Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 10:43 PM BST

PDB ID	:	2K7B
Title	:	NMR structure of Mg2+-bound CaBP1 N-domain
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Deposited on	:	2008-08-08

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

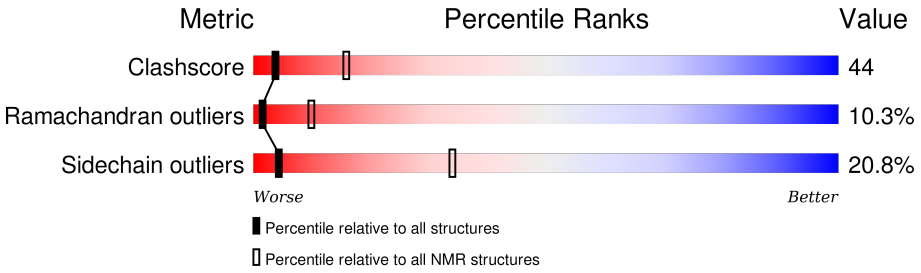
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	76	21% 62% 12% 5%

2 Ensemble composition and analysis

This entry contains 15 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:20-A:91 (72)	0.73	13

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 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1214 atoms, of which 592 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	76	1213	384	592	105	124	8	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
			Total	Mg
2	A	1	1	1

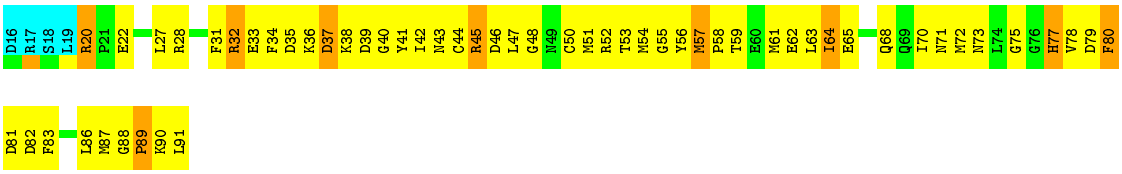
4 Residue-property plots

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: Calcium-binding protein 1

Chain A:



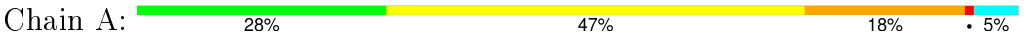
4.2 Scores per residue for each member of the ensemble

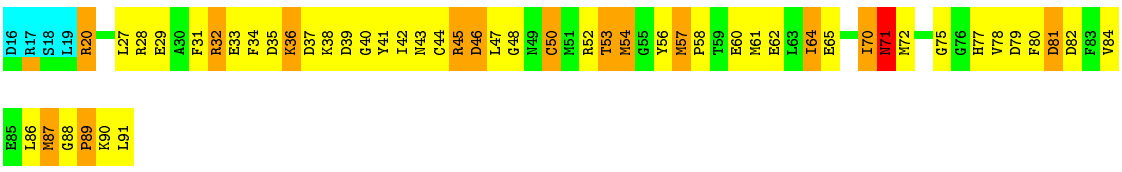
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Calcium-binding protein 1

Chain A:

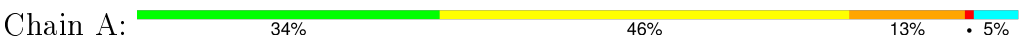


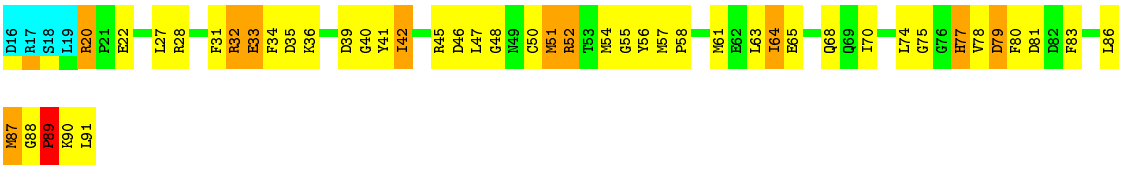


4.2.2 Score per residue for model 2

- Molecule 1: Calcium-binding protein 1

Chain A:

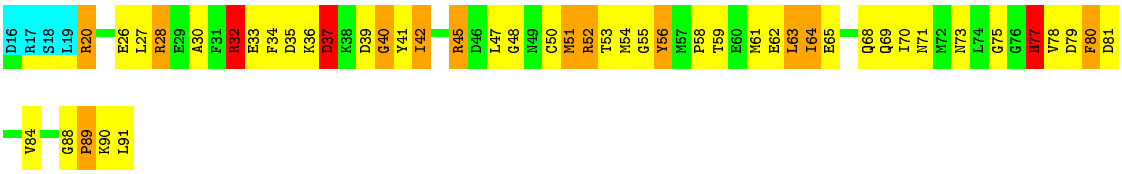




4.2.3 Score per residue for model 3

- Molecule 1: Calcium-binding protein 1

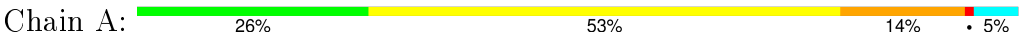
Chain A:

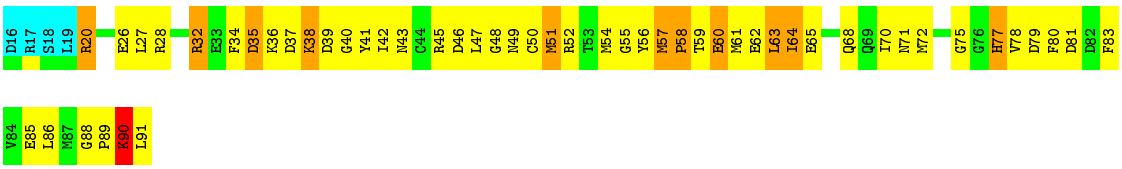


4.2.4 Score per residue for model 4

- Molecule 1: Calcium-binding protein 1

Chain A:

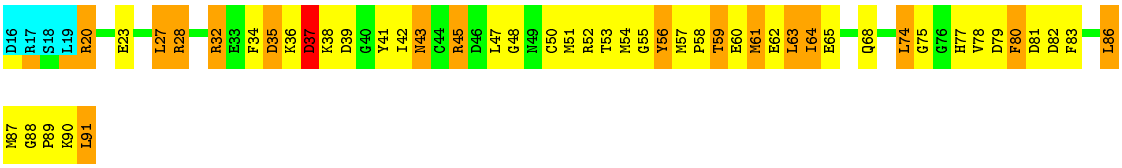




4.2.5 Score per residue for model 5

- Molecule 1: Calcium-binding protein 1

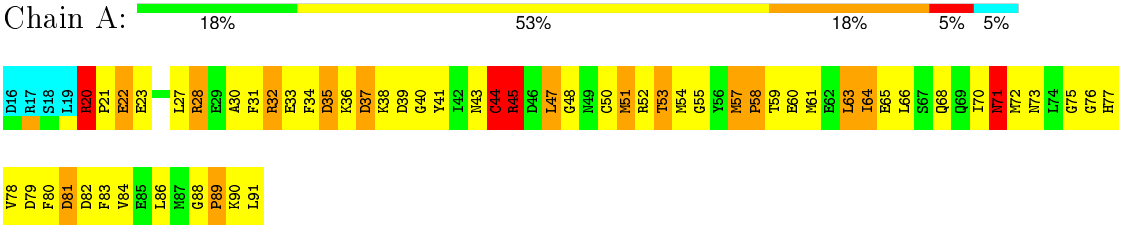
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Calcium-binding protein 1

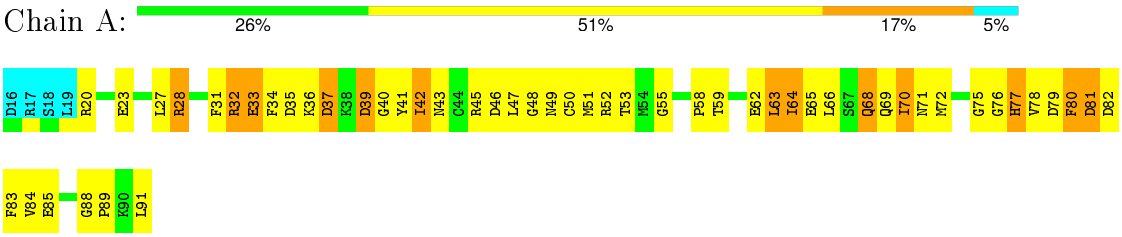
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Calcium-binding protein 1

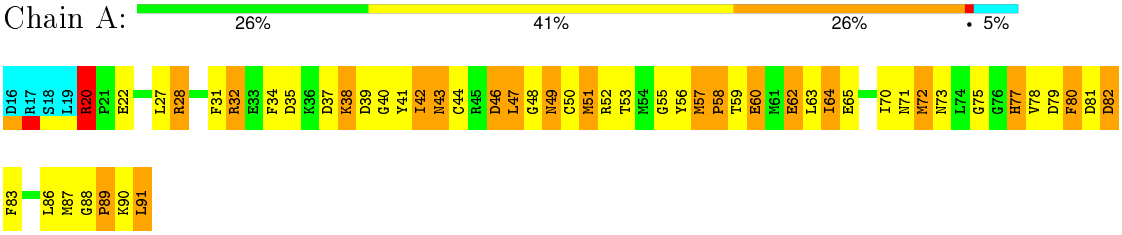
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: Calcium-binding protein 1

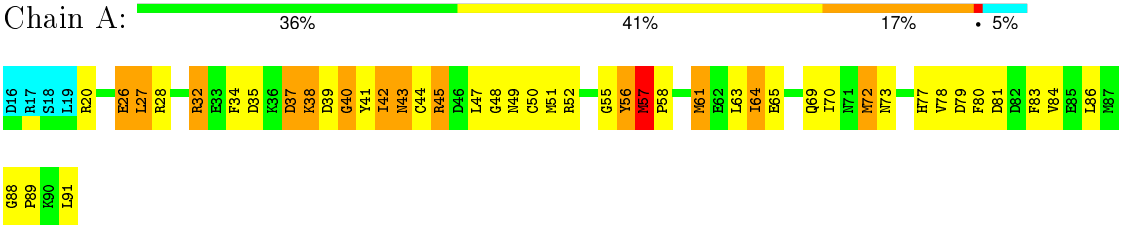
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: Calcium-binding protein 1

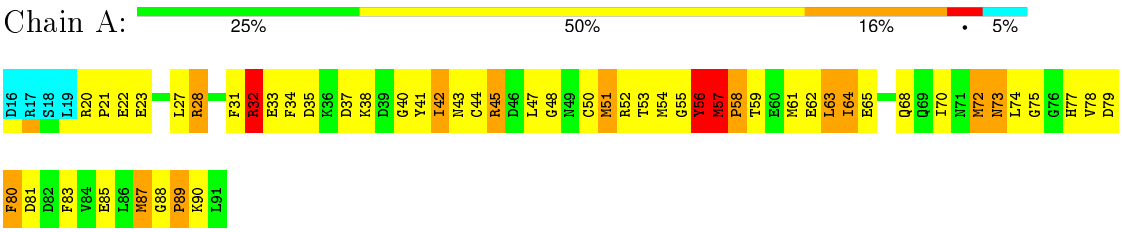
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Calcium-binding protein 1

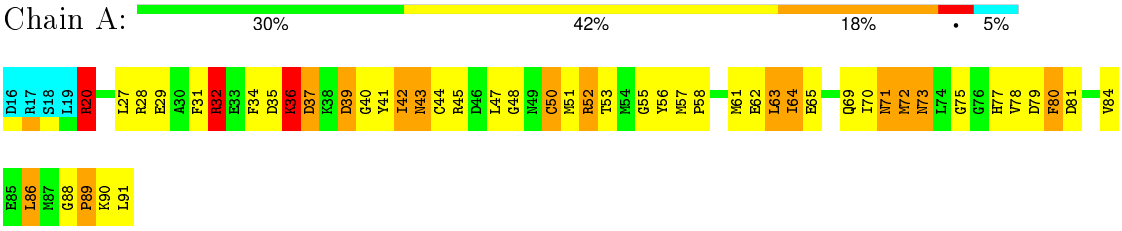
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Calcium-binding protein 1

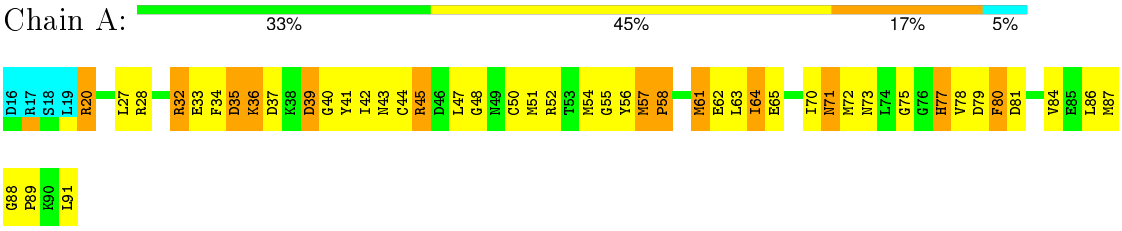
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Calcium-binding protein 1

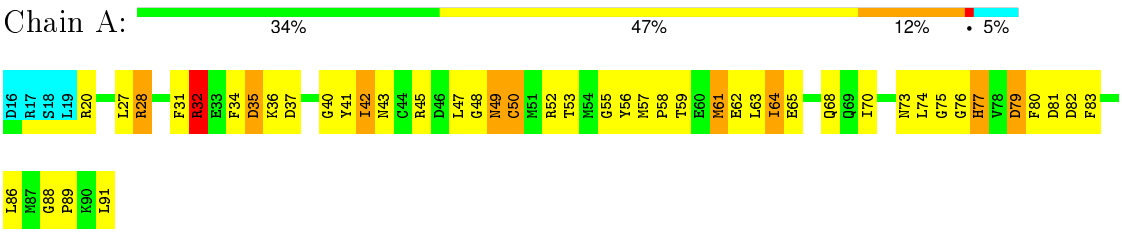
Chain A:



4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: Calcium-binding protein 1

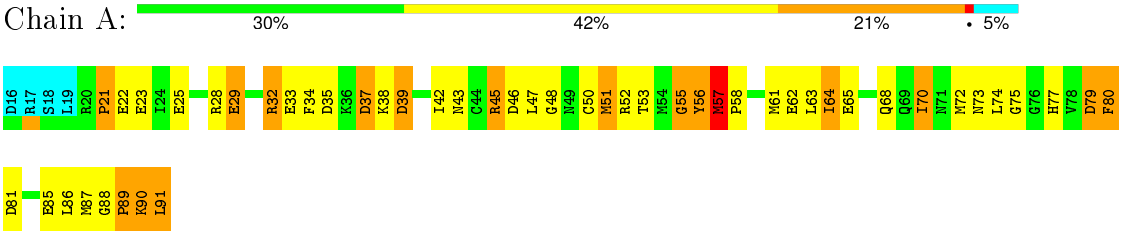
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Calcium-binding protein 1

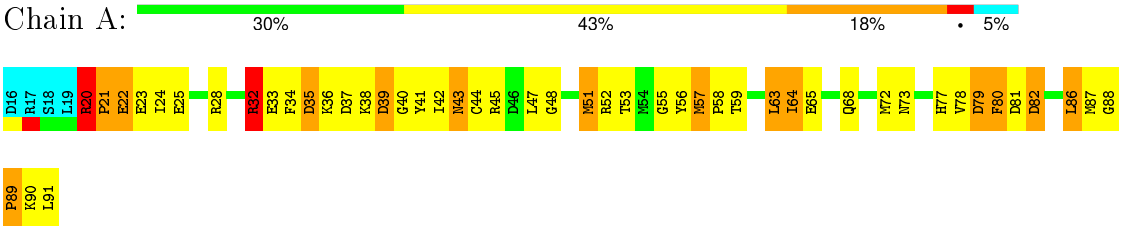
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Calcium-binding protein 1

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

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 15197
Number of chemical shift lists	1
Total number of shifts	1577
Number of shifts mapped to atoms	783
Number of unparsed shifts	0
Number of shifts with mapping errors	794
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.07±0.01	1±0/597 (0.2±0.0%)	1.19±0.01	0±0/798 (0.0±0.0%)
All	All	1.07	15/8955 (0.2%)	1.19	0/11970 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	4.5±0.6
All	All	0	67

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	77	HIS	CG-ND1	-6.25	1.25	1.38	14	15

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	32	ARG	Sidechain	15
1	A	52	ARG	Sidechain	14
1	A	28	ARG	Sidechain	13
1	A	45	ARG	Sidechain	13
1	A	20	ARG	Sidechain	12

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	588	559	559	51±6
All	All	8835	8385	8385	758

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 44.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LEU:HD13	1:A:63:LEU:H	1.01	1.15	5	1
1:A:59:THR:HG22	1:A:60:GLU:H	0.88	1.28	8	3
1:A:59:THR:HG22	1:A:60:GLU:N	0.86	1.85	4	2
1:A:63:LEU:HD23	1:A:64:ILE:H	0.83	1.33	8	1
1:A:91:LEU:N	1:A:91:LEU:HD22	0.82	1.89	9	2
1:A:57:MET:H	1:A:58:PRO:CD	0.81	1.88	9	6
1:A:43:ASN:N	1:A:43:ASN:ND2	0.79	2.30	8	2
1:A:74:LEU:HD12	1:A:74:LEU:O	0.78	1.78	5	1
1:A:34:PHE:CG	1:A:50:CYS:SG	0.78	2.76	8	2
1:A:42:ILE:HD12	1:A:47:LEU:HD11	0.78	1.54	5	8
1:A:57:MET:N	1:A:58:PRO:CD	0.77	2.48	10	10
1:A:63:LEU:HD23	1:A:64:ILE:N	0.76	1.96	8	1
1:A:42:ILE:HD12	1:A:47:LEU:CD2	0.75	2.11	8	6
1:A:57:MET:H	1:A:58:PRO:HD2	0.74	1.41	1	6
1:A:74:LEU:HD12	1:A:74:LEU:C	0.74	2.03	5	1
1:A:20:ARG:H	1:A:21:PRO:CD	0.74	1.95	15	1
1:A:31:PHE:CD2	1:A:42:ILE:HD11	0.74	2.18	11	3
1:A:88:GLY:N	1:A:89:PRO:CD	0.74	2.50	1	9
1:A:20:ARG:N	1:A:21:PRO:CD	0.74	2.50	15	1
1:A:34:PHE:CD2	1:A:50:CYS:SG	0.73	2.78	8	7
1:A:63:LEU:HD23	1:A:63:LEU:N	0.73	1.98	2	3
1:A:43:ASN:ND2	1:A:43:ASN:N	0.73	2.36	9	2
1:A:91:LEU:C	1:A:91:LEU:HD12	0.73	2.03	15	1
1:A:63:LEU:HD22	1:A:64:ILE:N	0.70	2.01	5	1
1:A:43:ASN:ND2	1:A:43:ASN:H	0.70	1.83	9	2
1:A:43:ASN:N	1:A:43:ASN:HD22	0.69	1.84	8	1
1:A:86:LEU:HD13	1:A:86:LEU:O	0.69	1.87	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ILE:HD12	1:A:47:LEU:HD21	0.69	1.63	10	5
1:A:91:LEU:CD2	1:A:91:LEU:N	0.68	2.56	9	1
1:A:64:ILE:HG22	1:A:65:GLU:N	0.68	2.04	5	15
1:A:56:TYR:CD1	1:A:56:TYR:N	0.68	2.58	3	1
1:A:31:PHE:CE2	1:A:42:ILE:HD11	0.67	2.24	11	2
1:A:59:THR:CG2	1:A:60:GLU:N	0.67	2.55	8	2
1:A:91:LEU:CD1	1:A:91:LEU:N	0.67	2.57	4	1
1:A:49:ASN:N	1:A:49:ASN:HD22	0.67	1.88	13	1
1:A:43:ASN:H	1:A:43:ASN:ND2	0.66	1.87	8	1
1:A:43:ASN:HD22	1:A:43:ASN:N	0.66	1.86	5	2
1:A:40:GLY:C	1:A:41:TYR:CD1	0.66	2.69	3	3
1:A:41:TYR:CD1	1:A:79:ASP:OD1	0.65	2.50	7	1
1:A:63:LEU:HD13	1:A:63:LEU:N	0.64	2.00	5	1
1:A:63:LEU:H	1:A:63:LEU:CD1	0.64	1.96	5	1
1:A:62:GLU:CD	1:A:63:LEU:N	0.64	2.51	11	1
1:A:54:MET:SD	1:A:87:MET:SD	0.64	2.95	10	1
1:A:64:ILE:CG2	1:A:65:GLU:N	0.63	2.62	5	9
1:A:41:TYR:CE2	1:A:79:ASP:OD2	0.63	2.51	3	1
1:A:59:THR:CG2	1:A:60:GLU:H	0.63	2.03	4	2
1:A:81:ASP:OD1	1:A:82:ASP:N	0.62	2.33	6	2
1:A:37:ASP:OD1	1:A:38:LYS:N	0.62	2.32	15	1
1:A:39:ASP:OD1	1:A:39:ASP:N	0.62	2.32	11	1
1:A:39:ASP:OD1	1:A:41:TYR:N	0.61	2.33	12	1
1:A:42:ILE:HD12	1:A:47:LEU:CD1	0.61	2.25	5	8
1:A:87:MET:HA	1:A:91:LEU:HD21	0.61	1.73	8	2
1:A:41:TYR:N	1:A:41:TYR:CD1	0.61	2.68	15	1
1:A:86:LEU:O	1:A:86:LEU:HD13	0.61	1.95	11	1
1:A:57:MET:N	1:A:58:PRO:HD2	0.61	2.11	13	7
1:A:63:LEU:H	1:A:63:LEU:HD23	0.60	1.55	12	3
1:A:57:MET:N	1:A:58:PRO:HD3	0.60	2.11	10	3
1:A:74:LEU:CD1	1:A:74:LEU:C	0.60	2.70	5	1
1:A:37:ASP:CG	1:A:38:LYS:N	0.60	2.52	9	1
1:A:28:ARG:HH12	1:A:32:ARG:NE	0.60	1.94	3	1
1:A:74:LEU:HD12	1:A:77:HIS:O	0.59	1.97	13	1
1:A:37:ASP:N	1:A:37:ASP:OD1	0.59	2.35	3	3
1:A:79:ASP:O	1:A:81:ASP:N	0.59	2.35	8	15
1:A:79:ASP:OD1	1:A:80:PHE:N	0.59	2.35	8	1
1:A:63:LEU:N	1:A:63:LEU:HD23	0.59	2.12	14	1
1:A:39:ASP:N	1:A:39:ASP:OD1	0.59	2.33	7	3
1:A:37:ASP:OD1	1:A:37:ASP:N	0.59	2.32	13	4
1:A:64:ILE:O	1:A:68:GLN:N	0.58	2.36	2	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:GLY:O	1:A:57:MET:N	0.58	2.36	9	5
1:A:88:GLY:O	1:A:90:LYS:N	0.58	2.37	10	7
1:A:47:LEU:O	1:A:50:CYS:N	0.58	2.36	12	14
1:A:49:ASN:ND2	1:A:49:ASN:N	0.58	2.50	13	1
1:A:87:MET:N	1:A:87:MET:SD	0.57	2.77	2	1
1:A:41:TYR:CB	1:A:77:HIS:CE1	0.57	2.87	3	1
1:A:34:PHE:CE2	1:A:50:CYS:SG	0.57	2.96	3	1
1:A:39:ASP:C	1:A:41:TYR:H	0.57	2.02	9	4
1:A:42:ILE:CD1	1:A:47:LEU:HD11	0.57	2.30	5	6
1:A:91:LEU:N	1:A:91:LEU:CD1	0.57	2.68	13	1
1:A:91:LEU:N	1:A:91:LEU:HD12	0.57	2.14	4	1
1:A:55:GLY:O	1:A:56:TYR:CD1	0.57	2.57	9	1
1:A:79:ASP:C	1:A:81:ASP:N	0.56	2.58	2	15
1:A:35:ASP:C	1:A:37:ASP:H	0.56	2.04	6	4
1:A:51:MET:O	1:A:55:GLY:N	0.56	2.38	15	8
1:A:88:GLY:C	1:A:90:LYS:H	0.56	2.04	6	7
1:A:71:ASN:C	1:A:71:ASN:ND2	0.56	2.57	1	1
1:A:37:ASP:OD2	1:A:38:LYS:N	0.56	2.38	9	1
1:A:91:LEU:C	1:A:91:LEU:CD1	0.56	2.74	15	1
1:A:88:GLY:N	1:A:89:PRO:HD2	0.56	2.13	1	14
1:A:42:ILE:HD12	1:A:47:LEU:HD23	0.56	1.76	8	1
1:A:52:ARG:NH2	1:A:60:GLU:OE2	0.56	2.39	1	1
1:A:35:ASP:O	1:A:37:ASP:N	0.56	2.38	6	4
1:A:41:TYR:CE1	1:A:79:ASP:OD2	0.56	2.59	6	2
1:A:34:PHE:O	1:A:36:LYS:N	0.55	2.39	5	3
1:A:70:ILE:O	1:A:72:MET:N	0.55	2.40	4	9
1:A:27:LEU:HD13	1:A:84:VAL:HG22	0.55	1.76	3	6
1:A:32:ARG:C	1:A:34:PHE:N	0.55	2.59	6	15
1:A:63:LEU:N	1:A:63:LEU:CD2	0.55	2.68	2	3
1:A:34:PHE:C	1:A:36:LYS:H	0.55	2.03	4	2
1:A:40:GLY:O	1:A:41:TYR:CD1	0.55	2.59	8	8
1:A:86:LEU:O	1:A:91:LEU:HD22	0.55	2.00	6	1
1:A:61:MET:SD	1:A:61:MET:N	0.55	2.80	13	1
1:A:81:ASP:CG	1:A:82:ASP:N	0.55	2.60	7	2
1:A:89:PRO:O	1:A:91:LEU:N	0.55	2.40	4	3
1:A:56:TYR:CD2	1:A:56:TYR:O	0.55	2.60	9	2
1:A:56:TYR:CG	1:A:56:TYR:O	0.55	2.58	1	2
1:A:32:ARG:O	1:A:35:ASP:N	0.55	2.39	13	14
1:A:32:ARG:O	1:A:34:PHE:N	0.55	2.40	2	14
1:A:43:ASN:O	1:A:45:ARG:N	0.55	2.40	9	6
1:A:35:ASP:C	1:A:37:ASP:N	0.54	2.59	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:ILE:O	1:A:74:LEU:N	0.54	2.40	14	1
1:A:79:ASP:OD1	1:A:79:ASP:N	0.54	2.40	12	2
1:A:63:LEU:CD2	1:A:64:ILE:N	0.54	2.71	5	2
1:A:32:ARG:CG	1:A:32:ARG:HH11	0.54	2.16	3	1
1:A:31:PHE:CE2	1:A:42:ILE:CD1	0.54	2.90	11	2
1:A:56:TYR:O	1:A:57:MET:CB	0.54	2.55	10	2
1:A:71:ASN:ND2	1:A:72:MET:N	0.54	2.56	1	1
1:A:62:GLU:CG	1:A:63:LEU:N	0.54	2.71	11	1
1:A:21:PRO:O	1:A:23:GLU:N	0.54	2.41	6	4
1:A:63:LEU:HD12	1:A:64:ILE:H	0.54	1.63	3	1
1:A:39:ASP:OD1	1:A:40:GLY:N	0.54	2.40	11	3
1:A:20:ARG:N	1:A:23:GLU:OE1	0.53	2.41	5	1
1:A:82:ASP:O	1:A:86:LEU:HD23	0.53	2.03	8	2
1:A:71:ASN:C	1:A:73:ASN:H	0.53	2.07	11	2
1:A:89:PRO:C	1:A:91:LEU:H	0.53	2.07	8	1
1:A:71:ASN:HD22	1:A:72:MET:N	0.53	2.02	1	1
1:A:70:ILE:O	1:A:73:ASN:N	0.53	2.40	8	6
1:A:90:LYS:C	1:A:91:LEU:HD12	0.53	2.24	1	1
1:A:39:ASP:O	1:A:41:TYR:CD2	0.53	2.62	2	2
1:A:43:ASN:C	1:A:45:ARG:N	0.52	2.63	10	6
1:A:39:ASP:C	1:A:41:TYR:N	0.52	2.62	8	4
1:A:48:GLY:HA2	1:A:63:LEU:HD22	0.52	1.80	6	1
1:A:71:ASN:ND2	1:A:71:ASN:O	0.52	2.42	12	2
1:A:52:ARG:O	1:A:56:TYR:N	0.52	2.42	11	1
1:A:43:ASN:ND2	1:A:76:GLY:O	0.52	2.42	6	2
1:A:46:ASP:O	1:A:50:CYS:N	0.52	2.42	14	2
1:A:20:ARG:N	1:A:21:PRO:HD2	0.52	2.20	15	1
1:A:32:ARG:HG3	1:A:33:GLU:N	0.52	2.19	15	1
1:A:56:TYR:O	1:A:56:TYR:CD2	0.52	2.62	8	1
1:A:79:ASP:C	1:A:81:ASP:H	0.52	2.08	8	9
1:A:27:LEU:CD2	1:A:83:PHE:CE2	0.52	2.92	5	5
1:A:70:ILE:HG23	1:A:73:ASN:HD21	0.52	1.65	10	1
1:A:20:ARG:H	1:A:21:PRO:HD2	0.52	1.65	15	1
1:A:71:ASN:ND2	1:A:71:ASN:C	0.52	2.64	6	1
1:A:63:LEU:HD22	1:A:64:ILE:H	0.51	1.63	5	1
1:A:70:ILE:CG1	1:A:82:ASP:OD2	0.51	2.59	1	1
1:A:63:LEU:H	1:A:63:LEU:CD2	0.51	2.18	12	2
1:A:43:ASN:N	1:A:43:ASN:OD1	0.51	2.44	11	1
1:A:85:GLU:O	1:A:89:PRO:CG	0.51	2.58	4	1
1:A:62:GLU:CD	1:A:62:GLU:C	0.51	2.69	11	1
1:A:84:VAL:O	1:A:88:GLY:N	0.51	2.44	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:LEU:HD23	1:A:91:LEU:H	0.51	1.66	14	1
1:A:35:ASP:OD2	1:A:36:LYS:N	0.51	2.44	12	1
1:A:88:GLY:C	1:A:90:LYS:N	0.51	2.64	14	6
1:A:76:GLY:O	1:A:77:HIS:CD2	0.51	2.64	13	2
1:A:87:MET:SD	1:A:87:MET:O	0.51	2.68	1	1
1:A:36:LYS:O	1:A:38:LYS:N	0.51	2.44	6	1
1:A:47:LEU:O	1:A:51:MET:N	0.50	2.38	15	7
1:A:37:ASP:CG	1:A:38:LYS:H	0.50	2.09	15	2
1:A:56:TYR:O	1:A:57:MET:SD	0.50	2.68	14	1
1:A:91:LEU:HD23	1:A:91:LEU:N	0.50	2.20	14	1
1:A:41:TYR:CD1	1:A:41:TYR:N	0.50	2.80	13	2
1:A:85:GLU:O	1:A:88:GLY:N	0.50	2.42	14	3
1:A:20:ARG:H	1:A:21:PRO:HD3	0.50	1.66	15	1
1:A:38:LYS:C	1:A:39:ASP:CG	0.50	2.70	14	1
1:A:36:LYS:O	1:A:37:ASP:CB	0.50	2.60	11	3
1:A:73:ASN:ND2	1:A:74:LEU:H	0.50	2.03	10	1
1:A:59:THR:OG1	1:A:62:GLU:CB	0.50	2.59	7	2
1:A:72:MET:CG	1:A:73:ASN:N	0.50	2.75	15	1
1:A:39:ASP:O	1:A:41:TYR:N	0.50	2.45	9	3
1:A:91:LEU:N	1:A:91:LEU:CD2	0.50	2.74	14	2
1:A:48:GLY:HA2	1:A:63:LEU:HD11	0.50	1.82	9	1
1:A:81:ASP:OD1	1:A:81:ASP:C	0.49	2.51	7	1
1:A:70:ILE:C	1:A:72:MET:N	0.49	2.64	4	9
1:A:63:LEU:HD12	1:A:64:ILE:N	0.49	2.22	3	1
1:A:51:MET:O	1:A:55:GLY:CA	0.49	2.61	12	1
1:A:47:LEU:O	1:A:48:GLY:C	0.49	2.51	12	15
1:A:35:ASP:OD2	1:A:37:ASP:C	0.49	2.51	3	1
1:A:28:ARG:HH12	1:A:32:ARG:HE	0.49	1.48	3	1
1:A:35:ASP:CG	1:A:36:LYS:N	0.49	2.64	12	1
1:A:37:ASP:O	1:A:38:LYS:CB	0.49	2.61	6	2
1:A:36:LYS:C	1:A:37:ASP:CG	0.49	2.71	3	1
1:A:26:GLU:CD	1:A:54:MET:SD	0.49	2.91	4	1
1:A:85:GLU:O	1:A:89:PRO:CD	0.48	2.61	4	1
1:A:47:LEU:CD2	1:A:47:LEU:N	0.48	2.76	9	1
1:A:57:MET:H	1:A:58:PRO:HD3	0.48	1.65	8	4
1:A:34:PHE:CD1	1:A:50:CYS:SG	0.48	2.99	5	2
1:A:41:TYR:CD1	1:A:79:ASP:CG	0.48	2.87	7	1
1:A:32:ARG:NH1	1:A:35:ASP:O	0.48	2.47	2	1
1:A:71:ASN:C	1:A:73:ASN:N	0.48	2.66	11	1
1:A:55:GLY:C	1:A:57:MET:N	0.48	2.66	13	5
1:A:43:ASN:OD1	1:A:46:ASP:N	0.48	2.43	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ASP:OD2	1:A:39:ASP:OD1	0.48	2.32	14	1
1:A:79:ASP:OD2	1:A:81:ASP:CG	0.47	2.52	10	1
1:A:40:GLY:C	1:A:41:TYR:CG	0.47	2.88	10	6
1:A:34:PHE:C	1:A:36:LYS:N	0.47	2.68	4	2
1:A:37:ASP:O	1:A:39:ASP:N	0.47	2.48	4	1
1:A:37:ASP:C	1:A:39:ASP:OD1	0.47	2.53	14	1
1:A:54:MET:SD	1:A:54:MET:C	0.47	2.92	1	1
1:A:34:PHE:CE2	1:A:50:CYS:CA	0.47	2.97	1	1
1:A:27:LEU:O	1:A:30:ALA:N	0.47	2.48	3	2
1:A:59:THR:O	1:A:63:LEU:CD2	0.47	2.63	15	1
1:A:36:LYS:CG	1:A:36:LYS:O	0.47	2.63	5	1
1:A:62:GLU:C	1:A:62:GLU:CD	0.47	2.74	8	1
1:A:27:LEU:HD22	1:A:83:PHE:CE2	0.47	2.45	13	2
1:A:56:TYR:CD1	1:A:56:TYR:O	0.47	2.68	10	1
1:A:43:ASN:C	1:A:45:ARG:H	0.47	2.13	10	3
1:A:41:TYR:HB2	1:A:77:HIS:CE1	0.46	2.45	3	1
1:A:79:ASP:N	1:A:79:ASP:OD1	0.46	2.46	9	1
1:A:63:LEU:N	1:A:63:LEU:HD12	0.46	2.25	3	2
1:A:62:GLU:C	1:A:64:ILE:N	0.46	2.65	5	5
1:A:36:LYS:HD2	1:A:36:LYS:N	0.46	2.25	11	1
1:A:70:ILE:C	1:A:72:MET:H	0.46	2.14	4	3
1:A:31:PHE:CD1	1:A:31:PHE:C	0.46	2.88	1	2
1:A:63:LEU:N	1:A:63:LEU:HD22	0.46	2.26	5	1
1:A:43:ASN:ND2	1:A:44:CYS:N	0.46	2.64	6	1
1:A:36:LYS:C	1:A:38:LYS:N	0.46	2.67	6	2
1:A:51:MET:C	1:A:53:THR:N	0.46	2.69	7	1
1:A:38:LYS:O	1:A:39:ASP:CB	0.46	2.61	15	1
1:A:66:LEU:CD1	1:A:66:LEU:N	0.46	2.78	6	1
1:A:89:PRO:C	1:A:91:LEU:N	0.46	2.68	8	2
1:A:53:THR:O	1:A:53:THR:CG2	0.46	2.64	8	2
1:A:86:LEU:C	1:A:87:MET:SD	0.46	2.94	2	1
1:A:79:ASP:O	1:A:80:PHE:C	0.45	2.55	3	7
1:A:21:PRO:C	1:A:23:GLU:N	0.45	2.67	6	1
1:A:31:PHE:HB2	1:A:83:PHE:CE2	0.45	2.46	2	5
1:A:21:PRO:O	1:A:22:GLU:C	0.45	2.55	14	2
1:A:31:PHE:CD1	1:A:31:PHE:O	0.45	2.70	1	2
1:A:72:MET:SD	1:A:72:MET:O	0.45	2.74	6	1
1:A:61:MET:SD	1:A:62:GLU:N	0.45	2.90	12	1
1:A:53:THR:CG2	1:A:53:THR:O	0.44	2.65	1	1
1:A:63:LEU:HG	1:A:64:ILE:N	0.44	2.28	2	2
1:A:70:ILE:O	1:A:73:ASN:ND2	0.44	2.50	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ARG:C	1:A:34:PHE:H	0.44	2.15	10	4
1:A:38:LYS:O	1:A:39:ASP:CG	0.44	2.55	15	1
1:A:79:ASP:OD2	1:A:81:ASP:N	0.44	2.42	10	1
1:A:41:TYR:CZ	1:A:79:ASP:OD2	0.44	2.71	3	1
1:A:57:MET:O	1:A:57:MET:SD	0.44	2.75	9	1
1:A:91:LEU:HD12	1:A:91:LEU:N	0.44	2.28	13	1
1:A:87:MET:O	1:A:88:GLY:C	0.44	2.56	15	3
1:A:64:ILE:O	1:A:68:GLN:CB	0.44	2.65	13	3
1:A:72:MET:N	1:A:72:MET:SD	0.44	2.90	9	1
1:A:57:MET:SD	1:A:57:MET:O	0.44	2.76	4	1
1:A:62:GLU:O	1:A:65:GLU:N	0.43	2.51	4	2
1:A:34:PHE:CE2	1:A:50:CYS:HA	0.43	2.48	1	2
1:A:50:CYS:SG	1:A:51:MET:N	0.43	2.90	11	1
1:A:51:MET:CE	1:A:86:LEU:HD12	0.43	2.43	15	1
1:A:47:LEU:O	1:A:49:ASN:N	0.43	2.51	9	1
1:A:59:THR:C	1:A:60:GLU:CG	0.43	2.86	5	1
1:A:70:ILE:CG2	1:A:73:ASN:HD21	0.43	2.26	10	1
1:A:32:ARG:O	1:A:33:GLU:C	0.43	2.57	1	4
1:A:88:GLY:C	1:A:91:LEU:HD11	0.43	2.34	1	1
1:A:55:GLY:O	1:A:56:TYR:C	0.43	2.55	14	4
1:A:53:THR:O	1:A:53:THR:HG22	0.43	2.13	8	1
1:A:56:TYR:O	1:A:56:TYR:CG	0.43	2.71	8	1
1:A:59:THR:HG21	1:A:62:GLU:OE1	0.43	2.14	3	1
1:A:63:LEU:O	1:A:66:LEU:N	0.43	2.52	7	1
1:A:31:PHE:CE2	1:A:42:ILE:HG12	0.43	2.49	8	3
1:A:25:GLU:OE2	1:A:29:GLU:OE1	0.43	2.37	14	1
1:A:88:GLY:O	1:A:91:LEU:HD11	0.43	2.14	1	1
1:A:39:ASP:OD1	1:A:39:ASP:C	0.43	2.58	12	1
1:A:46:ASP:O	1:A:49:ASN:N	0.43	2.51	8	1
1:A:83:PHE:CE1	1:A:87:MET:CE	0.43	3.02	5	1
1:A:82:ASP:O	1:A:86:LEU:N	0.42	2.52	1	2
1:A:59:THR:HG1	1:A:62:GLU:H	0.42	1.57	13	1
1:A:28:ARG:CG	1:A:32:ARG:HH12	0.42	2.26	10	1
1:A:20:ARG:O	1:A:20:ARG:CG	0.42	2.66	8	1
1:A:31:PHE:CD2	1:A:42:ILE:CD1	0.42	2.99	11	1
1:A:34:PHE:CZ	1:A:50:CYS:HA	0.42	2.49	5	1
1:A:88:GLY:O	1:A:91:LEU:CD2	0.42	2.67	5	1
1:A:31:PHE:CE2	1:A:42:ILE:CG1	0.42	3.02	7	1
1:A:63:LEU:HD12	1:A:63:LEU:N	0.42	2.29	11	2
1:A:74:LEU:HG	1:A:75:GLY:N	0.42	2.29	5	1
1:A:47:LEU:C	1:A:49:ASN:N	0.42	2.70	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ASP:C	1:A:35:ASP:OD1	0.42	2.57	15	1
1:A:32:ARG:NH1	1:A:32:ARG:HG2	0.42	2.30	3	1
1:A:28:ARG:HA	1:A:80:PHE:CE1	0.42	2.50	8	3
1:A:26:GLU:CA	1:A:26:GLU:OE1	0.42	2.67	9	1
1:A:63:LEU:N	1:A:63:LEU:CD1	0.42	2.72	5	1
1:A:68:GLN:O	1:A:69:GLN:C	0.42	2.58	7	1
1:A:90:LYS:NZ	1:A:90:LYS:CB	0.42	2.82	14	1
1:A:36:LYS:NZ	1:A:36:LYS:CB	0.42	2.83	7	1
1:A:59:THR:HG21	1:A:62:GLU:HB2	0.42	1.90	7	1
1:A:37:ASP:O	1:A:38:LYS:C	0.41	2.57	4	1
1:A:79:ASP:CG	1:A:80:PHE:N	0.41	2.73	8	1
1:A:20:ARG:C	1:A:22:GLU:H	0.41	2.18	2	1
1:A:79:ASP:OD1	1:A:82:ASP:OD1	0.41	2.38	15	1
1:A:91:LEU:N	1:A:91:LEU:HD23	0.41	2.29	8	1
1:A:87:MET:O	1:A:91:LEU:N	0.41	2.54	12	1
1:A:22:GLU:HG3	1:A:23:GLU:N	0.41	2.31	15	1
1:A:71:ASN:O	1:A:73:ASN:N	0.41	2.53	11	1
1:A:55:GLY:O	1:A:56:TYR:CB	0.41	2.68	5	1
1:A:20:ARG:O	1:A:24:ILE:CG1	0.41	2.68	15	1
1:A:43:ASN:O	1:A:44:CYS:C	0.41	2.56	8	1
1:A:70:ILE:HG22	1:A:71:ASN:N	0.41	2.30	1	1
1:A:54:MET:O	1:A:54:MET:SD	0.41	2.78	5	1
1:A:46:ASP:O	1:A:47:LEU:C	0.41	2.58	14	1
1:A:27:LEU:HD23	1:A:83:PHE:CE2	0.41	2.50	4	3
1:A:64:ILE:O	1:A:65:GLU:C	0.41	2.59	5	1
1:A:62:GLU:O	1:A:63:LEU:C	0.41	2.58	4	2
1:A:79:ASP:OD2	1:A:81:ASP:CB	0.41	2.69	10	1
1:A:87:MET:O	1:A:90:LYS:N	0.41	2.54	5	2
1:A:20:ARG:NH1	1:A:91:LEU:HD23	0.41	2.31	11	1
1:A:45:ARG:CG	1:A:46:ASP:N	0.41	2.84	2	1
1:A:61:MET:O	1:A:61:MET:CG	0.41	2.68	5	1
1:A:27:LEU:C	1:A:27:LEU:HD13	0.40	2.36	2	1
1:A:62:GLU:O	1:A:62:GLU:CD	0.40	2.59	8	1
1:A:69:GLN:O	1:A:70:ILE:C	0.40	2.60	11	1
1:A:43:ASN:N	1:A:46:ASP:OD2	0.40	2.41	7	1
1:A:63:LEU:CD2	1:A:63:LEU:C	0.40	2.90	5	1
1:A:89:PRO:O	1:A:90:LYS:C	0.40	2.60	4	1
1:A:37:ASP:OD1	1:A:37:ASP:C	0.40	2.60	1	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	71/76 (93%)	51±2 (72±3%)	13±2 (18±3%)	7±2 (10±2%)	1	10
All	All	1065/1140 (93%)	762 (72%)	193 (18%)	110 (10%)	1	10

All 22 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	80	PHE	15
1	A	75	GLY	12
1	A	89	PRO	9
1	A	58	PRO	8
1	A	61	MET	8
1	A	57	MET	7
1	A	33	GLU	6
1	A	71	ASN	6
1	A	35	ASP	6
1	A	44	CYS	5
1	A	37	ASP	5
1	A	38	LYS	4
1	A	56	TYR	3
1	A	40	GLY	3
1	A	55	GLY	2
1	A	22	GLU	2
1	A	21	PRO	2
1	A	36	LYS	2
1	A	39	ASP	2
1	A	60	GLU	1
1	A	73	ASN	1
1	A	90	LYS	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	65/69 (94%)	51±2 (79±4%)	14±2 (21±4%)	4 34
All	All	975/1035 (94%)	772 (79%)	203 (21%)	4 34

All 50 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	64	ILE	15
1	A	78	VAL	13
1	A	20	ARG	10
1	A	51	MET	9
1	A	53	THR	9
1	A	63	LEU	9
1	A	42	ILE	8
1	A	86	LEU	7
1	A	43	ASN	5
1	A	54	MET	5
1	A	32	ARG	5
1	A	72	MET	5
1	A	37	ASP	5
1	A	77	HIS	5
1	A	57	MET	5
1	A	61	MET	5
1	A	56	TYR	4
1	A	79	ASP	4
1	A	91	LEU	4
1	A	36	LYS	4
1	A	70	ILE	4
1	A	28	ARG	4
1	A	71	ASN	3
1	A	44	CYS	3
1	A	81	ASP	3
1	A	50	CYS	3
1	A	49	ASN	3
1	A	22	GLU	3
1	A	45	ARG	3
1	A	87	MET	3
1	A	39	ASP	3
1	A	29	GLU	3
1	A	90	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	74	LEU	2
1	A	47	LEU	2
1	A	73	ASN	2
1	A	46	ASP	2
1	A	27	LEU	2
1	A	26	GLU	2
1	A	82	ASP	2
1	A	52	ARG	2
1	A	69	GLN	2
1	A	89	PRO	1
1	A	68	GLN	1
1	A	25	GLU	1
1	A	62	GLU	1
1	A	59	THR	1
1	A	23	GLU	1
1	A	60	GLU	1
1	A	38	LYS	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

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

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 15197

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	1577
Number of shifts mapped to atoms	783
Number of unparsed shifts	0
Number of shifts with mapping errors	794
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- Residue not found in structure. All 794 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	158	PHE	HB2	2.24	0.04	2
A	146	ARG	HG2	1.66	0.04	2
A	147	ASP	N	119.49	0.2	1
A	125	ARG	CB	30.03	0.2	1
A	95	THR	CG2	21.86	0.2	1
A	119	ILE	HG22	0.12	0.04	1
A	12	LEU	HD11	0.84	0.04	2
A	165	MET	CB	31.29	0.2	1
A	139	ARG	HA	4.05	0.04	1
A	110	GLU	CB	29.06	0.2	1
A	103	GLU	HG2	2.93	0.04	2
A	129	ARG	C	179.01	0.2	1
A	97	ASP	HA	4.61	0.04	1
A	95	THR	HG22	1.24	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	121	THR	HG22	1.23	0.04	1
A	101	VAL	CA	66.17	0.2	1
A	161	PHE	CB	39.64	0.2	1
A	108	PHE	HD1	7.09	0.04	3
A	156	VAL	CG2	21.36	0.2	1
A	137	GLY	CA	45.37	0.2	1
A	93	ALA	CB	19.13	0.2	1
A	167	ARG	CA	57.8	0.2	1
A	119	ILE	C	174.37	0.2	1
A	107	ALA	HA	4.36	0.04	1
A	134	HIS	HA	4.61	0.04	1
A	160	GLU	CB	29.43	0.2	1
A	101	VAL	HG12	1.12	0.04	2
A	138	HIS	CB	30.11	0.2	1
A	107	ALA	HB3	1.8	0.04	1
A	98	MET	HA	4.49	0.04	1
A	97	ASP	CA	54.86	0.2	1
A	132	LEU	HD22	0.8	0.04	2
A	144	ILE	HD11	0.77	0.04	1
A	144	ILE	CB	38.24	0.2	1
A	129	ARG	CA	59.81	0.2	1
A	155	ARG	H	7.77	0.04	1
A	112	ASP	C	179.33	0.2	1
A	147	ASP	CA	56.75	0.2	1
A	108	PHE	CA	62.12	0.2	1
A	146	ARG	CB	30.41	0.2	1
A	135	GLN	CG	33.7	0.2	1
A	132	LEU	HD12	0.8	0.04	2
A	13	SER	C	174.72	0.2	1
A	114	ASN	CA	51.54	0.2	1
A	156	VAL	HG12	1.08	0.04	2
A	15	LYS	HG2	1.42	0.04	2
A	140	ASP	C	178.02	0.2	1
A	12	LEU	HB2	1.63	0.04	2
A	102	LYS	CE	42.27	0.2	1
A	97	ASP	C	176.06	0.2	1
A	148	VAL	CG1	21.61	0.2	1
A	136	VAL	C	176.08	0.2	1
A	163	ARG	N	120.57	0.2	1
A	99	ILE	HD12	0.84	0.04	1
A	148	VAL	HB	1.97	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	161	PHE	HA	4.11	0.04	1
A	144	ILE	H	7.5	0.04	1
A	109	ARG	CD	43.69	0.2	1
A	142	GLU	HB2	2.06	0.04	2
A	143	GLU	HB2	2.12	0.04	2
A	141	ILE	HG21	0.91	0.04	1
A	128	MET	HG2	2.15	0.04	2
A	159	GLU	N	117.53	0.2	1
A	155	ARG	CA	54.85	0.2	1
A	94	GLU	HA	4.4	0.04	1
A	105	ARG	H	8.89	0.04	1
A	96	ALA	HB2	1.42	0.04	1
A	108	PHE	HB2	3.19	0.04	2
A	92	LEU	C	177.44	0.2	1
A	100	GLY	C	174.55	0.2	1
A	103	GLU	HB2	2.02	0.04	2
A	14	ARG	HB2	2.02	0.04	2
A	125	ARG	N	118.42	0.2	1
A	157	ASP	HA	5.54	0.04	1
A	143	GLU	H	7.71	0.04	1
A	112	ASP	CA	52.12	0.2	1
A	131	LEU	HD22	1.0	0.04	2
A	132	LEU	HB3	1.76	0.04	2
A	148	VAL	HG13	0.82	0.04	2
A	119	ILE	HG13	0.99	0.04	1
A	120	SER	H	9.05	0.04	1
A	161	PHE	HB3	3.12	0.04	2
A	162	VAL	HG22	0.62	0.04	2
A	118	GLU	N	117.13	0.2	1
A	132	LEU	CD2	25.74	0.2	1
A	12	LEU	CD2	25.32	0.2	1
A	113	THR	N	114.63	0.2	1
A	166	SER	C	173.18	0.2	1
A	130	LYS	CE	40.87	0.2	1
A	105	ARG	CB	29.45	0.2	1
A	104	LEU	C	178.81	0.2	1
A	131	LEU	C	178.35	0.2	1
A	94	GLU	HB2	2.37	0.04	2
A	155	ARG	N	118.55	0.2	1
A	124	LEU	HD11	1.07	0.04	2
A	141	ILE	HD12	0.78	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	117	GLY	C	173.52	0.2	1
A	143	GLU	CB	29.49	0.2	1
A	126	GLU	HG2	2.33	0.04	2
A	167	ARG	HB2	1.8	0.04	2
A	150	LEU	CB	42.52	0.2	1
A	164	MET	CA	58.29	0.2	1
A	146	ARG	N	119.6	0.2	1
A	138	HIS	CA	53.94	0.2	1
A	97	ASP	H	8.29	0.04	1
A	124	LEU	HD21	0.94	0.04	2
A	148	VAL	HG23	0.9	0.04	2
A	145	ILE	HD12	0.73	0.04	1
A	12	LEU	N	122.66	0.2	1
A	166	SER	CA	58.68	0.2	1
A	145	ILE	N	116.95	0.2	1
A	121	THR	CA	66.38	0.2	1
A	162	VAL	HG13	0.26	0.04	2
A	135	GLN	H	8.09	0.04	1
A	144	ILE	CG1	28.82	0.2	1
A	94	GLU	HG2	2.36	0.04	2
A	121	THR	HG21	1.23	0.04	1
A	129	ARG	HB2	1.9	0.04	2
A	161	PHE	C	176.37	0.2	1
A	101	VAL	CB	31.8	0.2	1
A	131	LEU	HD13	0.97	0.04	2
A	117	GLY	CA	45.79	0.2	1
A	114	ASN	HB3	2.86	0.04	2
A	118	GLU	CA	54.0	0.2	1
A	126	GLU	HB2	1.84	0.04	2
A	101	VAL	HG21	1.07	0.04	2
A	104	LEU	HB2	2.32	0.04	2
A	124	LEU	CA	57.98	0.2	1
A	164	MET	HB2	2.0	0.04	2
A	138	HIS	C	179.51	0.2	1
A	109	ARG	HB2	1.93	0.04	2
A	160	GLU	CG	35.85	0.2	1
A	101	VAL	HG11	1.12	0.04	2
A	13	SER	CA	58.67	0.2	1
A	12	LEU	HD23	0.89	0.04	2
A	106	ASP	CA	57.42	0.2	1
A	97	ASP	CB	41.13	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	93	ALA	HA	4.26	0.04	1
A	134	HIS	C	175.7	0.2	1
A	144	ILE	HD12	0.77	0.04	1
A	137	GLY	HA2	4.03	0.04	2
A	129	ARG	CD	37.09	0.2	1
A	115	GLY	HA2	3.85	0.04	2
A	164	MET	N	120.87	0.2	1
A	119	ILE	CD1	13.15	0.2	1
A	135	GLN	CB	29.63	0.2	1
A	156	VAL	HG11	1.08	0.04	2
A	145	ILE	CA	64.36	0.2	1
A	98	MET	CG	32.07	0.2	1
A	110	GLU	HB2	1.95	0.04	2
A	102	LYS	CB	32.21	0.2	1
A	109	ARG	H	8.33	0.04	1
A	165	MET	HB2	1.63	0.04	2
A	134	HIS	CA	56.86	0.2	1
A	117	GLY	N	113.21	0.2	1
A	15	LYS	HD2	1.68	0.04	2
A	158	PHE	H	8.4	0.04	1
A	107	ALA	C	178.48	0.2	1
A	125	ARG	HB2	1.91	0.04	2
A	142	GLU	C	179.24	0.2	1
A	94	GLU	N	118.94	0.2	1
A	124	LEU	N	120.01	0.2	1
A	99	ILE	CB	38.57	0.2	1
A	118	GLU	HB2	2.11	0.04	2
A	109	ARG	CG	27.73	0.2	1
A	117	GLY	HA3	3.73	0.04	2
A	93	ALA	HB2	1.49	0.04	1
A	144	ILE	HG21	0.87	0.04	1
A	105	ARG	HG2	1.39	0.04	2
A	103	GLU	HA	4.19	0.04	1
A	113	THR	HB	4.35	0.04	1
A	125	ARG	HG3	1.63	0.04	2
A	96	ALA	HB1	1.42	0.04	1
A	116	ASP	HB2	1.85	0.04	2
A	99	ILE	HG23	0.96	0.04	1
A	94	GLU	C	176.9	0.2	1
A	160	GLU	H	8.21	0.04	1
A	131	LEU	HD21	1.0	0.04	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	139	ARG	CA	58.38	0.2	1
A	15	LYS	CB	32.91	0.2	1
A	141	ILE	CG2	17.85	0.2	1
A	108	PHE	H	8.61	0.04	1
A	128	MET	CA	59.86	0.2	1
A	96	ALA	H	8.3	0.04	1
A	125	ARG	H	7.99	0.04	1
A	118	GLU	HG2	2.17	0.04	2
A	104	LEU	HD12	0.7	0.04	2
A	155	ARG	CB	34.25	0.2	1
A	134	HIS	HD2	7.008	0.04	1
A	100	GLY	HA3	4.27	0.04	2
A	162	VAL	HG21	0.62	0.04	2
A	142	GLU	CB	28.62	0.2	1
A	104	LEU	HD23	0.76	0.04	2
A	156	VAL	H	9.0	0.04	1
A	94	GLU	CA	56.88	0.2	1
A	102	LYS	HE2	2.61	0.04	2
A	106	ASP	HA	4.41	0.04	1
A	92	LEU	CD2	25.29	0.2	1
A	149	ASP	CA	55.86	0.2	1
A	14	ARG	CB	32.64	0.2	1
A	96	ALA	C	177.46	0.2	1
A	124	LEU	HD12	1.07	0.04	2
A	92	LEU	CG	27.0	0.2	1
A	156	VAL	N	118.17	0.2	1
A	124	LEU	CD2	26.93	0.2	1
A	153	ASP	HB2	2.66	0.04	2
A	102	LYS	HA	4.01	0.04	1
A	161	PHE	HD1	7.08	0.04	3
A	125	ARG	HA	3.66	0.04	1
A	112	ASP	HB2	2.61	0.04	2
A	113	THR	C	175.34	0.2	1
A	113	THR	CG2	22.45	0.2	1
A	111	PHE	HB3	3.0	0.04	2
A	157	ASP	C	176.1	0.2	1
A	141	ILE	C	177.1	0.2	1
A	165	MET	N	114.48	0.2	1
A	103	GLU	CA	60.54	0.2	1
A	128	MET	N	115.47	0.2	1
A	93	ALA	C	177.96	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	110	GLU	N	117.7	0.2	1
A	162	VAL	HA	2.97	0.04	1
A	131	LEU	HB2	1.82	0.04	2
A	102	LYS	N	121.87	0.2	1
A	112	ASP	H	7.7	0.04	1
A	116	ASP	HA	4.68	0.04	1
A	98	MET	H	8.11	0.04	1
A	162	VAL	CG2	21.3	0.2	1
A	93	ALA	N	121.93	0.2	1
A	124	LEU	CB	41.65	0.2	1
A	131	LEU	CG	26.86	0.2	1
A	130	LYS	CA	59.26	0.2	1
A	152	GLY	HA3	3.92	0.04	2
A	101	VAL	HA	3.86	0.04	1
A	156	VAL	HG21	0.92	0.04	2
A	159	GLU	CG	37.14	0.2	1
A	157	ASP	CA	51.93	0.2	1
A	13	SER	H	8.26	0.04	1
A	92	LEU	HD13	0.73	0.04	2
A	125	ARG	HD2	3.22	0.04	2
A	121	THR	CG2	23.8	0.2	1
A	142	GLU	HA	3.96	0.04	1
A	102	LYS	HB2	1.84	0.04	2
A	98	MET	C	176.22	0.2	1
A	158	PHE	HB3	2.58	0.04	2
A	122	SER	C	177.19	0.2	1
A	123	GLU	HA	4.02	0.04	1
A	13	SER	HB2	3.87	0.04	2
A	119	ILE	HG23	0.12	0.04	1
A	165	MET	CA	54.48	0.2	1
A	132	LEU	N	115.8	0.2	1
A	98	MET	CB	33.36	0.2	1
A	115	GLY	CA	47.74	0.2	1
A	102	LYS	C	178.27	0.2	1
A	110	GLU	CA	58.78	0.2	1
A	103	GLU	HG3	2.84	0.04	2
A	124	LEU	H	8.72	0.04	1
A	95	THR	HG23	1.24	0.04	1
A	109	ARG	HD2	3.21	0.04	2
A	122	SER	H	8.17	0.04	1
A	13	SER	CB	64.03	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	138	HIS	HB3	3.34	0.04	2
A	116	ASP	CB	40.62	0.2	1
A	139	ARG	HB2	1.73	0.04	2
A	14	ARG	N	122.72	0.2	1
A	101	VAL	C	177.42	0.2	1
A	107	ALA	HB2	1.8	0.04	1
A	105	ARG	HA	3.9	0.04	1
A	132	LEU	HD23	0.8	0.04	2
A	113	THR	HA	4.0	0.04	1
A	92	LEU	HG	1.6	0.04	1
A	131	LEU	HB3	1.5	0.04	2
A	132	LEU	HD11	0.8	0.04	2
A	146	ARG	C	178.62	0.2	1
A	15	LYS	C	176.14	0.2	1
A	123	GLU	H	7.48	0.04	1
A	139	ARG	CB	33.24	0.2	1
A	15	LYS	CG	24.8	0.2	1
A	130	LYS	HD3	1.52	0.04	2
A	141	ILE	CG1	28.98	0.2	1
A	115	GLY	N	108.95	0.2	1
A	158	PHE	C	176.29	0.2	1
A	128	MET	CB	33.3	0.2	1
A	98	MET	N	119.8	0.2	1
A	163	ARG	H	7.66	0.04	1
A	145	ILE	HG21	0.68	0.04	1
A	161	PHE	HE1	6.94	0.04	3
A	116	ASP	H	8.32	0.04	1
A	123	GLU	CG	37.25	0.2	1
A	104	LEU	H	8.19	0.04	1
A	131	LEU	H	8.04	0.04	1
A	138	HIS	HA	4.11	0.04	1
A	142	GLU	CG	36.07	0.2	1
A	131	LEU	HG	1.63	0.04	1
A	123	GLU	HB2	1.93	0.04	2
A	99	ILE	HD13	0.84	0.04	1
A	113	THR	CB	68.67	0.2	1
A	105	ARG	N	121.3	0.2	1
A	15	LYS	HB2	1.76	0.04	2
A	151	ASN	N	124.94	0.2	1
A	14	ARG	CA	56.4	0.2	1
A	95	THR	C	174.65	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	136	VAL	CA	62.38	0.2	1
A	119	ILE	HD11	0.3	0.04	1
A	99	ILE	HG13	1.17	0.04	1
A	104	LEU	HA	4.34	0.04	1
A	139	ARG	H	8.24	0.04	1
A	143	GLU	N	118.3	0.2	1
A	124	LEU	CD1	24.14	0.2	1
A	112	ASP	HA	5.29	0.04	1
A	165	MET	HB3	1.89	0.04	2
A	164	MET	CG	32.49	0.2	1
A	121	THR	H	8.67	0.04	1
A	131	LEU	HD11	0.97	0.04	2
A	145	ILE	HA	3.7	0.04	1
A	140	ASP	CB	41.05	0.2	1
A	118	GLU	H	7.91	0.04	1
A	12	LEU	CB	42.37	0.2	1
A	132	LEU	CB	42.88	0.2	1
A	132	LEU	HB2	1.42	0.04	2
A	162	VAL	HB	1.73	0.04	1
A	161	PHE	CA	61.13	0.2	1
A	113	THR	H	8.03	0.04	1
A	119	ILE	HG12	1.36	0.04	1
A	159	GLU	C	179.53	0.2	1
A	101	VAL	N	119.81	0.2	1
A	111	PHE	H	7.19	0.04	1
A	99	ILE	HA	4.06	0.04	1
A	162	VAL	CG1	23.64	0.2	1
A	137	GLY	N	111.75	0.2	1
A	13	SER	N	115.72	0.2	1
A	124	LEU	CG	27.16	0.2	1
A	136	VAL	HG13	0.92	0.04	2
A	130	LYS	CD	25.57	0.2	1
A	105	ARG	CA	60.06	0.2	1
A	136	VAL	N	119.06	0.2	1
A	160	GLU	HG2	2.39	0.04	2
A	157	ASP	CB	41.97	0.2	1
A	159	GLU	HB3	2.31	0.04	2
A	111	PHE	HD1	7.41	0.04	3
A	108	PHE	HE1	7.42	0.04	3
A	97	ASP	N	118.64	0.2	1
A	131	LEU	CD1	23.26	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	124	LEU	HA	3.83	0.04	1
A	143	GLU	CA	58.89	0.2	1
A	106	ASP	C	179.01	0.2	1
A	101	VAL	CG1	22.35	0.2	1
A	132	LEU	H	8.36	0.04	1
A	135	GLN	N	119.42	0.2	1
A	99	ILE	CA	62.14	0.2	1
A	128	MET	HA	3.94	0.04	1
A	104	LEU	CD2	26.75	0.2	1
A	145	ILE	HD11	0.73	0.04	1
A	165	MET	HA	4.47	0.04	1
A	141	ILE	HA	3.74	0.04	1
A	92	LEU	HB2	1.63	0.04	2
A	127	ALA	C	179.65	0.2	1
A	131	LEU	N	117.21	0.2	1
A	95	THR	H	8.02	0.04	1
A	118	GLU	C	174.78	0.2	1
A	130	LYS	HA	4.12	0.04	1
A	114	ASN	HB2	3.27	0.04	2
A	143	GLU	C	178.5	0.2	1
A	103	GLU	H	8.21	0.04	1
A	157	ASP	H	8.31	0.04	1
A	101	VAL	HG22	1.07	0.04	2
A	156	VAL	HB	2.25	0.04	1
A	121	THR	C	176.9	0.2	1
A	104	LEU	HB3	1.58	0.04	2
A	129	ARG	H	8.05	0.04	1
A	120	SER	CA	56.78	0.2	1
A	166	SER	N	114.61	0.2	1
A	106	ASP	CB	40.06	0.2	1
A	97	ASP	HB2	2.6	0.04	2
A	92	LEU	N	118.11	0.2	1
A	144	ILE	HD13	0.77	0.04	1
A	129	ARG	CG	27.88	0.2	1
A	166	SER	H	7.46	0.04	1
A	124	LEU	C	177.73	0.2	1
A	129	ARG	HG2	1.8	0.04	2
A	135	GLN	CA	56.48	0.2	1
A	98	MET	HG2	2.61	0.04	2
A	132	LEU	HA	4.44	0.04	1
A	15	LYS	CD	29.02	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	153	ASP	HA	4.7	0.04	1
A	117	GLY	H	10.54	0.04	1
A	92	LEU	HA	4.17	0.04	1
A	128	MET	CG	33.08	0.2	1
A	98	MET	HB2	2.07	0.04	2
A	94	GLU	H	8.12	0.04	1
A	111	PHE	HA	4.34	0.04	1
A	145	ILE	CG1	28.7	0.2	1
A	136	VAL	HG21	0.93	0.04	2
A	113	THR	CA	64.49	0.2	1
A	128	MET	C	178.23	0.2	1
A	107	ALA	CB	18.48	0.2	1
A	160	GLU	HA	4.19	0.04	1
A	106	ASP	H	8.44	0.04	1
A	141	ILE	HD11	0.78	0.04	1
A	117	GLY	HA2	4.36	0.04	2
A	145	ILE	H	7.92	0.04	1
A	155	ARG	C	176.09	0.2	1
A	93	ALA	HB3	1.49	0.04	1
A	144	ILE	HG22	0.87	0.04	1
A	106	ASP	HB2	2.82	0.04	2
A	134	HIS	HB2	3.16	0.04	2
A	148	VAL	CB	34.4	0.2	1
A	121	THR	HA	3.88	0.04	1
A	100	GLY	CA	45.31	0.2	1
A	149	ASP	HB2	1.69	0.04	2
A	144	ILE	C	178.19	0.2	1
A	146	ARG	CG	27.05	0.2	1
A	145	ILE	HB	1.85	0.04	1
A	145	ILE	HG12	1.75	0.04	1
A	107	ALA	H	7.99	0.04	1
A	103	GLU	CG	37.72	0.2	1
A	12	LEU	CA	55.83	0.2	1
A	148	VAL	HG11	0.82	0.04	2
A	141	ILE	HG12	1.72	0.04	1
A	118	GLU	HG3	2.07	0.04	2
A	104	LEU	HD13	0.7	0.04	2
A	146	ARG	HD2	3.25	0.04	2
A	100	GLY	HA2	4.0	0.04	2
A	104	LEU	HD22	0.76	0.04	2
A	141	ILE	H	8.02	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	164	MET	CB	32.87	0.2	1
A	104	LEU	CA	58.59	0.2	1
A	131	LEU	CA	57.01	0.2	1
A	130	LYS	CG	21.48	0.2	1
A	148	VAL	C	175.85	0.2	1
A	126	GLU	CA	58.74	0.2	1
A	127	ALA	H	8.11	0.04	1
A	143	GLU	HG2	2.33	0.04	2
A	106	ASP	N	119.61	0.2	1
A	124	LEU	HD13	1.07	0.04	2
A	150	LEU	HB2	1.61	0.04	2
A	13	SER	HA	4.43	0.04	1
A	100	GLY	N	113.55	0.2	1
A	165	MET	H	7.49	0.04	1
A	124	LEU	HD23	0.94	0.04	2
A	148	VAL	HG21	0.9	0.04	2
A	122	SER	CA	61.12	0.2	1
A	162	VAL	C	179.09	0.2	1
A	111	PHE	HB2	2.39	0.04	2
A	162	VAL	HG11	0.26	0.04	2
A	141	ILE	HB	1.96	0.04	1
A	162	VAL	N	117.76	0.2	1
A	127	ALA	CB	17.47	0.2	1
A	93	ALA	H	7.44	0.04	1
A	126	GLU	C	178.84	0.2	1
A	157	ASP	HB2	2.85	0.04	2
A	148	VAL	HG22	0.9	0.04	2
A	123	GLU	N	124.62	0.2	1
A	141	ILE	CD1	13.33	0.2	1
A	151	ASN	HA	4.48	0.04	1
A	107	ALA	N	122.25	0.2	1
A	154	GLY	C	173.83	0.2	1
A	95	THR	HB	4.33	0.04	1
A	123	GLU	HG2	2.32	0.04	2
A	104	LEU	N	120.09	0.2	1
A	116	ASP	N	117.82	0.2	1
A	139	ARG	N	117.77	0.2	1
A	109	ARG	N	115.26	0.2	1
A	133	GLY	CA	46.52	0.2	1
A	120	SER	CB	65.98	0.2	1
A	126	GLU	N	116.99	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	156	VAL	HG22	0.92	0.04	2
A	12	LEU	HD21	0.89	0.04	2
A	15	LYS	HE2	3.01	0.04	2
A	146	ARG	H	7.73	0.04	1
A	92	LEU	HD21	0.75	0.04	2
A	166	SER	HB2	3.87	0.04	2
A	92	LEU	HD12	0.73	0.04	2
A	133	GLY	HA3	3.88	0.04	2
A	105	ARG	HD3	2.84	0.04	2
A	140	ASP	CA	55.51	0.2	1
A	102	LYS	HB3	1.96	0.04	2
A	151	ASN	H	8.03	0.04	1
A	127	ALA	HB1	1.01	0.04	1
A	167	ARG	HD2	3.17	0.04	2
A	154	GLY	CA	46.43	0.2	1
A	125	ARG	CD	42.77	0.2	1
A	12	LEU	HD13	0.84	0.04	2
A	145	ILE	HG23	0.68	0.04	1
A	99	ILE	C	176.02	0.2	1
A	98	MET	CA	55.87	0.2	1
A	127	ALA	HB3	1.01	0.04	1
A	99	ILE	CD1	13.45	0.2	1
A	158	PHE	CA	61.85	0.2	1
A	107	ALA	CA	55.05	0.2	1
A	136	VAL	CG2	21.58	0.2	1
A	131	LEU	HA	4.28	0.04	1
A	138	HIS	HB2	3.12	0.04	2
A	116	ASP	CA	53.03	0.2	1
A	115	GLY	C	174.45	0.2	1
A	133	GLY	N	107.88	0.2	1
A	119	ILE	CA	59.47	0.2	1
A	137	GLY	H	8.61	0.04	1
A	124	LEU	HB2	1.38	0.04	2
A	140	ASP	HA	4.53	0.04	1
A	120	SER	HB2	4.7	0.04	2
A	121	THR	HB	4.22	0.04	1
A	113	THR	HG23	1.27	0.04	1
A	136	VAL	H	7.92	0.04	1
A	146	ARG	CD	43.29	0.2	1
A	154	GLY	HA2	4.12	0.04	2
A	145	ILE	CD1	13.27	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	127	ALA	HA	3.53	0.04	1
A	130	LYS	HD2	1.67	0.04	2
A	114	ASN	C	176.25	0.2	1
A	12	LEU	HA	4.35	0.04	1
A	143	GLU	HA	3.98	0.04	1
A	102	LYS	CG	25.08	0.2	1
A	96	ALA	HA	4.32	0.04	1
A	99	ILE	HB	1.82	0.04	1
A	104	LEU	HD21	0.76	0.04	2
A	160	GLU	C	178.2	0.2	1
A	155	ARG	HA	5.02	0.04	1
A	167	ARG	N	127.14	0.2	1
A	142	GLU	CA	58.92	0.2	1
A	109	ARG	CB	30.03	0.2	1
A	163	ARG	CA	60.21	0.2	1
A	150	LEU	HA	4.41	0.04	1
A	141	ILE	HG23	0.91	0.04	1
A	119	ILE	HD12	0.3	0.04	1
A	157	ASP	N	124.52	0.2	1
A	99	ILE	HG12	1.56	0.04	1
A	124	LEU	HG	1.6	0.04	1
A	99	ILE	H	8.21	0.04	1
A	133	GLY	H	7.83	0.04	1
A	129	ARG	N	118.98	0.2	1
A	108	PHE	N	118.51	0.2	1
A	167	ARG	HA	4.12	0.04	1
A	162	VAL	CB	31.28	0.2	1
A	114	ASN	N	115.05	0.2	1
A	103	GLU	C	180.47	0.2	1
A	101	VAL	H	8.27	0.04	1
A	132	LEU	CA	55.18	0.2	1
A	144	ILE	HB	1.94	0.04	1
A	159	GLU	HA	3.62	0.04	1
A	92	LEU	CD1	23.03	0.2	1
A	113	THR	HG21	1.27	0.04	1
A	126	GLU	HA	3.94	0.04	1
A	130	LYS	C	178.5	0.2	1
A	96	ALA	CB	19.44	0.2	1
A	163	ARG	C	179.64	0.2	1
A	136	VAL	HG12	0.92	0.04	2
A	166	SER	HA	4.53	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	159	GLU	CA	59.88	0.2	1
A	136	VAL	HG22	0.93	0.04	2
A	167	ARG	H	7.49	0.04	1
A	120	SER	C	175.83	0.2	1
A	162	VAL	H	8.23	0.04	1
A	92	LEU	CB	41.99	0.2	1
A	135	GLN	HB3	1.97	0.04	2
A	143	GLU	HB3	2.32	0.04	2
A	14	ARG	H	8.22	0.04	1
A	101	VAL	CG2	21.36	0.2	1
A	109	ARG	HA	3.97	0.04	1
A	125	ARG	C	178.29	0.2	1
A	157	ASP	HB3	3.33	0.04	2
A	159	GLU	HB2	2.08	0.04	2
A	119	ILE	CG1	23.97	0.2	1
A	110	GLU	HG3	1.95	0.04	2
A	104	LEU	CD1	24.18	0.2	1
A	164	MET	H	8.29	0.04	1
A	107	ALA	HB1	1.8	0.04	1
A	141	ILE	CA	64.38	0.2	1
A	119	ILE	HB	2.28	0.04	1
A	105	ARG	HB2	1.91	0.04	2
A	95	THR	HG21	1.24	0.04	1
A	121	THR	HG23	1.23	0.04	1
A	156	VAL	CG1	22.15	0.2	1
A	118	GLU	CG	36.54	0.2	1
A	164	MET	HG2	2.59	0.04	2
A	148	VAL	CA	62.51	0.2	1
A	101	VAL	HG23	1.07	0.04	2
A	92	LEU	HD11	0.73	0.04	2
A	156	VAL	HA	4.68	0.04	1
A	131	LEU	CD2	26.19	0.2	1
A	167	ARG	CB	31.3	0.2	1
A	92	LEU	H	7.86	0.04	1
A	136	VAL	HB	2.07	0.04	1
A	118	GLU	HB3	1.78	0.04	2
A	101	VAL	HG13	1.12	0.04	2
A	105	ARG	C	178.68	0.2	1
A	163	ARG	CB	30.09	0.2	1
A	97	ASP	HB3	2.75	0.04	2
A	110	GLU	HA	3.73	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	129	ARG	HG3	1.53	0.04	2
A	108	PHE	CB	40.21	0.2	1
A	146	ARG	CA	58.87	0.2	1
A	132	LEU	HD13	0.8	0.04	2
A	114	ASN	CB	36.77	0.2	1
A	129	ARG	HA	3.87	0.04	1
A	15	LYS	CE	42.25	0.2	1
A	156	VAL	HG13	1.08	0.04	2
A	142	GLU	H	8.1	0.04	1
A	121	THR	N	112.12	0.2	1
A	122	SER	HA	4.23	0.04	1
A	164	MET	HA	4.05	0.04	1
A	102	LYS	CD	29.28	0.2	1
A	109	ARG	HG2	1.78	0.04	2
A	161	PHE	N	122.01	0.2	1
A	99	ILE	HD11	0.84	0.04	1
A	144	ILE	CD1	13.6	0.2	1
A	95	THR	CA	62.08	0.2	1
A	151	ASN	HB2	2.82	0.04	2
A	144	ILE	HG23	0.87	0.04	1
A	125	ARG	CA	60.6	0.2	1
A	150	LEU	C	176.35	0.2	1
A	104	LEU	HG	1.62	0.04	1
A	108	PHE	C	177.02	0.2	1
A	114	ASN	H	7.81	0.04	1
A	96	ALA	HB3	1.42	0.04	1
A	99	ILE	HG21	0.96	0.04	1
A	126	GLU	H	7.19	0.04	1
A	108	PHE	HB3	3.04	0.04	2
A	159	GLU	H	8.12	0.04	1
A	103	GLU	HB3	2.37	0.04	2
A	131	LEU	HD23	1.0	0.04	2
A	15	LYS	HA	4.29	0.04	1
A	148	VAL	HG12	0.82	0.04	2
A	136	VAL	CG1	21.0	0.2	1
A	123	GLU	CB	29.93	0.2	1
A	113	THR	HG22	1.27	0.04	1
A	146	ARG	HA	4.12	0.04	1
A	150	LEU	CA	54.95	0.2	1
A	161	PHE	HB2	3.35	0.04	2
A	112	ASP	CB	38.8	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	162	VAL	HG23	0.62	0.04	2
A	132	LEU	CD1	22.64	0.2	1
A	144	ILE	HG12	1.72	0.04	1
A	94	GLU	CG	36.45	0.2	1
A	104	LEU	CB	41.94	0.2	1
A	159	GLU	HG2	2.32	0.04	2
A	130	LYS	HB2	2.1	0.04	2
A	131	LEU	CB	43.47	0.2	1
A	164	MET	C	177.54	0.2	1
A	120	SER	N	117.9	0.2	1
A	126	GLU	CB	29.04	0.2	1
A	159	GLU	CB	28.93	0.2	1
A	141	ILE	HD13	0.78	0.04	1
A	126	GLU	HG3	2.43	0.04	2
A	156	VAL	CA	61.0	0.2	1
A	114	ASN	HA	4.78	0.04	1
A	140	ASP	HB2	2.7	0.04	2
A	156	VAL	C	175.05	0.2	1
A	124	LEU	HD22	0.94	0.04	2
A	147	ASP	HA	4.66	0.04	1
A	119	ILE	CG2	16.0	0.2	1
A	122	SER	CB	61.95	0.2	1
A	108	PHE	HA	3.54	0.04	1
A	145	ILE	HD13	0.73	0.04	1
A	99	ILE	CG1	27.77	0.2	1
A	121	THR	CB	67.9	0.2	1
A	128	MET	HB2	2.5	0.04	2
A	127	ALA	CA	55.07	0.2	1
A	153	ASP	CA	54.35	0.2	1
A	119	ILE	HA	5.01	0.04	1
A	142	GLU	HG2	2.35	0.04	2
A	127	ALA	N	123.88	0.2	1
A	131	LEU	HD12	0.97	0.04	2
A	155	ARG	HB2	1.69	0.04	2
A	118	GLU	CB	34.52	0.2	1
A	95	THR	HA	4.4	0.04	1
A	160	GLU	HB2	2.02	0.04	2
A	136	VAL	HA	4.14	0.04	1
A	149	ASP	N	122.62	0.2	1
A	105	ARG	CD	42.99	0.2	1
A	120	SER	HA	5.03	0.04	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	112	ASP	N	120.32	0.2	1
A	111	PHE	CB	39.7	0.2	1
A	156	VAL	HG23	0.92	0.04	2
A	12	LEU	HD22	0.89	0.04	2
A	116	ASP	C	177.28	0.2	1
A	92	LEU	HD22	0.75	0.04	2
A	133	GLY	HA2	4.09	0.04	2
A	137	GLY	HA3	3.95	0.04	2
A	105	ARG	HD2	2.93	0.04	2
A	145	ILE	C	177.29	0.2	1
A	163	ARG	HA	3.86	0.04	1
A	135	GLN	C	175.71	0.2	1
A	129	ARG	HD2	3.12	0.04	2
A	119	ILE	H	9.36	0.04	1
A	128	MET	H	8.6	0.04	1
A	125	ARG	CG	28.92	0.2	1
A	119	ILE	HG21	0.12	0.04	1
A	12	LEU	HD12	0.84	0.04	2
A	165	MET	CG	31.98	0.2	1
A	103	GLU	N	118.76	0.2	1
A	145	ILE	CB	37.62	0.2	1
A	147	ASP	H	8.37	0.04	1
A	153	ASP	N	118.37	0.2	1
A	165	MET	C	176.89	0.2	1
A	110	GLU	HB3	1.4	0.04	2
A	110	GLU	CG	35.57	0.2	1
A	152	GLY	CA	46.34	0.2	1
A	127	ALA	HB2	1.01	0.04	1
A	102	LYS	CA	60.37	0.2	1
A	134	HIS	CB	30.29	0.2	1
A	158	PHE	CB	38.76	0.2	1
A	142	GLU	N	118.1	0.2	1
A	149	ASP	HA	4.27	0.04	1
A	93	ALA	CA	53.17	0.2	1
A	95	THR	CB	69.99	0.2	1
A	130	LYS	N	119.17	0.2	1
A	160	GLU	CA	60.26	0.2	1
A	119	ILE	CB	40.85	0.2	1
A	93	ALA	HB1	1.49	0.04	1
A	138	HIS	HD2	7.023	0.04	1
A	123	GLU	C	177.94	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	141	ILE	N	121.75	0.2	1
A	132	LEU	HD21	0.8	0.04	2
A	118	GLU	HA	5.51	0.04	1
A	144	ILE	CA	64.61	0.2	1
A	129	ARG	CB	29.98	0.2	1
A	125	ARG	HG2	1.41	0.04	2
A	99	ILE	HG22	0.96	0.04	1
A	12	LEU	H	8.31	0.04	1
A	147	ASP	HB2	2.81	0.04	2
A	147	ASP	CB	41.48	0.2	1
A	135	GLN	HA	4.36	0.04	1
A	154	GLY	HA3	3.78	0.04	2
A	109	ARG	C	178.2	0.2	1
A	162	VAL	HG12	0.26	0.04	2
A	122	SER	N	116.87	0.2	1
A	15	LYS	CA	56.43	0.2	1
A	146	ARG	HB2	1.9	0.04	2
A	12	LEU	CG	26.71	0.2	1
A	102	LYS	H	8.49	0.04	1
A	95	THR	N	113.59	0.2	1
A	145	ILE	HG22	0.68	0.04	1
A	123	GLU	CA	58.83	0.2	1
A	104	LEU	HD11	0.7	0.04	2
A	148	VAL	CG2	21.0	0.2	1
A	132	LEU	C	178.63	0.2	1
A	135	GLN	HG2	2.18	0.04	2
A	153	ASP	H	8.22	0.04	1
A	94	GLU	CB	30.45	0.2	1
A	99	ILE	N	122.28	0.2	1
A	104	LEU	CG	26.72	0.2	1
A	96	ALA	N	125.55	0.2	1
A	109	ARG	CA	59.07	0.2	1
A	149	ASP	CB	42.05	0.2	1
A	160	GLU	N	120.94	0.2	1
A	126	GLU	CG	36.03	0.2	1
A	14	ARG	HA	4.06	0.04	1
A	111	PHE	N	114.23	0.2	1
A	141	ILE	HG22	0.91	0.04	1
A	119	ILE	HD13	0.3	0.04	1
A	100	GLY	H	8.61	0.04	1
A	145	ILE	CG2	17.57	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	144	ILE	N	119.83	0.2	1
A	130	LYS	H	7.83	0.04	1
A	156	VAL	CB	34.93	0.2	1
A	115	GLY	H	7.74	0.04	1
A	158	PHE	HA	3.41	0.04	1
A	136	VAL	CB	32.86	0.2	1
A	162	VAL	CA	66.89	0.2	1
A	111	PHE	C	175.69	0.2	1
A	112	ASP	HB3	1.77	0.04	2
A	130	LYS	HE2	3.08	0.04	2
A	99	ILE	CG2	17.98	0.2	1
A	102	LYS	HG2	1.47	0.04	2
A	103	GLU	CB	29.05	0.2	1
A	144	ILE	HA	3.78	0.04	1
A	153	ASP	CB	41.41	0.2	1
A	141	ILE	CB	38.05	0.2	1
A	92	LEU	HD23	0.75	0.04	2
A	149	ASP	H	8.6	0.04	1
A	158	PHE	N	119.14	0.2	1
A	148	VAL	HA	4.12	0.04	1
A	144	ILE	CG2	17.63	0.2	1
A	122	SER	HB2	3.9	0.04	2
A	164	MET	HB3	2.18	0.04	2
A	110	GLU	H	7.52	0.04	1
A	92	LEU	CA	55.82	0.2	1
A	12	LEU	CD1	23.54	0.2	1
A	96	ALA	CA	53.07	0.2	1
A	136	VAL	HG11	0.92	0.04	2
A	130	LYS	CB	32.73	0.2	1
A	105	ARG	CG	27.23	0.2	1
A	152	GLY	HA2	4.22	0.04	2
A	151	ASN	CA	55.17	0.2	1
A	166	SER	CB	64.0	0.2	1
A	101	VAL	HB	2.19	0.04	1
A	111	PHE	CA	60.23	0.2	1
A	163	ARG	HB2	1.91	0.04	2
A	161	PHE	H	8.4	0.04	1
A	119	ILE	N	119.36	0.2	1
A	136	VAL	HG23	0.93	0.04	2
A	110	GLU	C	177.46	0.2	1
A	135	GLN	HB2	2.11	0.04	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	143	GLU	CG	36.52	0.2	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	156	-0.37 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	142	0.10 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	140	-0.32 ± 0.12	None needed (< 0.5 ppm)
^{15}N	145	0.53 ± 0.28	None needed (imprecise)

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 80%, i.e. 735 atoms were assigned a chemical shift out of a possible 914. 8 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	349/354 (99%)	141/141 (100%)	139/144 (97%)	69/69 (100%)
Sidechain	349/501 (70%)	218/295 (74%)	131/182 (72%)	0/24 (0%)
Aromatic	37/59 (63%)	29/32 (91%)	8/26 (31%)	0/1 (0%)
Overall	735/914 (80%)	388/468 (83%)	278/352 (79%)	69/94 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 779 atoms were assigned a chemical shift out of a possible 968. 9 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	369/374 (99%)	149/149 (100%)	147/152 (97%)	73/73 (100%)
Sidechain	373/535 (70%)	233/315 (74%)	140/193 (73%)	0/27 (0%)
Aromatic	37/59 (63%)	29/32 (91%)	8/26 (31%)	0/1 (0%)
Overall	779/968 (80%)	411/496 (83%)	295/371 (80%)	73/101 (72%)

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	129	ARG	CD	37.09	47.57 – 38.77	-6.9

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: