Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2KM6
BMRB ID	:	16263
Title	:	NMR structure of the NLRP7 Pyrin domain
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Deposited on	:	2009-07-21

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

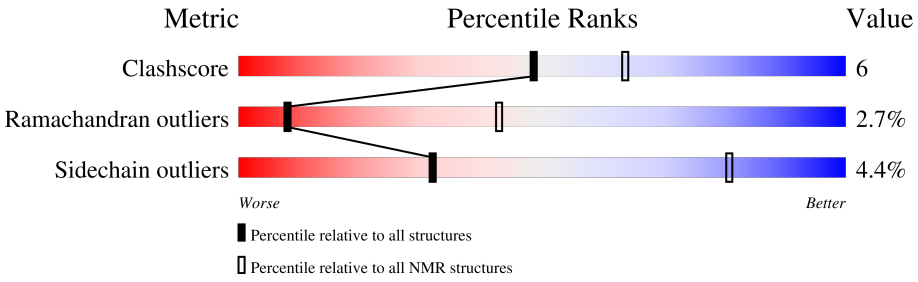
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 91%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	106	58% 14% 18% 9%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:9-A:34, A:43-A:93 (77)	0.42	10

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

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

The models can be grouped into 4 clusters and 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1538 atoms, of which 764 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NACHT, LRR and PYD domains-containing protein 7.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	96	1538	489	764	121	158	6	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q8WX94
A	2	HIS	-	expression tag	UNP Q8WX94
A	99	LEU	-	expression tag	UNP Q8WX94
A	100	GLU	-	expression tag	UNP Q8WX94
A	101	HIS	-	expression tag	UNP Q8WX94
A	102	HIS	-	expression tag	UNP Q8WX94
A	103	HIS	-	expression tag	UNP Q8WX94
A	104	HIS	-	expression tag	UNP Q8WX94
A	105	HIS	-	expression tag	UNP Q8WX94
A	106	HIS	-	expression tag	UNP Q8WX94

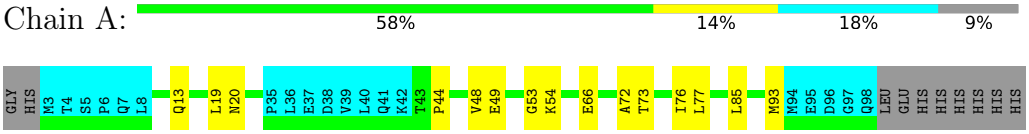
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: NACHT, LRR and PYD domains-containing protein 7

Chain A:



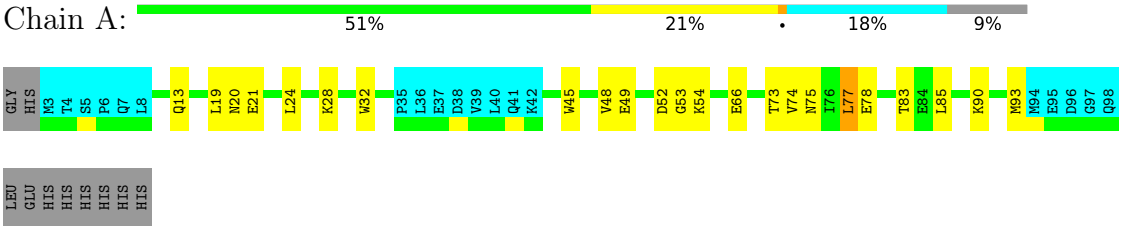
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

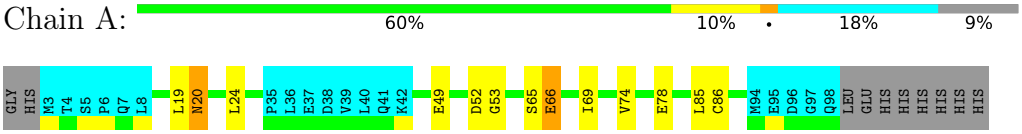
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

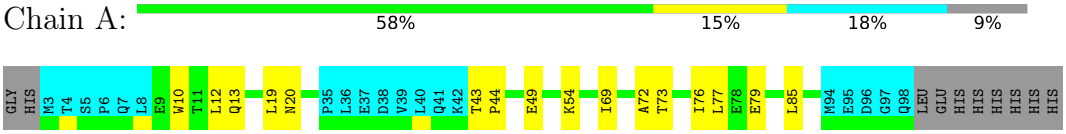
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

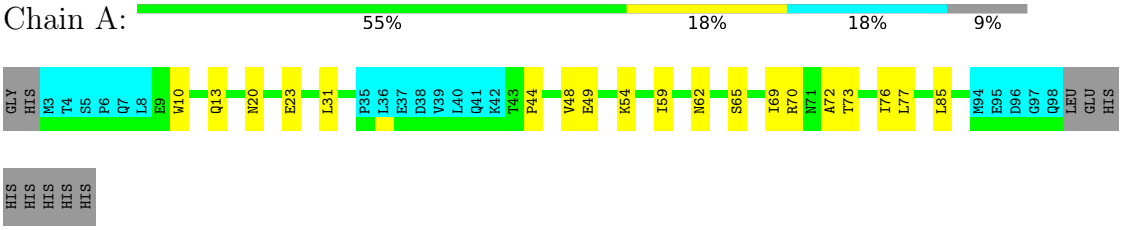
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

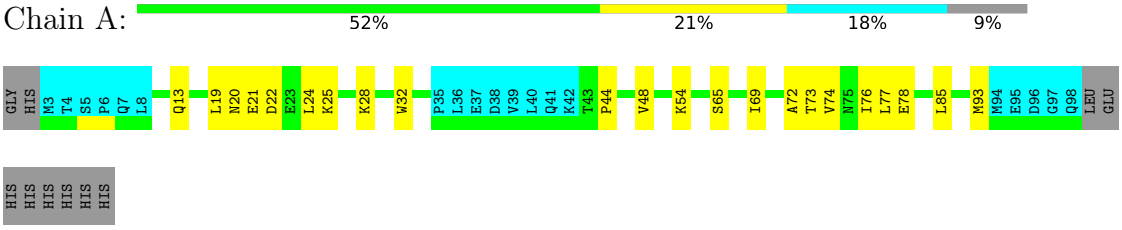
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

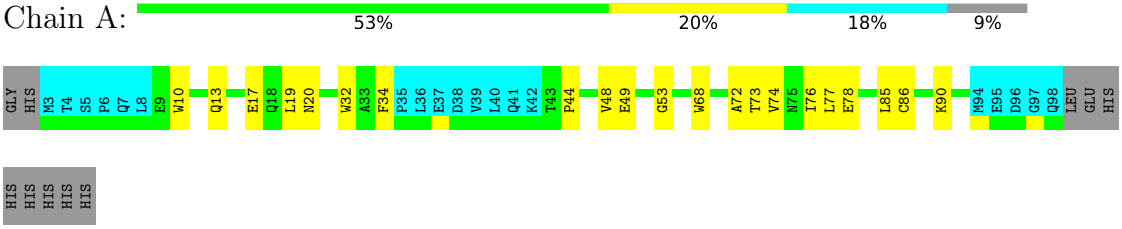
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

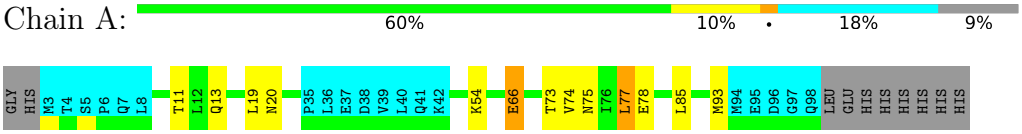
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

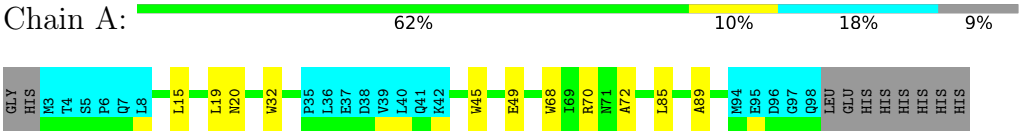
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

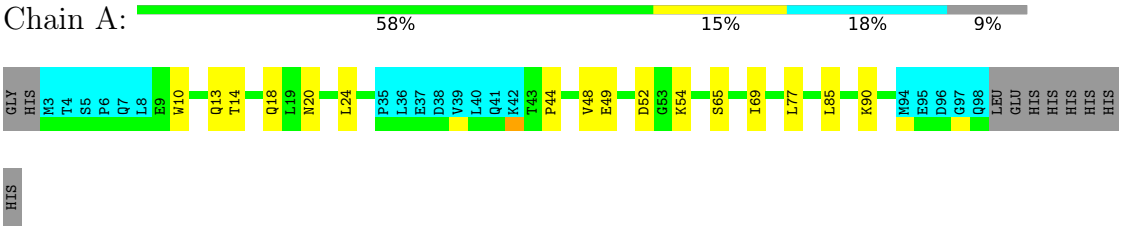
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

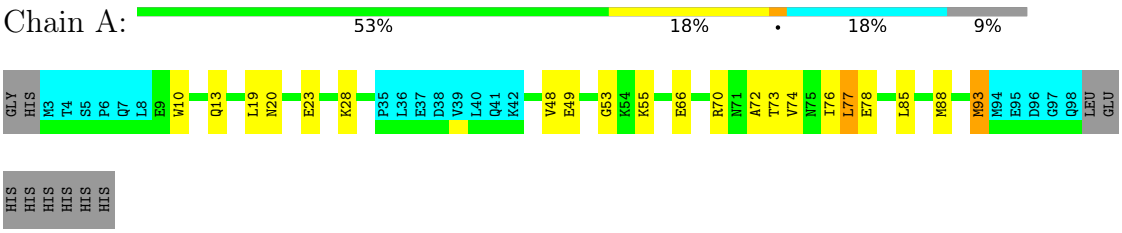
Chain A:



4.2.10 Score per residue for model 10 (medoid)

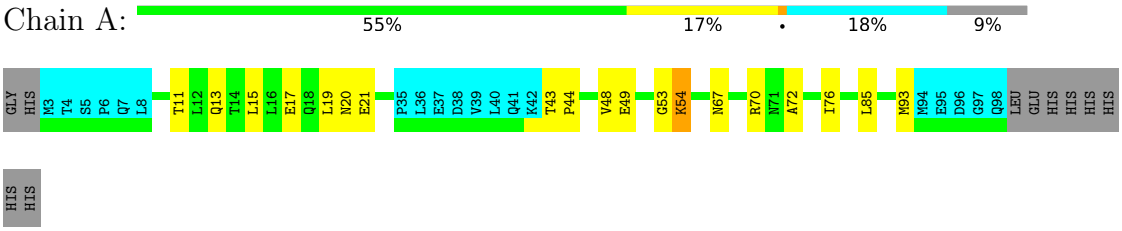
• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

Chain A:



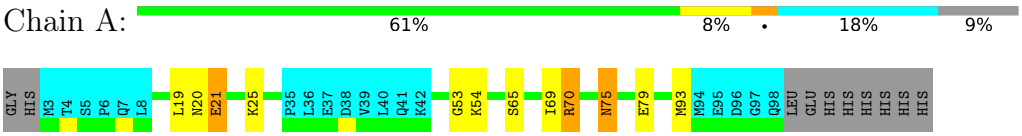
4.2.11 Score per residue for model 11

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7



4.2.12 Score per residue for model 12

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7



4.2.13 Score per residue for model 13

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

4.2.14 Score per residue for model 14

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

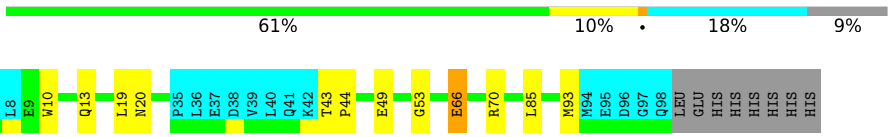
4.2.15 Score per residue for model 15

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

4.2.16 Score per residue for model 16

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

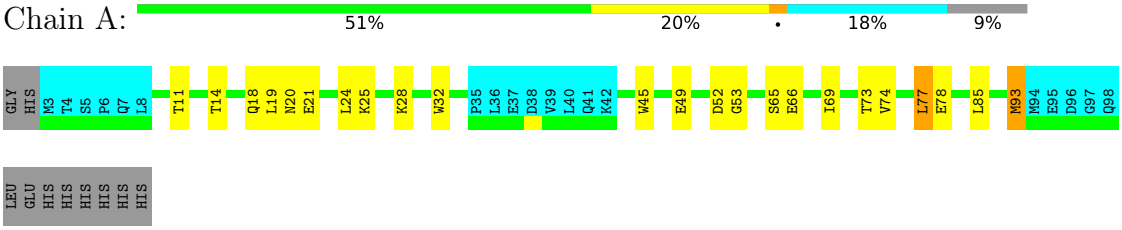
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

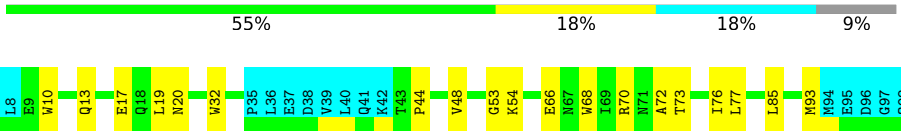
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

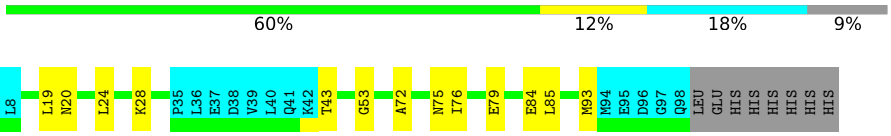
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

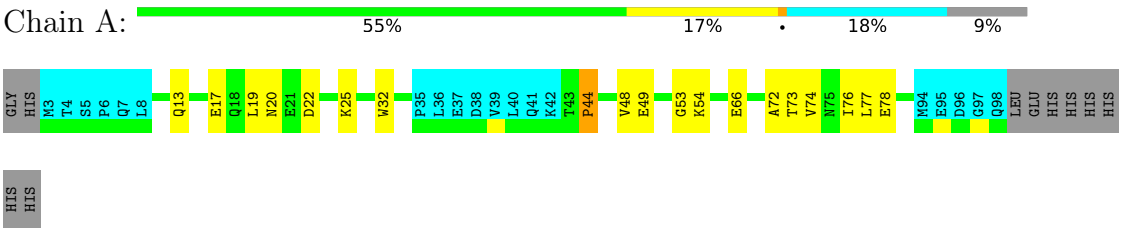
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: NACHT, LRR and PYD domains-containing protein 7

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
CYANA	structure solution	2.1
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1231
Number of shifts mapped to atoms	1202
Number of unparsed shifts	0
Number of shifts with mapping errors	29
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality

6.1 Standard geometry

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.2±0.4
All	All	0	4

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	70	ARG	Sidechain	4

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	626	618	618	8±2
All	All	12520	12360	12360	154

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:GLN:NE2	1:A:54:LYS:HG3	0.60	2.11	4	6
1:A:72:ALA:O	1:A:76:ILE:HG12	0.55	2.02	15	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:TRP:CZ3	1:A:72:ALA:HB2	0.55	2.36	8	2
1:A:73:THR:O	1:A:77:LEU:HD13	0.53	2.04	15	7
1:A:10:TRP:O	1:A:13:GLN:HG2	0.53	2.04	6	5
1:A:28:LYS:HE2	1:A:48:VAL:O	0.52	2.05	14	2
1:A:22:ASP:HA	1:A:25:LYS:HD3	0.51	1.81	20	2
1:A:24:LEU:O	1:A:28:LYS:HG3	0.51	2.06	19	4
1:A:85:LEU:H	1:A:85:LEU:HD23	0.50	1.66	10	17
1:A:19:LEU:O	1:A:19:LEU:HG	0.50	2.07	5	18
1:A:73:THR:O	1:A:77:LEU:HD12	0.50	2.07	14	5
1:A:74:VAL:O	1:A:78:GLU:HG2	0.49	2.08	6	5
1:A:73:THR:O	1:A:77:LEU:HG	0.49	2.08	5	1
1:A:65:SER:O	1:A:69:ILE:HG13	0.48	2.08	12	7
1:A:74:VAL:HG13	1:A:86:CYS:SG	0.48	2.49	2	1
1:A:93:MET:CE	1:A:93:MET:HA	0.47	2.39	17	1
1:A:75:ASN:O	1:A:79:GLU:HG2	0.47	2.08	12	2
1:A:24:LEU:CD2	1:A:52:ASP:HA	0.47	2.39	17	5
1:A:44:PRO:O	1:A:48:VAL:HG13	0.47	2.10	15	9
1:A:45:TRP:NE1	1:A:49:GLU:HG3	0.47	2.25	17	2
1:A:11:THR:CG2	1:A:93:MET:HG2	0.47	2.40	7	2
1:A:93:MET:HA	1:A:93:MET:HE2	0.46	1.87	17	1
1:A:67:ASN:OD1	1:A:70:ARG:HD3	0.46	2.10	11	1
1:A:13:GLN:O	1:A:17:GLU:HG3	0.46	2.11	6	5
1:A:11:THR:O	1:A:15:LEU:HG	0.45	2.12	13	2
1:A:20:ASN:HA	1:A:24:LEU:HB2	0.45	1.89	13	2
1:A:74:VAL:O	1:A:78:GLU:HG3	0.44	2.12	14	4
1:A:86:CYS:O	1:A:90:LYS:HG3	0.44	2.13	14	2
1:A:12:LEU:HD21	1:A:69:ILE:HG21	0.44	1.90	3	1
1:A:10:TRP:HA	1:A:13:GLN:HG2	0.43	1.89	4	3
1:A:86:CYS:O	1:A:90:LYS:HG2	0.43	2.13	6	1
1:A:14:THR:O	1:A:18:GLN:HG3	0.43	2.13	17	2
1:A:75:ASN:O	1:A:79:GLU:HG3	0.43	2.14	15	1
1:A:15:LEU:HD11	1:A:89:ALA:HB2	0.42	1.91	8	2
1:A:34:PHE:CZ	1:A:68:TRP:HH2	0.42	2.32	6	2
1:A:21:GLU:O	1:A:25:LYS:HE2	0.42	2.14	12	1
1:A:54:LYS:HE2	1:A:54:LYS:O	0.42	2.13	11	1
1:A:45:TRP:HA	1:A:48:VAL:HG22	0.42	1.92	1	1
1:A:70:ARG:HA	1:A:93:MET:SD	0.41	2.55	10	2
1:A:85:LEU:O	1:A:88:MET:HB3	0.41	2.15	10	2
1:A:45:TRP:CD1	1:A:49:GLU:HG3	0.41	2.51	1	1
1:A:84:GLU:H	1:A:84:GLU:CD	0.41	2.19	19	1
1:A:59:ILE:O	1:A:62:ASN:HB3	0.40	2.16	4	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	77/106 (73%)	70±1 (91±1%)	5±1 (7±2%)	2±1 (3±1%)	8 43
All	All	1540/2120 (73%)	1397 (91%)	101 (7%)	42 (3%)	8 43

All 5 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	20	ASN	20
1	A	53	GLY	11
1	A	21	GLU	4
1	A	43	THR	4
1	A	44	PRO	3

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	70/97 (72%)	67±1 (96±2%)	3±1 (4±2%)	32 81
All	All	1400/1940 (72%)	1339 (96%)	61 (4%)	32 81

All 15 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	49	GLU	12
1	A	66	GLU	9
1	A	93	MET	9
1	A	32	TRP	8
1	A	54	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	77	LEU	5
1	A	75	ASN	3
1	A	23	GLU	2
1	A	83	THR	1
1	A	79	GLU	1
1	A	85	LEU	1
1	A	55	LYS	1
1	A	21	GLU	1
1	A	31	LEU	1
1	A	25	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 monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	1231
Number of shifts mapped to atoms	1202
Number of unparsed shifts	0
Number of shifts with mapping errors	29
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- No matching atom found in the structure. All 29 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	LEU	H	8.071	0.010	.
1	A	99	LEU	HA	4.08	0.015	.
1	A	99	LEU	HB2	1.444	0.015	.
1	A	99	LEU	HB3	1.362	0.015	.
1	A	99	LEU	HD11	0.739	0.015	.
1	A	99	LEU	HD12	0.739	0.015	.
1	A	99	LEU	HD13	0.739	0.015	.
1	A	99	LEU	HD21	0.675	0.015	.
1	A	99	LEU	HD22	0.675	0.015	.
1	A	99	LEU	HD23	0.675	0.015	.
1	A	99	LEU	HG	1.421	0.015	.
1	A	99	LEU	C	177.358	0.070	.
1	A	99	LEU	CA	55.469	0.250	.
1	A	99	LEU	CB	42.061	0.250	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	LEU	CD1	24.821	0.250	.
1	A	99	LEU	CD2	23.385	0.250	.
1	A	99	LEU	CG	26.976	0.250	.
1	A	99	LEU	N	121.996	0.050	.
1	A	100	GLU	H	8.153	0.010	.
1	A	100	GLU	HA	3.994	0.015	.
1	A	100	GLU	HB2	1.72	0.015	.
1	A	100	GLU	HB3	1.72	0.015	.
1	A	100	GLU	HG2	2.024	0.015	.
1	A	100	GLU	HG3	1.983	0.015	.
1	A	100	GLU	C	176.171	0.070	.
1	A	100	GLU	CA	56.427	0.250	.
1	A	100	GLU	CB	30.089	0.250	.
1	A	100	GLU	CG	35.835	0.250	.
1	A	100	GLU	N	120.271	0.050	.

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	98	-0.43 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	96	0.30 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	96	-0.19 ± 0.10	None needed (< 0.5 ppm)
^{15}N	91	0.80 ± 0.22	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 973 atoms were assigned a chemical shift out of a possible 1069. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	382/384 (99%)	153/154 (99%)	154/154 (100%)	75/76 (99%)
Sidechain	564/617 (91%)	384/400 (96%)	173/200 (86%)	7/17 (41%)
Aromatic	27/68 (40%)	27/34 (79%)	0/30 (0%)	0/4 (0%)
Overall	973/1069 (91%)	564/588 (96%)	327/384 (85%)	82/97 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1202 atoms were assigned a chemical shift out of a possible

1322. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	466/476 (98%)	187/191 (98%)	190/192 (99%)	89/93 (96%)
Sidechain	709/778 (91%)	482/504 (96%)	217/253 (86%)	10/21 (48%)
Aromatic	27/68 (40%)	27/34 (79%)	0/30 (0%)	0/4 (0%)
Overall	1202/1322 (91%)	696/729 (95%)	407/475 (86%)	99/118 (84%)

7.1.4 Statistically unusual chemical shifts (i)

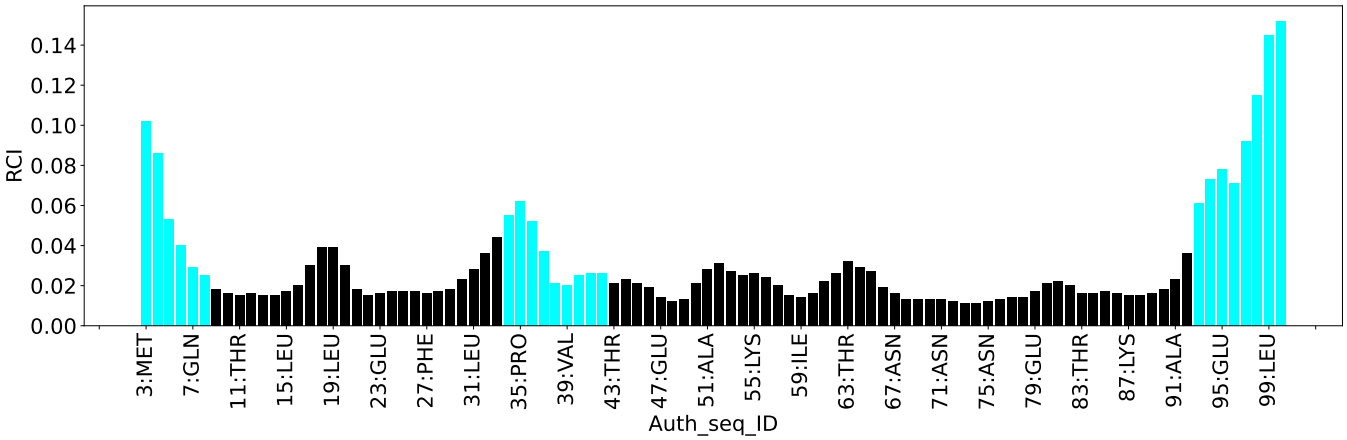
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	72	ALA	HB1	-0.29	0.14 – 2.58	-6.8
1	A	72	ALA	HB2	-0.29	0.14 – 2.58	-6.8
1	A	72	ALA	HB3	-0.29	0.14 – 2.58	-6.8

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1670
Intra-residue (|i-j|=0)	503
Sequential (|i-j|=1)	361
Medium range (|i-j|>1 and |i-j|<5)	448
Long range (|i-j|≥5)	358
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	17
Number of restraints per residue	15.8
Number of long range restraints per residue[1]	3.4

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	13.2	0.2
0.2-0.5 (Medium)	0.6	0.31
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

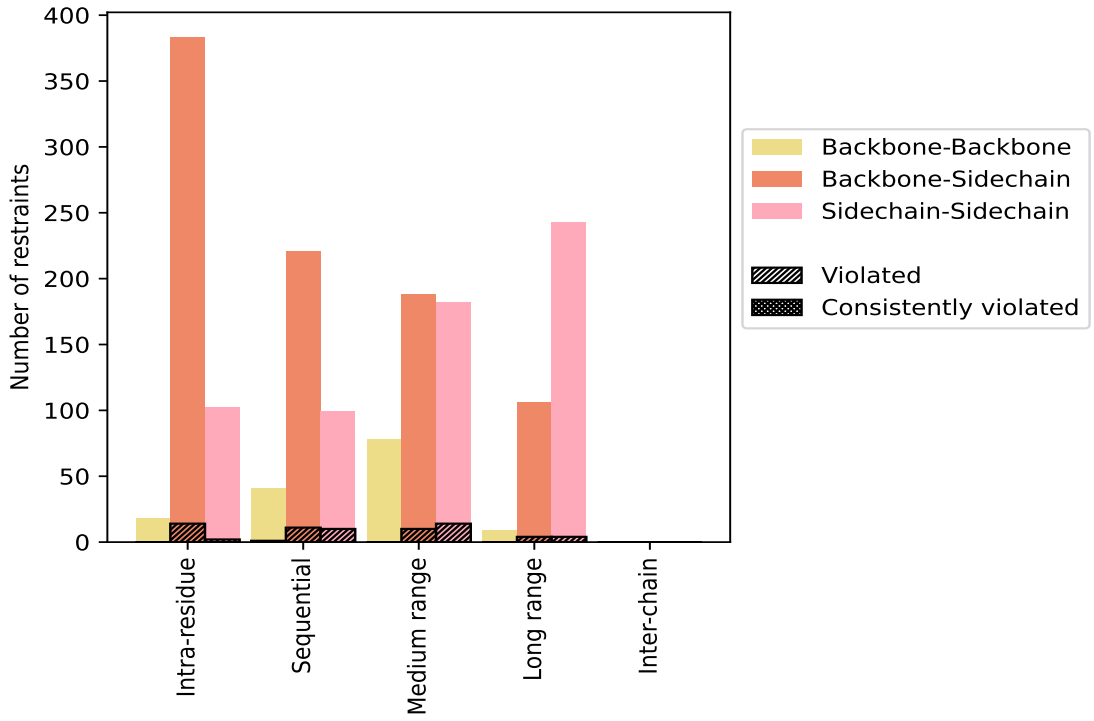
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	503	30.1	16	3.2	1.0	0	0.0	0.0
Backbone-Backbone	18	1.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	383	22.9	14	3.7	0.8	0	0.0	0.0
Sidechain-Sidechain	102	6.1	2	2.0	0.1	0	0.0	0.0
Sequential (|i-j|=1)	361	21.6	22	6.1	1.3	0	0.0	0.0
Backbone-Backbone	41	2.5	1	2.4	0.1	0	0.0	0.0
Backbone-Sidechain	221	13.2	11	5.0	0.7	0	0.0	0.0
Sidechain-Sidechain	99	5.9	10	10.1	0.6	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	448	26.8	24	5.4	1.4	0	0.0	0.0
Backbone-Backbone	78	4.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	188	11.3	10	5.3	0.6	0	0.0	0.0
Sidechain-Sidechain	182	10.9	14	7.7	0.8	0	0.0	0.0
Long range (|i-j|≥5)	358	21.4	8	2.2	0.5	0	0.0	0.0
Backbone-Backbone	9	0.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	106	6.3	4	3.8	0.2	0	0.0	0.0
Sidechain-Sidechain	243	14.6	4	1.6	0.2	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1670	100.0	70	4.2	4.2	0	0.0	0.0
Backbone-Backbone	146	8.7	1	0.7	0.1	0	0.0	0.0
Backbone-Sidechain	898	53.8	39	4.3	2.3	0	0.0	0.0
Sidechain-Sidechain	626	37.5	30	4.8	1.8	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	1	4	1	2	0	8	0.14	0.2	0.03	0.13
2	2	2	1	3	0	8	0.14	0.19	0.03	0.14
3	2	4	8	2	0	16	0.13	0.19	0.03	0.12
4	2	6	4	2	0	14	0.14	0.23	0.03	0.13
5	2	5	6	4	0	17	0.14	0.26	0.04	0.12
6	3	4	4	1	0	12	0.14	0.19	0.03	0.13
7	5	3	2	4	0	14	0.15	0.24	0.04	0.13
8	4	4	7	2	0	17	0.13	0.2	0.03	0.12
9	4	1	6	5	0	16	0.15	0.21	0.03	0.14
10	6	6	1	2	0	15	0.13	0.17	0.02	0.13
11	3	6	3	4	0	16	0.14	0.22	0.03	0.12

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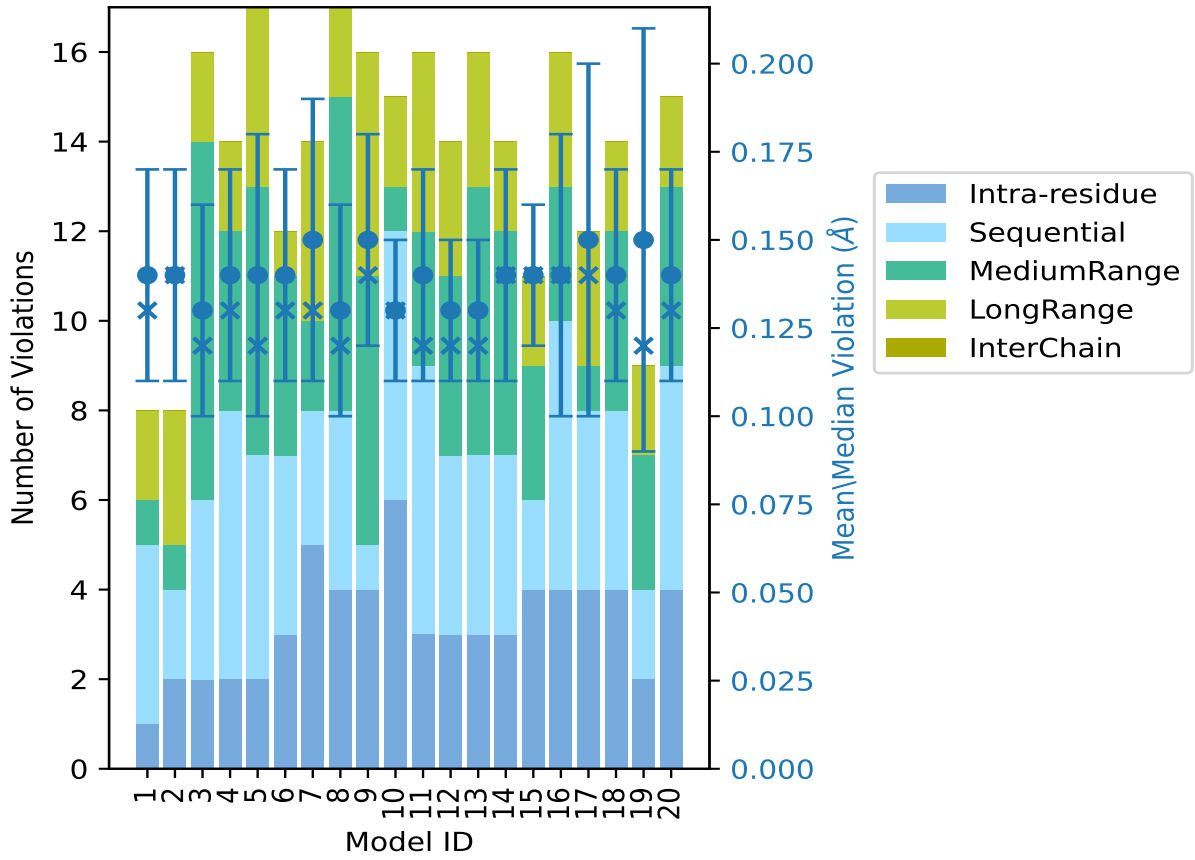
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	3	4	4	3	0	14	0.13	0.18	0.02	0.12
13	3	4	6	3	0	16	0.13	0.19	0.02	0.12
14	3	4	5	2	0	14	0.14	0.22	0.03	0.14
15	4	2	3	2	0	11	0.14	0.18	0.02	0.14
16	4	6	3	3	0	16	0.14	0.26	0.04	0.14
17	4	4	1	3	0	12	0.15	0.31	0.05	0.14
18	4	4	4	2	0	14	0.14	0.19	0.03	0.13
19	2	2	3	2	0	9	0.15	0.29	0.06	0.12
20	4	5	4	2	0	15	0.14	0.2	0.03	0.13

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

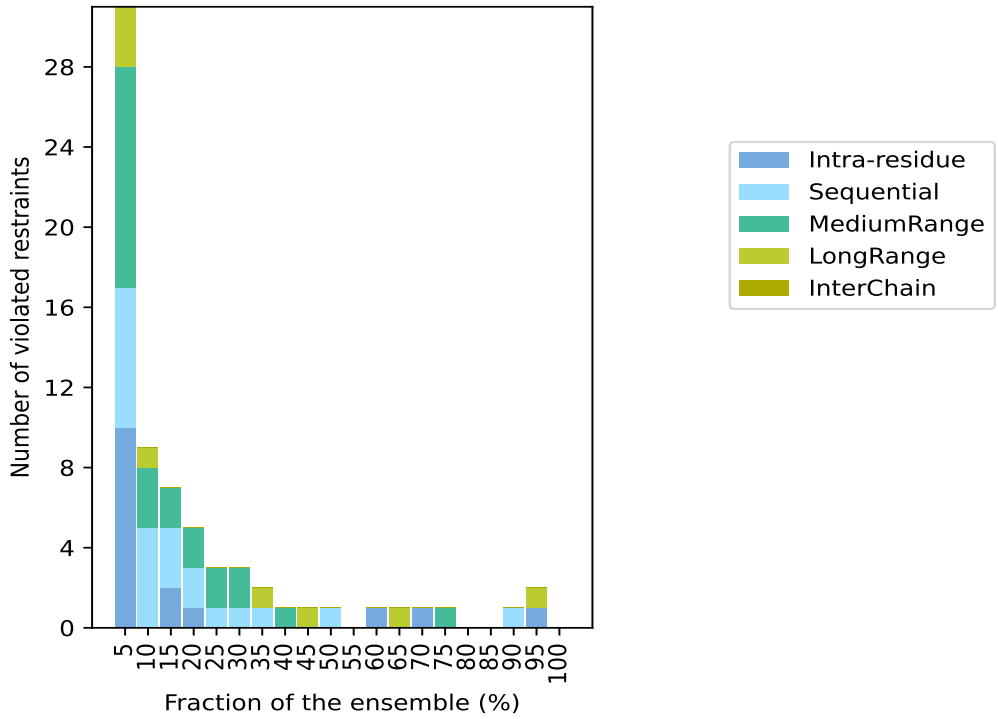
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1600(IR:487, SQ:339, MR:424, LR:350, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
10	7	11	3	0	31	1	5.0
0	5	3	1	0	9	2	10.0
2	3	2	0	0	7	3	15.0
1	2	2	0	0	5	4	20.0
0	1	2	0	0	3	5	25.0
0	1	2	0	0	3	6	30.0
0	1	0	1	0	2	7	35.0
0	0	1	0	0	1	8	40.0
0	0	0	1	0	1	9	45.0
0	1	0	0	0	1	10	50.0
0	0	0	0	0	0	11	55.0
1	0	0	0	0	1	12	60.0
0	0	0	1	0	1	13	65.0
1	0	0	0	0	1	14	70.0
0	0	1	0	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	1	0	0	0	1	18	90.0
1	0	0	1	0	2	19	95.0
0	0	0	0	0	0	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

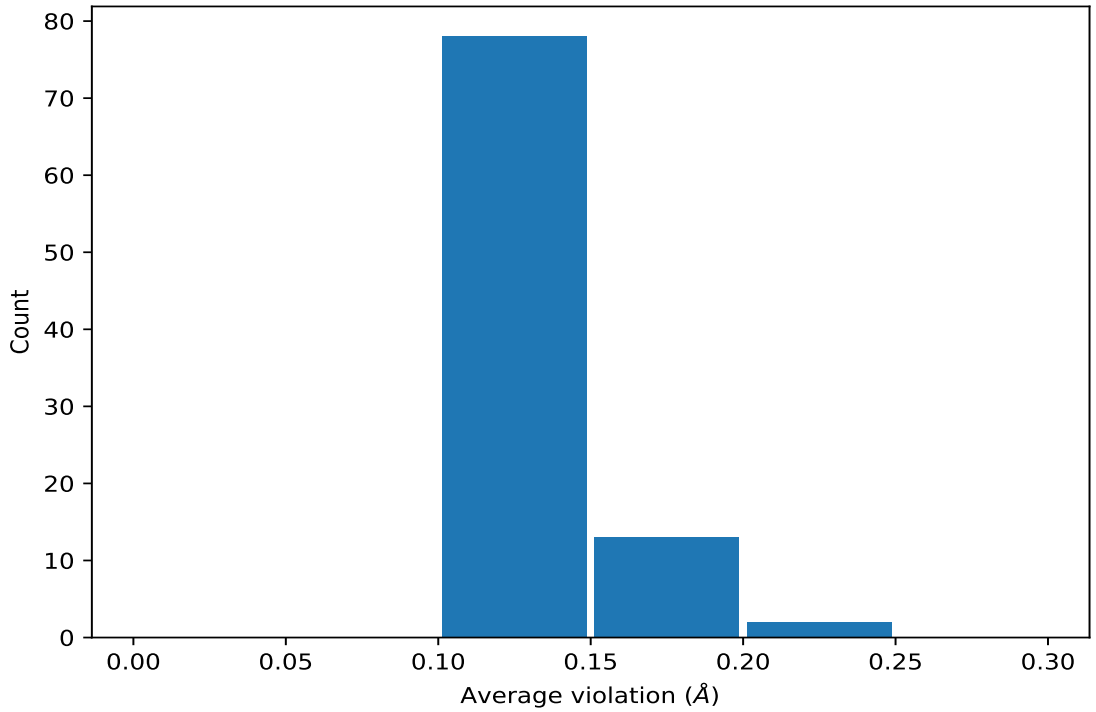
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	19	0.17	0.01	0.17
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	19	0.17	0.01	0.17
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	19	0.17	0.01	0.17
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	19	0.13	0.01	0.13
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	18	0.14	0.02	0.13
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	15	0.14	0.02	0.13
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	15	0.14	0.02	0.13
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	15	0.14	0.02	0.13
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	15	0.14	0.02	0.13
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	14	0.17	0.03	0.18
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	13	0.15	0.02	0.14
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	13	0.15	0.02	0.14
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	13	0.15	0.02	0.14
(1,66)	1:A:29:SER:H	1:A:29:SER:HB3	12	0.13	0.01	0.13
(1,930)	1:A:49:GLU:HG2	1:A:50:GLU:HA	10	0.17	0.05	0.16
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD21	9	0.13	0.04	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD22	9	0.13	0.04	0.13
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD23	9	0.13	0.04	0.13
(1,1288)	1:A:73:THR:HA	1:A:77:LEU:HG	8	0.15	0.02	0.15
(1,801)	1:A:12:LEU:HA	1:A:93:MET:HB2	7	0.12	0.01	0.12
(1,63)	1:A:26:SER:HB3	1:A:27:PHE:HB3	7	0.11	0.0	0.11
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB2	6	0.14	0.02	0.15
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB3	6	0.14	0.02	0.15
(1,65)	1:A:29:SER:HB3	1:A:30:LEU:H	6	0.12	0.01	0.11
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG2	6	0.11	0.01	0.11
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG3	6	0.11	0.01	0.11
(1,895)	1:A:36:LEU:HB2	1:A:37:GLU:HG3	5	0.13	0.02	0.12
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD11	5	0.12	0.01	0.12
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD12	5	0.12	0.01	0.12
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD13	5	0.12	0.01	0.12
(1,121)	1:A:45:TRP:HA	1:A:48:VAL:HB	5	0.12	0.01	0.11
(1,483)	1:A:39:VAL:H	1:A:39:VAL:HB	4	0.18	0.02	0.18
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD11	4	0.14	0.02	0.14
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD12	4	0.14	0.02	0.14
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD13	4	0.14	0.02	0.14
(1,763)	1:A:89:ALA:HB1	1:A:92:GLU:HG3	4	0.12	0.01	0.12
(1,763)	1:A:89:ALA:HB2	1:A:92:GLU:HG3	4	0.12	0.01	0.12
(1,763)	1:A:89:ALA:HB3	1:A:92:GLU:HG3	4	0.12	0.01	0.12
(1,1344)	1:A:19:LEU:HD11	1:A:20:ASN:HD21	4	0.12	0.01	0.12
(1,1344)	1:A:19:LEU:HD12	1:A:20:ASN:HD21	4	0.12	0.01	0.12
(1,1344)	1:A:19:LEU:HD13	1:A:20:ASN:HD21	4	0.12	0.01	0.12
(1,1088)	1:A:91:ALA:HA	1:A:92:GLU:HB2	4	0.11	0.0	0.11
(1,283)	1:A:54:LYS:HA	1:A:54:LYS:HE2	3	0.16	0.07	0.11
(1,283)	1:A:54:LYS:HA	1:A:54:LYS:HE3	3	0.16	0.07	0.11
(1,3)	1:A:4:THR:HB	1:A:5:SER:H	3	0.16	0.04	0.13
(1,301)	1:A:8:LEU:HB3	1:A:8:LEU:HG	3	0.12	0.0	0.12
(1,1369)	1:A:8:LEU:HD11	1:A:9:GLU:HB2	3	0.12	0.01	0.12
(1,1369)	1:A:8:LEU:HD11	1:A:9:GLU:HB3	3	0.12	0.01	0.12
(1,1369)	1:A:8:LEU:HD12	1:A:9:GLU:HB2	3	0.12	0.01	0.12
(1,1369)	1:A:8:LEU:HD12	1:A:9:GLU:HB3	3	0.12	0.01	0.12
(1,1369)	1:A:8:LEU:HD13	1:A:9:GLU:HB2	3	0.12	0.01	0.12
(1,1369)	1:A:8:LEU:HD13	1:A:9:GLU:HB3	3	0.12	0.01	0.12
(1,1369)	1:A:8:LEU:HD21	1:A:9:GLU:HB2	3	0.12	0.01	0.12
(1,1369)	1:A:8:LEU:HD21	1:A:9:GLU:HB3	3	0.12	0.01	0.12
(1,1369)	1:A:8:LEU:HD22	1:A:9:GLU:HB2	3	0.12	0.01	0.12
(1,1369)	1:A:8:LEU:HD22	1:A:9:GLU:HB3	3	0.12	0.01	0.12
(1,1369)	1:A:8:LEU:HD23	1:A:9:GLU:HB2	3	0.12	0.01	0.12
(1,1369)	1:A:8:LEU:HD23	1:A:9:GLU:HB3	3	0.12	0.01	0.12

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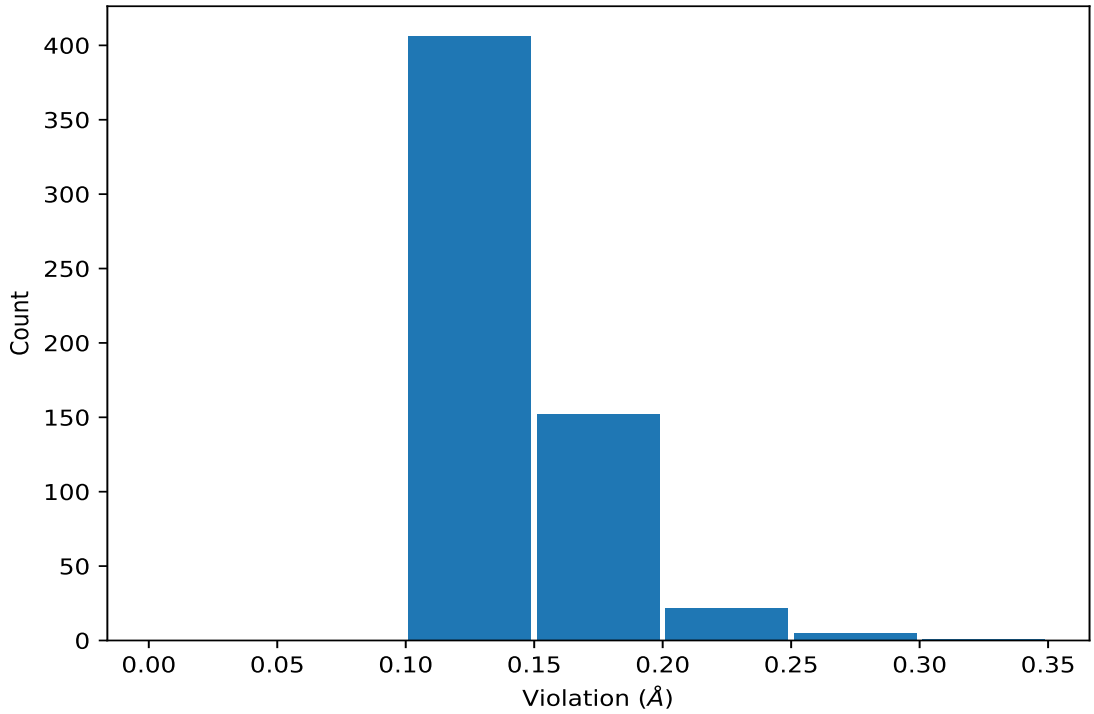
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,420)	1:A:91:ALA:HB1	1:A:92:GLU:HG3	3	0.12	0.0	0.12
(1,420)	1:A:91:ALA:HB2	1:A:92:GLU:HG3	3	0.12	0.0	0.12
(1,420)	1:A:91:ALA:HB3	1:A:92:GLU:HG3	3	0.12	0.0	0.12
(1,958)	1:A:42:LYS:HE2	1:A:44:PRO:HD2	3	0.11	0.0	0.11
(1,958)	1:A:42:LYS:HE3	1:A:44:PRO:HD2	3	0.11	0.0	0.11
(1,1335)	1:A:83:THR:HG21	1:A:87:LYS:HE2	3	0.11	0.0	0.11
(1,1335)	1:A:83:THR:HG21	1:A:87:LYS:HE3	3	0.11	0.0	0.11
(1,1335)	1:A:83:THR:HG22	1:A:87:LYS:HE2	3	0.11	0.0	0.11
(1,1335)	1:A:83:THR:HG22	1:A:87:LYS:HE3	3	0.11	0.0	0.11
(1,1335)	1:A:83:THR:HG23	1:A:87:LYS:HE2	3	0.11	0.0	0.11
(1,1335)	1:A:83:THR:HG23	1:A:87:LYS:HE3	3	0.11	0.0	0.11
(1,1442)	1:A:21:GLU:HG2	1:A:22:ASP:HA	2	0.23	0.03	0.23
(1,1442)	1:A:21:GLU:HG3	1:A:22:ASP:HA	2	0.23	0.03	0.23
(1,1001)	1:A:92:GLU:HB3	1:A:93:MET:HG3	2	0.14	0.02	0.14
(1,1085)	1:A:89:ALA:HA	1:A:92:GLU:HG2	2	0.14	0.01	0.14
(1,660)	1:A:82:LEU:HD21	1:A:83:THR:H	2	0.13	0.02	0.13
(1,660)	1:A:82:LEU:HD22	1:A:83:THR:H	2	0.13	0.02	0.13
(1,660)	1:A:82:LEU:HD23	1:A:83:THR:H	2	0.13	0.02	0.13
(1,1368)	1:A:8:LEU:HD11	1:A:9:GLU:HA	2	0.12	0.01	0.12
(1,1368)	1:A:8:LEU:HD12	1:A:9:GLU:HA	2	0.12	0.01	0.12
(1,1368)	1:A:8:LEU:HD13	1:A:9:GLU:HA	2	0.12	0.01	0.12
(1,1368)	1:A:8:LEU:HD21	1:A:9:GLU:HA	2	0.12	0.01	0.12
(1,1368)	1:A:8:LEU:HD22	1:A:9:GLU:HA	2	0.12	0.01	0.12
(1,1368)	1:A:8:LEU:HD23	1:A:9:GLU:HA	2	0.12	0.01	0.12
(1,78)	1:A:29:SER:HA	1:A:32:TRP:HE3	2	0.12	0.0	0.12
(1,443)	1:A:11:THR:HB	1:A:93:MET:HG2	2	0.12	0.0	0.12
(1,1535)	1:A:42:LYS:HG2	1:A:43:THR:HG21	2	0.12	0.0	0.12
(1,1535)	1:A:42:LYS:HG2	1:A:43:THR:HG22	2	0.12	0.0	0.12
(1,1535)	1:A:42:LYS:HG2	1:A:43:THR:HG23	2	0.12	0.0	0.12
(1,1535)	1:A:42:LYS:HG3	1:A:43:THR:HG21	2	0.12	0.0	0.12
(1,1535)	1:A:42:LYS:HG3	1:A:43:THR:HG22	2	0.12	0.0	0.12
(1,1535)	1:A:42:LYS:HG3	1:A:43:THR:HG23	2	0.12	0.0	0.12
(1,633)	1:A:34:PHE:HZ	1:A:36:LEU:HD11	2	0.11	0.0	0.11
(1,633)	1:A:34:PHE:HZ	1:A:36:LEU:HD12	2	0.11	0.0	0.11
(1,633)	1:A:34:PHE:HZ	1:A:36:LEU:HD13	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:A:25:LYS:HA	1:A:25:LYS:HG2	17	0.31
(1,930)	1:A:49:GLU:HG2	1:A:50:GLU:HA	19	0.29
(1,283)	1:A:54:LYS:HA	1:A:54:LYS:HE2	16	0.26
(1,283)	1:A:54:LYS:HA	1:A:54:LYS:HE3	16	0.26
(1,1442)	1:A:21:GLU:HG2	1:A:22:ASP:HA	5	0.26
(1,1442)	1:A:21:GLU:HG3	1:A:22:ASP:HA	5	0.26
(1,2)	1:A:4:THR:H	1:A:4:THR:HB	7	0.24
(1,1103)	1:A:95:GLU:HG2	1:A:96:ASP:HB2	4	0.23
(1,1103)	1:A:95:GLU:HG2	1:A:96:ASP:HB3	4	0.23
(1,1103)	1:A:95:GLU:HG3	1:A:96:ASP:HB2	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1103)	1:A:95:GLU:HG3	1:A:96:ASP:HB3	4	0.23
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD21	5	0.23
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD22	5	0.23
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD23	5	0.23
(1,930)	1:A:49:GLU:HG2	1:A:50:GLU:HA	11	0.22
(1,3)	1:A:4:THR:HB	1:A:5:SER:H	14	0.22
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	16	0.21
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	9	0.21
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	9	0.21
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	9	0.21
(1,675)	1:A:73:THR:H	1:A:73:THR:HG21	8	0.2
(1,675)	1:A:73:THR:H	1:A:73:THR:HG22	8	0.2
(1,675)	1:A:73:THR:H	1:A:73:THR:HG23	8	0.2
(1,483)	1:A:39:VAL:H	1:A:39:VAL:HB	9	0.2
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	7	0.2
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	20	0.2
(1,1442)	1:A:21:GLU:HG2	1:A:22:ASP:HA	1	0.2
(1,1442)	1:A:21:GLU:HG3	1:A:22:ASP:HA	1	0.2
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	6	0.19
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	18	0.19
(1,930)	1:A:49:GLU:HG2	1:A:50:GLU:HA	6	0.19
(1,930)	1:A:49:GLU:HG2	1:A:50:GLU:HA	13	0.19
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	11	0.19
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	11	0.19
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	11	0.19
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	11	0.19
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	3	0.19
(1,1441)	1:A:21:GLU:HA	1:A:21:GLU:HG2	7	0.19
(1,1441)	1:A:21:GLU:HA	1:A:21:GLU:HG3	7	0.19
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	2	0.19
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	2	0.19
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	2	0.19
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	18	0.19
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	18	0.19
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	18	0.19
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	4	0.18
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	4	0.18
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	4	0.18
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	4	0.18
(1,805)	1:A:12:LEU:HD11	1:A:93:MET:HA	9	0.18
(1,805)	1:A:12:LEU:HD12	1:A:93:MET:HA	9	0.18
(1,805)	1:A:12:LEU:HD13	1:A:93:MET:HA	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,805)	1:A:12:LEU:HD21	1:A:93:MET:HA	9	0.18
(1,805)	1:A:12:LEU:HD22	1:A:93:MET:HA	9	0.18
(1,805)	1:A:12:LEU:HD23	1:A:93:MET:HA	9	0.18
(1,483)	1:A:39:VAL:H	1:A:39:VAL:HB	20	0.18
(1,422)	1:A:9:GLU:HA	1:A:9:GLU:HG3	12	0.18
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	9	0.18
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	14	0.18
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	15	0.18
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	18	0.18
(1,318)	1:A:22:ASP:HB2	1:A:25:LYS:HE2	20	0.18
(1,318)	1:A:22:ASP:HB2	1:A:25:LYS:HE3	20	0.18
(1,318)	1:A:22:ASP:HB3	1:A:25:LYS:HE2	20	0.18
(1,318)	1:A:22:ASP:HB3	1:A:25:LYS:HE3	20	0.18
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	17	0.18
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	17	0.18
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	17	0.18
(1,1288)	1:A:73:THR:HA	1:A:77:LEU:HG	3	0.18
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	7	0.18
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	7	0.18
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	7	0.18
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	8	0.18
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	8	0.18
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	8	0.18
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	11	0.18
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	11	0.18
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	11	0.18
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	12	0.18
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	12	0.18
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	12	0.18
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	19	0.18
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	19	0.18
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	19	0.18
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	20	0.18
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	20	0.18
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	20	0.18
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	7	0.17
(1,895)	1:A:36:LEU:HB2	1:A:37:GLU:HG3	17	0.17
(1,483)	1:A:39:VAL:H	1:A:39:VAL:HB	8	0.17
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	2	0.17
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	10	0.17
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB2	3	0.17
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB3	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	1:A:73:THR:HA	1:A:77:LEU:HG	15	0.17
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	1	0.17
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	1	0.17
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	1	0.17
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	9	0.17
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	9	0.17
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	9	0.17
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	8	0.16
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	14	0.16
(1,930)	1:A:49:GLU:HG2	1:A:50:GLU:HA	4	0.16
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	13	0.16
(1,409)	1:A:50:GLU:HA	1:A:50:GLU:HG2	17	0.16
(1,409)	1:A:50:GLU:HA	1:A:50:GLU:HG3	17	0.16
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB2	4	0.16
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB3	4	0.16
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	2	0.16
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	2	0.16
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	2	0.16
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	13	0.16
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	13	0.16
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	13	0.16
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD11	4	0.16
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD12	4	0.16
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD13	4	0.16
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD11	6	0.16
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD12	6	0.16
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD13	6	0.16
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	3	0.16
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	3	0.16
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	3	0.16
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	10	0.16
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	10	0.16
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	10	0.16
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	13	0.16
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	13	0.16
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	13	0.16
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	15	0.16
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	15	0.16
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	15	0.16
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	16	0.16
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	16	0.16
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	17	0.16
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	17	0.16
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	17	0.16
(1,1001)	1:A:92:GLU:HB3	1:A:93:MET:HG3	10	0.16
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD11	16	0.15
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD12	16	0.15
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD13	16	0.15
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	11	0.15
(1,930)	1:A:49:GLU:HG2	1:A:50:GLU:HA	14	0.15
(1,895)	1:A:36:LEU:HB2	1:A:37:GLU:HG3	10	0.15
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	1	0.15
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	1	0.15
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	1	0.15
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	1	0.15
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	9	0.15
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	9	0.15
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	9	0.15
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	9	0.15
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	19	0.15
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	19	0.15
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	19	0.15
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	19	0.15
(1,660)	1:A:82:LEU:HD21	1:A:83:THR:H	16	0.15
(1,660)	1:A:82:LEU:HD22	1:A:83:THR:H	16	0.15
(1,660)	1:A:82:LEU:HD23	1:A:83:THR:H	16	0.15
(1,483)	1:A:39:VAL:H	1:A:39:VAL:HB	10	0.15
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	6	0.15
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB2	9	0.15
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB3	9	0.15
(1,1288)	1:A:73:THR:HA	1:A:77:LEU:HG	13	0.15
(1,1288)	1:A:73:THR:HA	1:A:77:LEU:HG	20	0.15
(1,127)	1:A:32:TRP:HA	1:A:32:TRP:HE3	15	0.15
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	5	0.15
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	5	0.15
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	5	0.15
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	6	0.15
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	6	0.15
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	6	0.15
(1,1141)	1:A:19:LEU:HD21	1:A:53:GLY:HA2	14	0.15
(1,1141)	1:A:19:LEU:HD22	1:A:53:GLY:HA2	14	0.15
(1,1141)	1:A:19:LEU:HD23	1:A:53:GLY:HA2	14	0.15
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD21	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD22	16	0.15
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD23	16	0.15
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	15	0.14
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	17	0.14
(1,930)	1:A:49:GLU:HG2	1:A:50:GLU:HA	10	0.14
(1,930)	1:A:49:GLU:HG2	1:A:50:GLU:HA	15	0.14
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	15	0.14
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	15	0.14
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	15	0.14
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	15	0.14
(1,801)	1:A:12:LEU:HA	1:A:93:MET:HB2	7	0.14
(1,763)	1:A:89:ALA:HB1	1:A:92:GLU:HG3	11	0.14
(1,763)	1:A:89:ALA:HB2	1:A:92:GLU:HG3	11	0.14
(1,763)	1:A:89:ALA:HB3	1:A:92:GLU:HG3	11	0.14
(1,66)	1:A:29:SER:H	1:A:29:SER:HB3	5	0.14
(1,66)	1:A:29:SER:H	1:A:29:SER:HB3	11	0.14
(1,66)	1:A:29:SER:H	1:A:29:SER:HB3	13	0.14
(1,66)	1:A:29:SER:H	1:A:29:SER:HB3	16	0.14
(1,65)	1:A:29:SER:HB3	1:A:30:LEU:H	14	0.14
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	2	0.14
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	5	0.14
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	8	0.14
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	13	0.14
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	15	0.14
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	17	0.14
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	20	0.14
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB2	8	0.14
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB3	8	0.14
(1,1344)	1:A:19:LEU:HD11	1:A:20:ASN:HD21	9	0.14
(1,1344)	1:A:19:LEU:HD12	1:A:20:ASN:HD21	9	0.14
(1,1344)	1:A:19:LEU:HD13	1:A:20:ASN:HD21	9	0.14
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	14	0.14
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	14	0.14
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	14	0.14
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	16	0.14
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	16	0.14
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	16	0.14
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	20	0.14
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	20	0.14
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	20	0.14
(1,1288)	1:A:73:THR:HA	1:A:77:LEU:HG	4	0.14
(1,1288)	1:A:73:THR:HA	1:A:77:LEU:HG	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:A:89:ALA:HA	1:A:92:GLU:HG2	12	0.14
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD11	18	0.13
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD12	18	0.13
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD13	18	0.13
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	1	0.13
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	2	0.13
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	5	0.13
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	10	0.13
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	20	0.13
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	3	0.13
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	3	0.13
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	3	0.13
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	3	0.13
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	6	0.13
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	6	0.13
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	6	0.13
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	6	0.13
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	18	0.13
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	18	0.13
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	18	0.13
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	18	0.13
(1,801)	1:A:12:LEU:HA	1:A:93:MET:HB2	4	0.13
(1,801)	1:A:12:LEU:HA	1:A:93:MET:HB2	15	0.13
(1,66)	1:A:29:SER:H	1:A:29:SER:HB3	8	0.13
(1,66)	1:A:29:SER:H	1:A:29:SER:HB3	10	0.13
(1,66)	1:A:29:SER:H	1:A:29:SER:HB3	12	0.13
(1,66)	1:A:29:SER:H	1:A:29:SER:HB3	17	0.13
(1,66)	1:A:29:SER:H	1:A:29:SER:HB3	18	0.13
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	1	0.13
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	4	0.13
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	6	0.13
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	7	0.13
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	10	0.13
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	11	0.13
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	12	0.13
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	14	0.13
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	18	0.13
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG2	18	0.13
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG3	18	0.13
(1,3)	1:A:4:THR:HB	1:A:5:SER:H	16	0.13
(1,287)	1:A:38:ASP:HB2	1:A:39:VAL:H	8	0.13
(1,287)	1:A:38:ASP:HB3	1:A:39:VAL:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1638)	1:A:85:LEU:HG	1:A:88:MET:HB2	20	0.13
(1,1638)	1:A:85:LEU:HG	1:A:88:MET:HB3	20	0.13
(1,1530)	1:A:41:GLN:H	1:A:41:GLN:HB2	10	0.13
(1,1530)	1:A:41:GLN:H	1:A:41:GLN:HB3	10	0.13
(1,1369)	1:A:8:LEU:HD11	1:A:9:GLU:HB2	4	0.13
(1,1369)	1:A:8:LEU:HD11	1:A:9:GLU:HB3	4	0.13
(1,1369)	1:A:8:LEU:HD12	1:A:9:GLU:HB2	4	0.13
(1,1369)	1:A:8:LEU:HD12	1:A:9:GLU:HB3	4	0.13
(1,1369)	1:A:8:LEU:HD13	1:A:9:GLU:HB2	4	0.13
(1,1369)	1:A:8:LEU:HD13	1:A:9:GLU:HB3	4	0.13
(1,1369)	1:A:8:LEU:HD21	1:A:9:GLU:HB2	4	0.13
(1,1369)	1:A:8:LEU:HD21	1:A:9:GLU:HB3	4	0.13
(1,1369)	1:A:8:LEU:HD22	1:A:9:GLU:HB2	4	0.13
(1,1369)	1:A:8:LEU:HD22	1:A:9:GLU:HB3	4	0.13
(1,1369)	1:A:8:LEU:HD23	1:A:9:GLU:HB2	4	0.13
(1,1369)	1:A:8:LEU:HD23	1:A:9:GLU:HB3	4	0.13
(1,1368)	1:A:8:LEU:HD11	1:A:9:GLU:HA	5	0.13
(1,1368)	1:A:8:LEU:HD12	1:A:9:GLU:HA	5	0.13
(1,1368)	1:A:8:LEU:HD13	1:A:9:GLU:HA	5	0.13
(1,1368)	1:A:8:LEU:HD21	1:A:9:GLU:HA	5	0.13
(1,1368)	1:A:8:LEU:HD22	1:A:9:GLU:HA	5	0.13
(1,1368)	1:A:8:LEU:HD23	1:A:9:GLU:HA	5	0.13
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	4	0.13
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	4	0.13
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	4	0.13
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	5	0.13
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	5	0.13
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	5	0.13
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	7	0.13
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	7	0.13
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	7	0.13
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	10	0.13
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	10	0.13
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	10	0.13
(1,1288)	1:A:73:THR:HA	1:A:77:LEU:HG	6	0.13
(1,121)	1:A:45:TRP:HA	1:A:48:VAL:HB	9	0.13
(1,1101)	1:A:95:GLU:H	1:A:96:ASP:HA	16	0.13
(1,1085)	1:A:89:ALA:HA	1:A:92:GLU:HG2	14	0.13
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD21	9	0.13
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD22	9	0.13
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD23	9	0.13
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD21	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD22	11	0.13
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD23	11	0.13
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD21	19	0.13
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD22	19	0.13
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD23	19	0.13
(1,958)	1:A:42:LYS:HE2	1:A:44:PRO:HD2	9	0.12
(1,958)	1:A:42:LYS:HE3	1:A:44:PRO:HD2	9	0.12
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD11	13	0.12
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD12	13	0.12
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD13	13	0.12
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	12	0.12
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	13	0.12
(1,930)	1:A:49:GLU:HG2	1:A:50:GLU:HA	2	0.12
(1,895)	1:A:36:LEU:HB2	1:A:37:GLU:HG3	1	0.12
(1,895)	1:A:36:LEU:HB2	1:A:37:GLU:HG3	8	0.12
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	7	0.12
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	7	0.12
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	7	0.12
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	7	0.12
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	12	0.12
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	12	0.12
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	12	0.12
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	12	0.12
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	13	0.12
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	13	0.12
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	13	0.12
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	13	0.12
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	14	0.12
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	14	0.12
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	14	0.12
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	14	0.12
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	16	0.12
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	16	0.12
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	16	0.12
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	16	0.12
(1,801)	1:A:12:LEU:HA	1:A:93:MET:HB2	9	0.12
(1,801)	1:A:12:LEU:HA	1:A:93:MET:HB2	18	0.12
(1,78)	1:A:29:SER:HA	1:A:32:TRP:HE3	13	0.12
(1,763)	1:A:89:ALA:HB1	1:A:92:GLU:HG3	5	0.12
(1,763)	1:A:89:ALA:HB2	1:A:92:GLU:HG3	5	0.12
(1,763)	1:A:89:ALA:HB3	1:A:92:GLU:HG3	5	0.12
(1,676)	1:A:72:ALA:HB1	1:A:73:THR:HG21	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:A:72:ALA:HB1	1:A:73:THR:HG22	8	0.12
(1,676)	1:A:72:ALA:HB1	1:A:73:THR:HG23	8	0.12
(1,676)	1:A:72:ALA:HB2	1:A:73:THR:HG21	8	0.12
(1,676)	1:A:72:ALA:HB2	1:A:73:THR:HG22	8	0.12
(1,676)	1:A:72:ALA:HB2	1:A:73:THR:HG23	8	0.12
(1,676)	1:A:72:ALA:HB3	1:A:73:THR:HG21	8	0.12
(1,676)	1:A:72:ALA:HB3	1:A:73:THR:HG22	8	0.12
(1,676)	1:A:72:ALA:HB3	1:A:73:THR:HG23	8	0.12
(1,66)	1:A:29:SER:H	1:A:29:SER:HB3	20	0.12
(1,65)	1:A:29:SER:HB3	1:A:30:LEU:H	11	0.12
(1,63)	1:A:26:SER:HB3	1:A:27:PHE:HB3	7	0.12
(1,63)	1:A:26:SER:HB3	1:A:27:PHE:HB3	20	0.12
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	9	0.12
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	16	0.12
(1,62)	1:A:26:SER:H	1:A:26:SER:HB3	19	0.12
(1,446)	1:A:13:GLN:HG2	1:A:54:LYS:HG3	11	0.12
(1,446)	1:A:13:GLN:HG3	1:A:54:LYS:HG3	11	0.12
(1,443)	1:A:11:THR:HB	1:A:93:MET:HG2	12	0.12
(1,420)	1:A:91:ALA:HB1	1:A:92:GLU:HG3	4	0.12
(1,420)	1:A:91:ALA:HB2	1:A:92:GLU:HG3	4	0.12
(1,420)	1:A:91:ALA:HB3	1:A:92:GLU:HG3	4	0.12
(1,420)	1:A:91:ALA:HB1	1:A:92:GLU:HG3	11	0.12
(1,420)	1:A:91:ALA:HB2	1:A:92:GLU:HG3	11	0.12
(1,420)	1:A:91:ALA:HB3	1:A:92:GLU:HG3	11	0.12
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	4	0.12
(1,301)	1:A:8:LEU:HB3	1:A:8:LEU:HG	6	0.12
(1,301)	1:A:8:LEU:HB3	1:A:8:LEU:HG	18	0.12
(1,301)	1:A:8:LEU:HB3	1:A:8:LEU:HG	19	0.12
(1,3)	1:A:4:THR:HB	1:A:5:SER:H	12	0.12
(1,222)	1:A:43:THR:H	1:A:44:PRO:HD3	3	0.12
(1,1657)	1:A:91:ALA:HA	1:A:94:MET:HG2	11	0.12
(1,1657)	1:A:91:ALA:HA	1:A:94:MET:HG3	11	0.12
(1,1535)	1:A:42:LYS:HG2	1:A:43:THR:HG21	13	0.12
(1,1535)	1:A:42:LYS:HG2	1:A:43:THR:HG22	13	0.12
(1,1535)	1:A:42:LYS:HG2	1:A:43:THR:HG23	13	0.12
(1,1535)	1:A:42:LYS:HG3	1:A:43:THR:HG21	13	0.12
(1,1535)	1:A:42:LYS:HG3	1:A:43:THR:HG22	13	0.12
(1,1535)	1:A:42:LYS:HG3	1:A:43:THR:HG23	13	0.12
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB2	5	0.12
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB3	5	0.12
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB2	14	0.12
(1,1378)	1:A:10:TRP:HA	1:A:13:GLN:HB3	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	1:A:8:LEU:HD11	1:A:9:GLU:HB2	18	0.12
(1,1369)	1:A:8:LEU:HD11	1:A:9:GLU:HB3	18	0.12
(1,1369)	1:A:8:LEU:HD12	1:A:9:GLU:HB2	18	0.12
(1,1369)	1:A:8:LEU:HD12	1:A:9:GLU:HB3	18	0.12
(1,1369)	1:A:8:LEU:HD13	1:A:9:GLU:HB2	18	0.12
(1,1369)	1:A:8:LEU:HD13	1:A:9:GLU:HB3	18	0.12
(1,1369)	1:A:8:LEU:HD21	1:A:9:GLU:HB2	18	0.12
(1,1369)	1:A:8:LEU:HD21	1:A:9:GLU:HB3	18	0.12
(1,1369)	1:A:8:LEU:HD22	1:A:9:GLU:HB2	18	0.12
(1,1369)	1:A:8:LEU:HD22	1:A:9:GLU:HB3	18	0.12
(1,1369)	1:A:8:LEU:HD23	1:A:9:GLU:HB2	18	0.12
(1,1369)	1:A:8:LEU:HD23	1:A:9:GLU:HB3	18	0.12
(1,1344)	1:A:19:LEU:HD11	1:A:20:ASN:HD21	11	0.12
(1,1344)	1:A:19:LEU:HD12	1:A:20:ASN:HD21	11	0.12
(1,1344)	1:A:19:LEU:HD13	1:A:20:ASN:HD21	11	0.12
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	1	0.12
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	1	0.12
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	1	0.12
(1,1341)	1:A:15:LEU:HD21	1:A:86:CYS:HB3	3	0.12
(1,1341)	1:A:15:LEU:HD22	1:A:86:CYS:HB3	3	0.12
(1,1341)	1:A:15:LEU:HD23	1:A:86:CYS:HB3	3	0.12
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD11	13	0.12
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD12	13	0.12
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD13	13	0.12
(1,1288)	1:A:73:THR:HA	1:A:77:LEU:HG	8	0.12
(1,121)	1:A:45:TRP:HA	1:A:48:VAL:HB	3	0.12
(1,1157)	1:A:89:ALA:H	1:A:90:LYS:HD2	4	0.12
(1,1157)	1:A:89:ALA:H	1:A:90:LYS:HD3	4	0.12
(1,1120)	1:A:4:THR:HB	1:A:7:GLN:HA	14	0.12
(1,1088)	1:A:91:ALA:HA	1:A:92:GLU:HB2	6	0.12
(1,958)	1:A:42:LYS:HE2	1:A:44:PRO:HD2	3	0.11
(1,958)	1:A:42:LYS:HE3	1:A:44:PRO:HD2	3	0.11
(1,958)	1:A:42:LYS:HE2	1:A:44:PRO:HD2	12	0.11
(1,958)	1:A:42:LYS:HE3	1:A:44:PRO:HD2	12	0.11
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD11	8	0.11
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD12	8	0.11
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD13	8	0.11
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD11	17	0.11
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD12	17	0.11
(1,956)	1:A:55:LYS:HG2	1:A:59:ILE:HD13	17	0.11
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	3	0.11
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:A:54:LYS:HG3	1:A:55:LYS:HA	16	0.11
(1,930)	1:A:49:GLU:HG2	1:A:50:GLU:HA	20	0.11
(1,895)	1:A:36:LEU:HB2	1:A:37:GLU:HG3	5	0.11
(1,874)	1:A:29:SER:HB2	1:A:30:LEU:HD11	3	0.11
(1,874)	1:A:29:SER:HB2	1:A:30:LEU:HD12	3	0.11
(1,874)	1:A:29:SER:HB2	1:A:30:LEU:HD13	3	0.11
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD2	8	0.11
(1,855)	1:A:23:GLU:HG2	1:A:25:LYS:HD3	8	0.11
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD2	8	0.11
(1,855)	1:A:23:GLU:HG3	1:A:25:LYS:HD3	8	0.11
(1,801)	1:A:12:LEU:HA	1:A:93:MET:HB2	5	0.11
(1,801)	1:A:12:LEU:HA	1:A:93:MET:HB2	13	0.11
(1,78)	1:A:29:SER:HA	1:A:32:TRP:HE3	8	0.11
(1,763)	1:A:89:ALA:HB1	1:A:92:GLU:HG3	9	0.11
(1,763)	1:A:89:ALA:HB2	1:A:92:GLU:HG3	9	0.11
(1,763)	1:A:89:ALA:HB3	1:A:92:GLU:HG3	9	0.11
(1,763)	1:A:89:ALA:HB1	1:A:92:GLU:HG3	19	0.11
(1,763)	1:A:89:ALA:HB2	1:A:92:GLU:HG3	19	0.11
(1,763)	1:A:89:ALA:HB3	1:A:92:GLU:HG3	19	0.11
(1,731)	1:A:56:LEU:H	1:A:59:ILE:HD11	10	0.11
(1,731)	1:A:56:LEU:H	1:A:59:ILE:HD12	10	0.11
(1,731)	1:A:56:LEU:H	1:A:59:ILE:HD13	10	0.11
(1,73)	1:A:26:SER:HB2	1:A:30:LEU:HD11	3	0.11
(1,73)	1:A:26:SER:HB2	1:A:30:LEU:HD12	3	0.11
(1,73)	1:A:26:SER:HB2	1:A:30:LEU:HD13	3	0.11
(1,707)	1:A:69:ILE:HG21	1:A:73:THR:HB	8	0.11
(1,707)	1:A:69:ILE:HG22	1:A:73:THR:HB	8	0.11
(1,707)	1:A:69:ILE:HG23	1:A:73:THR:HB	8	0.11
(1,660)	1:A:82:LEU:HD21	1:A:83:THR:H	7	0.11
(1,660)	1:A:82:LEU:HD22	1:A:83:THR:H	7	0.11
(1,660)	1:A:82:LEU:HD23	1:A:83:THR:H	7	0.11
(1,66)	1:A:29:SER:H	1:A:29:SER:HB3	7	0.11
(1,66)	1:A:29:SER:H	1:A:29:SER:HB3	14	0.11
(1,65)	1:A:29:SER:HB3	1:A:30:LEU:H	10	0.11
(1,65)	1:A:29:SER:HB3	1:A:30:LEU:H	13	0.11
(1,65)	1:A:29:SER:HB3	1:A:30:LEU:H	16	0.11
(1,65)	1:A:29:SER:HB3	1:A:30:LEU:H	18	0.11
(1,633)	1:A:34:PHE:HZ	1:A:36:LEU:HD11	3	0.11
(1,633)	1:A:34:PHE:HZ	1:A:36:LEU:HD12	3	0.11
(1,633)	1:A:34:PHE:HZ	1:A:36:LEU:HD13	3	0.11
(1,633)	1:A:34:PHE:HZ	1:A:36:LEU:HD11	6	0.11
(1,633)	1:A:34:PHE:HZ	1:A:36:LEU:HD12	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:A:34:PHE:HZ	1:A:36:LEU:HD13	6	0.11
(1,63)	1:A:26:SER:HB3	1:A:27:PHE:HB3	1	0.11
(1,63)	1:A:26:SER:HB3	1:A:27:PHE:HB3	6	0.11
(1,63)	1:A:26:SER:HB3	1:A:27:PHE:HB3	16	0.11
(1,63)	1:A:26:SER:HB3	1:A:27:PHE:HB3	17	0.11
(1,63)	1:A:26:SER:HB3	1:A:27:PHE:HB3	19	0.11
(1,547)	1:A:45:TRP:HE1	1:A:49:GLU:HB2	5	0.11
(1,443)	1:A:11:THR:HB	1:A:93:MET:HG2	8	0.11
(1,420)	1:A:91:ALA:HB1	1:A:92:GLU:HG3	10	0.11
(1,420)	1:A:91:ALA:HB2	1:A:92:GLU:HG3	10	0.11
(1,420)	1:A:91:ALA:HB3	1:A:92:GLU:HG3	10	0.11
(1,418)	1:A:49:GLU:HA	1:A:49:GLU:HG3	11	0.11
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG2	3	0.11
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG3	3	0.11
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG2	5	0.11
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG3	5	0.11
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG2	13	0.11
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG3	13	0.11
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG2	14	0.11
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG3	14	0.11
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG2	15	0.11
(1,404)	1:A:20:ASN:HD21	1:A:23:GLU:HG3	15	0.11
(1,319)	1:A:96:ASP:H	1:A:96:ASP:HB2	15	0.11
(1,319)	1:A:96:ASP:H	1:A:96:ASP:HB3	15	0.11
(1,283)	1:A:54:LYS:HA	1:A:54:LYS:HE2	3	0.11
(1,283)	1:A:54:LYS:HA	1:A:54:LYS:HE3	3	0.11
(1,283)	1:A:54:LYS:HA	1:A:54:LYS:HE2	9	0.11
(1,283)	1:A:54:LYS:HA	1:A:54:LYS:HE3	9	0.11
(1,271)	1:A:25:LYS:HG3	1:A:25:LYS:HE2	10	0.11
(1,271)	1:A:25:LYS:HG3	1:A:25:LYS:HE3	10	0.11
(1,193)	1:A:15:LEU:HD11	1:A:89:ALA:HA	11	0.11
(1,193)	1:A:15:LEU:HD12	1:A:89:ALA:HA	11	0.11
(1,193)	1:A:15:LEU:HD13	1:A:89:ALA:HA	11	0.11
(1,1535)	1:A:42:LYS:HG2	1:A:43:THR:HG21	5	0.11
(1,1535)	1:A:42:LYS:HG2	1:A:43:THR:HG22	5	0.11
(1,1535)	1:A:42:LYS:HG2	1:A:43:THR:HG23	5	0.11
(1,1535)	1:A:42:LYS:HG3	1:A:43:THR:HG21	5	0.11
(1,1535)	1:A:42:LYS:HG3	1:A:43:THR:HG22	5	0.11
(1,1535)	1:A:42:LYS:HG3	1:A:43:THR:HG23	5	0.11
(1,1369)	1:A:8:LEU:HD11	1:A:9:GLU:HB2	12	0.11
(1,1369)	1:A:8:LEU:HD11	1:A:9:GLU:HB3	12	0.11
(1,1369)	1:A:8:LEU:HD12	1:A:9:GLU:HB2	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	1:A:8:LEU:HD12	1:A:9:GLU:HB3	12	0.11
(1,1369)	1:A:8:LEU:HD13	1:A:9:GLU:HB2	12	0.11
(1,1369)	1:A:8:LEU:HD13	1:A:9:GLU:HB3	12	0.11
(1,1369)	1:A:8:LEU:HD21	1:A:9:GLU:HB2	12	0.11
(1,1369)	1:A:8:LEU:HD21	1:A:9:GLU:HB3	12	0.11
(1,1369)	1:A:8:LEU:HD22	1:A:9:GLU:HB2	12	0.11
(1,1369)	1:A:8:LEU:HD22	1:A:9:GLU:HB3	12	0.11
(1,1369)	1:A:8:LEU:HD23	1:A:9:GLU:HB2	12	0.11
(1,1369)	1:A:8:LEU:HD23	1:A:9:GLU:HB3	12	0.11
(1,1368)	1:A:8:LEU:HD11	1:A:9:GLU:HA	20	0.11
(1,1368)	1:A:8:LEU:HD12	1:A:9:GLU:HA	20	0.11
(1,1368)	1:A:8:LEU:HD13	1:A:9:GLU:HA	20	0.11
(1,1368)	1:A:8:LEU:HD21	1:A:9:GLU:HA	20	0.11
(1,1368)	1:A:8:LEU:HD22	1:A:9:GLU:HA	20	0.11
(1,1368)	1:A:8:LEU:HD23	1:A:9:GLU:HA	20	0.11
(1,1344)	1:A:19:LEU:HD11	1:A:20:ASN:HD21	3	0.11
(1,1344)	1:A:19:LEU:HD12	1:A:20:ASN:HD21	3	0.11
(1,1344)	1:A:19:LEU:HD13	1:A:20:ASN:HD21	3	0.11
(1,1344)	1:A:19:LEU:HD11	1:A:20:ASN:HD21	20	0.11
(1,1344)	1:A:19:LEU:HD12	1:A:20:ASN:HD21	20	0.11
(1,1344)	1:A:19:LEU:HD13	1:A:20:ASN:HD21	20	0.11
(1,1335)	1:A:83:THR:HG21	1:A:87:LYS:HE2	5	0.11
(1,1335)	1:A:83:THR:HG21	1:A:87:LYS:HE3	5	0.11
(1,1335)	1:A:83:THR:HG22	1:A:87:LYS:HE2	5	0.11
(1,1335)	1:A:83:THR:HG22	1:A:87:LYS:HE3	5	0.11
(1,1335)	1:A:83:THR:HG23	1:A:87:LYS:HE2	5	0.11
(1,1335)	1:A:83:THR:HG23	1:A:87:LYS:HE3	5	0.11
(1,1335)	1:A:83:THR:HG21	1:A:87:LYS:HE2	9	0.11
(1,1335)	1:A:83:THR:HG21	1:A:87:LYS:HE3	9	0.11
(1,1335)	1:A:83:THR:HG22	1:A:87:LYS:HE2	9	0.11
(1,1335)	1:A:83:THR:HG22	1:A:87:LYS:HE3	9	0.11
(1,1335)	1:A:83:THR:HG23	1:A:87:LYS:HE2	9	0.11
(1,1335)	1:A:83:THR:HG23	1:A:87:LYS:HE3	9	0.11
(1,1335)	1:A:83:THR:HG21	1:A:87:LYS:HE2	19	0.11
(1,1335)	1:A:83:THR:HG21	1:A:87:LYS:HE3	19	0.11
(1,1335)	1:A:83:THR:HG22	1:A:87:LYS:HE2	19	0.11
(1,1335)	1:A:83:THR:HG22	1:A:87:LYS:HE3	19	0.11
(1,1335)	1:A:83:THR:HG23	1:A:87:LYS:HE2	19	0.11
(1,1335)	1:A:83:THR:HG23	1:A:87:LYS:HE3	19	0.11
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD11	20	0.11
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD12	20	0.11
(1,1290)	1:A:73:THR:HA	1:A:76:ILE:HD13	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1221)	1:A:10:TRP:HD1	1:A:14:THR:HG21	5	0.11
(1,1221)	1:A:10:TRP:HD1	1:A:14:THR:HG22	5	0.11
(1,1221)	1:A:10:TRP:HD1	1:A:14:THR:HG23	5	0.11
(1,121)	1:A:45:TRP:HA	1:A:48:VAL:HB	2	0.11
(1,121)	1:A:45:TRP:HA	1:A:48:VAL:HB	7	0.11
(1,121)	1:A:45:TRP:HA	1:A:48:VAL:HB	12	0.11
(1,116)	1:A:84:GLU:HA	1:A:87:LYS:HE2	8	0.11
(1,116)	1:A:84:GLU:HA	1:A:87:LYS:HE3	8	0.11
(1,1091)	1:A:87:LYS:HE2	1:A:91:ALA:HB1	16	0.11
(1,1091)	1:A:87:LYS:HE2	1:A:91:ALA:HB2	16	0.11
(1,1091)	1:A:87:LYS:HE2	1:A:91:ALA:HB3	16	0.11
(1,1091)	1:A:87:LYS:HE3	1:A:91:ALA:HB1	16	0.11
(1,1091)	1:A:87:LYS:HE3	1:A:91:ALA:HB2	16	0.11
(1,1091)	1:A:87:LYS:HE3	1:A:91:ALA:HB3	16	0.11
(1,1088)	1:A:91:ALA:HA	1:A:92:GLU:HB2	12	0.11
(1,1088)	1:A:91:ALA:HA	1:A:92:GLU:HB2	17	0.11
(1,1088)	1:A:91:ALA:HA	1:A:92:GLU:HB2	18	0.11
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD21	2	0.11
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD22	2	0.11
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD23	2	0.11
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD21	7	0.11
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD22	7	0.11
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD23	7	0.11
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD21	12	0.11
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD22	12	0.11
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD23	12	0.11
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD21	17	0.11
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD22	17	0.11
(1,1064)	1:A:77:LEU:HG	1:A:82:LEU:HD23	17	0.11
(1,1001)	1:A:92:GLU:HB3	1:A:93:MET:HG3	11	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found