Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 08:02 PM EDT

PDB ID	:	2MY1
BMRB ID	:	25439
Title	:	Solution structure of Bud31p
Authors	:	van Roon, A.M.; Yang, J.; Mathieu, D.; Bermel, W.; Nagai, K.; Neuhaus, D.
Deposited on	:	2015-01-19

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

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

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

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

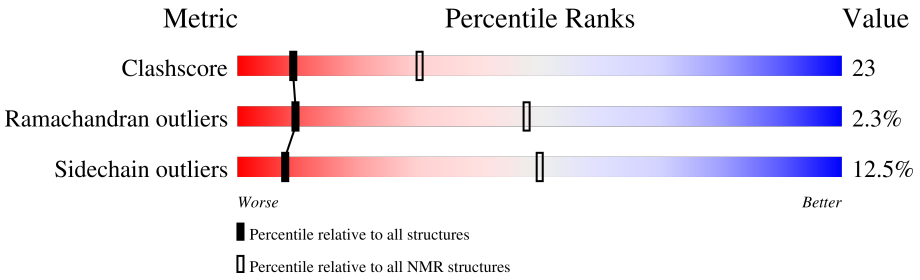
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 78%.

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	159	52% 25% . 19%

2 Ensemble composition and analysis (i)

This entry contains 35 models. Model 2 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:12-A:36, A:45-A:110, A:119-A:155 (128)	0.61	2

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 6 clusters and 5 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2614 atoms, of which 1314 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	159	2611	810	1314	242	235	10	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P25337
A	0	GLY	-	expression tag	UNP P25337
A	1	SER	-	expression tag	UNP P25337

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	3	3	3

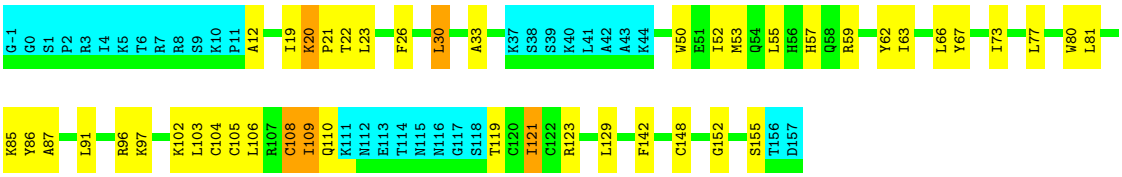
4 Residue-property plots

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: Pre-mRNA-splicing factor BUD31

Chain A:



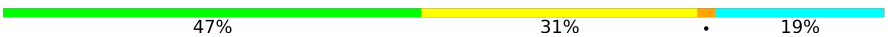
4.2 Scores per residue for each member of the ensemble

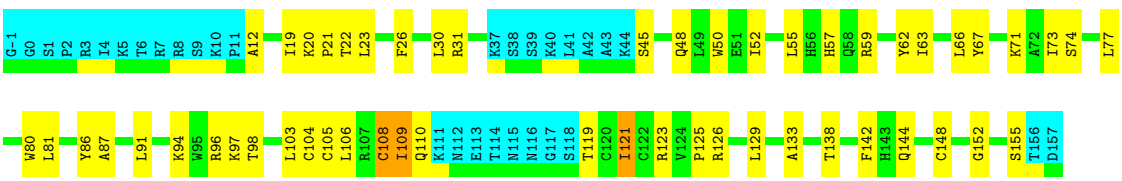
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Pre-mRNA-splicing factor BUD31

Chain A:

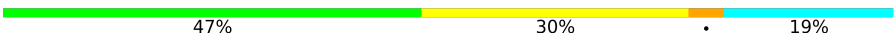


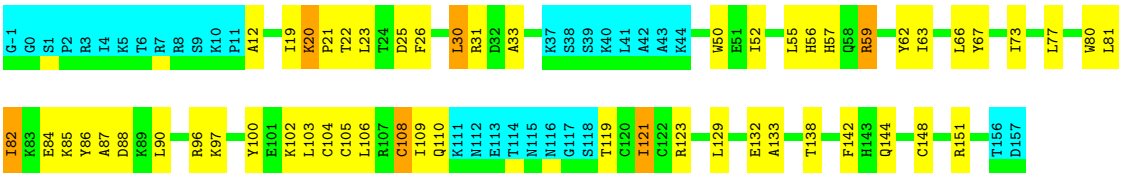


4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Pre-mRNA-splicing factor BUD31

Chain A:

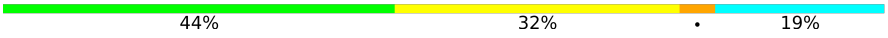


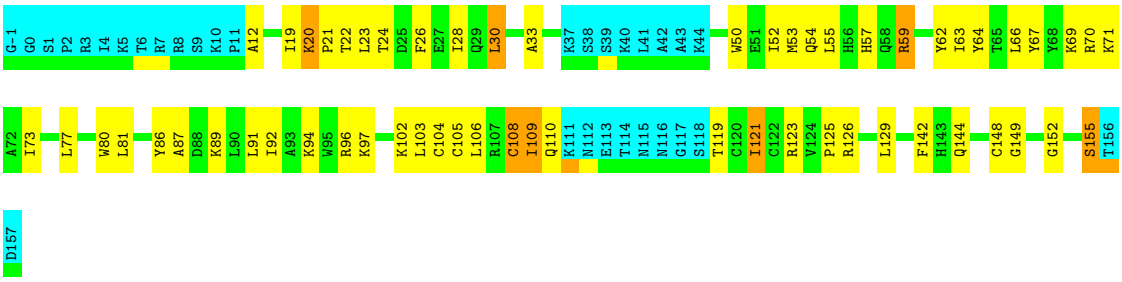


4.2.3 Score per residue for model 3

• Molecule 1: Pre-mRNA-splicing factor BUD31

Chain A:

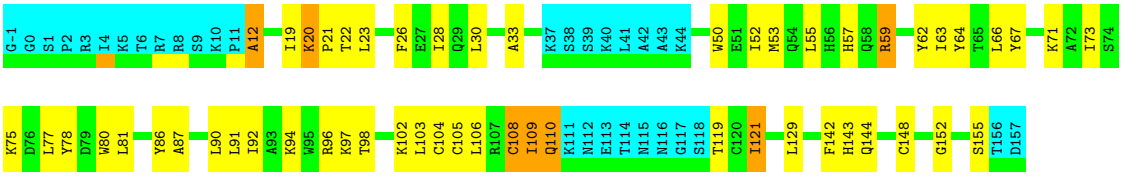




4.2.4 Score per residue for model 4

• Molecule 1: Pre-mRNA-splicing factor BUD31

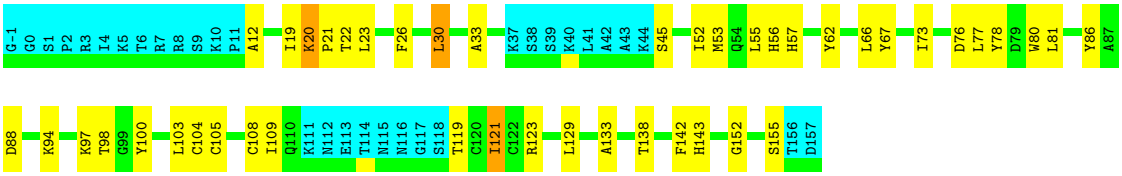
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Pre-mRNA-splicing factor BUD31

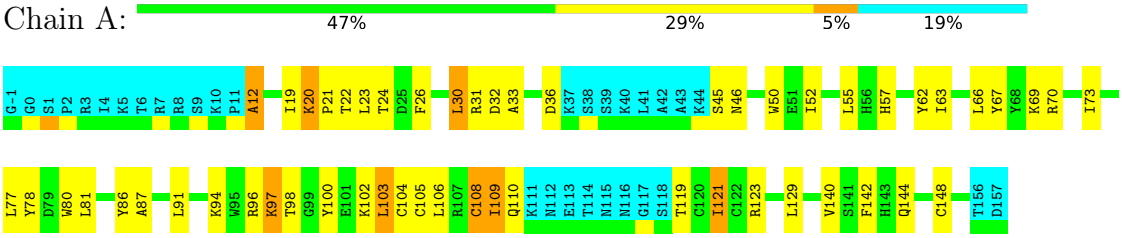
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Pre-mRNA-splicing factor BUD31

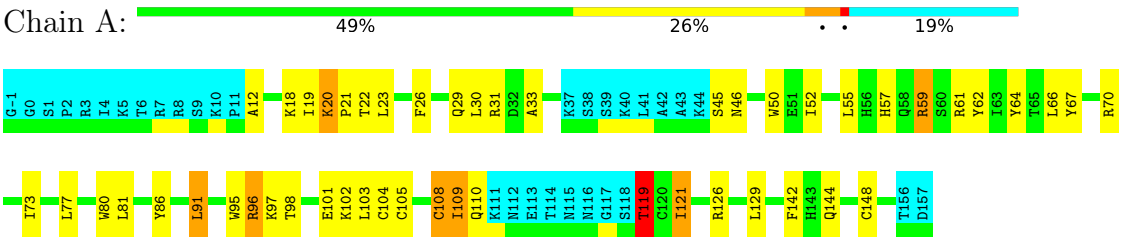
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Pre-mRNA-splicing factor BUD31

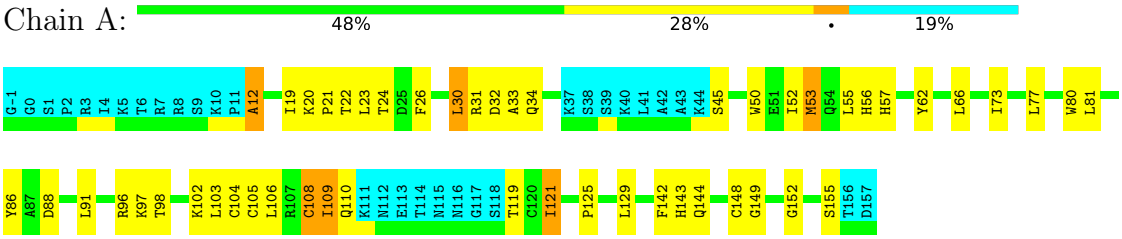
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Pre-mRNA-splicing factor BUD31

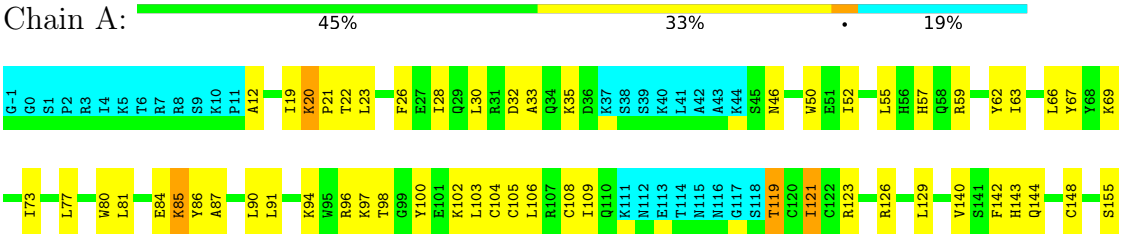
Chain A:



4.2.9 Score per residue for model 9

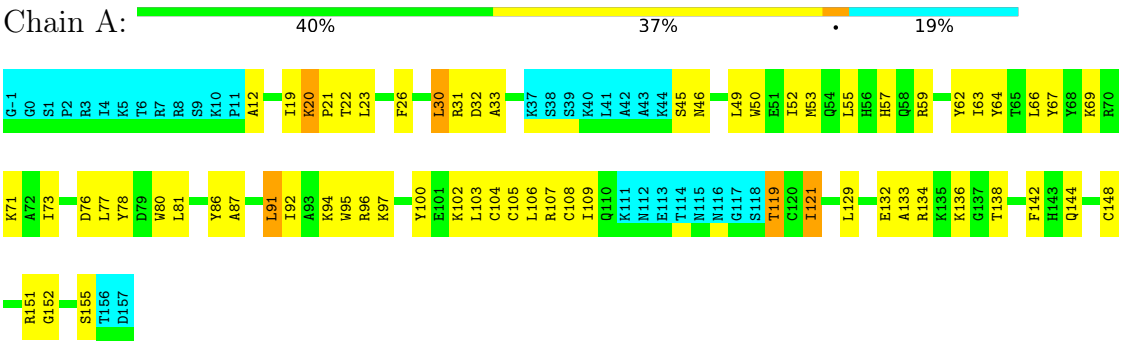
• Molecule 1: Pre-mRNA-splicing factor BUD31

Chain A:



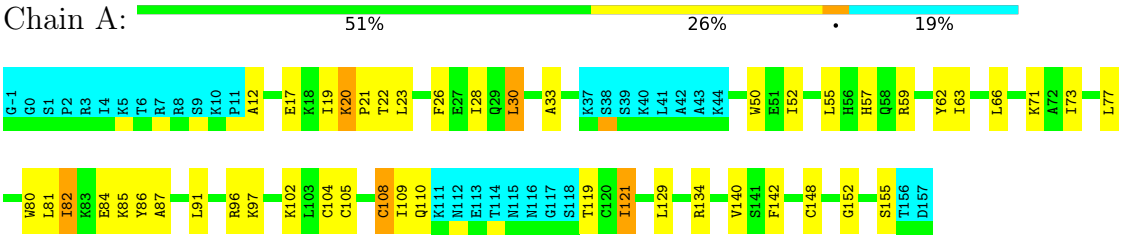
4.2.10 Score per residue for model 10

• Molecule 1: Pre-mRNA-splicing factor BUD31



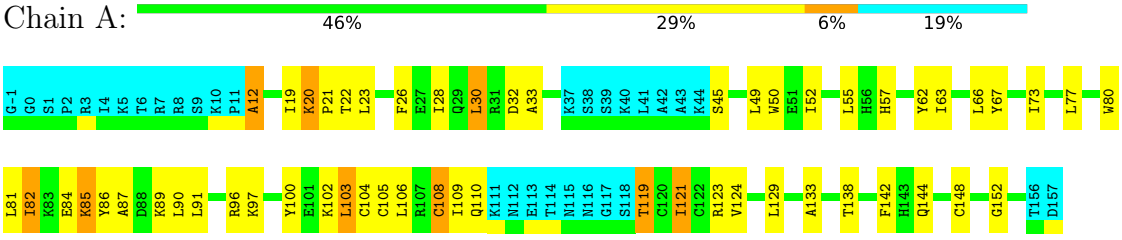
4.2.11 Score per residue for model 11

• Molecule 1: Pre-mRNA-splicing factor BUD31



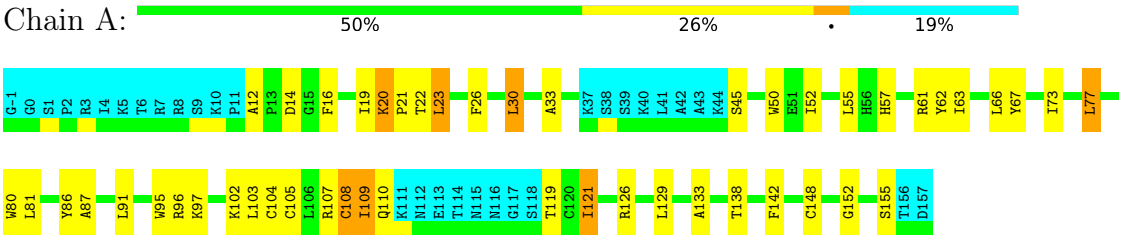
4.2.12 Score per residue for model 12

• Molecule 1: Pre-mRNA-splicing factor BUD31



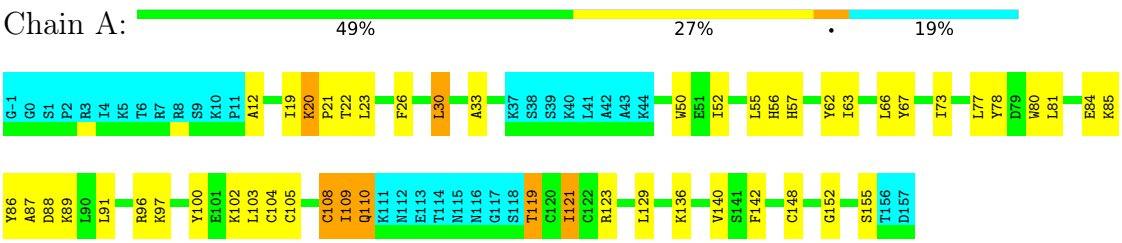
4.2.13 Score per residue for model 13

• Molecule 1: Pre-mRNA-splicing factor BUD31



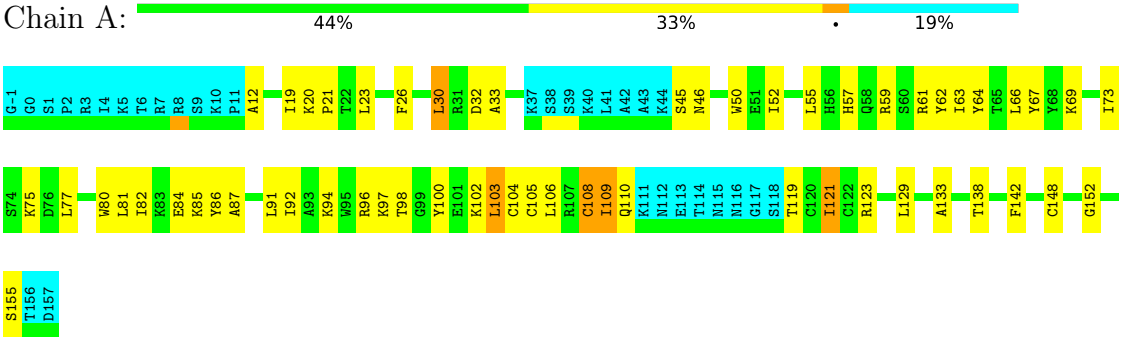
4.2.14 Score per residue for model 14

• Molecule 1: Pre-mRNA-splicing factor BUD31



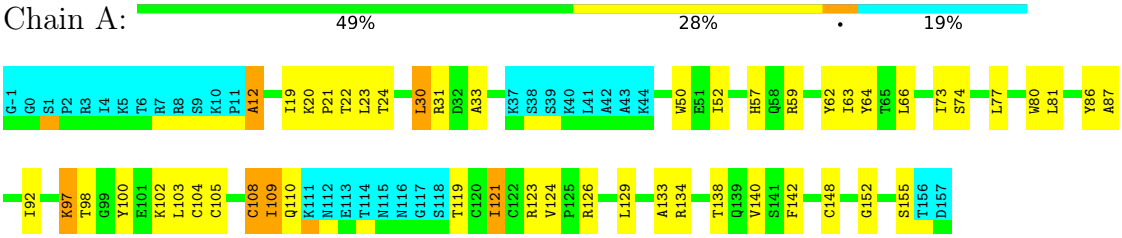
4.2.15 Score per residue for model 15

• Molecule 1: Pre-mRNA-splicing factor BUD31



4.2.16 Score per residue for model 16

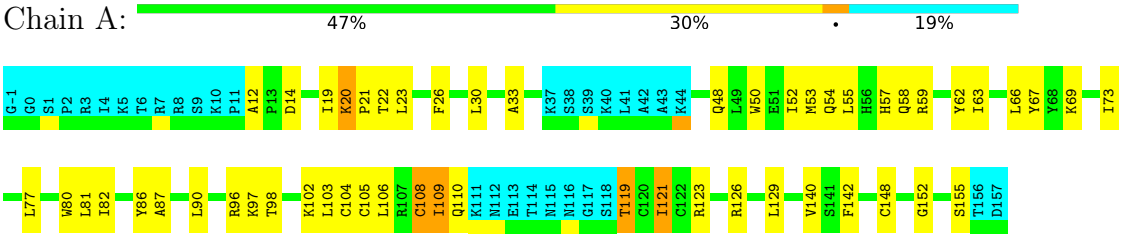
• Molecule 1: Pre-mRNA-splicing factor BUD31



4.2.17 Score per residue for model 17

• Molecule 1: Pre-mRNA-splicing factor BUD31

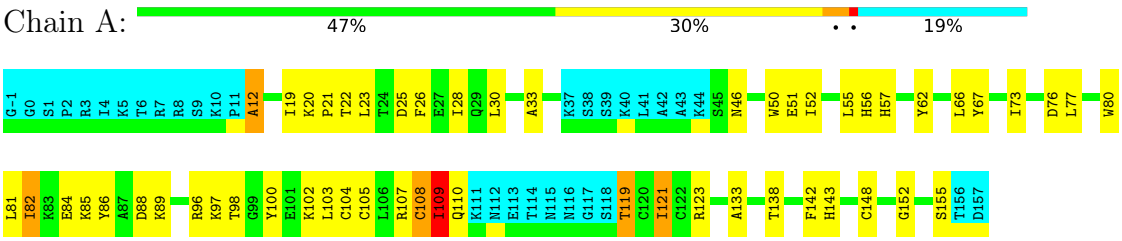
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Pre-mRNA-splicing factor BUD31

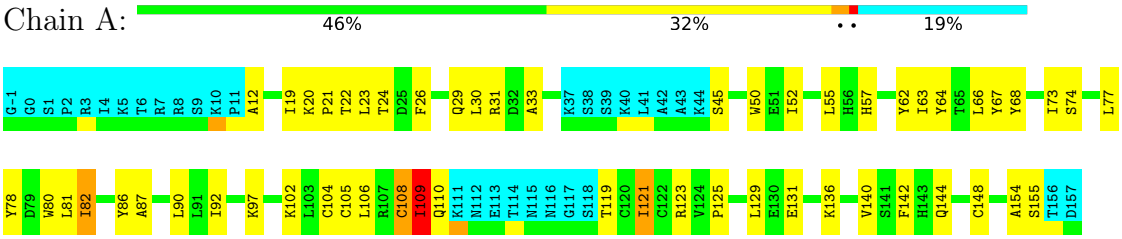
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Pre-mRNA-splicing factor BUD31

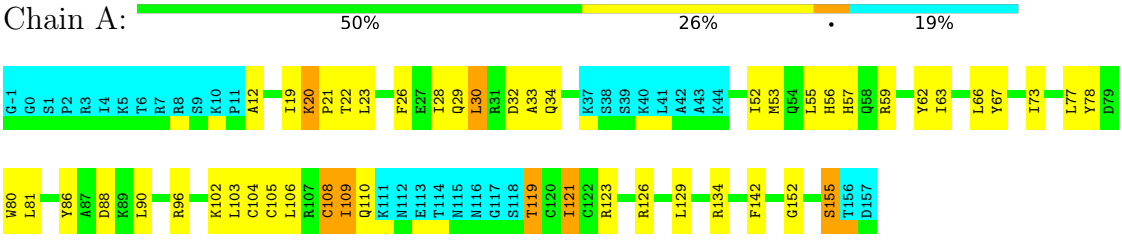
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Pre-mRNA-splicing factor BUD31

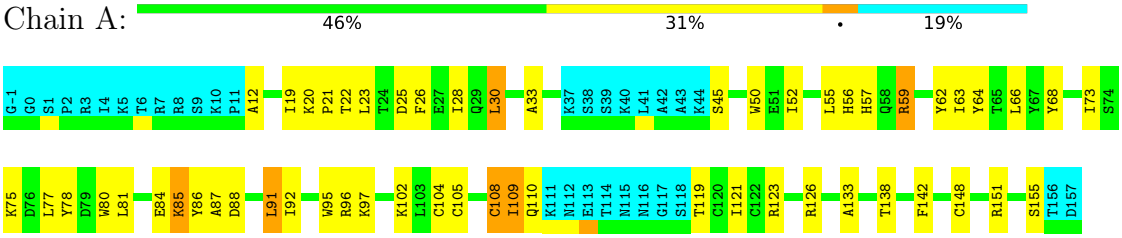
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: Pre-mRNA-splicing factor BUD31

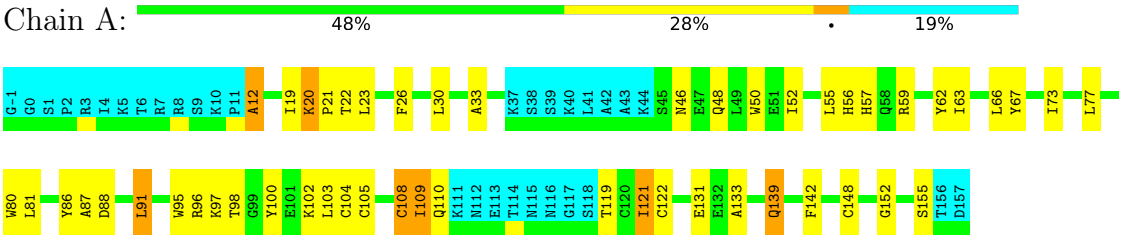
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: Pre-mRNA-splicing factor BUD31

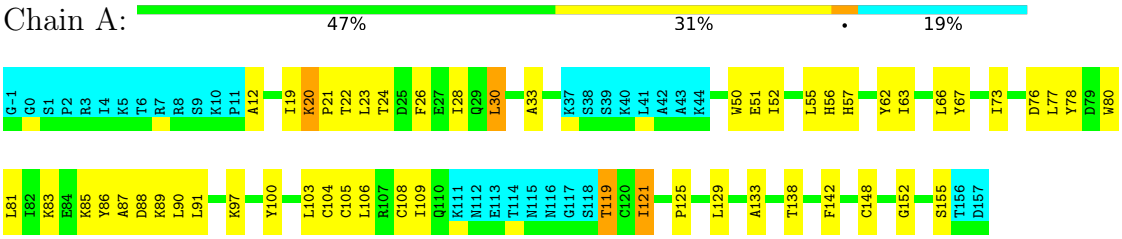
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: Pre-mRNA-splicing factor BUD31

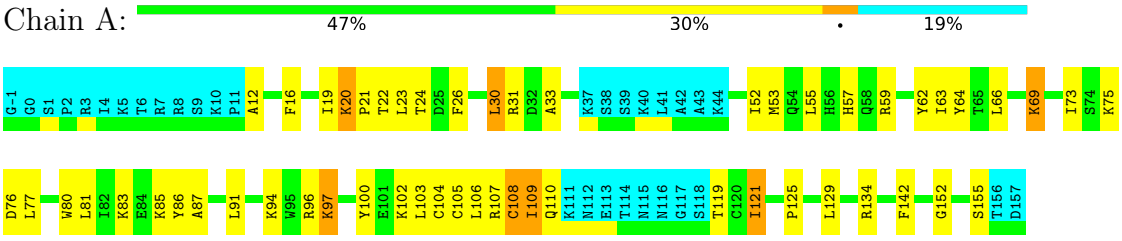
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: Pre-mRNA-splicing factor BUD31

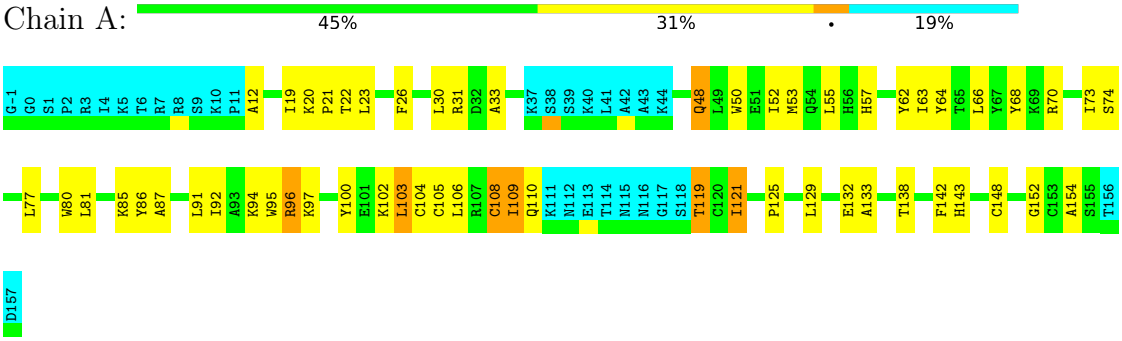
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: Pre-mRNA-splicing factor BUD31

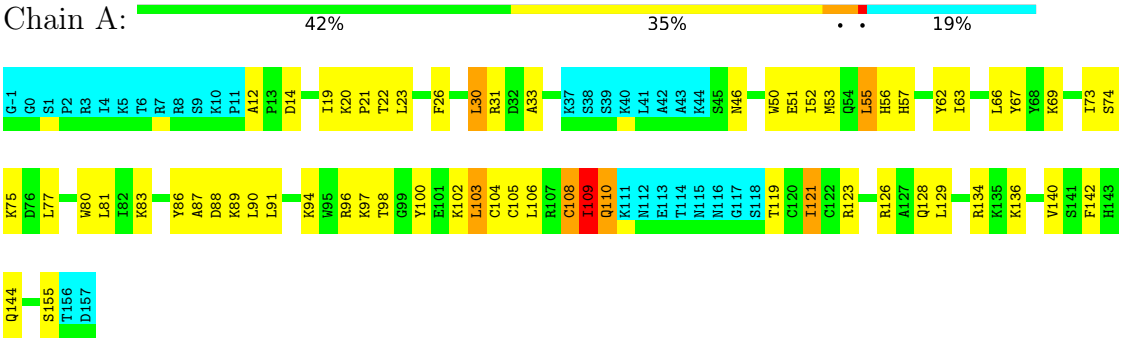
Chain A:



4.2.26 Score per residue for model 26

• Molecule 1: Pre-mRNA-splicing factor BUD31

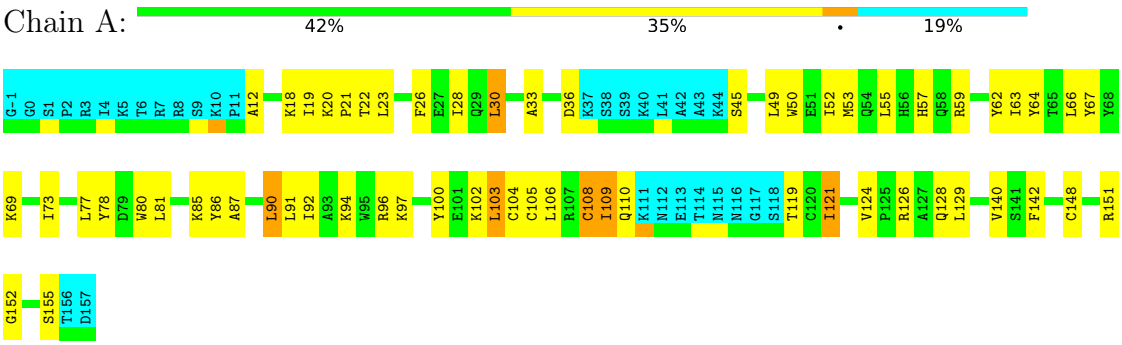
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: Pre-mRNA-splicing factor BUD31

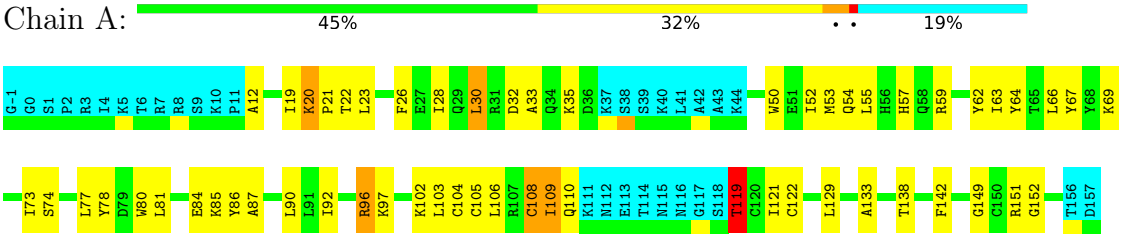
Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: Pre-mRNA-splicing factor BUD31

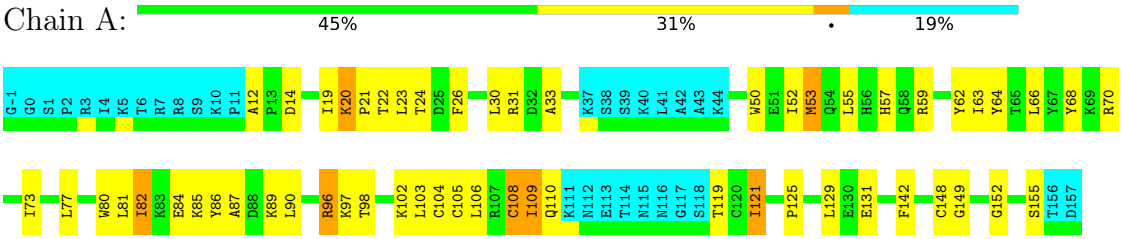
Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: Pre-mRNA-splicing factor BUD31

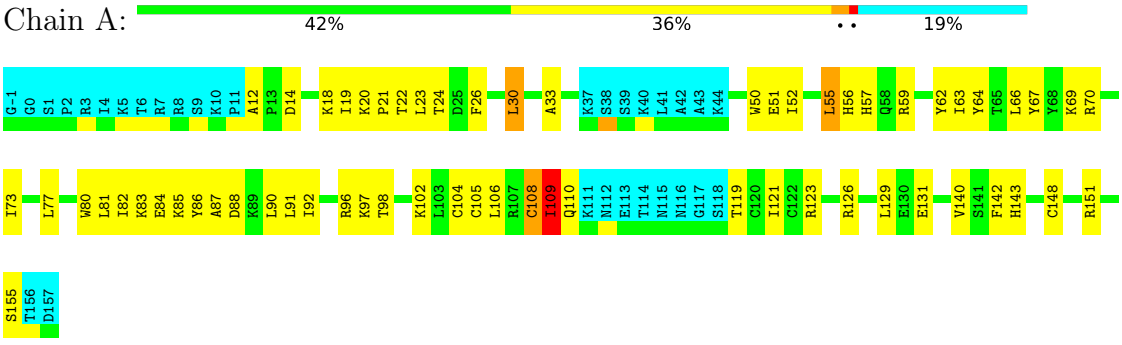
Chain A:



4.2.30 Score per residue for model 30

• Molecule 1: Pre-mRNA-splicing factor BUD31

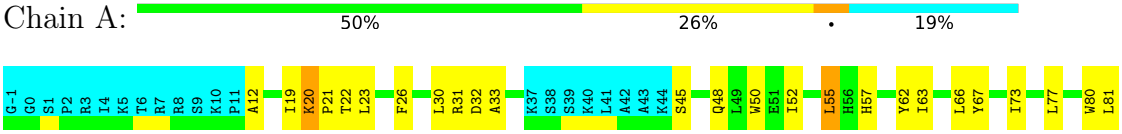
Chain A:

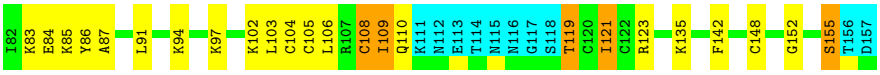


4.2.31 Score per residue for model 31

• Molecule 1: Pre-mRNA-splicing factor BUD31

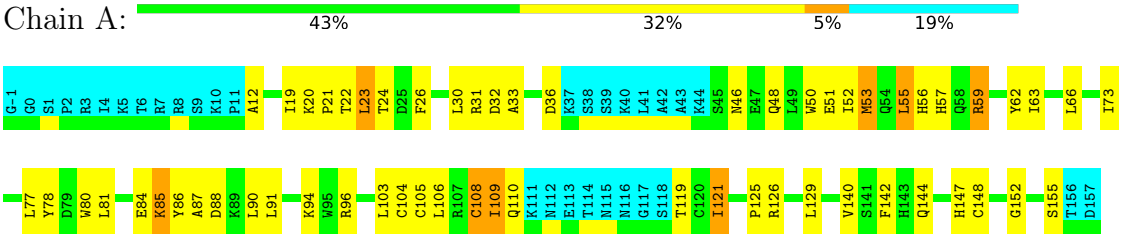
Chain A:





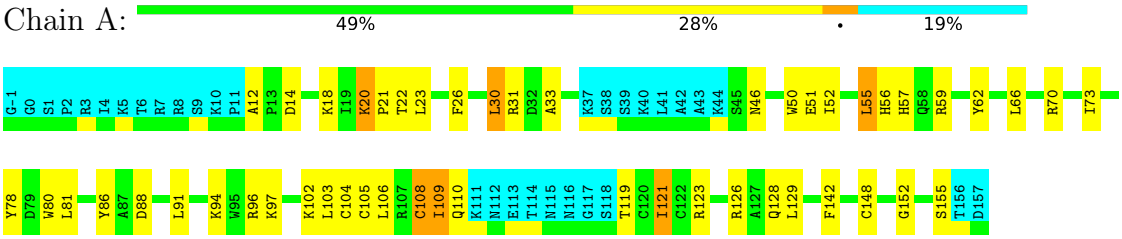
4.2.32 Score per residue for model 32

• Molecule 1: Pre-mRNA-splicing factor BUD31



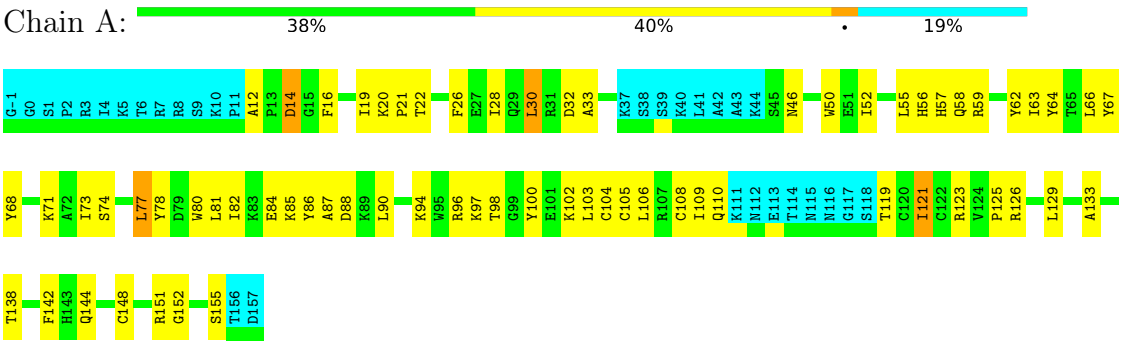
4.2.33 Score per residue for model 33

• Molecule 1: Pre-mRNA-splicing factor BUD31



4.2.34 Score per residue for model 34

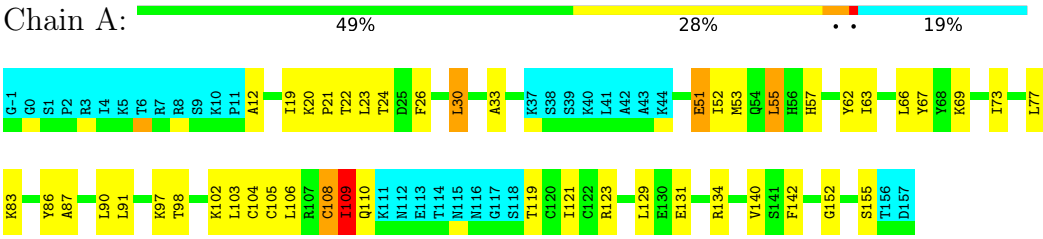
• Molecule 1: Pre-mRNA-splicing factor BUD31



4.2.35 Score per residue for model 35

• Molecule 1: Pre-mRNA-splicing factor BUD31

Chain A:


49%
28%
19%
G-1 G0 S1 P2 R3 I4 K5 T6 R7 R8 S9 K10 P11 A12 I19 K20 P21 T22 L23 T24 D25 F26 L30 A33 K37 S38 S39 K40 L41 A42 A43 K44 E51 I52 M53 Q54 L55 H56 H57 Y62 I63 L66 Y67 Y68 K69 I73 L77 W80 L81 I82
K83 Y86 A87 L90 L91 K97 T98 K102 L103 C104 C105 L106 R107 C108 I109 Q110 K111 N112 E113 T114 N115 N116 G117 S118 T119 C120 I121 C122 R123 L129 E130 E131 R134 V140 S141 F142 G152 S155 T156 D157

5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 35 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.28
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	1698
Number of shifts mapped to atoms	1698
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

6 Model quality

6.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.09±0.00	0±0/1088 (0.0± 0.0%)	1.19±0.00	1±0/1461 (0.1± 0.0%)
All	All	1.09	0/38080 (0.0%)	1.19	30/51135 (0.1%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	108	CYS	N-CA-CB	-5.58	100.55	110.60	31	30

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	1065	1066	1066	49±4
All	All	37380	37310	37310	1704

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 23.

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:LEU:HD11	1:A:52:ILE:HG23	1.05	1.26	13	15
1:A:22:THR:HG21	1:A:62:TYR:CE2	0.86	2.05	32	34
1:A:121:ILE:HD12	1:A:142:PHE:CD1	0.86	2.06	15	17
1:A:63:ILE:HD12	1:A:87:ALA:HB2	0.84	1.47	26	29
1:A:30:LEU:CD1	1:A:52:ILE:HG23	0.83	2.03	29	15
1:A:103:LEU:HD12	1:A:109:ILE:HD13	0.82	1.48	33	1
1:A:103:LEU:HD13	1:A:109:ILE:HD13	0.81	1.53	28	11
1:A:30:LEU:HD12	1:A:55:LEU:HD23	0.78	1.55	35	3
1:A:19:ILE:O	1:A:23:LEU:HD12	0.77	1.79	20	31
1:A:103:LEU:HD11	1:A:105:CYS:O	0.76	1.81	3	12
1:A:12:ALA:HB2	1:A:80:TRP:CH2	0.75	2.16	34	35
1:A:121:ILE:O	1:A:121:ILE:HD13	0.75	1.81	27	31
1:A:30:LEU:HD21	1:A:52:ILE:HG23	0.75	1.59	30	19
1:A:121:ILE:HD11	1:A:129:LEU:HD11	0.74	1.59	2	23
1:A:133:ALA:HB1	1:A:138:THR:O	0.73	1.84	15	14
1:A:103:LEU:HD13	1:A:109:ILE:CD1	0.72	2.15	20	12
1:A:121:ILE:HD12	1:A:142:PHE:CG	0.72	2.19	19	30
1:A:51:GLU:O	1:A:55:LEU:HD22	0.72	1.84	26	4
1:A:81:LEU:HD22	1:A:86:TYR:CD2	0.71	2.20	31	14
1:A:19:ILE:HD12	1:A:23:LEU:HD11	0.71	1.61	17	27
1:A:90:LEU:HD23	1:A:106:LEU:HD13	0.71	1.60	35	10
1:A:90:LEU:HD23	1:A:106:LEU:HD22	0.70	1.61	29	5
1:A:109:ILE:O	1:A:119:THR:HG21	0.69	1.87	23	5
1:A:30:LEU:CD2	1:A:52:ILE:HG23	0.69	2.17	33	19
1:A:110:GLN:C	1:A:119:THR:HG23	0.68	2.08	14	27
1:A:30:LEU:HD11	1:A:52:ILE:CG2	0.68	2.16	1	11
1:A:19:ILE:HG22	1:A:62:TYR:OH	0.68	1.88	15	24
1:A:91:LEU:HA	1:A:106:LEU:HD21	0.67	1.67	1	13
1:A:26:PHE:CD2	1:A:55:LEU:HD12	0.67	2.24	32	4
1:A:26:PHE:CD2	1:A:55:LEU:HD22	0.66	2.26	28	23
1:A:121:ILE:HG23	1:A:142:PHE:CE1	0.66	2.25	27	35
1:A:30:LEU:CG	1:A:52:ILE:HG23	0.65	2.22	27	21
1:A:73:ILE:HG13	1:A:77:LEU:HD23	0.65	1.69	12	31
1:A:103:LEU:HD12	1:A:109:ILE:CD1	0.64	2.21	33	1
1:A:26:PHE:CD1	1:A:55:LEU:HD22	0.64	2.28	23	5
1:A:30:LEU:CD1	1:A:55:LEU:HD23	0.63	2.23	35	3
1:A:90:LEU:CD2	1:A:106:LEU:HD22	0.62	2.25	29	2
1:A:103:LEU:HB2	1:A:109:ILE:HD13	0.62	1.71	10	2
1:A:91:LEU:HD12	1:A:95:TRP:CZ3	0.62	2.29	21	4
1:A:91:LEU:HD21	1:A:95:TRP:CH2	0.61	2.31	25	2
1:A:91:LEU:CA	1:A:106:LEU:HD21	0.60	2.25	1	6
1:A:129:LEU:O	1:A:140:VAL:HG11	0.60	1.96	30	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:HD21	1:A:52:ILE:CG2	0.60	2.25	26	18
1:A:78:TYR:HA	1:A:81:LEU:HD12	0.60	1.74	5	11
1:A:19:ILE:HD12	1:A:23:LEU:CD1	0.59	2.26	2	21
1:A:30:LEU:HD12	1:A:55:LEU:HD12	0.59	1.75	6	1
1:A:66:LEU:CD1	1:A:73:ILE:HG21	0.59	2.28	35	33
1:A:103:LEU:HD12	1:A:104:CYS:N	0.58	2.13	35	1
1:A:12:ALA:HB2	1:A:80:TRP:CZ2	0.58	2.32	32	35
1:A:110:GLN:O	1:A:119:THR:HG23	0.58	1.99	35	19
1:A:121:ILE:HD12	1:A:142:PHE:CD2	0.58	2.34	3	19
1:A:30:LEU:HG	1:A:52:ILE:HG23	0.58	1.76	27	15
1:A:12:ALA:HB2	1:A:80:TRP:CZ3	0.57	2.34	13	27
1:A:33:ALA:CB	1:A:52:ILE:HD11	0.57	2.28	24	23
1:A:105:CYS:HB2	1:A:108:CYS:HB2	0.55	1.77	23	35
1:A:66:LEU:HD12	1:A:67:TYR:N	0.54	2.17	6	26
1:A:91:LEU:N	1:A:106:LEU:HD11	0.54	2.18	9	2
1:A:124:VAL:HG13	1:A:128:GLN:CD	0.54	2.23	27	1
1:A:125:PRO:O	1:A:129:LEU:HD12	0.53	2.02	24	8
1:A:66:LEU:HD12	1:A:73:ILE:HG21	0.53	1.81	30	22
1:A:125:PRO:HD3	1:A:154:ALA:HB1	0.53	1.81	19	2
1:A:23:LEU:HD13	1:A:86:TYR:HE2	0.52	1.64	11	16
1:A:30:LEU:HD23	1:A:34:GLN:HG3	0.52	1.81	8	1
1:A:121:ILE:HD11	1:A:129:LEU:CD1	0.51	2.36	17	15
1:A:30:LEU:HD12	1:A:55:LEU:CD1	0.51	2.35	6	1
1:A:66:LEU:HD12	1:A:66:LEU:C	0.51	2.26	27	35
1:A:23:LEU:HD13	1:A:86:TYR:CE2	0.51	2.41	11	12
1:A:121:ILE:HD13	1:A:121:ILE:C	0.50	2.26	34	31
1:A:16:PHE:N	1:A:77:LEU:HD21	0.50	2.21	13	2
1:A:28:ILE:N	1:A:28:ILE:HD12	0.50	2.22	3	12
1:A:26:PHE:CE2	1:A:55:LEU:HD12	0.50	2.42	31	5
1:A:64:TYR:CD1	1:A:68:TYR:CD2	0.50	3.00	19	4
1:A:100:TYR:HB3	1:A:103:LEU:HD23	0.48	1.85	25	16
1:A:23:LEU:HD22	1:A:86:TYR:CD2	0.48	2.43	20	7
1:A:33:ALA:HB3	1:A:52:ILE:CG1	0.48	2.38	31	27
1:A:57:HIS:CD2	1:A:91:LEU:HD21	0.48	2.43	12	5
1:A:81:LEU:CD2	1:A:86:TYR:CD2	0.48	2.97	26	34
1:A:81:LEU:HD23	1:A:86:TYR:CE2	0.48	2.44	12	9
1:A:33:ALA:HB1	1:A:48:GLN:O	0.47	2.09	31	1
1:A:90:LEU:HD12	1:A:106:LEU:CD2	0.47	2.39	27	1
1:A:29:GLN:OE1	1:A:55:LEU:HD21	0.47	2.10	20	1
1:A:56:HIS:NE2	1:A:88:ASP:CB	0.47	2.78	22	3
1:A:91:LEU:HD11	1:A:103:LEU:HD11	0.47	1.86	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:ILE:HD12	1:A:87:ALA:HB3	0.46	1.87	11	3
1:A:64:TYR:CE1	1:A:92:ILE:HG23	0.46	2.45	4	9
1:A:91:LEU:HD11	1:A:103:LEU:HD21	0.46	1.86	33	1
1:A:82:ILE:CD1	1:A:87:ALA:HB3	0.46	2.40	17	1
1:A:50:TRP:CD1	1:A:148:CYS:HA	0.46	2.45	25	28
1:A:121:ILE:CG2	1:A:142:PHE:CE1	0.46	2.98	27	34
1:A:103:LEU:C	1:A:103:LEU:HD12	0.46	2.31	24	13
1:A:33:ALA:HB3	1:A:52:ILE:HD11	0.46	1.87	27	9
1:A:121:ILE:CD1	1:A:129:LEU:HD11	0.46	2.41	13	3
1:A:81:LEU:HD23	1:A:86:TYR:CD2	0.46	2.46	27	8
1:A:82:ILE:HD11	1:A:89:LYS:N	0.46	2.25	18	3
1:A:64:TYR:OH	1:A:96:ARG:NE	0.46	2.49	29	1
1:A:50:TRP:CE3	1:A:149:GLY:CA	0.46	2.99	29	4
1:A:57:HIS:NE2	1:A:91:LEU:HD21	0.46	2.26	26	3
1:A:91:LEU:CD1	1:A:95:TRP:CZ3	0.46	2.99	22	4
1:A:56:HIS:NE2	1:A:88:ASP:N	0.45	2.64	20	1
1:A:91:LEU:CD1	1:A:103:LEU:HD21	0.45	2.41	33	1
1:A:57:HIS:NE2	1:A:104:CYS:O	0.45	2.48	32	31
1:A:63:ILE:CG2	1:A:78:TYR:CD1	0.45	3.00	20	3
1:A:81:LEU:HD22	1:A:86:TYR:CE2	0.45	2.46	31	3
1:A:64:TYR:CE1	1:A:92:ILE:CG2	0.45	2.99	30	5
1:A:108:CYS:O	1:A:109:ILE:HG23	0.45	2.12	17	19
1:A:49:LEU:HD23	1:A:52:ILE:HD12	0.45	1.89	10	3
1:A:26:PHE:CD2	1:A:59:ARG:CD	0.45	2.99	20	5
1:A:26:PHE:CD1	1:A:59:ARG:CD	0.45	3.00	4	1
1:A:124:VAL:HG12	1:A:129:LEU:HG	0.45	1.89	12	1
1:A:16:PHE:HB2	1:A:77:LEU:HD11	0.45	1.87	24	1
1:A:94:LYS:HB3	1:A:103:LEU:HD22	0.45	1.88	10	2
1:A:62:TYR:CE1	1:A:66:LEU:CD2	0.45	3.00	21	1
1:A:57:HIS:CE1	1:A:104:CYS:O	0.45	2.70	3	34
1:A:67:TYR:CE2	1:A:78:TYR:CD2	0.45	3.05	10	1
1:A:22:THR:HG21	1:A:62:TYR:CD2	0.45	2.46	22	1
1:A:73:ILE:CG1	1:A:77:LEU:HD23	0.45	2.40	10	19
1:A:64:TYR:OH	1:A:96:ARG:NH1	0.44	2.50	28	3
1:A:20:LYS:N	1:A:21:PRO:CD	0.44	2.81	22	35
1:A:103:LEU:C	1:A:103:LEU:HD23	0.44	2.32	33	1
1:A:110:GLN:CA	1:A:119:THR:HG23	0.44	2.42	12	1
1:A:94:LYS:CD	1:A:100:TYR:CZ	0.44	3.01	27	3
1:A:33:ALA:CB	1:A:52:ILE:CG1	0.44	2.96	26	32
1:A:64:TYR:CE2	1:A:68:TYR:CD2	0.44	3.05	34	1
1:A:81:LEU:CD2	1:A:86:TYR:CE2	0.43	3.01	22	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:LEU:HD12	1:A:95:TRP:CE3	0.43	2.48	10	1
1:A:33:ALA:HB1	1:A:48:GLN:HG2	0.43	1.89	31	2
1:A:53:MET:HE1	1:A:147:HIS:O	0.43	2.14	32	1
1:A:94:LYS:CD	1:A:106:LEU:CD2	0.43	2.97	10	11
1:A:19:ILE:CG2	1:A:62:TYR:OH	0.43	2.64	21	2
1:A:50:TRP:CD1	1:A:50:TRP:N	0.43	2.86	3	5
1:A:91:LEU:CD2	1:A:95:TRP:CZ3	0.43	3.01	25	1
1:A:50:TRP:O	1:A:53:MET:HE3	0.43	2.14	29	1
1:A:78:TYR:CE1	1:A:82:ILE:CD1	0.43	3.02	34	2
1:A:56:HIS:NE2	1:A:88:ASP:HB2	0.42	2.29	33	12
1:A:63:ILE:CG2	1:A:78:TYR:CE1	0.42	3.02	20	2
1:A:66:LEU:HD12	1:A:73:ILE:CG2	0.42	2.44	10	4
1:A:45:SER:OG	1:A:46:ASN:N	0.42	2.52	10	2
1:A:108:CYS:C	1:A:109:ILE:HG23	0.42	2.35	32	19
1:A:121:ILE:CD1	1:A:142:PHE:CG	0.42	3.01	2	13
1:A:66:LEU:CD1	1:A:73:ILE:CG2	0.42	2.97	24	22
1:A:26:PHE:CE1	1:A:55:LEU:HD22	0.42	2.50	1	2
1:A:84:GLU:O	1:A:85:LYS:CB	0.42	2.68	34	14
1:A:63:ILE:HD11	1:A:86:TYR:HB3	0.42	1.90	30	2
1:A:46:ASN:O	1:A:50:TRP:CD1	0.42	2.73	22	6
1:A:108:CYS:O	1:A:109:ILE:CG2	0.42	2.68	35	9
1:A:26:PHE:CD2	1:A:59:ARG:HD3	0.42	2.50	32	4
1:A:26:PHE:CE2	1:A:55:LEU:HD22	0.42	2.49	18	2
1:A:46:ASN:O	1:A:50:TRP:CG	0.42	2.73	18	2
1:A:63:ILE:HG22	1:A:78:TYR:CE1	0.41	2.50	34	1
1:A:26:PHE:CD2	1:A:59:ARG:HD2	0.41	2.51	28	2
1:A:56:HIS:NE2	1:A:88:ASP:OD2	0.41	2.53	26	1
1:A:64:TYR:CE1	1:A:68:TYR:CD2	0.41	3.08	29	1
1:A:62:TYR:O	1:A:66:LEU:HD23	0.41	2.15	21	1
1:A:26:PHE:CE1	1:A:55:LEU:HD12	0.41	2.50	26	1
1:A:26:PHE:CG	1:A:59:ARG:CD	0.41	3.04	7	1
1:A:81:LEU:O	1:A:86:TYR:CD1	0.41	2.73	14	2
1:A:69:LYS:CD	1:A:69:LYS:N	0.41	2.84	24	1
1:A:73:ILE:CD1	1:A:77:LEU:HD23	0.41	2.46	24	1
1:A:30:LEU:HD23	1:A:34:GLN:CG	0.41	2.46	8	1
1:A:19:ILE:HD11	1:A:81:LEU:CD2	0.41	2.46	34	1
1:A:94:LYS:HD3	1:A:106:LEU:HD23	0.41	1.93	4	1
1:A:64:TYR:OH	1:A:96:ARG:CD	0.41	2.69	25	1
1:A:50:TRP:CZ3	1:A:144:GLN:OE1	0.41	2.74	34	1
1:A:133:ALA:HB1	1:A:139:GLN:CA	0.40	2.46	22	1
1:A:94:LYS:CE	1:A:100:TYR:CZ	0.40	3.04	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ASN:OD1	1:A:50:TRP:CZ2	0.40	2.75	6	1
1:A:66:LEU:HD11	1:A:73:ILE:CD1	0.40	2.46	13	1
1:A:94:LYS:HD2	1:A:100:TYR:CZ	0.40	2.52	27	1
1:A:129:LEU:CD1	1:A:142:PHE:CB	0.40	3.00	28	1
1:A:63:ILE:HD12	1:A:87:ALA:CB	0.40	2.41	30	1
1:A:53:MET:CE	1:A:148:CYS:HB2	0.40	2.47	8	1
1:A:122:CYS:HA	1:A:142:PHE:CE2	0.40	2.52	22	2

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	128/159 (81%)	111±2 (87±2%)	14±2 (11±2%)	3±1 (2±1%)	9	48
All	All	4480/5565 (81%)	3894 (87%)	483 (11%)	103 (2%)	9	48

All 8 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	97	LYS	32
1	A	109	ILE	30
1	A	152	GLY	27
1	A	12	ALA	7
1	A	14	ASP	3
1	A	119	THR	2
1	A	139	GLN	1
1	A	85	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	115/141 (82%)	101±3 (87±3%)	14±3 (13±3%)	8 50
All	All	4025/4935 (82%)	3520 (87%)	505 (13%)	8 50

All 59 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	121	ILE	31
1	A	102	LYS	31
1	A	155	SER	29
1	A	96	ARG	28
1	A	30	LEU	23
1	A	123	ARG	21
1	A	20	LYS	21
1	A	59	ARG	20
1	A	98	THR	17
1	A	31	ARG	15
1	A	126	ARG	15
1	A	53	MET	15
1	A	144	GLN	13
1	A	69	LYS	12
1	A	119	THR	12
1	A	24	THR	11
1	A	32	ASP	11
1	A	45	SER	10
1	A	82	ILE	9
1	A	74	SER	7
1	A	151	ARG	7
1	A	70	ARG	7
1	A	143	HIS	7
1	A	103	LEU	7
1	A	85	LYS	7
1	A	134	ARG	7
1	A	71	LYS	6
1	A	83	LYS	6
1	A	55	LEU	6
1	A	48	GLN	5
1	A	75	LYS	5
1	A	76	ASP	5
1	A	14	ASP	5
1	A	109	ILE	5
1	A	131	GLU	5
1	A	89	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	97	LYS	4
1	A	18	LYS	4
1	A	91	LEU	4
1	A	107	ARG	4
1	A	136	LYS	4
1	A	51	GLU	4
1	A	25	ASP	3
1	A	132	GLU	3
1	A	54	GLN	3
1	A	110	GLN	3
1	A	61	ARG	3
1	A	23	LEU	3
1	A	77	LEU	3
1	A	36	ASP	2
1	A	29	GLN	2
1	A	35	LYS	2
1	A	58	GLN	2
1	A	128	GLN	2
1	A	101	GLU	1
1	A	17	GLU	1
1	A	34	GLN	1
1	A	90	LEU	1
1	A	135	LYS	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 75% 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	1698
Number of shifts mapped to atoms	1698
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	158	-0.45 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	149	0.16 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	151	-0.30 ± 0.28	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 78%, i.e. 1437 atoms were assigned a chemical shift out of a possible 1847. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	507/639 (79%)	256/258 (99%)	127/256 (50%)	124/125 (99%)
Sidechain	792/1051 (75%)	540/675 (80%)	242/322 (75%)	10/54 (19%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	138/157 (88%)	69/77 (90%)	66/73 (90%)	3/7 (43%)
Overall	1437/1847 (78%)	865/1010 (86%)	435/651 (67%)	137/186 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 1698 atoms were assigned a chemical shift out of a possible 2250. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	626/793 (79%)	317/321 (99%)	158/318 (50%)	151/154 (98%)
Sidechain	934/1300 (72%)	636/832 (76%)	285/396 (72%)	13/72 (18%)
Aromatic	138/157 (88%)	69/77 (90%)	66/73 (90%)	3/7 (43%)
Overall	1698/2250 (75%)	1022/1230 (83%)	509/787 (65%)	167/233 (72%)

7.1.4 Statistically unusual chemical shifts (i)

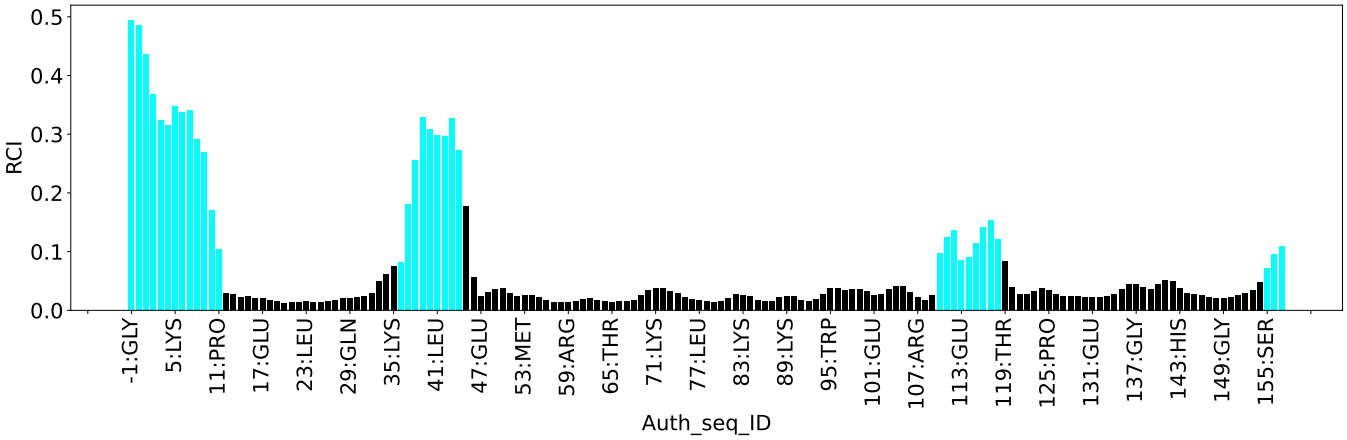
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	84	GLU	HG2	0.50	1.24 – 3.30	-8.6
1	A	84	GLU	HG3	1.07	1.20 – 3.30	-5.6
1	A	12	ALA	HB1	0.01	0.14 – 2.58	-5.5
1	A	12	ALA	HB2	0.01	0.14 – 2.58	-5.5
1	A	12	ALA	HB3	0.01	0.14 – 2.58	-5.5
1	A	91	LEU	HG	-0.20	-0.13 – 3.16	-5.2

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
0.5
0.4
0.3
0.2
0.1
0.0
-1:GLY
5:LYS
11:PRO
17:GLU
23:LEU
29:GLN
35:LYS
41:LEU
47:GLU
53:MET
59:ARG
65:THR
71:LYS
77:LEU
83:LYS
89:LYS
95:TRP
101:GLU
107:ARG
113:GLU
119:THR
125:PRO
131:GLU
137:GLY
143:HIS
149:GLY
155: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	1874
Intra-residue (|i-j|=0)	676
Sequential (|i-j|=1)	408
Medium range (|i-j|>1 and |i-j|<5)	389
Long range (|i-j|≥5)	353
Inter-chain	0
Hydrogen bond restraints	30
Disulfide bond restraints	18
Total dihedral-angle restraints	197
Number of unmapped restraints	1
Number of restraints per residue	13.0
Number of long range restraints per residue[1]	2.3

[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)	18.6	0.2
0.2-0.5 (Medium)	1.6	0.32
>0.5 (Large)	None	None

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.2	1.2
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

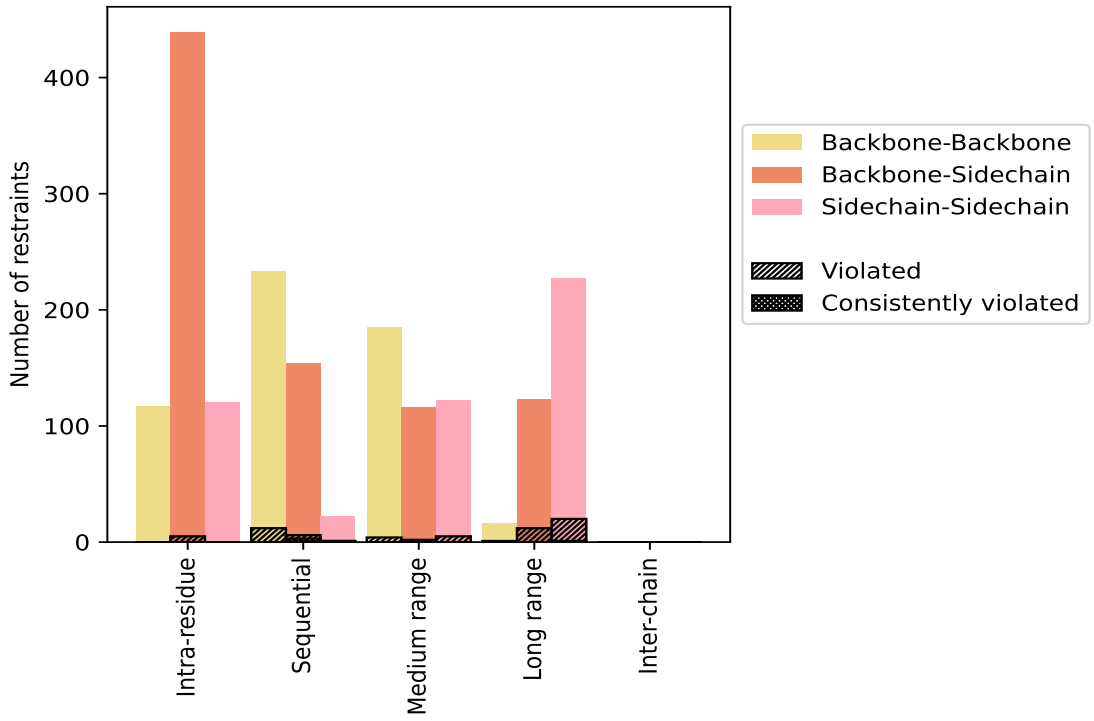
9.1 Summary of distance violations (i)

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)	676	36.1	5	0.7	0.3	0	0.0	0.0
Backbone-Backbone	117	6.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	439	23.4	5	1.1	0.3	0	0.0	0.0
Sidechain-Sidechain	120	6.4	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	408	21.8	19	4.7	1.0	4	1.0	0.2
Backbone-Backbone	233	12.4	12	5.2	0.6	0	0.0	0.0
Backbone-Sidechain	154	8.2	6	3.9	0.3	3	1.9	0.2
Sidechain-Sidechain	21	1.1	1	4.8	0.1	1	4.8	0.1
Medium range (|i-j|>1 & |i-j|<5)	389	20.8	11	2.8	0.6	0	0.0	0.0
Backbone-Backbone	155	8.3	4	2.6	0.2	0	0.0	0.0
Backbone-Sidechain	116	6.2	2	1.7	0.1	0	0.0	0.0
Sidechain-Sidechain	118	6.3	5	4.2	0.3	0	0.0	0.0
Long range (|i-j|≥5)	353	18.8	32	9.1	1.7	1	0.3	0.1
Backbone-Backbone	16	0.9	1	6.2	0.1	0	0.0	0.0
Backbone-Sidechain	123	6.6	12	9.8	0.6	0	0.0	0.0
Sidechain-Sidechain	214	11.4	19	8.9	1.0	1	0.5	0.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	30	1.6	0	0.0	0.0	0	0.0	0.0
Disulfide bond	18	1.0	1	5.6	0.1	0	0.0	0.0
Total	1874	100.0	68	3.6	3.6	5	0.3	0.3
Backbone-Backbone	551	29.4	17	3.1	0.9	0	0.0	0.0
Backbone-Sidechain	832	44.4	25	3.0	1.3	3	0.4	0.2
Sidechain-Sidechain	491	26.2	26	5.3	1.4	2	0.4	0.1

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	3	5	2	9	0	19	0.14	0.23	0.03	0.13
2	1	8	3	7	0	19	0.13	0.22	0.03	0.13
3	3	7	2	11	0	23	0.14	0.3	0.04	0.13
4	3	5	1	7	0	16	0.14	0.23	0.03	0.15
5	3	6	0	10	0	19	0.14	0.22	0.03	0.13
6	2	5	1	6	0	14	0.15	0.23	0.03	0.14
7	2	7	2	10	0	21	0.14	0.23	0.03	0.13
8	3	7	4	14	0	28	0.14	0.32	0.04	0.12
9	3	6	2	5	0	16	0.14	0.22	0.03	0.13
10	2	6	0	13	0	21	0.15	0.26	0.04	0.13
11	2	6	1	7	0	16	0.15	0.22	0.03	0.14

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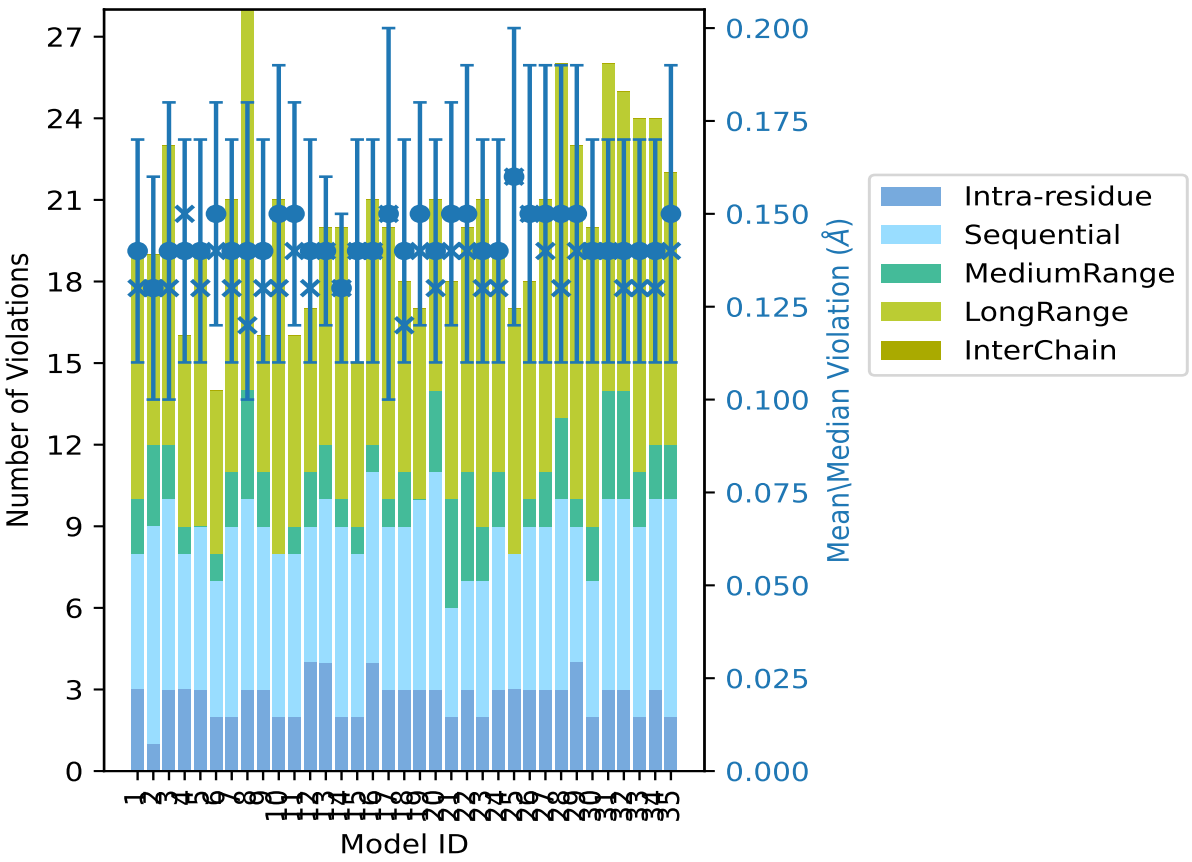
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	4	5	2	6	0	17	0.14	0.22	0.03	0.13
13	4	6	2	8	0	20	0.14	0.22	0.02	0.14
14	2	7	1	10	0	20	0.13	0.2	0.02	0.13
15	2	6	1	6	0	15	0.14	0.21	0.03	0.14
16	4	7	1	9	0	21	0.14	0.22	0.03	0.14
17	3	6	1	10	0	20	0.15	0.31	0.05	0.15
18	3	6	2	7	0	18	0.14	0.22	0.03	0.12
19	3	7	0	7	0	17	0.15	0.22	0.03	0.14
20	3	8	3	7	0	21	0.14	0.21	0.03	0.13
21	2	4	4	8	0	18	0.15	0.23	0.03	0.14
22	3	4	4	9	0	20	0.15	0.24	0.04	0.14
23	2	5	2	12	0	21	0.14	0.22	0.03	0.13
24	3	6	2	8	0	19	0.14	0.23	0.03	0.13
25	3	5	0	9	0	17	0.16	0.23	0.04	0.16
26	3	6	1	8	0	18	0.15	0.23	0.04	0.15
27	3	6	2	10	0	21	0.15	0.22	0.04	0.14
28	3	7	3	13	0	26	0.15	0.31	0.04	0.13
29	4	5	1	13	0	23	0.15	0.31	0.04	0.14
30	2	5	2	11	0	20	0.14	0.22	0.03	0.14
31	3	7	4	12	0	26	0.14	0.23	0.03	0.14
32	3	7	4	11	0	25	0.14	0.21	0.03	0.13
33	2	7	2	13	0	24	0.14	0.21	0.03	0.13
34	3	7	2	12	0	24	0.14	0.2	0.03	0.13
35	2	8	2	10	0	22	0.15	0.23	0.04	0.14

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1759(IR:671, SQ:389, MR:378, LR:321, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	3	0	2	0	6	1	2.9
0	6	1	2	0	9	2	5.7
0	3	2	7	0	12	3	8.6
0	1	2	3	0	6	4	11.4
0	0	1	2	0	3	5	14.3
0	0	0	2	0	2	6	17.1

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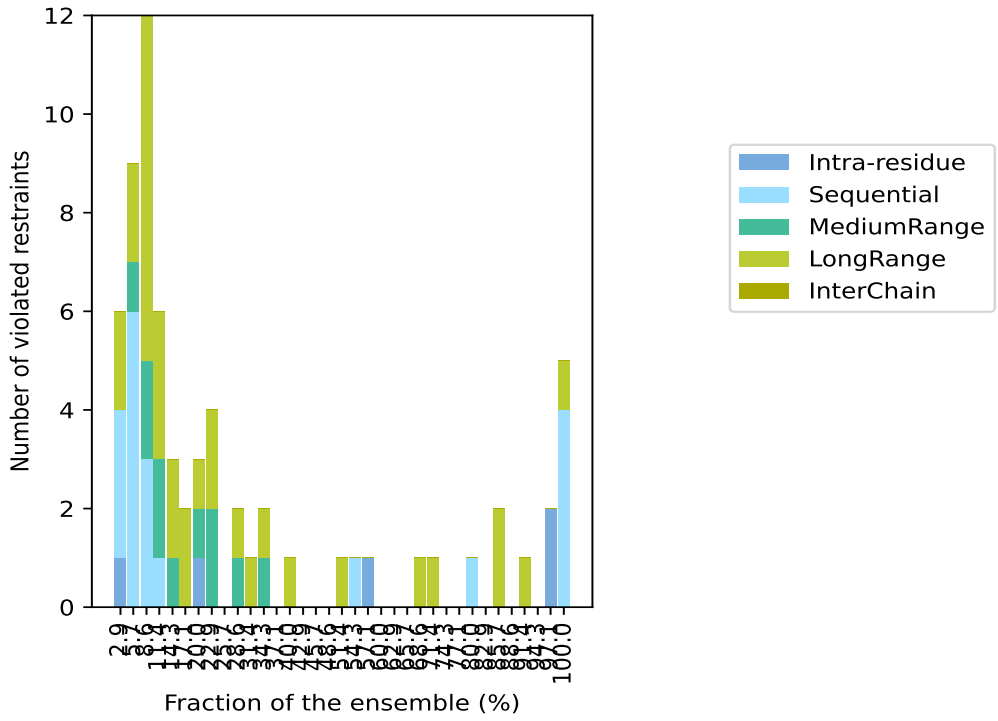
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	0	1	1	0	3	7	20.0
0	0	2	2	0	4	8	22.9
0	0	0	0	0	0	9	25.7
0	0	1	1	0	2	10	28.6
0	0	0	1	0	1	11	31.4
0	0	1	1	0	2	12	34.3
0	0	0	0	0	0	13	37.1
0	0	0	1	0	1	14	40.0
0	0	0	0	0	0	15	42.9
0	0	0	0	0	0	16	45.7
0	0	0	0	0	0	17	48.6
0	0	0	1	0	1	18	51.4
0	1	0	0	0	1	19	54.3
1	0	0	0	0	1	20	57.1
0	0	0	0	0	0	21	60.0
0	0	0	0	0	0	22	62.9
0	0	0	0	0	0	23	65.7
0	0	0	1	0	1	24	68.6
0	0	0	1	0	1	25	71.4
0	0	0	0	0	0	26	74.3
0	0	0	0	0	0	27	77.1
0	1	0	0	0	1	28	80.0
0	0	0	0	0	0	29	82.9
0	0	0	2	0	2	30	85.7
0	0	0	0	0	0	31	88.6
0	0	0	1	0	1	32	91.4
0	0	0	0	0	0	33	94.3
2	0	0	0	0	2	34	97.1
0	4	0	1	0	5	35	100.0

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

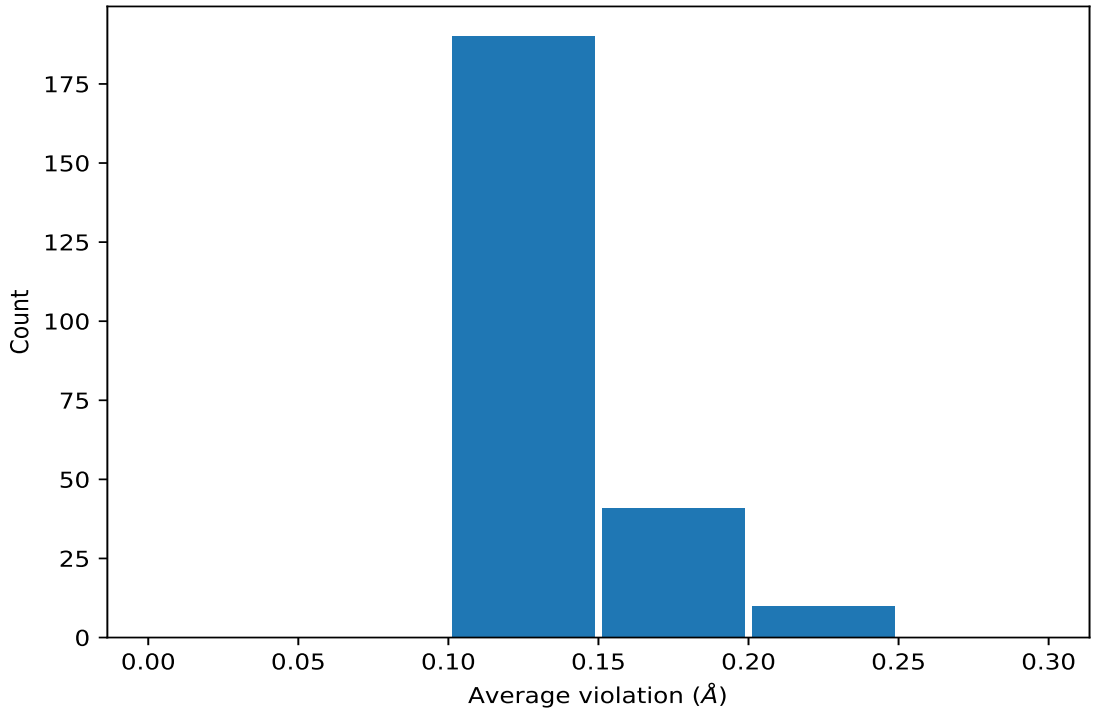
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	35	0.22	0.01	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	35	0.22	0.01	0.22
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	35	0.17	0.01	0.17
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	35	0.17	0.01	0.17
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	35	0.16	0.02	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	35	0.14	0.01	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	35	0.14	0.01	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	35	0.14	0.01	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	35	0.14	0.01	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	35	0.14	0.01	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	35	0.14	0.01	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	35	0.14	0.01	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	35	0.14	0.01	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	35	0.14	0.01	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	35	0.14	0.01	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	35	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	35	0.14	0.01	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	35	0.14	0.01	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	35	0.14	0.01	0.14
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	34	0.18	0.06	0.15
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	34	0.15	0.03	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	32	0.15	0.02	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	32	0.15	0.02	0.16
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	30	0.14	0.02	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	30	0.14	0.02	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	30	0.14	0.02	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	30	0.14	0.02	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	30	0.14	0.02	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	30	0.14	0.02	0.15
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	30	0.13	0.01	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	30	0.13	0.01	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	30	0.13	0.01	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	30	0.13	0.01	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	30	0.13	0.01	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	30	0.13	0.01	0.13
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	28	0.12	0.01	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	25	0.13	0.02	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	25	0.13	0.02	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	25	0.13	0.02	0.13
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	24	0.15	0.03	0.15
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	24	0.15	0.03	0.15
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	20	0.12	0.01	0.12
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	19	0.11	0.0	0.11
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	18	0.12	0.01	0.12
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	14	0.12	0.02	0.11
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG21	12	0.13	0.02	0.12
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG22	12	0.13	0.02	0.12
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG23	12	0.13	0.02	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG21	12	0.13	0.02	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG22	12	0.13	0.02	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG23	12	0.13	0.02	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG21	12	0.13	0.02	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG22	12	0.13	0.02	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG23	12	0.13	0.02	0.12
(1,287)	1:A:28:ILE:HA	1:A:31:ARG:H	12	0.11	0.01	0.11
(1,1317)	1:A:108:CYS:HB2	1:A:120:CYS:HB3	11	0.12	0.01	0.12
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD1	10	0.12	0.01	0.11
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD2	10	0.12	0.01	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD1	10	0.12	0.01	0.11
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD2	10	0.12	0.01	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD11	10	0.11	0.0	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD12	10	0.11	0.0	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD13	10	0.11	0.0	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD11	10	0.11	0.0	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD12	10	0.11	0.0	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD13	10	0.11	0.0	0.11
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD11	8	0.17	0.03	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD12	8	0.17	0.03	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD13	8	0.17	0.03	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD21	8	0.17	0.03	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD22	8	0.17	0.03	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD23	8	0.17	0.03	0.16
(1,559)	1:A:53:MET:HB3	1:A:148:CYS:HB3	8	0.15	0.05	0.13
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE1	8	0.12	0.01	0.12
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE2	8	0.12	0.01	0.12
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE1	8	0.12	0.01	0.12
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE2	8	0.12	0.01	0.12
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD2	8	0.12	0.0	0.12
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD3	8	0.12	0.0	0.12
(1,1587)	1:A:132:GLU:HA	1:A:132:GLU:HB3	7	0.15	0.0	0.15
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD11	7	0.12	0.01	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD12	7	0.12	0.01	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD13	7	0.12	0.01	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD11	7	0.12	0.01	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD12	7	0.12	0.01	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD13	7	0.12	0.01	0.11
(1,303)	1:A:29:GLN:HA	1:A:32:ASP:H	7	0.11	0.0	0.11
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB2	6	0.21	0.02	0.22
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB3	6	0.21	0.02	0.22
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB2	6	0.21	0.02	0.22
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB3	6	0.21	0.02	0.22
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB2	6	0.21	0.02	0.22
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB3	6	0.21	0.02	0.22
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD11	6	0.12	0.01	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD12	6	0.12	0.01	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD13	6	0.12	0.01	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD21	6	0.12	0.01	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD22	6	0.12	0.01	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD23	6	0.12	0.01	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD11	6	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD12	6	0.12	0.01	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD13	6	0.12	0.01	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD21	6	0.12	0.01	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD22	6	0.12	0.01	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD23	6	0.12	0.01	0.12
(1,563)	1:A:53:MET:HE1	1:A:148:CYS:HB3	5	0.16	0.01	0.16
(1,563)	1:A:53:MET:HE2	1:A:148:CYS:HB3	5	0.16	0.01	0.16
(1,563)	1:A:53:MET:HE3	1:A:148:CYS:HB3	5	0.16	0.01	0.16
(1,1421)	1:A:121:ILE:HG21	1:A:142:PHE:HA	5	0.14	0.02	0.14
(1,1421)	1:A:121:ILE:HG22	1:A:142:PHE:HA	5	0.14	0.02	0.14
(1,1421)	1:A:121:ILE:HG23	1:A:142:PHE:HA	5	0.14	0.02	0.14
(1,503)	1:A:50:TRP:HA	1:A:53:MET:H	5	0.13	0.01	0.13
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG11	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG12	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG13	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG21	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG22	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG23	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG11	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG12	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG13	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG21	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG22	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG23	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG11	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG12	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG13	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG21	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG22	4	0.19	0.01	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG23	4	0.19	0.01	0.19
(1,1433)	1:A:121:ILE:HG21	1:A:145:CYS:HB2	4	0.12	0.02	0.12
(1,1433)	1:A:121:ILE:HG22	1:A:145:CYS:HB2	4	0.12	0.02	0.12
(1,1433)	1:A:121:ILE:HG23	1:A:145:CYS:HB2	4	0.12	0.02	0.12
(1,1698)	1:A:142:PHE:HE1	1:A:145:CYS:H	4	0.12	0.0	0.12
(1,1698)	1:A:142:PHE:HE2	1:A:145:CYS:H	4	0.12	0.0	0.12
(1,509)	1:A:50:TRP:HE1	1:A:146:VAL:HA	4	0.11	0.0	0.11
(1,788)	1:A:67:TYR:HE1	1:A:75:LYS:H	4	0.11	0.0	0.11
(1,788)	1:A:67:TYR:HE2	1:A:75:LYS:H	4	0.11	0.0	0.11
(1,1821)	1:A:156:THR:HA	1:A:157:ASP:H	4	0.11	0.0	0.11
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD11	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD12	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD13	3	0.14	0.0	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD21	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD22	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD23	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD11	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD12	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD13	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD21	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD22	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD23	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD11	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD12	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD13	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD21	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD22	3	0.14	0.0	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD23	3	0.14	0.0	0.14
(1,414)	1:A:42:ALA:HB1	1:A:43:ALA:H	3	0.13	0.02	0.14
(1,414)	1:A:42:ALA:HB2	1:A:43:ALA:H	3	0.13	0.02	0.14
(1,414)	1:A:42:ALA:HB3	1:A:43:ALA:H	3	0.13	0.02	0.14
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD11	3	0.13	0.01	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD12	3	0.13	0.01	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD13	3	0.13	0.01	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD21	3	0.13	0.01	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD22	3	0.13	0.01	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD23	3	0.13	0.01	0.12
(1,1256)	1:A:103:LEU:HB2	1:A:109:ILE:HD11	3	0.13	0.02	0.12
(1,1256)	1:A:103:LEU:HB2	1:A:109:ILE:HD12	3	0.13	0.02	0.12
(1,1256)	1:A:103:LEU:HB2	1:A:109:ILE:HD13	3	0.13	0.02	0.12
(1,1256)	1:A:103:LEU:HB3	1:A:109:ILE:HD11	3	0.13	0.02	0.12
(1,1256)	1:A:103:LEU:HB3	1:A:109:ILE:HD12	3	0.13	0.02	0.12
(1,1256)	1:A:103:LEU:HB3	1:A:109:ILE:HD13	3	0.13	0.02	0.12
(1,61)	1:A:14:ASP:H	1:A:15:GLY:H	3	0.12	0.01	0.13
(1,1335)	1:A:109:ILE:HA	1:A:119:THR:HG21	3	0.12	0.01	0.12
(1,1335)	1:A:109:ILE:HA	1:A:119:THR:HG22	3	0.12	0.01	0.12
(1,1335)	1:A:109:ILE:HA	1:A:119:THR:HG23	3	0.12	0.01	0.12
(1,488)	1:A:49:LEU:HB2	1:A:53:MET:HE1	3	0.12	0.01	0.12
(1,488)	1:A:49:LEU:HB2	1:A:53:MET:HE2	3	0.12	0.01	0.12
(1,488)	1:A:49:LEU:HB2	1:A:53:MET:HE3	3	0.12	0.01	0.12
(1,488)	1:A:49:LEU:HB3	1:A:53:MET:HE1	3	0.12	0.01	0.12
(1,488)	1:A:49:LEU:HB3	1:A:53:MET:HE2	3	0.12	0.01	0.12
(1,488)	1:A:49:LEU:HB3	1:A:53:MET:HE3	3	0.12	0.01	0.12
(1,353)	1:A:32:ASP:HA	1:A:35:LYS:H	3	0.12	0.01	0.11
(1,610)	1:A:57:HIS:HE1	1:A:104:CYS:HB2	3	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,610)	1:A:57:HIS:HE1	1:A:104:CYS:HB3	3	0.12	0.0	0.12
(1,1102)	1:A:91:LEU:HD11	1:A:106:LEU:HB2	3	0.11	0.0	0.11
(1,1102)	1:A:91:LEU:HD11	1:A:106:LEU:HB3	3	0.11	0.0	0.11
(1,1102)	1:A:91:LEU:HD12	1:A:106:LEU:HB2	3	0.11	0.0	0.11
(1,1102)	1:A:91:LEU:HD12	1:A:106:LEU:HB3	3	0.11	0.0	0.11
(1,1102)	1:A:91:LEU:HD13	1:A:106:LEU:HB2	3	0.11	0.0	0.11
(1,1102)	1:A:91:LEU:HD13	1:A:106:LEU:HB3	3	0.11	0.0	0.11
(1,1102)	1:A:91:LEU:HD21	1:A:106:LEU:HB2	3	0.11	0.0	0.11
(1,1102)	1:A:91:LEU:HD21	1:A:106:LEU:HB3	3	0.11	0.0	0.11
(1,1102)	1:A:91:LEU:HD22	1:A:106:LEU:HB2	3	0.11	0.0	0.11
(1,1102)	1:A:91:LEU:HD22	1:A:106:LEU:HB3	3	0.11	0.0	0.11
(1,1102)	1:A:91:LEU:HD23	1:A:106:LEU:HB2	3	0.11	0.0	0.11
(1,1102)	1:A:91:LEU:HD23	1:A:106:LEU:HB3	3	0.11	0.0	0.11
(3,18)	1:A:120:CYS:SG	1:A:145:CYS:SG	3	0.11	0.0	0.11
(1,17)	1:A:4:ILE:HA	1:A:5:LYS:H	3	0.11	0.0	0.11
(1,857)	1:A:73:ILE:HG21	1:A:78:TYR:HB2	3	0.11	0.0	0.11
(1,857)	1:A:73:ILE:HG21	1:A:78:TYR:HB3	3	0.11	0.0	0.11
(1,857)	1:A:73:ILE:HG22	1:A:78:TYR:HB2	3	0.11	0.0	0.11
(1,857)	1:A:73:ILE:HG22	1:A:78:TYR:HB3	3	0.11	0.0	0.11
(1,857)	1:A:73:ILE:HG23	1:A:78:TYR:HB2	3	0.11	0.0	0.11
(1,857)	1:A:73:ILE:HG23	1:A:78:TYR:HB3	3	0.11	0.0	0.11
(1,1356)	1:A:112:ASN:HB2	1:A:113:GLU:H	2	0.22	0.02	0.22
(1,1356)	1:A:112:ASN:HB3	1:A:113:GLU:H	2	0.22	0.02	0.22
(1,418)	1:A:43:ALA:HB1	1:A:44:LYS:H	2	0.17	0.0	0.17
(1,418)	1:A:43:ALA:HB2	1:A:44:LYS:H	2	0.17	0.0	0.17
(1,418)	1:A:43:ALA:HB3	1:A:44:LYS:H	2	0.17	0.0	0.17
(1,30)	1:A:11:PRO:HA	1:A:12:ALA:H	2	0.12	0.0	0.12
(1,326)	1:A:30:LEU:HA	1:A:52:ILE:HD11	2	0.12	0.0	0.12
(1,326)	1:A:30:LEU:HA	1:A:52:ILE:HD12	2	0.12	0.0	0.12
(1,326)	1:A:30:LEU:HA	1:A:52:ILE:HD13	2	0.12	0.0	0.12
(1,7)	1:A:3:ARG:HA	1:A:4:ILE:H	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD11	1:A:33:ALA:HB1	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD11	1:A:33:ALA:HB2	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD11	1:A:33:ALA:HB3	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD12	1:A:33:ALA:HB1	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD12	1:A:33:ALA:HB2	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD12	1:A:33:ALA:HB3	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD13	1:A:33:ALA:HB1	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD13	1:A:33:ALA:HB2	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD13	1:A:33:ALA:HB3	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD21	1:A:33:ALA:HB1	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD21	1:A:33:ALA:HB2	2	0.11	0.0	0.11

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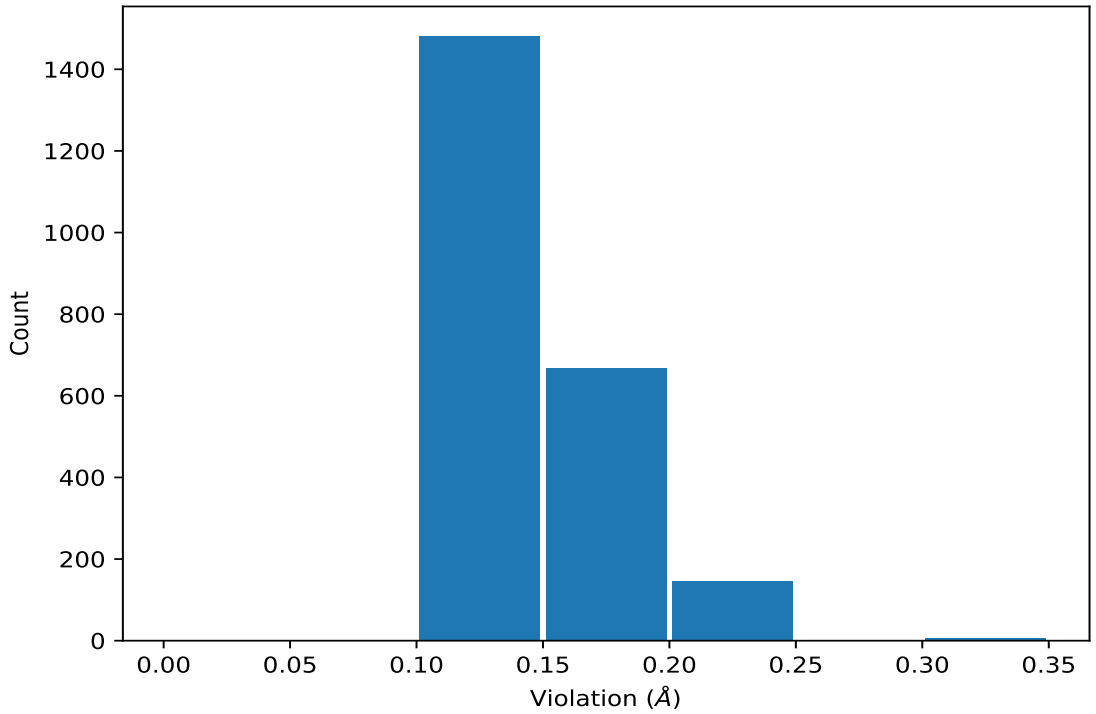
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,324)	1:A:30:LEU:HD21	1:A:33:ALA:HB3	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD22	1:A:33:ALA:HB1	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD22	1:A:33:ALA:HB2	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD22	1:A:33:ALA:HB3	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD23	1:A:33:ALA:HB1	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD23	1:A:33:ALA:HB2	2	0.11	0.0	0.11
(1,324)	1:A:30:LEU:HD23	1:A:33:ALA:HB3	2	0.11	0.0	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD11	2	0.11	0.0	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD12	2	0.11	0.0	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD13	2	0.11	0.0	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD21	2	0.11	0.0	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD22	2	0.11	0.0	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD23	2	0.11	0.0	0.11
(1,1358)	1:A:113:GLU:HA	1:A:114:THR:H	2	0.11	0.0	0.11
(1,1713)	1:A:143:HIS:HA	1:A:144:GLN:H	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	8	0.32
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	17	0.31
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	28	0.31
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	29	0.31
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	3	0.3
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	10	0.26
(1,1664)	1:A:139:GLN:H	1:A:139:GLN:HB2	22	0.24
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD11	26	0.23
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD12	26	0.23
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD13	26	0.23
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD21	26	0.23
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD22	26	0.23
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD23	26	0.23
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	25	0.23
(1,1356)	1:A:112:ASN:HB2	1:A:113:GLU:H	35	0.23
(1,1356)	1:A:112:ASN:HB3	1:A:113:GLU:H	35	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	1	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	1	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	3	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	3	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	4	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	4	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	6	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	6	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	7	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	7	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	8	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	8	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	17	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	17	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	21	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	21	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	22	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	22	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	24	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	24	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	26	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	26	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	31	0.23
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	31	0.23
(1,559)	1:A:53:MET:HB3	1:A:148:CYS:HB3	10	0.22
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB2	1	0.22
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB3	1	0.22
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB2	1	0.22
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB3	1	0.22
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB2	1	0.22
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB3	1	0.22
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB2	17	0.22
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB3	17	0.22
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB2	17	0.22
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB3	17	0.22
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB2	17	0.22
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB3	17	0.22
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB2	25	0.22
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB3	25	0.22
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB2	25	0.22
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB3	25	0.22
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB2	25	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB3	25	0.22
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	27	0.22
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	27	0.22
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	35	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	2	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	2	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	5	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	5	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	9	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	9	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	10	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	10	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	11	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	11	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	12	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	12	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	13	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	13	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	16	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	16	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	18	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	18	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	19	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	19	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	23	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	23	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	25	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	25	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	27	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	27	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	29	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	29	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	30	0.22
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	30	0.22
(1,559)	1:A:53:MET:HB3	1:A:148:CYS:HB3	25	0.21
(1,559)	1:A:53:MET:HB3	1:A:148:CYS:HB3	27	0.21
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB2	31	0.21
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB3	31	0.21
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB2	31	0.21
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB3	31	0.21
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB2	31	0.21
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB3	31	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB2	32	0.21
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB3	32	0.21
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB2	32	0.21
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB3	32	0.21
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB2	32	0.21
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB3	32	0.21
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	21	0.21
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	19	0.21
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	24	0.21
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	15	0.21
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	15	0.21
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	20	0.21
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	20	0.21
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	28	0.21
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	28	0.21
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	33	0.21
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	33	0.21
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	35	0.21
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	35	0.21
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	27	0.2
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	32	0.2
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	35	0.2
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	28	0.2
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	28	0.2
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	28	0.2
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG11	35	0.2
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG12	35	0.2
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG13	35	0.2
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG21	35	0.2
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG22	35	0.2
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG23	35	0.2
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG11	35	0.2
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG12	35	0.2
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG13	35	0.2
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG21	35	0.2
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG22	35	0.2
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG23	35	0.2
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG11	35	0.2
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG12	35	0.2
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG13	35	0.2
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG21	35	0.2
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG22	35	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG23	35	0.2
(1,1356)	1:A:112:ASN:HB2	1:A:113:GLU:H	34	0.2
(1,1356)	1:A:112:ASN:HB3	1:A:113:GLU:H	34	0.2
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	14	0.2
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	14	0.2
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	32	0.2
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	32	0.2
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD1	34	0.2
(1,1019)	1:A:85:LYS:HA	1:A:86:TYR:HD2	34	0.2
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	18	0.2
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	18	0.2
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD11	35	0.19
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD12	35	0.19
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD13	35	0.19
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD21	35	0.19
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD22	35	0.19
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD23	35	0.19
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	21	0.19
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	21	0.19
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	30	0.19
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	30	0.19
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	30	0.19
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	34	0.19
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	34	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG11	28	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG12	28	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG13	28	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG21	28	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG22	28	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG23	28	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG11	28	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG12	28	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG13	28	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG21	28	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG22	28	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG23	28	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG11	28	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG12	28	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG13	28	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG21	28	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG22	28	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG23	28	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG11	30	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG12	30	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG13	30	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG21	30	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG22	30	0.19
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG23	30	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG11	30	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG12	30	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG13	30	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG21	30	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG22	30	0.19
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG23	30	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG11	30	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG12	30	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG13	30	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG21	30	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG22	30	0.19
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG23	30	0.19
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	18	0.19
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	12	0.19
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	12	0.19
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	15	0.19
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	15	0.19
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	35	0.19
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	35	0.19
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG21	31	0.18
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG22	31	0.18
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG23	31	0.18
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG21	31	0.18
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG22	31	0.18
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG23	31	0.18
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG21	31	0.18
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG22	31	0.18
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG23	31	0.18
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	4	0.18
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	26	0.18
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	33	0.18
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	1	0.18
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	1	0.18
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	8	0.18
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	8	0.18
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	12	0.18
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	17	0.18
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	17	0.18
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	20	0.18
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	20	0.18
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	32	0.18
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	32	0.18
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	19	0.18
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	19	0.18
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	19	0.18
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	19	0.18
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	19	0.18
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	19	0.18
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG11	21	0.18
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG12	21	0.18
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG13	21	0.18
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG21	21	0.18
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG22	21	0.18
(1,1420)	1:A:121:ILE:HD11	1:A:124:VAL:HG23	21	0.18
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG11	21	0.18
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG12	21	0.18
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG13	21	0.18
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG21	21	0.18
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG22	21	0.18
(1,1420)	1:A:121:ILE:HD12	1:A:124:VAL:HG23	21	0.18
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG11	21	0.18
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG12	21	0.18
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG13	21	0.18
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG21	21	0.18
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG22	21	0.18
(1,1420)	1:A:121:ILE:HD13	1:A:124:VAL:HG23	21	0.18
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	5	0.18
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	25	0.18
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	26	0.18
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	27	0.18
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	2	0.18
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	2	0.18
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	11	0.18
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	11	0.18
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	16	0.18
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	16	0.18
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	20	0.18
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	29	0.18
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	29	0.18
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	30	0.18
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	30	0.18
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	34	0.18
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	34	0.18
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	8	0.17
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	8	0.17
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	8	0.17
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	8	0.17
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	8	0.17
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	8	0.17
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	15	0.17
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	15	0.17
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	15	0.17
(1,563)	1:A:53:MET:HE1	1:A:148:CYS:HB3	8	0.17
(1,563)	1:A:53:MET:HE2	1:A:148:CYS:HB3	8	0.17
(1,563)	1:A:53:MET:HE3	1:A:148:CYS:HB3	8	0.17
(1,563)	1:A:53:MET:HE1	1:A:148:CYS:HB3	17	0.17
(1,563)	1:A:53:MET:HE2	1:A:148:CYS:HB3	17	0.17
(1,563)	1:A:53:MET:HE3	1:A:148:CYS:HB3	17	0.17
(1,418)	1:A:43:ALA:HB1	1:A:44:LYS:H	11	0.17
(1,418)	1:A:43:ALA:HB2	1:A:44:LYS:H	11	0.17
(1,418)	1:A:43:ALA:HB3	1:A:44:LYS:H	11	0.17
(1,418)	1:A:43:ALA:HB1	1:A:44:LYS:H	31	0.17
(1,418)	1:A:43:ALA:HB2	1:A:44:LYS:H	31	0.17
(1,418)	1:A:43:ALA:HB3	1:A:44:LYS:H	31	0.17
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG21	32	0.17
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG22	32	0.17
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG23	32	0.17
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG21	32	0.17
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG22	32	0.17
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG23	32	0.17
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG21	32	0.17
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG22	32	0.17
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG23	32	0.17
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB2	22	0.17
(1,366)	1:A:33:ALA:HB1	1:A:48:GLN:HB3	22	0.17
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB2	22	0.17
(1,366)	1:A:33:ALA:HB2	1:A:48:GLN:HB3	22	0.17
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB2	22	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:A:33:ALA:HB3	1:A:48:GLN:HB3	22	0.17
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD11	31	0.17
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD12	31	0.17
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD13	31	0.17
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD21	31	0.17
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD22	31	0.17
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD23	31	0.17
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD11	33	0.17
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD12	33	0.17
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD13	33	0.17
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD21	33	0.17
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD22	33	0.17
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD23	33	0.17
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	11	0.17
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	11	0.17
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	15	0.17
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	15	0.17
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	18	0.17
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	18	0.17
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	35	0.17
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	35	0.17
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	23	0.17
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	23	0.17
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	23	0.17
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	23	0.17
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	23	0.17
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	23	0.17
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	23	0.17
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	23	0.17
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	23	0.17
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	23	0.17
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	23	0.17
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	23	0.17
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	16	0.17
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	13	0.17
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	13	0.17
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	22	0.17
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	22	0.17
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	23	0.17
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	23	0.17
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	28	0.17
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	28	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	5	0.17
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	5	0.17
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	5	0.17
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	5	0.17
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	5	0.17
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	5	0.17
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	10	0.17
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	10	0.17
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	10	0.17
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	10	0.17
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	10	0.17
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	10	0.17
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	16	0.17
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	16	0.17
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	16	0.17
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	16	0.17
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	16	0.17
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	16	0.17
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	25	0.17
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	25	0.17
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	25	0.17
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	25	0.17
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	25	0.17
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	25	0.17
(1,1421)	1:A:121:ILE:HG21	1:A:142:PHE:HA	21	0.17
(1,1421)	1:A:121:ILE:HG22	1:A:142:PHE:HA	21	0.17
(1,1421)	1:A:121:ILE:HG23	1:A:142:PHE:HA	21	0.17
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	2	0.17
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	6	0.17
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	12	0.17
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	16	0.17
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	30	0.17
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	26	0.17
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	26	0.17
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	27	0.17
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	27	0.17
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	6	0.17
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	6	0.17
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	7	0.17
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	7	0.17
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	8	0.17
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	14	0.17
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	14	0.17
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	17	0.17
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	17	0.17
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	19	0.17
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	19	0.17
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	23	0.17
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	23	0.17
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	25	0.17
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	25	0.17
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	28	0.17
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	28	0.17
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	31	0.17
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	31	0.17
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	32	0.17
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	32	0.17
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	33	0.17
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	33	0.17
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	29	0.16
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	29	0.16
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	29	0.16
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	29	0.16
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	29	0.16
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	29	0.16
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	4	0.16
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	4	0.16
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	4	0.16
(1,563)	1:A:53:MET:HE1	1:A:148:CYS:HB3	28	0.16
(1,563)	1:A:53:MET:HE2	1:A:148:CYS:HB3	28	0.16
(1,563)	1:A:53:MET:HE3	1:A:148:CYS:HB3	28	0.16
(1,563)	1:A:53:MET:HE1	1:A:148:CYS:HB3	29	0.16
(1,563)	1:A:53:MET:HE2	1:A:148:CYS:HB3	29	0.16
(1,563)	1:A:53:MET:HE3	1:A:148:CYS:HB3	29	0.16
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	33	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD11	30	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD12	30	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD13	30	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD21	30	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD22	30	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD23	30	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD11	32	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD12	32	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD13	32	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD21	32	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD22	32	0.16
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD23	32	0.16
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	20	0.16
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	24	0.16
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	6	0.16
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	6	0.16
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	9	0.16
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	9	0.16
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	14	0.16
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	14	0.16
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	1	0.16
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	1	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	1	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	1	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	1	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	1	0.16
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	1	0.16
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	1	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	1	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	1	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	1	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	1	0.16
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	5	0.16
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	5	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	5	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	5	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	5	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	5	0.16
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	5	0.16
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	5	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	5	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	5	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	5	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	5	0.16
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	7	0.16
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	7	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	7	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	7	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	7	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	7	0.16
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	7	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	7	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	7	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	7	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	7	0.16
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	12	0.16
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	12	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	12	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	12	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	12	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	12	0.16
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	12	0.16
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	12	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	12	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	12	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	12	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	12	0.16
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	18	0.16
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	18	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	18	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	18	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	18	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	18	0.16
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	18	0.16
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	18	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	18	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	18	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	18	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	18	0.16
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	21	0.16
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	21	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	21	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	21	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	21	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	21	0.16
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	21	0.16
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	21	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	21	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	21	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	21	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	21	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	34	0.16
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	34	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	34	0.16
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	34	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	34	0.16
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	34	0.16
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	34	0.16
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	34	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	34	0.16
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	34	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	34	0.16
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	34	0.16
(1,1587)	1:A:132:GLU:HA	1:A:132:GLU:HB3	12	0.16
(1,1587)	1:A:132:GLU:HA	1:A:132:GLU:HB3	16	0.16
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	5	0.16
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	8	0.16
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	10	0.16
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	20	0.16
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	23	0.16
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	24	0.16
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	27	0.16
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	29	0.16
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	31	0.16
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	34	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	3	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	3	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	4	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	4	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	5	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	5	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	10	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	10	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	25	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	25	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	29	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	29	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	31	0.16
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	31	0.16
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	3	0.16
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	3	0.16
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	3	0.16
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	3	0.16
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	3	0.16
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	26	0.16
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	26	0.16
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	26	0.16
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	26	0.16
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	26	0.16
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	26	0.16
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	33	0.16
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	33	0.16
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	33	0.16
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	33	0.16
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	33	0.16
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	33	0.16
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	17	0.16
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	7	0.16
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	8	0.16
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	11	0.16
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	22	0.16
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	29	0.16
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	3	0.16
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	3	0.16
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	9	0.16
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	9	0.16
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	13	0.16
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	13	0.16
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	16	0.16
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	16	0.16
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	19	0.16
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	19	0.16
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	25	0.16
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	25	0.16
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	1	0.16
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	1	0.16
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	3	0.16
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	3	0.16
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	5	0.16
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	5	0.16
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	21	0.16
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	21	0.16
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	22	0.16
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	22	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	27	0.16
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	27	0.16
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	1	0.15
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	1	0.15
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	1	0.15
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	1	0.15
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	1	0.15
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	1	0.15
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	20	0.15
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	20	0.15
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	20	0.15
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	20	0.15
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	20	0.15
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	20	0.15
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	3	0.15
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	3	0.15
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	3	0.15
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	16	0.15
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	16	0.15
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	16	0.15
(1,563)	1:A:53:MET:HE1	1:A:148:CYS:HB3	3	0.15
(1,563)	1:A:53:MET:HE2	1:A:148:CYS:HB3	3	0.15
(1,563)	1:A:53:MET:HE3	1:A:148:CYS:HB3	3	0.15
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	3	0.15
(1,414)	1:A:42:ALA:HB1	1:A:43:ALA:H	5	0.15
(1,414)	1:A:42:ALA:HB2	1:A:43:ALA:H	5	0.15
(1,414)	1:A:42:ALA:HB3	1:A:43:ALA:H	5	0.15
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	19	0.15
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	31	0.15
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	7	0.15
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	7	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	4	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	4	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	4	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	4	0.15
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	4	0.15
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	4	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	4	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	4	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	4	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	4	0.15
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	4	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	13	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	13	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	13	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	13	0.15
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	13	0.15
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	13	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	13	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	13	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	13	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	13	0.15
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	13	0.15
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	13	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	16	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	16	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	16	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	16	0.15
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	16	0.15
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	16	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	16	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	16	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	16	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	16	0.15
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	16	0.15
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	16	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	20	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	20	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	20	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	20	0.15
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	20	0.15
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	20	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	20	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	20	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	20	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	20	0.15
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	20	0.15
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	20	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	22	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	22	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	22	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	22	0.15
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	22	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	22	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	22	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	22	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	22	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	22	0.15
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	22	0.15
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	22	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	27	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	27	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	27	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	27	0.15
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	27	0.15
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	27	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	27	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	27	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	27	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	27	0.15
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	27	0.15
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	27	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	28	0.15
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	28	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	28	0.15
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	28	0.15
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	28	0.15
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	28	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	28	0.15
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	28	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	28	0.15
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	28	0.15
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	28	0.15
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	28	0.15
(1,1587)	1:A:132:GLU:HA	1:A:132:GLU:HB3	9	0.15
(1,1587)	1:A:132:GLU:HA	1:A:132:GLU:HB3	13	0.15
(1,1587)	1:A:132:GLU:HA	1:A:132:GLU:HB3	27	0.15
(1,1587)	1:A:132:GLU:HA	1:A:132:GLU:HB3	28	0.15
(1,1587)	1:A:132:GLU:HA	1:A:132:GLU:HB3	29	0.15
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	6	0.15
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	9	0.15
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	11	0.15
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	12	0.15
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	13	0.15
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	19	0.15
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	25	0.15
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	26	0.15
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	7	0.15
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	7	0.15
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	14	0.15
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	14	0.15
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	16	0.15
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	16	0.15
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	26	0.15
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	26	0.15
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	33	0.15
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	33	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	4	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	4	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	4	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	4	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	4	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	4	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	17	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	17	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	17	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	17	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	17	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	17	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	23	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	23	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	23	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	23	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	23	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	23	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	24	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	24	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	24	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	24	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	24	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	24	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	29	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	29	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	29	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	29	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	29	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	29	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	31	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	31	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	31	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	31	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	31	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	31	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	32	0.15
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	32	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	32	0.15
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	32	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	32	0.15
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	32	0.15
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	8	0.15
(1,1317)	1:A:108:CYS:HB2	1:A:120:CYS:HB3	23	0.15
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	13	0.15
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	14	0.15
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	15	0.15
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	17	0.15
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	21	0.15
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	28	0.15
(1,1256)	1:A:103:LEU:HB2	1:A:109:ILE:HD11	3	0.15
(1,1256)	1:A:103:LEU:HB2	1:A:109:ILE:HD12	3	0.15
(1,1256)	1:A:103:LEU:HB2	1:A:109:ILE:HD13	3	0.15
(1,1256)	1:A:103:LEU:HB3	1:A:109:ILE:HD11	3	0.15
(1,1256)	1:A:103:LEU:HB3	1:A:109:ILE:HD12	3	0.15
(1,1256)	1:A:103:LEU:HB3	1:A:109:ILE:HD13	3	0.15
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	1	0.15
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	1	0.15
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	4	0.15
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	4	0.15
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	6	0.15
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	6	0.15
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	10	0.15
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	10	0.15
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	24	0.15
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	24	0.15
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	4	0.15
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	4	0.15
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	9	0.15
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	9	0.15
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	10	0.15
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	13	0.15
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	13	0.15
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	24	0.15
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	24	0.15
(1,1004)	1:A:84:GLU:HB2	1:A:85:LYS:H	26	0.15
(1,1004)	1:A:84:GLU:HB3	1:A:85:LYS:H	26	0.15
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	11	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	11	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	11	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	11	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	11	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	11	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	13	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	13	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	13	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	13	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	13	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	13	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	19	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	19	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	19	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	19	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	19	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	19	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	23	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	23	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	23	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	23	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	23	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	23	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	33	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	33	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	33	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	33	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	33	0.14
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	33	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	2	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	2	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	2	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	11	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	11	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	19	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	19	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	19	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	29	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	29	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	29	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	30	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	30	0.14
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	30	0.14
(1,559)	1:A:53:MET:HB3	1:A:148:CYS:HB3	8	0.14
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	13	0.14
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	14	0.14
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	27	0.14
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	34	0.14
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	29	0.14
(1,503)	1:A:50:TRP:HA	1:A:53:MET:H	31	0.14
(1,503)	1:A:50:TRP:HA	1:A:53:MET:H	32	0.14
(1,414)	1:A:42:ALA:HB1	1:A:43:ALA:H	15	0.14
(1,414)	1:A:42:ALA:HB2	1:A:43:ALA:H	15	0.14
(1,414)	1:A:42:ALA:HB3	1:A:43:ALA:H	15	0.14
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG21	30	0.14
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG22	30	0.14
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG23	30	0.14
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG21	30	0.14
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG22	30	0.14
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG23	30	0.14
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG21	30	0.14
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG22	30	0.14
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG23	30	0.14
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD11	31	0.14
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD12	31	0.14
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD13	31	0.14
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD21	31	0.14
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD22	31	0.14
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD23	31	0.14
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD11	16	0.14
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD12	16	0.14
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD13	16	0.14
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD21	16	0.14
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD22	16	0.14
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD23	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	6	0.14
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	7	0.14
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	13	0.14
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	15	0.14
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	16	0.14
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	2	0.14
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	2	0.14
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	22	0.14
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	22	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	6	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	6	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	6	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	6	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	6	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	6	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	6	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	6	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	6	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	6	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	6	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	6	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	8	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	8	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	8	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	8	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	8	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	8	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	8	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	8	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	8	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	8	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	8	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	8	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	9	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	9	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	9	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	9	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	9	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	9	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	9	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	9	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	9	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	9	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	9	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	10	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	10	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	10	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	10	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	10	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	10	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	10	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	10	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	10	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	10	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	10	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	10	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	11	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	11	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	11	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	11	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	11	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	11	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	11	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	11	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	11	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	11	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	11	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	11	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	14	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	14	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	14	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	14	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	14	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	14	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	14	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	14	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	14	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	14	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	14	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	14	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	17	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	17	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	17	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	17	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	17	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	17	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	17	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	17	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	17	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	17	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	17	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	19	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	19	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	19	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	19	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	19	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	19	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	19	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	19	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	19	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	19	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	19	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	19	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	24	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	24	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	24	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	24	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	24	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	24	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	24	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	24	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	24	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	24	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	24	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	24	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	26	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	26	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	26	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	26	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	26	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	26	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	26	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	26	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	26	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	26	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	26	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	26	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	29	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	29	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	29	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	29	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	29	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	29	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	29	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	29	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	29	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	29	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	29	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	29	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	31	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	31	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	31	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	31	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	31	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	31	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	31	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	31	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	31	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	31	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	31	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	31	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	32	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	32	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	32	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	32	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	32	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	32	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	32	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	32	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	32	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	32	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	32	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	32	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	33	0.14
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	33	0.14
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	33	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	33	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	33	0.14
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	33	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	33	0.14
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	33	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	33	0.14
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	33	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	33	0.14
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	33	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD11	13	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD12	13	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD13	13	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD21	13	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD22	13	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD23	13	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD11	13	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD12	13	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD13	13	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD21	13	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD22	13	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD23	13	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD11	13	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD12	13	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD13	13	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD21	13	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD22	13	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD23	13	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD11	34	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD12	34	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD13	34	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD21	34	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD22	34	0.14
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD23	34	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD11	34	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD12	34	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD13	34	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD21	34	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD22	34	0.14
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD23	34	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD11	34	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD12	34	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD13	34	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD21	34	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD22	34	0.14
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD23	34	0.14
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	1	0.14
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	2	0.14
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	3	0.14
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	4	0.14
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	7	0.14
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	14	0.14
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	15	0.14
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	18	0.14
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	22	0.14
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	32	0.14
(1,1448)	1:A:122:CYS:HB2	1:A:142:PHE:HZ	33	0.14
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	24	0.14
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	24	0.14
(1,1433)	1:A:121:ILE:HG21	1:A:145:CYS:HB2	21	0.14
(1,1433)	1:A:121:ILE:HG22	1:A:145:CYS:HB2	21	0.14
(1,1433)	1:A:121:ILE:HG23	1:A:145:CYS:HB2	21	0.14
(1,1433)	1:A:121:ILE:HG21	1:A:145:CYS:HB2	35	0.14
(1,1433)	1:A:121:ILE:HG22	1:A:145:CYS:HB2	35	0.14
(1,1433)	1:A:121:ILE:HG23	1:A:145:CYS:HB2	35	0.14
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	1	0.14
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	1	0.14
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	1	0.14
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	1	0.14
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	1	0.14
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	1	0.14
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	8	0.14
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	8	0.14
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	8	0.14
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	8	0.14
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	8	0.14
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	8	0.14
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	12	0.14
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	12	0.14
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	12	0.14
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	12	0.14
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	12	0.14
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	12	0.14
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	13	0.14
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	13	0.14
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	13	0.14
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	13	0.14
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	13	0.14
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	20	0.14
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	20	0.14
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	20	0.14
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	20	0.14
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	20	0.14
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	20	0.14
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	34	0.14
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	34	0.14
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	34	0.14
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	34	0.14
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	34	0.14
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	34	0.14
(1,1421)	1:A:121:ILE:HG21	1:A:142:PHE:HA	30	0.14
(1,1421)	1:A:121:ILE:HG22	1:A:142:PHE:HA	30	0.14
(1,1421)	1:A:121:ILE:HG23	1:A:142:PHE:HA	30	0.14
(1,1421)	1:A:121:ILE:HG21	1:A:142:PHE:HA	35	0.14
(1,1421)	1:A:121:ILE:HG22	1:A:142:PHE:HA	35	0.14
(1,1421)	1:A:121:ILE:HG23	1:A:142:PHE:HA	35	0.14
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	29	0.14
(1,1335)	1:A:109:ILE:HA	1:A:119:THR:HG21	34	0.14
(1,1335)	1:A:109:ILE:HA	1:A:119:THR:HG22	34	0.14
(1,1335)	1:A:109:ILE:HA	1:A:119:THR:HG23	34	0.14
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	20	0.14
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD1	20	0.14
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD2	20	0.14
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD1	20	0.14
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD2	20	0.14
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD11	10	0.14
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD12	10	0.14
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD13	10	0.14
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD21	10	0.14
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD22	10	0.14
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD23	10	0.14
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD11	10	0.14
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD12	10	0.14
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD13	10	0.14
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD21	10	0.14
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD22	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD23	10	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	7	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	7	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	11	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	11	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	17	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	17	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	21	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	21	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	22	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	22	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	23	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	23	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	28	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	28	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	29	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	29	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	31	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	31	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	33	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	33	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	35	0.14
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	35	0.14
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE1	22	0.14
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE2	22	0.14
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE1	22	0.14
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE2	22	0.14
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	2	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	2	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	2	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	2	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	2	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	2	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	4	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	4	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	4	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	4	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	4	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	4	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	7	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	7	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	7	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	7	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	7	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	14	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	14	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	14	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	14	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	14	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	14	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	16	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	16	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	16	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	16	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	16	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	16	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	18	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	18	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	18	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	18	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	18	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	18	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	21	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	21	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	21	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	21	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	21	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	21	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	22	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	22	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	22	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	22	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	22	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	22	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	25	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	25	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	25	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	25	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	25	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	25	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	32	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	32	0.13
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	32	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	32	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	32	0.13
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	32	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	1	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	1	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	1	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	7	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	7	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	7	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	23	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	23	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	23	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	24	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	24	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	24	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	25	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	25	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	25	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	27	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	27	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	27	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	32	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	32	0.13
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	32	0.13
(1,61)	1:A:14:ASP:H	1:A:15:GLY:H	13	0.13
(1,61)	1:A:14:ASP:H	1:A:15:GLY:H	34	0.13
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	6	0.13
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	16	0.13
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	32	0.13
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	28	0.13
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	31	0.13
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	33	0.13
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	34	0.13
(1,503)	1:A:50:TRP:HA	1:A:53:MET:H	26	0.13
(1,488)	1:A:49:LEU:HB2	1:A:53:MET:HE1	29	0.13
(1,488)	1:A:49:LEU:HB2	1:A:53:MET:HE2	29	0.13
(1,488)	1:A:49:LEU:HB2	1:A:53:MET:HE3	29	0.13
(1,488)	1:A:49:LEU:HB3	1:A:53:MET:HE1	29	0.13
(1,488)	1:A:49:LEU:HB3	1:A:53:MET:HE2	29	0.13
(1,488)	1:A:49:LEU:HB3	1:A:53:MET:HE3	29	0.13
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG21	7	0.13
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG22	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG23	7	0.13
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG21	7	0.13
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG22	7	0.13
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG23	7	0.13
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG21	7	0.13
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG22	7	0.13
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG23	7	0.13
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG21	26	0.13
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG22	26	0.13
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG23	26	0.13
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG21	26	0.13
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG22	26	0.13
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG23	26	0.13
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG21	26	0.13
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG22	26	0.13
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG23	26	0.13
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG21	33	0.13
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG22	33	0.13
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG23	33	0.13
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG21	33	0.13
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG22	33	0.13
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG23	33	0.13
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG21	33	0.13
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG22	33	0.13
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG23	33	0.13
(1,353)	1:A:32:ASP:HA	1:A:35:LYS:H	22	0.13
(1,287)	1:A:28:ILE:HA	1:A:31:ARG:H	20	0.13
(1,287)	1:A:28:ILE:HA	1:A:31:ARG:H	23	0.13
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	1	0.13
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	5	0.13
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	9	0.13
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	11	0.13
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	14	0.13
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	21	0.13
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	30	0.13
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	34	0.13
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	10	0.13
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	10	0.13
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	16	0.13
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	16	0.13
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	23	0.13
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	23	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	25	0.13
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	25	0.13
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	1	0.13
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	4	0.13
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	19	0.13
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	20	0.13
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	24	0.13
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	31	0.13
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	2	0.13
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	2	0.13
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	2	0.13
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	2	0.13
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	2	0.13
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	2	0.13
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	2	0.13
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	2	0.13
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	2	0.13
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	2	0.13
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	2	0.13
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	2	0.13
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	3	0.13
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	3	0.13
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	3	0.13
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	3	0.13
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	3	0.13
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	3	0.13
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	3	0.13
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	3	0.13
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	3	0.13
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	3	0.13
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	3	0.13
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	3	0.13
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	15	0.13
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	15	0.13
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	15	0.13
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	15	0.13
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	15	0.13
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	15	0.13
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	15	0.13
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	15	0.13
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	15	0.13
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	15	0.13
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	15	0.13
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	25	0.13
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	25	0.13
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	25	0.13
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	25	0.13
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	25	0.13
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	25	0.13
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	25	0.13
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	25	0.13
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	25	0.13
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	25	0.13
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	25	0.13
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	25	0.13
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	35	0.13
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	35	0.13
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	35	0.13
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	35	0.13
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	35	0.13
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	35	0.13
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	35	0.13
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	35	0.13
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	35	0.13
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	35	0.13
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	35	0.13
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	35	0.13
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD11	27	0.13
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD12	27	0.13
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD13	27	0.13
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD21	27	0.13
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD22	27	0.13
(1,149)	1:A:19:ILE:HG21	1:A:77:LEU:HD23	27	0.13
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD11	27	0.13
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD12	27	0.13
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD13	27	0.13
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD21	27	0.13
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD22	27	0.13
(1,149)	1:A:19:ILE:HG22	1:A:77:LEU:HD23	27	0.13
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD11	27	0.13
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD12	27	0.13
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD13	27	0.13
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD21	27	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD22	27	0.13
(1,149)	1:A:19:ILE:HG23	1:A:77:LEU:HD23	27	0.13
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	11	0.13
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	11	0.13
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	15	0.13
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	15	0.13
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	18	0.13
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	18	0.13
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	19	0.13
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	19	0.13
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	2	0.13
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	2	0.13
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	2	0.13
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	2	0.13
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	2	0.13
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	2	0.13
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	6	0.13
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	6	0.13
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	6	0.13
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	6	0.13
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	6	0.13
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	6	0.13
(1,1421)	1:A:121:ILE:HG21	1:A:142:PHE:HA	28	0.13
(1,1421)	1:A:121:ILE:HG22	1:A:142:PHE:HA	28	0.13
(1,1421)	1:A:121:ILE:HG23	1:A:142:PHE:HA	28	0.13
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	28	0.13
(1,1317)	1:A:108:CYS:HB2	1:A:120:CYS:HB3	5	0.13
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	1	0.13
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	9	0.13
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	31	0.13
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	32	0.13
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	35	0.13
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD11	13	0.13
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD12	13	0.13
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD13	13	0.13
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD11	13	0.13
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD12	13	0.13
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD13	13	0.13
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD11	20	0.13
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD12	20	0.13
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD13	20	0.13
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD11	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD12	20	0.13
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD13	20	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	2	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	2	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	5	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	5	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	8	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	8	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	12	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	12	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	14	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	14	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	20	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	20	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	30	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	30	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	32	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	32	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	34	0.13
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	34	0.13
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE1	8	0.13
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE2	8	0.13
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE1	8	0.13
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE2	8	0.13
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE1	21	0.13
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE2	21	0.13
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE1	21	0.13
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE2	21	0.13
(3,18)	1:A:120:CYS:SG	1:A:145:CYS:SG	34	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	12	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	12	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	12	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	12	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	12	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	12	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	24	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	24	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	24	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	24	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	24	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	24	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	27	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	27	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	27	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	27	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	27	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	27	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	31	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	31	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	31	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	31	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	31	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	31	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	34	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	34	0.12
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	34	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	34	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	34	0.12
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	34	0.12
(1,788)	1:A:67:TYR:HE1	1:A:75:LYS:H	24	0.12
(1,788)	1:A:67:TYR:HE2	1:A:75:LYS:H	24	0.12
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD2	2	0.12
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD3	2	0.12
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD2	8	0.12
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD3	8	0.12
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD2	13	0.12
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD3	13	0.12
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD2	32	0.12
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD3	32	0.12
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD11	23	0.12
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD12	23	0.12
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD13	23	0.12
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD11	23	0.12
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD12	23	0.12
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD13	23	0.12
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD11	29	0.12
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD12	29	0.12
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD13	29	0.12
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD11	29	0.12
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD12	29	0.12
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD13	29	0.12
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD11	30	0.12
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD12	30	0.12
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD13	30	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD11	30	0.12
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD12	30	0.12
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD13	30	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	10	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	10	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	10	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	20	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	20	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	20	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	21	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	21	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	21	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	28	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	28	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	28	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	34	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	34	0.12
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	34	0.12
(1,610)	1:A:57:HIS:HE1	1:A:104:CYS:HB2	3	0.12
(1,610)	1:A:57:HIS:HE1	1:A:104:CYS:HB3	3	0.12
(1,610)	1:A:57:HIS:HE1	1:A:104:CYS:HB2	29	0.12
(1,610)	1:A:57:HIS:HE1	1:A:104:CYS:HB3	29	0.12
(1,559)	1:A:53:MET:HB3	1:A:148:CYS:HB3	17	0.12
(1,559)	1:A:53:MET:HB3	1:A:148:CYS:HB3	28	0.12
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	8	0.12
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	11	0.12
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	19	0.12
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	24	0.12
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	31	0.12
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	35	0.12
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	8	0.12
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	17	0.12
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	24	0.12
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	32	0.12
(1,509)	1:A:50:TRP:HE1	1:A:146:VAL:HA	8	0.12
(1,503)	1:A:50:TRP:HA	1:A:53:MET:H	33	0.12
(1,488)	1:A:49:LEU:HB2	1:A:53:MET:HE1	17	0.12
(1,488)	1:A:49:LEU:HB2	1:A:53:MET:HE2	17	0.12
(1,488)	1:A:49:LEU:HB2	1:A:53:MET:HE3	17	0.12
(1,488)	1:A:49:LEU:HB3	1:A:53:MET:HE1	17	0.12
(1,488)	1:A:49:LEU:HB3	1:A:53:MET:HE2	17	0.12
(1,488)	1:A:49:LEU:HB3	1:A:53:MET:HE3	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG21	2	0.12
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG22	2	0.12
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG23	2	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG21	2	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG22	2	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG23	2	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG21	2	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG22	2	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG23	2	0.12
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG21	5	0.12
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG22	5	0.12
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG23	5	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG21	5	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG22	5	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG23	5	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG21	5	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG22	5	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG23	5	0.12
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG21	10	0.12
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG22	10	0.12
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG23	10	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG21	10	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG22	10	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG23	10	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG21	10	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG22	10	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG23	10	0.12
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG21	35	0.12
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG22	35	0.12
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG23	35	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG21	35	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG22	35	0.12
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG23	35	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG21	35	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG22	35	0.12
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG23	35	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD11	32	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD12	32	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD13	32	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD21	32	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD22	32	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD23	32	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD11	35	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD12	35	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD13	35	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD21	35	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD22	35	0.12
(1,331)	1:A:30:LEU:H	1:A:55:LEU:HD23	35	0.12
(1,326)	1:A:30:LEU:HA	1:A:52:ILE:HD11	30	0.12
(1,326)	1:A:30:LEU:HA	1:A:52:ILE:HD12	30	0.12
(1,326)	1:A:30:LEU:HA	1:A:52:ILE:HD13	30	0.12
(1,303)	1:A:29:GLN:HA	1:A:32:ASP:H	3	0.12
(1,303)	1:A:29:GLN:HA	1:A:32:ASP:H	27	0.12
(1,303)	1:A:29:GLN:HA	1:A:32:ASP:H	28	0.12
(1,30)	1:A:11:PRO:HA	1:A:12:ALA:H	14	0.12
(1,287)	1:A:28:ILE:HA	1:A:31:ARG:H	27	0.12
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	12	0.12
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	22	0.12
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	23	0.12
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	34	0.12
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	34	0.12
(1,1698)	1:A:142:PHE:HE1	1:A:145:CYS:H	6	0.12
(1,1698)	1:A:142:PHE:HE2	1:A:145:CYS:H	6	0.12
(1,1698)	1:A:142:PHE:HE1	1:A:145:CYS:H	9	0.12
(1,1698)	1:A:142:PHE:HE2	1:A:145:CYS:H	9	0.12
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	3	0.12
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	13	0.12
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	16	0.12
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	23	0.12
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	26	0.12
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	29	0.12
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	32	0.12
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB2	30	0.12
(1,1679)	1:A:140:VAL:HG11	1:A:141:SER:HB3	30	0.12
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB2	30	0.12
(1,1679)	1:A:140:VAL:HG12	1:A:141:SER:HB3	30	0.12
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB2	30	0.12
(1,1679)	1:A:140:VAL:HG13	1:A:141:SER:HB3	30	0.12
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB2	30	0.12
(1,1679)	1:A:140:VAL:HG21	1:A:141:SER:HB3	30	0.12
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB2	30	0.12
(1,1679)	1:A:140:VAL:HG22	1:A:141:SER:HB3	30	0.12
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB2	30	0.12
(1,1679)	1:A:140:VAL:HG23	1:A:141:SER:HB3	30	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	2	0.12
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	2	0.12
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	6	0.12
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	6	0.12
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	7	0.12
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	7	0.12
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	7	0.12
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	7	0.12
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	7	0.12
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	7	0.12
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	9	0.12
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	9	0.12
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	9	0.12
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	9	0.12
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	9	0.12
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	9	0.12
(1,1421)	1:A:121:ILE:HG21	1:A:142:PHE:HA	27	0.12
(1,1421)	1:A:121:ILE:HG22	1:A:142:PHE:HA	27	0.12
(1,1421)	1:A:121:ILE:HG23	1:A:142:PHE:HA	27	0.12
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	14	0.12
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	22	0.12
(1,1335)	1:A:109:ILE:HA	1:A:119:THR:HG21	10	0.12
(1,1335)	1:A:109:ILE:HA	1:A:119:THR:HG22	10	0.12
(1,1335)	1:A:109:ILE:HA	1:A:119:THR:HG23	10	0.12
(1,1317)	1:A:108:CYS:HB2	1:A:120:CYS:HB3	7	0.12
(1,1317)	1:A:108:CYS:HB2	1:A:120:CYS:HB3	10	0.12
(1,1317)	1:A:108:CYS:HB2	1:A:120:CYS:HB3	12	0.12
(1,1317)	1:A:108:CYS:HB2	1:A:120:CYS:HB3	22	0.12
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	3	0.12
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	4	0.12
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	10	0.12
(1,1256)	1:A:103:LEU:HB2	1:A:109:ILE:HD11	28	0.12
(1,1256)	1:A:103:LEU:HB2	1:A:109:ILE:HD12	28	0.12
(1,1256)	1:A:103:LEU:HB2	1:A:109:ILE:HD13	28	0.12
(1,1256)	1:A:103:LEU:HB3	1:A:109:ILE:HD11	28	0.12
(1,1256)	1:A:103:LEU:HB3	1:A:109:ILE:HD12	28	0.12
(1,1256)	1:A:103:LEU:HB3	1:A:109:ILE:HD13	28	0.12
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD1	7	0.12
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD2	7	0.12
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD1	7	0.12
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD2	7	0.12
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD1	22	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD2	22	0.12
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD1	22	0.12
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD2	22	0.12
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD1	24	0.12
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD2	24	0.12
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD1	24	0.12
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD2	24	0.12
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD11	28	0.12
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD12	28	0.12
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD13	28	0.12
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD11	28	0.12
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD12	28	0.12
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD13	28	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD11	24	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD12	24	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD13	24	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD21	24	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD22	24	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD23	24	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD11	24	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD12	24	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD13	24	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD21	24	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD22	24	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD23	24	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD11	31	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD12	31	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD13	31	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD21	31	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD22	31	0.12
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD23	31	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD11	31	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD12	31	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD13	31	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD21	31	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD22	31	0.12
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD23	31	0.12
(1,1102)	1:A:91:LEU:HD11	1:A:106:LEU:HB2	5	0.12
(1,1102)	1:A:91:LEU:HD11	1:A:106:LEU:HB3	5	0.12
(1,1102)	1:A:91:LEU:HD12	1:A:106:LEU:HB2	5	0.12
(1,1102)	1:A:91:LEU:HD12	1:A:106:LEU:HB3	5	0.12
(1,1102)	1:A:91:LEU:HD13	1:A:106:LEU:HB2	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1102)	1:A:91:LEU:HD13	1:A:106:LEU:HB3	5	0.12
(1,1102)	1:A:91:LEU:HD21	1:A:106:LEU:HB2	5	0.12
(1,1102)	1:A:91:LEU:HD21	1:A:106:LEU:HB3	5	0.12
(1,1102)	1:A:91:LEU:HD22	1:A:106:LEU:HB2	5	0.12
(1,1102)	1:A:91:LEU:HD22	1:A:106:LEU:HB3	5	0.12
(1,1102)	1:A:91:LEU:HD23	1:A:106:LEU:HB2	5	0.12
(1,1102)	1:A:91:LEU:HD23	1:A:106:LEU:HB3	5	0.12
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	15	0.12
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	15	0.12
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD1	18	0.12
(1,1016)	1:A:85:LYS:H	1:A:86:TYR:HD2	18	0.12
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE1	18	0.12
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE2	18	0.12
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE1	18	0.12
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE2	18	0.12
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE1	31	0.12
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE2	31	0.12
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE1	31	0.12
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE2	31	0.12
(3,18)	1:A:120:CYS:SG	1:A:145:CYS:SG	10	0.11
(3,18)	1:A:120:CYS:SG	1:A:145:CYS:SG	23	0.11
(1,857)	1:A:73:ILE:HG21	1:A:78:TYR:HB2	14	0.11
(1,857)	1:A:73:ILE:HG21	1:A:78:TYR:HB3	14	0.11
(1,857)	1:A:73:ILE:HG22	1:A:78:TYR:HB2	14	0.11
(1,857)	1:A:73:ILE:HG22	1:A:78:TYR:HB3	14	0.11
(1,857)	1:A:73:ILE:HG23	1:A:78:TYR:HB2	14	0.11
(1,857)	1:A:73:ILE:HG23	1:A:78:TYR:HB3	14	0.11
(1,857)	1:A:73:ILE:HG21	1:A:78:TYR:HB2	17	0.11
(1,857)	1:A:73:ILE:HG21	1:A:78:TYR:HB3	17	0.11
(1,857)	1:A:73:ILE:HG22	1:A:78:TYR:HB2	17	0.11
(1,857)	1:A:73:ILE:HG22	1:A:78:TYR:HB3	17	0.11
(1,857)	1:A:73:ILE:HG23	1:A:78:TYR:HB2	17	0.11
(1,857)	1:A:73:ILE:HG23	1:A:78:TYR:HB3	17	0.11
(1,857)	1:A:73:ILE:HG21	1:A:78:TYR:HB2	33	0.11
(1,857)	1:A:73:ILE:HG21	1:A:78:TYR:HB3	33	0.11
(1,857)	1:A:73:ILE:HG22	1:A:78:TYR:HB2	33	0.11
(1,857)	1:A:73:ILE:HG22	1:A:78:TYR:HB3	33	0.11
(1,857)	1:A:73:ILE:HG23	1:A:78:TYR:HB2	33	0.11
(1,857)	1:A:73:ILE:HG23	1:A:78:TYR:HB3	33	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	3	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	3	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	3	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	3	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	3	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	5	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	5	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	5	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	5	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	5	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	5	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	6	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	6	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	6	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	6	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	6	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	6	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	9	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	9	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	9	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	9	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	9	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	9	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	10	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	10	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	10	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	10	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	10	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	10	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD11	26	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD12	26	0.11
(1,808)	1:A:68:TYR:HD1	1:A:92:ILE:HD13	26	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD11	26	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD12	26	0.11
(1,808)	1:A:68:TYR:HD2	1:A:92:ILE:HD13	26	0.11
(1,788)	1:A:67:TYR:HE1	1:A:75:LYS:H	5	0.11
(1,788)	1:A:67:TYR:HE2	1:A:75:LYS:H	5	0.11
(1,788)	1:A:67:TYR:HE1	1:A:75:LYS:H	21	0.11
(1,788)	1:A:67:TYR:HE2	1:A:75:LYS:H	21	0.11
(1,788)	1:A:67:TYR:HE1	1:A:75:LYS:H	32	0.11
(1,788)	1:A:67:TYR:HE2	1:A:75:LYS:H	32	0.11
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD2	1	0.11
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD3	1	0.11
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD2	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD3	14	0.11
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD2	22	0.11
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD3	22	0.11
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD2	33	0.11
(1,753)	1:A:66:LEU:HA	1:A:69:LYS:HD3	33	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD11	7	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD12	7	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD13	7	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD11	7	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD12	7	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD13	7	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD11	8	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD12	8	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD13	8	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD11	8	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD12	8	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD13	8	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD11	10	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD12	10	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD13	10	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD11	10	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD12	10	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD13	10	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD11	16	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD12	16	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD13	16	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD11	16	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD12	16	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD13	16	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD11	20	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD12	20	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD13	20	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD11	20	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD12	20	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD13	20	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD11	25	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD12	25	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD13	25	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD11	25	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD12	25	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD13	25	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD11	28	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD12	28	0.11
(1,719)	1:A:64:TYR:HE1	1:A:92:ILE:HD13	28	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD11	28	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD12	28	0.11
(1,719)	1:A:64:TYR:HE2	1:A:92:ILE:HD13	28	0.11
(1,7)	1:A:3:ARG:HA	1:A:4:ILE:H	2	0.11
(1,7)	1:A:3:ARG:HA	1:A:4:ILE:H	16	0.11
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	8	0.11
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	8	0.11
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	8	0.11
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	14	0.11
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	14	0.11
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	14	0.11
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	22	0.11
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	22	0.11
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	22	0.11
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD11	33	0.11
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD12	33	0.11
(1,636)	1:A:60:SER:H	1:A:92:ILE:HD13	33	0.11
(1,610)	1:A:57:HIS:HE1	1:A:104:CYS:HB2	28	0.11
(1,610)	1:A:57:HIS:HE1	1:A:104:CYS:HB3	28	0.11
(1,61)	1:A:14:ASP:H	1:A:15:GLY:H	33	0.11
(1,559)	1:A:53:MET:HB3	1:A:148:CYS:HB3	3	0.11
(1,559)	1:A:53:MET:HB3	1:A:148:CYS:HB3	33	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	2	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	3	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	4	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	5	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	7	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	9	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	10	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	12	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	17	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	18	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	20	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	26	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	28	0.11
(1,52)	1:A:13:PRO:HA	1:A:14:ASP:H	30	0.11
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	1	0.11
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	5	0.11
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	13	0.11
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	18	0.11
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	23	0.11
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	26	0.11
(1,514)	1:A:50:TRP:HH2	1:A:146:VAL:HA	35	0.11
(1,509)	1:A:50:TRP:HE1	1:A:146:VAL:HA	3	0.11
(1,509)	1:A:50:TRP:HE1	1:A:146:VAL:HA	19	0.11
(1,509)	1:A:50:TRP:HE1	1:A:146:VAL:HA	33	0.11
(1,503)	1:A:50:TRP:HA	1:A:53:MET:H	35	0.11
(1,488)	1:A:49:LEU:HB2	1:A:53:MET:HE1	8	0.11
(1,488)	1:A:49:LEU:HB2	1:A:53:MET:HE2	8	0.11
(1,488)	1:A:49:LEU:HB2	1:A:53:MET:HE3	8	0.11
(1,488)	1:A:49:LEU:HB3	1:A:53:MET:HE1	8	0.11
(1,488)	1:A:49:LEU:HB3	1:A:53:MET:HE2	8	0.11
(1,488)	1:A:49:LEU:HB3	1:A:53:MET:HE3	8	0.11
(1,45)	1:A:12:ALA:HB1	1:A:80:TRP:HE3	34	0.11
(1,45)	1:A:12:ALA:HB2	1:A:80:TRP:HE3	34	0.11
(1,45)	1:A:12:ALA:HB3	1:A:80:TRP:HE3	34	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	1	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	2	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	7	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	8	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	10	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	14	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	15	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	16	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	17	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	19	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	20	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	23	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	24	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	26	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	28	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	29	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	31	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	32	0.11
(1,425)	1:A:45:SER:HA	1:A:46:ASN:H	35	0.11
(1,414)	1:A:42:ALA:HB1	1:A:43:ALA:H	25	0.11
(1,414)	1:A:42:ALA:HB2	1:A:43:ALA:H	25	0.11
(1,414)	1:A:42:ALA:HB3	1:A:43:ALA:H	25	0.11
(1,386)	1:A:34:GLN:HA	1:A:52:ILE:HD11	17	0.11
(1,386)	1:A:34:GLN:HA	1:A:52:ILE:HD12	17	0.11
(1,386)	1:A:34:GLN:HA	1:A:52:ILE:HD13	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG21	8	0.11
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG22	8	0.11
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG23	8	0.11
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG21	8	0.11
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG22	8	0.11
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG23	8	0.11
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG21	8	0.11
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG22	8	0.11
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG23	8	0.11
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG21	23	0.11
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG22	23	0.11
(1,374)	1:A:33:ALA:HB1	1:A:52:ILE:HG23	23	0.11
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG21	23	0.11
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG22	23	0.11
(1,374)	1:A:33:ALA:HB2	1:A:52:ILE:HG23	23	0.11
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG21	23	0.11
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG22	23	0.11
(1,374)	1:A:33:ALA:HB3	1:A:52:ILE:HG23	23	0.11
(1,353)	1:A:32:ASP:HA	1:A:35:LYS:H	1	0.11
(1,353)	1:A:32:ASP:HA	1:A:35:LYS:H	31	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD11	30	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD12	30	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD13	30	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD21	30	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD22	30	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD23	30	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD11	33	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD12	33	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD13	33	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD21	33	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD22	33	0.11
(1,332)	1:A:30:LEU:HA	1:A:55:LEU:HD23	33	0.11
(1,326)	1:A:30:LEU:HA	1:A:52:ILE:HD11	26	0.11
(1,326)	1:A:30:LEU:HA	1:A:52:ILE:HD12	26	0.11
(1,326)	1:A:30:LEU:HA	1:A:52:ILE:HD13	26	0.11
(1,324)	1:A:30:LEU:HD11	1:A:33:ALA:HB1	31	0.11
(1,324)	1:A:30:LEU:HD11	1:A:33:ALA:HB2	31	0.11
(1,324)	1:A:30:LEU:HD11	1:A:33:ALA:HB3	31	0.11
(1,324)	1:A:30:LEU:HD12	1:A:33:ALA:HB1	31	0.11
(1,324)	1:A:30:LEU:HD12	1:A:33:ALA:HB2	31	0.11
(1,324)	1:A:30:LEU:HD12	1:A:33:ALA:HB3	31	0.11
(1,324)	1:A:30:LEU:HD13	1:A:33:ALA:HB1	31	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,324)	1:A:30:LEU:HD13	1:A:33:ALA:HB2	31	0.11
(1,324)	1:A:30:LEU:HD13	1:A:33:ALA:HB3	31	0.11
(1,324)	1:A:30:LEU:HD21	1:A:33:ALA:HB1	31	0.11
(1,324)	1:A:30:LEU:HD21	1:A:33:ALA:HB2	31	0.11
(1,324)	1:A:30:LEU:HD21	1:A:33:ALA:HB3	31	0.11
(1,324)	1:A:30:LEU:HD22	1:A:33:ALA:HB1	31	0.11
(1,324)	1:A:30:LEU:HD22	1:A:33:ALA:HB2	31	0.11
(1,324)	1:A:30:LEU:HD22	1:A:33:ALA:HB3	31	0.11
(1,324)	1:A:30:LEU:HD23	1:A:33:ALA:HB1	31	0.11
(1,324)	1:A:30:LEU:HD23	1:A:33:ALA:HB2	31	0.11
(1,324)	1:A:30:LEU:HD23	1:A:33:ALA:HB3	31	0.11
(1,324)	1:A:30:LEU:HD11	1:A:33:ALA:HB1	32	0.11
(1,324)	1:A:30:LEU:HD11	1:A:33:ALA:HB2	32	0.11
(1,324)	1:A:30:LEU:HD11	1:A:33:ALA:HB3	32	0.11
(1,324)	1:A:30:LEU:HD12	1:A:33:ALA:HB1	32	0.11
(1,324)	1:A:30:LEU:HD12	1:A:33:ALA:HB2	32	0.11
(1,324)	1:A:30:LEU:HD12	1:A:33:ALA:HB3	32	0.11
(1,324)	1:A:30:LEU:HD13	1:A:33:ALA:HB1	32	0.11
(1,324)	1:A:30:LEU:HD13	1:A:33:ALA:HB2	32	0.11
(1,324)	1:A:30:LEU:HD13	1:A:33:ALA:HB3	32	0.11
(1,324)	1:A:30:LEU:HD21	1:A:33:ALA:HB1	32	0.11
(1,324)	1:A:30:LEU:HD21	1:A:33:ALA:HB2	32	0.11
(1,324)	1:A:30:LEU:HD21	1:A:33:ALA:HB3	32	0.11
(1,324)	1:A:30:LEU:HD22	1:A:33:ALA:HB1	32	0.11
(1,324)	1:A:30:LEU:HD22	1:A:33:ALA:HB2	32	0.11
(1,324)	1:A:30:LEU:HD22	1:A:33:ALA:HB3	32	0.11
(1,324)	1:A:30:LEU:HD23	1:A:33:ALA:HB1	32	0.11
(1,324)	1:A:30:LEU:HD23	1:A:33:ALA:HB2	32	0.11
(1,324)	1:A:30:LEU:HD23	1:A:33:ALA:HB3	32	0.11
(1,303)	1:A:29:GLN:HA	1:A:32:ASP:H	20	0.11
(1,303)	1:A:29:GLN:HA	1:A:32:ASP:H	21	0.11
(1,303)	1:A:29:GLN:HA	1:A:32:ASP:H	23	0.11
(1,303)	1:A:29:GLN:HA	1:A:32:ASP:H	34	0.11
(1,30)	1:A:11:PRO:HA	1:A:12:ALA:H	9	0.11
(1,287)	1:A:28:ILE:HA	1:A:31:ARG:H	3	0.11
(1,287)	1:A:28:ILE:HA	1:A:31:ARG:H	4	0.11
(1,287)	1:A:28:ILE:HA	1:A:31:ARG:H	9	0.11
(1,287)	1:A:28:ILE:HA	1:A:31:ARG:H	11	0.11
(1,287)	1:A:28:ILE:HA	1:A:31:ARG:H	12	0.11
(1,287)	1:A:28:ILE:HA	1:A:31:ARG:H	18	0.11
(1,287)	1:A:28:ILE:HA	1:A:31:ARG:H	21	0.11
(1,287)	1:A:28:ILE:HA	1:A:31:ARG:H	28	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	1:A:28:ILE:HA	1:A:31:ARG:H	34	0.11
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD11	23	0.11
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD12	23	0.11
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD13	23	0.11
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD21	23	0.11
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD22	23	0.11
(1,256)	1:A:26:PHE:HZ	1:A:55:LEU:HD23	23	0.11
(1,1821)	1:A:156:THR:HA	1:A:157:ASP:H	2	0.11
(1,1821)	1:A:156:THR:HA	1:A:157:ASP:H	3	0.11
(1,1821)	1:A:156:THR:HA	1:A:157:ASP:H	7	0.11
(1,1821)	1:A:156:THR:HA	1:A:157:ASP:H	20	0.11
(1,1772)	1:A:148:CYS:H	1:A:148:CYS:HB3	18	0.11
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	8	0.11
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	8	0.11
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	13	0.11
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	13	0.11
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	19	0.11
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	19	0.11
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	29	0.11
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	29	0.11
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA2	31	0.11
(1,1736)	1:A:144:GLN:HA	1:A:152:GLY:HA3	31	0.11
(1,1724)	1:A:144:GLN:HA	1:A:145:CYS:H	27	0.11
(1,1713)	1:A:143:HIS:HA	1:A:144:GLN:H	8	0.11
(1,1713)	1:A:143:HIS:HA	1:A:144:GLN:H	19	0.11
(1,17)	1:A:4:ILE:HA	1:A:5:LYS:H	18	0.11
(1,17)	1:A:4:ILE:HA	1:A:5:LYS:H	28	0.11
(1,17)	1:A:4:ILE:HA	1:A:5:LYS:H	32	0.11
(1,1698)	1:A:142:PHE:HE1	1:A:145:CYS:H	2	0.11
(1,1698)	1:A:142:PHE:HE2	1:A:145:CYS:H	2	0.11
(1,1698)	1:A:142:PHE:HE1	1:A:145:CYS:H	7	0.11
(1,1698)	1:A:142:PHE:HE2	1:A:145:CYS:H	7	0.11
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	5	0.11
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	8	0.11
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	12	0.11
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	17	0.11
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	18	0.11
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	25	0.11
(1,1688)	1:A:142:PHE:H	1:A:142:PHE:HB2	34	0.11
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	30	0.11
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	30	0.11
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD1	35	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1442)	1:A:122:CYS:HA	1:A:142:PHE:HD2	35	0.11
(1,1433)	1:A:121:ILE:HG21	1:A:145:CYS:HB2	27	0.11
(1,1433)	1:A:121:ILE:HG22	1:A:145:CYS:HB2	27	0.11
(1,1433)	1:A:121:ILE:HG23	1:A:145:CYS:HB2	27	0.11
(1,1433)	1:A:121:ILE:HG21	1:A:145:CYS:HB2	30	0.11
(1,1433)	1:A:121:ILE:HG22	1:A:145:CYS:HB2	30	0.11
(1,1433)	1:A:121:ILE:HG23	1:A:145:CYS:HB2	30	0.11
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	11	0.11
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	11	0.11
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	11	0.11
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	11	0.11
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	11	0.11
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	11	0.11
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	14	0.11
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	14	0.11
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	14	0.11
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	14	0.11
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	14	0.11
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	14	0.11
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	15	0.11
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	15	0.11
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	15	0.11
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	15	0.11
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	15	0.11
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	15	0.11
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	18	0.11
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	18	0.11
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	18	0.11
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	18	0.11
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	18	0.11
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	18	0.11
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE1	22	0.11
(1,1429)	1:A:121:ILE:HD11	1:A:142:PHE:HE2	22	0.11
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE1	22	0.11
(1,1429)	1:A:121:ILE:HD12	1:A:142:PHE:HE2	22	0.11
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE1	22	0.11
(1,1429)	1:A:121:ILE:HD13	1:A:142:PHE:HE2	22	0.11
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	7	0.11
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	11	0.11
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	12	0.11
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	16	0.11
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	21	0.11
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	31	0.11
(1,1398)	1:A:120:CYS:HA	1:A:147:HIS:HD2	35	0.11
(1,1377)	1:A:118:SER:HA	1:A:119:THR:H	20	0.11
(1,1358)	1:A:113:GLU:HA	1:A:114:THR:H	3	0.11
(1,1358)	1:A:113:GLU:HA	1:A:114:THR:H	33	0.11
(1,1335)	1:A:109:ILE:HA	1:A:119:THR:HG21	5	0.11
(1,1335)	1:A:109:ILE:HA	1:A:119:THR:HG22	5	0.11
(1,1335)	1:A:109:ILE:HA	1:A:119:THR:HG23	5	0.11
(1,1317)	1:A:108:CYS:HB2	1:A:120:CYS:HB3	9	0.11
(1,1317)	1:A:108:CYS:HB2	1:A:120:CYS:HB3	14	0.11
(1,1317)	1:A:108:CYS:HB2	1:A:120:CYS:HB3	15	0.11
(1,1317)	1:A:108:CYS:HB2	1:A:120:CYS:HB3	33	0.11
(1,1317)	1:A:108:CYS:HB2	1:A:120:CYS:HB3	34	0.11
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	33	0.11
(1,1260)	1:A:104:CYS:H	1:A:104:CYS:HB3	34	0.11
(1,1256)	1:A:103:LEU:HB2	1:A:109:ILE:HD11	29	0.11
(1,1256)	1:A:103:LEU:HB2	1:A:109:ILE:HD12	29	0.11
(1,1256)	1:A:103:LEU:HB2	1:A:109:ILE:HD13	29	0.11
(1,1256)	1:A:103:LEU:HB3	1:A:109:ILE:HD11	29	0.11
(1,1256)	1:A:103:LEU:HB3	1:A:109:ILE:HD12	29	0.11
(1,1256)	1:A:103:LEU:HB3	1:A:109:ILE:HD13	29	0.11
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD1	2	0.11
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD2	2	0.11
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD1	2	0.11
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD2	2	0.11
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD1	8	0.11
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD2	8	0.11
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD1	8	0.11
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD2	8	0.11
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD1	13	0.11
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD2	13	0.11
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD1	13	0.11
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD2	13	0.11
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD1	16	0.11
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD2	16	0.11
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD1	16	0.11
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD2	16	0.11
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD1	30	0.11
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD2	30	0.11
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD1	30	0.11
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD2	30	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD1	32	0.11
(1,1189)	1:A:97:LYS:HG2	1:A:100:TYR:HD2	32	0.11
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD1	32	0.11
(1,1189)	1:A:97:LYS:HG3	1:A:100:TYR:HD2	32	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD11	1	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD12	1	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD13	1	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD11	1	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD12	1	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD13	1	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD11	8	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD12	8	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD13	8	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD11	8	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD12	8	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD13	8	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD11	27	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD12	27	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD13	27	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD11	27	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD12	27	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD13	27	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD11	29	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD12	29	0.11
(1,1154)	1:A:94:LYS:HG2	1:A:109:ILE:HD13	29	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD11	29	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD12	29	0.11
(1,1154)	1:A:94:LYS:HG3	1:A:109:ILE:HD13	29	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD11	1	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD12	1	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD13	1	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD21	1	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD22	1	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD23	1	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD11	1	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD12	1	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD13	1	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD21	1	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD22	1	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD23	1	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD11	4	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD12	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD13	4	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD21	4	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD22	4	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD23	4	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD11	4	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD12	4	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD13	4	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD21	4	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD22	4	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD23	4	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD11	6	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD12	6	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD13	6	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD21	6	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD22	6	0.11
(1,1151)	1:A:94:LYS:HB2	1:A:106:LEU:HD23	6	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD11	6	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD12	6	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD13	6	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD21	6	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD22	6	0.11
(1,1151)	1:A:94:LYS:HB3	1:A:106:LEU:HD23	6	0.11
(1,1102)	1:A:91:LEU:HD11	1:A:106:LEU:HB2	4	0.11
(1,1102)	1:A:91:LEU:HD11	1:A:106:LEU:HB3	4	0.11
(1,1102)	1:A:91:LEU:HD12	1:A:106:LEU:HB2	4	0.11
(1,1102)	1:A:91:LEU:HD12	1:A:106:LEU:HB3	4	0.11
(1,1102)	1:A:91:LEU:HD13	1:A:106:LEU:HB2	4	0.11
(1,1102)	1:A:91:LEU:HD13	1:A:106:LEU:HB3	4	0.11
(1,1102)	1:A:91:LEU:HD21	1:A:106:LEU:HB2	4	0.11
(1,1102)	1:A:91:LEU:HD21	1:A:106:LEU:HB3	4	0.11
(1,1102)	1:A:91:LEU:HD22	1:A:106:LEU:HB2	4	0.11
(1,1102)	1:A:91:LEU:HD22	1:A:106:LEU:HB3	4	0.11
(1,1102)	1:A:91:LEU:HD23	1:A:106:LEU:HB2	4	0.11
(1,1102)	1:A:91:LEU:HD23	1:A:106:LEU:HB3	4	0.11
(1,1102)	1:A:91:LEU:HD11	1:A:106:LEU:HB2	27	0.11
(1,1102)	1:A:91:LEU:HD11	1:A:106:LEU:HB3	27	0.11
(1,1102)	1:A:91:LEU:HD12	1:A:106:LEU:HB2	27	0.11
(1,1102)	1:A:91:LEU:HD12	1:A:106:LEU:HB3	27	0.11
(1,1102)	1:A:91:LEU:HD13	1:A:106:LEU:HB2	27	0.11
(1,1102)	1:A:91:LEU:HD13	1:A:106:LEU:HB3	27	0.11
(1,1102)	1:A:91:LEU:HD21	1:A:106:LEU:HB2	27	0.11
(1,1102)	1:A:91:LEU:HD21	1:A:106:LEU:HB3	27	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1102)	1:A:91:LEU:HD22	1:A:106:LEU:HB2	27	0.11
(1,1102)	1:A:91:LEU:HD22	1:A:106:LEU:HB3	27	0.11
(1,1102)	1:A:91:LEU:HD23	1:A:106:LEU:HB2	27	0.11
(1,1102)	1:A:91:LEU:HD23	1:A:106:LEU:HB3	27	0.11
(1,1029)	1:A:86:TYR:HA	1:A:87:ALA:H	35	0.11
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE1	12	0.11
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE2	12	0.11
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE1	12	0.11
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE2	12	0.11
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE1	15	0.11
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE2	15	0.11
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE1	15	0.11
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE2	15	0.11
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE1	24	0.11
(1,1011)	1:A:84:GLU:HG2	1:A:86:TYR:HE2	24	0.11
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE1	24	0.11
(1,1011)	1:A:84:GLU:HG3	1:A:86:TYR:HE2	24	0.11

10 Dihedral-angle violation analysis

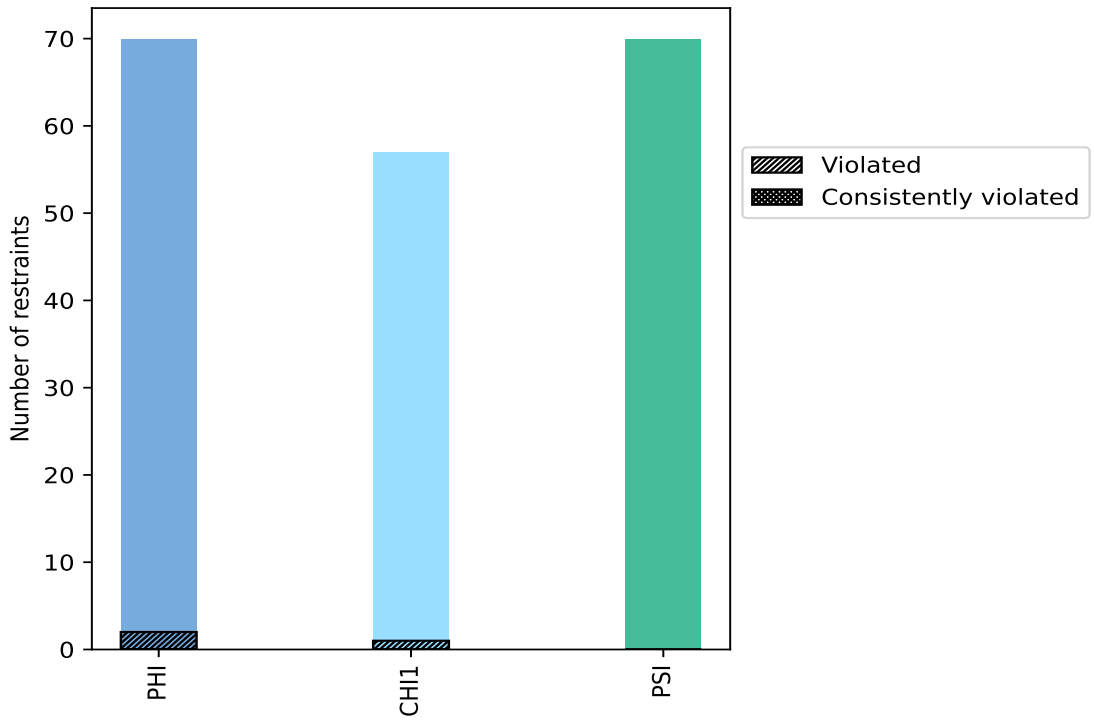
10.1 Summary of dihedral-angle violations

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]
PHI	70	35.5	2	2.9	1.0	0	0.0	0.0
CHI1	57	28.9	1	1.8	0.5	0	0.0	0.0
PSI	70	35.5	0	0.0	0.0	0	0.0	0.0
Total	197	100.0	3	1.5	1.5	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



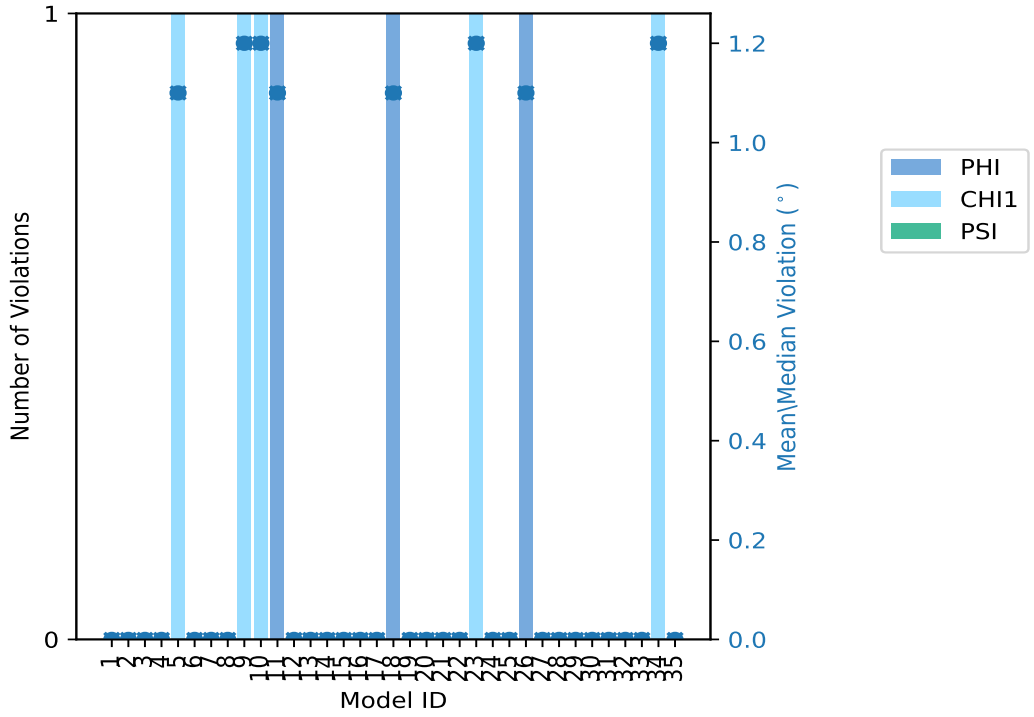
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations				Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	CHI1	PSI	Total				
1	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0.0	0.0	0.0	0.0
5	0	1	0	1	1.1	1.1	0.0	1.1
6	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0.0	0.0	0.0	0.0
9	0	1	0	1	1.2	1.2	0.0	1.2
10	0	1	0	1	1.2	1.2	0.0	1.2
11	1	0	0	1	1.1	1.1	0.0	1.1
12	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0	0.0	0.0	0.0	0.0
18	1	0	0	1	1.1	1.1	0.0	1.1
19	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
21	0	0	0	0	0.0	0.0	0.0	0.0
22	0	0	0	0	0.0	0.0	0.0	0.0
23	0	1	0	1	1.2	1.2	0.0	1.2
24	0	0	0	0	0.0	0.0	0.0	0.0
25	0	0	0	0	0.0	0.0	0.0	0.0
26	1	0	0	1	1.1	1.1	0.0	1.1
27	0	0	0	0	0.0	0.0	0.0	0.0
28	0	0	0	0	0.0	0.0	0.0	0.0
29	0	0	0	0	0.0	0.0	0.0	0.0
30	0	0	0	0	0.0	0.0	0.0	0.0
31	0	0	0	0	0.0	0.0	0.0	0.0
32	0	0	0	0	0.0	0.0	0.0	0.0
33	0	0	0	0	0.0	0.0	0.0	0.0
34	0	1	0	1	1.2	1.2	0.0	1.2
35	0	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints				Fraction of the ensemble	
PHI	CHI1	PSI	Total	Count[1]	%
1	0	0	1	1	2.9
1	0	0	1	2	5.7
0	0	0	0	3	8.6
0	0	0	0	4	11.4
0	1	0	1	5	14.3
0	0	0	0	6	17.1
0	0	0	0	7	20.0
0	0	0	0	8	22.9
0	0	0	0	9	25.7
0	0	0	0	10	28.6
0	0	0	0	11	31.4

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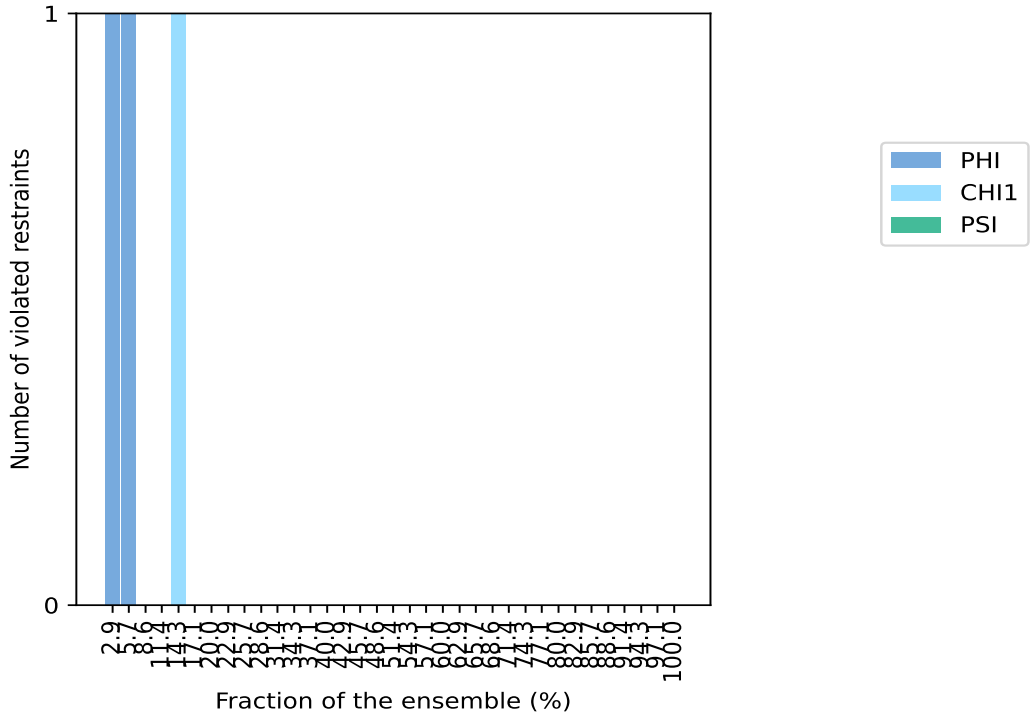
Number of violated restraints				Fraction of the ensemble	
PHI	CHI1	PSI	Total	Count[1]	%
0	0	0	0	12	34.3
0	0	0	0	13	37.1
0	0	0	0	14	40.0
0	0	0	0	15	42.9
0	0	0	0	16	45.7
0	0	0	0	17	48.6
0	0	0	0	18	51.4
0	0	0	0	19	54.3
0	0	0	0	20	57.1
0	0	0	0	21	60.0
0	0	0	0	22	62.9
0	0	0	0	23	65.7
0	0	0	0	24	68.6
0	0	0	0	25	71.4
0	0	0	0	26	74.3
0	0	0	0	27	77.1
0	0	0	0	28	80.0
0	0	0	0	29	82.9
0	0	0	0	30	85.7
0	0	0	0	31	88.6
0	0	0	0	32	91.4
0	0	0	0	33	94.3
0	0	0	0	34	97.1
0	0	0	0	35	100.0

[1] Number of models with violations

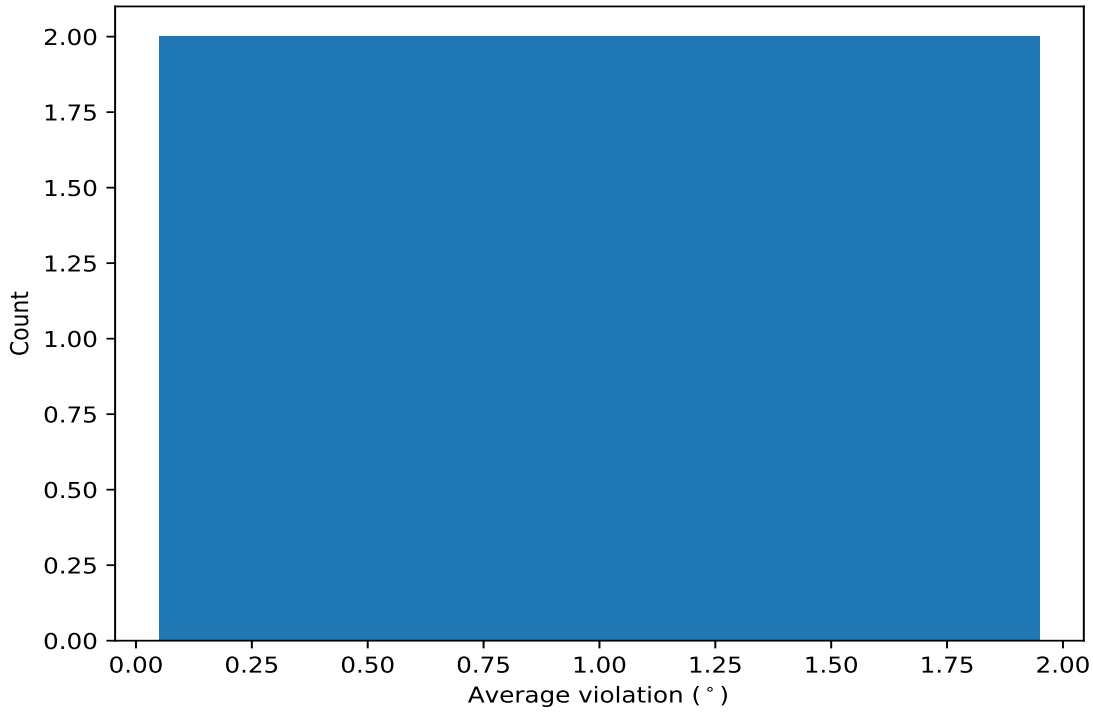
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle restraints

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

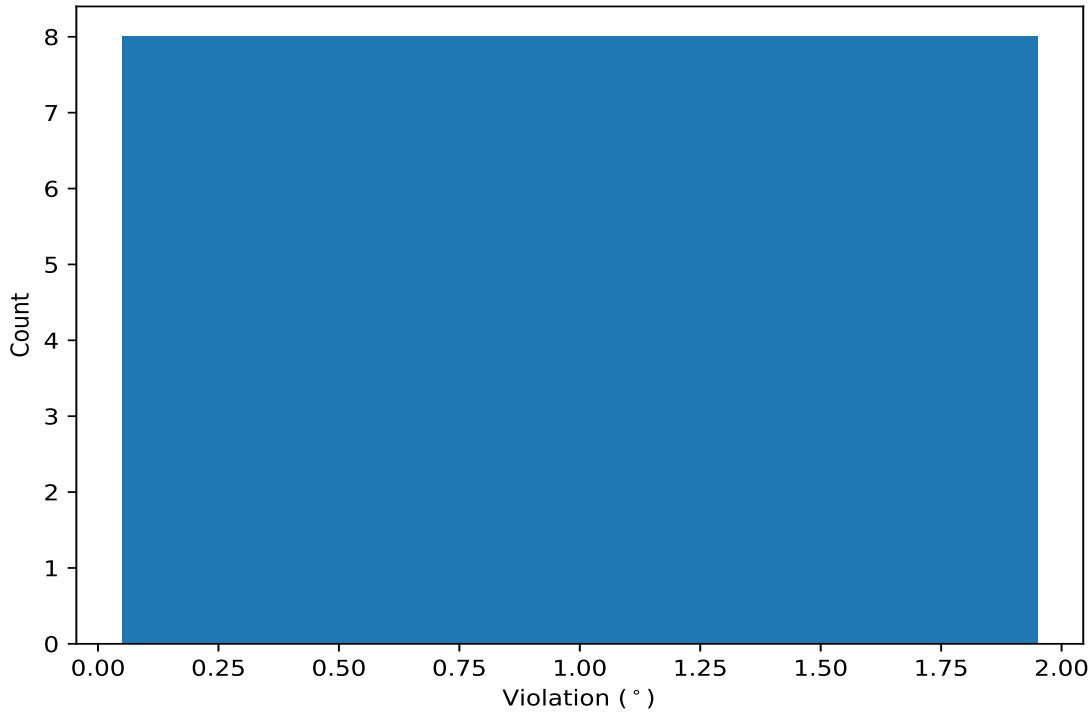
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,44)	1:A:108:CYS:N	1:A:108:CYS:CA	1:A:108:CYS:CB	1:A:108:CYS:SG	5	1.18	0.04	1.2
(1,134)	1:A:65:THR:C	1:A:66:LEU:N	1:A:66:LEU:CA	1:A:66:LEU:C	2	1.1	0.0	1.1

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,44)	1:A:108:CYS:N	1:A:108:CYS:CA	1:A:108:CYS:CB	1:A:108:CYS:SG	9	1.2
(1,44)	1:A:108:CYS:N	1:A:108:CYS:CA	1:A:108:CYS:CB	1:A:108:CYS:SG	10	1.2
(1,44)	1:A:108:CYS:N	1:A:108:CYS:CA	1:A:108:CYS:CB	1:A:108:CYS:SG	23	1.2
(1,44)	1:A:108:CYS:N	1:A:108:CYS:CA	1:A:108:CYS:CB	1:A:108:CYS:SG	34	1.2
(1,44)	1:A:108:CYS:N	1:A:108:CYS:CA	1:A:108:CYS:CB	1:A:108:CYS:SG	5	1.1
(1,136)	1:A:66:LEU:C	1:A:67:TYR:N	1:A:67:TYR:CA	1:A:67:TYR:C	26	1.1
(1,134)	1:A:65:THR:C	1:A:66:LEU:N	1:A:66:LEU:CA	1:A:66:LEU:C	11	1.1
(1,134)	1:A:65:THR:C	1:A:66:LEU:N	1:A:66:LEU:CA	1:A:66:LEU:C	18	1.1