Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2M3W
BMRB ID	:	17857
Title	:	Protein structure determination from a set of 4D NOESY
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Deposited on	:	2013-01-28

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:

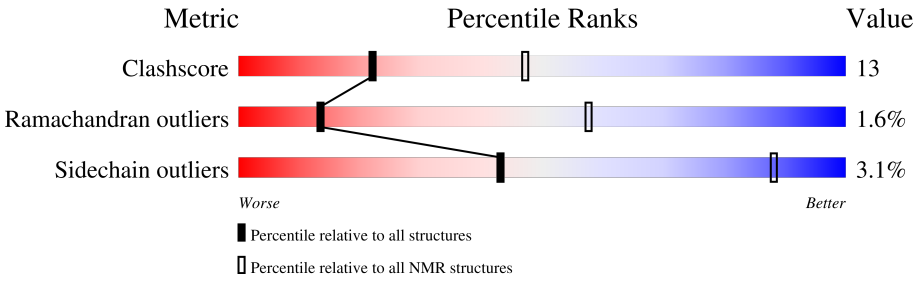
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 48%.

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	93	67% 15% 18%
1	B	93	65% 17% 18%

2 Ensemble composition and analysis

This entry contains 20 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:3-A:19, A:28-A:86, B:3-B:19, B:28-B:86 (152)	0.61	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 5 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2880 atoms, of which 1416 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein S100-A1.

Mol	Chain	Residues	Atoms						Trace
1	A	93	Total	C	H	N	O	S	0
			1440	461	708	116	152	3	
1	B	93	Total	C	H	N	O	S	0
			1440	461	708	116	152	3	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLN	GLU	engineered mutation	UNP P23297
B	32	GLN	GLU	engineered mutation	UNP P23297

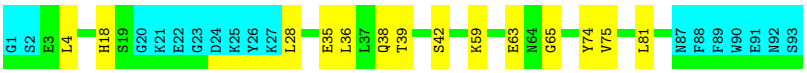
4 Residue-property plots

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: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

Chain B:

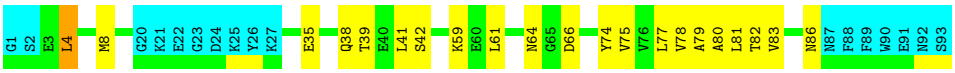
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

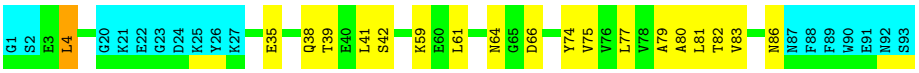
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

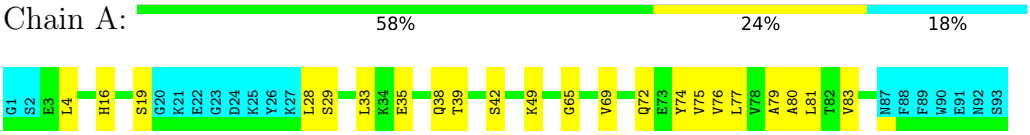
Chain B:



4.2.2 Score per residue for model 2

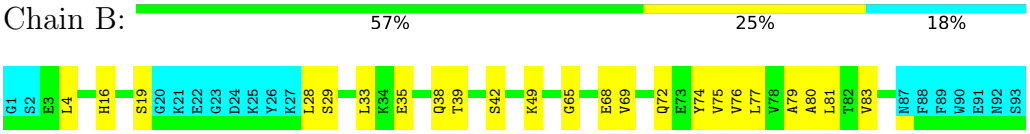
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

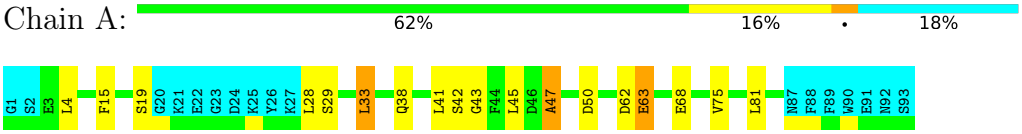
Chain B:



4.2.3 Score per residue for model 3

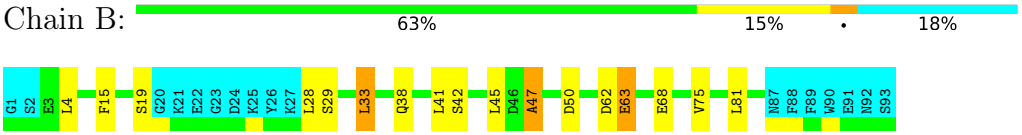
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

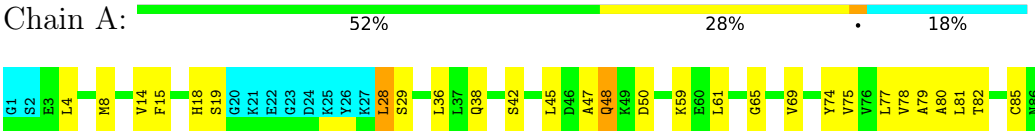
Chain B:



4.2.4 Score per residue for model 4

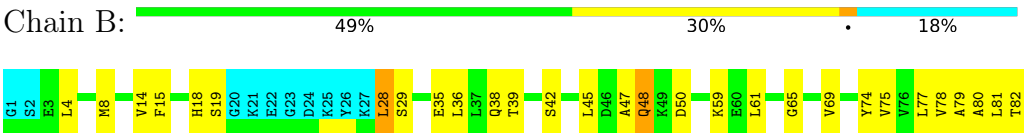
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

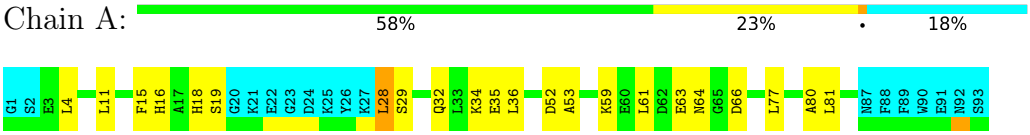
Chain B:



4.2.5 Score per residue for model 5

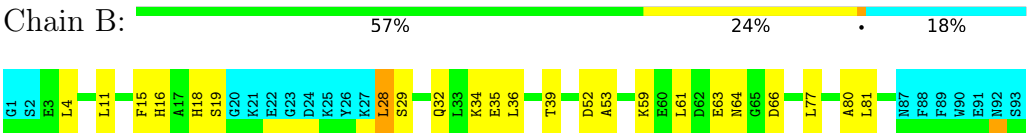
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

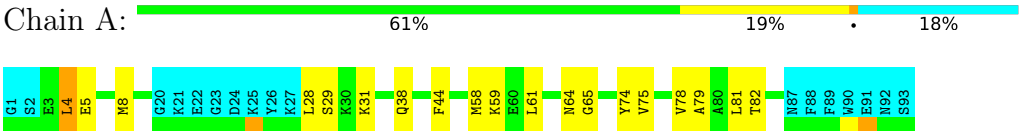
Chain B:



4.2.6 Score per residue for model 6

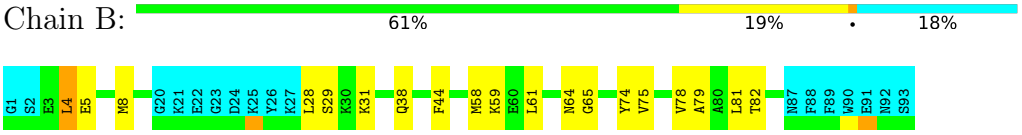
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

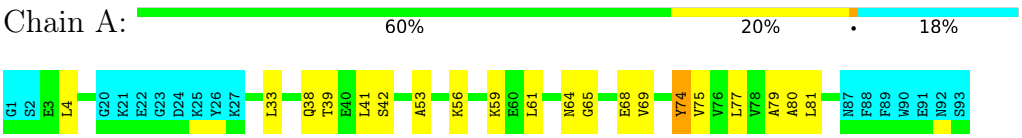
Chain B:



4.2.7 Score per residue for model 7

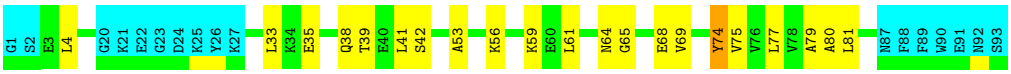
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

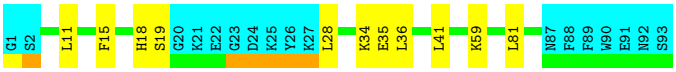
Chain B:



4.2.8 Score per residue for model 8

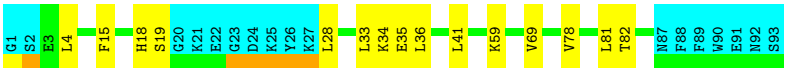
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

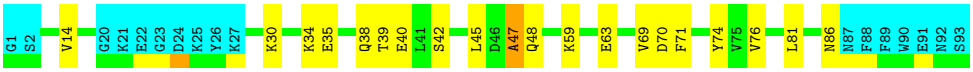
Chain B:



4.2.9 Score per residue for model 9

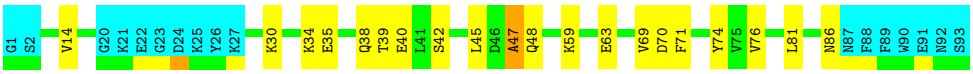
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

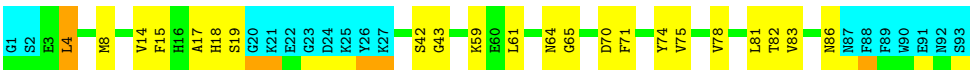
Chain B:



4.2.10 Score per residue for model 10

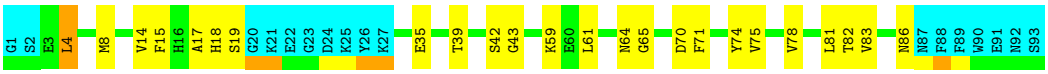
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

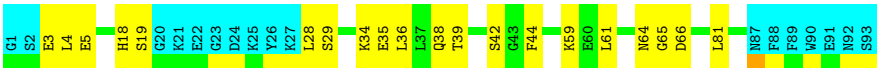
Chain B:



4.2.11 Score per residue for model 11

• Molecule 1: Protein S100-A1

Chain A:



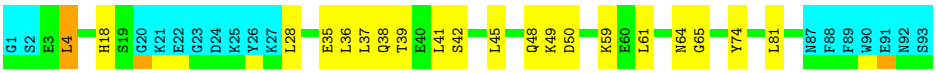
• Molecule 1: Protein S100-A1

Chain B:

4.2.12 Score per residue for model 12 (medoid)

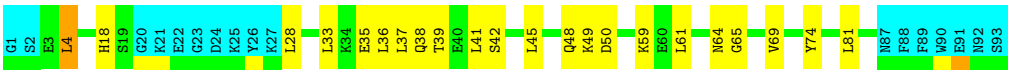
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

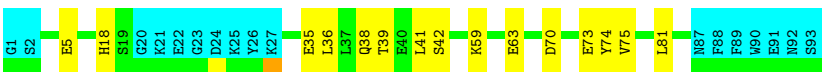
Chain B:



4.2.13 Score per residue for model 13

• Molecule 1: Protein S100-A1

Chain A:



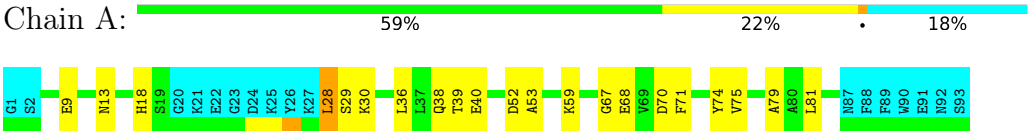
• Molecule 1: Protein S100-A1

Chain B:

4.2.14 Score per residue for model 14

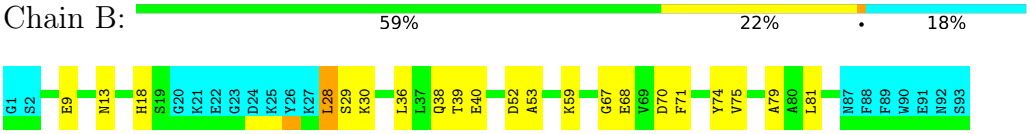
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

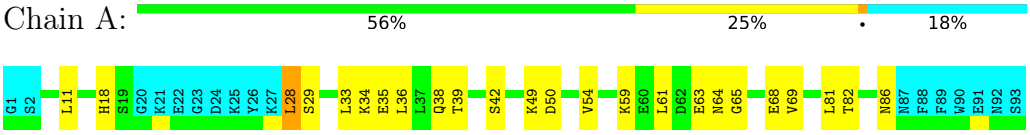
Chain B:



4.2.15 Score per residue for model 15

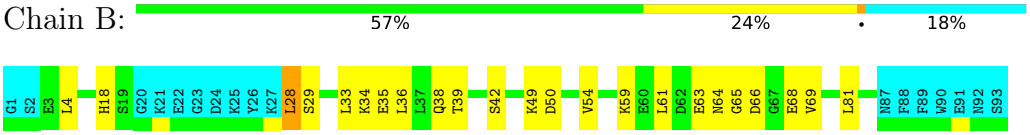
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

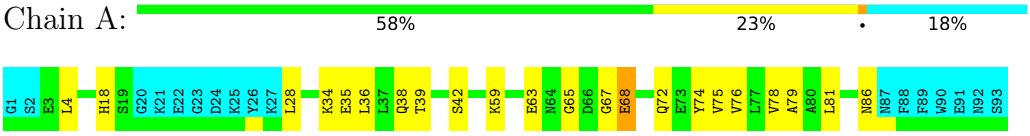
Chain B:



4.2.16 Score per residue for model 16

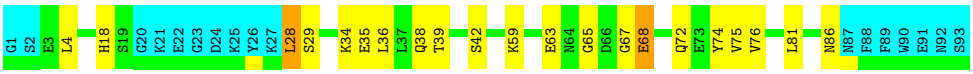
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

Chain B:



4.2.17 Score per residue for model 17

• Molecule 1: Protein S100-A1

Chain A:

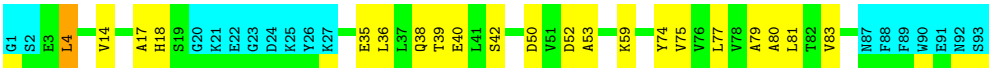
• Molecule 1: Protein S100-A1

Chain B:

4.2.18 Score per residue for model 18

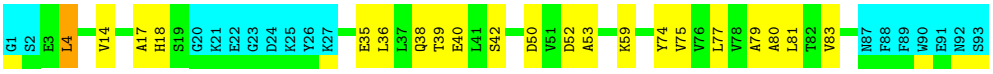
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

Chain B:



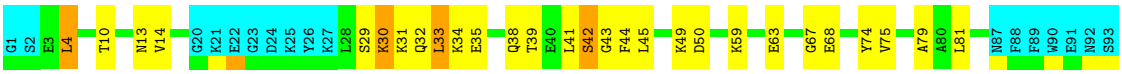
4.2.19 Score per residue for model 19

• Molecule 1: Protein S100-A1

Chain A:

• Molecule 1: Protein S100-A1

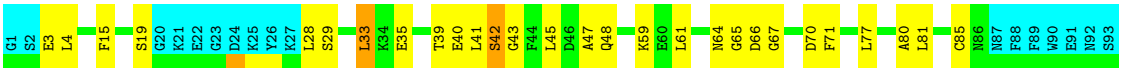
Chain B:



4.2.20 Score per residue for model 20

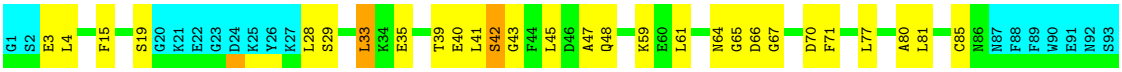
• Molecule 1: Protein S100-A1

Chain A:



• Molecule 1: Protein S100-A1

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 97 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1179
Number of shifts mapped to atoms	1179
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	48%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	590	585	583	16±3
1	B	590	585	583	17±4
All	All	23600	23400	23320	601

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LYS:HZ2	1:A:68:GLU:N	0.67	1.88	14	1
1:B:30:LYS:NZ	1:B:68:GLU:N	0.66	2.44	14	2
1:B:30:LYS:HZ2	1:B:68:GLU:N	0.66	1.88	14	1
1:A:30:LYS:NZ	1:A:68:GLU:N	0.66	2.44	14	2
1:A:38:GLN:O	1:A:42:SER:N	0.59	2.36	2	14
1:B:38:GLN:O	1:B:42:SER:N	0.59	2.36	4	14
1:B:38:GLN:NE2	1:B:58:MET:SD	0.59	2.76	6	1
1:A:13:ASN:OD1	1:A:14:VAL:N	0.59	2.36	19	1
1:B:13:ASN:OD1	1:B:14:VAL:N	0.59	2.36	19	1
1:B:52:ASP:OD1	1:B:53:ALA:N	0.59	2.36	14	3
1:A:38:GLN:NE2	1:A:58:MET:SD	0.59	2.76	6	1
1:B:41:LEU:O	1:B:43:GLY:N	0.59	2.36	20	2
1:B:48:GLN:OE1	1:B:48:GLN:N	0.58	2.36	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:GLN:N	1:A:48:GLN:OE1	0.58	2.36	4	1
1:B:29:SER:O	1:B:32:GLN:N	0.58	2.36	19	1
1:B:41:LEU:HD12	1:B:41:LEU:N	0.58	2.14	7	3
1:A:74:TYR:OH	1:B:4:LEU:HD11	0.58	1.98	7	7
1:B:10:THR:O	1:B:13:ASN:ND2	0.58	2.36	19	1
1:A:4:LEU:HD11	1:B:74:TYR:OH	0.58	1.98	7	7
1:A:52:ASP:OD1	1:A:53:ALA:N	0.58	2.36	14	3
1:A:41:LEU:O	1:A:43:GLY:N	0.58	2.36	20	2
1:A:81:LEU:N	1:A:81:LEU:HD22	0.57	2.14	18	2
1:A:10:THR:O	1:A:13:ASN:ND2	0.57	2.36	19	1
1:B:81:LEU:HD22	1:B:81:LEU:N	0.57	2.14	18	1
1:A:76:VAL:HG22	1:B:76:VAL:HG22	0.57	1.76	16	2
1:A:75:VAL:HG11	1:B:79:ALA:HB2	0.57	1.77	19	7
1:A:8:MET:SD	1:B:82:THR:OG1	0.56	2.64	6	4
1:A:41:LEU:N	1:A:41:LEU:HD12	0.56	2.14	7	4
1:A:29:SER:O	1:A:32:GLN:N	0.56	2.37	19	1
1:B:81:LEU:HD12	1:B:81:LEU:N	0.56	2.16	9	17
1:A:79:ALA:HB2	1:B:75:VAL:HG11	0.56	1.77	19	7
1:A:82:THR:OG1	1:B:8:MET:SD	0.56	2.64	6	3
1:A:81:LEU:HD12	1:A:81:LEU:N	0.56	2.16	9	17
1:B:28:LEU:HD13	1:B:29:SER:N	0.56	2.16	15	5
1:A:81:LEU:N	1:A:81:LEU:CD2	0.56	2.69	18	2
1:B:81:LEU:N	1:B:81:LEU:CD2	0.55	2.69	18	2
1:A:18:HIS:CG	1:A:36:LEU:HD13	0.55	2.36	15	5
1:B:18:HIS:CG	1:B:36:LEU:HD13	0.55	2.36	15	6
1:A:41:LEU:N	1:A:41:LEU:CD2	0.55	2.70	8	2
1:B:41:LEU:N	1:B:41:LEU:CD2	0.55	2.70	8	2
1:B:35:GLU:OE1	1:B:36:LEU:N	0.55	2.40	11	1
1:A:28:LEU:HD13	1:A:29:SER:N	0.55	2.16	15	4
1:A:35:GLU:OE1	1:A:36:LEU:N	0.54	2.40	11	1
1:A:45:LEU:HD13	1:A:48:GLN:NE2	0.54	2.18	20	1
1:B:15:PHE:CE1	1:B:19:SER:CB	0.54	2.91	10	1
1:B:70:ASP:N	1:B:73:GLU:OE2	0.54	2.40	13	1
1:A:33:LEU:HD22	1:A:69:VAL:HG21	0.54	1.80	15	2
1:B:41:LEU:N	1:B:41:LEU:CD1	0.54	2.72	7	2
1:A:15:PHE:CE1	1:A:19:SER:CB	0.54	2.91	10	1
1:B:45:LEU:HD13	1:B:48:GLN:NE2	0.54	2.18	20	1
1:A:70:ASP:N	1:A:73:GLU:OE2	0.53	2.40	13	1
1:A:66:ASP:OD1	1:A:67:GLY:N	0.53	2.41	20	1
1:B:66:ASP:OD1	1:B:67:GLY:N	0.53	2.41	20	1
1:A:4:LEU:CD1	1:B:74:TYR:OH	0.53	2.56	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:N	1:A:41:LEU:CD1	0.53	2.72	7	2
1:B:4:LEU:HD23	1:B:4:LEU:O	0.53	2.03	3	9
1:A:68:GLU:N	1:A:68:GLU:CD	0.53	2.62	3	5
1:B:33:LEU:HD22	1:B:69:VAL:HG21	0.53	1.80	15	4
1:A:74:TYR:OH	1:B:4:LEU:CD1	0.53	2.56	2	5
1:B:68:GLU:N	1:B:68:GLU:CD	0.53	2.62	3	5
1:A:15:PHE:CE2	1:A:19:SER:CB	0.53	2.92	8	1
1:A:41:LEU:N	1:A:41:LEU:HD22	0.53	2.19	8	2
1:B:41:LEU:N	1:B:41:LEU:HD22	0.53	2.19	8	2
1:B:33:LEU:HD13	1:B:33:LEU:O	0.53	2.03	20	2
1:A:33:LEU:O	1:A:33:LEU:HD13	0.53	2.04	20	1
1:A:4:LEU:O	1:A:4:LEU:HD23	0.52	2.05	1	9
1:A:34:LYS:CG	1:A:35:GLU:N	0.52	2.73	19	6
1:B:38:GLN:CG	1:B:39:THR:N	0.52	2.73	7	7
1:B:15:PHE:CE2	1:B:19:SER:CB	0.52	2.92	8	1
1:B:18:HIS:CD2	1:B:36:LEU:HD13	0.52	2.40	16	7
1:A:15:PHE:O	1:A:19:SER:N	0.52	2.42	3	3
1:B:15:PHE:O	1:B:19:SER:N	0.52	2.42	3	3
1:A:18:HIS:CD2	1:A:36:LEU:HD13	0.52	2.40	16	7
1:B:34:LYS:CG	1:B:35:GLU:N	0.52	2.73	19	7
1:A:41:LEU:C	1:A:43:GLY:N	0.51	2.63	20	2
1:A:81:LEU:N	1:A:81:LEU:CD1	0.51	2.74	3	11
1:B:81:LEU:N	1:B:81:LEU:CD1	0.51	2.74	3	12
1:B:34:LYS:O	1:B:38:GLN:NE2	0.51	2.44	9	1
1:A:14:VAL:HG13	1:A:15:PHE:N	0.51	2.21	4	1
1:A:38:GLN:CG	1:A:39:THR:N	0.51	2.73	7	7
1:A:34:LYS:O	1:A:38:GLN:NE2	0.51	2.44	9	1
1:A:30:LYS:HZ2	1:A:67:GLY:C	0.51	2.08	14	1
1:A:79:ALA:O	1:A:83:VAL:HG23	0.50	2.06	18	3
1:B:79:ALA:O	1:B:83:VAL:HG23	0.50	2.06	18	3
1:B:41:LEU:C	1:B:43:GLY:N	0.50	2.63	20	2
1:B:14:VAL:CG1	1:B:15:PHE:N	0.50	2.75	4	1
1:B:15:PHE:CD2	1:B:19:SER:OG	0.50	2.64	5	1
1:A:14:VAL:CG1	1:A:40:GLU:OE2	0.50	2.60	9	1
1:A:74:TYR:OH	1:B:4:LEU:HD22	0.50	2.07	4	1
1:B:30:LYS:HZ2	1:B:67:GLY:C	0.50	2.09	14	1
1:B:14:VAL:HG13	1:B:15:PHE:N	0.50	2.21	4	1
1:A:28:LEU:HD23	1:A:29:SER:N	0.49	2.21	11	5
1:A:74:TYR:C	1:A:74:TYR:CD1	0.49	2.85	17	3
1:B:28:LEU:HD23	1:B:29:SER:N	0.49	2.21	11	5
1:B:14:VAL:CG1	1:B:40:GLU:OE2	0.49	2.60	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:CG1	1:A:15:PHE:N	0.49	2.75	4	1
1:A:15:PHE:CD2	1:A:19:SER:OG	0.49	2.65	5	1
1:B:81:LEU:N	1:B:81:LEU:HD22	0.49	2.21	19	1
1:A:61:LEU:O	1:A:64:ASN:O	0.49	2.30	15	9
1:B:74:TYR:CD1	1:B:74:TYR:C	0.49	2.85	17	4
1:B:61:LEU:O	1:B:64:ASN:O	0.49	2.30	15	9
1:B:78:VAL:O	1:B:82:THR:OG1	0.49	2.31	4	4
1:A:4:LEU:HD22	1:B:74:TYR:OH	0.49	2.07	4	1
1:A:15:PHE:O	1:A:19:SER:OG	0.49	2.31	5	2
1:A:41:LEU:CD1	1:A:41:LEU:N	0.49	2.76	1	1
1:B:15:PHE:O	1:B:19:SER:OG	0.49	2.31	5	1
1:A:35:GLU:O	1:A:39:THR:OG1	0.48	2.31	9	11
1:B:39:THR:HG23	1:B:40:GLU:N	0.48	2.23	14	1
1:A:78:VAL:O	1:A:82:THR:OG1	0.48	2.31	6	4
1:B:41:LEU:CD1	1:B:41:LEU:N	0.48	2.76	1	1
1:B:77:LEU:O	1:B:80:ALA:N	0.48	2.45	5	7
1:A:9:GLU:O	1:A:13:ASN:OD1	0.48	2.31	14	1
1:B:35:GLU:O	1:B:39:THR:OG1	0.48	2.31	17	15
1:B:41:LEU:N	1:B:41:LEU:HD12	0.48	2.23	1	1
1:B:16:HIS:O	1:B:19:SER:OG	0.48	2.32	2	1
1:A:49:LYS:O	1:A:50:ASP:OD1	0.48	2.32	12	1
1:A:77:LEU:O	1:A:80:ALA:N	0.48	2.45	5	7
1:A:5:GLU:CD	1:B:44:PHE:CE1	0.48	2.87	11	3
1:B:42:SER:OG	1:B:43:GLY:N	0.48	2.47	10	1
1:B:49:LYS:O	1:B:50:ASP:OD1	0.48	2.32	12	1
1:B:9:GLU:O	1:B:13:ASN:OD1	0.48	2.31	14	1
1:A:39:THR:HG23	1:A:40:GLU:N	0.47	2.23	14	1
1:A:42:SER:OG	1:A:43:GLY:N	0.47	2.47	10	1
1:A:29:SER:O	1:A:31:LYS:N	0.47	2.47	19	1
1:B:49:LYS:N	1:B:49:LYS:CD	0.47	2.77	15	1
1:A:35:GLU:O	1:A:39:THR:CB	0.47	2.63	9	9
1:B:35:GLU:O	1:B:39:THR:CB	0.47	2.63	1	9
1:B:14:VAL:O	1:B:17:ALA:HB3	0.47	2.09	10	2
1:B:29:SER:O	1:B:31:LYS:N	0.47	2.47	19	1
1:A:74:TYR:CD1	1:A:74:TYR:C	0.47	2.88	12	3
1:A:53:ALA:O	1:A:56:LYS:N	0.47	2.47	7	1
1:A:50:ASP:O	1:A:54:VAL:HG23	0.47	2.10	15	1
1:B:82:THR:HG22	1:B:86:ASN:ND2	0.47	2.24	1	1
1:B:53:ALA:O	1:B:56:LYS:N	0.47	2.47	7	1
1:A:14:VAL:O	1:A:17:ALA:HB3	0.47	2.09	10	2
1:A:49:LYS:N	1:A:49:LYS:CD	0.47	2.77	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:PHE:CE1	1:B:5:GLU:CD	0.47	2.88	11	2
1:B:74:TYR:C	1:B:74:TYR:CD1	0.47	2.88	13	2
1:A:39:THR:CG2	1:A:40:GLU:N	0.47	2.78	14	1
1:A:16:HIS:O	1:A:19:SER:OG	0.47	2.31	2	1
1:A:83:VAL:O	1:A:86:ASN:O	0.46	2.34	1	2
1:A:47:ALA:O	1:A:85:CYS:SG	0.46	2.71	20	2
1:A:5:GLU:OE2	1:B:44:PHE:CD1	0.46	2.69	11	1
1:A:82:THR:HG22	1:A:86:ASN:ND2	0.46	2.24	1	1
1:B:50:ASP:O	1:B:54:VAL:HG23	0.46	2.10	15	1
1:B:83:VAL:O	1:B:86:ASN:O	0.46	2.34	1	2
1:B:39:THR:CG2	1:B:40:GLU:N	0.46	2.78	14	1
1:A:44:PHE:CD1	1:B:5:GLU:OE2	0.45	2.70	11	1
1:B:47:ALA:O	1:B:85:CYS:SG	0.45	2.71	20	2
1:B:37:LEU:HD21	1:B:81:LEU:HD11	0.45	1.89	12	1
1:A:75:VAL:HG12	1:B:75:VAL:HG12	0.45	1.89	18	7
1:A:28:LEU:CD2	1:A:29:SER:O	0.45	2.65	3	1
1:B:72:GLN:O	1:B:75:VAL:N	0.45	2.50	2	2
1:A:70:ASP:CG	1:A:71:PHE:H	0.45	2.15	9	4
1:A:59:LYS:O	1:A:63:GLU:OE2	0.45	2.34	17	1
1:B:50:ASP:OD2	1:B:53:ALA:HB2	0.45	2.12	17	1
1:A:45:LEU:HD12	1:A:45:LEU:N	0.45	2.27	19	1
1:B:45:LEU:N	1:B:45:LEU:HD12	0.45	2.27	19	1
1:B:59:LYS:O	1:B:63:GLU:OE2	0.45	2.34	17	1
1:A:35:GLU:OE1	1:A:35:GLU:C	0.45	2.56	11	1
1:A:36:LEU:HD11	1:A:40:GLU:OE2	0.45	2.11	14	1
1:B:36:LEU:HD11	1:B:40:GLU:OE2	0.45	2.11	14	1
1:A:28:LEU:HD23	1:A:28:LEU:C	0.44	2.32	3	2
1:B:28:LEU:HD23	1:B:28:LEU:C	0.44	2.32	6	2
1:A:13:ASN:OD1	1:A:13:ASN:C	0.44	2.55	19	1
1:B:33:LEU:C	1:B:33:LEU:CD1	0.44	2.86	3	2
1:A:45:LEU:O	1:A:48:GLN:CD	0.44	2.56	4	1
1:A:50:ASP:OD2	1:A:53:ALA:HB2	0.44	2.12	17	1
1:B:45:LEU:C	1:B:47:ALA:H	0.44	2.16	9	2
1:B:45:LEU:O	1:B:48:GLN:CD	0.44	2.56	4	1
1:B:35:GLU:OE1	1:B:35:GLU:C	0.44	2.56	11	1
1:A:15:PHE:CD2	1:A:19:SER:CB	0.44	3.01	8	1
1:A:37:LEU:HD21	1:A:81:LEU:HD11	0.44	1.89	12	1
1:A:33:LEU:C	1:A:33:LEU:CD1	0.44	2.86	3	2
1:B:70:ASP:CG	1:B:71:PHE:H	0.44	2.15	9	4
1:B:13:ASN:OD1	1:B:13:ASN:C	0.44	2.55	19	1
1:A:33:LEU:C	1:A:33:LEU:HD13	0.44	2.33	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:LEU:CD2	1:B:29:SER:O	0.44	2.65	3	1
1:B:28:LEU:O	1:B:69:VAL:HG22	0.44	2.12	4	1
1:B:68:GLU:N	1:B:68:GLU:OE1	0.44	2.51	14	1
1:A:67:GLY:C	1:A:68:GLU:OE1	0.44	2.56	16	1
1:A:72:GLN:O	1:A:75:VAL:N	0.44	2.50	2	2
1:A:45:LEU:C	1:A:47:ALA:H	0.44	2.16	3	2
1:B:38:GLN:O	1:B:42:SER:OG	0.44	2.31	12	1
1:B:67:GLY:C	1:B:68:GLU:OE1	0.44	2.56	16	2
1:B:30:LYS:NZ	1:B:69:VAL:CG1	0.43	2.81	9	1
1:B:15:PHE:CD2	1:B:19:SER:CB	0.43	3.01	8	1
1:A:30:LYS:NZ	1:A:69:VAL:CG1	0.43	2.81	9	1
1:A:68:GLU:N	1:A:68:GLU:OE1	0.43	2.51	14	1
1:A:68:GLU:OE1	1:A:68:GLU:C	0.43	2.56	7	1
1:A:40:GLU:C	1:A:42:SER:H	0.43	2.17	20	1
1:B:3:GLU:H	1:B:3:GLU:CD	0.43	2.17	20	2
1:A:3:GLU:H	1:A:3:GLU:CD	0.43	2.16	20	2
1:A:28:LEU:O	1:A:69:VAL:HG22	0.43	2.12	4	1
1:B:33:LEU:C	1:B:33:LEU:HD13	0.43	2.33	19	2
1:B:68:GLU:OE1	1:B:68:GLU:C	0.42	2.56	7	1
1:A:4:LEU:C	1:A:4:LEU:CD2	0.42	2.88	11	1
1:A:66:ASP:OD1	1:A:66:ASP:C	0.42	2.57	11	3
1:A:30:LYS:HZ3	1:A:67:GLY:C	0.42	2.17	17	1
1:B:4:LEU:C	1:B:4:LEU:CD2	0.42	2.87	11	1
1:B:29:SER:O	1:B:30:LYS:C	0.42	2.57	19	1
1:B:40:GLU:C	1:B:42:SER:H	0.42	2.17	20	1
1:A:68:GLU:OE1	1:A:69:VAL:N	0.42	2.52	7	1
1:A:11:LEU:HD23	1:B:4:LEU:CD1	0.42	2.45	5	3
1:A:33:LEU:HD21	1:A:77:LEU:CD1	0.42	2.45	7	1
1:B:30:LYS:HZ3	1:B:67:GLY:C	0.42	2.17	17	1
1:A:29:SER:C	1:A:31:LYS:N	0.42	2.72	19	1
1:B:33:LEU:HD21	1:B:77:LEU:CD1	0.42	2.45	7	1
1:B:68:GLU:OE1	1:B:69:VAL:N	0.42	2.52	7	1
1:A:33:LEU:O	1:A:34:LYS:C	0.42	2.58	19	1
1:B:61:LEU:O	1:B:65:GLY:N	0.41	2.53	4	1
1:B:29:SER:C	1:B:31:LYS:N	0.41	2.72	19	1
1:B:66:ASP:OD1	1:B:66:ASP:C	0.41	2.58	5	3
1:A:41:LEU:O	1:A:44:PHE:N	0.41	2.53	19	1
1:B:28:LEU:C	1:B:28:LEU:CD1	0.41	2.89	17	2
1:A:61:LEU:O	1:A:65:GLY:N	0.41	2.53	4	1
1:B:16:HIS:ND1	1:B:16:HIS:O	0.41	2.54	5	1
1:A:29:SER:O	1:A:30:LYS:C	0.41	2.57	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:41:LEU:O	1:B:44:PHE:N	0.41	2.53	19	1
1:A:62:ASP:O	1:A:63:GLU:C	0.41	2.59	3	1
1:A:70:ASP:OD1	1:A:71:PHE:N	0.41	2.52	14	1
1:A:4:LEU:HD23	1:A:4:LEU:C	0.41	2.36	20	1
1:A:4:LEU:C	1:A:4:LEU:HD23	0.41	2.35	11	1
1:B:4:LEU:C	1:B:4:LEU:HD23	0.41	2.35	11	1
1:B:33:LEU:O	1:B:34:LYS:C	0.41	2.59	19	2
1:B:4:LEU:HD23	1:B:4:LEU:C	0.41	2.36	20	1
1:B:45:LEU:O	1:B:48:GLN:OE1	0.41	2.39	12	1
1:B:41:LEU:C	1:B:43:GLY:H	0.41	2.19	20	1
1:A:16:HIS:ND1	1:A:16:HIS:O	0.41	2.54	5	1
1:B:62:ASP:O	1:B:63:GLU:C	0.40	2.59	3	1
1:A:4:LEU:CD1	1:B:11:LEU:HD23	0.40	2.45	5	1
1:A:45:LEU:O	1:A:48:GLN:OE1	0.40	2.39	12	1
1:A:28:LEU:C	1:A:28:LEU:CD1	0.40	2.89	17	1
1:A:41:LEU:C	1:A:43:GLY:H	0.40	2.20	3	1
1:B:66:ASP:C	1:B:66:ASP:OD1	0.40	2.59	15	1
1:B:68:GLU:CD	1:B:68:GLU:C	0.40	2.80	2	1
1:A:28:LEU:CD1	1:A:28:LEU:C	0.40	2.89	5	1
1:A:82:THR:CG2	1:A:86:ASN:ND2	0.40	2.85	15	1
1:A:78:VAL:HG23	1:A:79:ALA:N	0.40	2.31	16	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	76/93 (82%)	69±2 (91±2%)	5±2 (7±2%)	1±1 (2±1%)	13	57
1	B	76/93 (82%)	69±2 (91±2%)	5±2 (7±3%)	1±1 (2±1%)	13	57
All	All	3040/3720 (82%)	2774 (91%)	218 (7%)	48 (2%)	13	57

All 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	65	GLY	10
1	B	65	GLY	10
1	A	63	GLU	8
1	B	63	GLU	8
1	A	47	ALA	2
1	B	47	ALA	2
1	A	42	SER	2
1	B	42	SER	2
1	A	48	GLN	1
1	B	48	GLN	1
1	A	30	LYS	1
1	B	30	LYS	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	66/80 (82%)	64±1 (97±1%)	2±1 (3±1%)	43 88
1	B	66/80 (82%)	64±1 (97±1%)	2±1 (3±1%)	43 88
All	All	2640/3200 (82%)	2558 (97%)	82 (3%)	43 88

All 20 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	59	LYS	18
1	B	59	LYS	18
1	A	28	LEU	8
1	B	28	LEU	8
1	A	4	LEU	6
1	B	4	LEU	6
1	A	33	LEU	3
1	B	33	LEU	3
1	A	48	GLN	1
1	B	48	GLN	1
1	A	31	LYS	1
1	B	31	LYS	1
1	A	74	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	B	74	TYR	1
1	A	76	VAL	1
1	B	76	VAL	1
1	A	68	GLU	1
1	B	68	GLU	1
1	A	63	GLU	1
1	B	63	GLU	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 48% for the well-defined parts and 48% 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	1179
Number of shifts mapped to atoms	1179
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	93	-0.57 ± 0.19	Should be checked
$^{13}C_{\beta}$	87	0.02 ± 0.15	None needed (< 0.5 ppm)
$^{13}C'$	90	-0.32 ± 0.11	None needed (< 0.5 ppm)
^{15}N	91	0.42 ± 0.36	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 48%, i.e. 976 atoms were assigned a chemical shift out of a possible 2032. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	381/766 (50%)	155/310 (50%)	150/304 (49%)	76/152 (50%)
Sidechain	549/1156 (47%)	376/752 (50%)	166/378 (44%)	7/26 (27%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	46/110 (42%)	23/54 (43%)	23/48 (48%)	0/8 (0%)
Overall	976/2032 (48%)	554/1116 (50%)	339/730 (46%)	83/186 (45%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 48%, i.e. 1179 atoms were assigned a chemical shift out of a possible 2468. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	464/942 (49%)	190/384 (49%)	183/372 (49%)	91/186 (49%)
Sidechain	630/1334 (47%)	430/860 (50%)	191/438 (44%)	9/36 (25%)
Aromatic	85/192 (44%)	43/94 (46%)	41/88 (47%)	1/10 (10%)
Overall	1179/2468 (48%)	663/1338 (50%)	415/898 (46%)	101/232 (44%)

7.1.4 Statistically unusual chemical shifts (i)

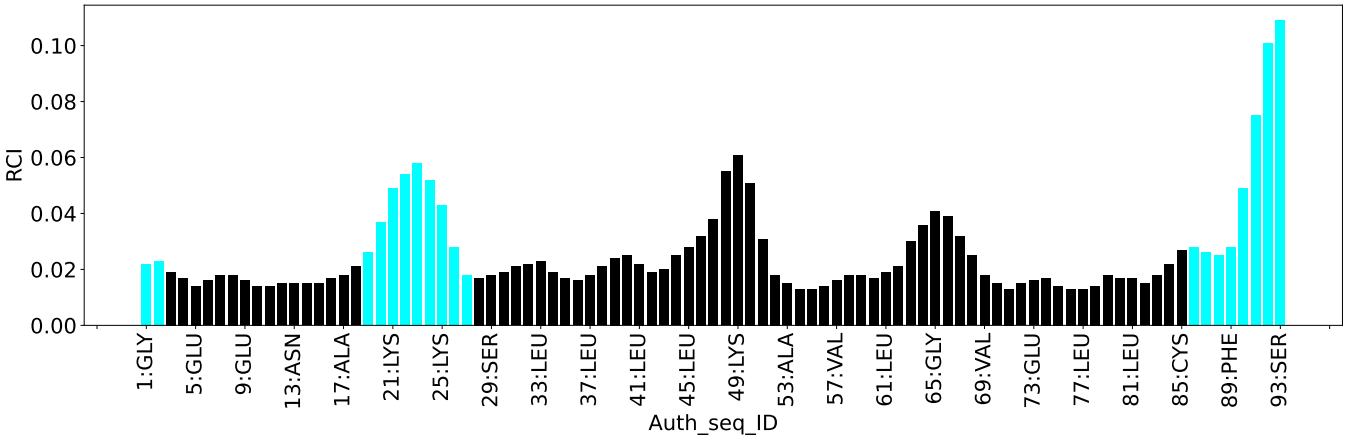
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	5	GLU	HG3	0.46	1.20 – 3.30	-8.5
1	A	49	LYS	HB2	0.45	0.58 – 2.97	-5.6
1	A	49	LYS	HB3	0.37	0.46 – 3.04	-5.4

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
0.00
0.02
0.04
0.06
0.08
0.10
1:GLY
5:GLU
9:GLU
13:ASN
17:ALA
21:LYS
25:LYS
29:SER
33:LEU
37:LEU
41:LEU
45:LEU
49:LYS
53:ALA
57:VAL
61:LEU
65:GLY
69:VAL
73:GLU
77:LEU
81:LEU
85:CYS
89:PHE
93:SER
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	4043
Intra-residue (|i-j|=0)	1076
Sequential (|i-j|=1)	790
Medium range (|i-j|>1 and |i-j|<5)	886
Long range (|i-j|≥5)	770
Inter-chain	413
Hydrogen bond restraints	108
Disulfide bond restraints	0
Total dihedral-angle restraints	208
Number of unmapped restraints	0
Number of restraints per residue	22.9
Number of long range restraints per residue[1]	4.2

[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)	0.9	0.2
0.2-0.5 (Medium)	0.8	0.49
>0.5 (Large)	24.1	4.2

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)

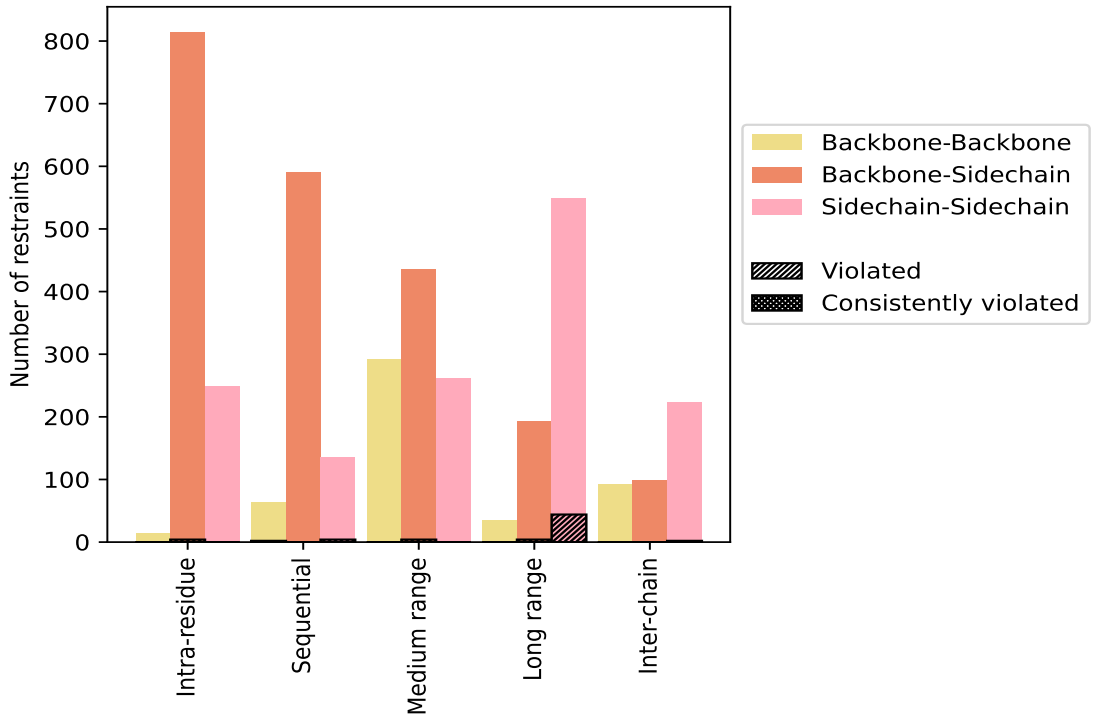
9.1 Summary of distance violations (i)

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)	1076	26.6	4	0.4	0.1	0	0.0	0.0
Backbone-Backbone	14	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	814	20.1	4	0.5	0.1	0	0.0	0.0
Sidechain-Sidechain	248	6.1	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	790	19.5	6	0.8	0.1	0	0.0	0.0
Backbone-Backbone	64	1.6	2	3.1	0.0	0	0.0	0.0
Backbone-Sidechain	590	14.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	136	3.4	4	2.9	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	886	21.9	4	0.5	0.1	0	0.0	0.0
Backbone-Backbone	188	4.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	436	10.8	4	0.9	0.1	0	0.0	0.0
Sidechain-Sidechain	262	6.5	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	770	19.0	48	6.2	1.2	0	0.0	0.0
Backbone-Backbone	30	0.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	192	4.7	4	2.1	0.1	0	0.0	0.0
Sidechain-Sidechain	548	13.6	44	8.0	1.1	0	0.0	0.0
Inter-chain	413	10.2	2	0.5	0.0	0	0.0	0.0
Backbone-Backbone	92	2.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	98	2.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	223	5.5	2	0.9	0.0	0	0.0	0.0
Hydrogen bond	108	2.7	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	4043	100.0	64	1.6	1.6	0	0.0	0.0
Backbone-Backbone	496	12.3	2	0.4	0.0	0	0.0	0.0
Backbone-Sidechain	2130	52.7	12	0.6	0.3	0	0.0	0.0
Sidechain-Sidechain	1417	35.0	50	3.5	1.2	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	4	0	2	0	0	6	0.13	0.14	0.0	0.13
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	4	2	44	0	50	1.68	4.18	0.96	1.3
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	4	2	44	0	50	1.66	3.63	0.82	1.48
7	0	4	2	44	2	52	1.45	3.62	0.84	1.27
8	2	4	2	42	0	50	1.71	4.2	1.03	1.43
9	0	4	2	44	0	50	1.65	4.16	0.99	1.19
10	0	0	0	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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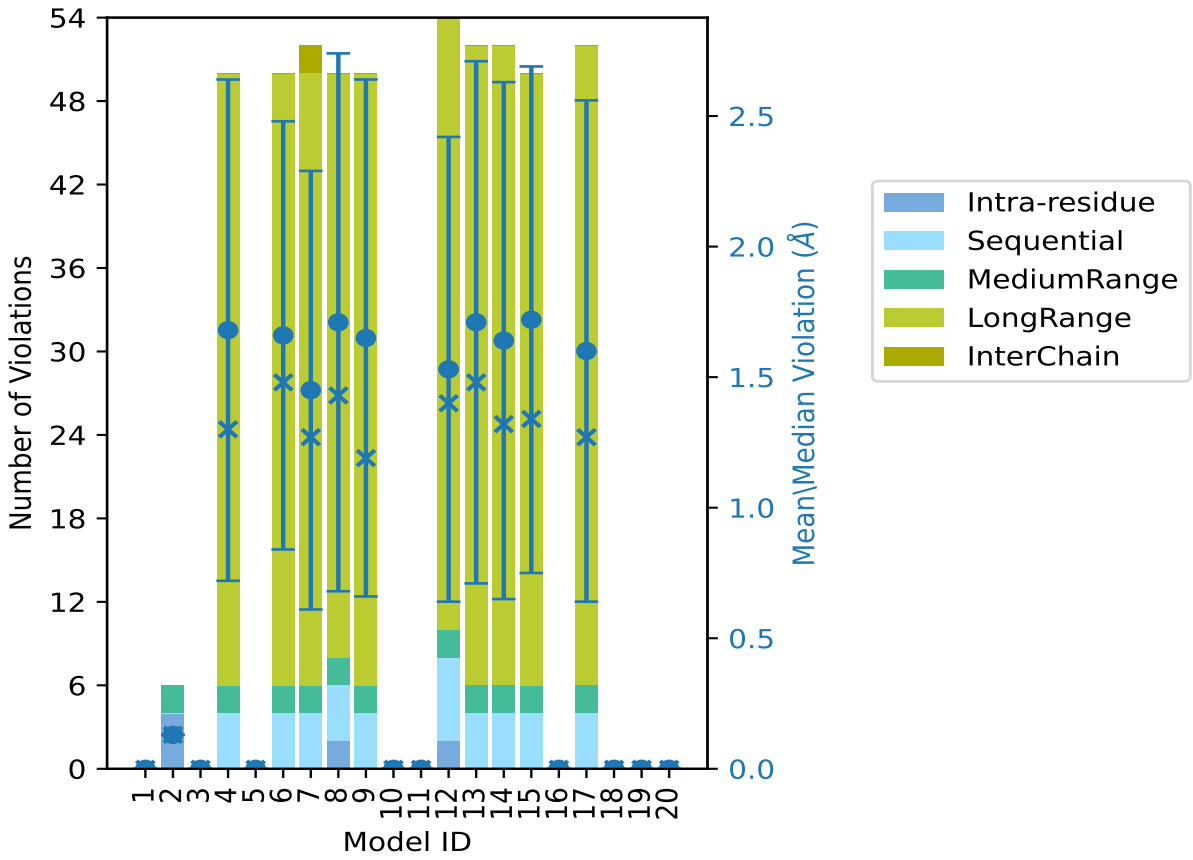
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	2	6	2	44	0	54	1.53	3.59	0.89	1.4
13	0	4	2	46	0	52	1.71	4.16	1.0	1.48
14	0	4	2	46	0	52	1.64	4.12	0.99	1.32
15	0	4	2	44	0	50	1.72	4.19	0.97	1.34
16	0	0	0	0	0	0	0.0	0.0	0.0	0.0
17	0	4	2	46	0	52	1.6	4.01	0.96	1.27
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

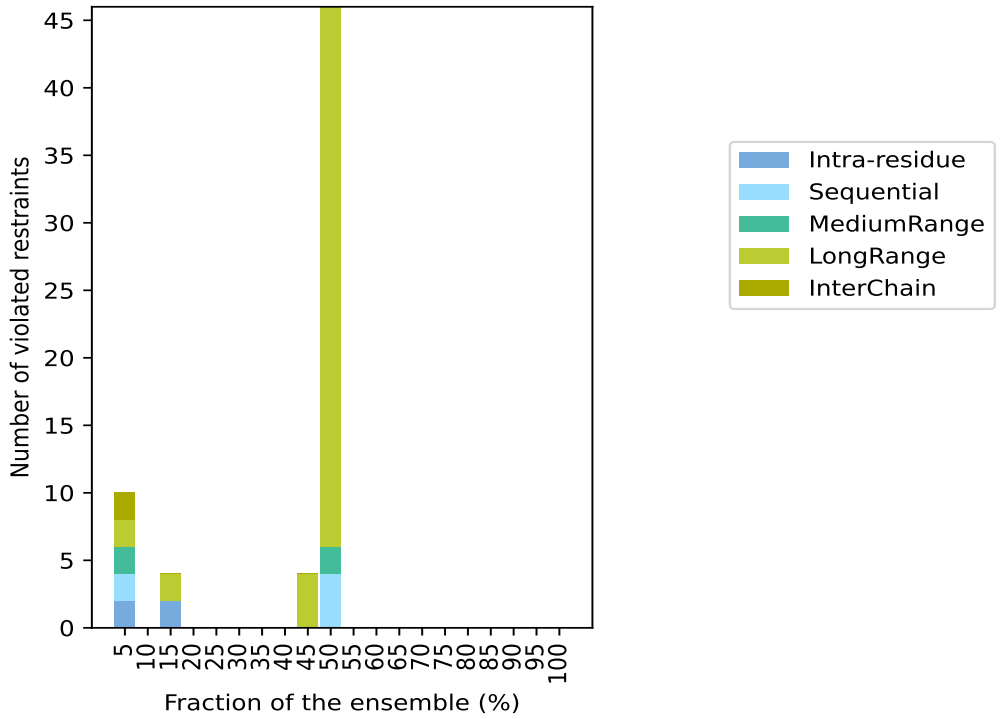
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3871(IR:1072, SQ:784, MR:882, LR:722, IC:411) 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]	%
2	2	2	2	2	10	1	5.0
0	0	0	0	0	0	2	10.0
2	0	0	2	0	4	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	4	0	4	9	45.0
0	4	2	40	0	46	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

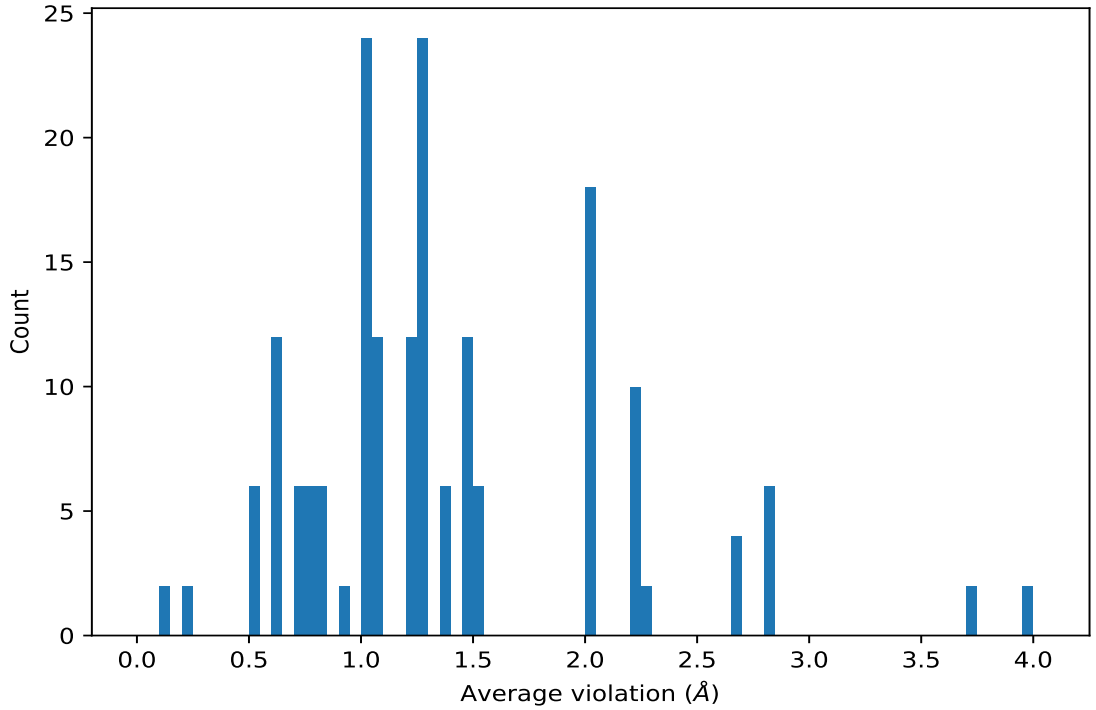
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (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)
(1,1088)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	10	3.99	0.25	4.14
(1,2849)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	10	3.98	0.25	4.14
(1,1082)	1:A:11:LEU:HG	1:A:74:TYR:HE2	10	3.7	0.28	3.78
(1,2843)	1:B:11:LEU:HG	1:B:74:TYR:HE2	10	3.7	0.28	3.78
(1,1084)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	10	2.82	0.24	2.9
(1,1084)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	10	2.82	0.24	2.9
(1,1084)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	10	2.82	0.24	2.9
(1,2845)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	10	2.82	0.24	2.9
(1,2845)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	10	2.82	0.24	2.9
(1,2845)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	10	2.82	0.24	2.9
(1,1144)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	10	2.67	0.23	2.81
(1,1144)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	10	2.67	0.23	2.81
(1,2905)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	10	2.67	0.23	2.81
(1,2905)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	10	2.67	0.23	2.81
(1,2848)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	10	2.27	0.25	2.42
(1,1087)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	10	2.26	0.25	2.42

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1077)	1:A:36:LEU:HG	1:A:74:TYR:HD1	10	2.24	0.21	2.14
(1,2838)	1:B:36:LEU:HG	1:B:74:TYR:HD1	10	2.24	0.21	2.14
(1,1090)	1:A:11:LEU:HA	1:A:74:TYR:HE2	10	2.23	0.27	2.27
(1,2851)	1:B:11:LEU:HA	1:B:74:TYR:HE2	10	2.22	0.27	2.27
(1,2841)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	10	2.2	0.19	2.13
(1,2841)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	10	2.2	0.19	2.13
(1,2841)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	10	2.2	0.19	2.13
(1,1080)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	10	2.2	0.19	2.13
(1,1080)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	10	2.2	0.19	2.13
(1,1080)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	10	2.2	0.19	2.13
(1,1079)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	10	2.02	0.19	1.95
(1,1079)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	10	2.02	0.19	1.95
(1,1079)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	10	2.02	0.19	1.95
(1,2840)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	10	2.02	0.19	1.95
(1,2840)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	10	2.02	0.19	1.95
(1,2840)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	10	2.02	0.19	1.95
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG11	10	2.02	0.2	2.12
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG12	10	2.02	0.2	2.12
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG13	10	2.02	0.2	2.12
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG21	10	2.02	0.2	2.12
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG22	10	2.02	0.2	2.12
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG23	10	2.02	0.2	2.12
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG11	10	2.02	0.2	2.12
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG12	10	2.02	0.2	2.12
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG13	10	2.02	0.2	2.12
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG21	10	2.02	0.2	2.12
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG22	10	2.02	0.2	2.12
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG23	10	2.02	0.2	2.12
(1,1081)	1:A:69:VAL:HG21	1:A:74:TYR:HD1	10	1.5	0.16	1.57
(1,1081)	1:A:69:VAL:HG22	1:A:74:TYR:HD1	10	1.5	0.16	1.57
(1,1081)	1:A:69:VAL:HG23	1:A:74:TYR:HD1	10	1.5	0.16	1.57
(1,2842)	1:B:69:VAL:HG21	1:B:74:TYR:HD1	10	1.5	0.16	1.56
(1,2842)	1:B:69:VAL:HG22	1:B:74:TYR:HD1	10	1.5	0.16	1.56
(1,2842)	1:B:69:VAL:HG23	1:B:74:TYR:HD1	10	1.5	0.16	1.56
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG11	10	1.48	0.11	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG12	10	1.48	0.11	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG13	10	1.48	0.11	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG21	10	1.48	0.11	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG22	10	1.48	0.11	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG23	10	1.48	0.11	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG11	10	1.48	0.11	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG12	10	1.48	0.11	1.54

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG13	10	1.48	0.11	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG21	10	1.48	0.11	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG22	10	1.48	0.11	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG23	10	1.48	0.11	1.54
(1,2847)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	10	1.37	0.25	1.27
(1,2847)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	10	1.37	0.25	1.27
(1,2847)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	10	1.37	0.25	1.27
(1,1086)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	10	1.37	0.25	1.27
(1,1086)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	10	1.37	0.25	1.27
(1,1086)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	10	1.37	0.25	1.27
(1,3090)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	10	1.28	0.14	1.28
(1,3090)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	10	1.28	0.14	1.28
(1,3090)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	10	1.28	0.14	1.28
(1,3090)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	10	1.28	0.14	1.28
(1,3090)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	10	1.28	0.14	1.28
(1,3090)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	10	1.28	0.14	1.28
(1,1329)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	10	1.28	0.14	1.28
(1,1329)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	10	1.28	0.14	1.28
(1,1329)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	10	1.28	0.14	1.28
(1,1329)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	10	1.28	0.14	1.28
(1,1329)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	10	1.28	0.14	1.28
(1,1329)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	10	1.28	0.14	1.28
(1,1293)	1:A:33:LEU:HD11	1:A:74:TYR:HE1	10	1.28	0.14	1.27
(1,1293)	1:A:33:LEU:HD12	1:A:74:TYR:HE1	10	1.28	0.14	1.27
(1,1293)	1:A:33:LEU:HD13	1:A:74:TYR:HE1	10	1.28	0.14	1.27
(1,1293)	1:A:33:LEU:HD21	1:A:74:TYR:HE1	10	1.28	0.14	1.27
(1,1293)	1:A:33:LEU:HD22	1:A:74:TYR:HE1	10	1.28	0.14	1.27
(1,1293)	1:A:33:LEU:HD23	1:A:74:TYR:HE1	10	1.28	0.14	1.27
(1,3054)	1:B:33:LEU:HD11	1:B:74:TYR:HE1	10	1.28	0.14	1.27
(1,3054)	1:B:33:LEU:HD12	1:B:74:TYR:HE1	10	1.28	0.14	1.27
(1,3054)	1:B:33:LEU:HD13	1:B:74:TYR:HE1	10	1.28	0.14	1.27
(1,3054)	1:B:33:LEU:HD21	1:B:74:TYR:HE1	10	1.28	0.14	1.27
(1,3054)	1:B:33:LEU:HD22	1:B:74:TYR:HE1	10	1.28	0.14	1.27
(1,3054)	1:B:33:LEU:HD23	1:B:74:TYR:HE1	10	1.28	0.14	1.27
(1,3053)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	10	1.23	0.16	1.2
(1,3053)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	10	1.23	0.16	1.2
(1,3053)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	10	1.23	0.16	1.2
(1,3053)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	10	1.23	0.16	1.2
(1,3053)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	10	1.23	0.16	1.2
(1,3053)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	10	1.23	0.16	1.2
(1,1292)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	10	1.23	0.16	1.2
(1,1292)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	10	1.23	0.16	1.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1292)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	10	1.23	0.16	1.2
(1,1292)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	10	1.23	0.16	1.2
(1,1292)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	10	1.23	0.16	1.2
(1,1292)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	10	1.23	0.16	1.2
(1,1149)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	10	1.08	0.23	1.16
(1,1149)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	10	1.08	0.23	1.16
(1,1149)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	10	1.08	0.23	1.16
(1,1149)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	10	1.08	0.23	1.16
(1,1149)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	10	1.08	0.23	1.16
(1,1149)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	10	1.08	0.23	1.16
(1,2910)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	10	1.08	0.23	1.16
(1,2910)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	10	1.08	0.23	1.16
(1,2910)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	10	1.08	0.23	1.16
(1,2910)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	10	1.08	0.23	1.16
(1,2910)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	10	1.08	0.23	1.16
(1,2910)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	10	1.08	0.23	1.16
(1,1330)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	10	1.03	0.17	1.02
(1,1330)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	10	1.03	0.17	1.02
(1,1330)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	10	1.03	0.17	1.02
(1,1330)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	10	1.03	0.17	1.02
(1,1330)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	10	1.03	0.17	1.02
(1,1330)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	10	1.03	0.17	1.02
(1,3091)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	10	1.03	0.17	1.02
(1,3091)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	10	1.03	0.17	1.02
(1,3091)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	10	1.03	0.17	1.02
(1,3091)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	10	1.03	0.17	1.02
(1,3091)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	10	1.03	0.17	1.02
(1,3091)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	10	1.03	0.17	1.02
(1,1150)	1:A:11:LEU:HD11	1:A:74:TYR:HD2	10	1.02	0.1	1.04
(1,1150)	1:A:11:LEU:HD12	1:A:74:TYR:HD2	10	1.02	0.1	1.04
(1,1150)	1:A:11:LEU:HD13	1:A:74:TYR:HD2	10	1.02	0.1	1.04
(1,1150)	1:A:11:LEU:HD21	1:A:74:TYR:HD2	10	1.02	0.1	1.04
(1,1150)	1:A:11:LEU:HD22	1:A:74:TYR:HD2	10	1.02	0.1	1.04
(1,1150)	1:A:11:LEU:HD23	1:A:74:TYR:HD2	10	1.02	0.1	1.04
(1,2911)	1:B:11:LEU:HD11	1:B:74:TYR:HD2	10	1.02	0.1	1.04
(1,2911)	1:B:11:LEU:HD12	1:B:74:TYR:HD2	10	1.02	0.1	1.04
(1,2911)	1:B:11:LEU:HD13	1:B:74:TYR:HD2	10	1.02	0.1	1.04
(1,2911)	1:B:11:LEU:HD21	1:B:74:TYR:HD2	10	1.02	0.1	1.04
(1,2911)	1:B:11:LEU:HD22	1:B:74:TYR:HD2	10	1.02	0.1	1.04
(1,2911)	1:B:11:LEU:HD23	1:B:74:TYR:HD2	10	1.02	0.1	1.04
(1,1075)	1:A:71:PHE:HA	1:A:74:TYR:HD2	10	0.91	0.14	0.89
(1,2836)	1:B:71:PHE:HA	1:B:74:TYR:HD2	10	0.91	0.14	0.89

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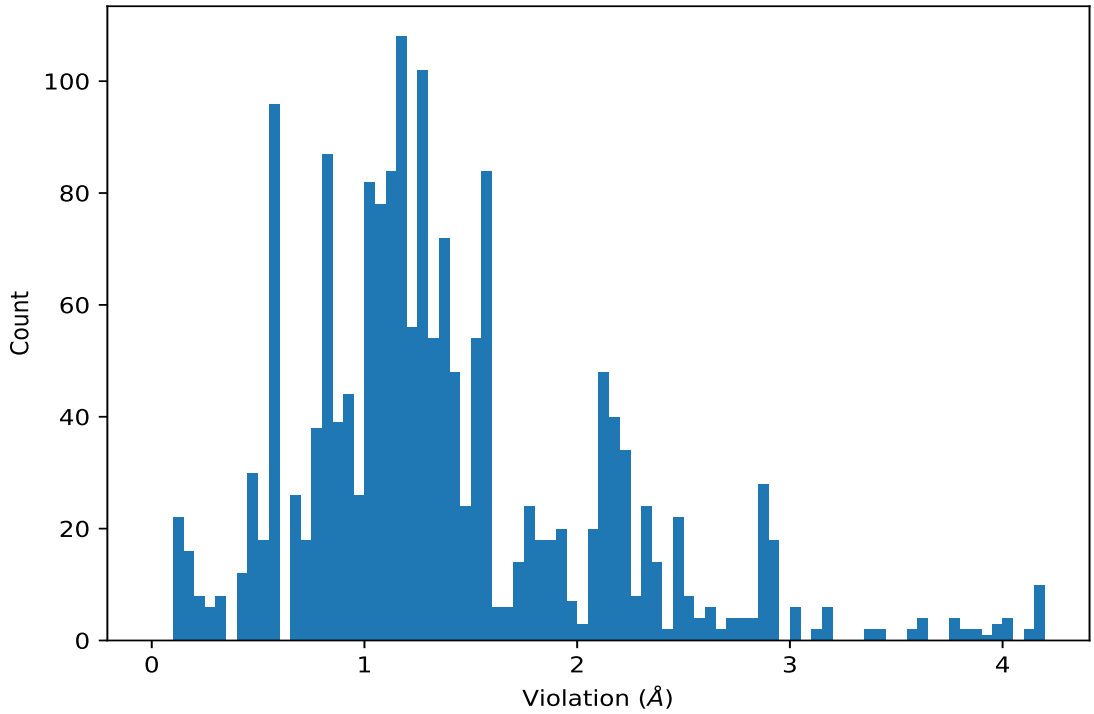
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2839)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	10	0.81	0.15	0.8
(1,2839)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	10	0.81	0.15	0.8
(1,2839)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	10	0.81	0.15	0.8
(1,1078)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	10	0.81	0.15	0.8
(1,1078)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	10	0.81	0.15	0.8
(1,1078)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	10	0.81	0.15	0.8
(1,2837)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	10	0.78	0.17	0.77
(1,2837)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	10	0.78	0.17	0.77
(1,2837)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	10	0.78	0.17	0.77
(1,1076)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	10	0.78	0.17	0.77
(1,1076)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	10	0.78	0.17	0.77
(1,1076)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	10	0.78	0.17	0.77
(1,1083)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	10	0.73	0.18	0.73
(1,1083)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	10	0.73	0.18	0.73
(1,1083)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	10	0.73	0.18	0.73
(1,2844)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	10	0.73	0.18	0.73
(1,2844)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	10	0.73	0.18	0.73
(1,2844)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	10	0.73	0.18	0.73
(1,1345)	1:A:37:LEU:HD11	1:A:74:TYR:HE1	9	0.6	0.35	0.53
(1,1345)	1:A:37:LEU:HD12	1:A:74:TYR:HE1	9	0.6	0.35	0.53
(1,1345)	1:A:37:LEU:HD13	1:A:74:TYR:HE1	9	0.6	0.35	0.53
(1,1345)	1:A:37:LEU:HD21	1:A:74:TYR:HE1	9	0.6	0.35	0.53
(1,1345)	1:A:37:LEU:HD22	1:A:74:TYR:HE1	9	0.6	0.35	0.53
(1,1345)	1:A:37:LEU:HD23	1:A:74:TYR:HE1	9	0.6	0.35	0.53
(1,3106)	1:B:37:LEU:HD11	1:B:74:TYR:HE1	9	0.6	0.35	0.53
(1,3106)	1:B:37:LEU:HD12	1:B:74:TYR:HE1	9	0.6	0.35	0.53
(1,3106)	1:B:37:LEU:HD13	1:B:74:TYR:HE1	9	0.6	0.35	0.53
(1,3106)	1:B:37:LEU:HD21	1:B:74:TYR:HE1	9	0.6	0.35	0.53
(1,3106)	1:B:37:LEU:HD22	1:B:74:TYR:HE1	9	0.6	0.35	0.53
(1,3106)	1:B:37:LEU:HD23	1:B:74:TYR:HE1	9	0.6	0.35	0.53
(1,1085)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	9	0.54	0.18	0.57
(1,1085)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	9	0.54	0.18	0.57
(1,1085)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	9	0.54	0.18	0.57
(1,2846)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	9	0.54	0.18	0.57
(1,2846)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	9	0.54	0.18	0.57
(1,2846)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	9	0.54	0.18	0.57
(1,1089)	1:A:15:PHE:HA	1:A:74:TYR:HE1	3	0.22	0.08	0.17
(1,2850)	1:B:15:PHE:HA	1:B:74:TYR:HE1	3	0.22	0.08	0.17
(1,247)	1:A:38:GLN:H	1:A:38:GLN:HG3	3	0.12	0.01	0.11
(1,2008)	1:B:38:GLN:H	1:B:38:GLN:HG3	3	0.12	0.01	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)
(1,2849)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	8	4.2
(1,1088)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	8	4.2
(1,2849)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	15	4.19
(1,1088)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	15	4.19
(1,2849)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	4	4.18
(1,1088)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	4	4.18
(1,2849)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	9	4.16
(1,1088)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	9	4.16
(1,1088)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	13	4.16
(1,2849)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	13	4.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2849)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	14	4.12
(1,1088)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	14	4.12
(1,2843)	1:B:11:LEU:HG	1:B:74:TYR:HE2	8	4.03
(1,1082)	1:A:11:LEU:HG	1:A:74:TYR:HE2	8	4.03
(1,2849)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	17	4.01
(1,1088)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	17	4.01
(1,2843)	1:B:11:LEU:HG	1:B:74:TYR:HE2	15	3.96
(1,1082)	1:A:11:LEU:HG	1:A:74:TYR:HE2	15	3.96
(1,1082)	1:A:11:LEU:HG	1:A:74:TYR:HE2	13	3.95
(1,2843)	1:B:11:LEU:HG	1:B:74:TYR:HE2	13	3.94
(1,2843)	1:B:11:LEU:HG	1:B:74:TYR:HE2	9	3.85
(1,1082)	1:A:11:LEU:HG	1:A:74:TYR:HE2	9	3.85
(1,2843)	1:B:11:LEU:HG	1:B:74:TYR:HE2	14	3.81
(1,1082)	1:A:11:LEU:HG	1:A:74:TYR:HE2	14	3.81
(1,2843)	1:B:11:LEU:HG	1:B:74:TYR:HE2	17	3.76
(1,1082)	1:A:11:LEU:HG	1:A:74:TYR:HE2	17	3.76
(1,2843)	1:B:11:LEU:HG	1:B:74:TYR:HE2	4	3.75
(1,1082)	1:A:11:LEU:HG	1:A:74:TYR:HE2	4	3.75
(1,2849)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	6	3.63
(1,1088)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	6	3.63
(1,2849)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	7	3.62
(1,1088)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	7	3.62
(1,1088)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	12	3.59
(1,2849)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	12	3.58
(1,2843)	1:B:11:LEU:HG	1:B:74:TYR:HE2	6	3.44
(1,1082)	1:A:11:LEU:HG	1:A:74:TYR:HE2	6	3.44
(1,2843)	1:B:11:LEU:HG	1:B:74:TYR:HE2	12	3.37
(1,1082)	1:A:11:LEU:HG	1:A:74:TYR:HE2	12	3.37
(1,2845)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	13	3.17
(1,2845)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	13	3.17
(1,2845)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	13	3.17
(1,1084)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	13	3.17
(1,1084)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	13	3.17
(1,1084)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	13	3.17
(1,2843)	1:B:11:LEU:HG	1:B:74:TYR:HE2	7	3.12
(1,1082)	1:A:11:LEU:HG	1:A:74:TYR:HE2	7	3.12
(1,2845)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	8	3.03
(1,2845)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	8	3.03
(1,2845)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	8	3.03
(1,1084)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	8	3.03
(1,1084)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	8	3.03
(1,1084)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	8	3.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2845)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	15	2.94
(1,2845)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	15	2.94
(1,2845)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	15	2.94
(1,1084)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	15	2.94
(1,1084)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	15	2.94
(1,1084)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	15	2.94
(1,2845)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	17	2.93
(1,2845)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	17	2.93
(1,2845)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	17	2.93
(1,1084)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	17	2.93
(1,1084)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	17	2.93
(1,1084)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	17	2.93
(1,2845)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	14	2.92
(1,2845)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	14	2.92
(1,2845)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	14	2.92
(1,1084)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	14	2.92
(1,1084)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	14	2.92
(1,1084)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	14	2.92
(1,2845)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	4	2.89
(1,2845)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	4	2.89
(1,2845)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	4	2.89
(1,1084)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	4	2.89
(1,1084)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	4	2.89
(1,1084)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	4	2.89
(1,2845)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	9	2.87
(1,2845)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	9	2.87
(1,2845)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	9	2.87
(1,1084)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	9	2.87
(1,1084)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	9	2.87
(1,1084)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	9	2.87
(1,2905)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	4	2.86
(1,2905)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	4	2.86
(1,2905)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	8	2.86
(1,2905)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	8	2.86
(1,1144)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	4	2.86
(1,1144)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	4	2.86
(1,1144)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	8	2.86
(1,1144)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	8	2.86
(1,2905)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	13	2.85
(1,2905)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	13	2.85
(1,2905)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	15	2.85
(1,2905)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	15	2.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	13	2.85
(1,1144)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	13	2.85
(1,1144)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	15	2.85
(1,1144)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	15	2.85
(1,2905)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	9	2.83
(1,2905)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	9	2.83
(1,1144)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	9	2.83
(1,1144)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	9	2.83
(1,2905)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	14	2.79
(1,2905)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	14	2.79
(1,1144)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	14	2.79
(1,1144)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	14	2.79
(1,2905)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	17	2.7
(1,2905)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	17	2.7
(1,1144)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	17	2.7
(1,1144)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	17	2.7
(1,2838)	1:B:36:LEU:HG	1:B:74:TYR:HD1	6	2.66
(1,1077)	1:A:36:LEU:HG	1:A:74:TYR:HD1	6	2.66
(1,2845)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	12	2.63
(1,2845)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	12	2.63
(1,2845)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	12	2.63
(1,1084)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	12	2.63
(1,1084)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	12	2.63
(1,1084)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	12	2.63
(1,2851)	1:B:11:LEU:HA	1:B:74:TYR:HE2	15	2.57
(1,2838)	1:B:36:LEU:HG	1:B:74:TYR:HD1	12	2.57
(1,1090)	1:A:11:LEU:HA	1:A:74:TYR:HE2	15	2.57
(1,1077)	1:A:36:LEU:HG	1:A:74:TYR:HD1	12	2.57
(1,2841)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	6	2.55
(1,2841)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	6	2.55
(1,2841)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	6	2.55
(1,1080)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	6	2.55
(1,1080)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	6	2.55
(1,1080)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	6	2.55
(1,2851)	1:B:11:LEU:HA	1:B:74:TYR:HE2	8	2.53
(1,1090)	1:A:11:LEU:HA	1:A:74:TYR:HE2	8	2.53
(1,2845)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	6	2.49
(1,2845)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	6	2.49
(1,2845)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	6	2.49
(1,1084)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	6	2.49
(1,1084)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	6	2.49
(1,1084)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	6	2.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2841)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	12	2.48
(1,2841)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	12	2.48
(1,2841)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	12	2.48
(1,2848)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	4	2.47
(1,2848)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	8	2.47
(1,1087)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	4	2.47
(1,1080)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	12	2.47
(1,1080)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	12	2.47
(1,1080)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	12	2.47
(1,2851)	1:B:11:LEU:HA	1:B:74:TYR:HE2	9	2.46
(1,2848)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	13	2.46
(1,1090)	1:A:11:LEU:HA	1:A:74:TYR:HE2	9	2.46
(1,1087)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	8	2.46
(1,1087)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	13	2.46
(1,2848)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	15	2.45
(1,1087)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	15	2.45
(1,2848)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	9	2.43
(1,1087)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	9	2.43
(1,2848)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	14	2.4
(1,2840)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	8	2.4
(1,2840)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	8	2.4
(1,2840)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	8	2.4
(1,1087)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	14	2.4
(1,1079)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	8	2.4
(1,1079)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	8	2.4
(1,1079)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	8	2.4
(1,2851)	1:B:11:LEU:HA	1:B:74:TYR:HE2	14	2.39
(1,1090)	1:A:11:LEU:HA	1:A:74:TYR:HE2	14	2.39
(1,2905)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	7	2.35
(1,2905)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	7	2.35
(1,1144)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	7	2.35
(1,1144)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	7	2.35
(1,2841)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	7	2.34
(1,2841)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	7	2.34
(1,2841)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	7	2.34
(1,1080)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	7	2.34
(1,1080)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	7	2.34
(1,1080)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	7	2.34
(1,2905)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	6	2.33
(1,2905)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	6	2.33
(1,2851)	1:B:11:LEU:HA	1:B:74:TYR:HE2	4	2.33
(1,2845)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	7	2.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2845)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	7	2.33
(1,2845)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	7	2.33
(1,1144)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	6	2.33
(1,1144)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	6	2.33
(1,1090)	1:A:11:LEU:HA	1:A:74:TYR:HE2	4	2.33
(1,1084)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	7	2.33
(1,1084)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	7	2.33
(1,1084)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	7	2.33
(1,2905)	1:B:11:LEU:HB2	1:B:74:TYR:HE2	12	2.32
(1,2905)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	12	2.32
(1,2838)	1:B:36:LEU:HG	1:B:74:TYR:HD1	7	2.32
(1,1144)	1:A:11:LEU:HB2	1:A:74:TYR:HE2	12	2.32
(1,1144)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	12	2.32
(1,1077)	1:A:36:LEU:HG	1:A:74:TYR:HD1	7	2.32
(1,2848)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	17	2.3
(1,1087)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	17	2.3
(1,2840)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	13	2.26
(1,2840)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	13	2.26
(1,2840)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	13	2.26
(1,1079)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	13	2.26
(1,1079)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	13	2.26
(1,1079)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	13	2.26
(1,2838)	1:B:36:LEU:HG	1:B:74:TYR:HD1	14	2.24
(1,1077)	1:A:36:LEU:HG	1:A:74:TYR:HD1	14	2.24
(1,2841)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	14	2.22
(1,2841)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	14	2.22
(1,2841)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	14	2.22
(1,1080)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	14	2.22
(1,1080)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	14	2.22
(1,1080)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	14	2.22
(1,2851)	1:B:11:LEU:HA	1:B:74:TYR:HE2	13	2.21
(1,1090)	1:A:11:LEU:HA	1:A:74:TYR:HE2	13	2.21
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG11	8	2.2
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG12	8	2.2
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG13	8	2.2
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG21	8	2.2
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG22	8	2.2
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG23	8	2.2
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG11	13	2.2
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG12	13	2.2
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG13	13	2.2
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG21	13	2.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG22	13	2.2
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG23	13	2.2
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG11	8	2.2
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG12	8	2.2
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG13	8	2.2
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG21	8	2.2
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG22	8	2.2
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG23	8	2.2
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG11	13	2.2
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG12	13	2.2
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG13	13	2.2
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG21	13	2.2
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG22	13	2.2
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG23	13	2.2
(1,1090)	1:A:11:LEU:HA	1:A:74:TYR:HE2	17	2.18
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG11	17	2.17
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG12	17	2.17
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG13	17	2.17
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG21	17	2.17
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG22	17	2.17
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG23	17	2.17
(1,2851)	1:B:11:LEU:HA	1:B:74:TYR:HE2	17	2.17
(1,2840)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	15	2.17
(1,2840)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	15	2.17
(1,2840)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	15	2.17
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG11	17	2.17
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG12	17	2.17
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG13	17	2.17
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG21	17	2.17
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG22	17	2.17
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG23	17	2.17
(1,1079)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	15	2.17
(1,1079)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	15	2.17
(1,1079)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	15	2.17
(1,2841)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	13	2.16
(1,2841)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	13	2.16
(1,2841)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	13	2.16
(1,1080)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	13	2.16
(1,1080)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	13	2.16
(1,1080)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	13	2.16
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG11	15	2.15
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG12	15	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG13	15	2.15
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG21	15	2.15
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG22	15	2.15
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG23	15	2.15
(1,2838)	1:B:36:LEU:HG	1:B:74:TYR:HD1	13	2.15
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG11	15	2.15
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG12	15	2.15
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG13	15	2.15
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG21	15	2.15
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG22	15	2.15
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG23	15	2.15
(1,1077)	1:A:36:LEU:HG	1:A:74:TYR:HD1	13	2.15
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG11	4	2.14
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG12	4	2.14
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG13	4	2.14
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG21	4	2.14
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG22	4	2.14
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG23	4	2.14
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG11	4	2.14
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG12	4	2.14
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG13	4	2.14
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG21	4	2.14
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG22	4	2.14
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG23	4	2.14
(1,2838)	1:B:36:LEU:HG	1:B:74:TYR:HD1	4	2.13
(1,1077)	1:A:36:LEU:HG	1:A:74:TYR:HD1	4	2.13
(1,2838)	1:B:36:LEU:HG	1:B:74:TYR:HD1	15	2.12
(1,2838)	1:B:36:LEU:HG	1:B:74:TYR:HD1	17	2.12
(1,1077)	1:A:36:LEU:HG	1:A:74:TYR:HD1	15	2.12
(1,1077)	1:A:36:LEU:HG	1:A:74:TYR:HD1	17	2.12
(1,2841)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	9	2.11
(1,2841)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	9	2.11
(1,2841)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	9	2.11
(1,2841)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	17	2.11
(1,2841)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	17	2.11
(1,2841)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	17	2.11
(1,1080)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	9	2.11
(1,1080)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	9	2.11
(1,1080)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	9	2.11
(1,1080)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	17	2.11
(1,1080)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	17	2.11
(1,1080)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	17	2.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG11	14	2.1
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG12	14	2.1
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG13	14	2.1
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG21	14	2.1
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG22	14	2.1
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG23	14	2.1
(1,2840)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	12	2.1
(1,2840)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	12	2.1
(1,2840)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	12	2.1
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG11	14	2.1
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG12	14	2.1
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG13	14	2.1
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG21	14	2.1
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG22	14	2.1
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG23	14	2.1
(1,1079)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	12	2.1
(1,1079)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	12	2.1
(1,1079)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	12	2.1
(1,2841)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	4	2.09
(1,2841)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	4	2.09
(1,2841)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	4	2.09
(1,1080)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	4	2.09
(1,1080)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	4	2.09
(1,1080)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	4	2.09
(1,2838)	1:B:36:LEU:HG	1:B:74:TYR:HD1	9	2.08
(1,1077)	1:A:36:LEU:HG	1:A:74:TYR:HD1	9	2.08
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG11	9	2.06
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG12	9	2.06
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG13	9	2.06
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG21	9	2.06
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG22	9	2.06
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG23	9	2.06
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG11	9	2.06
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG12	9	2.06
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG13	9	2.06
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG21	9	2.06
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG22	9	2.06
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG23	9	2.06
(1,2841)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	15	2.0
(1,2841)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	15	2.0
(1,2841)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	15	2.0
(1,2851)	1:B:11:LEU:HA	1:B:74:TYR:HE2	6	1.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:A:11:LEU:HA	1:A:74:TYR:HE2	6	1.99
(1,1080)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	15	1.99
(1,1080)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	15	1.99
(1,1080)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	15	1.99
(1,2838)	1:B:36:LEU:HG	1:B:74:TYR:HD1	8	1.97
(1,1077)	1:A:36:LEU:HG	1:A:74:TYR:HD1	8	1.97
(1,2840)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	9	1.95
(1,2840)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	9	1.95
(1,2840)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	9	1.95
(1,2840)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	14	1.95
(1,2840)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	14	1.95
(1,2840)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	14	1.95
(1,1079)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	9	1.95
(1,1079)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	9	1.95
(1,1079)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	9	1.95
(1,1079)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	14	1.95
(1,1079)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	14	1.95
(1,1079)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	14	1.95
(1,2848)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	7	1.92
(1,2841)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	8	1.92
(1,2841)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	8	1.92
(1,2841)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	8	1.92
(1,1087)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	7	1.92
(1,1080)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	8	1.92
(1,1080)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	8	1.92
(1,1080)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	8	1.92
(1,2840)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	7	1.9
(1,2840)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	7	1.9
(1,2840)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	7	1.9
(1,1079)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	7	1.9
(1,1079)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	7	1.9
(1,1079)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	7	1.9
(1,2848)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	6	1.88
(1,2848)	1:B:11:LEU:HB3	1:B:74:TYR:HE2	12	1.88
(1,1087)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	6	1.88
(1,1087)	1:A:11:LEU:HB3	1:A:74:TYR:HE2	12	1.88
(1,2840)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	17	1.87
(1,2840)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	17	1.87
(1,2840)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	17	1.87
(1,1079)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	17	1.87
(1,1079)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	17	1.87
(1,1079)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	17	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2851)	1:B:11:LEU:HA	1:B:74:TYR:HE2	7	1.86
(1,1090)	1:A:11:LEU:HA	1:A:74:TYR:HE2	7	1.86
(1,2840)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	6	1.84
(1,2840)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	6	1.84
(1,2840)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	6	1.84
(1,1079)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	6	1.84
(1,1079)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	6	1.84
(1,1079)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	6	1.84
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG11	12	1.82
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG12	12	1.82
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG13	12	1.82
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG21	12	1.82
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG22	12	1.82
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG23	12	1.82
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG11	12	1.82
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG12	12	1.82
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG13	12	1.82
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG21	12	1.82
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG22	12	1.82
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG23	12	1.82
(1,2840)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	4	1.78
(1,2840)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	4	1.78
(1,2840)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	4	1.78
(1,1079)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	4	1.78
(1,1079)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	4	1.78
(1,1079)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	4	1.78
(1,2847)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	6	1.77
(1,2847)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	6	1.77
(1,2847)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	6	1.77
(1,1086)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	6	1.77
(1,1086)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	6	1.77
(1,1086)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	6	1.77
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG11	6	1.76
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG12	6	1.76
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG13	6	1.76
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG21	6	1.76
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG22	6	1.76
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG23	6	1.76
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG11	6	1.76
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG12	6	1.76
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG13	6	1.76
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG21	6	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG22	6	1.76
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG23	6	1.76
(1,2851)	1:B:11:LEU:HA	1:B:74:TYR:HE2	12	1.74
(1,2847)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	12	1.74
(1,2847)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	12	1.74
(1,2847)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	12	1.74
(1,2842)	1:B:69:VAL:HG21	1:B:74:TYR:HD1	4	1.74
(1,2842)	1:B:69:VAL:HG22	1:B:74:TYR:HD1	4	1.74
(1,2842)	1:B:69:VAL:HG23	1:B:74:TYR:HD1	4	1.74
(1,1090)	1:A:11:LEU:HA	1:A:74:TYR:HE2	12	1.74
(1,1086)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	12	1.74
(1,1086)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	12	1.74
(1,1086)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	12	1.74
(1,1081)	1:A:69:VAL:HG21	1:A:74:TYR:HD1	4	1.74
(1,1081)	1:A:69:VAL:HG22	1:A:74:TYR:HD1	4	1.74
(1,1081)	1:A:69:VAL:HG23	1:A:74:TYR:HD1	4	1.74
(1,2847)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	7	1.68
(1,2847)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	7	1.68
(1,2847)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	7	1.68
(1,1086)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	7	1.68
(1,1086)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	7	1.68
(1,1086)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	7	1.68
(1,2842)	1:B:69:VAL:HG21	1:B:74:TYR:HD1	14	1.61
(1,2842)	1:B:69:VAL:HG22	1:B:74:TYR:HD1	14	1.61
(1,2842)	1:B:69:VAL:HG23	1:B:74:TYR:HD1	14	1.61
(1,1081)	1:A:69:VAL:HG21	1:A:74:TYR:HD1	14	1.61
(1,1081)	1:A:69:VAL:HG22	1:A:74:TYR:HD1	14	1.61
(1,1081)	1:A:69:VAL:HG23	1:A:74:TYR:HD1	14	1.61
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG11	13	1.59
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG12	13	1.59
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG13	13	1.59
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG21	13	1.59
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG22	13	1.59
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG23	13	1.59
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG11	7	1.59
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG12	7	1.59
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG13	7	1.59
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG21	7	1.59
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG22	7	1.59
(1,3339)	1:B:74:TYR:HE2	1:B:75:VAL:HG23	7	1.59
(1,2842)	1:B:69:VAL:HG21	1:B:74:TYR:HD1	6	1.59
(1,2842)	1:B:69:VAL:HG22	1:B:74:TYR:HD1	6	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2842)	1:B:69:VAL:HG23	1:B:74:TYR:HD1	6	1.59
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG11	13	1.59
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG12	13	1.59
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG13	13	1.59
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG21	13	1.59
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG22	13	1.59
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG23	13	1.59
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG11	7	1.59
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG12	7	1.59
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG13	7	1.59
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG21	7	1.59
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG22	7	1.59
(1,1578)	1:A:74:TYR:HE2	1:A:75:VAL:HG23	7	1.59
(1,1081)	1:A:69:VAL:HG21	1:A:74:TYR:HD1	6	1.59
(1,1081)	1:A:69:VAL:HG22	1:A:74:TYR:HD1	6	1.59
(1,1081)	1:A:69:VAL:HG23	1:A:74:TYR:HD1	6	1.59
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG11	8	1.58
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG12	8	1.58
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG13	8	1.58
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG21	8	1.58
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG22	8	1.58
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG23	8	1.58
(1,3090)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	12	1.58
(1,3090)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	12	1.58
(1,3090)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	12	1.58
(1,3090)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	12	1.58
(1,3090)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	12	1.58
(1,3090)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	12	1.58
(1,2842)	1:B:69:VAL:HG21	1:B:74:TYR:HD1	17	1.58
(1,2842)	1:B:69:VAL:HG22	1:B:74:TYR:HD1	17	1.58
(1,2842)	1:B:69:VAL:HG23	1:B:74:TYR:HD1	17	1.58
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG11	8	1.58
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG12	8	1.58
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG13	8	1.58
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG21	8	1.58
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG22	8	1.58
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG23	8	1.58
(1,1329)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	12	1.58
(1,1329)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	12	1.58
(1,1329)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	12	1.58
(1,1329)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	12	1.58
(1,1329)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	12	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	12	1.58
(1,2842)	1:B:69:VAL:HG21	1:B:74:TYR:HD1	13	1.57
(1,2842)	1:B:69:VAL:HG22	1:B:74:TYR:HD1	13	1.57
(1,2842)	1:B:69:VAL:HG23	1:B:74:TYR:HD1	13	1.57
(1,1081)	1:A:69:VAL:HG21	1:A:74:TYR:HD1	8	1.57
(1,1081)	1:A:69:VAL:HG22	1:A:74:TYR:HD1	8	1.57
(1,1081)	1:A:69:VAL:HG23	1:A:74:TYR:HD1	8	1.57
(1,1081)	1:A:69:VAL:HG21	1:A:74:TYR:HD1	13	1.57
(1,1081)	1:A:69:VAL:HG22	1:A:74:TYR:HD1	13	1.57
(1,1081)	1:A:69:VAL:HG23	1:A:74:TYR:HD1	13	1.57
(1,1081)	1:A:69:VAL:HG21	1:A:74:TYR:HD1	17	1.57
(1,1081)	1:A:69:VAL:HG22	1:A:74:TYR:HD1	17	1.57
(1,1081)	1:A:69:VAL:HG23	1:A:74:TYR:HD1	17	1.57
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG11	17	1.56
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG12	17	1.56
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG13	17	1.56
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG21	17	1.56
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG22	17	1.56
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG23	17	1.56
(1,2842)	1:B:69:VAL:HG21	1:B:74:TYR:HD1	8	1.56
(1,2842)	1:B:69:VAL:HG22	1:B:74:TYR:HD1	8	1.56
(1,2842)	1:B:69:VAL:HG23	1:B:74:TYR:HD1	8	1.56
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG11	17	1.56
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG12	17	1.56
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG13	17	1.56
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG21	17	1.56
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG22	17	1.56
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG23	17	1.56
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG11	4	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG12	4	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG13	4	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG21	4	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG22	4	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG23	4	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG11	15	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG12	15	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG13	15	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG21	15	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG22	15	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG23	15	1.54
(1,3054)	1:B:33:LEU:HD11	1:B:74:TYR:HE1	13	1.54
(1,3054)	1:B:33:LEU:HD12	1:B:74:TYR:HE1	13	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3054)	1:B:33:LEU:HD13	1:B:74:TYR:HE1	13	1.54
(1,3054)	1:B:33:LEU:HD21	1:B:74:TYR:HE1	13	1.54
(1,3054)	1:B:33:LEU:HD22	1:B:74:TYR:HE1	13	1.54
(1,3054)	1:B:33:LEU:HD23	1:B:74:TYR:HE1	13	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG11	4	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG12	4	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG13	4	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG21	4	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG22	4	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG23	4	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG11	15	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG12	15	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG13	15	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG21	15	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG22	15	1.54
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG23	15	1.54
(1,1293)	1:A:33:LEU:HD11	1:A:74:TYR:HE1	13	1.54
(1,1293)	1:A:33:LEU:HD12	1:A:74:TYR:HE1	13	1.54
(1,1293)	1:A:33:LEU:HD13	1:A:74:TYR:HE1	13	1.54
(1,1293)	1:A:33:LEU:HD21	1:A:74:TYR:HE1	13	1.54
(1,1293)	1:A:33:LEU:HD22	1:A:74:TYR:HE1	13	1.54
(1,1293)	1:A:33:LEU:HD23	1:A:74:TYR:HE1	13	1.54
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG11	14	1.53
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG12	14	1.53
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG13	14	1.53
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG21	14	1.53
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG22	14	1.53
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG23	14	1.53
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG11	14	1.53
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG12	14	1.53
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG13	14	1.53
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG21	14	1.53
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG22	14	1.53
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG23	14	1.53
(1,2842)	1:B:69:VAL:HG21	1:B:74:TYR:HD1	12	1.52
(1,2842)	1:B:69:VAL:HG22	1:B:74:TYR:HD1	12	1.52
(1,2842)	1:B:69:VAL:HG23	1:B:74:TYR:HD1	12	1.52
(1,1081)	1:A:69:VAL:HG21	1:A:74:TYR:HD1	12	1.52
(1,1081)	1:A:69:VAL:HG22	1:A:74:TYR:HD1	12	1.52
(1,1081)	1:A:69:VAL:HG23	1:A:74:TYR:HD1	12	1.52
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG11	9	1.49
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG12	9	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG13	9	1.49
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG21	9	1.49
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG22	9	1.49
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG23	9	1.49
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG11	9	1.49
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG12	9	1.49
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG13	9	1.49
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG21	9	1.49
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG22	9	1.49
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG23	9	1.49
(1,3106)	1:B:37:LEU:HD11	1:B:74:TYR:HE1	6	1.48
(1,3106)	1:B:37:LEU:HD12	1:B:74:TYR:HE1	6	1.48
(1,3106)	1:B:37:LEU:HD13	1:B:74:TYR:HE1	6	1.48
(1,3106)	1:B:37:LEU:HD21	1:B:74:TYR:HE1	6	1.48
(1,3106)	1:B:37:LEU:HD22	1:B:74:TYR:HE1	6	1.48
(1,3106)	1:B:37:LEU:HD23	1:B:74:TYR:HE1	6	1.48
(1,1345)	1:A:37:LEU:HD11	1:A:74:TYR:HE1	6	1.48
(1,1345)	1:A:37:LEU:HD12	1:A:74:TYR:HE1	6	1.48
(1,1345)	1:A:37:LEU:HD13	1:A:74:TYR:HE1	6	1.48
(1,1345)	1:A:37:LEU:HD21	1:A:74:TYR:HE1	6	1.48
(1,1345)	1:A:37:LEU:HD22	1:A:74:TYR:HE1	6	1.48
(1,1345)	1:A:37:LEU:HD23	1:A:74:TYR:HE1	6	1.48
(1,3090)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	6	1.44
(1,3090)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	6	1.44
(1,3090)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	6	1.44
(1,3090)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	6	1.44
(1,3090)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	6	1.44
(1,3090)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	6	1.44
(1,3053)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	15	1.44
(1,3053)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	15	1.44
(1,3053)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	15	1.44
(1,3053)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	15	1.44
(1,3053)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	15	1.44
(1,3053)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	15	1.44
(1,1292)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	15	1.44
(1,1292)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	15	1.44
(1,1292)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	15	1.44
(1,1292)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	15	1.44
(1,1292)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	15	1.44
(1,1292)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	15	1.44
(1,3053)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	8	1.43
(1,3053)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	8	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3053)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	8	1.43
(1,3053)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	8	1.43
(1,3053)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	8	1.43
(1,3053)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	8	1.43
(1,3053)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	13	1.43
(1,3053)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	13	1.43
(1,3053)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	13	1.43
(1,3053)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	13	1.43
(1,3053)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	13	1.43
(1,3053)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	13	1.43
(1,1329)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	6	1.43
(1,1329)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	6	1.43
(1,1329)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	6	1.43
(1,1329)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	6	1.43
(1,1329)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	6	1.43
(1,1329)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	6	1.43
(1,1292)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	8	1.43
(1,1292)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	8	1.43
(1,1292)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	8	1.43
(1,1292)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	8	1.43
(1,1292)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	8	1.43
(1,1292)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	8	1.43
(1,1292)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	13	1.42
(1,1292)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	13	1.42
(1,1292)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	13	1.42
(1,1292)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	13	1.42
(1,1292)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	13	1.42
(1,1292)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	13	1.42
(1,3054)	1:B:33:LEU:HD11	1:B:74:TYR:HE1	12	1.4
(1,3054)	1:B:33:LEU:HD12	1:B:74:TYR:HE1	12	1.4
(1,3054)	1:B:33:LEU:HD13	1:B:74:TYR:HE1	12	1.4
(1,3054)	1:B:33:LEU:HD21	1:B:74:TYR:HE1	12	1.4
(1,3054)	1:B:33:LEU:HD22	1:B:74:TYR:HE1	12	1.4
(1,3054)	1:B:33:LEU:HD23	1:B:74:TYR:HE1	12	1.4
(1,1293)	1:A:33:LEU:HD11	1:A:74:TYR:HE1	12	1.4
(1,1293)	1:A:33:LEU:HD12	1:A:74:TYR:HE1	12	1.4
(1,1293)	1:A:33:LEU:HD13	1:A:74:TYR:HE1	12	1.4
(1,1293)	1:A:33:LEU:HD21	1:A:74:TYR:HE1	12	1.4
(1,1293)	1:A:33:LEU:HD22	1:A:74:TYR:HE1	12	1.4
(1,1293)	1:A:33:LEU:HD23	1:A:74:TYR:HE1	12	1.4
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG11	12	1.39
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG12	12	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG13	12	1.39
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG21	12	1.39
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG22	12	1.39
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG23	12	1.39
(1,3054)	1:B:33:LEU:HD11	1:B:74:TYR:HE1	8	1.39
(1,3054)	1:B:33:LEU:HD12	1:B:74:TYR:HE1	8	1.39
(1,3054)	1:B:33:LEU:HD13	1:B:74:TYR:HE1	8	1.39
(1,3054)	1:B:33:LEU:HD21	1:B:74:TYR:HE1	8	1.39
(1,3054)	1:B:33:LEU:HD22	1:B:74:TYR:HE1	8	1.39
(1,3054)	1:B:33:LEU:HD23	1:B:74:TYR:HE1	8	1.39
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG11	12	1.39
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG12	12	1.39
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG13	12	1.39
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG21	12	1.39
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG22	12	1.39
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG23	12	1.39
(1,1293)	1:A:33:LEU:HD11	1:A:74:TYR:HE1	8	1.39
(1,1293)	1:A:33:LEU:HD12	1:A:74:TYR:HE1	8	1.39
(1,1293)	1:A:33:LEU:HD13	1:A:74:TYR:HE1	8	1.39
(1,1293)	1:A:33:LEU:HD21	1:A:74:TYR:HE1	8	1.39
(1,1293)	1:A:33:LEU:HD22	1:A:74:TYR:HE1	8	1.39
(1,1293)	1:A:33:LEU:HD23	1:A:74:TYR:HE1	8	1.39
(1,3091)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	12	1.37
(1,3091)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	12	1.37
(1,3091)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	12	1.37
(1,3091)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	12	1.37
(1,3091)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	12	1.37
(1,3091)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	12	1.37
(1,2842)	1:B:69:VAL:HG21	1:B:74:TYR:HD1	9	1.37
(1,2842)	1:B:69:VAL:HG22	1:B:74:TYR:HD1	9	1.37
(1,2842)	1:B:69:VAL:HG23	1:B:74:TYR:HD1	9	1.37
(1,1330)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	12	1.37
(1,1330)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	12	1.37
(1,1330)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	12	1.37
(1,1330)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	12	1.37
(1,1330)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	12	1.37
(1,1330)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	12	1.37
(1,1081)	1:A:69:VAL:HG21	1:A:74:TYR:HD1	9	1.37
(1,1081)	1:A:69:VAL:HG22	1:A:74:TYR:HD1	9	1.37
(1,1081)	1:A:69:VAL:HG23	1:A:74:TYR:HD1	9	1.37
(1,2910)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	13	1.36
(1,2910)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	13	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2910)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	13	1.36
(1,2910)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	13	1.36
(1,2910)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	13	1.36
(1,2910)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	13	1.36
(1,2847)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	14	1.36
(1,2847)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	14	1.36
(1,2847)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	14	1.36
(1,1149)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	13	1.36
(1,1149)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	13	1.36
(1,1149)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	13	1.36
(1,1149)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	13	1.36
(1,1149)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	13	1.36
(1,1149)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	13	1.36
(1,1086)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	14	1.36
(1,1086)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	14	1.36
(1,1086)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	14	1.36
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG11	6	1.34
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG12	6	1.34
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG13	6	1.34
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG21	6	1.34
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG22	6	1.34
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG23	6	1.34
(1,3054)	1:B:33:LEU:HD11	1:B:74:TYR:HE1	15	1.34
(1,3054)	1:B:33:LEU:HD12	1:B:74:TYR:HE1	15	1.34
(1,3054)	1:B:33:LEU:HD13	1:B:74:TYR:HE1	15	1.34
(1,3054)	1:B:33:LEU:HD21	1:B:74:TYR:HE1	15	1.34
(1,3054)	1:B:33:LEU:HD22	1:B:74:TYR:HE1	15	1.34
(1,3054)	1:B:33:LEU:HD23	1:B:74:TYR:HE1	15	1.34
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG11	6	1.34
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG12	6	1.34
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG13	6	1.34
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG21	6	1.34
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG22	6	1.34
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG23	6	1.34
(1,1293)	1:A:33:LEU:HD11	1:A:74:TYR:HE1	15	1.34
(1,1293)	1:A:33:LEU:HD12	1:A:74:TYR:HE1	15	1.34
(1,1293)	1:A:33:LEU:HD13	1:A:74:TYR:HE1	15	1.34
(1,1293)	1:A:33:LEU:HD21	1:A:74:TYR:HE1	15	1.34
(1,1293)	1:A:33:LEU:HD22	1:A:74:TYR:HE1	15	1.34
(1,1293)	1:A:33:LEU:HD23	1:A:74:TYR:HE1	15	1.34
(1,2910)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	8	1.32
(1,2910)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	8	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2910)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	8	1.32
(1,2910)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	8	1.32
(1,2910)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	8	1.32
(1,2910)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	8	1.32
(1,1149)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	8	1.32
(1,1149)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	8	1.32
(1,1149)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	8	1.32
(1,1149)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	8	1.32
(1,1149)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	8	1.32
(1,1149)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	8	1.32
(1,3090)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	4	1.3
(1,3090)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	4	1.3
(1,3090)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	4	1.3
(1,3090)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	4	1.3
(1,3090)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	4	1.3
(1,3090)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	4	1.3
(1,3090)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	17	1.3
(1,3090)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	17	1.3
(1,3090)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	17	1.3
(1,3090)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	17	1.3
(1,3090)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	17	1.3
(1,3090)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	17	1.3
(1,1329)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	4	1.3
(1,1329)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	4	1.3
(1,1329)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	4	1.3
(1,1329)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	4	1.3
(1,1329)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	4	1.3
(1,1329)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	4	1.3
(1,3053)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	12	1.29
(1,3053)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	12	1.29
(1,3053)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	12	1.29
(1,3053)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	12	1.29
(1,3053)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	12	1.29
(1,3053)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	12	1.29
(1,1329)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	17	1.29
(1,1329)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	17	1.29
(1,1329)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	17	1.29
(1,1329)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	17	1.29
(1,1329)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	17	1.29
(1,1329)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	17	1.29
(1,1292)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	12	1.29
(1,1292)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	12	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1292)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	12	1.29
(1,1292)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	12	1.29
(1,1292)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	12	1.29
(1,1292)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	12	1.29
(1,3090)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	7	1.28
(1,3090)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	7	1.28
(1,3090)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	7	1.28
(1,3090)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	7	1.28
(1,3090)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	7	1.28
(1,3090)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	7	1.28
(1,3090)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	14	1.28
(1,3090)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	14	1.28
(1,3090)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	14	1.28
(1,3090)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	14	1.28
(1,3090)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	14	1.28
(1,3090)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	14	1.28
(1,2847)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	4	1.28
(1,2847)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	4	1.28
(1,2847)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	4	1.28
(1,1329)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	7	1.28
(1,1329)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	7	1.28
(1,1329)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	7	1.28
(1,1329)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	7	1.28
(1,1329)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	7	1.28
(1,1329)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	7	1.28
(1,1329)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	14	1.28
(1,1329)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	14	1.28
(1,1329)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	14	1.28
(1,1329)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	14	1.28
(1,1329)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	14	1.28
(1,1329)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	14	1.28
(1,1086)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	4	1.28
(1,1086)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	4	1.28
(1,1086)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	4	1.28
(1,3054)	1:B:33:LEU:HD11	1:B:74:TYR:HE1	6	1.27
(1,3054)	1:B:33:LEU:HD12	1:B:74:TYR:HE1	6	1.27
(1,3054)	1:B:33:LEU:HD13	1:B:74:TYR:HE1	6	1.27
(1,3054)	1:B:33:LEU:HD21	1:B:74:TYR:HE1	6	1.27
(1,3054)	1:B:33:LEU:HD22	1:B:74:TYR:HE1	6	1.27
(1,3054)	1:B:33:LEU:HD23	1:B:74:TYR:HE1	6	1.27
(1,3054)	1:B:33:LEU:HD11	1:B:74:TYR:HE1	7	1.27
(1,3054)	1:B:33:LEU:HD12	1:B:74:TYR:HE1	7	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3054)	1:B:33:LEU:HD13	1:B:74:TYR:HE1	7	1.27
(1,3054)	1:B:33:LEU:HD21	1:B:74:TYR:HE1	7	1.27
(1,3054)	1:B:33:LEU:HD22	1:B:74:TYR:HE1	7	1.27
(1,3054)	1:B:33:LEU:HD23	1:B:74:TYR:HE1	7	1.27
(1,1293)	1:A:33:LEU:HD11	1:A:74:TYR:HE1	6	1.27
(1,1293)	1:A:33:LEU:HD12	1:A:74:TYR:HE1	6	1.27
(1,1293)	1:A:33:LEU:HD13	1:A:74:TYR:HE1	6	1.27
(1,1293)	1:A:33:LEU:HD21	1:A:74:TYR:HE1	6	1.27
(1,1293)	1:A:33:LEU:HD22	1:A:74:TYR:HE1	6	1.27
(1,1293)	1:A:33:LEU:HD23	1:A:74:TYR:HE1	6	1.27
(1,1293)	1:A:33:LEU:HD11	1:A:74:TYR:HE1	7	1.27
(1,1293)	1:A:33:LEU:HD12	1:A:74:TYR:HE1	7	1.27
(1,1293)	1:A:33:LEU:HD13	1:A:74:TYR:HE1	7	1.27
(1,1293)	1:A:33:LEU:HD21	1:A:74:TYR:HE1	7	1.27
(1,1293)	1:A:33:LEU:HD22	1:A:74:TYR:HE1	7	1.27
(1,1293)	1:A:33:LEU:HD23	1:A:74:TYR:HE1	7	1.27
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG11	7	1.26
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG12	7	1.26
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG13	7	1.26
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG21	7	1.26
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG22	7	1.26
(1,3340)	1:B:74:TYR:HD2	1:B:75:VAL:HG23	7	1.26
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG11	7	1.26
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG12	7	1.26
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG13	7	1.26
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG21	7	1.26
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG22	7	1.26
(1,1579)	1:A:74:TYR:HD2	1:A:75:VAL:HG23	7	1.26
(1,3053)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	14	1.25
(1,3053)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	14	1.25
(1,3053)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	14	1.25
(1,3053)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	14	1.25
(1,3053)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	14	1.25
(1,3053)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	14	1.25
(1,2847)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	17	1.25
(1,2847)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	17	1.25
(1,2847)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	17	1.25
(1,1292)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	14	1.25
(1,1292)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	14	1.25
(1,1292)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	14	1.25
(1,1292)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	14	1.25
(1,1292)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	14	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1292)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	14	1.25
(1,1086)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	17	1.25
(1,1086)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	17	1.25
(1,1086)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	17	1.25
(1,2911)	1:B:11:LEU:HD11	1:B:74:TYR:HD2	13	1.24
(1,2911)	1:B:11:LEU:HD12	1:B:74:TYR:HD2	13	1.24
(1,2911)	1:B:11:LEU:HD13	1:B:74:TYR:HD2	13	1.24
(1,2911)	1:B:11:LEU:HD21	1:B:74:TYR:HD2	13	1.24
(1,2911)	1:B:11:LEU:HD22	1:B:74:TYR:HD2	13	1.24
(1,2911)	1:B:11:LEU:HD23	1:B:74:TYR:HD2	13	1.24
(1,2910)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	15	1.24
(1,2910)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	15	1.24
(1,2910)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	15	1.24
(1,2910)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	15	1.24
(1,2910)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	15	1.24
(1,2910)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	15	1.24
(1,2847)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	13	1.24
(1,2847)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	13	1.24
(1,2847)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	13	1.24
(1,1150)	1:A:11:LEU:HD11	1:A:74:TYR:HD2	13	1.24
(1,1150)	1:A:11:LEU:HD12	1:A:74:TYR:HD2	13	1.24
(1,1150)	1:A:11:LEU:HD13	1:A:74:TYR:HD2	13	1.24
(1,1150)	1:A:11:LEU:HD21	1:A:74:TYR:HD2	13	1.24
(1,1150)	1:A:11:LEU:HD22	1:A:74:TYR:HD2	13	1.24
(1,1150)	1:A:11:LEU:HD23	1:A:74:TYR:HD2	13	1.24
(1,1149)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	15	1.24
(1,1149)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	15	1.24
(1,1149)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	15	1.24
(1,1149)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	15	1.24
(1,1149)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	15	1.24
(1,1149)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	15	1.24
(1,1086)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	13	1.24
(1,1086)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	13	1.24
(1,1086)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	13	1.24
(1,3090)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	13	1.23
(1,3090)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	13	1.23
(1,3090)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	13	1.23
(1,3090)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	13	1.23
(1,3090)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	13	1.23
(1,3090)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	13	1.23
(1,2842)	1:B:69:VAL:HG21	1:B:74:TYR:HD1	15	1.23
(1,2842)	1:B:69:VAL:HG22	1:B:74:TYR:HD1	15	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2842)	1:B:69:VAL:HG23	1:B:74:TYR:HD1	15	1.23
(1,1329)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	13	1.23
(1,1329)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	13	1.23
(1,1329)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	13	1.23
(1,1329)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	13	1.23
(1,1329)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	13	1.23
(1,1329)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	13	1.23
(1,1081)	1:A:69:VAL:HG21	1:A:74:TYR:HD1	15	1.23
(1,1081)	1:A:69:VAL:HG22	1:A:74:TYR:HD1	15	1.23
(1,1081)	1:A:69:VAL:HG23	1:A:74:TYR:HD1	15	1.23
(1,2842)	1:B:69:VAL:HG21	1:B:74:TYR:HD1	7	1.22
(1,2842)	1:B:69:VAL:HG22	1:B:74:TYR:HD1	7	1.22
(1,2842)	1:B:69:VAL:HG23	1:B:74:TYR:HD1	7	1.22
(1,1081)	1:A:69:VAL:HG21	1:A:74:TYR:HD1	7	1.22
(1,1081)	1:A:69:VAL:HG22	1:A:74:TYR:HD1	7	1.22
(1,1081)	1:A:69:VAL:HG23	1:A:74:TYR:HD1	7	1.22
(1,1075)	1:A:71:PHE:HA	1:A:74:TYR:HD2	6	1.22
(1,2836)	1:B:71:PHE:HA	1:B:74:TYR:HD2	6	1.21
(1,3054)	1:B:33:LEU:HD11	1:B:74:TYR:HE1	14	1.2
(1,3054)	1:B:33:LEU:HD12	1:B:74:TYR:HE1	14	1.2
(1,3054)	1:B:33:LEU:HD13	1:B:74:TYR:HE1	14	1.2
(1,3054)	1:B:33:LEU:HD21	1:B:74:TYR:HE1	14	1.2
(1,3054)	1:B:33:LEU:HD22	1:B:74:TYR:HE1	14	1.2
(1,3054)	1:B:33:LEU:HD23	1:B:74:TYR:HE1	14	1.2
(1,1293)	1:A:33:LEU:HD11	1:A:74:TYR:HE1	14	1.2
(1,1293)	1:A:33:LEU:HD12	1:A:74:TYR:HE1	14	1.2
(1,1293)	1:A:33:LEU:HD13	1:A:74:TYR:HE1	14	1.2
(1,1293)	1:A:33:LEU:HD21	1:A:74:TYR:HE1	14	1.2
(1,1293)	1:A:33:LEU:HD22	1:A:74:TYR:HE1	14	1.2
(1,1293)	1:A:33:LEU:HD23	1:A:74:TYR:HE1	14	1.2
(1,3091)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	6	1.19
(1,3091)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	6	1.19
(1,3091)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	6	1.19
(1,3091)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	6	1.19
(1,3091)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	6	1.19
(1,3091)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	6	1.19
(1,3054)	1:B:33:LEU:HD11	1:B:74:TYR:HE1	9	1.19
(1,3054)	1:B:33:LEU:HD12	1:B:74:TYR:HE1	9	1.19
(1,3054)	1:B:33:LEU:HD13	1:B:74:TYR:HE1	9	1.19
(1,3054)	1:B:33:LEU:HD21	1:B:74:TYR:HE1	9	1.19
(1,3054)	1:B:33:LEU:HD22	1:B:74:TYR:HE1	9	1.19
(1,3054)	1:B:33:LEU:HD23	1:B:74:TYR:HE1	9	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	6	1.19
(1,1330)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	6	1.19
(1,1330)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	6	1.19
(1,1330)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	6	1.19
(1,1330)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	6	1.19
(1,1330)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	6	1.19
(1,1330)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	7	1.19
(1,1330)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	7	1.19
(1,1330)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	7	1.19
(1,1330)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	7	1.19
(1,1330)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	7	1.19
(1,1330)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	7	1.19
(1,1293)	1:A:33:LEU:HD11	1:A:74:TYR:HE1	9	1.19
(1,1293)	1:A:33:LEU:HD12	1:A:74:TYR:HE1	9	1.19
(1,1293)	1:A:33:LEU:HD13	1:A:74:TYR:HE1	9	1.19
(1,1293)	1:A:33:LEU:HD21	1:A:74:TYR:HE1	9	1.19
(1,1293)	1:A:33:LEU:HD22	1:A:74:TYR:HE1	9	1.19
(1,1293)	1:A:33:LEU:HD23	1:A:74:TYR:HE1	9	1.19
(1,3091)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	7	1.18
(1,3091)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	7	1.18
(1,3091)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	7	1.18
(1,3091)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	7	1.18
(1,3091)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	7	1.18
(1,3091)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	7	1.18
(1,3090)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	15	1.18
(1,3090)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	15	1.18
(1,3090)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	15	1.18
(1,3090)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	15	1.18
(1,3090)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	15	1.18
(1,3090)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	15	1.18
(1,2847)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	9	1.18
(1,2847)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	9	1.18
(1,2847)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	9	1.18
(1,1329)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	15	1.18
(1,1329)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	15	1.18
(1,1329)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	15	1.18
(1,1329)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	15	1.18
(1,1329)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	15	1.18
(1,1329)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	15	1.18
(1,2910)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	14	1.17
(1,2910)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	14	1.17
(1,2910)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	14	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2910)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	14	1.17
(1,2910)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	14	1.17
(1,2910)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	14	1.17
(1,2910)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	17	1.17
(1,2910)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	17	1.17
(1,2910)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	17	1.17
(1,2910)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	17	1.17
(1,2910)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	17	1.17
(1,2910)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	17	1.17
(1,1149)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	14	1.17
(1,1149)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	14	1.17
(1,1149)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	14	1.17
(1,1149)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	14	1.17
(1,1149)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	14	1.17
(1,1149)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	14	1.17
(1,1149)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	17	1.17
(1,1149)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	17	1.17
(1,1149)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	17	1.17
(1,1149)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	17	1.17
(1,1149)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	17	1.17
(1,1149)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	17	1.17
(1,1086)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	9	1.17
(1,1086)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	9	1.17
(1,1086)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	9	1.17
(1,2910)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	9	1.16
(1,2910)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	9	1.16
(1,2910)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	9	1.16
(1,2910)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	9	1.16
(1,2910)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	9	1.16
(1,2910)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	9	1.16
(1,1292)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	9	1.16
(1,1292)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	9	1.16
(1,1292)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	9	1.16
(1,1292)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	9	1.16
(1,1292)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	9	1.16
(1,1292)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	9	1.16
(1,1149)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	9	1.16
(1,1149)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	9	1.16
(1,1149)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	9	1.16
(1,1149)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	9	1.16
(1,1149)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	9	1.16
(1,1149)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	9	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3090)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	9	1.15
(1,3090)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	9	1.15
(1,3090)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	9	1.15
(1,3090)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	9	1.15
(1,3090)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	9	1.15
(1,3090)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	9	1.15
(1,3053)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	6	1.15
(1,3053)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	6	1.15
(1,3053)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	6	1.15
(1,3053)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	6	1.15
(1,3053)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	6	1.15
(1,3053)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	6	1.15
(1,3053)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	9	1.15
(1,3053)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	9	1.15
(1,3053)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	9	1.15
(1,3053)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	9	1.15
(1,3053)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	9	1.15
(1,3053)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	9	1.15
(1,2839)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	12	1.15
(1,2839)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	12	1.15
(1,2839)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	12	1.15
(1,1329)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	9	1.15
(1,1329)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	9	1.15
(1,1329)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	9	1.15
(1,1329)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	9	1.15
(1,1329)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	9	1.15
(1,1329)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	9	1.15
(1,1292)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	6	1.15
(1,1292)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	6	1.15
(1,1292)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	6	1.15
(1,1292)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	6	1.15
(1,1292)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	6	1.15
(1,1292)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	6	1.15
(1,1078)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	12	1.15
(1,1078)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	12	1.15
(1,1078)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	12	1.15
(1,2911)	1:B:11:LEU:HD11	1:B:74:TYR:HD2	8	1.12
(1,2911)	1:B:11:LEU:HD12	1:B:74:TYR:HD2	8	1.12
(1,2911)	1:B:11:LEU:HD13	1:B:74:TYR:HD2	8	1.12
(1,2911)	1:B:11:LEU:HD21	1:B:74:TYR:HD2	8	1.12
(1,2911)	1:B:11:LEU:HD22	1:B:74:TYR:HD2	8	1.12
(1,2911)	1:B:11:LEU:HD23	1:B:74:TYR:HD2	8	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1150)	1:A:11:LEU:HD11	1:A:74:TYR:HD2	8	1.12
(1,1150)	1:A:11:LEU:HD12	1:A:74:TYR:HD2	8	1.12
(1,1150)	1:A:11:LEU:HD13	1:A:74:TYR:HD2	8	1.12
(1,1150)	1:A:11:LEU:HD21	1:A:74:TYR:HD2	8	1.12
(1,1150)	1:A:11:LEU:HD22	1:A:74:TYR:HD2	8	1.12
(1,1150)	1:A:11:LEU:HD23	1:A:74:TYR:HD2	8	1.12
(1,3054)	1:B:33:LEU:HD11	1:B:74:TYR:HE1	17	1.11
(1,3054)	1:B:33:LEU:HD12	1:B:74:TYR:HE1	17	1.11
(1,3054)	1:B:33:LEU:HD13	1:B:74:TYR:HE1	17	1.11
(1,3054)	1:B:33:LEU:HD21	1:B:74:TYR:HE1	17	1.11
(1,3054)	1:B:33:LEU:HD22	1:B:74:TYR:HE1	17	1.11
(1,3054)	1:B:33:LEU:HD23	1:B:74:TYR:HE1	17	1.11
(1,2910)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	4	1.11
(1,2910)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	4	1.11
(1,2910)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	4	1.11
(1,2910)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	4	1.11
(1,2910)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	4	1.11
(1,2910)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	4	1.11
(1,2847)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	8	1.11
(1,2847)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	8	1.11
(1,2847)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	8	1.11
(1,1293)	1:A:33:LEU:HD11	1:A:74:TYR:HE1	17	1.11
(1,1293)	1:A:33:LEU:HD12	1:A:74:TYR:HE1	17	1.11
(1,1293)	1:A:33:LEU:HD13	1:A:74:TYR:HE1	17	1.11
(1,1293)	1:A:33:LEU:HD21	1:A:74:TYR:HE1	17	1.11
(1,1293)	1:A:33:LEU:HD22	1:A:74:TYR:HE1	17	1.11
(1,1293)	1:A:33:LEU:HD23	1:A:74:TYR:HE1	17	1.11
(1,1149)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	4	1.11
(1,1149)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	4	1.11
(1,1149)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	4	1.11
(1,1149)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	4	1.11
(1,1149)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	4	1.11
(1,1149)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	4	1.11
(1,1086)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	8	1.11
(1,1086)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	8	1.11
(1,1086)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	8	1.11
(1,1083)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	12	1.11
(1,1083)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	12	1.11
(1,1083)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	12	1.11
(1,2844)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	12	1.1
(1,2844)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	12	1.1
(1,2844)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	12	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2847)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	15	1.09
(1,2847)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	15	1.09
(1,2847)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	15	1.09
(1,1086)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	15	1.09
(1,1086)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	15	1.09
(1,1086)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	15	1.09
(1,3091)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	4	1.08
(1,3091)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	4	1.08
(1,3091)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	4	1.08
(1,3091)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	4	1.08
(1,3091)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	4	1.08
(1,3091)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	4	1.08
(1,1330)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	4	1.08
(1,1330)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	4	1.08
(1,1330)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	4	1.08
(1,1330)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	4	1.08
(1,1330)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	4	1.08
(1,1330)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	4	1.08
(1,3090)	1:B:36:LEU:HD11	1:B:74:TYR:HD1	8	1.07
(1,3090)	1:B:36:LEU:HD12	1:B:74:TYR:HD1	8	1.07
(1,3090)	1:B:36:LEU:HD13	1:B:74:TYR:HD1	8	1.07
(1,3090)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	8	1.07
(1,3090)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	8	1.07
(1,3090)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	8	1.07
(1,3054)	1:B:33:LEU:HD11	1:B:74:TYR:HE1	4	1.07
(1,3054)	1:B:33:LEU:HD12	1:B:74:TYR:HE1	4	1.07
(1,3054)	1:B:33:LEU:HD13	1:B:74:TYR:HE1	4	1.07
(1,3054)	1:B:33:LEU:HD21	1:B:74:TYR:HE1	4	1.07
(1,3054)	1:B:33:LEU:HD22	1:B:74:TYR:HE1	4	1.07
(1,3054)	1:B:33:LEU:HD23	1:B:74:TYR:HE1	4	1.07
(1,1329)	1:A:36:LEU:HD11	1:A:74:TYR:HD1	8	1.07
(1,1329)	1:A:36:LEU:HD12	1:A:74:TYR:HD1	8	1.07
(1,1329)	1:A:36:LEU:HD13	1:A:74:TYR:HD1	8	1.07
(1,1329)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	8	1.07
(1,1329)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	8	1.07
(1,1329)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	8	1.07
(1,1293)	1:A:33:LEU:HD11	1:A:74:TYR:HE1	4	1.07
(1,1293)	1:A:33:LEU:HD12	1:A:74:TYR:HE1	4	1.07
(1,1293)	1:A:33:LEU:HD13	1:A:74:TYR:HE1	4	1.07
(1,1293)	1:A:33:LEU:HD21	1:A:74:TYR:HE1	4	1.07
(1,1293)	1:A:33:LEU:HD22	1:A:74:TYR:HE1	4	1.07
(1,1293)	1:A:33:LEU:HD23	1:A:74:TYR:HE1	4	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3053)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	17	1.06
(1,3053)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	17	1.06
(1,3053)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	17	1.06
(1,3053)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	17	1.06
(1,3053)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	17	1.06
(1,3053)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	17	1.06
(1,1292)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	17	1.06
(1,1292)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	17	1.06
(1,1292)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	17	1.06
(1,1292)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	17	1.06
(1,1292)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	17	1.06
(1,1292)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	17	1.06
(1,3053)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	7	1.05
(1,3053)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	7	1.05
(1,3053)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	7	1.05
(1,3053)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	7	1.05
(1,3053)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	7	1.05
(1,3053)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	7	1.05
(1,2911)	1:B:11:LEU:HD11	1:B:74:TYR:HD2	15	1.05
(1,2911)	1:B:11:LEU:HD12	1:B:74:TYR:HD2	15	1.05
(1,2911)	1:B:11:LEU:HD13	1:B:74:TYR:HD2	15	1.05
(1,2911)	1:B:11:LEU:HD21	1:B:74:TYR:HD2	15	1.05
(1,2911)	1:B:11:LEU:HD22	1:B:74:TYR:HD2	15	1.05
(1,2911)	1:B:11:LEU:HD23	1:B:74:TYR:HD2	15	1.05
(1,1292)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	7	1.05
(1,1292)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	7	1.05
(1,1292)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	7	1.05
(1,1292)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	7	1.05
(1,1292)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	7	1.05
(1,1292)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	7	1.05
(1,1150)	1:A:11:LEU:HD11	1:A:74:TYR:HD2	15	1.05
(1,1150)	1:A:11:LEU:HD12	1:A:74:TYR:HD2	15	1.05
(1,1150)	1:A:11:LEU:HD13	1:A:74:TYR:HD2	15	1.05
(1,1150)	1:A:11:LEU:HD21	1:A:74:TYR:HD2	15	1.05
(1,1150)	1:A:11:LEU:HD22	1:A:74:TYR:HD2	15	1.05
(1,1150)	1:A:11:LEU:HD23	1:A:74:TYR:HD2	15	1.05
(1,2911)	1:B:11:LEU:HD11	1:B:74:TYR:HD2	9	1.04
(1,2911)	1:B:11:LEU:HD12	1:B:74:TYR:HD2	9	1.04
(1,2911)	1:B:11:LEU:HD13	1:B:74:TYR:HD2	9	1.04
(1,2911)	1:B:11:LEU:HD21	1:B:74:TYR:HD2	9	1.04
(1,2911)	1:B:11:LEU:HD22	1:B:74:TYR:HD2	9	1.04
(1,2911)	1:B:11:LEU:HD23	1:B:74:TYR:HD2	9	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2911)	1:B:11:LEU:HD11	1:B:74:TYR:HD2	14	1.04
(1,2911)	1:B:11:LEU:HD12	1:B:74:TYR:HD2	14	1.04
(1,2911)	1:B:11:LEU:HD13	1:B:74:TYR:HD2	14	1.04
(1,2911)	1:B:11:LEU:HD21	1:B:74:TYR:HD2	14	1.04
(1,2911)	1:B:11:LEU:HD22	1:B:74:TYR:HD2	14	1.04
(1,2911)	1:B:11:LEU:HD23	1:B:74:TYR:HD2	14	1.04
(1,2837)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	15	1.04
(1,2837)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	15	1.04
(1,2837)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	15	1.04
(1,1150)	1:A:11:LEU:HD11	1:A:74:TYR:HD2	9	1.04
(1,1150)	1:A:11:LEU:HD12	1:A:74:TYR:HD2	9	1.04
(1,1150)	1:A:11:LEU:HD13	1:A:74:TYR:HD2	9	1.04
(1,1150)	1:A:11:LEU:HD21	1:A:74:TYR:HD2	9	1.04
(1,1150)	1:A:11:LEU:HD22	1:A:74:TYR:HD2	9	1.04
(1,1150)	1:A:11:LEU:HD23	1:A:74:TYR:HD2	9	1.04
(1,1150)	1:A:11:LEU:HD11	1:A:74:TYR:HD2	14	1.04
(1,1150)	1:A:11:LEU:HD12	1:A:74:TYR:HD2	14	1.04
(1,1150)	1:A:11:LEU:HD13	1:A:74:TYR:HD2	14	1.04
(1,1150)	1:A:11:LEU:HD21	1:A:74:TYR:HD2	14	1.04
(1,1150)	1:A:11:LEU:HD22	1:A:74:TYR:HD2	14	1.04
(1,1150)	1:A:11:LEU:HD23	1:A:74:TYR:HD2	14	1.04
(1,1076)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	15	1.04
(1,1076)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	15	1.04
(1,1076)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	15	1.04
(1,3091)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	17	1.03
(1,3091)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	17	1.03
(1,3091)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	17	1.03
(1,3091)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	17	1.03
(1,3091)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	17	1.03
(1,3091)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	17	1.03
(1,3053)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	4	1.03
(1,3053)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	4	1.03
(1,3053)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	4	1.03
(1,3053)	1:B:33:LEU:HD21	1:B:74:TYR:HD1	4	1.03
(1,3053)	1:B:33:LEU:HD22	1:B:74:TYR:HD1	4	1.03
(1,3053)	1:B:33:LEU:HD23	1:B:74:TYR:HD1	4	1.03
(1,2911)	1:B:11:LEU:HD11	1:B:74:TYR:HD2	17	1.03
(1,2911)	1:B:11:LEU:HD12	1:B:74:TYR:HD2	17	1.03
(1,2911)	1:B:11:LEU:HD13	1:B:74:TYR:HD2	17	1.03
(1,2911)	1:B:11:LEU:HD21	1:B:74:TYR:HD2	17	1.03
(1,2911)	1:B:11:LEU:HD22	1:B:74:TYR:HD2	17	1.03
(1,2911)	1:B:11:LEU:HD23	1:B:74:TYR:HD2	17	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	17	1.03
(1,1330)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	17	1.03
(1,1330)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	17	1.03
(1,1330)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	17	1.03
(1,1330)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	17	1.03
(1,1330)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	17	1.03
(1,1150)	1:A:11:LEU:HD11	1:A:74:TYR:HD2	17	1.03
(1,1150)	1:A:11:LEU:HD12	1:A:74:TYR:HD2	17	1.03
(1,1150)	1:A:11:LEU:HD13	1:A:74:TYR:HD2	17	1.03
(1,1150)	1:A:11:LEU:HD21	1:A:74:TYR:HD2	17	1.03
(1,1150)	1:A:11:LEU:HD22	1:A:74:TYR:HD2	17	1.03
(1,1150)	1:A:11:LEU:HD23	1:A:74:TYR:HD2	17	1.03
(1,2836)	1:B:71:PHE:HA	1:B:74:TYR:HD2	9	1.02
(1,1292)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	4	1.02
(1,1292)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	4	1.02
(1,1292)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	4	1.02
(1,1292)	1:A:33:LEU:HD21	1:A:74:TYR:HD1	4	1.02
(1,1292)	1:A:33:LEU:HD22	1:A:74:TYR:HD1	4	1.02
(1,1292)	1:A:33:LEU:HD23	1:A:74:TYR:HD1	4	1.02
(1,1075)	1:A:71:PHE:HA	1:A:74:TYR:HD2	9	1.02
(1,2836)	1:B:71:PHE:HA	1:B:74:TYR:HD2	4	1.01
(1,1075)	1:A:71:PHE:HA	1:A:74:TYR:HD2	4	1.01
(1,3091)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	14	1.0
(1,3091)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	14	1.0
(1,3091)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	14	1.0
(1,3091)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	14	1.0
(1,3091)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	14	1.0
(1,3091)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	14	1.0
(1,1330)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	14	1.0
(1,1330)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	14	1.0
(1,1330)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	14	1.0
(1,1330)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	14	1.0
(1,1330)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	14	1.0
(1,1330)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	14	1.0
(1,2837)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	13	0.99
(1,2837)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	13	0.99
(1,2837)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	13	0.99
(1,1076)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	13	0.99
(1,1076)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	13	0.99
(1,1076)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	13	0.99
(1,2911)	1:B:11:LEU:HD11	1:B:74:TYR:HD2	4	0.96
(1,2911)	1:B:11:LEU:HD12	1:B:74:TYR:HD2	4	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2911)	1:B:11:LEU:HD13	1:B:74:TYR:HD2	4	0.96
(1,2911)	1:B:11:LEU:HD21	1:B:74:TYR:HD2	4	0.96
(1,2911)	1:B:11:LEU:HD22	1:B:74:TYR:HD2	4	0.96
(1,2911)	1:B:11:LEU:HD23	1:B:74:TYR:HD2	4	0.96
(1,2837)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	8	0.96
(1,2837)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	8	0.96
(1,2837)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	8	0.96
(1,2836)	1:B:71:PHE:HA	1:B:74:TYR:HD2	13	0.96
(1,1150)	1:A:11:LEU:HD11	1:A:74:TYR:HD2	4	0.96
(1,1150)	1:A:11:LEU:HD12	1:A:74:TYR:HD2	4	0.96
(1,1150)	1:A:11:LEU:HD13	1:A:74:TYR:HD2	4	0.96
(1,1150)	1:A:11:LEU:HD21	1:A:74:TYR:HD2	4	0.96
(1,1150)	1:A:11:LEU:HD22	1:A:74:TYR:HD2	4	0.96
(1,1150)	1:A:11:LEU:HD23	1:A:74:TYR:HD2	4	0.96
(1,1076)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	8	0.96
(1,1076)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	8	0.96
(1,1076)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	8	0.96
(1,1075)	1:A:71:PHE:HA	1:A:74:TYR:HD2	13	0.96
(1,2911)	1:B:11:LEU:HD11	1:B:74:TYR:HD2	6	0.95
(1,2911)	1:B:11:LEU:HD12	1:B:74:TYR:HD2	6	0.95
(1,2911)	1:B:11:LEU:HD13	1:B:74:TYR:HD2	6	0.95
(1,2911)	1:B:11:LEU:HD21	1:B:74:TYR:HD2	6	0.95
(1,2911)	1:B:11:LEU:HD22	1:B:74:TYR:HD2	6	0.95
(1,2911)	1:B:11:LEU:HD23	1:B:74:TYR:HD2	6	0.95
(1,2911)	1:B:11:LEU:HD11	1:B:74:TYR:HD2	12	0.95
(1,2911)	1:B:11:LEU:HD12	1:B:74:TYR:HD2	12	0.95
(1,2911)	1:B:11:LEU:HD13	1:B:74:TYR:HD2	12	0.95
(1,2911)	1:B:11:LEU:HD21	1:B:74:TYR:HD2	12	0.95
(1,2911)	1:B:11:LEU:HD22	1:B:74:TYR:HD2	12	0.95
(1,2911)	1:B:11:LEU:HD23	1:B:74:TYR:HD2	12	0.95
(1,1150)	1:A:11:LEU:HD11	1:A:74:TYR:HD2	6	0.95
(1,1150)	1:A:11:LEU:HD12	1:A:74:TYR:HD2	6	0.95
(1,1150)	1:A:11:LEU:HD13	1:A:74:TYR:HD2	6	0.95
(1,1150)	1:A:11:LEU:HD21	1:A:74:TYR:HD2	6	0.95
(1,1150)	1:A:11:LEU:HD22	1:A:74:TYR:HD2	6	0.95
(1,1150)	1:A:11:LEU:HD23	1:A:74:TYR:HD2	6	0.95
(1,1150)	1:A:11:LEU:HD11	1:A:74:TYR:HD2	12	0.95
(1,1150)	1:A:11:LEU:HD12	1:A:74:TYR:HD2	12	0.95
(1,1150)	1:A:11:LEU:HD13	1:A:74:TYR:HD2	12	0.95
(1,1150)	1:A:11:LEU:HD21	1:A:74:TYR:HD2	12	0.95
(1,1150)	1:A:11:LEU:HD22	1:A:74:TYR:HD2	12	0.95
(1,1150)	1:A:11:LEU:HD23	1:A:74:TYR:HD2	12	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2839)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	6	0.94
(1,2839)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	6	0.94
(1,2839)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	6	0.94
(1,1078)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	6	0.94
(1,1078)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	6	0.94
(1,1078)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	6	0.94
(1,2836)	1:B:71:PHE:HA	1:B:74:TYR:HD2	15	0.93
(1,1075)	1:A:71:PHE:HA	1:A:74:TYR:HD2	15	0.93
(1,3091)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	13	0.92
(1,3091)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	13	0.92
(1,3091)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	13	0.92
(1,3091)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	13	0.92
(1,3091)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	13	0.92
(1,3091)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	13	0.92
(1,1330)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	13	0.92
(1,1330)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	13	0.92
(1,1330)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	13	0.92
(1,1330)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	13	0.92
(1,1330)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	13	0.92
(1,1330)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	13	0.92
(1,2910)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	12	0.89
(1,2910)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	12	0.89
(1,2910)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	12	0.89
(1,2910)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	12	0.89
(1,2910)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	12	0.89
(1,2910)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	12	0.89
(1,1149)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	12	0.89
(1,1149)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	12	0.89
(1,1149)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	12	0.89
(1,1149)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	12	0.89
(1,1149)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	12	0.89
(1,1149)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	12	0.89
(1,3091)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	15	0.87
(1,3091)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	15	0.87
(1,3091)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	15	0.87
(1,3091)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	15	0.87
(1,3091)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	15	0.87
(1,3091)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	15	0.87
(1,2839)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	4	0.87
(1,2839)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	4	0.87
(1,2839)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	4	0.87
(1,1330)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	15	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	15	0.87
(1,1330)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	15	0.87
(1,1330)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	15	0.87
(1,1330)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	15	0.87
(1,1330)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	15	0.87
(1,1078)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	4	0.87
(1,1078)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	4	0.87
(1,1078)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	4	0.87
(1,2839)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	17	0.86
(1,2839)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	17	0.86
(1,2839)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	17	0.86
(1,1330)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	8	0.86
(1,1330)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	8	0.86
(1,1330)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	8	0.86
(1,1330)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	8	0.86
(1,1330)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	8	0.86
(1,1330)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	8	0.86
(1,3091)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	8	0.85
(1,3091)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	8	0.85
(1,3091)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	8	0.85
(1,3091)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	8	0.85
(1,3091)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	8	0.85
(1,3091)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	8	0.85
(1,2844)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	4	0.85
(1,2844)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	4	0.85
(1,2844)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	4	0.85
(1,2837)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	12	0.85
(1,2837)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	12	0.85
(1,2837)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	12	0.85
(1,2836)	1:B:71:PHE:HA	1:B:74:TYR:HD2	7	0.85
(1,2836)	1:B:71:PHE:HA	1:B:74:TYR:HD2	12	0.85
(1,1083)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	4	0.85
(1,1083)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	4	0.85
(1,1083)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	4	0.85
(1,1078)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	17	0.85
(1,1078)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	17	0.85
(1,1078)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	17	0.85
(1,1075)	1:A:71:PHE:HA	1:A:74:TYR:HD2	7	0.85
(1,1075)	1:A:71:PHE:HA	1:A:74:TYR:HD2	12	0.85
(1,1076)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	12	0.84
(1,1076)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	12	0.84
(1,1076)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	12	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2911)	1:B:11:LEU:HD11	1:B:74:TYR:HD2	7	0.83
(1,2911)	1:B:11:LEU:HD12	1:B:74:TYR:HD2	7	0.83
(1,2911)	1:B:11:LEU:HD13	1:B:74:TYR:HD2	7	0.83
(1,2911)	1:B:11:LEU:HD21	1:B:74:TYR:HD2	7	0.83
(1,2911)	1:B:11:LEU:HD22	1:B:74:TYR:HD2	7	0.83
(1,2911)	1:B:11:LEU:HD23	1:B:74:TYR:HD2	7	0.83
(1,2844)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	7	0.83
(1,2844)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	7	0.83
(1,2844)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	7	0.83
(1,2837)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	14	0.83
(1,2837)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	14	0.83
(1,2837)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	14	0.83
(1,1150)	1:A:11:LEU:HD11	1:A:74:TYR:HD2	7	0.83
(1,1150)	1:A:11:LEU:HD12	1:A:74:TYR:HD2	7	0.83
(1,1150)	1:A:11:LEU:HD13	1:A:74:TYR:HD2	7	0.83
(1,1150)	1:A:11:LEU:HD21	1:A:74:TYR:HD2	7	0.83
(1,1150)	1:A:11:LEU:HD22	1:A:74:TYR:HD2	7	0.83
(1,1150)	1:A:11:LEU:HD23	1:A:74:TYR:HD2	7	0.83
(1,1083)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	7	0.83
(1,1083)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	7	0.83
(1,1083)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	7	0.83
(1,1076)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	14	0.83
(1,1076)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	14	0.83
(1,1076)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	14	0.83
(1,3091)	1:B:36:LEU:HD11	1:B:74:TYR:HE1	9	0.82
(1,3091)	1:B:36:LEU:HD12	1:B:74:TYR:HE1	9	0.82
(1,3091)	1:B:36:LEU:HD13	1:B:74:TYR:HE1	9	0.82
(1,3091)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	9	0.82
(1,3091)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	9	0.82
(1,3091)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	9	0.82
(1,2910)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	6	0.82
(1,2910)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	6	0.82
(1,2910)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	6	0.82
(1,2910)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	6	0.82
(1,2910)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	6	0.82
(1,2910)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	6	0.82
(1,2836)	1:B:71:PHE:HA	1:B:74:TYR:HD2	8	0.82
(1,1330)	1:A:36:LEU:HD11	1:A:74:TYR:HE1	9	0.82
(1,1330)	1:A:36:LEU:HD12	1:A:74:TYR:HE1	9	0.82
(1,1330)	1:A:36:LEU:HD13	1:A:74:TYR:HE1	9	0.82
(1,1330)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	9	0.82
(1,1330)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	9	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	9	0.82
(1,1149)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	6	0.82
(1,1149)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	6	0.82
(1,1149)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	6	0.82
(1,1149)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	6	0.82
(1,1149)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	6	0.82
(1,1149)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	6	0.82
(1,1075)	1:A:71:PHE:HA	1:A:74:TYR:HD2	8	0.82
(1,2844)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	6	0.81
(1,2844)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	6	0.81
(1,2844)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	6	0.81
(1,2839)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	14	0.81
(1,2839)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	14	0.81
(1,2839)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	14	0.81
(1,1083)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	6	0.81
(1,1083)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	6	0.81
(1,1083)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	6	0.81
(1,1078)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	14	0.81
(1,1078)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	14	0.81
(1,1078)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	14	0.81
(1,3106)	1:B:37:LEU:HD11	1:B:74:TYR:HE1	15	0.78
(1,3106)	1:B:37:LEU:HD12	1:B:74:TYR:HE1	15	0.78
(1,3106)	1:B:37:LEU:HD13	1:B:74:TYR:HE1	15	0.78
(1,3106)	1:B:37:LEU:HD21	1:B:74:TYR:HE1	15	0.78
(1,3106)	1:B:37:LEU:HD22	1:B:74:TYR:HE1	15	0.78
(1,3106)	1:B:37:LEU:HD23	1:B:74:TYR:HE1	15	0.78
(1,2844)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	17	0.78
(1,2844)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	17	0.78
(1,2844)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	17	0.78
(1,2839)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	7	0.78
(1,2839)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	7	0.78
(1,2839)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	7	0.78
(1,2836)	1:B:71:PHE:HA	1:B:74:TYR:HD2	14	0.78
(1,1345)	1:A:37:LEU:HD11	1:A:74:TYR:HE1	15	0.78
(1,1345)	1:A:37:LEU:HD12	1:A:74:TYR:HE1	15	0.78
(1,1345)	1:A:37:LEU:HD13	1:A:74:TYR:HE1	15	0.78
(1,1345)	1:A:37:LEU:HD21	1:A:74:TYR:HE1	15	0.78
(1,1345)	1:A:37:LEU:HD22	1:A:74:TYR:HE1	15	0.78
(1,1345)	1:A:37:LEU:HD23	1:A:74:TYR:HE1	15	0.78
(1,1083)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	17	0.78
(1,1083)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	17	0.78
(1,1083)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	17	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	7	0.78
(1,1078)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	7	0.78
(1,1078)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	7	0.78
(1,1075)	1:A:71:PHE:HA	1:A:74:TYR:HD2	14	0.78
(1,2846)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	13	0.77
(1,2846)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	13	0.77
(1,2846)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	13	0.77
(1,1085)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	13	0.77
(1,1085)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	13	0.77
(1,1085)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	13	0.77
(1,2839)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	13	0.75
(1,2839)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	13	0.75
(1,2839)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	13	0.75
(1,1078)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	13	0.75
(1,1078)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	13	0.75
(1,1078)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	13	0.75
(1,2846)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	8	0.74
(1,2846)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	8	0.74
(1,2846)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	8	0.74
(1,1085)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	8	0.74
(1,1085)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	8	0.74
(1,1085)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	8	0.74
(1,2839)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	15	0.73
(1,2839)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	15	0.73
(1,2839)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	15	0.73
(1,1078)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	15	0.73
(1,1078)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	15	0.73
(1,1078)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	15	0.73
(1,2837)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	6	0.72
(1,2837)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	6	0.72
(1,2837)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	6	0.72
(1,1076)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	6	0.72
(1,1076)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	6	0.72
(1,1076)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	6	0.72
(1,2837)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	9	0.7
(1,2837)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	9	0.7
(1,2837)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	9	0.7
(1,2836)	1:B:71:PHE:HA	1:B:74:TYR:HD2	17	0.7
(1,1076)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	9	0.7
(1,1076)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	9	0.7
(1,1076)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	9	0.7
(1,1075)	1:A:71:PHE:HA	1:A:74:TYR:HD2	17	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2844)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	14	0.68
(1,2844)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	14	0.68
(1,2844)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	14	0.68
(1,1083)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	14	0.68
(1,1083)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	14	0.68
(1,1083)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	14	0.68
(1,2846)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	15	0.66
(1,2846)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	15	0.66
(1,2846)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	15	0.66
(1,2839)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	9	0.66
(1,2839)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	9	0.66
(1,2839)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	9	0.66
(1,1085)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	15	0.66
(1,1085)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	15	0.66
(1,1085)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	15	0.66
(1,1078)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	9	0.66
(1,1078)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	9	0.66
(1,1078)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	9	0.66
(1,2844)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	13	0.6
(1,2844)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	13	0.6
(1,2844)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	13	0.6
(1,2844)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	15	0.6
(1,2844)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	15	0.6
(1,2844)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	15	0.6
(1,1083)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	13	0.6
(1,1083)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	13	0.6
(1,1083)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	13	0.6
(1,1083)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	15	0.6
(1,1083)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	15	0.6
(1,1083)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	15	0.6
(1,2839)	1:B:36:LEU:HD21	1:B:74:TYR:HD1	8	0.59
(1,2839)	1:B:36:LEU:HD22	1:B:74:TYR:HD1	8	0.59
(1,2839)	1:B:36:LEU:HD23	1:B:74:TYR:HD1	8	0.59
(1,2837)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	17	0.59
(1,2837)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	17	0.59
(1,2837)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	17	0.59
(1,1078)	1:A:36:LEU:HD21	1:A:74:TYR:HD1	8	0.59
(1,1078)	1:A:36:LEU:HD22	1:A:74:TYR:HD1	8	0.59
(1,1078)	1:A:36:LEU:HD23	1:A:74:TYR:HD1	8	0.59
(1,1076)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	17	0.59
(1,1076)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	17	0.59
(1,1076)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	17	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2846)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	14	0.58
(1,2846)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	14	0.58
(1,2846)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	14	0.58
(1,2837)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	7	0.58
(1,2837)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	7	0.58
(1,2837)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	7	0.58
(1,1085)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	14	0.58
(1,1085)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	14	0.58
(1,1085)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	14	0.58
(1,1076)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	7	0.58
(1,1076)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	7	0.58
(1,1076)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	7	0.58
(1,3106)	1:B:37:LEU:HD11	1:B:74:TYR:HE1	7	0.57
(1,3106)	1:B:37:LEU:HD12	1:B:74:TYR:HE1	7	0.57
(1,3106)	1:B:37:LEU:HD13	1:B:74:TYR:HE1	7	0.57
(1,3106)	1:B:37:LEU:HD21	1:B:74:TYR:HE1	7	0.57
(1,3106)	1:B:37:LEU:HD22	1:B:74:TYR:HE1	7	0.57
(1,3106)	1:B:37:LEU:HD23	1:B:74:TYR:HE1	7	0.57
(1,3106)	1:B:37:LEU:HD11	1:B:74:TYR:HE1	9	0.57
(1,3106)	1:B:37:LEU:HD12	1:B:74:TYR:HE1	9	0.57
(1,3106)	1:B:37:LEU:HD13	1:B:74:TYR:HE1	9	0.57
(1,3106)	1:B:37:LEU:HD21	1:B:74:TYR:HE1	9	0.57
(1,3106)	1:B:37:LEU:HD22	1:B:74:TYR:HE1	9	0.57
(1,3106)	1:B:37:LEU:HD23	1:B:74:TYR:HE1	9	0.57
(1,2910)	1:B:11:LEU:HD11	1:B:74:TYR:HE2	7	0.57
(1,2910)	1:B:11:LEU:HD12	1:B:74:TYR:HE2	7	0.57
(1,2910)	1:B:11:LEU:HD13	1:B:74:TYR:HE2	7	0.57
(1,2910)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	7	0.57
(1,2910)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	7	0.57
(1,2910)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	7	0.57
(1,2846)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	17	0.57
(1,2846)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	17	0.57
(1,2846)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	17	0.57
(1,2837)	1:B:33:LEU:HD11	1:B:74:TYR:HD1	4	0.57
(1,2837)	1:B:33:LEU:HD12	1:B:74:TYR:HD1	4	0.57
(1,2837)	1:B:33:LEU:HD13	1:B:74:TYR:HD1	4	0.57
(1,1345)	1:A:37:LEU:HD11	1:A:74:TYR:HE1	7	0.57
(1,1345)	1:A:37:LEU:HD12	1:A:74:TYR:HE1	7	0.57
(1,1345)	1:A:37:LEU:HD13	1:A:74:TYR:HE1	7	0.57
(1,1345)	1:A:37:LEU:HD21	1:A:74:TYR:HE1	7	0.57
(1,1345)	1:A:37:LEU:HD22	1:A:74:TYR:HE1	7	0.57
(1,1345)	1:A:37:LEU:HD23	1:A:74:TYR:HE1	7	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:A:37:LEU:HD11	1:A:74:TYR:HE1	9	0.57
(1,1345)	1:A:37:LEU:HD12	1:A:74:TYR:HE1	9	0.57
(1,1345)	1:A:37:LEU:HD13	1:A:74:TYR:HE1	9	0.57
(1,1345)	1:A:37:LEU:HD21	1:A:74:TYR:HE1	9	0.57
(1,1345)	1:A:37:LEU:HD22	1:A:74:TYR:HE1	9	0.57
(1,1345)	1:A:37:LEU:HD23	1:A:74:TYR:HE1	9	0.57
(1,1149)	1:A:11:LEU:HD11	1:A:74:TYR:HE2	7	0.57
(1,1149)	1:A:11:LEU:HD12	1:A:74:TYR:HE2	7	0.57
(1,1149)	1:A:11:LEU:HD13	1:A:74:TYR:HE2	7	0.57
(1,1149)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	7	0.57
(1,1149)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	7	0.57
(1,1149)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	7	0.57
(1,1085)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	17	0.57
(1,1085)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	17	0.57
(1,1085)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	17	0.57
(1,1076)	1:A:33:LEU:HD11	1:A:74:TYR:HD1	4	0.57
(1,1076)	1:A:33:LEU:HD12	1:A:74:TYR:HD1	4	0.57
(1,1076)	1:A:33:LEU:HD13	1:A:74:TYR:HD1	4	0.57
(1,2846)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	9	0.56
(1,2846)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	9	0.56
(1,2846)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	9	0.56
(1,1085)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	9	0.56
(1,1085)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	9	0.56
(1,1085)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	9	0.56
(1,1083)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	8	0.56
(1,1083)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	8	0.56
(1,1083)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	8	0.56
(1,2844)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	8	0.55
(1,2844)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	8	0.55
(1,2844)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	8	0.55
(1,3106)	1:B:37:LEU:HD11	1:B:74:TYR:HE1	4	0.53
(1,3106)	1:B:37:LEU:HD12	1:B:74:TYR:HE1	4	0.53
(1,3106)	1:B:37:LEU:HD13	1:B:74:TYR:HE1	4	0.53
(1,3106)	1:B:37:LEU:HD21	1:B:74:TYR:HE1	4	0.53
(1,3106)	1:B:37:LEU:HD22	1:B:74:TYR:HE1	4	0.53
(1,3106)	1:B:37:LEU:HD23	1:B:74:TYR:HE1	4	0.53
(1,1345)	1:A:37:LEU:HD11	1:A:74:TYR:HE1	4	0.53
(1,1345)	1:A:37:LEU:HD12	1:A:74:TYR:HE1	4	0.53
(1,1345)	1:A:37:LEU:HD13	1:A:74:TYR:HE1	4	0.53
(1,1345)	1:A:37:LEU:HD21	1:A:74:TYR:HE1	4	0.53
(1,1345)	1:A:37:LEU:HD22	1:A:74:TYR:HE1	4	0.53
(1,1345)	1:A:37:LEU:HD23	1:A:74:TYR:HE1	4	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2846)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	4	0.51
(1,2846)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	4	0.51
(1,2846)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	4	0.51
(1,1085)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	4	0.51
(1,1085)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	4	0.51
(1,1085)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	4	0.51
(1,3106)	1:B:37:LEU:HD11	1:B:74:TYR:HE1	17	0.49
(1,3106)	1:B:37:LEU:HD12	1:B:74:TYR:HE1	17	0.49
(1,3106)	1:B:37:LEU:HD13	1:B:74:TYR:HE1	17	0.49
(1,3106)	1:B:37:LEU:HD21	1:B:74:TYR:HE1	17	0.49
(1,3106)	1:B:37:LEU:HD22	1:B:74:TYR:HE1	17	0.49
(1,3106)	1:B:37:LEU:HD23	1:B:74:TYR:HE1	17	0.49
(1,1345)	1:A:37:LEU:HD11	1:A:74:TYR:HE1	17	0.49
(1,1345)	1:A:37:LEU:HD12	1:A:74:TYR:HE1	17	0.49
(1,1345)	1:A:37:LEU:HD13	1:A:74:TYR:HE1	17	0.49
(1,1345)	1:A:37:LEU:HD21	1:A:74:TYR:HE1	17	0.49
(1,1345)	1:A:37:LEU:HD22	1:A:74:TYR:HE1	17	0.49
(1,1345)	1:A:37:LEU:HD23	1:A:74:TYR:HE1	17	0.49
(1,2844)	1:B:36:LEU:HD21	1:B:74:TYR:HE1	9	0.46
(1,2844)	1:B:36:LEU:HD22	1:B:74:TYR:HE1	9	0.46
(1,2844)	1:B:36:LEU:HD23	1:B:74:TYR:HE1	9	0.46
(1,1083)	1:A:36:LEU:HD21	1:A:74:TYR:HE1	9	0.46
(1,1083)	1:A:36:LEU:HD22	1:A:74:TYR:HE1	9	0.46
(1,1083)	1:A:36:LEU:HD23	1:A:74:TYR:HE1	9	0.46
(1,3106)	1:B:37:LEU:HD11	1:B:74:TYR:HE1	14	0.45
(1,3106)	1:B:37:LEU:HD12	1:B:74:TYR:HE1	14	0.45
(1,3106)	1:B:37:LEU:HD13	1:B:74:TYR:HE1	14	0.45
(1,3106)	1:B:37:LEU:HD21	1:B:74:TYR:HE1	14	0.45
(1,3106)	1:B:37:LEU:HD22	1:B:74:TYR:HE1	14	0.45
(1,3106)	1:B:37:LEU:HD23	1:B:74:TYR:HE1	14	0.45
(1,1345)	1:A:37:LEU:HD11	1:A:74:TYR:HE1	14	0.45
(1,1345)	1:A:37:LEU:HD12	1:A:74:TYR:HE1	14	0.45
(1,1345)	1:A:37:LEU:HD13	1:A:74:TYR:HE1	14	0.45
(1,1345)	1:A:37:LEU:HD21	1:A:74:TYR:HE1	14	0.45
(1,1345)	1:A:37:LEU:HD22	1:A:74:TYR:HE1	14	0.45
(1,1345)	1:A:37:LEU:HD23	1:A:74:TYR:HE1	14	0.45
(1,3106)	1:B:37:LEU:HD11	1:B:74:TYR:HE1	13	0.42
(1,3106)	1:B:37:LEU:HD12	1:B:74:TYR:HE1	13	0.42
(1,3106)	1:B:37:LEU:HD13	1:B:74:TYR:HE1	13	0.42
(1,3106)	1:B:37:LEU:HD21	1:B:74:TYR:HE1	13	0.42
(1,3106)	1:B:37:LEU:HD22	1:B:74:TYR:HE1	13	0.42
(1,3106)	1:B:37:LEU:HD23	1:B:74:TYR:HE1	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:A:37:LEU:HD11	1:A:74:TYR:HE1	13	0.42
(1,1345)	1:A:37:LEU:HD12	1:A:74:TYR:HE1	13	0.42
(1,1345)	1:A:37:LEU:HD13	1:A:74:TYR:HE1	13	0.42
(1,1345)	1:A:37:LEU:HD21	1:A:74:TYR:HE1	13	0.42
(1,1345)	1:A:37:LEU:HD22	1:A:74:TYR:HE1	13	0.42
(1,1345)	1:A:37:LEU:HD23	1:A:74:TYR:HE1	13	0.42
(1,3834)	1:A:4:LEU:HD21	1:B:74:TYR:HE1	7	0.35
(1,3834)	1:A:4:LEU:HD22	1:B:74:TYR:HE1	7	0.35
(1,3834)	1:A:4:LEU:HD23	1:B:74:TYR:HE1	7	0.35
(1,3835)	1:A:74:TYR:HE1	1:B:4:LEU:HD21	7	0.34
(1,3835)	1:A:74:TYR:HE1	1:B:4:LEU:HD22	7	0.34
(1,3835)	1:A:74:TYR:HE1	1:B:4:LEU:HD23	7	0.34
(1,2850)	1:B:15:PHE:HA	1:B:74:TYR:HE1	17	0.33
(1,1089)	1:A:15:PHE:HA	1:A:74:TYR:HE1	17	0.33
(1,2846)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	12	0.28
(1,2846)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	12	0.28
(1,2846)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	12	0.28
(1,1085)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	12	0.28
(1,1085)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	12	0.28
(1,1085)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	12	0.28
(1,2846)	1:B:11:LEU:HD21	1:B:74:TYR:HE2	6	0.22
(1,2846)	1:B:11:LEU:HD22	1:B:74:TYR:HE2	6	0.22
(1,2846)	1:B:11:LEU:HD23	1:B:74:TYR:HE2	6	0.22
(1,1085)	1:A:11:LEU:HD21	1:A:74:TYR:HE2	6	0.22
(1,1085)	1:A:11:LEU:HD22	1:A:74:TYR:HE2	6	0.22
(1,1085)	1:A:11:LEU:HD23	1:A:74:TYR:HE2	6	0.22
(1,309)	1:A:47:ALA:HA	1:A:48:GLN:H	12	0.21
(1,2070)	1:B:47:ALA:HA	1:B:48:GLN:H	12	0.2
(1,2850)	1:B:15:PHE:HA	1:B:74:TYR:HE1	13	0.17
(1,2850)	1:B:15:PHE:HA	1:B:74:TYR:HE1	14	0.17
(1,1089)	1:A:15:PHE:HA	1:A:74:TYR:HE1	13	0.17
(1,1089)	1:A:15:PHE:HA	1:A:74:TYR:HE1	14	0.17
(1,2933)	1:B:14:VAL:HG11	1:B:74:TYR:HE1	7	0.16
(1,2933)	1:B:14:VAL:HG12	1:B:74:TYR:HE1	7	0.16
(1,2933)	1:B:14:VAL:HG13	1:B:74:TYR:HE1	7	0.16
(1,2933)	1:B:14:VAL:HG21	1:B:74:TYR:HE1	7	0.16
(1,2933)	1:B:14:VAL:HG22	1:B:74:TYR:HE1	7	0.16
(1,2933)	1:B:14:VAL:HG23	1:B:74:TYR:HE1	7	0.16
(1,1172)	1:A:14:VAL:HG11	1:A:74:TYR:HE1	7	0.16
(1,1172)	1:A:14:VAL:HG12	1:A:74:TYR:HE1	7	0.16
(1,1172)	1:A:14:VAL:HG13	1:A:74:TYR:HE1	7	0.16
(1,1172)	1:A:14:VAL:HG21	1:A:74:TYR:HE1	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:A:14:VAL:HG22	1:A:74:TYR:HE1	7	0.16
(1,1172)	1:A:14:VAL:HG23	1:A:74:TYR:HE1	7	0.16
(1,396)	1:A:59:LYS:H	1:A:59:LYS:HG3	2	0.14
(1,2157)	1:B:59:LYS:H	1:B:59:LYS:HG3	2	0.14
(1,916)	1:A:56:LYS:HA	1:A:59:LYS:HG2	2	0.13
(1,2677)	1:B:56:LYS:HA	1:B:59:LYS:HG2	2	0.13
(1,247)	1:A:38:GLN:H	1:A:38:GLN:HG3	2	0.13
(1,2008)	1:B:38:GLN:H	1:B:38:GLN:HG3	2	0.13
(1,3106)	1:B:37:LEU:HD11	1:B:74:TYR:HE1	12	0.12
(1,3106)	1:B:37:LEU:HD12	1:B:74:TYR:HE1	12	0.12
(1,3106)	1:B:37:LEU:HD13	1:B:74:TYR:HE1	12	0.12
(1,3106)	1:B:37:LEU:HD21	1:B:74:TYR:HE1	12	0.12
(1,3106)	1:B:37:LEU:HD22	1:B:74:TYR:HE1	12	0.12
(1,3106)	1:B:37:LEU:HD23	1:B:74:TYR:HE1	12	0.12
(1,1345)	1:A:37:LEU:HD11	1:A:74:TYR:HE1	12	0.12
(1,1345)	1:A:37:LEU:HD12	1:A:74:TYR:HE1	12	0.12
(1,1345)	1:A:37:LEU:HD13	1:A:74:TYR:HE1	12	0.12
(1,1345)	1:A:37:LEU:HD21	1:A:74:TYR:HE1	12	0.12
(1,1345)	1:A:37:LEU:HD22	1:A:74:TYR:HE1	12	0.12
(1,1345)	1:A:37:LEU:HD23	1:A:74:TYR:HE1	12	0.12
(1,247)	1:A:38:GLN:H	1:A:38:GLN:HG3	8	0.11
(1,247)	1:A:38:GLN:H	1:A:38:GLN:HG3	12	0.11
(1,2008)	1:B:38:GLN:H	1:B:38:GLN:HG3	8	0.11
(1,2008)	1:B:38:GLN:H	1:B:38:GLN:HG3	12	0.11

10 Dihedral-angle violation analysis

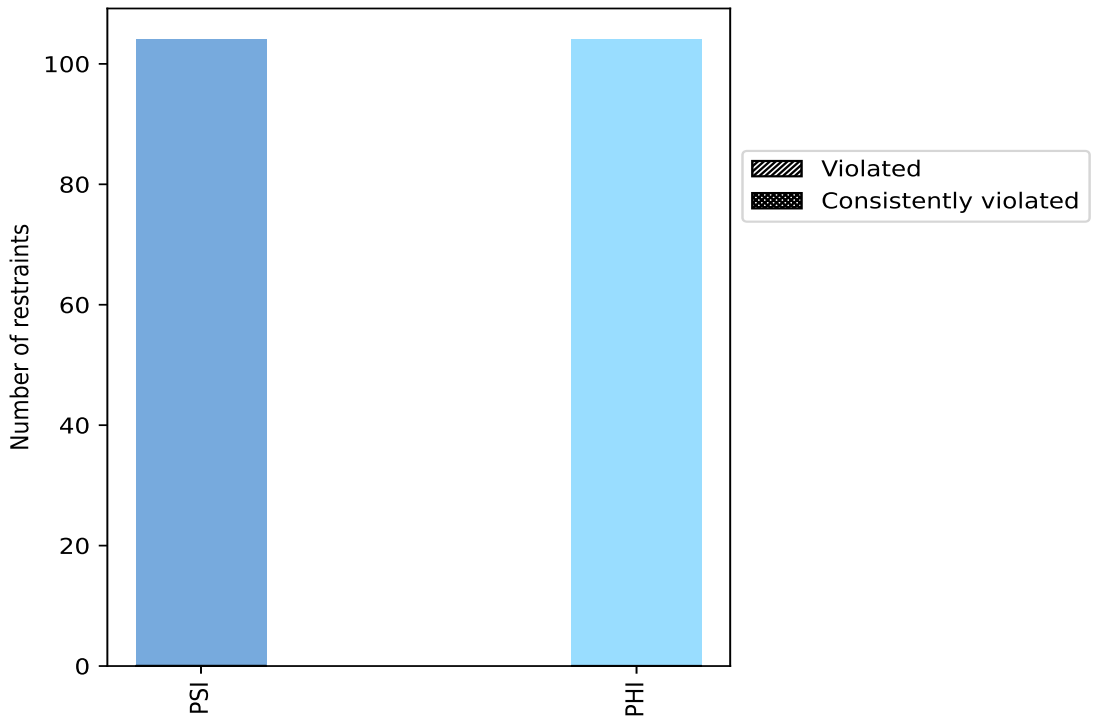
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	104	50.0	0	0.0	0.0	0	0.0	0.0
PHI	104	50.0	0	0.0	0.0	0	0.0	0.0
Total	208	100.0	0	0.0	0.0	0	0.0	0.0

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

No violations found

10.3 Dihedral-angle violation statistics for the ensemble (i)

No violations found

10.4 Most violated dihedral-angle restraints in the ensemble (i)

No violations found

10.5 All violated dihedral-angle restraints (i)

No violations found