Full wwPDB NMR Structure Validation Report

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PDB ID	:	1P9J
BMRB ID	:	5801
Title	:	Solution structure and dynamics of the EGF/TGF-alpha chimera T1E
Authors	:	Wingens, M.; Walma, T.; Van Ingen, H.; Stortelers, C.; Van Leeuwen, J.E.; Van Zoelen, E.J.; Vuister, G.W.
Deposited on	:	2003-05-12

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:

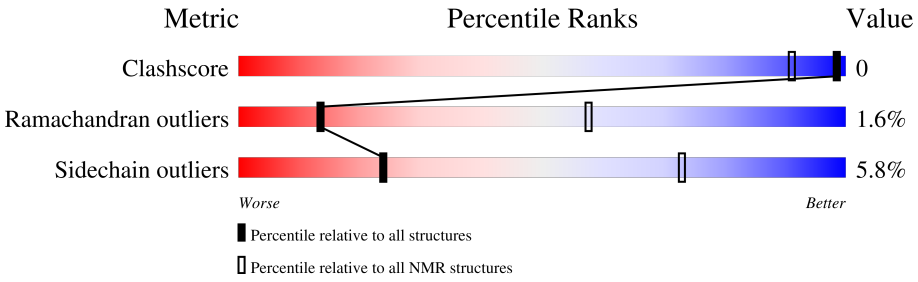
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 55%.

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	54	96%

2 Ensemble composition and analysis (i)

This entry contains 36 models. Model 12 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:1-A:54 (54)	2.02	12

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 8 single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 7, 10, 12, 14, 15, 19, 22, 24, 25, 26, 28, 30, 32, 34, 35
2	6, 8, 16, 20, 27, 29, 36
3	1, 2, 11, 17, 23, 31
Single-model clusters	9; 13; 18; 21; 33

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 846 atoms, of which 404 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	54	846	281	404	73	81	7	0

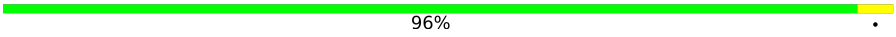
4 Residue-property plots

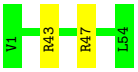
4.1 Average score per residue in the NMR ensemble

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: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

Chain A:





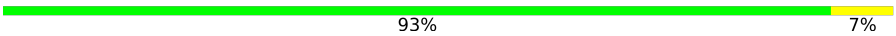
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

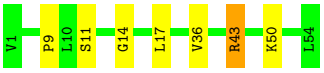
Chain A:



4.2.2 Score per residue for model 2

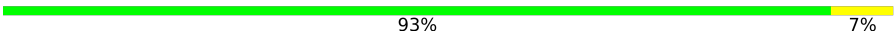
• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

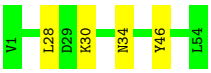
Chain A:



4.2.3 Score per residue for model 3

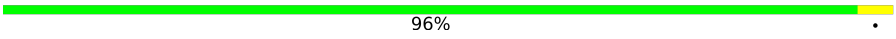
• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

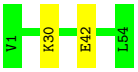
Chain A: 



4.2.4 Score per residue for model 4

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

Chain A: 



4.2.5 Score per residue for model 5

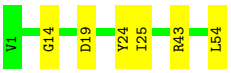
• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

Chain A: 

4.2.6 Score per residue for model 6

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

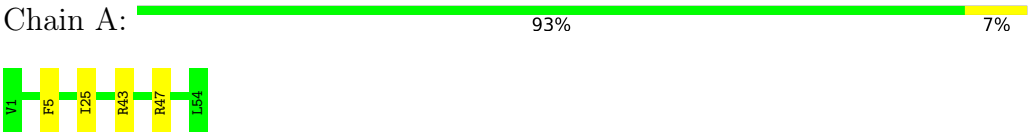
Chain A: 



4.2.7 Score per residue for model 7

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

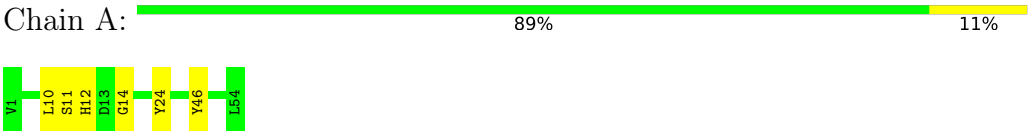
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

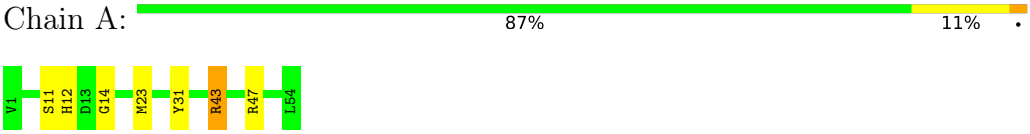
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

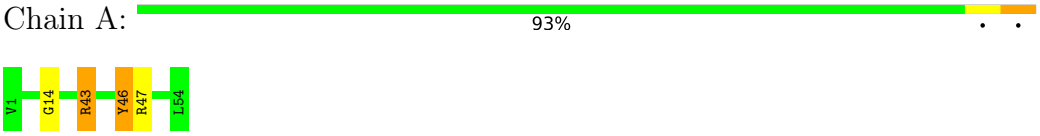
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

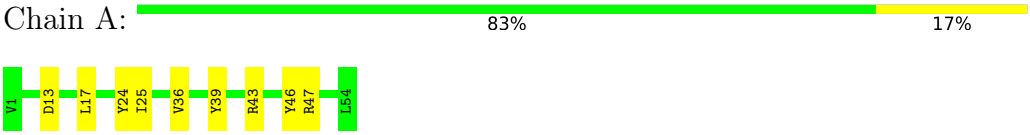
Chain A:



4.2.11 Score per residue for model 11

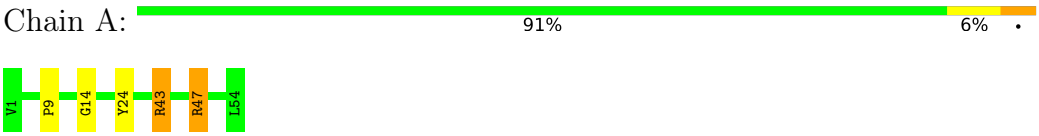
• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

Chain A:



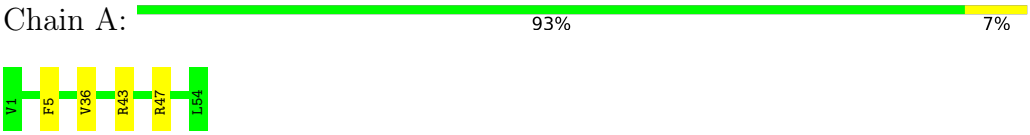
4.2.12 Score per residue for model 12 (medoid)

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

Chain A: 

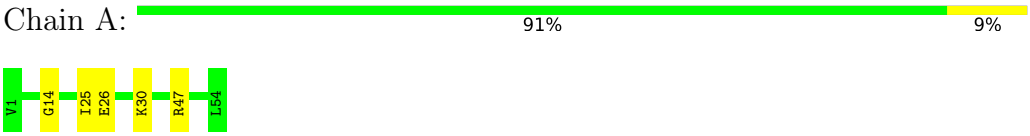
4.2.13 Score per residue for model 13

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

Chain A: 

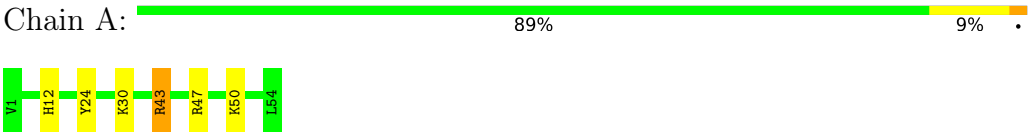
4.2.14 Score per residue for model 14

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

Chain A: 

4.2.15 Score per residue for model 15

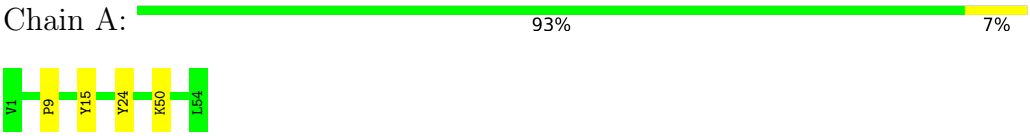
• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

Chain A: 

4.2.16 Score per residue for model 16

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

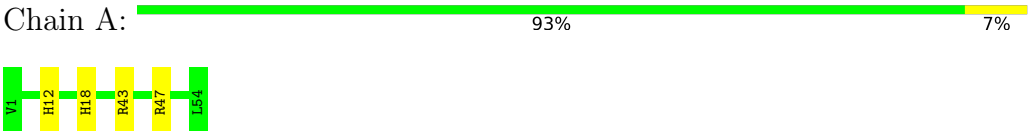
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

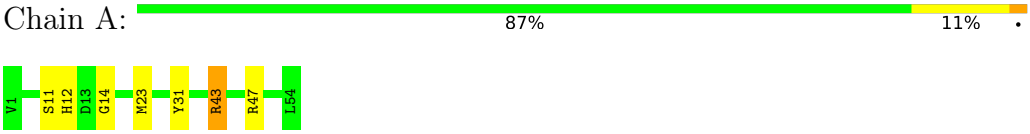
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

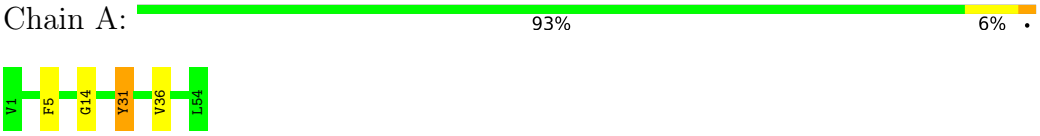
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

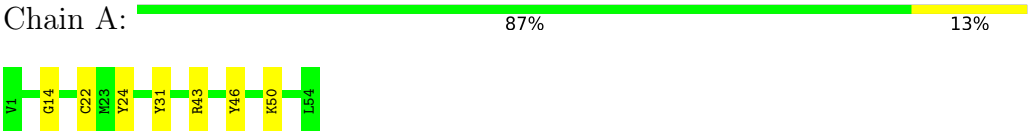
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

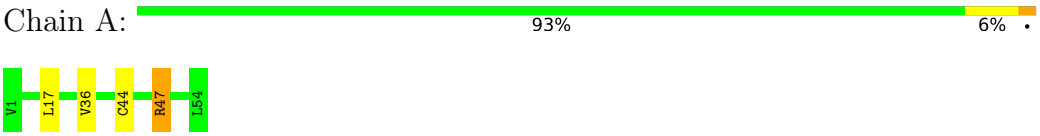
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

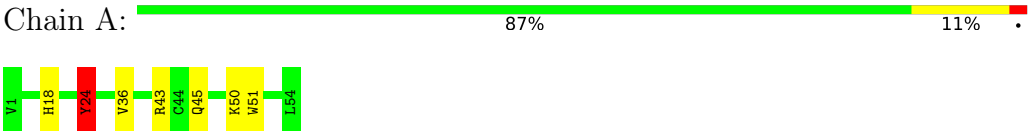
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

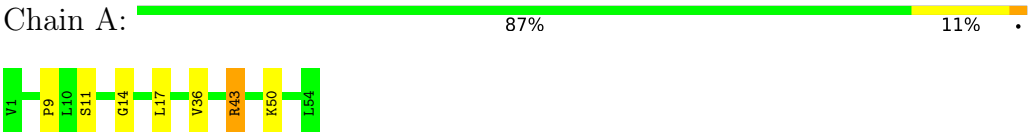
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

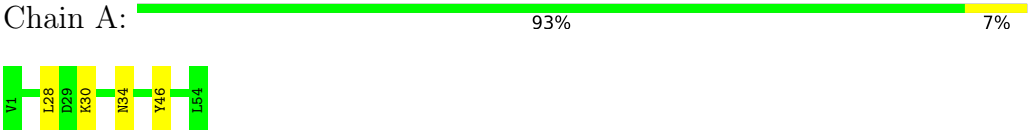
Chain A:



4.2.24 Score per residue for model 24

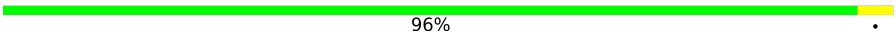
• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

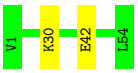
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

Chain A: 



4.2.26 Score per residue for model 26

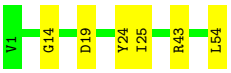
• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

Chain A: 

4.2.27 Score per residue for model 27

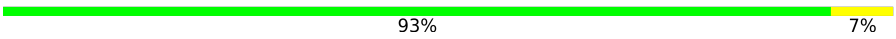
• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

Chain A: 



4.2.28 Score per residue for model 28

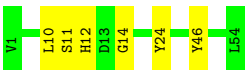
• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

Chain A: 

4.2.29 Score per residue for model 29

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

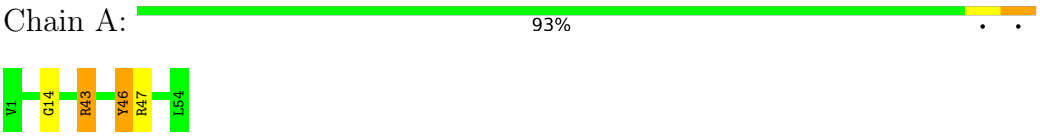
Chain A: 



4.2.30 Score per residue for model 30

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

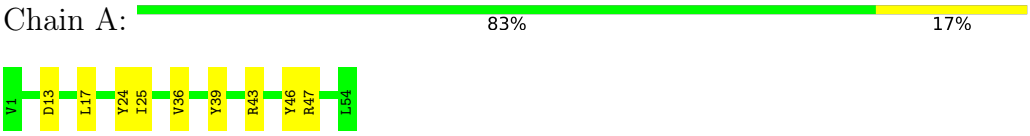
Chain A:



4.2.31 Score per residue for model 31

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

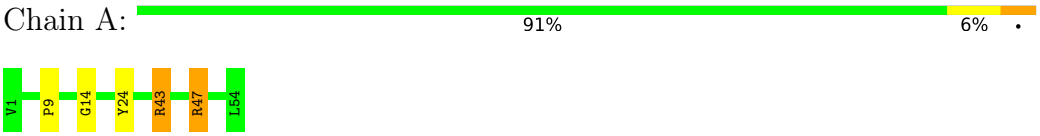
Chain A:



4.2.32 Score per residue for model 32

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

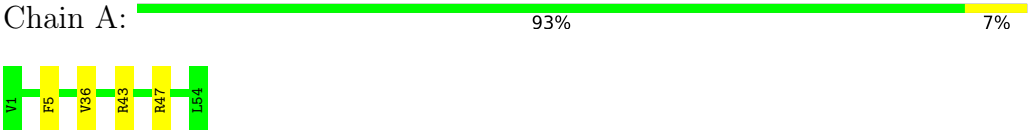
Chain A:



4.2.33 Score per residue for model 33

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

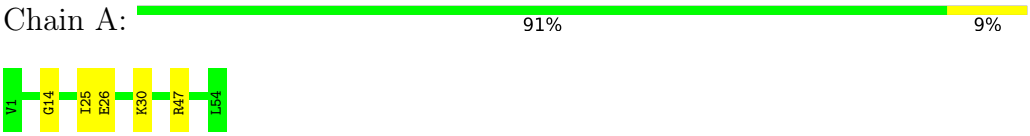
Chain A:



4.2.34 Score per residue for model 34

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

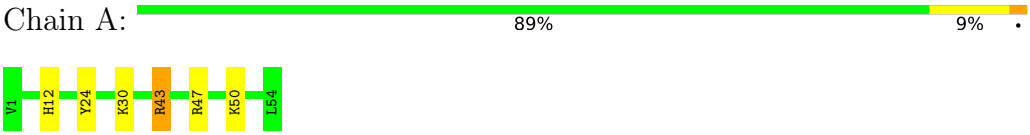
Chain A:



4.2.35 Score per residue for model 35

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

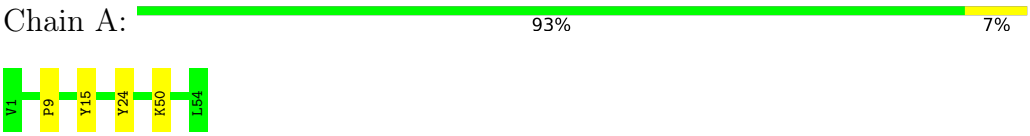
Chain A:



4.2.36 Score per residue for model 36

• Molecule 1: chimera of Epidermal growth factor(EGF) and Transforming growth factor alpha (TGF-alpha)

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry followed by brief molecular dynamics run in water.*.

Of the 98 calculated structures, 36 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	3.851
CHARMM	refinement	22

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	402
Number of shifts mapped to atoms	402
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	55%

6 Model quality

6.1 Standard geometry

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	0.99±0.00	0±0/455 (0.0± 0.0%)	1.08±0.07	2±1/616 (0.3± 0.2%)
All	All	0.99	0/16380 (0.0%)	1.08	69/22176 (0.3%)

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	0.6±0.6
All	All	0	21

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	24	TYR	CB-CG-CD2	-11.05	114.37	121.00	22	14
1	A	31	TYR	CB-CG-CD2	-10.50	114.70	121.00	19	1
1	A	24	TYR	CB-CG-CD1	9.12	126.47	121.00	22	8
1	A	46	TYR	CB-CG-CD2	-9.02	115.59	121.00	8	7
1	A	31	TYR	CB-CG-CD1	8.86	126.31	121.00	19	1
1	A	47	ARG	NE-CZ-NH1	8.38	124.49	120.30	11	17
1	A	46	TYR	CB-CG-CD1	7.77	125.66	121.00	8	3
1	A	43	ARG	NE-CZ-NH2	-7.02	116.79	120.30	9	4
1	A	43	ARG	NE-CZ-NH1	6.75	123.68	120.30	1	10
1	A	47	ARG	NE-CZ-NH2	-5.49	117.55	120.30	14	2
1	A	50	LYS	N-CA-CB	-5.21	101.23	110.60	2	2

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	43	ARG	Sidechain	10
1	A	11	SER	Peptide	4
1	A	47	ARG	Sidechain	2
1	A	46	TYR	Sidechain	2
1	A	39	TYR	Sidechain	2
1	A	24	TYR	Sidechain	1

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	442	404	401	0±0
All	All	15912	14544	14436	2

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:HIS:HE1	1:A:45:GLN:O	0.42	1.98	22	1
1:A:18:HIS:CE1	1:A:45:GLN:O	0.40	2.73	22	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	52/54 (96%)	47±1 (91±3%)	4±1 (8±3%)	1±1 (2±1%)	13	57
All	All	1872/1944 (96%)	1695 (91%)	147 (8%)	30 (2%)	13	57

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occur-

rence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	14	GLY	16
1	A	9	PRO	8
1	A	12	HIS	6

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	48/48 (100%)	45±1 (94±2%)	3±1 (6±2%)	24	73
All	All	1728/1728 (100%)	1628 (94%)	100 (6%)	24	73

All 28 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	43	ARG	12
1	A	25	ILE	10
1	A	36	VAL	9
1	A	30	LYS	8
1	A	50	LYS	6
1	A	17	LEU	5
1	A	5	PHE	5
1	A	19	ASP	4
1	A	31	TYR	4
1	A	22	CYS	3
1	A	47	ARG	3
1	A	12	HIS	2
1	A	18	HIS	2
1	A	11	SER	2
1	A	28	LEU	2
1	A	34	ASN	2
1	A	46	TYR	2
1	A	42	GLU	2
1	A	45	GLN	2
1	A	54	LEU	2
1	A	10	LEU	2
1	A	23	MET	2

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Mol	Chain	Res	Type	Models (Total)
1	A	13	ASP	2
1	A	26	GLU	2
1	A	15	TYR	2
1	A	44	CYS	1
1	A	24	TYR	1
1	A	51	TRP	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 55% for the well-defined parts and 55% 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	402
Number of shifts mapped to atoms	402
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	53	-0.60 ± 0.94	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 55%, i.e. 401 atoms were assigned a chemical shift out of a possible 727. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	163/272 (60%)	110/111 (99%)	0/108 (0%)	53/53 (100%)
Sidechain	206/352 (59%)	205/229 (90%)	0/112 (0%)	1/11 (9%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	32/103 (31%)	30/49 (61%)	0/46 (0%)	2/8 (25%)
Overall	401/727 (55%)	345/389 (89%)	0/266 (0%)	56/72 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 55%, i.e. 401 atoms were assigned a chemical shift out of a possible 727. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	163/272 (60%)	110/111 (99%)	0/108 (0%)	53/53 (100%)
Sidechain	206/352 (59%)	205/229 (90%)	0/112 (0%)	1/11 (9%)
Aromatic	32/103 (31%)	30/49 (61%)	0/46 (0%)	2/8 (25%)
Overall	401/727 (55%)	345/389 (89%)	0/266 (0%)	56/72 (78%)

7.1.4 Statistically unusual chemical shifts (i)

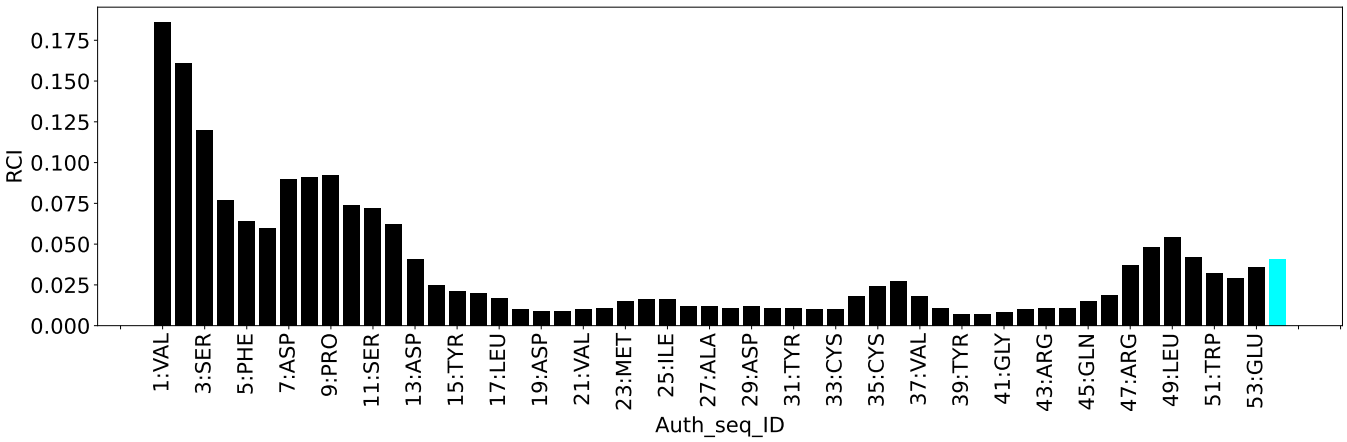
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	41	GLY	N	127.71	91.59 – 127.52	5.0

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:


RCI
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
1:VAL
3:SER
5:PHE
7:ASP
9:PRO
11:SER
13:ASP
15:TYR
17:LEU
19:ASP
21:VAL
23:MET
25:ILE
27:ALA
29:ASP
31:TYR
33:CYS
35:CYS
37:VAL
39:TYR
41:GLY
43:ARG
45:GLN
47:ARG
49:LEU
51:TRP
53:GLU
Auth_seq_ID

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	660
Intra-residue (|i-j|=0)	308
Sequential (|i-j|=1)	193
Medium range (|i-j|>1 and |i-j|<5)	68
Long range (|i-j|≥5)	91
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	4
Number of restraints per residue	12.2
Number of long range restraints per residue[1]	1.7

[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)	6.3	0.2
0.2-0.5 (Medium)	2.2	0.39
>0.5 (Large)	0.7	1.68

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)

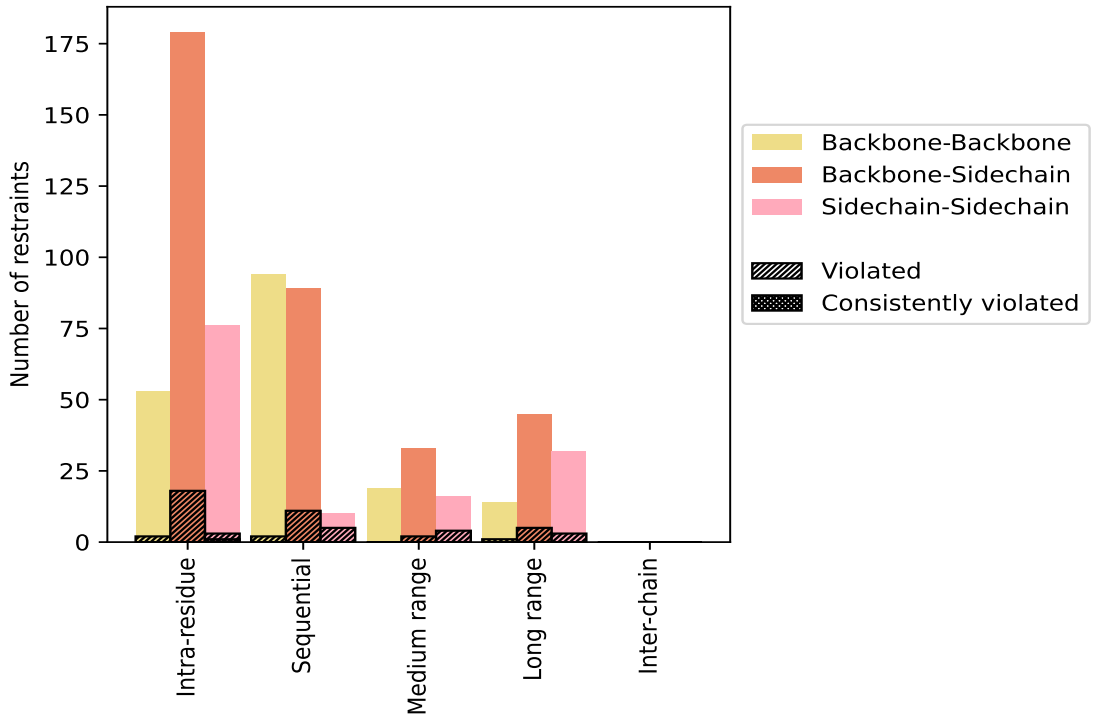
9.1 Summary of distance violations (i)

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)	308	46.7	23	7.5	3.5	1	0.3	0.2
Backbone-Backbone	53	8.0	2	3.8	0.3	0	0.0	0.0
Backbone-Sidechain	179	27.1	18	10.1	2.7	0	0.0	0.0
Sidechain-Sidechain	76	11.5	3	3.9	0.5	1	1.3	0.2
Sequential (|i-j|=1)	193	29.2	18	9.3	2.7	0	0.0	0.0
Backbone-Backbone	94	14.2	2	2.1	0.3	0	0.0	0.0
Backbone-Sidechain	89	13.5	11	12.4	1.7	0	0.0	0.0
Sidechain-Sidechain	10	1.5	5	50.0	0.8	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	68	10.3	6	8.8	0.9	0	0.0	0.0
Backbone-Backbone	19	2.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	33	5.0	2	6.1	0.3	0	0.0	0.0
Sidechain-Sidechain	16	2.4	4	25.0	0.6	0	0.0	0.0
Long range (|i-j|≥5)	91	13.8	9	9.9	1.4	0	0.0	0.0
Backbone-Backbone	14	2.1	1	7.1	0.2	0	0.0	0.0
Backbone-Sidechain	45	6.8	5	11.1	0.8	0	0.0	0.0
Sidechain-Sidechain	32	4.8	3	9.4	0.5	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	660	100.0	56	8.5	8.5	1	0.2	0.2
Backbone-Backbone	180	27.3	5	2.8	0.8	0	0.0	0.0
Backbone-Sidechain	346	52.4	36	10.4	5.5	0	0.0	0.0
Sidechain-Sidechain	134	20.3	15	11.2	2.3	1	0.7	0.2

[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	3	3	1	1	0	8	0.16	0.35	0.08	0.13
2	4	2	2	1	0	9	0.2	0.37	0.09	0.15
3	3	0	2	2	0	7	0.29	0.81	0.23	0.18
4	6	1	0	1	0	8	0.31	1.06	0.29	0.18
5	3	2	4	2	0	11	0.28	1.49	0.39	0.17
6	4	3	1	0	0	8	0.19	0.37	0.08	0.16
7	4	3	0	1	0	8	0.33	1.38	0.41	0.15
8	4	4	1	1	0	10	0.3	1.57	0.43	0.12
9	5	1	0	5	0	11	0.31	1.62	0.42	0.15
10	5	3	1	2	0	11	0.22	0.69	0.17	0.13
11	5	4	2	1	0	12	0.16	0.35	0.06	0.15

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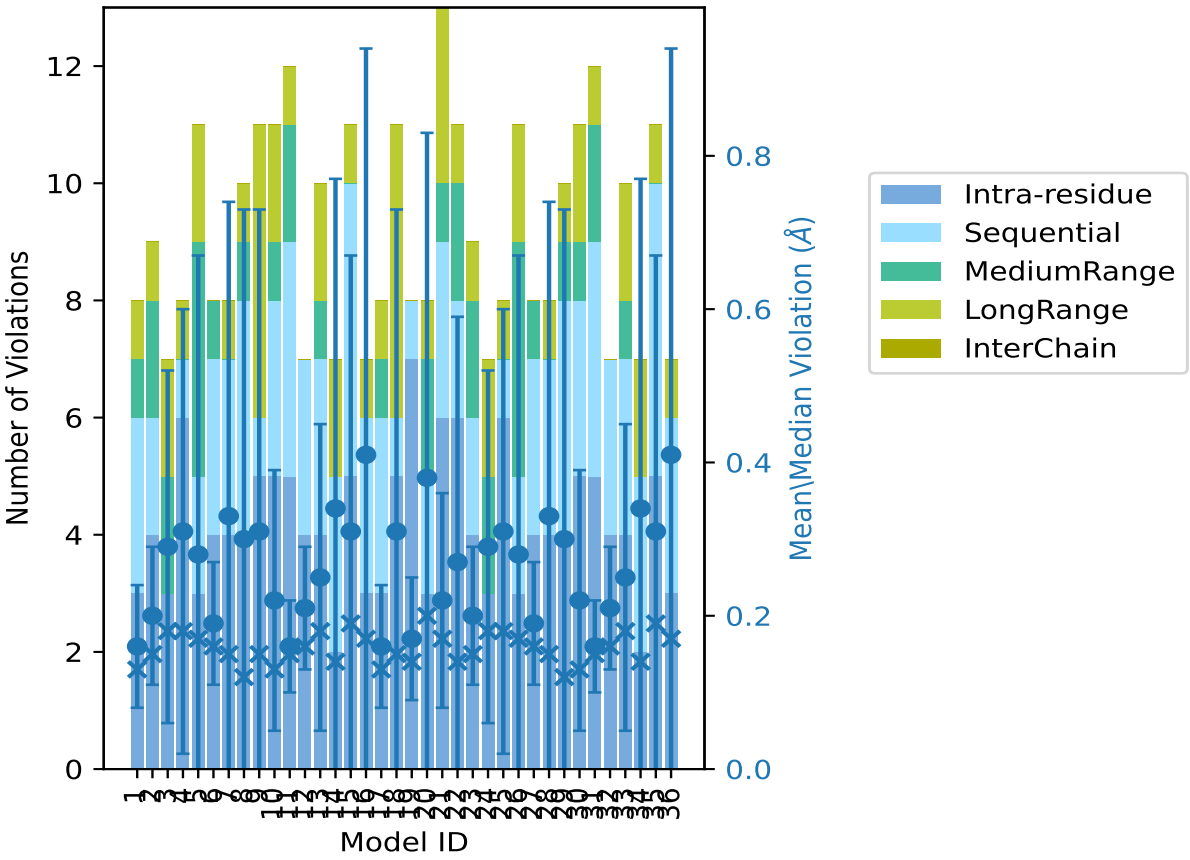
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	4	3	0	0	0	7	0.21	0.37	0.08	0.16
13	4	3	1	2	0	10	0.25	0.8	0.2	0.18
14	2	3	0	2	0	7	0.34	1.39	0.43	0.14
15	5	5	0	1	0	11	0.31	1.42	0.36	0.19
16	3	3	0	1	0	7	0.41	1.68	0.53	0.17
17	3	3	1	1	0	8	0.16	0.35	0.08	0.13
18	5	1	0	5	0	11	0.31	1.62	0.42	0.15
19	7	1	0	0	0	8	0.17	0.38	0.08	0.14
20	3	2	2	1	0	8	0.38	1.55	0.45	0.2
21	6	3	1	3	0	13	0.22	0.64	0.14	0.17
22	6	2	2	1	0	11	0.27	1.27	0.32	0.14
23	4	2	2	1	0	9	0.2	0.37	0.09	0.15
24	3	0	2	2	0	7	0.29	0.81	0.23	0.18
25	6	1	0	1	0	8	0.31	1.06	0.29	0.18
26	3	2	4	2	0	11	0.28	1.49	0.39	0.17
27	4	3	1	0	0	8	0.19	0.37	0.08	0.16
28	4	3	0	1	0	8	0.33	1.38	0.41	0.15
29	4	4	1	1	0	10	0.3	1.57	0.43	0.12
30	5	3	1	2	0	11	0.22	0.69	0.17	0.13
31	5	4	2	1	0	12	0.16	0.35	0.06	0.15
32	4	3	0	0	0	7	0.21	0.37	0.08	0.16
33	4	3	1	2	0	10	0.25	0.8	0.2	0.18
34	2	3	0	2	0	7	0.34	1.39	0.43	0.14
35	5	5	0	1	0	11	0.31	1.42	0.36	0.19
36	3	3	0	1	0	7	0.41	1.68	0.53	0.17

[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

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, 604(IR:285, SQ:175, MR:62, LR:82, 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]	%
3	0	0	0	0	3	1	2.8
4	9	1	5	0	19	2	5.6
4	1	1	1	0	7	3	8.3
4	2	0	1	0	7	4	11.1
1	1	0	0	0	2	5	13.9
0	0	2	0	0	2	6	16.7

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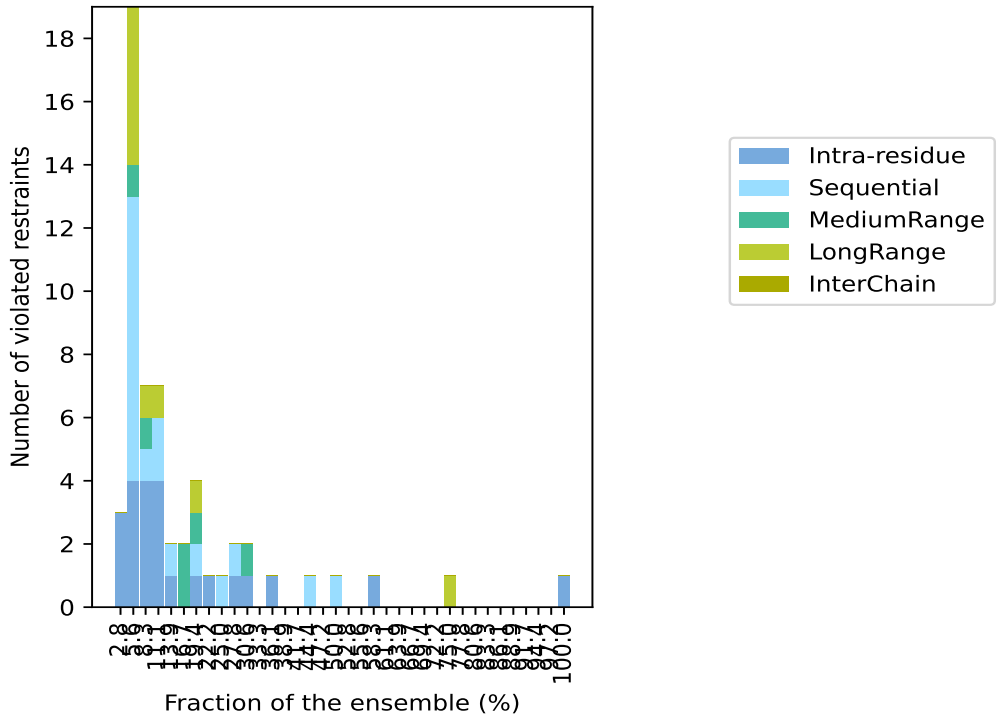
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	1	1	1	0	4	7	19.4
1	0	0	0	0	1	8	22.2
0	1	0	0	0	1	9	25.0
1	1	0	0	0	2	10	27.8
1	0	1	0	0	2	11	30.6
0	0	0	0	0	0	12	33.3
1	0	0	0	0	1	13	36.1
0	0	0	0	0	0	14	38.9
0	0	0	0	0	0	15	41.7
0	1	0	0	0	1	16	44.4
0	0	0	0	0	0	17	47.2
0	1	0	0	0	1	18	50.0
0	0	0	0	0	0	19	52.8
0	0	0	0	0	0	20	55.6
1	0	0	0	0	1	21	58.3
0	0	0	0	0	0	22	61.1
0	0	0	0	0	0	23	63.9
0	0	0	0	0	0	24	66.7
0	0	0	0	0	0	25	69.4
0	0	0	0	0	0	26	72.2
0	0	0	1	0	1	27	75.0
0	0	0	0	0	0	28	77.8
0	0	0	0	0	0	29	80.6
0	0	0	0	0	0	30	83.3
0	0	0	0	0	0	31	86.1
0	0	0	0	0	0	32	88.9
0	0	0	0	0	0	33	91.7
0	0	0	0	0	0	34	94.4
0	0	0	0	0	0	35	97.2
1	0	0	0	0	1	36	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

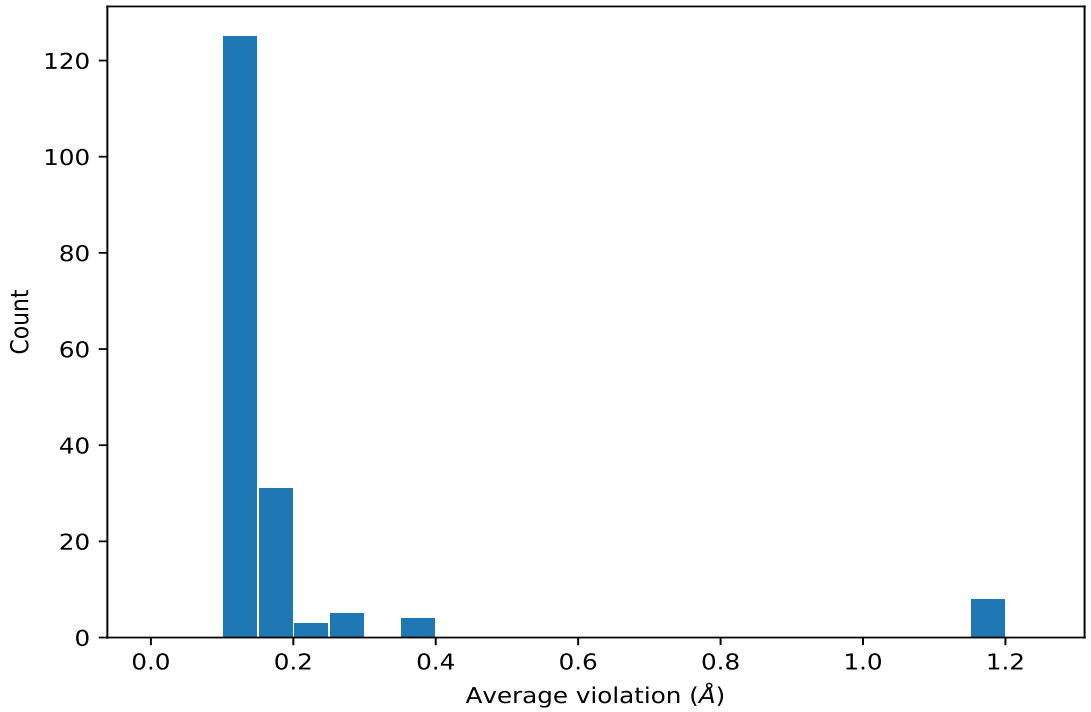
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (i)

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)
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	36	0.37	0.01	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	36	0.37	0.01	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	36	0.37	0.01	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	36	0.37	0.01	0.37
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	27	1.18	0.42	1.38
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	27	1.18	0.42	1.38
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	27	1.18	0.42	1.38
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	27	1.18	0.42	1.38
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	27	1.18	0.42	1.38
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	27	1.18	0.42	1.38
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	27	1.18	0.42	1.38
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	27	1.18	0.42	1.38
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	21	0.25	0.02	0.25
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	21	0.25	0.02	0.25
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	21	0.25	0.02	0.25
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	18	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	18	0.14	0.02	0.13
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	16	0.13	0.01	0.12
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	16	0.13	0.01	0.12
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	13	0.18	0.03	0.17
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	13	0.18	0.03	0.17
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE2	11	0.16	0.03	0.17
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE3	11	0.16	0.03	0.17
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE2	11	0.16	0.03	0.17
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE3	11	0.16	0.03	0.17
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD11	11	0.13	0.01	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD12	11	0.13	0.01	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD13	11	0.13	0.01	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD21	11	0.13	0.01	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD22	11	0.13	0.01	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD23	11	0.13	0.01	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD11	11	0.13	0.01	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD12	11	0.13	0.01	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD13	11	0.13	0.01	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD21	11	0.13	0.01	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD22	11	0.13	0.01	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD23	11	0.13	0.01	0.13
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD1	10	0.17	0.01	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD2	10	0.17	0.01	0.17
(1,310)	1:A:36:VAL:HB	1:A:37:VAL:H	10	0.14	0.04	0.11
(1,266)	1:A:30:LYS:HD2	1:A:31:TYR:H	9	0.17	0.04	0.17
(1,266)	1:A:30:LYS:HD3	1:A:31:TYR:H	9	0.17	0.04	0.17
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD2	8	0.16	0.03	0.16
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD3	8	0.16	0.03	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD11	7	0.15	0.02	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD12	7	0.15	0.02	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD13	7	0.15	0.02	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD21	7	0.15	0.02	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD22	7	0.15	0.02	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD23	7	0.15	0.02	0.16
(1,397)	1:A:43:ARG:HG2	1:A:45:GLN:H	7	0.15	0.02	0.15
(1,397)	1:A:43:ARG:HG3	1:A:45:GLN:H	7	0.15	0.02	0.15
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE1	7	0.15	0.03	0.17
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE2	7	0.15	0.03	0.17
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD11	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD12	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD13	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD21	7	0.12	0.01	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD22	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD23	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD11	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD12	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD13	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD21	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD22	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD23	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD11	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD12	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD13	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD21	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD22	7	0.12	0.01	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD23	7	0.12	0.01	0.11
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB2	6	0.13	0.03	0.12
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB3	6	0.13	0.03	0.12
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB2	6	0.13	0.03	0.12
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB3	6	0.13	0.03	0.12
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG2	6	0.13	0.02	0.12
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG3	6	0.13	0.02	0.12
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG2	6	0.13	0.02	0.12
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG3	6	0.13	0.02	0.12
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD11	5	0.17	0.06	0.14
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD12	5	0.17	0.06	0.14
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD13	5	0.17	0.06	0.14
(1,421)	1:A:45:GLN:HE21	1:A:46:TYR:HD1	5	0.16	0.04	0.15
(1,421)	1:A:45:GLN:HE21	1:A:46:TYR:HD2	5	0.16	0.04	0.15
(1,421)	1:A:45:GLN:HE22	1:A:46:TYR:HD1	5	0.16	0.04	0.15
(1,421)	1:A:45:GLN:HE22	1:A:46:TYR:HD2	5	0.16	0.04	0.15
(1,195)	1:A:25:ILE:HG12	1:A:25:ILE:H	4	0.26	0.02	0.26
(1,195)	1:A:25:ILE:HG13	1:A:25:ILE:H	4	0.26	0.02	0.26
(1,472)	1:A:50:LYS:HD2	1:A:50:LYS:H	4	0.15	0.0	0.15
(1,472)	1:A:50:LYS:HD3	1:A:50:LYS:H	4	0.15	0.0	0.15
(1,513)	1:A:53:GLU:H	1:A:54:LEU:H	4	0.15	0.03	0.15
(2,34)	1:A:18:HIS:H	1:A:45:GLN:HE21	4	0.14	0.03	0.14
(2,34)	1:A:18:HIS:H	1:A:45:GLN:HE22	4	0.14	0.03	0.14
(1,254)	1:A:30:LYS:HB2	1:A:30:LYS:H	4	0.13	0.01	0.13
(1,254)	1:A:30:LYS:HB3	1:A:30:LYS:H	4	0.13	0.01	0.13
(1,343)	1:A:39:TYR:H	1:A:40:ILE:HG12	4	0.12	0.01	0.12
(1,343)	1:A:39:TYR:H	1:A:40:ILE:HG13	4	0.12	0.01	0.12
(1,487)	1:A:51:TRP:HB2	1:A:51:TRP:HD1	4	0.12	0.01	0.12
(1,487)	1:A:51:TRP:HB3	1:A:51:TRP:HD1	4	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,419)	1:A:45:GLN:HB2	1:A:46:TYR:HD1	3	0.17	0.07	0.12
(1,419)	1:A:45:GLN:HB2	1:A:46:TYR:HD2	3	0.17	0.07	0.12
(1,419)	1:A:45:GLN:HB3	1:A:46:TYR:HD1	3	0.17	0.07	0.12
(1,419)	1:A:45:GLN:HB3	1:A:46:TYR:HD2	3	0.17	0.07	0.12
(1,26)	1:A:5:PHE:HA	1:A:5:PHE:HD1	3	0.16	0.0	0.16
(1,26)	1:A:5:PHE:HA	1:A:5:PHE:HD2	3	0.16	0.0	0.16
(1,189)	1:A:25:ILE:HB	1:A:25:ILE:H	3	0.15	0.0	0.15
(1,367)	1:A:40:ILE:HG12	1:A:46:TYR:HE1	3	0.14	0.0	0.14
(1,367)	1:A:40:ILE:HG12	1:A:46:TYR:HE2	3	0.14	0.0	0.14
(1,367)	1:A:40:ILE:HG13	1:A:46:TYR:HE1	3	0.14	0.0	0.14
(1,367)	1:A:40:ILE:HG13	1:A:46:TYR:HE2	3	0.14	0.0	0.14
(1,232)	1:A:28:LEU:HG	1:A:28:LEU:H	3	0.13	0.01	0.14
(2,121)	1:A:42:GLU:H	1:A:45:GLN:HE21	3	0.13	0.03	0.11
(2,121)	1:A:42:GLU:H	1:A:45:GLN:HE22	3	0.13	0.03	0.11
(1,9)	1:A:2:VAL:HA	1:A:2:VAL:H	3	0.11	0.0	0.11
(1,476)	1:A:50:LYS:HG2	1:A:50:LYS:H	2	0.23	0.0	0.23
(1,476)	1:A:50:LYS:HG3	1:A:50:LYS:H	2	0.23	0.0	0.23
(1,11)	1:A:2:VAL:HB	1:A:2:VAL:H	2	0.22	0.0	0.22
(1,260)	1:A:30:LYS:HG2	1:A:30:LYS:H	2	0.17	0.0	0.17
(1,260)	1:A:30:LYS:HG3	1:A:30:LYS:H	2	0.17	0.0	0.17
(1,422)	1:A:45:GLN:HE21	1:A:46:TYR:HE1	2	0.16	0.0	0.16
(1,422)	1:A:45:GLN:HE21	1:A:46:TYR:HE2	2	0.16	0.0	0.16
(1,422)	1:A:45:GLN:HE22	1:A:46:TYR:HE1	2	0.16	0.0	0.16
(1,422)	1:A:45:GLN:HE22	1:A:46:TYR:HE2	2	0.16	0.0	0.16
(1,158)	1:A:23:MET:HB2	1:A:24:TYR:H	2	0.15	0.0	0.15
(1,158)	1:A:23:MET:HB3	1:A:24:TYR:H	2	0.15	0.0	0.15
(1,315)	1:A:36:VAL:HG11	1:A:39:TYR:HE1	2	0.15	0.0	0.15
(1,315)	1:A:36:VAL:HG11	1:A:39:TYR:HE2	2	0.15	0.0	0.15
(1,315)	1:A:36:VAL:HG12	1:A:39:TYR:HE1	2	0.15	0.0	0.15
(1,315)	1:A:36:VAL:HG12	1:A:39:TYR:HE2	2	0.15	0.0	0.15
(1,315)	1:A:36:VAL:HG13	1:A:39:TYR:HE1	2	0.15	0.0	0.15
(1,315)	1:A:36:VAL:HG13	1:A:39:TYR:HE2	2	0.15	0.0	0.15
(1,315)	1:A:36:VAL:HG21	1:A:39:TYR:HE1	2	0.15	0.0	0.15
(1,315)	1:A:36:VAL:HG21	1:A:39:TYR:HE2	2	0.15	0.0	0.15
(1,315)	1:A:36:VAL:HG22	1:A:39:TYR:HE1	2	0.15	0.0	0.15
(1,315)	1:A:36:VAL:HG22	1:A:39:TYR:HE2	2	0.15	0.0	0.15
(1,315)	1:A:36:VAL:HG23	1:A:39:TYR:HE1	2	0.15	0.0	0.15
(1,315)	1:A:36:VAL:HG23	1:A:39:TYR:HE2	2	0.15	0.0	0.15
(1,65)	1:A:10:LEU:HB2	1:A:11:SER:H	2	0.14	0.0	0.14
(1,65)	1:A:10:LEU:HB3	1:A:11:SER:H	2	0.14	0.0	0.14
(1,331)	1:A:38:GLY:HA2	1:A:39:TYR:HD1	2	0.14	0.0	0.14
(1,331)	1:A:38:GLY:HA2	1:A:39:TYR:HD2	2	0.14	0.0	0.14

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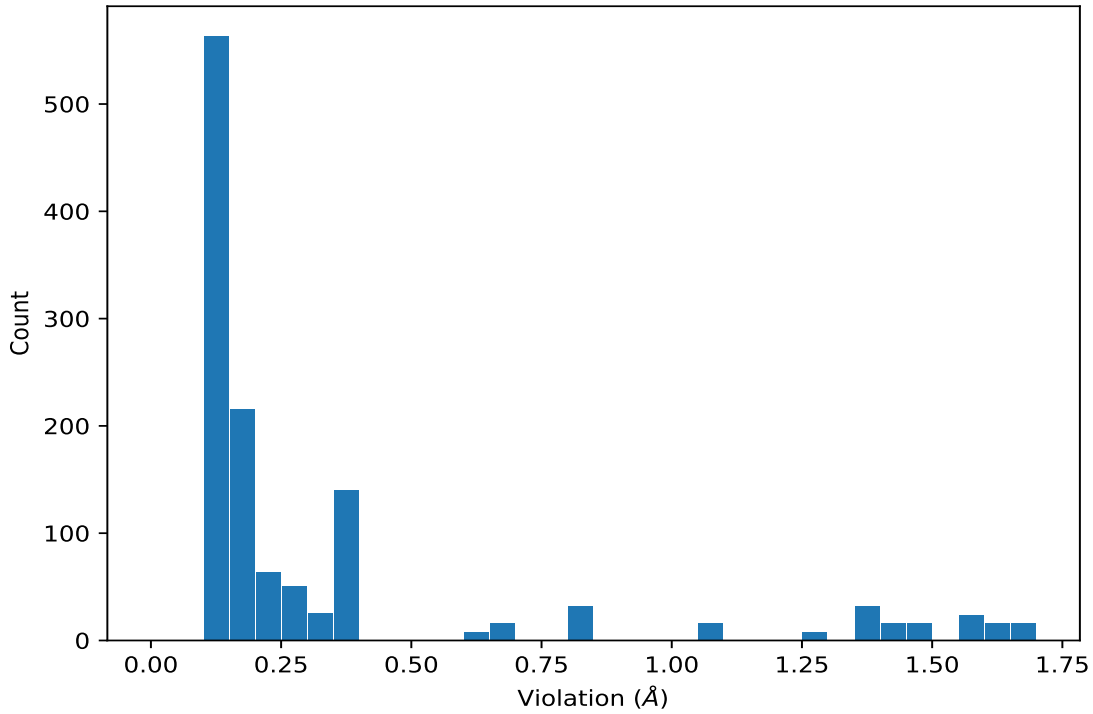
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,331)	1:A:38:GLY:HA3	1:A:39:TYR:HD1	2	0.14	0.0	0.14
(1,331)	1:A:38:GLY:HA3	1:A:39:TYR:HD2	2	0.14	0.0	0.14
(1,348)	1:A:39:TYR:HD1	1:A:48:ASP:H	2	0.14	0.0	0.14
(1,348)	1:A:39:TYR:HD2	1:A:48:ASP:H	2	0.14	0.0	0.14
(2,8)	1:A:6:ASN:HB2	1:A:24:TYR:HD1	2	0.14	0.0	0.14
(2,8)	1:A:6:ASN:HB2	1:A:24:TYR:HD2	2	0.14	0.0	0.14
(2,8)	1:A:6:ASN:HB3	1:A:24:TYR:HD1	2	0.14	0.0	0.14
(2,8)	1:A:6:ASN:HB3	1:A:24:TYR:HD2	2	0.14	0.0	0.14
(1,263)	1:A:30:LYS:HA	1:A:31:TYR:HD1	2	0.13	0.01	0.13
(1,263)	1:A:30:LYS:HA	1:A:31:TYR:HD2	2	0.13	0.01	0.13
(1,395)	1:A:43:ARG:H	1:A:44:CYS:H	2	0.13	0.0	0.13
(1,497)	1:A:51:TRP:HZ2	1:A:52:TRP:HE1	2	0.13	0.0	0.13
(1,106)	1:A:17:LEU:HD11	1:A:18:HIS:H	2	0.12	0.0	0.12
(1,106)	1:A:17:LEU:HD12	1:A:18:HIS:H	2	0.12	0.0	0.12
(1,106)	1:A:17:LEU:HD13	1:A:18:HIS:H	2	0.12	0.0	0.12
(1,106)	1:A:17:LEU:HD21	1:A:18:HIS:H	2	0.12	0.0	0.12
(1,106)	1:A:17:LEU:HD22	1:A:18:HIS:H	2	0.12	0.0	0.12
(1,106)	1:A:17:LEU:HD23	1:A:18:HIS:H	2	0.12	0.0	0.12
(1,51)	1:A:8:CYS:HA	1:A:9:PRO:HD2	2	0.11	0.0	0.11
(1,51)	1:A:8:CYS:HA	1:A:9:PRO:HD3	2	0.11	0.0	0.11
(1,339)	1:A:39:TYR:HD1	1:A:39:TYR:H	2	0.11	0.0	0.11
(1,339)	1:A:39:TYR:HD2	1:A:39:TYR:H	2	0.11	0.0	0.11
(1,366)	1:A:40:ILE:HG12	1:A:46:TYR:HD1	2	0.11	0.0	0.11
(1,366)	1:A:40:ILE:HG12	1:A:46:TYR:HD2	2	0.11	0.0	0.11
(1,366)	1:A:40:ILE:HG13	1:A:46:TYR:HD1	2	0.11	0.0	0.11
(1,366)	1:A:40:ILE:HG13	1:A:46:TYR:HD2	2	0.11	0.0	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD11	2	0.11	0.0	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD12	2	0.11	0.0	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD13	2	0.11	0.0	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD21	2	0.11	0.0	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD22	2	0.11	0.0	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD23	2	0.11	0.0	0.11
(2,30)	1:A:17:LEU:HA	1:A:45:GLN:HE21	2	0.11	0.0	0.11
(2,30)	1:A:17:LEU:HA	1:A:45:GLN:HE22	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)
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	16	1.68
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	16	1.68
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	16	1.68
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	16	1.68
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	16	1.68
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	16	1.68
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	16	1.68
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	16	1.68
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	36	1.68
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	36	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	36	1.68
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	36	1.68
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	36	1.68
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	36	1.68
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	36	1.68
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	36	1.68
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	9	1.62
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	9	1.62
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	9	1.62
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	9	1.62
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	9	1.62
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	9	1.62
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	9	1.62
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	9	1.62
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	18	1.62
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	18	1.62
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	18	1.62
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	18	1.62
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	18	1.62
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	18	1.62
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	18	1.62
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	18	1.62
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	8	1.57
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	8	1.57
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	8	1.57
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	8	1.57
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	8	1.57
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	8	1.57
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	8	1.57
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	8	1.57
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	29	1.57
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	29	1.57
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	29	1.57
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	29	1.57
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	29	1.57
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	29	1.57
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	29	1.57
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	29	1.57
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	20	1.55
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	20	1.55
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	20	1.55
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	20	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	20	1.55
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	20	1.55
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	20	1.55
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	20	1.55
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	5	1.49
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	5	1.49
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	5	1.49
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	5	1.49
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	5	1.49
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	5	1.49
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	5	1.49
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	5	1.49
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	26	1.49
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	26	1.49
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	26	1.49
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	26	1.49
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	26	1.49
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	26	1.49
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	26	1.49
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	26	1.49
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	15	1.42
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	15	1.42
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	15	1.42
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	15	1.42
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	15	1.42
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	15	1.42
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	15	1.42
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	15	1.42
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	35	1.42
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	35	1.42
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	35	1.42
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	35	1.42
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	35	1.42
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	35	1.42
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	35	1.42
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	35	1.42
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	14	1.39
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	14	1.39
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	14	1.39
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	14	1.39
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	14	1.39
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	14	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	14	1.39
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	14	1.39
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	34	1.39
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	34	1.39
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	34	1.39
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	34	1.39
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	34	1.39
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	34	1.39
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	34	1.39
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	34	1.39
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	7	1.38
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	7	1.38
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	7	1.38
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	7	1.38
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	7	1.38
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	7	1.38
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	7	1.38
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	7	1.38
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	28	1.38
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	28	1.38
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	28	1.38
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	28	1.38
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	28	1.38
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	28	1.38
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	28	1.38
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	28	1.38
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	22	1.27
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	22	1.27
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	22	1.27
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	22	1.27
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	22	1.27
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	22	1.27
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	22	1.27
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	22	1.27
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	4	1.06
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	4	1.06
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	4	1.06
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	4	1.06
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	4	1.06
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	4	1.06
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	4	1.06
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	4	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	25	1.06
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	25	1.06
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	25	1.06
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	25	1.06
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	25	1.06
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	25	1.06
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	25	1.06
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	25	1.06
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	3	0.81
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	3	0.81
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	3	0.81
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	3	0.81
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	3	0.81
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	3	0.81
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	3	0.81
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	3	0.81
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	24	0.81
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	24	0.81
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	24	0.81
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	24	0.81
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	24	0.81
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	24	0.81
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	24	0.81
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	24	0.81
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	13	0.8
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	13	0.8
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	13	0.8
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	13	0.8
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	13	0.8
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	13	0.8
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	13	0.8
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	13	0.8
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	33	0.8
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	33	0.8
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	33	0.8
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	33	0.8
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	33	0.8
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	33	0.8
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	33	0.8
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	33	0.8
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	10	0.69
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	10	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	10	0.69
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	10	0.69
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	10	0.69
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	10	0.69
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	10	0.69
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	10	0.69
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	30	0.69
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	30	0.69
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	30	0.69
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	30	0.69
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	30	0.69
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	30	0.69
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	30	0.69
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	30	0.69
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	21	0.64
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	21	0.64
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	21	0.64
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	21	0.64
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	21	0.64
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	21	0.64
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	21	0.64
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	21	0.64
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	7	0.39
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	7	0.39
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	7	0.39
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	7	0.39
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	28	0.39
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	28	0.39
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	28	0.39
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	28	0.39
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	3	0.38
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	3	0.38
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	3	0.38
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	3	0.38
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	16	0.38
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	16	0.38
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	16	0.38
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	16	0.38
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	19	0.38
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	19	0.38
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	19	0.38
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	24	0.38
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	24	0.38
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	24	0.38
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	24	0.38
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	36	0.38
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	36	0.38
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	36	0.38
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	36	0.38
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	2	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	2	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	2	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	2	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	4	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	4	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	4	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	4	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	6	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	6	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	6	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	6	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	8	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	8	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	8	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	8	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	12	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	12	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	12	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	12	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	13	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	13	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	13	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	13	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	15	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	15	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	15	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	15	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	23	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	23	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	23	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	23	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	25	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	25	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	25	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	25	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	27	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	27	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	27	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	27	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	29	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	29	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	29	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	29	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	32	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	32	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	32	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	32	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	33	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	33	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	33	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	33	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	35	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	35	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	35	0.37
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	35	0.37
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	5	0.36
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	5	0.36
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	5	0.36
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	5	0.36
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	9	0.36
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	9	0.36
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	9	0.36
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	9	0.36
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	18	0.36
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	18	0.36
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	18	0.36
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	18	0.36
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	20	0.36
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	20	0.36
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	20	0.36
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	20	0.36
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	21	0.36
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	21	0.36
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	21	0.36
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	21	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	26	0.36
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	26	0.36
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	26	0.36
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	26	0.36
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	1	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	1	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	1	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	1	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	10	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	10	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	10	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	10	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	11	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	11	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	11	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	11	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	14	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	14	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	14	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	14	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	17	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	17	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	17	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	17	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	30	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	30	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	30	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	30	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	31	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	31	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	31	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	31	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	34	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	34	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	34	0.35
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	34	0.35
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE1	22	0.34
(1,168)	1:A:24:TYR:HB2	1:A:24:TYR:HE2	22	0.34
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE1	22	0.34
(1,168)	1:A:24:TYR:HB3	1:A:24:TYR:HE2	22	0.34
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	2	0.31
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	2	0.31
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	2	0.31
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	2	0.31
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	2	0.31
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	2	0.31
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	2	0.31
(1,7)	1:A:1:VAL:HA	1:A:28:LEU:HA	23	0.31
(1,7)	1:A:1:VAL:HB	1:A:28:LEU:HA	23	0.31
(1,7)	1:A:1:VAL:HG11	1:A:28:LEU:HA	23	0.31
(1,7)	1:A:1:VAL:HG12	1:A:28:LEU:HA	23	0.31
(1,7)	1:A:1:VAL:HG13	1:A:28:LEU:HA	23	0.31
(1,7)	1:A:1:VAL:HG21	1:A:28:LEU:HA	23	0.31
(1,7)	1:A:1:VAL:HG22	1:A:28:LEU:HA	23	0.31
(1,7)	1:A:1:VAL:HG23	1:A:28:LEU:HA	23	0.31
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	15	0.3
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	15	0.3
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	15	0.3
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	35	0.3
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	35	0.3
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	35	0.3
(1,195)	1:A:25:ILE:HG12	1:A:25:ILE:H	10	0.28
(1,195)	1:A:25:ILE:HG13	1:A:25:ILE:H	10	0.28
(1,195)	1:A:25:ILE:HG12	1:A:25:ILE:H	30	0.28
(1,195)	1:A:25:ILE:HG13	1:A:25:ILE:H	30	0.28
(1,419)	1:A:45:GLN:HB2	1:A:46:TYR:HD1	20	0.26
(1,419)	1:A:45:GLN:HB2	1:A:46:TYR:HD2	20	0.26
(1,419)	1:A:45:GLN:HB3	1:A:46:TYR:HD1	20	0.26
(1,419)	1:A:45:GLN:HB3	1:A:46:TYR:HD2	20	0.26
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	4	0.26
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	4	0.26
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	4	0.26
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	12	0.26
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	12	0.26
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	12	0.26
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	13	0.26
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	13	0.26
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	13	0.26
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	16	0.26
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	16	0.26
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	16	0.26
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	25	0.26
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	25	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	25	0.26
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	32	0.26
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	32	0.26
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	32	0.26
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	33	0.26
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	33	0.26
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	33	0.26
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	36	0.26
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	36	0.26
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	36	0.26
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	3	0.25
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	3	0.25
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	3	0.25
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	22	0.25
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	22	0.25
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	22	0.25
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	24	0.25
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	24	0.25
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	24	0.25
(1,195)	1:A:25:ILE:HG12	1:A:25:ILE:H	8	0.25
(1,195)	1:A:25:ILE:HG13	1:A:25:ILE:H	8	0.25
(1,195)	1:A:25:ILE:HG12	1:A:25:ILE:H	29	0.25
(1,195)	1:A:25:ILE:HG13	1:A:25:ILE:H	29	0.25
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD11	12	0.25
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD12	12	0.25
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD13	12	0.25
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD11	32	0.25
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD12	32	0.25
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD13	32	0.25
(1,421)	1:A:45:GLN:HE21	1:A:46:TYR:HD1	21	0.24
(1,421)	1:A:45:GLN:HE21	1:A:46:TYR:HD2	21	0.24
(1,421)	1:A:45:GLN:HE22	1:A:46:TYR:HD1	21	0.24
(1,421)	1:A:45:GLN:HE22	1:A:46:TYR:HD2	21	0.24
(1,266)	1:A:30:LYS:HD2	1:A:31:TYR:H	21	0.24
(1,266)	1:A:30:LYS:HD3	1:A:31:TYR:H	21	0.24
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	2	0.24
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	2	0.24
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	2	0.24
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	21	0.24
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	21	0.24
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	21	0.24
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	23	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	23	0.24
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	23	0.24
(1,476)	1:A:50:LYS:HG2	1:A:50:LYS:H	2	0.23
(1,476)	1:A:50:LYS:HG3	1:A:50:LYS:H	2	0.23
(1,476)	1:A:50:LYS:HG2	1:A:50:LYS:H	23	0.23
(1,476)	1:A:50:LYS:HG3	1:A:50:LYS:H	23	0.23
(1,471)	1:A:50:LYS:HD2	1:A:50:LYS:HA	22	0.23
(1,471)	1:A:50:LYS:HD3	1:A:50:LYS:HA	22	0.23
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	1	0.23
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	1	0.23
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	1	0.23
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	9	0.23
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	9	0.23
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	9	0.23
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	17	0.23
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	17	0.23
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	17	0.23
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	18	0.23
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	18	0.23
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	18	0.23
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	9	0.22
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	9	0.22
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	18	0.22
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	18	0.22
(1,11)	1:A:2:VAL:HB	1:A:2:VAL:H	6	0.22
(1,11)	1:A:2:VAL:HB	1:A:2:VAL:H	27	0.22
(1,310)	1:A:36:VAL:HB	1:A:37:VAL:H	15	0.21
(1,310)	1:A:36:VAL:HB	1:A:37:VAL:H	35	0.21
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	6	0.21
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	6	0.21
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	27	0.21
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	27	0.21
(1,198)	1:A:25:ILE:HG21	1:A:25:ILE:H	20	0.21
(1,198)	1:A:25:ILE:HG22	1:A:25:ILE:H	20	0.21
(1,198)	1:A:25:ILE:HG23	1:A:25:ILE:H	20	0.21
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE2	11	0.2
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE3	11	0.2
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE2	11	0.2
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE3	11	0.2
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE2	31	0.2
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE3	31	0.2
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE2	31	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE3	31	0.2
(1,266)	1:A:30:LYS:HD2	1:A:31:TYR:H	4	0.2
(1,266)	1:A:30:LYS:HD3	1:A:31:TYR:H	4	0.2
(1,266)	1:A:30:LYS:HD2	1:A:31:TYR:H	25	0.2
(1,266)	1:A:30:LYS:HD3	1:A:31:TYR:H	25	0.2
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	7	0.2
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	7	0.2
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	28	0.2
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	28	0.2
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE1	13	0.19
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE2	13	0.19
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE1	33	0.19
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE2	33	0.19
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE2	15	0.19
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE3	15	0.19
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE2	15	0.19
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE3	15	0.19
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE2	35	0.19
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE3	35	0.19
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE2	35	0.19
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE3	35	0.19
(1,397)	1:A:43:ARG:HG2	1:A:45:GLN:H	13	0.19
(1,397)	1:A:43:ARG:HG3	1:A:45:GLN:H	13	0.19
(1,397)	1:A:43:ARG:HG2	1:A:45:GLN:H	33	0.19
(1,397)	1:A:43:ARG:HG3	1:A:45:GLN:H	33	0.19
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD2	15	0.19
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD3	15	0.19
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD2	35	0.19
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD3	35	0.19
(2,34)	1:A:18:HIS:H	1:A:45:GLN:HE21	9	0.18
(2,34)	1:A:18:HIS:H	1:A:45:GLN:HE22	9	0.18
(2,34)	1:A:18:HIS:H	1:A:45:GLN:HE21	18	0.18
(2,34)	1:A:18:HIS:H	1:A:45:GLN:HE22	18	0.18
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	14	0.18
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	14	0.18
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	20	0.18
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	20	0.18
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	34	0.18
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	34	0.18
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD1	10	0.18
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD2	10	0.18
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD1	30	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD2	30	0.18
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD2	3	0.18
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD3	3	0.18
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD2	24	0.18
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD3	24	0.18
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE1	5	0.17
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE2	5	0.17
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE1	26	0.17
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE2	26	0.17
(2,121)	1:A:42:GLU:H	1:A:45:GLN:HE21	20	0.17
(2,121)	1:A:42:GLU:H	1:A:45:GLN:HE22	20	0.17
(1,513)	1:A:53:GLU:H	1:A:54:LEU:H	11	0.17
(1,513)	1:A:53:GLU:H	1:A:54:LEU:H	31	0.17
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE2	5	0.17
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE3	5	0.17
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE2	5	0.17
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE3	5	0.17
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE2	26	0.17
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE3	26	0.17
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE2	26	0.17
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE3	26	0.17
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB2	6	0.17
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB3	6	0.17
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB2	6	0.17
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB3	6	0.17
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB2	27	0.17
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB3	27	0.17
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB2	27	0.17
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB3	27	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD1	4	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD2	4	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD1	5	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD2	5	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD1	13	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD2	13	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD1	21	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD2	21	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD1	25	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD2	25	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD1	26	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD2	26	0.17
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD1	33	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD2	33	0.17
(1,266)	1:A:30:LYS:HD2	1:A:31:TYR:H	5	0.17
(1,266)	1:A:30:LYS:HD3	1:A:31:TYR:H	5	0.17
(1,266)	1:A:30:LYS:HD2	1:A:31:TYR:H	26	0.17
(1,266)	1:A:30:LYS:HD3	1:A:31:TYR:H	26	0.17
(1,260)	1:A:30:LYS:HG2	1:A:30:LYS:H	4	0.17
(1,260)	1:A:30:LYS:HG3	1:A:30:LYS:H	4	0.17
(1,260)	1:A:30:LYS:HG2	1:A:30:LYS:H	25	0.17
(1,260)	1:A:30:LYS:HG3	1:A:30:LYS:H	25	0.17
(1,26)	1:A:5:PHE:HA	1:A:5:PHE:HD1	21	0.17
(1,26)	1:A:5:PHE:HA	1:A:5:PHE:HD2	21	0.17
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	16	0.17
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	16	0.17
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	19	0.17
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	19	0.17
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	36	0.17
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	36	0.17
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD11	11	0.17
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD12	11	0.17
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD13	11	0.17
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD21	11	0.17
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD22	11	0.17
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD23	11	0.17
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD11	31	0.17
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD12	31	0.17
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD13	31	0.17
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD21	31	0.17
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD22	31	0.17
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD23	31	0.17
(1,82)	1:A:15:TYR:HA	1:A:15:TYR:HD1	19	0.16
(1,82)	1:A:15:TYR:HA	1:A:15:TYR:HD2	19	0.16
(1,422)	1:A:45:GLN:HE21	1:A:46:TYR:HE1	16	0.16
(1,422)	1:A:45:GLN:HE21	1:A:46:TYR:HE2	16	0.16
(1,422)	1:A:45:GLN:HE22	1:A:46:TYR:HE1	16	0.16
(1,422)	1:A:45:GLN:HE22	1:A:46:TYR:HE2	16	0.16
(1,422)	1:A:45:GLN:HE21	1:A:46:TYR:HE1	36	0.16
(1,422)	1:A:45:GLN:HE21	1:A:46:TYR:HE2	36	0.16
(1,422)	1:A:45:GLN:HE22	1:A:46:TYR:HE1	36	0.16
(1,422)	1:A:45:GLN:HE22	1:A:46:TYR:HE2	36	0.16
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG2	3	0.16
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG3	3	0.16
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG2	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG3	3	0.16
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG2	24	0.16
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG3	24	0.16
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG2	24	0.16
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG3	24	0.16
(1,26)	1:A:5:PHE:HA	1:A:5:PHE:HD1	10	0.16
(1,26)	1:A:5:PHE:HA	1:A:5:PHE:HD2	10	0.16
(1,26)	1:A:5:PHE:HA	1:A:5:PHE:HD1	30	0.16
(1,26)	1:A:5:PHE:HA	1:A:5:PHE:HD2	30	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD11	12	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD12	12	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD13	12	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD21	12	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD22	12	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD23	12	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD11	22	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD12	22	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD13	22	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD21	22	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD22	22	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD23	22	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD11	32	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD12	32	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD13	32	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD21	32	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD22	32	0.16
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD23	32	0.16
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	15	0.15
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	15	0.15
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	35	0.15
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	35	0.15
(1,472)	1:A:50:LYS:HD2	1:A:50:LYS:H	2	0.15
(1,472)	1:A:50:LYS:HD3	1:A:50:LYS:H	2	0.15
(1,472)	1:A:50:LYS:HD2	1:A:50:LYS:H	9	0.15
(1,472)	1:A:50:LYS:HD3	1:A:50:LYS:H	9	0.15
(1,472)	1:A:50:LYS:HD2	1:A:50:LYS:H	18	0.15
(1,472)	1:A:50:LYS:HD3	1:A:50:LYS:H	18	0.15
(1,472)	1:A:50:LYS:HD2	1:A:50:LYS:H	23	0.15
(1,472)	1:A:50:LYS:HD3	1:A:50:LYS:H	23	0.15
(1,421)	1:A:45:GLN:HE21	1:A:46:TYR:HD1	13	0.15
(1,421)	1:A:45:GLN:HE21	1:A:46:TYR:HD2	13	0.15
(1,421)	1:A:45:GLN:HE22	1:A:46:TYR:HD1	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,421)	1:A:45:GLN:HE22	1:A:46:TYR:HD2	13	0.15
(1,421)	1:A:45:GLN:HE21	1:A:46:TYR:HD1	33	0.15
(1,421)	1:A:45:GLN:HE21	1:A:46:TYR:HD2	33	0.15
(1,421)	1:A:45:GLN:HE22	1:A:46:TYR:HD1	33	0.15
(1,421)	1:A:45:GLN:HE22	1:A:46:TYR:HD2	33	0.15
(1,397)	1:A:43:ARG:HG2	1:A:45:GLN:H	11	0.15
(1,397)	1:A:43:ARG:HG3	1:A:45:GLN:H	11	0.15
(1,397)	1:A:43:ARG:HG2	1:A:45:GLN:H	31	0.15
(1,397)	1:A:43:ARG:HG3	1:A:45:GLN:H	31	0.15
(1,315)	1:A:36:VAL:HG11	1:A:39:TYR:HE1	11	0.15
(1,315)	1:A:36:VAL:HG11	1:A:39:TYR:HE2	11	0.15
(1,315)	1:A:36:VAL:HG12	1:A:39:TYR:HE1	11	0.15
(1,315)	1:A:36:VAL:HG12	1:A:39:TYR:HE2	11	0.15
(1,315)	1:A:36:VAL:HG13	1:A:39:TYR:HE1	11	0.15
(1,315)	1:A:36:VAL:HG13	1:A:39:TYR:HE2	11	0.15
(1,315)	1:A:36:VAL:HG21	1:A:39:TYR:HE1	11	0.15
(1,315)	1:A:36:VAL:HG21	1:A:39:TYR:HE2	11	0.15
(1,315)	1:A:36:VAL:HG22	1:A:39:TYR:HE1	11	0.15
(1,315)	1:A:36:VAL:HG22	1:A:39:TYR:HE2	11	0.15
(1,315)	1:A:36:VAL:HG23	1:A:39:TYR:HE1	11	0.15
(1,315)	1:A:36:VAL:HG23	1:A:39:TYR:HE2	11	0.15
(1,315)	1:A:36:VAL:HG11	1:A:39:TYR:HE1	31	0.15
(1,315)	1:A:36:VAL:HG11	1:A:39:TYR:HE2	31	0.15
(1,315)	1:A:36:VAL:HG12	1:A:39:TYR:HE1	31	0.15
(1,315)	1:A:36:VAL:HG12	1:A:39:TYR:HE2	31	0.15
(1,315)	1:A:36:VAL:HG13	1:A:39:TYR:HE1	31	0.15
(1,315)	1:A:36:VAL:HG13	1:A:39:TYR:HE2	31	0.15
(1,315)	1:A:36:VAL:HG21	1:A:39:TYR:HE1	31	0.15
(1,315)	1:A:36:VAL:HG21	1:A:39:TYR:HE2	31	0.15
(1,315)	1:A:36:VAL:HG22	1:A:39:TYR:HE1	31	0.15
(1,315)	1:A:36:VAL:HG22	1:A:39:TYR:HE2	31	0.15
(1,315)	1:A:36:VAL:HG23	1:A:39:TYR:HE1	31	0.15
(1,315)	1:A:36:VAL:HG23	1:A:39:TYR:HE2	31	0.15
(1,310)	1:A:36:VAL:HB	1:A:37:VAL:H	6	0.15
(1,310)	1:A:36:VAL:HB	1:A:37:VAL:H	27	0.15
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	12	0.15
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	12	0.15
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	15	0.15
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	15	0.15
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	32	0.15
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	32	0.15
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	35	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	35	0.15
(1,266)	1:A:30:LYS:HD2	1:A:31:TYR:H	12	0.15
(1,266)	1:A:30:LYS:HD3	1:A:31:TYR:H	12	0.15
(1,266)	1:A:30:LYS:HD2	1:A:31:TYR:H	32	0.15
(1,266)	1:A:30:LYS:HD3	1:A:31:TYR:H	32	0.15
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	11	0.15
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	11	0.15
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	31	0.15
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	31	0.15
(1,189)	1:A:25:ILE:HB	1:A:25:ILE:H	7	0.15
(1,189)	1:A:25:ILE:HB	1:A:25:ILE:H	28	0.15
(1,158)	1:A:23:MET:HB2	1:A:24:TYR:H	12	0.15
(1,158)	1:A:23:MET:HB3	1:A:24:TYR:H	12	0.15
(1,158)	1:A:23:MET:HB2	1:A:24:TYR:H	32	0.15
(1,158)	1:A:23:MET:HB3	1:A:24:TYR:H	32	0.15
(2,8)	1:A:6:ASN:HB2	1:A:24:TYR:HD1	9	0.14
(2,8)	1:A:6:ASN:HB2	1:A:24:TYR:HD2	9	0.14
(2,8)	1:A:6:ASN:HB3	1:A:24:TYR:HD1	9	0.14
(2,8)	1:A:6:ASN:HB3	1:A:24:TYR:HD2	9	0.14
(2,8)	1:A:6:ASN:HB2	1:A:24:TYR:HD1	18	0.14
(2,8)	1:A:6:ASN:HB2	1:A:24:TYR:HD2	18	0.14
(2,8)	1:A:6:ASN:HB3	1:A:24:TYR:HD1	18	0.14
(2,8)	1:A:6:ASN:HB3	1:A:24:TYR:HD2	18	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD11	5	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD12	5	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD13	5	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD21	5	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD22	5	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD23	5	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD11	5	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD12	5	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD13	5	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD21	5	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD22	5	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD23	5	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD11	20	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD12	20	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD13	20	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD21	20	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD22	20	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD23	20	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD11	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD12	20	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD13	20	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD21	20	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD22	20	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD23	20	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD11	21	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD12	21	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD13	21	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD21	21	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD22	21	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD23	21	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD11	21	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD12	21	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD13	21	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD21	21	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD22	21	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD23	21	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD11	26	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD12	26	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD13	26	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD21	26	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD22	26	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD23	26	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD11	26	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD12	26	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD13	26	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD21	26	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD22	26	0.14
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD23	26	0.14
(1,65)	1:A:10:LEU:HB2	1:A:11:SER:H	8	0.14
(1,65)	1:A:10:LEU:HB3	1:A:11:SER:H	8	0.14
(1,65)	1:A:10:LEU:HB2	1:A:11:SER:H	29	0.14
(1,65)	1:A:10:LEU:HB3	1:A:11:SER:H	29	0.14
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	1	0.14
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	1	0.14
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	7	0.14
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	7	0.14
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	17	0.14
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	17	0.14
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	28	0.14
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	28	0.14
(1,397)	1:A:43:ARG:HG2	1:A:45:GLN:H	22	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:A:43:ARG:HG3	1:A:45:GLN:H	22	0.14
(1,367)	1:A:40:ILE:HG12	1:A:46:TYR:HE1	9	0.14
(1,367)	1:A:40:ILE:HG12	1:A:46:TYR:HE2	9	0.14
(1,367)	1:A:40:ILE:HG13	1:A:46:TYR:HE1	9	0.14
(1,367)	1:A:40:ILE:HG13	1:A:46:TYR:HE2	9	0.14
(1,367)	1:A:40:ILE:HG12	1:A:46:TYR:HE1	18	0.14
(1,367)	1:A:40:ILE:HG12	1:A:46:TYR:HE2	18	0.14
(1,367)	1:A:40:ILE:HG13	1:A:46:TYR:HE1	18	0.14
(1,367)	1:A:40:ILE:HG13	1:A:46:TYR:HE2	18	0.14
(1,348)	1:A:39:TYR:HD1	1:A:48:ASP:H	11	0.14
(1,348)	1:A:39:TYR:HD2	1:A:48:ASP:H	11	0.14
(1,348)	1:A:39:TYR:HD1	1:A:48:ASP:H	31	0.14
(1,348)	1:A:39:TYR:HD2	1:A:48:ASP:H	31	0.14
(1,331)	1:A:38:GLY:HA2	1:A:39:TYR:HD1	11	0.14
(1,331)	1:A:38:GLY:HA2	1:A:39:TYR:HD2	11	0.14
(1,331)	1:A:38:GLY:HA3	1:A:39:TYR:HD1	11	0.14
(1,331)	1:A:38:GLY:HA3	1:A:39:TYR:HD2	11	0.14
(1,331)	1:A:38:GLY:HA2	1:A:39:TYR:HD1	31	0.14
(1,331)	1:A:38:GLY:HA2	1:A:39:TYR:HD2	31	0.14
(1,331)	1:A:38:GLY:HA3	1:A:39:TYR:HD1	31	0.14
(1,331)	1:A:38:GLY:HA3	1:A:39:TYR:HD2	31	0.14
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD1	19	0.14
(1,270)	1:A:31:TYR:HA	1:A:31:TYR:HD2	19	0.14
(1,263)	1:A:30:LYS:HA	1:A:31:TYR:HD1	19	0.14
(1,263)	1:A:30:LYS:HA	1:A:31:TYR:HD2	19	0.14
(1,254)	1:A:30:LYS:HB2	1:A:30:LYS:H	15	0.14
(1,254)	1:A:30:LYS:HB3	1:A:30:LYS:H	15	0.14
(1,254)	1:A:30:LYS:HB2	1:A:30:LYS:H	35	0.14
(1,254)	1:A:30:LYS:HB3	1:A:30:LYS:H	35	0.14
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD2	14	0.14
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD3	14	0.14
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD2	34	0.14
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD3	34	0.14
(1,232)	1:A:28:LEU:HG	1:A:28:LEU:H	6	0.14
(1,232)	1:A:28:LEU:HG	1:A:28:LEU:H	27	0.14
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD11	21	0.14
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD12	21	0.14
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD13	21	0.14
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD21	21	0.14
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD22	21	0.14
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD23	21	0.14
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD11	21	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD12	21	0.14
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD13	21	0.14
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD21	21	0.14
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD22	21	0.14
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD23	21	0.14
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD11	21	0.14
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD12	21	0.14
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD13	21	0.14
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD21	21	0.14
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD22	21	0.14
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD23	21	0.14
(1,189)	1:A:25:ILE:HB	1:A:25:ILE:H	19	0.14
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD11	19	0.14
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD12	19	0.14
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD13	19	0.14
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD11	2	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD12	2	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD13	2	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD21	2	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD22	2	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD23	2	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD11	2	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD12	2	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD13	2	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD21	2	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD22	2	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD23	2	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD11	10	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD12	10	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD13	10	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD21	10	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD22	10	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD23	10	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD11	10	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD12	10	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD13	10	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD21	10	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD22	10	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD23	10	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD11	22	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD12	22	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD13	22	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD21	22	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD22	22	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD23	22	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD11	22	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD12	22	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD13	22	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD21	22	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD22	22	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD23	22	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD11	23	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD12	23	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD13	23	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD21	23	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD22	23	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD23	23	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD11	23	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD12	23	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD13	23	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD21	23	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD22	23	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD23	23	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD11	30	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD12	30	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD13	30	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD21	30	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD22	30	0.13
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD23	30	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD11	30	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD12	30	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD13	30	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD21	30	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD22	30	0.13
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD23	30	0.13
(1,497)	1:A:51:TRP:HZ2	1:A:52:TRP:HE1	13	0.13
(1,497)	1:A:51:TRP:HZ2	1:A:52:TRP:HE1	33	0.13
(1,487)	1:A:51:TRP:HB2	1:A:51:TRP:HD1	13	0.13
(1,487)	1:A:51:TRP:HB3	1:A:51:TRP:HD1	13	0.13
(1,487)	1:A:51:TRP:HB2	1:A:51:TRP:HD1	33	0.13
(1,487)	1:A:51:TRP:HB3	1:A:51:TRP:HD1	33	0.13
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE2	8	0.13
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE3	8	0.13
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE2	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE3	8	0.13
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE2	10	0.13
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE3	10	0.13
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE2	10	0.13
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE3	10	0.13
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE2	29	0.13
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE3	29	0.13
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE2	29	0.13
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE3	29	0.13
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE2	30	0.13
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE3	30	0.13
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE2	30	0.13
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE3	30	0.13
(1,397)	1:A:43:ARG:HG2	1:A:45:GLN:H	1	0.13
(1,397)	1:A:43:ARG:HG3	1:A:45:GLN:H	1	0.13
(1,397)	1:A:43:ARG:HG2	1:A:45:GLN:H	17	0.13
(1,397)	1:A:43:ARG:HG3	1:A:45:GLN:H	17	0.13
(1,395)	1:A:43:ARG:H	1:A:44:CYS:H	11	0.13
(1,395)	1:A:43:ARG:H	1:A:44:CYS:H	31	0.13
(1,367)	1:A:40:ILE:HG12	1:A:46:TYR:HE1	21	0.13
(1,367)	1:A:40:ILE:HG12	1:A:46:TYR:HE2	21	0.13
(1,367)	1:A:40:ILE:HG13	1:A:46:TYR:HE1	21	0.13
(1,367)	1:A:40:ILE:HG13	1:A:46:TYR:HE2	21	0.13
(1,343)	1:A:39:TYR:H	1:A:40:ILE:HG12	7	0.13
(1,343)	1:A:39:TYR:H	1:A:40:ILE:HG13	7	0.13
(1,343)	1:A:39:TYR:H	1:A:40:ILE:HG12	28	0.13
(1,343)	1:A:39:TYR:H	1:A:40:ILE:HG13	28	0.13
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	1	0.13
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	1	0.13
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	6	0.13
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	6	0.13
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	17	0.13
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	17	0.13
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	27	0.13
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	27	0.13
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	20	0.13
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	20	0.13
(1,256)	1:A:30:LYS:HD2	1:A:30:LYS:H	22	0.13
(1,256)	1:A:30:LYS:HD3	1:A:30:LYS:H	22	0.13
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD11	9	0.13
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD12	9	0.13
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD13	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD21	9	0.13
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD22	9	0.13
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD23	9	0.13
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD11	18	0.13
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD12	18	0.13
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD13	18	0.13
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD21	18	0.13
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD22	18	0.13
(1,231)	1:A:28:LEU:HA	1:A:28:LEU:HD23	18	0.13
(1,133)	1:A:21:VAL:HA	1:A:21:VAL:H	21	0.13
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE1	10	0.12
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE2	10	0.12
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE1	21	0.12
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE2	21	0.12
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE1	30	0.12
(2,64)	1:A:24:TYR:H	1:A:31:TYR:HE2	30	0.12
(1,9)	1:A:2:VAL:HA	1:A:2:VAL:H	21	0.12
(1,513)	1:A:53:GLU:H	1:A:54:LEU:H	10	0.12
(1,513)	1:A:53:GLU:H	1:A:54:LEU:H	30	0.12
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	2	0.12
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	2	0.12
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	6	0.12
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	6	0.12
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	9	0.12
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	9	0.12
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	18	0.12
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	18	0.12
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	22	0.12
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	22	0.12
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	23	0.12
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	23	0.12
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	27	0.12
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	27	0.12
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE2	19	0.12
(1,469)	1:A:50:LYS:HB2	1:A:50:LYS:HE3	19	0.12
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE2	19	0.12
(1,469)	1:A:50:LYS:HB3	1:A:50:LYS:HE3	19	0.12
(1,421)	1:A:45:GLN:HE21	1:A:46:TYR:HD1	16	0.12
(1,421)	1:A:45:GLN:HE21	1:A:46:TYR:HD2	16	0.12
(1,421)	1:A:45:GLN:HE22	1:A:46:TYR:HD1	16	0.12
(1,421)	1:A:45:GLN:HE22	1:A:46:TYR:HD2	16	0.12
(1,421)	1:A:45:GLN:HE21	1:A:46:TYR:HD1	36	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,421)	1:A:45:GLN:HE21	1:A:46:TYR:HD2	36	0.12
(1,421)	1:A:45:GLN:HE22	1:A:46:TYR:HD1	36	0.12
(1,421)	1:A:45:GLN:HE22	1:A:46:TYR:HD2	36	0.12
(1,419)	1:A:45:GLN:HB2	1:A:46:TYR:HD1	8	0.12
(1,419)	1:A:45:GLN:HB2	1:A:46:TYR:HD2	8	0.12
(1,419)	1:A:45:GLN:HB3	1:A:46:TYR:HD1	8	0.12
(1,419)	1:A:45:GLN:HB3	1:A:46:TYR:HD2	8	0.12
(1,419)	1:A:45:GLN:HB2	1:A:46:TYR:HD1	29	0.12
(1,419)	1:A:45:GLN:HB2	1:A:46:TYR:HD2	29	0.12
(1,419)	1:A:45:GLN:HB3	1:A:46:TYR:HD1	29	0.12
(1,419)	1:A:45:GLN:HB3	1:A:46:TYR:HD2	29	0.12
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG2	2	0.12
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG3	2	0.12
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG2	2	0.12
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG3	2	0.12
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG2	5	0.12
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG3	5	0.12
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG2	5	0.12
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG3	5	0.12
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG2	23	0.12
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG3	23	0.12
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG2	23	0.12
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG3	23	0.12
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG2	26	0.12
(1,400)	1:A:43:ARG:HG2	1:A:45:GLN:HG3	26	0.12
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG2	26	0.12
(1,400)	1:A:43:ARG:HG3	1:A:45:GLN:HG3	26	0.12
(1,343)	1:A:39:TYR:H	1:A:40:ILE:HG12	15	0.12
(1,343)	1:A:39:TYR:H	1:A:40:ILE:HG13	15	0.12
(1,343)	1:A:39:TYR:H	1:A:40:ILE:HG12	35	0.12
(1,343)	1:A:39:TYR:H	1:A:40:ILE:HG13	35	0.12
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB2	8	0.12
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB3	8	0.12
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB2	8	0.12
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB3	8	0.12
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB2	29	0.12
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB3	29	0.12
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB2	29	0.12
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB3	29	0.12
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	8	0.12
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	8	0.12
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	11	0.12
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	14	0.12
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	14	0.12
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	29	0.12
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	29	0.12
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	31	0.12
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	31	0.12
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	34	0.12
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	34	0.12
(1,263)	1:A:30:LYS:HA	1:A:31:TYR:HD1	22	0.12
(1,263)	1:A:30:LYS:HA	1:A:31:TYR:HD2	22	0.12
(1,254)	1:A:30:LYS:HB2	1:A:30:LYS:H	4	0.12
(1,254)	1:A:30:LYS:HB3	1:A:30:LYS:H	4	0.12
(1,254)	1:A:30:LYS:HB2	1:A:30:LYS:H	25	0.12
(1,254)	1:A:30:LYS:HB3	1:A:30:LYS:H	25	0.12
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD2	4	0.12
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD3	4	0.12
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD2	25	0.12
(1,252)	1:A:30:LYS:HA	1:A:30:LYS:HD3	25	0.12
(1,232)	1:A:28:LEU:HG	1:A:28:LEU:H	22	0.12
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD11	15	0.12
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD12	15	0.12
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD13	15	0.12
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD21	15	0.12
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD22	15	0.12
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD23	15	0.12
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD11	15	0.12
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD12	15	0.12
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD13	15	0.12
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD21	15	0.12
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD22	15	0.12
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD23	15	0.12
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD11	15	0.12
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD12	15	0.12
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD13	15	0.12
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD21	15	0.12
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD22	15	0.12
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD23	15	0.12
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD11	35	0.12
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD12	35	0.12
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD13	35	0.12
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD21	35	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD22	35	0.12
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD23	35	0.12
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD11	35	0.12
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD12	35	0.12
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD13	35	0.12
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD21	35	0.12
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD22	35	0.12
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD23	35	0.12
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD11	35	0.12
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD12	35	0.12
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD13	35	0.12
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD21	35	0.12
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD22	35	0.12
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD23	35	0.12
(1,106)	1:A:17:LEU:HD11	1:A:18:HIS:H	8	0.12
(1,106)	1:A:17:LEU:HD12	1:A:18:HIS:H	8	0.12
(1,106)	1:A:17:LEU:HD13	1:A:18:HIS:H	8	0.12
(1,106)	1:A:17:LEU:HD21	1:A:18:HIS:H	8	0.12
(1,106)	1:A:17:LEU:HD22	1:A:18:HIS:H	8	0.12
(1,106)	1:A:17:LEU:HD23	1:A:18:HIS:H	8	0.12
(1,106)	1:A:17:LEU:HD11	1:A:18:HIS:H	29	0.12
(1,106)	1:A:17:LEU:HD12	1:A:18:HIS:H	29	0.12
(1,106)	1:A:17:LEU:HD13	1:A:18:HIS:H	29	0.12
(1,106)	1:A:17:LEU:HD21	1:A:18:HIS:H	29	0.12
(1,106)	1:A:17:LEU:HD22	1:A:18:HIS:H	29	0.12
(1,106)	1:A:17:LEU:HD23	1:A:18:HIS:H	29	0.12
(2,34)	1:A:18:HIS:H	1:A:45:GLN:HE21	3	0.11
(2,34)	1:A:18:HIS:H	1:A:45:GLN:HE22	3	0.11
(2,34)	1:A:18:HIS:H	1:A:45:GLN:HE21	24	0.11
(2,34)	1:A:18:HIS:H	1:A:45:GLN:HE22	24	0.11
(2,30)	1:A:17:LEU:HA	1:A:45:GLN:HE21	14	0.11
(2,30)	1:A:17:LEU:HA	1:A:45:GLN:HE22	14	0.11
(2,30)	1:A:17:LEU:HA	1:A:45:GLN:HE21	34	0.11
(2,30)	1:A:17:LEU:HA	1:A:45:GLN:HE22	34	0.11
(2,121)	1:A:42:GLU:H	1:A:45:GLN:HE21	5	0.11
(2,121)	1:A:42:GLU:H	1:A:45:GLN:HE22	5	0.11
(2,121)	1:A:42:GLU:H	1:A:45:GLN:HE21	26	0.11
(2,121)	1:A:42:GLU:H	1:A:45:GLN:HE22	26	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD11	1	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD12	1	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD13	1	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD21	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD22	1	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD23	1	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD11	17	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD12	17	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD13	17	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD21	17	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD22	17	0.11
(2,1)	1:A:2:VAL:H	1:A:28:LEU:HD23	17	0.11
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD11	3	0.11
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD12	3	0.11
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD13	3	0.11
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD21	3	0.11
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD22	3	0.11
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD23	3	0.11
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD11	3	0.11
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD12	3	0.11
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD13	3	0.11
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD21	3	0.11
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD22	3	0.11
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD23	3	0.11
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD11	24	0.11
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD12	24	0.11
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD13	24	0.11
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD21	24	0.11
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD22	24	0.11
(1,93)	1:A:15:TYR:HE1	1:A:17:LEU:HD23	24	0.11
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD11	24	0.11
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD12	24	0.11
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD13	24	0.11
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD21	24	0.11
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD22	24	0.11
(1,93)	1:A:15:TYR:HE2	1:A:17:LEU:HD23	24	0.11
(1,9)	1:A:2:VAL:HA	1:A:2:VAL:H	1	0.11
(1,9)	1:A:2:VAL:HA	1:A:2:VAL:H	17	0.11
(1,51)	1:A:8:CYS:HA	1:A:9:PRO:HD2	14	0.11
(1,51)	1:A:8:CYS:HA	1:A:9:PRO:HD3	14	0.11
(1,51)	1:A:8:CYS:HA	1:A:9:PRO:HD2	34	0.11
(1,51)	1:A:8:CYS:HA	1:A:9:PRO:HD3	34	0.11
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	10	0.11
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	10	0.11
(1,496)	1:A:51:TRP:HB2	1:A:52:TRP:H	30	0.11
(1,496)	1:A:51:TRP:HB3	1:A:52:TRP:H	30	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,487)	1:A:51:TRP:HB2	1:A:51:TRP:HD1	8	0.11
(1,487)	1:A:51:TRP:HB3	1:A:51:TRP:HD1	8	0.11
(1,487)	1:A:51:TRP:HB2	1:A:51:TRP:HD1	29	0.11
(1,487)	1:A:51:TRP:HB3	1:A:51:TRP:HD1	29	0.11
(1,366)	1:A:40:ILE:HG12	1:A:46:TYR:HD1	9	0.11
(1,366)	1:A:40:ILE:HG12	1:A:46:TYR:HD2	9	0.11
(1,366)	1:A:40:ILE:HG13	1:A:46:TYR:HD1	9	0.11
(1,366)	1:A:40:ILE:HG13	1:A:46:TYR:HD2	9	0.11
(1,366)	1:A:40:ILE:HG12	1:A:46:TYR:HD1	18	0.11
(1,366)	1:A:40:ILE:HG12	1:A:46:TYR:HD2	18	0.11
(1,366)	1:A:40:ILE:HG13	1:A:46:TYR:HD1	18	0.11
(1,366)	1:A:40:ILE:HG13	1:A:46:TYR:HD2	18	0.11
(1,339)	1:A:39:TYR:HD1	1:A:39:TYR:H	11	0.11
(1,339)	1:A:39:TYR:HD2	1:A:39:TYR:H	11	0.11
(1,339)	1:A:39:TYR:HD1	1:A:39:TYR:H	31	0.11
(1,339)	1:A:39:TYR:HD2	1:A:39:TYR:H	31	0.11
(1,310)	1:A:36:VAL:HB	1:A:37:VAL:H	1	0.11
(1,310)	1:A:36:VAL:HB	1:A:37:VAL:H	5	0.11
(1,310)	1:A:36:VAL:HB	1:A:37:VAL:H	16	0.11
(1,310)	1:A:36:VAL:HB	1:A:37:VAL:H	17	0.11
(1,310)	1:A:36:VAL:HB	1:A:37:VAL:H	26	0.11
(1,310)	1:A:36:VAL:HB	1:A:37:VAL:H	36	0.11
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB2	5	0.11
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB3	5	0.11
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB2	5	0.11
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB3	5	0.11
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB2	26	0.11
(1,302)	1:A:35:CYS:HB2	1:A:39:TYR:HB3	26	0.11
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB2	26	0.11
(1,302)	1:A:35:CYS:HB3	1:A:39:TYR:HB3	26	0.11
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	2	0.11
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	2	0.11
(1,279)	1:A:31:TYR:HD1	1:A:32:ALA:HA	23	0.11
(1,279)	1:A:31:TYR:HD2	1:A:32:ALA:HA	23	0.11
(1,266)	1:A:30:LYS:HD2	1:A:31:TYR:H	7	0.11
(1,266)	1:A:30:LYS:HD3	1:A:31:TYR:H	7	0.11
(1,266)	1:A:30:LYS:HD2	1:A:31:TYR:H	28	0.11
(1,266)	1:A:30:LYS:HD3	1:A:31:TYR:H	28	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD11	10	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD12	10	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD13	10	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD21	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD22	10	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD23	10	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD11	10	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD12	10	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD13	10	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD21	10	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD22	10	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD23	10	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD11	10	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD12	10	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD13	10	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD21	10	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD22	10	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD23	10	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD11	13	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD12	13	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD13	13	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD21	13	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD22	13	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD23	13	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD11	13	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD12	13	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD13	13	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD21	13	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD22	13	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD23	13	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD11	13	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD12	13	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD13	13	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD21	13	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD22	13	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD23	13	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD11	30	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD12	30	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD13	30	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD21	30	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD22	30	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD23	30	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD11	30	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD12	30	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD13	30	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD21	30	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD22	30	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD23	30	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD11	30	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD12	30	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD13	30	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD21	30	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD22	30	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD23	30	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD11	33	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD12	33	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD13	33	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD21	33	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD22	33	0.11
(1,225)	1:A:27:ALA:HB1	1:A:28:LEU:HD23	33	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD11	33	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD12	33	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD13	33	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD21	33	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD22	33	0.11
(1,225)	1:A:27:ALA:HB2	1:A:28:LEU:HD23	33	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD11	33	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD12	33	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD13	33	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD21	33	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD22	33	0.11
(1,225)	1:A:27:ALA:HB3	1:A:28:LEU:HD23	33	0.11
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD11	7	0.11
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD12	7	0.11
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD13	7	0.11
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD11	28	0.11
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD12	28	0.11
(1,186)	1:A:25:ILE:HA	1:A:25:ILE:HD13	28	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found