (3%)	5/196 (3%)	0/167 (0%)	5/7 (71%)
Overall	1893/2590 (73%)	946/1333 (71%)	749/1003 (75%)	198/254 (78%)

#### 7.2.4 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	392	THR	HG22	-1.19	2.29 – -0.01	-10.1
1	A	392	THR	HG23	-1.19	2.29 – -0.01	-10.1
1	A	392	THR	HG21	-1.19	2.29 – -0.01	-10.1
1	A	450	GLU	HG3	0.81	3.31 – 1.21	-6.9
1	A	298	ILE	HG21	-0.94	2.13 – -0.57	-6.4
1	A	298	ILE	HG23	-0.94	2.13 – -0.57	-6.4
1	A	298	ILE	HG22	-0.94	2.13 – -0.57	-6.4
1	A	410	MET	CG	24.07	38.33 – 25.73	-6.3
1	A	134	PRO	CB	24.69	37.79 – 25.89	-6.0
1	A	128	PRO	HA	2.46	6.05 – 2.75	-5.9
1	A	425	ILE	HG21	-0.79	2.13 – -0.57	-5.8
1	A	425	ILE	HG23	-0.79	2.13 – -0.57	-5.8
1	A	425	ILE	HG22	-0.79	2.13 – -0.57	-5.8
1	A	106	THR	HB	2.35	5.82 – 2.52	-5.5
1	A	352	TYR	HB3	0.91	4.75 – 0.95	-5.1
1	A	448	GLN	HG3	0.83	3.75 – 0.85	-5.1
1	A	380	ILE	HD13	-0.79	2.13 – -0.77	-5.1
1	A	380	ILE	HD12	-0.79	2.13 – -0.77	-5.1
1	A	380	ILE	HD11	-0.79	2.13 – -0.77	-5.1

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

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

Random coil index (RCI) for chain A:

