Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 05:29 AM EDT

PDB ID	:	2L9N
BMRB ID	:	17479
Title	:	Structure of the human Shwachman-Bodian-Diamond syndrome (SBDS) protein
Authors	:	Hilcenko, C.; Freund, S.M.V.; Warren, A.J.
Deposited on	:	2011-02-21

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

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

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

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

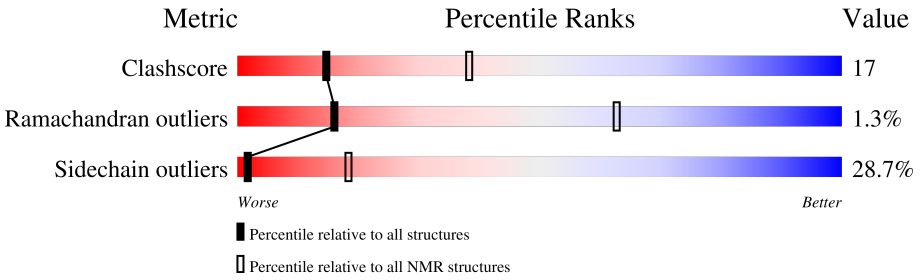
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 79%.

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	252	44% 40% . 13% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:15-A:40, A:46-A:94 (75)	0.47	1
2	A:95-A:169 (75)	1.03	16
3	A:171-A:238 (68)	0.86	17

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4129 atoms, of which 2114 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribosome maturation protein SBDS.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	250	4129	1272	2114	352	380	11	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9Y3A5
A	0	SER	-	expression tag	UNP Q9Y3A5

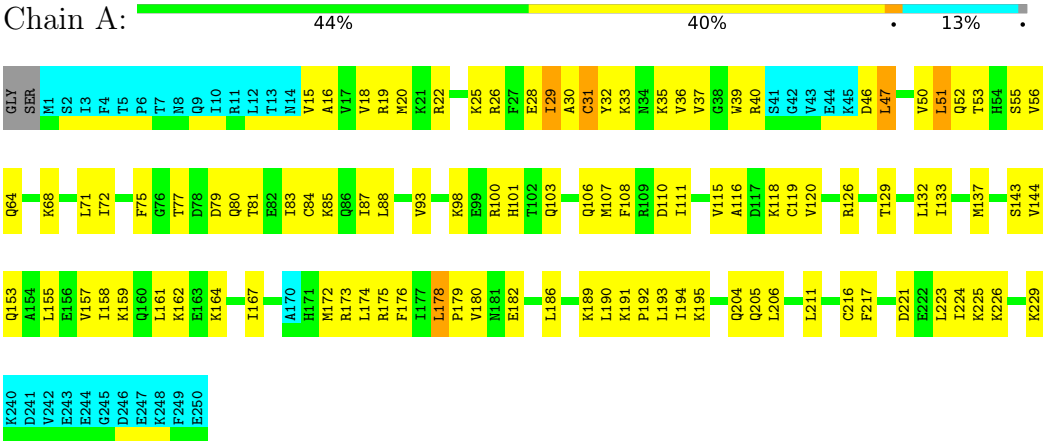
4 Residue-property plots

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: Ribosome maturation protein SBDS

Chain A:



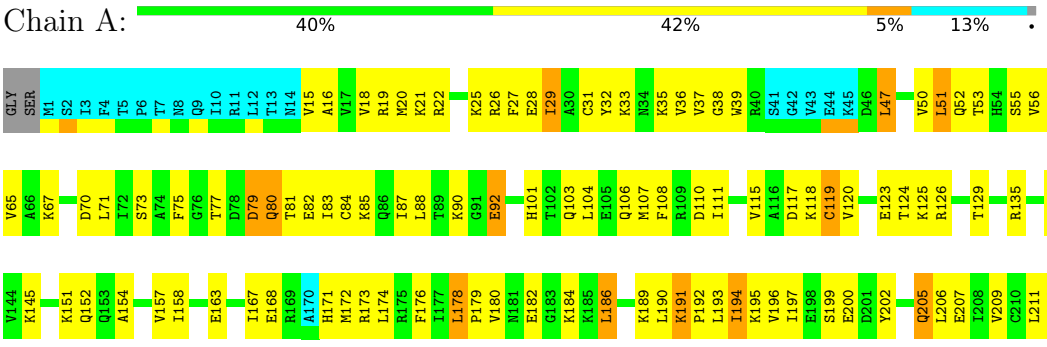
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

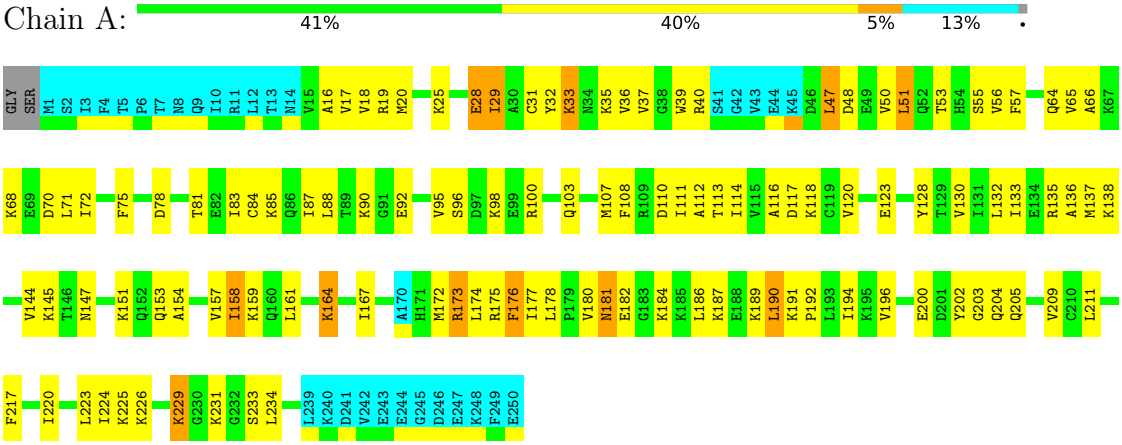
• Molecule 1: Ribosome maturation protein SBDS

Chain A:



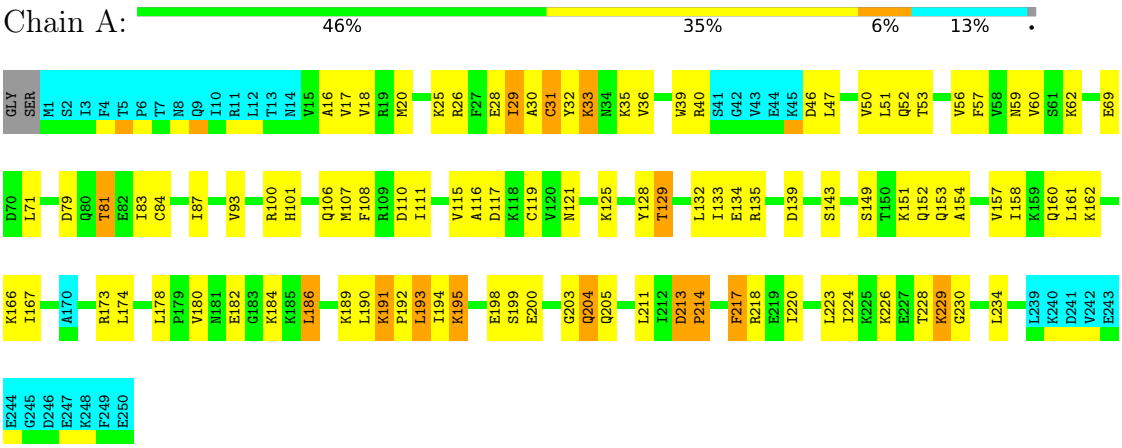
4.2.2 Score per residue for model 2

• Molecule 1: Ribosome maturation protein SBDS



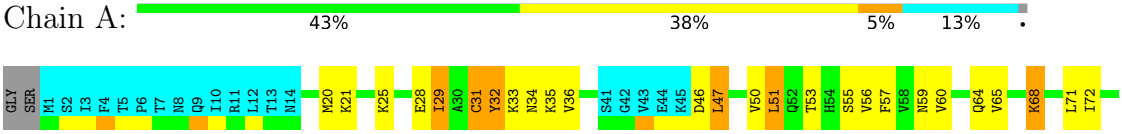
4.2.3 Score per residue for model 3

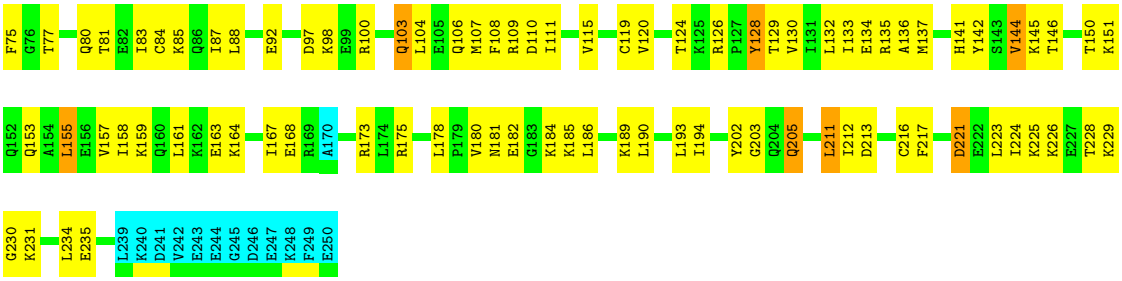
• Molecule 1: Ribosome maturation protein SBDS



4.2.4 Score per residue for model 4

• Molecule 1: Ribosome maturation protein SBDS

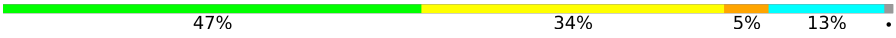


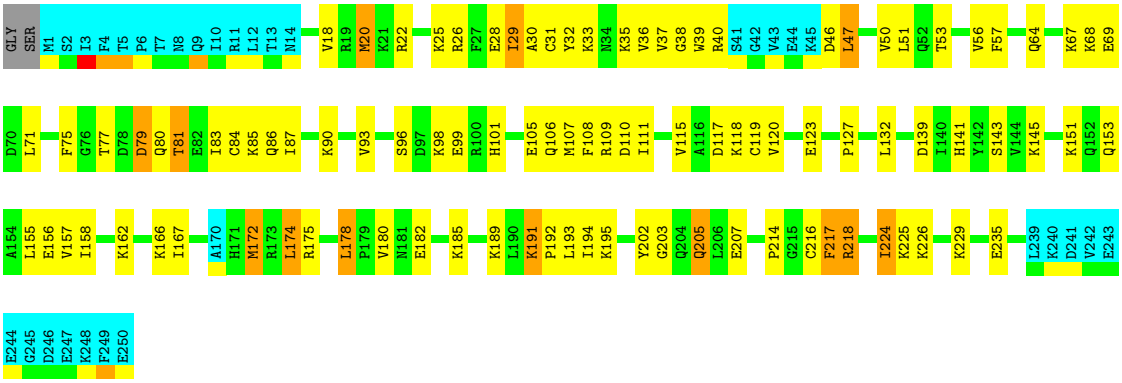


4.2.5 Score per residue for model 5

• Molecule 1: Ribosome maturation protein SBDS

Chain A:

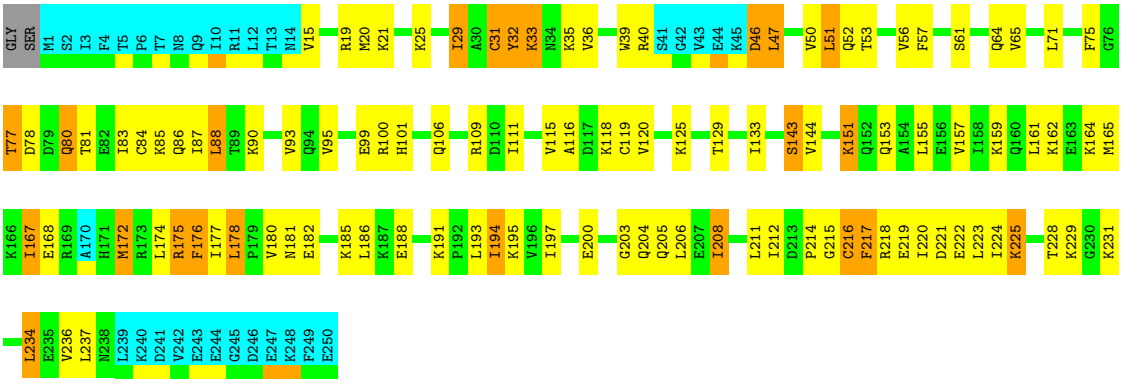




4.2.6 Score per residue for model 6

• Molecule 1: Ribosome maturation protein SBDS

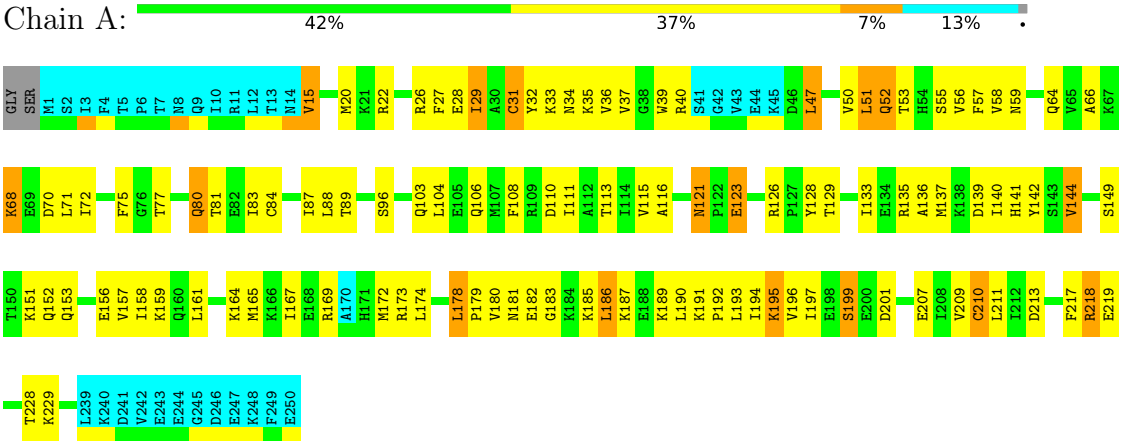
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Ribosome maturation protein SBDS

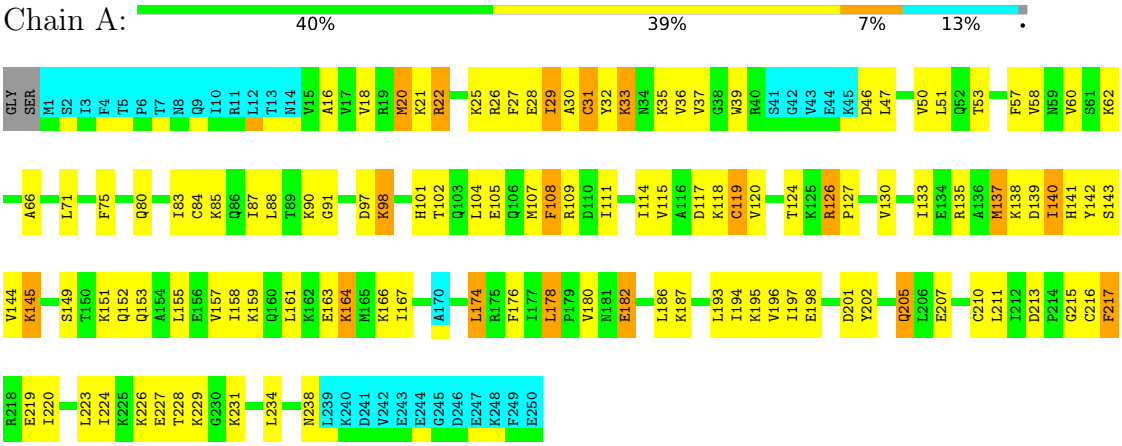
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Ribosome maturation protein SBDS

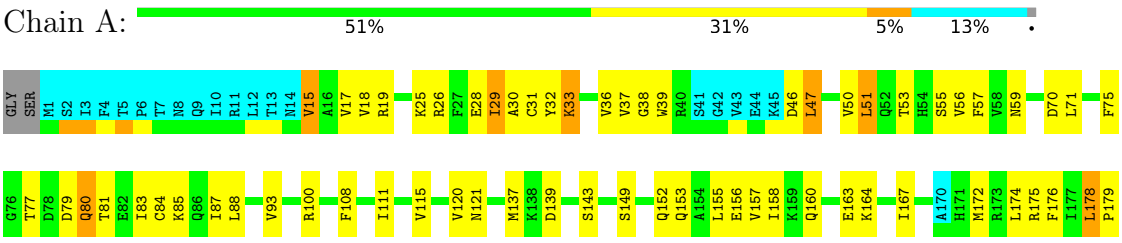
Chain A:



4.2.9 Score per residue for model 9

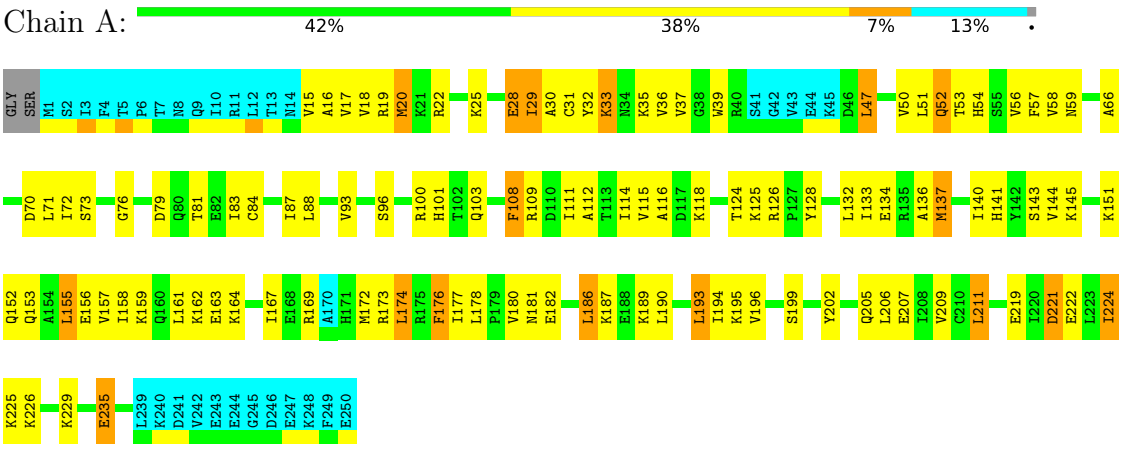
• Molecule 1: Ribosome maturation protein SBDS

Chain A:



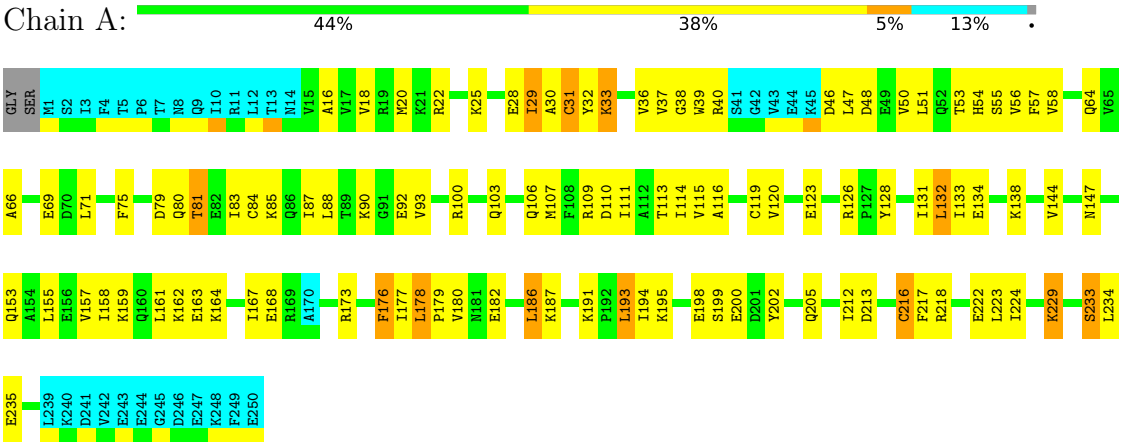
4.2.10 Score per residue for model 10

• Molecule 1: Ribosome maturation protein SBDS



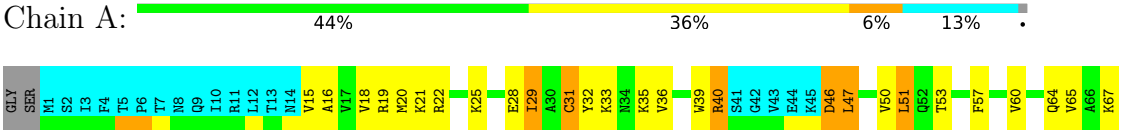
4.2.11 Score per residue for model 11

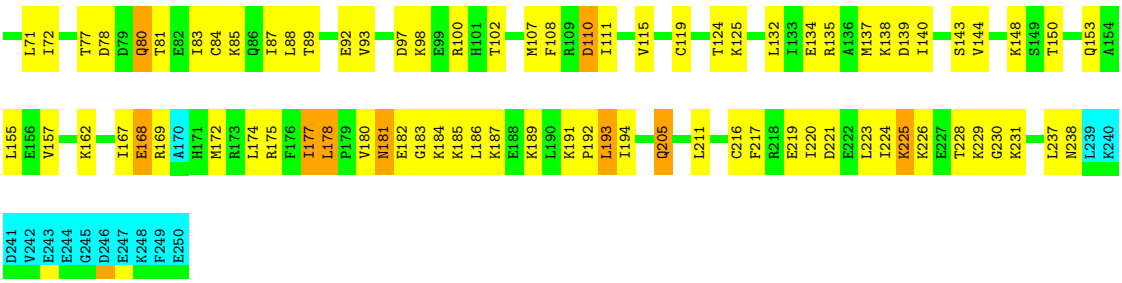
• Molecule 1: Ribosome maturation protein SBDS



4.2.12 Score per residue for model 12

• Molecule 1: Ribosome maturation protein SBDS

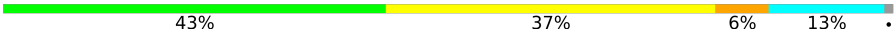


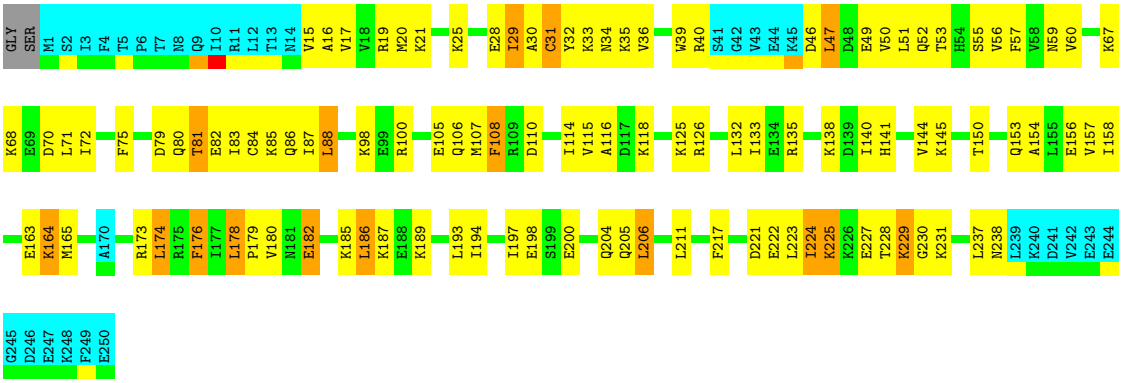


4.2.13 Score per residue for model 13

• Molecule 1: Ribosome maturation protein SBDS

Chain A:

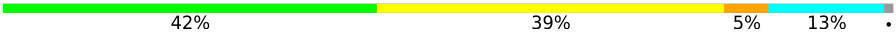


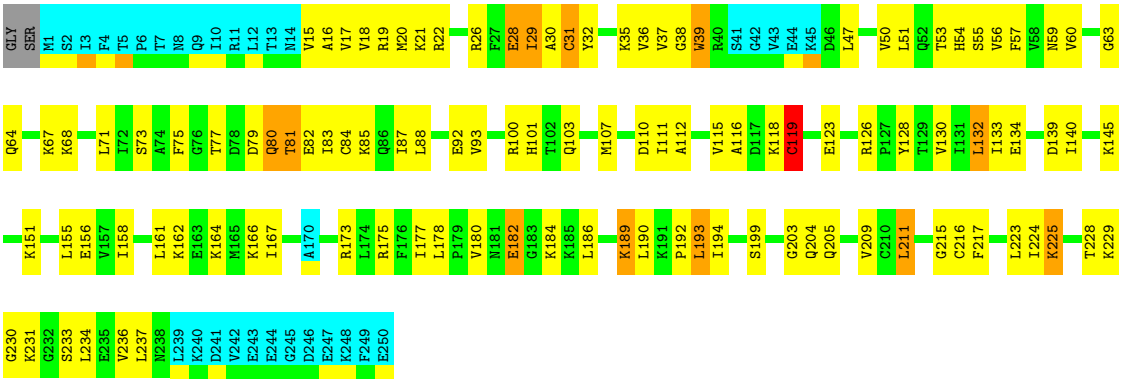


4.2.14 Score per residue for model 14

• Molecule 1: Ribosome maturation protein SBDS

Chain A:

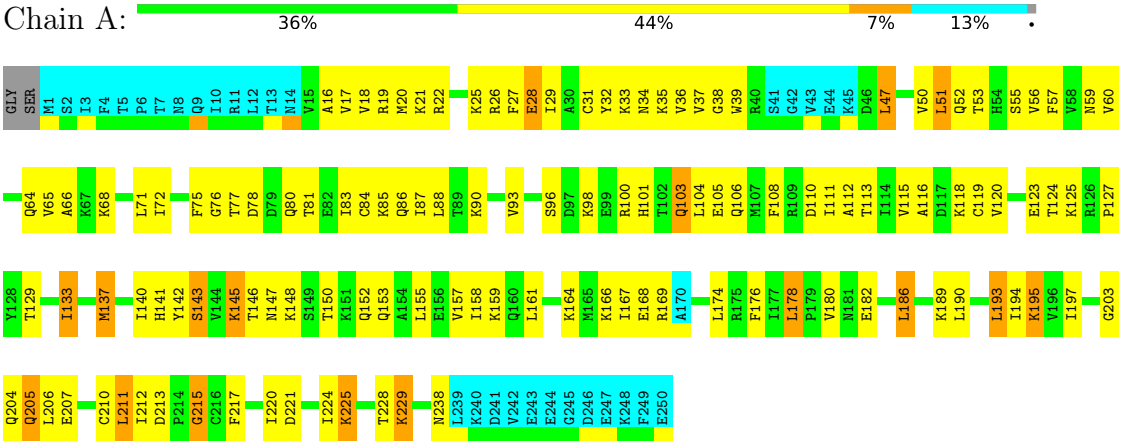




4.2.15 Score per residue for model 15

• Molecule 1: Ribosome maturation protein SBDS

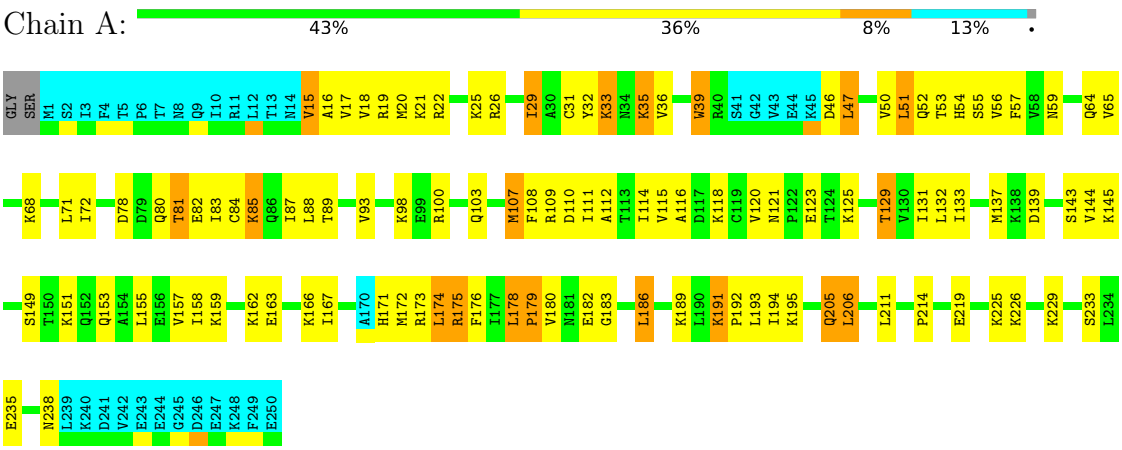
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Ribosome maturation protein SBDS

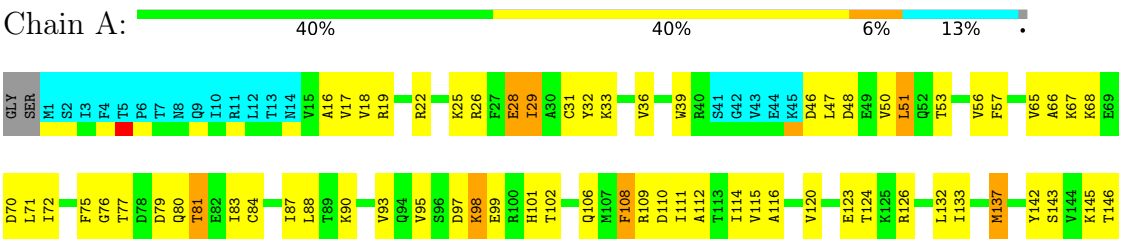
Chain A:

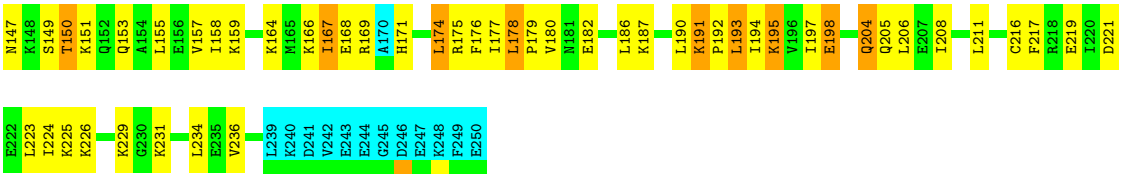


4.2.17 Score per residue for model 17

• Molecule 1: Ribosome maturation protein SBDS

Chain A:

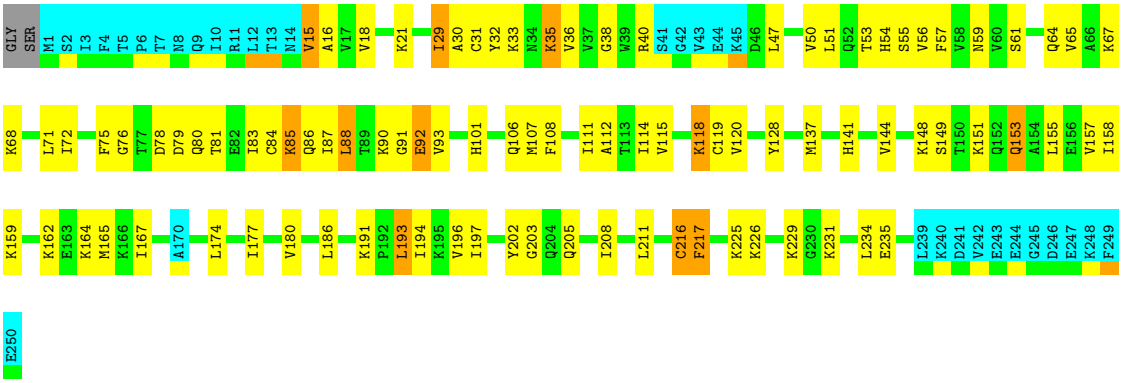




4.2.18 Score per residue for model 18

• Molecule 1: Ribosome maturation protein SBDS

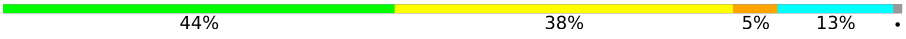
Chain A:

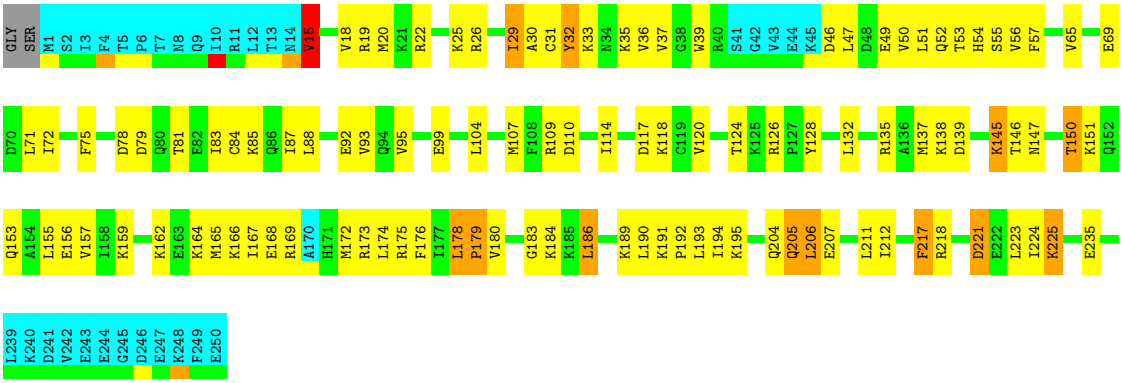


4.2.19 Score per residue for model 19

• Molecule 1: Ribosome maturation protein SBDS

Chain A:

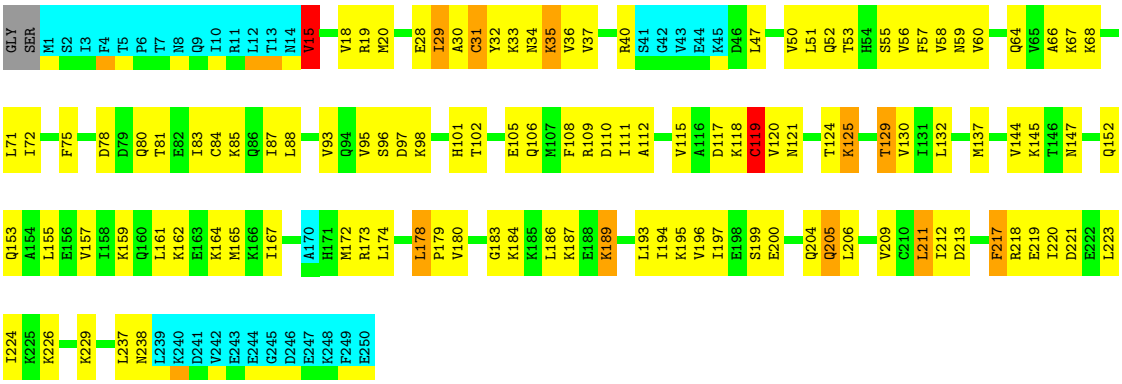




4.2.20 Score per residue for model 20

• Molecule 1: Ribosome maturation protein SBDS

Chain A:


GLY SER M1 S2 I3 F4 T5 P6 T7 N8 Q9 I10 R11 L12 T13 N14 V15 V18 R19 M20 E28 I29 A30 C31 Y32 K33 N34 K35 V36 V37 R40 S41 G42 V43 E44 K45 D46 L47 V50 L51 Q52 T53 H54 S55 V56 F57 V58 N59 V60 Q64 V65 A66 K67 K68
L71 I72 F75 D78 D79 Q80 T81 E82 I83 C84 K85 Q86 I87 L88 V93 Q94 V95 S96 D97 K98 H101 T102 E105 Q106 M107 F108 R109 D110 I111 A112 V115 A116 D117 K118 C119 V120 N121 T124 K125 T129 V130 I131 L132 M137 V144 K145 T146 N147 Q152
Q153 A154 L155 E156 V157 I158 K159 Q160 L161 K162 E163 K164 M165 K166 I167 A170 H171 M172 R173 L174 L178 P179 V180 G183 K184 K185 L186 K187 E188 K189 L193 I194 K195 V196 I197 E198 S199 E200 Q204 Q205 L206 V209 C210 L211 I212 D213 F217 R218 E219 I220 D221 E222 L223
I224 K225 K226 K229 L237 N238 L239 K240 D241 V242 E243 E244 G245 D246 E247 K248 F249 E250

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure calculation	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2846
Number of shifts mapped to atoms	2846
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1761	1866	1862	62±7
All	All	35220	37320	37240	1230

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:LEU:HD22	1:A:83:ILE:HD13	1.03	1.26	6	20
1:A:136:ALA:HB1	1:A:161:LEU:HD21	1.00	1.29	4	1
1:A:56:VAL:HG21	1:A:71:LEU:HD21	0.96	1.31	3	14
1:A:186:LEU:HD11	1:A:190:LEU:HD23	0.93	1.41	2	1
1:A:193:LEU:HD23	1:A:194:ILE:HG23	0.92	1.41	4	4
1:A:196:VAL:HG12	1:A:211:LEU:HD22	0.89	1.40	18	1
1:A:32:TYR:O	1:A:36:VAL:HG23	0.87	1.70	19	20
1:A:30:ALA:HB3	1:A:53:THR:HG22	0.85	1.45	14	9
1:A:51:LEU:HD11	1:A:84:CYS:CB	0.83	2.02	18	17
1:A:196:VAL:HG12	1:A:211:LEU:CD2	0.83	2.04	18	1
1:A:190:LEU:HD13	1:A:211:LEU:HD21	0.82	1.47	19	2
1:A:177:ILE:HD12	1:A:208:ILE:HG22	0.80	1.53	18	1
1:A:153:GLN:O	1:A:157:VAL:HG23	0.80	1.77	20	14
1:A:158:ILE:HG23	1:A:167:ILE:HG23	0.79	1.53	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:CYS:SG	1:A:50:VAL:HG22	0.78	2.19	20	5
1:A:47:LEU:HD12	1:A:51:LEU:HD12	0.78	1.52	14	4
1:A:33:LYS:O	1:A:37:VAL:HG23	0.78	1.78	15	1
1:A:29:ILE:HG21	1:A:84:CYS:SG	0.77	2.19	13	18
1:A:56:VAL:CG2	1:A:71:LEU:HD21	0.77	2.10	15	10
1:A:36:VAL:HG11	1:A:93:VAL:HG11	0.76	1.57	17	1
1:A:16:ALA:HB2	1:A:33:LYS:HG3	0.76	1.58	15	6
1:A:116:ALA:HB2	1:A:133:ILE:CD1	0.76	2.11	17	8
1:A:178:LEU:CD2	1:A:186:LEU:HD13	0.76	2.11	6	1
1:A:194:ILE:HD11	1:A:211:LEU:HB3	0.75	1.59	1	2
1:A:20:MET:HB2	1:A:87:ILE:HG23	0.75	1.59	1	16
1:A:178:LEU:CD2	1:A:186:LEU:HD22	0.74	2.12	8	2
1:A:111:ILE:O	1:A:115:VAL:HG23	0.74	1.83	6	16
1:A:39:TRP:CE3	1:A:50:VAL:HG11	0.73	2.18	16	2
1:A:20:MET:CB	1:A:87:ILE:HG23	0.73	2.13	14	9
1:A:30:ALA:HB3	1:A:53:THR:CB	0.73	2.13	19	2
1:A:116:ALA:HB2	1:A:133:ILE:HD11	0.73	1.58	2	1
1:A:186:LEU:HD12	1:A:190:LEU:HD11	0.73	1.60	14	1
1:A:18:VAL:HG22	1:A:93:VAL:HG12	0.73	1.61	17	1
1:A:187:LYS:CG	1:A:209:VAL:HG21	0.72	2.13	10	1
1:A:31:CYS:HB3	1:A:51:LEU:HD23	0.72	1.60	14	6
1:A:190:LEU:HD22	1:A:211:LEU:CD2	0.72	2.14	9	1
1:A:31:CYS:SG	1:A:36:VAL:HG21	0.72	2.24	17	10
1:A:114:ILE:HG23	1:A:118:LYS:HD2	0.72	1.59	16	2
1:A:35:LYS:CB	1:A:50:VAL:HG23	0.71	2.15	7	8
1:A:47:LEU:HG	1:A:81:THR:HG22	0.71	1.62	17	6
1:A:51:LEU:HD11	1:A:84:CYS:SG	0.71	2.26	6	13
1:A:18:VAL:HG22	1:A:93:VAL:HG23	0.70	1.60	11	3
1:A:112:ALA:HA	1:A:133:ILE:HG21	0.70	1.64	10	2
1:A:56:VAL:HG21	1:A:71:LEU:CD2	0.70	2.16	5	11
1:A:31:CYS:SG	1:A:88:LEU:HD21	0.70	2.27	4	4
1:A:115:VAL:HG13	1:A:167:ILE:HG21	0.69	1.63	18	2
1:A:47:LEU:HD21	1:A:85:LYS:HE3	0.69	1.64	4	4
1:A:30:ALA:HB3	1:A:53:THR:HB	0.69	1.63	19	1
1:A:196:VAL:HG13	1:A:209:VAL:HG23	0.69	1.63	2	1
1:A:210:CYS:C	1:A:211:LEU:HD12	0.69	2.08	7	2
1:A:177:ILE:C	1:A:178:LEU:HD13	0.69	2.08	11	1
1:A:119:CYS:SG	1:A:167:ILE:HD13	0.69	2.28	20	2
1:A:51:LEU:HD13	1:A:54:HIS:HA	0.68	1.63	19	4
1:A:186:LEU:CD1	1:A:190:LEU:HD23	0.68	2.17	2	1
1:A:178:LEU:HD11	1:A:186:LEU:CD2	0.68	2.18	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:GLN:HA	1:A:83:ILE:HD12	0.68	1.65	12	10
1:A:178:LEU:HD11	1:A:209:VAL:HG12	0.68	1.66	9	1
1:A:39:TRP:CH2	1:A:47:LEU:HD23	0.68	2.24	7	6
1:A:130:VAL:HA	1:A:133:ILE:HD12	0.68	1.65	4	3
1:A:31:CYS:SG	1:A:88:LEU:HD11	0.68	2.28	1	7
1:A:178:LEU:HD22	1:A:186:LEU:HB2	0.67	1.64	10	1
1:A:39:TRP:CZ3	1:A:50:VAL:HG11	0.67	2.24	13	3
1:A:112:ALA:O	1:A:133:ILE:HD13	0.67	1.88	2	2
1:A:158:ILE:HG23	1:A:167:ILE:CG2	0.67	2.20	14	2
1:A:194:ILE:HB	1:A:211:LEU:HD23	0.67	1.65	7	1
1:A:15:VAL:HG23	1:A:32:TYR:CD1	0.67	2.24	19	1
1:A:186:LEU:HD11	1:A:229:LYS:HG3	0.67	1.66	11	1
1:A:177:ILE:CG2	1:A:206:LEU:HD12	0.66	2.19	10	2
1:A:47:LEU:HD12	1:A:51:LEU:CD1	0.66	2.19	14	2
1:A:47:LEU:HD12	1:A:81:THR:HG22	0.66	1.65	16	1
1:A:220:ILE:O	1:A:224:ILE:HG22	0.66	1.90	20	5
1:A:111:ILE:CD1	1:A:144:VAL:HG11	0.66	2.21	6	1
1:A:193:LEU:HD11	1:A:224:ILE:HG21	0.66	1.68	17	4
1:A:178:LEU:HD23	1:A:229:LYS:HD2	0.66	1.67	2	1
1:A:33:LYS:O	1:A:37:VAL:HG22	0.66	1.91	5	2
1:A:51:LEU:HD11	1:A:84:CYS:HB3	0.66	1.66	18	1
1:A:35:LYS:HB2	1:A:50:VAL:HG23	0.65	1.66	7	4
1:A:197:ILE:HG21	1:A:212:ILE:CD1	0.65	2.21	15	1
1:A:83:ILE:HG22	1:A:87:ILE:HD11	0.65	1.69	18	8
1:A:140:ILE:O	1:A:140:ILE:HD13	0.65	1.91	8	1
1:A:224:ILE:HD12	1:A:225:LYS:N	0.65	2.06	9	5
1:A:71:LEU:HD22	1:A:83:ILE:CD1	0.65	2.22	16	5
1:A:178:LEU:HD11	1:A:186:LEU:HD22	0.65	1.69	1	3
1:A:189:LYS:HD3	1:A:224:ILE:HD11	0.65	1.67	10	2
1:A:47:LEU:CD1	1:A:81:THR:HG22	0.65	2.22	16	1
1:A:158:ILE:HG23	1:A:167:ILE:HB	0.65	1.69	18	2
1:A:72:ILE:HD11	1:A:78:ASP:OD1	0.65	1.91	20	7
1:A:217:PHE:CD1	1:A:220:ILE:HD13	0.65	2.26	3	1
1:A:57:PHE:CZ	1:A:65:VAL:HG22	0.64	2.27	1	10
1:A:111:ILE:HA	1:A:114:ILE:HD12	0.64	1.70	2	3
1:A:186:LEU:HD12	1:A:190:LEU:CD1	0.64	2.23	14	1
1:A:178:LEU:HD12	1:A:183:GLY:HA2	0.64	1.68	19	1
1:A:178:LEU:HB3	1:A:186:LEU:HD11	0.64	1.69	20	1
1:A:47:LEU:HD13	1:A:51:LEU:HB2	0.64	1.68	15	5
1:A:29:ILE:HG23	1:A:56:VAL:HA	0.64	1.69	4	6
1:A:193:LEU:HD23	1:A:194:ILE:HD11	0.64	1.70	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:ILE:HB	1:A:211:LEU:HD22	0.64	1.68	15	2
1:A:75:PHE:CE2	1:A:83:ILE:HG23	0.64	2.28	11	4
1:A:190:LEU:HD13	1:A:211:LEU:CD2	0.64	2.20	19	2
1:A:176:PHE:HB2	1:A:211:LEU:HD11	0.64	1.69	6	1
1:A:185:LYS:HE2	1:A:228:THR:HG23	0.64	1.67	7	1
1:A:178:LEU:HD12	1:A:207:GLU:O	0.64	1.92	7	1
1:A:16:ALA:HB3	1:A:31:CYS:O	0.63	1.92	8	10
1:A:18:VAL:HG11	1:A:88:LEU:HA	0.63	1.70	18	1
1:A:187:LYS:HG2	1:A:209:VAL:HG21	0.63	1.71	10	1
1:A:186:LEU:HD12	1:A:187:LYS:N	0.63	2.08	12	1
1:A:186:LEU:HD11	1:A:225:LYS:HA	0.63	1.68	16	1
1:A:35:LYS:HB3	1:A:50:VAL:HG23	0.63	1.70	4	10
1:A:178:LEU:HD12	1:A:178:LEU:N	0.63	2.09	2	2
1:A:158:ILE:HG22	1:A:167:ILE:CG1	0.63	2.24	17	1
1:A:180:VAL:HG22	1:A:205:GLN:HA	0.63	1.71	3	11
1:A:174:LEU:O	1:A:211:LEU:HD12	0.63	1.94	15	2
1:A:186:LEU:HD21	1:A:229:LYS:CD	0.63	2.24	11	1
1:A:15:VAL:HG22	1:A:31:CYS:O	0.63	1.94	20	2
1:A:194:ILE:HG13	1:A:211:LEU:HD22	0.62	1.71	20	1
1:A:120:VAL:HG12	1:A:127:PRO:N	0.62	2.10	8	1
1:A:84:CYS:O	1:A:88:LEU:HD13	0.62	1.94	12	5
1:A:211:LEU:HD11	1:A:221:ASP:OD2	0.62	1.94	4	1
1:A:51:LEU:HD21	1:A:84:CYS:HB3	0.62	1.70	9	1
1:A:154:ALA:O	1:A:158:ILE:HG23	0.62	1.94	1	1
1:A:158:ILE:HA	1:A:167:ILE:HG21	0.62	1.71	4	1
1:A:33:LYS:HG3	1:A:95:VAL:HG11	0.62	1.71	6	1
1:A:194:ILE:CD1	1:A:211:LEU:HD13	0.62	2.25	14	1
1:A:178:LEU:HD13	1:A:186:LEU:HB3	0.62	1.70	19	1
1:A:178:LEU:HD13	1:A:186:LEU:CB	0.61	2.25	19	1
1:A:179:PRO:HA	1:A:206:LEU:HD23	0.61	1.73	16	2
1:A:53:THR:HG21	1:A:57:PHE:CE1	0.61	2.29	14	17
1:A:112:ALA:HB1	1:A:133:ILE:CD1	0.61	2.25	15	1
1:A:37:VAL:HG22	1:A:147:ASN:O	0.61	1.95	19	1
1:A:31:CYS:HG	1:A:50:VAL:HG22	0.61	1.54	6	2
1:A:193:LEU:HD13	1:A:224:ILE:HD13	0.61	1.72	6	2
1:A:36:VAL:HG13	1:A:88:LEU:HG	0.61	1.73	14	3
1:A:112:ALA:HB1	1:A:130:VAL:HG12	0.60	1.70	20	1
1:A:180:VAL:HG12	1:A:205:GLN:C	0.60	2.16	11	3
1:A:211:LEU:HD11	1:A:225:LYS:HE3	0.60	1.73	10	1
1:A:47:LEU:HD21	1:A:85:LYS:CE	0.60	2.27	14	4
1:A:158:ILE:HG22	1:A:167:ILE:HD12	0.60	1.72	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:TYR:CD1	1:A:132:LEU:HD13	0.60	2.32	14	4
1:A:47:LEU:HD13	1:A:51:LEU:CB	0.60	2.26	15	1
1:A:33:LYS:O	1:A:37:VAL:HG13	0.60	1.97	9	3
1:A:158:ILE:HA	1:A:167:ILE:HD13	0.60	1.74	10	1
1:A:190:LEU:HD12	1:A:211:LEU:HD22	0.60	1.73	10	1
1:A:116:ALA:HB2	1:A:133:ILE:HD13	0.60	1.74	13	1
1:A:173:ARG:HG2	1:A:212:ILE:HD12	0.59	1.73	19	2
1:A:211:LEU:O	1:A:212:ILE:HD13	0.59	1.96	4	1
1:A:56:VAL:O	1:A:66:ALA:HB3	0.59	1.97	10	4
1:A:120:VAL:HG12	1:A:127:PRO:HA	0.59	1.72	15	2
1:A:144:VAL:HG13	1:A:153:GLN:HG2	0.59	1.74	12	1
1:A:37:VAL:HG23	1:A:147:ASN:HA	0.59	1.75	20	1
1:A:194:ILE:HD11	1:A:211:LEU:HD22	0.59	1.74	16	1
1:A:71:LEU:CD2	1:A:83:ILE:HD13	0.59	2.16	6	1
1:A:194:ILE:HD13	1:A:211:LEU:HB3	0.59	1.74	18	1
1:A:211:LEU:HD12	1:A:211:LEU:N	0.59	2.13	6	2
1:A:31:CYS:SG	1:A:36:VAL:HG22	0.59	2.38	19	2
1:A:180:VAL:HG12	1:A:205:GLN:CA	0.58	2.28	11	3
1:A:178:LEU:HD22	1:A:183:GLY:HA2	0.58	1.74	7	2
1:A:18:VAL:HG22	1:A:93:VAL:HA	0.58	1.74	18	3
1:A:197:ILE:HG22	1:A:210:CYS:O	0.58	1.98	15	1
1:A:114:ILE:HG23	1:A:118:LYS:HG3	0.58	1.74	19	1
1:A:142:TYR:CD2	1:A:144:VAL:HG22	0.58	2.33	7	1
1:A:18:VAL:CG2	1:A:93:VAL:HG23	0.58	2.28	11	1
1:A:30:ALA:HB3	1:A:53:THR:OG1	0.58	1.98	18	2
1:A:110:ASP:HB3	1:A:150:THR:HG21	0.58	1.76	12	1
1:A:233:SER:O	1:A:234:LEU:HD12	0.58	1.98	2	1
1:A:167:ILE:N	1:A:167:ILE:HD13	0.58	2.13	17	2
1:A:161:LEU:CB	1:A:167:ILE:HD11	0.58	2.28	10	1
1:A:157:VAL:HG12	1:A:161:LEU:HD12	0.58	1.75	10	3
1:A:29:ILE:HG22	1:A:56:VAL:HA	0.58	1.76	19	1
1:A:173:ARG:C	1:A:174:LEU:HD22	0.58	2.19	2	1
1:A:18:VAL:HG21	1:A:88:LEU:HD12	0.58	1.76	20	2
1:A:186:LEU:HD23	1:A:229:LYS:CD	0.58	2.29	3	1
1:A:129:THR:O	1:A:133:ILE:HD12	0.58	1.99	16	1
1:A:173:ARG:HG3	1:A:212:ILE:HG23	0.57	1.75	11	1
1:A:158:ILE:HG22	1:A:167:ILE:HG13	0.57	1.74	17	1
1:A:29:ILE:HG23	1:A:56:VAL:HG13	0.57	1.73	19	1
1:A:186:LEU:HD22	1:A:229:LYS:HG3	0.57	1.75	2	1
1:A:120:VAL:HG21	1:A:216:CYS:HB2	0.57	1.74	4	3
1:A:31:CYS:SG	1:A:51:LEU:HD23	0.57	2.39	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:196:VAL:HG13	1:A:209:VAL:CG1	0.57	2.29	20	1
1:A:137:MET:CE	1:A:161:LEU:HD11	0.57	2.29	15	1
1:A:158:ILE:HA	1:A:167:ILE:HD11	0.57	1.76	17	2
1:A:37:VAL:HG21	1:A:146:THR:O	0.57	1.99	19	1
1:A:30:ALA:HB3	1:A:53:THR:CG2	0.57	2.28	11	4
1:A:18:VAL:HG22	1:A:93:VAL:CG2	0.57	2.30	11	1
1:A:186:LEU:HD21	1:A:229:LYS:HD3	0.57	1.77	11	1
1:A:224:ILE:O	1:A:228:THR:HG23	0.57	2.00	8	3
1:A:120:VAL:HG11	1:A:216:CYS:HB2	0.57	1.76	18	2
1:A:178:LEU:HD21	1:A:207:GLU:OE1	0.57	2.00	15	1
1:A:18:VAL:HG11	1:A:87:ILE:O	0.57	2.00	17	1
1:A:178:LEU:HD22	1:A:178:LEU:N	0.57	2.15	1	2
1:A:194:ILE:CD1	1:A:211:LEU:HD23	0.56	2.30	2	1
1:A:114:ILE:HG23	1:A:118:LYS:HD3	0.56	1.76	18	1
1:A:47:LEU:HA	1:A:50:VAL:HG12	0.56	1.78	10	10
1:A:16:ALA:HB2	1:A:33:LYS:CG	0.56	2.30	12	4
1:A:111:ILE:HD11	1:A:153:GLN:OE1	0.56	1.99	11	1
1:A:186:LEU:HD23	1:A:190:LEU:HD11	0.56	1.76	1	2
1:A:93:VAL:HG13	1:A:93:VAL:O	0.56	2.00	9	8
1:A:118:LYS:O	1:A:120:VAL:HG13	0.56	2.00	15	1
1:A:120:VAL:HG21	1:A:216:CYS:HB3	0.56	1.76	5	1
1:A:47:LEU:HD21	1:A:85:LYS:HD2	0.56	1.78	18	2
1:A:111:ILE:HD13	1:A:137:MET:HE1	0.56	1.76	8	1
1:A:174:LEU:N	1:A:211:LEU:O	0.56	2.39	16	6
1:A:75:PHE:CD1	1:A:83:ILE:HG23	0.56	2.36	19	2
1:A:136:ALA:O	1:A:140:ILE:HG22	0.56	2.00	7	2
1:A:58:VAL:HG23	1:A:66:ALA:N	0.56	2.16	8	1
1:A:17:VAL:HG12	1:A:28:GLU:HG2	0.55	1.76	17	4
1:A:110:ASP:OD1	1:A:114:ILE:HD11	0.55	2.01	11	1
1:A:186:LEU:HD21	1:A:225:LYS:HG2	0.55	1.77	15	1
1:A:190:LEU:HD23	1:A:224:ILE:HD11	0.55	1.78	14	1
1:A:180:VAL:HG22	1:A:205:GLN:CA	0.55	2.32	20	10
1:A:56:VAL:CB	1:A:71:LEU:HD21	0.55	2.31	16	5
1:A:18:VAL:HG21	1:A:88:LEU:CD1	0.55	2.32	20	2
1:A:120:VAL:HG21	1:A:125:LYS:HE2	0.55	1.78	20	1
1:A:178:LEU:HD23	1:A:186:LEU:HB3	0.55	1.79	17	2
1:A:137:MET:HE1	1:A:157:VAL:HG13	0.55	1.79	10	1
1:A:178:LEU:HD12	1:A:183:GLY:CA	0.55	2.32	12	1
1:A:107:MET:HB3	1:A:144:VAL:HG11	0.55	1.77	16	1
1:A:196:VAL:HG13	1:A:209:VAL:CG2	0.55	2.29	2	1
1:A:144:VAL:HG13	1:A:153:GLN:OE1	0.55	2.01	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:MET:SD	1:A:174:LEU:HD21	0.55	2.42	5	1
1:A:178:LEU:HD13	1:A:178:LEU:N	0.55	2.15	11	1
1:A:177:ILE:N	1:A:177:ILE:HD13	0.55	2.16	12	1
1:A:186:LEU:HD23	1:A:190:LEU:CD1	0.55	2.31	15	1
1:A:110:ASP:OD2	1:A:150:THR:HG21	0.55	2.01	4	1
1:A:75:PHE:CZ	1:A:83:ILE:HG23	0.55	2.37	14	5
1:A:154:ALA:O	1:A:158:ILE:HG22	0.55	2.01	13	2
1:A:47:LEU:HD12	1:A:81:THR:CG2	0.55	2.32	16	1
1:A:75:PHE:CE1	1:A:83:ILE:HG23	0.54	2.37	19	4
1:A:189:LYS:HG3	1:A:228:THR:HG21	0.54	1.79	14	2
1:A:176:PHE:CE2	1:A:190:LEU:HD11	0.54	2.37	17	1
1:A:167:ILE:HD12	1:A:167:ILE:O	0.54	2.02	19	2
1:A:36:VAL:HG11	1:A:93:VAL:HG21	0.54	1.79	20	1
1:A:167:ILE:HD13	1:A:167:ILE:H	0.54	1.61	6	2
1:A:178:LEU:N	1:A:178:LEU:HD23	0.54	2.17	19	2
1:A:189:LYS:HD3	1:A:228:THR:HG21	0.54	1.79	12	1
1:A:47:LEU:HD21	1:A:85:LYS:HE2	0.54	1.78	11	4
1:A:119:CYS:HB3	1:A:167:ILE:HD11	0.54	1.79	14	2
1:A:33:LYS:O	1:A:37:VAL:HG12	0.54	2.03	10	2
1:A:51:LEU:HD11	1:A:84:CYS:HB2	0.54	1.79	18	1
1:A:29:ILE:HD11	1:A:88:LEU:CD1	0.54	2.33	16	1
1:A:193:LEU:HD21	1:A:220:ILE:HG22	0.54	1.80	12	2
1:A:140:ILE:HG22	1:A:140:ILE:O	0.54	2.03	13	3
1:A:53:THR:CG2	1:A:57:PHE:CE1	0.53	2.91	19	4
1:A:186:LEU:HD21	1:A:225:LYS:CG	0.53	2.33	15	1
1:A:18:VAL:HG13	1:A:92:GLU:C	0.53	2.24	11	4
1:A:98:LYS:O	1:A:102:THR:HG23	0.53	2.03	8	1
1:A:193:LEU:HD13	1:A:224:ILE:CD1	0.53	2.34	15	1
1:A:83:ILE:HG22	1:A:87:ILE:CD1	0.53	2.32	3	4
1:A:18:VAL:HG23	1:A:31:CYS:SG	0.53	2.44	10	8
1:A:178:LEU:HD12	1:A:183:GLY:HA3	0.53	1.80	20	2
1:A:29:ILE:HD11	1:A:87:ILE:CG2	0.52	2.33	5	1
1:A:18:VAL:HG22	1:A:93:VAL:HG13	0.52	1.81	14	1
1:A:32:TYR:O	1:A:36:VAL:CG2	0.52	2.57	15	14
1:A:217:PHE:CE1	1:A:220:ILE:HD11	0.52	2.39	8	1
1:A:116:ALA:HB2	1:A:133:ILE:CG1	0.52	2.35	10	1
1:A:98:LYS:O	1:A:102:THR:HG22	0.52	2.05	17	3
1:A:172:MET:HE2	1:A:218:ARG:HB2	0.52	1.81	5	1
1:A:174:LEU:HD11	1:A:218:ARG:HD3	0.52	1.81	7	1
1:A:211:LEU:C	1:A:212:ILE:HD12	0.52	2.24	15	1
1:A:174:LEU:HB3	1:A:211:LEU:HD13	0.52	1.81	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:178:LEU:CD1	1:A:186:LEU:HD22	0.52	2.34	11	2
1:A:180:VAL:HG12	1:A:205:GLN:HA	0.52	1.80	4	1
1:A:34:ASN:O	1:A:37:VAL:HG12	0.52	2.03	20	2
1:A:174:LEU:HD22	1:A:211:LEU:HD22	0.52	1.81	12	1
1:A:15:VAL:HG23	1:A:32:TYR:CE1	0.52	2.39	19	1
1:A:217:PHE:CD1	1:A:220:ILE:HD11	0.52	2.40	8	1
1:A:112:ALA:CB	1:A:130:VAL:HG12	0.52	2.34	20	1
1:A:189:LYS:CE	1:A:224:ILE:HD11	0.52	2.34	20	1
1:A:47:LEU:HD21	1:A:85:LYS:HG2	0.52	1.81	12	5
1:A:15:VAL:HG22	1:A:52:GLN:NE2	0.52	2.20	6	2
1:A:190:LEU:HD23	1:A:224:ILE:CD1	0.52	2.34	14	1
1:A:47:LEU:CD1	1:A:51:LEU:HD12	0.52	2.35	5	3
1:A:137:MET:CE	1:A:157:VAL:HG13	0.52	2.34	10	1
1:A:196:VAL:CG1	1:A:209:VAL:HG11	0.51	2.36	1	1
1:A:200:GLU:HB2	1:A:208:ILE:HD11	0.51	1.82	6	1
1:A:120:VAL:HG12	1:A:126:ARG:C	0.51	2.25	8	1
1:A:71:LEU:HD22	1:A:83:ILE:HD12	0.51	1.81	16	1
1:A:27:PHE:CD2	1:A:75:PHE:CE2	0.51	2.99	15	3
1:A:211:LEU:N	1:A:211:LEU:HD22	0.51	2.21	1	1
1:A:103:GLN:HB3	1:A:146:THR:HG21	0.51	1.83	15	2
1:A:155:LEU:HA	1:A:158:ILE:HD12	0.51	1.82	5	3
1:A:158:ILE:HA	1:A:167:ILE:HD12	0.51	1.82	16	2
1:A:196:VAL:C	1:A:197:ILE:HD12	0.51	2.25	20	1
1:A:180:VAL:HG23	1:A:205:GLN:O	0.51	2.06	2	2
1:A:174:LEU:CG	1:A:237:LEU:HD23	0.51	2.36	6	1
1:A:193:LEU:HD22	1:A:224:ILE:HG21	0.51	1.81	15	4
1:A:111:ILE:O	1:A:115:VAL:HG12	0.51	2.04	15	1
1:A:173:ARG:CG	1:A:212:ILE:HD12	0.51	2.36	1	1
1:A:193:LEU:CD1	1:A:224:ILE:HG21	0.50	2.36	4	3
1:A:211:LEU:HD23	1:A:221:ASP:OD2	0.50	2.05	6	1
1:A:29:ILE:CG2	1:A:56:VAL:HG13	0.50	2.36	19	1
1:A:186:LEU:HD23	1:A:229:LYS:HD2	0.50	1.83	3	1
1:A:84:CYS:O	1:A:88:LEU:HD23	0.50	2.06	18	1
1:A:190:LEU:HD21	1:A:221:ASP:OD1	0.50	2.06	17	2
1:A:111:ILE:HD13	1:A:144:VAL:HG11	0.50	1.83	6	1
1:A:113:THR:HG22	1:A:117:ASP:OD2	0.50	2.07	2	1
1:A:196:VAL:CG1	1:A:209:VAL:HG21	0.50	2.36	9	1
1:A:68:LYS:O	1:A:72:ILE:HD12	0.50	2.06	4	3
1:A:178:LEU:HD22	1:A:178:LEU:H	0.50	1.67	11	2
1:A:172:MET:HE3	1:A:174:LEU:HD11	0.50	1.82	5	1
1:A:199:SER:CB	1:A:209:VAL:HG22	0.50	2.37	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:LEU:HD12	1:A:228:THR:HG23	0.50	1.83	6	1
1:A:193:LEU:O	1:A:194:ILE:HG23	0.49	2.07	1	2
1:A:29:ILE:H	1:A:29:ILE:HD13	0.49	1.67	12	1
1:A:115:VAL:CG1	1:A:167:ILE:HG21	0.49	2.34	18	1
1:A:28:GLU:OE2	1:A:60:VAL:HG23	0.49	2.07	20	5
1:A:175:ARG:HD3	1:A:236:VAL:HG13	0.49	1.85	6	1
1:A:194:ILE:HD13	1:A:221:ASP:OD1	0.49	2.07	12	1
1:A:158:ILE:HG22	1:A:167:ILE:CD1	0.49	2.37	15	1
1:A:158:ILE:HD11	1:A:167:ILE:O	0.49	2.07	2	1
1:A:182:GLU:O	1:A:186:LEU:HD23	0.49	2.07	14	1
1:A:58:VAL:HG23	1:A:66:ALA:HB2	0.49	1.83	10	2
1:A:186:LEU:HD21	1:A:229:LYS:HG3	0.49	1.84	18	1
1:A:39:TRP:CH2	1:A:85:LYS:HD3	0.49	2.42	16	1
1:A:174:LEU:O	1:A:211:LEU:N	0.49	2.46	3	4
1:A:15:VAL:HG21	1:A:52:GLN:HG2	0.49	1.84	16	2
1:A:39:TRP:CH2	1:A:47:LEU:CD2	0.49	2.96	10	10
1:A:178:LEU:N	1:A:178:LEU:HD22	0.49	2.22	11	1
1:A:36:VAL:HG22	1:A:88:LEU:CD1	0.49	2.38	18	1
1:A:178:LEU:HG	1:A:186:LEU:HD13	0.49	1.84	11	1
1:A:186:LEU:HD21	1:A:229:LYS:HB3	0.49	1.84	13	1
1:A:178:LEU:HD11	1:A:207:GLU:HB3	0.49	1.85	5	1
1:A:17:VAL:HG11	1:A:28:GLU:OE2	0.49	2.08	9	1
1:A:194:ILE:HD11	1:A:221:ASP:CG	0.48	2.29	15	1
1:A:108:PHE:CE1	1:A:144:VAL:HG23	0.48	2.43	18	1
1:A:18:VAL:CG2	1:A:93:VAL:HG12	0.48	2.35	17	1
1:A:95:VAL:HG11	1:A:99:GLU:OE2	0.48	2.07	19	1
1:A:196:VAL:O	1:A:197:ILE:HG23	0.48	2.08	8	2
1:A:120:VAL:HG11	1:A:125:LYS:HE2	0.48	1.84	20	1
1:A:157:VAL:HG22	1:A:161:LEU:HD12	0.48	1.84	3	2
1:A:39:TRP:C	1:A:39:TRP:CD1	0.48	2.87	14	6
1:A:194:ILE:HG22	1:A:217:PHE:CD1	0.48	2.44	5	1
1:A:137:MET:HE1	1:A:161:LEU:HD11	0.48	1.86	15	1
1:A:142:TYR:CE2	1:A:144:VAL:HG22	0.48	2.44	8	1
1:A:47:LEU:CG	1:A:81:THR:HG22	0.48	2.38	17	2
1:A:109:ARG:O	1:A:113:THR:HG23	0.48	2.07	11	1
1:A:115:VAL:HG13	1:A:133:ILE:CD1	0.48	2.39	13	1
1:A:129:THR:OG1	1:A:132:LEU:HD23	0.48	2.08	20	1
1:A:142:TYR:HE2	1:A:144:VAL:HG22	0.48	1.68	8	1
1:A:190:LEU:HD12	1:A:194:ILE:CG2	0.48	2.39	10	1
1:A:18:VAL:HG22	1:A:93:VAL:CB	0.48	2.39	11	1
1:A:177:ILE:HD11	1:A:236:VAL:HG23	0.48	1.85	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:ILE:HG22	1:A:137:MET:HE2	0.47	1.86	2	1
1:A:15:VAL:CG2	1:A:32:TYR:CD1	0.47	2.97	19	1
1:A:29:ILE:HD11	1:A:88:LEU:HD12	0.47	1.86	2	5
1:A:178:LEU:O	1:A:178:LEU:HD12	0.47	2.09	5	1
1:A:186:LEU:HD11	1:A:229:LYS:HA	0.47	1.86	13	1
1:A:174:LEU:HD12	1:A:211:LEU:HB2	0.47	1.86	18	1
1:A:178:LEU:HD11	1:A:186:LEU:HD23	0.47	1.86	4	1
1:A:120:VAL:HG11	1:A:216:CYS:CB	0.47	2.39	9	1
1:A:194:ILE:HD11	1:A:211:LEU:HD13	0.47	1.85	20	1
1:A:180:VAL:HG22	1:A:205:GLN:C	0.47	2.30	16	3
1:A:180:VAL:HG13	1:A:204:GLN:C	0.47	2.30	13	5
1:A:180:VAL:HG23	1:A:181:ASN:N	0.47	2.24	12	2
1:A:110:ASP:O	1:A:113:THR:HG22	0.47	2.10	7	2
1:A:178:LEU:HD22	1:A:186:LEU:HD22	0.47	1.85	8	1
1:A:16:ALA:HB2	1:A:33:LYS:HB3	0.47	1.87	10	2
1:A:32:TYR:C	1:A:36:VAL:HG23	0.47	2.29	4	2
1:A:193:LEU:HD13	1:A:224:ILE:HG21	0.47	1.86	13	2
1:A:197:ILE:CD1	1:A:212:ILE:HD11	0.47	2.39	6	1
1:A:115:VAL:CG1	1:A:133:ILE:HD12	0.47	2.40	13	1
1:A:206:LEU:O	1:A:206:LEU:CD2	0.47	2.63	13	1
1:A:197:ILE:HD12	1:A:197:ILE:N	0.47	2.25	20	1
1:A:75:PHE:CE2	1:A:83:ILE:CG2	0.47	2.98	1	5
1:A:176:PHE:CE1	1:A:235:GLU:CB	0.47	2.98	10	1
1:A:186:LEU:HD12	1:A:186:LEU:C	0.47	2.29	12	1
1:A:189:LYS:CD	1:A:224:ILE:HD11	0.47	2.39	20	1
1:A:28:GLU:O	1:A:57:PHE:N	0.47	2.47	20	8
1:A:108:PHE:HA	1:A:111:ILE:HD12	0.47	1.85	8	2
1:A:199:SER:OG	1:A:209:VAL:HG22	0.47	2.09	7	1
1:A:178:LEU:HD11	1:A:209:VAL:CG1	0.47	2.40	9	1
1:A:191:LYS:N	1:A:192:PRO:CD	0.46	2.78	9	5
1:A:39:TRP:CZ3	1:A:47:LEU:CD2	0.46	2.98	6	1
1:A:161:LEU:HD12	1:A:167:ILE:HD11	0.46	1.86	7	2
1:A:18:VAL:HG13	1:A:92:GLU:O	0.46	2.10	18	1
1:A:112:ALA:HB1	1:A:130:VAL:CG1	0.46	2.41	20	1
1:A:56:VAL:HG11	1:A:71:LEU:HD21	0.46	1.86	18	3
1:A:57:PHE:CE2	1:A:65:VAL:HG22	0.46	2.45	19	2
1:A:161:LEU:HD23	1:A:164:LYS:NZ	0.46	2.25	8	1
1:A:29:ILE:HD13	1:A:88:LEU:CD1	0.46	2.40	9	1
1:A:161:LEU:HB2	1:A:167:ILE:HD11	0.46	1.86	10	1
1:A:224:ILE:HG23	1:A:225:LYS:N	0.46	2.26	6	3
1:A:107:MET:CE	1:A:150:THR:HG22	0.46	2.41	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:THR:OG1	1:A:132:LEU:HD12	0.46	2.11	3	1
1:A:29:ILE:HD13	1:A:88:LEU:HD13	0.46	1.88	9	1
1:A:85:LYS:CE	1:A:85:LYS:CA	0.46	2.94	16	1
1:A:185:LYS:HD3	1:A:228:THR:HG23	0.46	1.87	4	1
1:A:197:ILE:HG21	1:A:212:ILE:HD11	0.46	1.87	15	1
1:A:36:VAL:HG22	1:A:88:LEU:HD21	0.45	1.88	14	2
1:A:114:ILE:HG23	1:A:118:LYS:CG	0.45	2.40	19	1
1:A:33:LYS:HB2	1:A:95:VAL:HG11	0.45	1.89	20	1
1:A:15:VAL:HG12	1:A:16:ALA:N	0.45	2.26	1	2
1:A:50:VAL:HG13	1:A:51:LEU:N	0.45	2.27	14	9
1:A:178:LEU:HD23	1:A:182:GLU:HB3	0.45	1.89	10	1
1:A:115:VAL:HG13	1:A:133:ILE:HG21	0.45	1.87	15	1
1:A:136:ALA:HB1	1:A:164:LYS:CE	0.45	2.42	2	1
1:A:75:PHE:CE1	1:A:83:ILE:CG2	0.45	3.00	4	2
1:A:115:VAL:HG13	1:A:116:ALA:N	0.45	2.27	15	1
1:A:196:VAL:CG1	1:A:209:VAL:CG1	0.45	2.95	1	1
1:A:194:ILE:CG2	1:A:217:PHE:CD1	0.45	3.00	5	3
1:A:100:ARG:O	1:A:104:LEU:HD13	0.45	2.12	15	1
1:A:194:ILE:HG22	1:A:195:LYS:N	0.45	2.27	11	5
1:A:40:ARG:HA	1:A:89:THR:HG22	0.45	1.89	12	1
1:A:174:LEU:HD22	1:A:211:LEU:HD13	0.45	1.89	13	1
1:A:197:ILE:HD12	1:A:198:GLU:HB2	0.45	1.89	17	1
1:A:46:ASP:O	1:A:50:VAL:HG12	0.45	2.11	12	2
1:A:189:LYS:HE2	1:A:224:ILE:HD11	0.45	1.87	20	1
1:A:120:VAL:HG22	1:A:215:GLY:HA3	0.45	1.88	15	1
1:A:18:VAL:HB	1:A:29:ILE:HD11	0.45	1.89	19	1
1:A:22:ARG:CD	1:A:75:PHE:CZ	0.45	3.00	8	1
1:A:178:LEU:HD22	1:A:186:LEU:HD13	0.45	1.89	13	1
1:A:194:ILE:HD13	1:A:211:LEU:HD13	0.45	1.89	14	1
1:A:190:LEU:HD22	1:A:211:LEU:HD21	0.44	1.88	9	1
1:A:37:VAL:HG12	1:A:146:THR:O	0.44	2.12	15	1
1:A:36:VAL:HG22	1:A:88:LEU:CD2	0.44	2.42	17	1
1:A:111:ILE:CG2	1:A:112:ALA:N	0.44	2.79	17	2
1:A:180:VAL:HG13	1:A:181:ASN:N	0.44	2.27	7	3
1:A:196:VAL:HG12	1:A:211:LEU:HB3	0.44	1.88	10	1
1:A:18:VAL:HG12	1:A:87:ILE:HG22	0.44	1.90	19	1
1:A:196:VAL:HG13	1:A:209:VAL:HG11	0.44	1.89	20	1
1:A:72:ILE:HD11	1:A:78:ASP:CG	0.44	2.32	12	1
1:A:176:PHE:CD2	1:A:190:LEU:CD1	0.44	3.01	15	1
1:A:191:LYS:CB	1:A:192:PRO:CD	0.44	2.96	3	5
1:A:112:ALA:HB1	1:A:130:VAL:HG13	0.44	1.88	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:TYR:CE1	1:A:132:LEU:HD13	0.44	2.47	14	1
1:A:154:ALA:O	1:A:158:ILE:HD12	0.44	2.13	3	1
1:A:18:VAL:HG22	1:A:93:VAL:CA	0.44	2.43	11	3
1:A:53:THR:HG23	1:A:53:THR:O	0.44	2.13	5	2
1:A:18:VAL:HB	1:A:29:ILE:HD12	0.44	1.88	9	1
1:A:190:LEU:CD1	1:A:194:ILE:HG22	0.44	2.43	10	1
1:A:29:ILE:HD13	1:A:29:ILE:N	0.44	2.28	12	1
1:A:177:ILE:CD1	1:A:208:ILE:HG22	0.44	2.36	18	1
1:A:186:LEU:HD22	1:A:228:THR:CG2	0.44	2.42	3	1
1:A:158:ILE:HG23	1:A:159:LYS:N	0.43	2.28	2	1
1:A:161:LEU:HD22	1:A:164:LYS:HZ1	0.43	1.73	2	1
1:A:151:LYS:HG2	1:A:220:ILE:HD11	0.43	1.89	6	1
1:A:182:GLU:O	1:A:186:LEU:HD12	0.43	2.13	8	2
1:A:161:LEU:HB3	1:A:167:ILE:HD11	0.43	1.90	10	1
1:A:194:ILE:HD11	1:A:221:ASP:CB	0.43	2.42	15	1
1:A:225:LYS:HG3	1:A:226:LYS:N	0.43	2.28	17	1
1:A:120:VAL:HG11	1:A:215:GLY:O	0.43	2.13	1	1
1:A:116:ALA:HB2	1:A:133:ILE:HD12	0.43	1.89	3	1
1:A:72:ILE:O	1:A:76:GLY:N	0.43	2.51	10	4
1:A:133:ILE:CG2	1:A:137:MET:HE1	0.43	2.43	17	1
1:A:145:LYS:HD2	1:A:150:THR:HG23	0.43	1.90	17	1
1:A:157:VAL:HG13	1:A:158:ILE:N	0.43	2.29	8	5
1:A:186:LEU:HD13	1:A:228:THR:HB	0.43	1.90	4	1
1:A:211:LEU:HD13	1:A:221:ASP:OD2	0.43	2.13	19	1
1:A:17:VAL:HG13	1:A:60:VAL:HG21	0.43	1.90	14	3
1:A:58:VAL:CG2	1:A:66:ALA:HB2	0.43	2.43	20	2
1:A:196:VAL:CG1	1:A:209:VAL:CG2	0.43	2.96	9	1
1:A:140:ILE:O	1:A:141:HIS:CG	0.43	2.71	13	1
1:A:140:ILE:HD11	1:A:161:LEU:HD23	0.43	1.91	14	1
1:A:191:LYS:HA	1:A:196:VAL:HG21	0.43	1.90	1	1
1:A:196:VAL:CG1	1:A:209:VAL:HG23	0.43	2.41	2	1
1:A:178:LEU:HD12	1:A:233:SER:HB3	0.43	1.90	11	1
1:A:47:LEU:CD1	1:A:51:LEU:CD1	0.43	2.96	5	1
1:A:111:ILE:HD11	1:A:144:VAL:HG11	0.43	1.91	12	1
1:A:194:ILE:HD11	1:A:211:LEU:HD23	0.43	1.91	13	1
1:A:31:CYS:CB	1:A:36:VAL:CG2	0.43	2.96	18	1
1:A:213:ASP:CB	1:A:214:PRO:CD	0.43	2.97	3	1
1:A:174:LEU:HD21	1:A:237:LEU:CD2	0.43	2.43	6	1
1:A:116:ALA:HB1	1:A:128:TYR:O	0.43	2.14	10	1
1:A:85:LYS:CE	1:A:85:LYS:HA	0.43	2.42	16	1
1:A:111:ILE:HG23	1:A:112:ALA:N	0.43	2.29	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:THR:O	1:A:54:HIS:HB2	0.43	2.14	18	2
1:A:33:LYS:CG	1:A:95:VAL:HG11	0.43	2.41	6	2
1:A:15:VAL:HG22	1:A:32:TYR:HA	0.43	1.91	9	2
1:A:167:ILE:HG22	1:A:168:GLU:N	0.43	2.29	11	2
1:A:33:LYS:HD3	1:A:95:VAL:HG12	0.43	1.89	17	1
1:A:115:VAL:HG13	1:A:167:ILE:HG12	0.42	1.91	1	1
1:A:111:ILE:CG2	1:A:157:VAL:HG11	0.42	2.44	20	2
1:A:178:LEU:HD13	1:A:186:LEU:HD11	0.42	1.91	12	1
1:A:173:ARG:HG2	1:A:212:ILE:HG23	0.42	1.91	20	1
1:A:33:LYS:CB	1:A:95:VAL:HG12	0.42	2.44	2	1
1:A:37:VAL:HG23	1:A:38:GLY:N	0.42	2.28	11	2
1:A:31:CYS:SG	1:A:51:LEU:HD22	0.42	2.54	9	1
1:A:39:TRP:CD1	1:A:39:TRP:C	0.42	2.92	12	3
1:A:77:THR:O	1:A:78:ASP:CB	0.42	2.67	6	1
1:A:121:ASN:O	1:A:125:LYS:N	0.42	2.52	20	1
1:A:116:ALA:HB2	1:A:133:ILE:HG13	0.42	1.90	10	1
1:A:54:HIS:CD2	1:A:54:HIS:N	0.42	2.86	14	1
1:A:33:LYS:HB2	1:A:95:VAL:HG12	0.42	1.92	2	1
1:A:180:VAL:CG1	1:A:181:ASN:N	0.42	2.82	2	3
1:A:176:PHE:CD1	1:A:234:LEU:O	0.42	2.72	6	1
1:A:190:LEU:HB3	1:A:211:LEU:HD21	0.42	1.91	7	1
1:A:177:ILE:HG23	1:A:177:ILE:O	0.42	2.14	2	1
1:A:158:ILE:HD13	1:A:167:ILE:CD1	0.42	2.45	8	1
1:A:225:LYS:O	1:A:229:LYS:N	0.42	2.53	12	1
1:A:176:PHE:CE1	1:A:225:LYS:CE	0.42	3.02	13	1
1:A:18:VAL:O	1:A:28:GLU:HA	0.42	2.15	17	2
1:A:31:CYS:HB2	1:A:36:VAL:CG2	0.42	2.45	18	1
1:A:114:ILE:HG13	1:A:150:THR:HG22	0.42	1.92	19	1
1:A:16:ALA:HB2	1:A:33:LYS:HG2	0.42	1.92	17	1
1:A:18:VAL:CG2	1:A:31:CYS:SG	0.42	3.08	17	1
1:A:36:VAL:HG22	1:A:88:LEU:HD13	0.42	1.91	18	1
1:A:197:ILE:HD11	1:A:212:ILE:HD11	0.42	1.90	1	1
1:A:111:ILE:HD13	1:A:137:MET:CE	0.42	2.44	8	1
1:A:186:LEU:HD12	1:A:190:LEU:HG	0.42	1.91	3	1
1:A:178:LEU:CD1	1:A:209:VAL:HG12	0.42	2.43	9	1
1:A:140:ILE:HD11	1:A:164:LYS:HB2	0.42	1.91	13	1
1:A:201:ASP:CB	1:A:207:GLU:CG	0.41	2.98	8	2
1:A:87:ILE:O	1:A:91:GLY:N	0.41	2.53	18	2
1:A:178:LEU:CG	1:A:186:LEU:HD22	0.41	2.45	11	1
1:A:108:PHE:HD1	1:A:144:VAL:HG21	0.41	1.75	13	1
1:A:178:LEU:N	1:A:178:LEU:CD2	0.41	2.83	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:ILE:O	1:A:86:GLN:HG2	0.41	2.15	15	1
1:A:18:VAL:HG22	1:A:93:VAL:HG22	0.41	1.92	20	1
1:A:210:CYS:O	1:A:211:LEU:HD12	0.41	2.15	7	1
1:A:189:LYS:HD2	1:A:228:THR:HG21	0.41	1.92	9	1
1:A:75:PHE:CZ	1:A:83:ILE:CG2	0.41	3.03	14	1
1:A:144:VAL:HG12	1:A:145:LYS:N	0.41	2.30	2	1
1:A:174:LEU:HD21	1:A:237:LEU:HD23	0.41	1.91	6	1
1:A:194:ILE:HD12	1:A:194:ILE:C	0.41	2.35	18	2
1:A:211:LEU:HD22	1:A:221:ASP:OD1	0.41	2.16	13	1
1:A:107:MET:HE1	1:A:145:LYS:O	0.41	2.15	19	1
1:A:57:PHE:CE1	1:A:65:VAL:HG22	0.41	2.49	1	1
1:A:15:VAL:HG21	1:A:52:GLN:HG3	0.41	1.92	7	1
1:A:18:VAL:O	1:A:29:ILE:HD13	0.41	2.15	16	1
1:A:37:VAL:HG13	1:A:38:GLY:N	0.41	2.31	14	2
1:A:233:SER:O	1:A:234:LEU:HD22	0.41	2.15	14	1
1:A:194:ILE:CD1	1:A:211:LEU:HD22	0.41	2.44	16	1
1:A:108:PHE:CE2	1:A:144:VAL:HG21	0.41	2.51	20	1
1:A:193:LEU:O	1:A:217:PHE:CE1	0.41	2.74	6	1
1:A:121:ASN:O	1:A:123:GLU:N	0.41	2.54	7	1
1:A:194:ILE:HG21	1:A:211:LEU:HD13	0.41	1.93	10	1
1:A:177:ILE:HD11	1:A:236:VAL:CG2	0.41	2.46	14	1
1:A:196:VAL:HG12	1:A:211:LEU:HG	0.41	1.92	7	1
1:A:193:LEU:O	1:A:194:ILE:CG2	0.41	2.68	1	1
1:A:26:ARG:O	1:A:27:PHE:CD1	0.41	2.74	8	1
1:A:53:THR:O	1:A:53:THR:HG23	0.41	2.16	8	1
1:A:29:ILE:CD1	1:A:88:LEU:CD1	0.41	2.98	10	1
1:A:108:PHE:CD2	1:A:144:VAL:HG21	0.41	2.51	10	1
1:A:176:PHE:CZ	1:A:229:LYS:HD3	0.41	2.49	11	1
1:A:178:LEU:HG	1:A:186:LEU:HD22	0.41	1.93	11	1
1:A:174:LEU:HD13	1:A:175:ARG:H	0.41	1.75	16	1
1:A:31:CYS:HB3	1:A:36:VAL:HG21	0.41	1.93	7	1
1:A:212:ILE:HG22	1:A:213:ASP:N	0.41	2.31	9	1
1:A:75:PHE:CE2	1:A:83:ILE:HG21	0.40	2.51	1	1
1:A:16:ALA:HB2	1:A:33:LYS:HD2	0.40	1.91	11	1
1:A:177:ILE:HD13	1:A:177:ILE:H	0.40	1.76	12	1
1:A:193:LEU:O	1:A:217:PHE:CZ	0.40	2.75	20	1
1:A:178:LEU:HD21	1:A:186:LEU:HD22	0.40	1.91	6	1
1:A:211:LEU:N	1:A:211:LEU:CD1	0.40	2.84	6	1
1:A:193:LEU:HD23	1:A:194:ILE:CD1	0.40	2.45	8	1
1:A:191:LYS:N	1:A:192:PRO:HD2	0.40	2.30	12	1
1:A:212:ILE:HD12	1:A:212:ILE:N	0.40	2.31	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:PHE:CE1	1:A:143:SER:O	0.40	2.74	17	1
1:A:15:VAL:HG12	1:A:31:CYS:O	0.40	2.17	1	1
1:A:176:PHE:HD2	1:A:211:LEU:HD11	0.40	1.77	2	1
1:A:178:LEU:HD22	1:A:186:LEU:CB	0.40	2.45	8	1
1:A:193:LEU:HD23	1:A:221:ASP:OD1	0.40	2.16	10	1
1:A:27:PHE:CD2	1:A:75:PHE:CZ	0.40	3.10	15	1
1:A:120:VAL:HG11	1:A:216:CYS:H	0.40	1.77	17	1
1:A:32:TYR:O	1:A:36:VAL:N	0.40	2.54	4	1
1:A:168:GLU:O	1:A:215:GLY:HA2	0.40	2.16	15	1
1:A:133:ILE:CG2	1:A:137:MET:CE	0.40	2.99	17	1
1:A:167:ILE:N	1:A:167:ILE:CD1	0.40	2.83	17	1
1:A:176:PHE:CZ	1:A:235:GLU:HB3	0.40	2.52	1	1
1:A:128:TYR:CE1	1:A:132:LEU:HD22	0.40	2.52	4	1
1:A:214:PRO:O	1:A:216:CYS:N	0.40	2.54	6	1
1:A:174:LEU:O	1:A:211:LEU:HB2	0.40	2.17	15	1
1:A:171:HIS:HA	1:A:214:PRO:HA	0.40	1.92	16	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/252 (87%)	195±4 (90±2%)	20±4 (9±2%)	3±1 (1±1%)	16	63
All	All	4360/5040 (87%)	3905 (90%)	398 (9%)	57 (1%)	16	63

All 20 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	179	PRO	9
1	A	203	GLY	8
1	A	79	ASP	6
1	A	230	GLY	6
1	A	15	VAL	4
1	A	144	VAL	3

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Mol	Chain	Res	Type	Models (Total)
1	A	119	CYS	3
1	A	214	PRO	2
1	A	143	SER	2
1	A	215	GLY	2
1	A	145	LYS	2
1	A	238	ASN	2
1	A	194	ILE	1
1	A	123	GLU	1
1	A	124	THR	1
1	A	54	HIS	1
1	A	231	LYS	1
1	A	166	LYS	1
1	A	192	PRO	1
1	A	229	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	199/229 (87%)	142±6 (71±3%)	57±6 (29±3%)	2 18
All	All	3980/4580 (87%)	2837 (71%)	1143 (29%)	2 18

All 154 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	29	ILE	20
1	A	81	THR	19
1	A	217	PHE	18
1	A	25	LYS	16
1	A	229	LYS	16
1	A	178	LEU	15
1	A	182	GLU	15
1	A	164	LYS	15
1	A	151	LYS	14
1	A	155	LEU	14
1	A	19	ARG	13

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Mol	Chain	Res	Type	Models (Total)
1	A	33	LYS	13
1	A	55	SER	13
1	A	108	PHE	13
1	A	223	LEU	13
1	A	22	ARG	12
1	A	47	LEU	12
1	A	80	GLN	12
1	A	106	GLN	12
1	A	189	LYS	12
1	A	195	LYS	12
1	A	205	GLN	12
1	A	64	GLN	12
1	A	46	ASP	12
1	A	193	LEU	12
1	A	137	MET	12
1	A	159	LYS	12
1	A	101	HIS	11
1	A	107	MET	11
1	A	110	ASP	11
1	A	119	CYS	11
1	A	145	LYS	11
1	A	172	MET	11
1	A	100	ARG	11
1	A	59	ASN	11
1	A	162	LYS	11
1	A	21	LYS	10
1	A	26	ARG	10
1	A	51	LEU	10
1	A	77	THR	10
1	A	126	ARG	10
1	A	139	ASP	10
1	A	143	SER	10
1	A	225	LYS	10
1	A	40	ARG	10
1	A	68	LYS	10
1	A	175	ARG	10
1	A	226	LYS	10
1	A	31	CYS	10
1	A	90	LYS	9
1	A	103	GLN	9
1	A	118	LYS	9
1	A	125	LYS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	135	ARG	9
1	A	184	LYS	9
1	A	186	LEU	9
1	A	191	LYS	9
1	A	219	GLU	9
1	A	132	LEU	9
1	A	176	PHE	9
1	A	231	LYS	9
1	A	109	ARG	9
1	A	67	LYS	8
1	A	123	GLU	8
1	A	124	THR	8
1	A	129	THR	8
1	A	152	GLN	8
1	A	163	GLU	8
1	A	202	TYR	8
1	A	206	LEU	8
1	A	218	ARG	8
1	A	98	LYS	8
1	A	173	ARG	8
1	A	213	ASP	8
1	A	234	LEU	8
1	A	28	GLU	7
1	A	52	GLN	7
1	A	70	ASP	7
1	A	79	ASP	7
1	A	187	LYS	7
1	A	204	GLN	7
1	A	149	SER	7
1	A	166	LYS	7
1	A	141	HIS	7
1	A	235	GLU	7
1	A	156	GLU	7
1	A	174	LEU	7
1	A	216	CYS	7
1	A	92	GLU	6
1	A	117	ASP	6
1	A	168	GLU	6
1	A	199	SER	6
1	A	200	GLU	6
1	A	96	SER	6
1	A	138	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	134	GLU	6
1	A	165	MET	6
1	A	15	VAL	6
1	A	169	ARG	6
1	A	35	LYS	6
1	A	104	LEU	5
1	A	221	ASP	5
1	A	238	ASN	5
1	A	128	TYR	5
1	A	153	GLN	5
1	A	198	GLU	5
1	A	97	ASP	5
1	A	211	LEU	5
1	A	105	GLU	5
1	A	82	GLU	4
1	A	147	ASN	4
1	A	69	GLU	4
1	A	121	ASN	4
1	A	20	MET	4
1	A	86	GLN	4
1	A	185	LYS	4
1	A	222	GLU	4
1	A	237	LEU	4
1	A	62	LYS	3
1	A	73	SER	3
1	A	140	ILE	3
1	A	207	GLU	3
1	A	48	ASP	3
1	A	181	ASN	3
1	A	32	TYR	3
1	A	34	ASN	3
1	A	142	TYR	3
1	A	99	GLU	3
1	A	224	ILE	3
1	A	88	LEU	3
1	A	148	LYS	3
1	A	150	THR	3
1	A	171	HIS	2
1	A	160	GLN	2
1	A	61	SER	2
1	A	167	ILE	2
1	A	208	ILE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	89	THR	2
1	A	210	CYS	2
1	A	227	GLU	2
1	A	131	ILE	2
1	A	233	SER	2
1	A	49	GLU	2
1	A	197	ILE	2
1	A	39	TRP	2
1	A	85	LYS	2
1	A	158	ILE	1
1	A	190	LEU	1
1	A	188	GLU	1
1	A	194	ILE	1
1	A	114	ILE	1
1	A	177	ILE	1
1	A	133	ILE	1
1	A	146	THR	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 79% 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	2846
Number of shifts mapped to atoms	2846
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	18

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	243	-0.01 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	225	0.00 ± 0.06	None needed (< 0.5 ppm)
$^{13}C'$	214	-0.00 ± 0.07	None needed (< 0.5 ppm)
^{15}N	237	0.04 ± 0.32	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 79%, i.e. 2478 atoms were assigned a chemical shift out of a possible 3152. 0 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1038/1090 (95%)	432/441 (98%)	399/436 (92%)	207/213 (97%)
Sidechain	1406/1922 (73%)	962/1239 (78%)	436/599 (73%)	8/84 (10%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	34/140 (24%)	33/68 (49%)	0/63 (0%)	1/9 (11%)
Overall	2478/3152 (79%)	1427/1748 (82%)	835/1098 (76%)	216/306 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 2833 atoms were assigned a chemical shift out of a possible 3581. 0 out of 43 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1189/1250 (95%)	495/506 (98%)	457/500 (91%)	237/244 (97%)
Sidechain	1605/2171 (74%)	1099/1398 (79%)	496/680 (73%)	10/93 (11%)
Aromatic	39/160 (24%)	38/78 (49%)	0/73 (0%)	1/9 (11%)
Overall	2833/3581 (79%)	1632/1982 (82%)	953/1253 (76%)	248/346 (72%)

7.1.4 Statistically unusual chemical shifts (i)

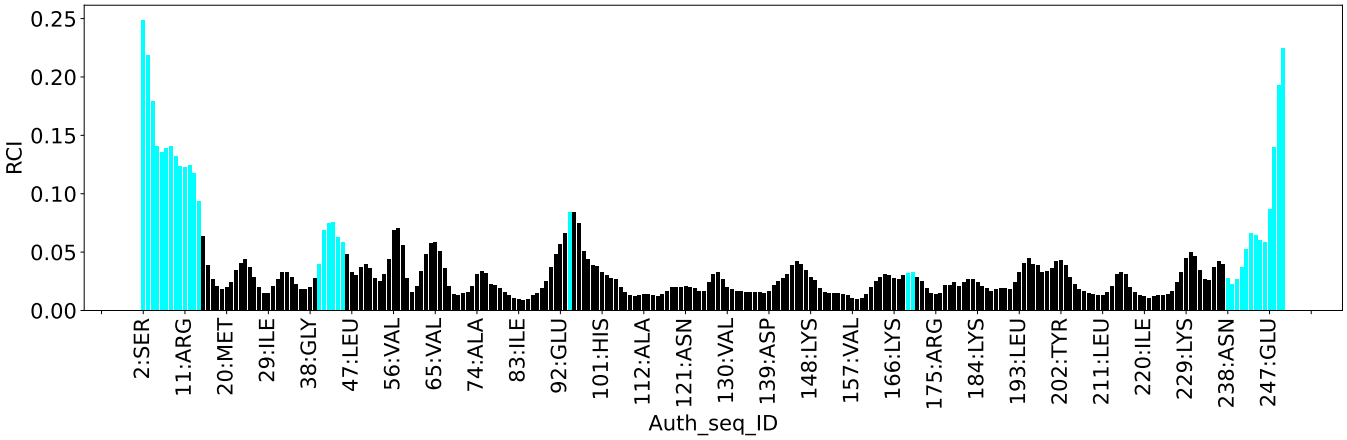
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	124	THR	HG1	4.91	0.08 – 2.19	17.9
1	A	89	THR	HG1	4.65	0.08 – 2.19	16.6
1	A	102	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	228	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	5	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	81	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	53	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	77	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	13	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	146	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	113	THR	HG1	4.63	0.08 – 2.19	16.6
1	A	150	THR	HG1	4.35	0.08 – 2.19	15.2
1	A	72	ILE	CG2	10.27	10.93 – 24.12	-5.5
1	A	52	GLN	HG2	0.93	1.01 – 3.62	-5.3
1	A	77	THR	CG2	15.78	16.06 – 27.03	-5.2
1	A	83	ILE	HG21	-0.61	-0.56 – 2.11	-5.2
1	A	83	ILE	HG22	-0.61	-0.56 – 2.11	-5.2
1	A	83	ILE	HG23	-0.61	-0.56 – 2.11	-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:



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	4005
Intra-residue (|i-j|=0)	1476
Sequential (|i-j|=1)	1117
Medium range (|i-j|>1 and |i-j|<5)	592
Long range (|i-j|≥5)	820
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	15.9
Number of long range restraints per residue[1]	3.3

[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)	4.0	0.2
0.2-0.5 (Medium)	9.1	0.5
>0.5 (Large)	2.8	1.69

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

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

9 Distance violation analysis (i)

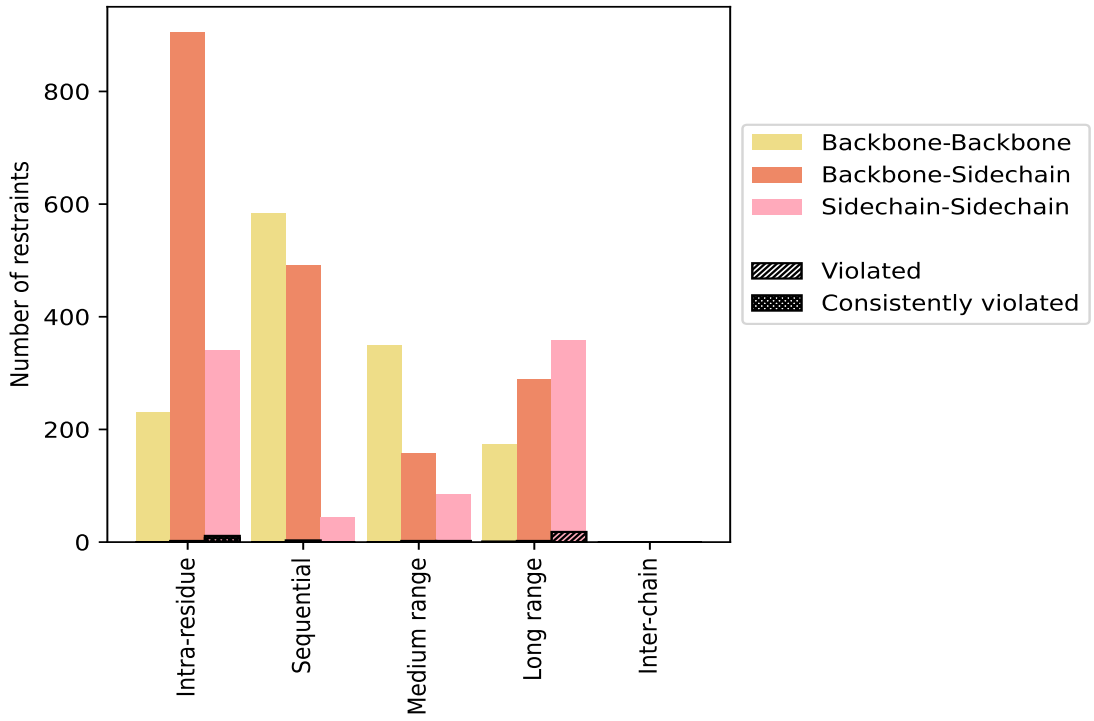
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	1476	36.9	13	0.9	0.3	7	0.5	0.2
Backbone-Backbone	230	5.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	905	22.6	2	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	341	8.5	11	3.2	0.3	7	2.1	0.2
Sequential (|i-j|=1)	1117	27.9	3	0.3	0.1	0	0.0	0.0
Backbone-Backbone	583	14.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	491	12.3	3	0.6	0.1	0	0.0	0.0
Sidechain-Sidechain	43	1.1	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	592	14.8	4	0.7	0.1	1	0.2	0.0
Backbone-Backbone	350	8.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	158	3.9	2	1.3	0.0	0	0.0	0.0
Sidechain-Sidechain	84	2.1	2	2.4	0.0	1	1.2	0.0
Long range (|i-j|≥5)	820	20.5	21	2.6	0.5	0	0.0	0.0
Backbone-Backbone	174	4.3	1	0.6	0.0	0	0.0	0.0
Backbone-Sidechain	288	7.2	2	0.7	0.0	0	0.0	0.0
Sidechain-Sidechain	358	8.9	18	5.0	0.4	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4005	100.0	41	1.0	1.0	8	0.2	0.2
Backbone-Backbone	1337	33.4	1	0.1	0.0	0	0.0	0.0
Backbone-Sidechain	1842	46.0	9	0.5	0.2	0	0.0	0.0
Sidechain-Sidechain	826	20.6	31	3.8	0.8	8	1.0	0.2

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	9	1	2	5	0	17	0.36	1.46	0.31	0.27
2	7	1	2	3	0	13	0.47	1.52	0.44	0.27
3	7	2	2	5	0	16	0.37	1.34	0.29	0.28
4	7	1	2	2	0	12	0.46	1.49	0.38	0.28
5	7	1	2	4	0	14	0.48	1.48	0.36	0.29
6	8	2	1	3	0	14	0.38	1.41	0.32	0.28
7	8	1	3	4	0	16	0.47	1.42	0.38	0.27
8	7	2	1	3	0	13	0.43	1.49	0.34	0.28
9	7	1	2	5	0	15	0.43	1.57	0.44	0.27
10	7	1	1	3	0	12	0.51	1.66	0.51	0.26
11	10	1	1	6	0	18	0.34	1.69	0.36	0.26

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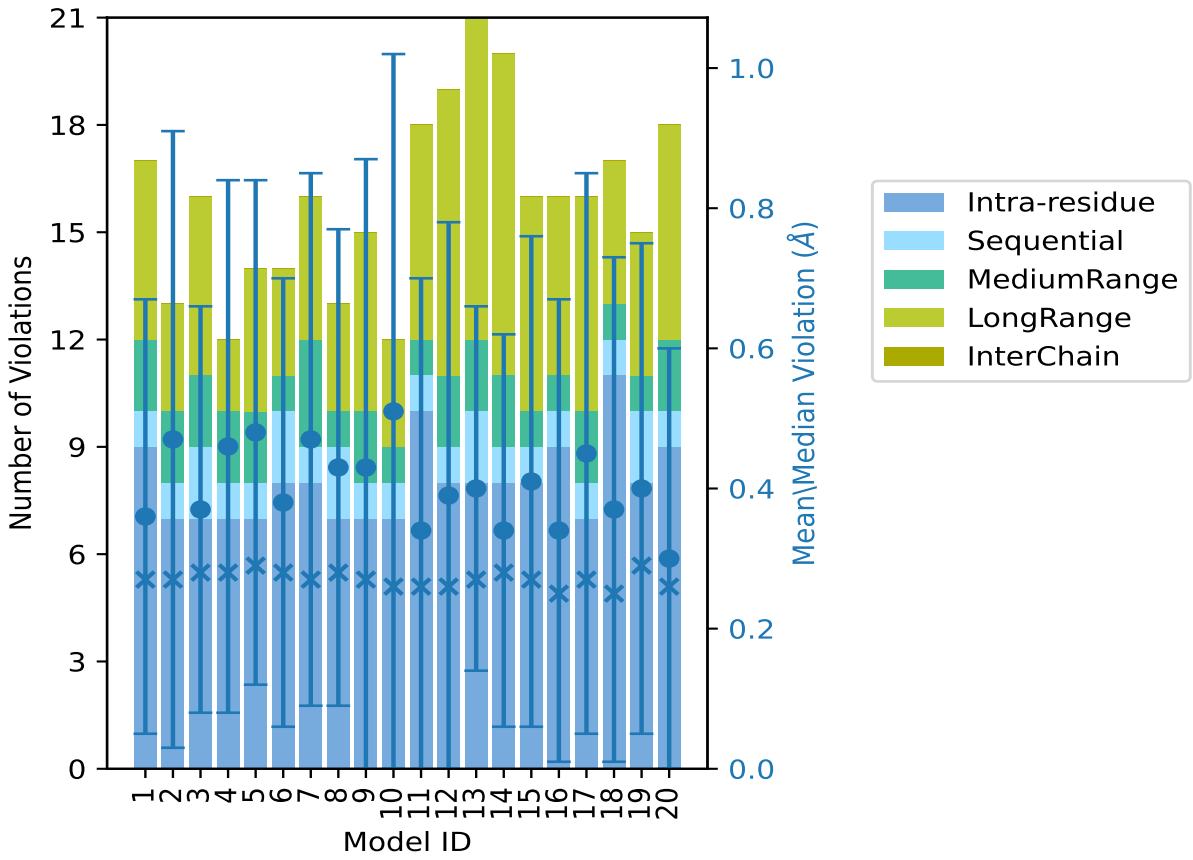
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	8	1	2	8	0	19	0.39	1.49	0.39	0.26
13	8	2	2	9	0	21	0.4	1.22	0.26	0.27
14	8	1	2	9	0	20	0.34	1.44	0.28	0.28
15	8	1	1	6	0	16	0.41	1.43	0.35	0.27
16	9	1	1	5	0	16	0.34	1.35	0.33	0.25
17	7	1	2	6	0	16	0.45	1.41	0.4	0.27
18	11	1	1	4	0	17	0.37	1.38	0.36	0.25
19	8	2	1	4	0	15	0.4	1.64	0.35	0.29
20	9	1	2	6	0	18	0.3	1.46	0.3	0.26

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

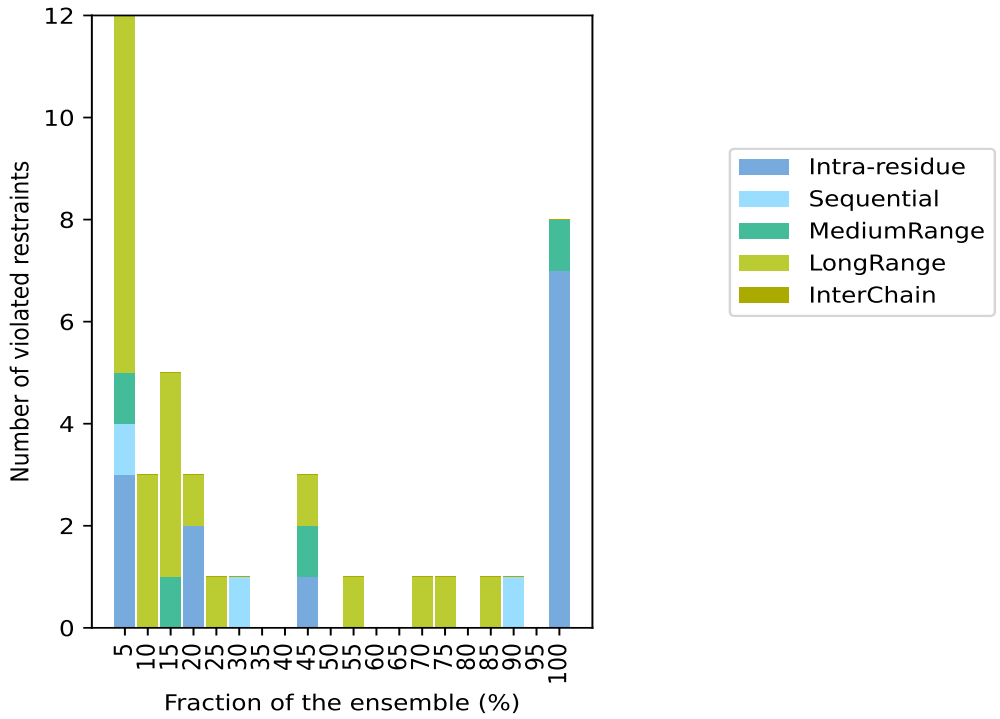
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3964(IR:1463, SQ:1114, MR:588, LR:799, IC:0) restraints are not violated in the ensemble.

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

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

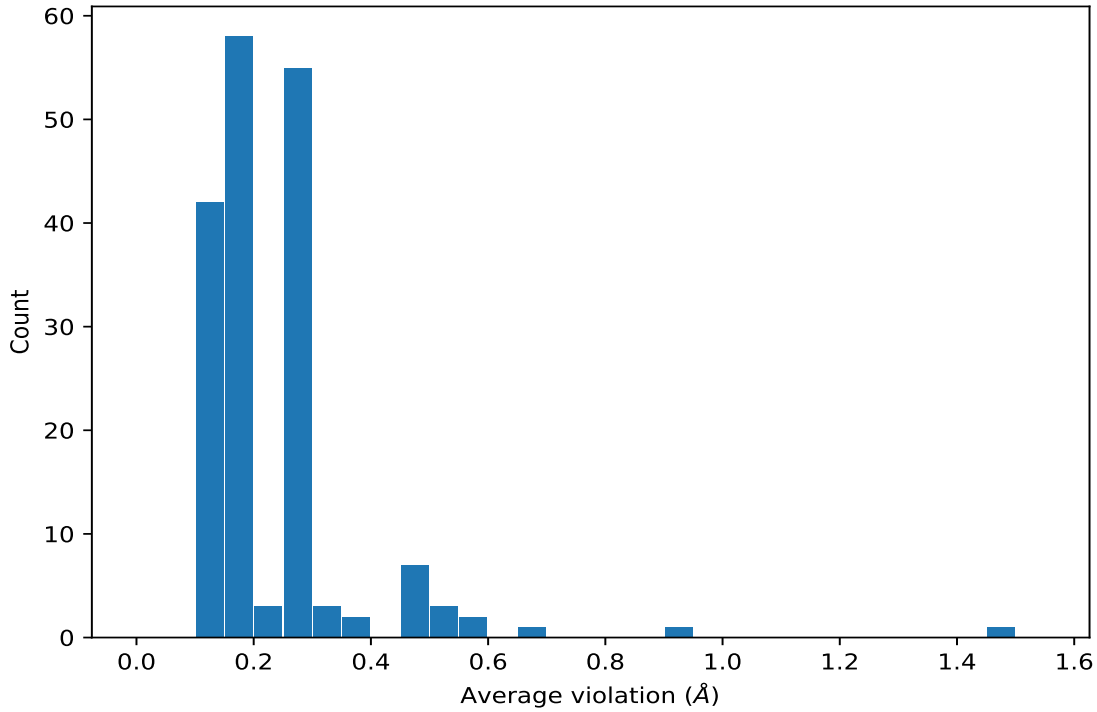
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	20	1.46	0.11	1.45
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	20	0.49	0.0	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	20	0.49	0.0	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	20	0.49	0.0	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	20	0.49	0.0	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	20	0.49	0.0	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	20	0.49	0.0	0.49
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	20	0.28	0.01	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	20	0.28	0.01	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	20	0.28	0.01	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	20	0.28	0.01	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	20	0.28	0.01	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	20	0.28	0.01	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	20	0.28	0.01	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	20	0.28	0.01	0.28
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	20	0.27	0.01	0.27

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	20	0.27	0.01	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	20	0.27	0.01	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	20	0.27	0.01	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	20	0.27	0.01	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	20	0.27	0.01	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	20	0.27	0.01	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	20	0.27	0.01	0.27
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	20	0.27	0.02	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	20	0.27	0.02	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	20	0.27	0.02	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	20	0.27	0.02	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	20	0.27	0.02	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	20	0.27	0.02	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	20	0.27	0.02	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	20	0.27	0.02	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	20	0.27	0.01	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	20	0.27	0.01	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	20	0.27	0.01	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	20	0.27	0.01	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	20	0.27	0.01	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	20	0.27	0.01	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	20	0.27	0.01	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	20	0.27	0.01	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	20	0.27	0.01	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	20	0.27	0.01	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	20	0.27	0.01	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	20	0.27	0.01	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	20	0.27	0.01	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	20	0.27	0.01	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	20	0.27	0.01	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	20	0.27	0.01	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	20	0.26	0.01	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	20	0.26	0.01	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	20	0.26	0.01	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	20	0.26	0.01	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	20	0.26	0.01	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	20	0.26	0.01	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	20	0.26	0.01	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	20	0.26	0.01	0.26
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	18	0.37	0.16	0.36
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	17	0.92	0.47	0.96
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	15	0.37	0.25	0.25

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	14	0.19	0.04	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	14	0.19	0.04	0.2
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD11	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD12	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD13	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD11	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD12	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD13	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD11	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD12	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD13	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD11	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD12	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD13	11	0.16	0.03	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD11	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD12	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD13	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD11	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD12	11	0.16	0.03	0.14
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD13	11	0.16	0.03	0.14
(1,2629)	1:A:239:LEU:HB2	1:A:241:ASP:H	9	0.53	0.23	0.6
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG12	9	0.16	0.03	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG13	9	0.16	0.03	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG21	9	0.16	0.03	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG22	9	0.16	0.03	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG23	9	0.16	0.03	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG12	9	0.16	0.03	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG13	9	0.16	0.03	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG21	9	0.16	0.03	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG22	9	0.16	0.03	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG23	9	0.16	0.03	0.16
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG12	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG13	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG21	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG22	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG23	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG12	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG13	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG21	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG22	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG23	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG12	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG13	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG21	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG22	9	0.15	0.04	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG23	9	0.15	0.04	0.14
(1,2575)	1:A:246:ASP:HB3	1:A:247:GLU:H	6	0.68	0.09	0.7
(1,3797)	1:A:140:ILE:HD11	1:A:160:GLN:HG2	5	0.24	0.15	0.17
(1,3797)	1:A:140:ILE:HD12	1:A:160:GLN:HG2	5	0.24	0.15	0.17
(1,3797)	1:A:140:ILE:HD13	1:A:160:GLN:HG2	5	0.24	0.15	0.17
(1,3295)	1:A:72:ILE:HG12	1:A:78:ASP:HB3	4	0.29	0.06	0.3
(1,3295)	1:A:72:ILE:HG13	1:A:78:ASP:HB3	4	0.29	0.06	0.3
(1,1047)	1:A:75:PHE:HB3	1:A:75:PHE:H	4	0.13	0.01	0.13
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG12	4	0.12	0.01	0.12
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG13	4	0.12	0.01	0.12
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG21	4	0.12	0.01	0.12

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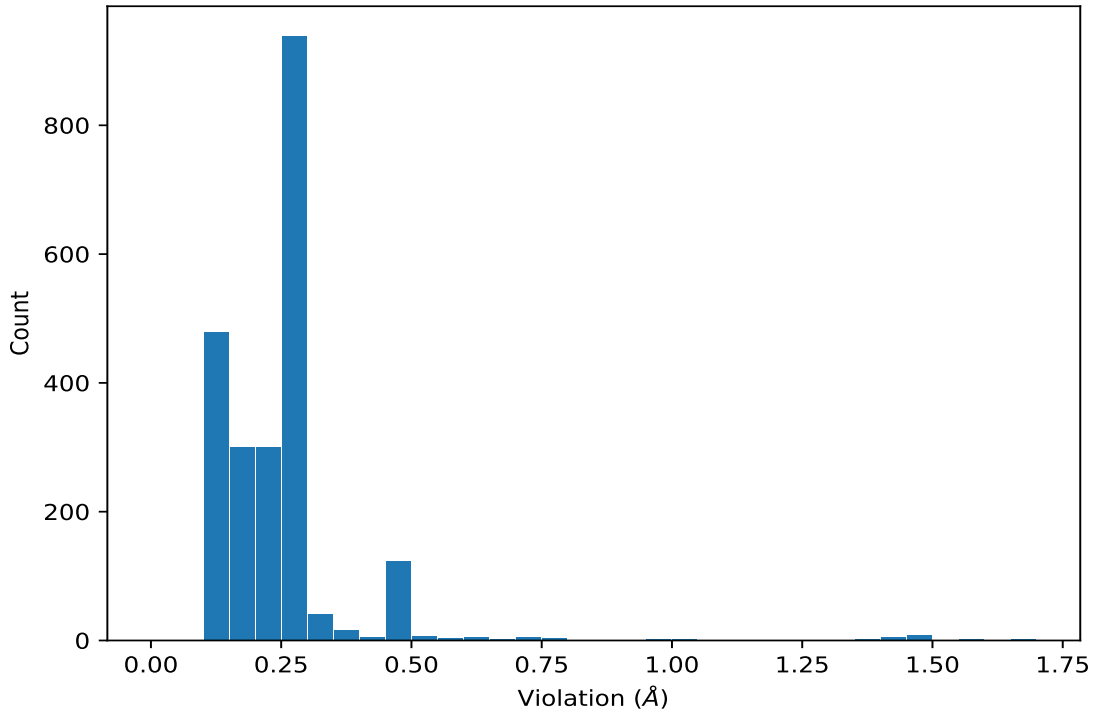
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG22	4	0.12	0.01	0.12
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG23	4	0.12	0.01	0.12
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG12	4	0.12	0.01	0.12
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG13	4	0.12	0.01	0.12
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG21	4	0.12	0.01	0.12
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG22	4	0.12	0.01	0.12
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG23	4	0.12	0.01	0.12
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG12	4	0.12	0.01	0.12
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG13	4	0.12	0.01	0.12
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG21	4	0.12	0.01	0.12
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG22	4	0.12	0.01	0.12
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG23	4	0.12	0.01	0.12
(1,3838)	1:A:226:LYS:HG2	1:A:231:LYS:HB2	3	0.51	0.19	0.55
(1,3838)	1:A:226:LYS:HG3	1:A:231:LYS:HB2	3	0.51	0.19	0.55
(1,2936)	1:A:67:LYS:HB3	1:A:70:ASP:H	3	0.47	0.41	0.22
(1,3261)	1:A:55:SER:HB3	1:A:65:VAL:HG21	3	0.33	0.06	0.31
(1,3261)	1:A:55:SER:HB3	1:A:65:VAL:HG22	3	0.33	0.06	0.31
(1,3261)	1:A:55:SER:HB3	1:A:65:VAL:HG23	3	0.33	0.06	0.31
(1,3320)	1:A:85:LYS:HE2	1:A:47:LEU:HD21	3	0.13	0.01	0.13
(1,3320)	1:A:85:LYS:HE2	1:A:47:LEU:HD22	3	0.13	0.01	0.13
(1,3320)	1:A:85:LYS:HE2	1:A:47:LEU:HD23	3	0.13	0.01	0.13
(1,3320)	1:A:85:LYS:HE3	1:A:47:LEU:HD21	3	0.13	0.01	0.13
(1,3320)	1:A:85:LYS:HE3	1:A:47:LEU:HD22	3	0.13	0.01	0.13
(1,3320)	1:A:85:LYS:HE3	1:A:47:LEU:HD23	3	0.13	0.01	0.13
(1,3990)	1:A:211:LEU:HA	1:A:174:LEU:HA	3	0.11	0.0	0.11
(1,3837)	1:A:226:LYS:HE2	1:A:231:LYS:HB2	2	0.56	0.19	0.56
(1,3837)	1:A:226:LYS:HE3	1:A:231:LYS:HB2	2	0.56	0.19	0.56
(1,3798)	1:A:140:ILE:HG12	1:A:160:GLN:HG2	2	0.28	0.08	0.28
(1,3798)	1:A:140:ILE:HG13	1:A:160:GLN:HG2	2	0.28	0.08	0.28
(1,3798)	1:A:140:ILE:HG21	1:A:160:GLN:HG2	2	0.28	0.08	0.28
(1,3798)	1:A:140:ILE:HG22	1:A:160:GLN:HG2	2	0.28	0.08	0.28
(1,3798)	1:A:140:ILE:HG23	1:A:160:GLN:HG2	2	0.28	0.08	0.28
(1,3806)	1:A:201:ASP:HB2	1:A:207:GLU:HG2	2	0.11	0.0	0.11
(1,3806)	1:A:201:ASP:HB2	1:A:207:GLU:HG3	2	0.11	0.0	0.11
(1,3806)	1:A:201:ASP:HB3	1:A:207:GLU:HG2	2	0.11	0.0	0.11
(1,3806)	1:A:201:ASP:HB3	1:A:207:GLU:HG3	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)
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	11	1.69
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	10	1.66
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	19	1.64
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	10	1.58
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	9	1.57
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	2	1.52
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	12	1.49
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	4	1.49
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	8	1.49
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	9	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	5	1.48
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	2	1.47
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	1	1.46
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	20	1.46
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	14	1.44
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	15	1.43
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	7	1.42
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	6	1.41
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	17	1.41
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	17	1.4
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	18	1.38
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	12	1.36
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	16	1.35
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	3	1.34
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	18	1.26
(1,2714)	1:A:57:PHE:HZ	1:A:55:SER:HB3	13	1.22
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	15	1.16
(1,2936)	1:A:67:LYS:HB3	1:A:70:ASP:H	7	1.04
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	7	1.01
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	16	0.99
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	4	0.96
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	5	0.95
(1,2629)	1:A:239:LEU:HB2	1:A:241:ASP:H	17	0.9
(1,2575)	1:A:246:ASP:HB3	1:A:247:GLU:H	7	0.79
(1,3837)	1:A:226:LYS:HE2	1:A:231:LYS:HB2	13	0.75
(1,3837)	1:A:226:LYS:HE3	1:A:231:LYS:HB2	13	0.75
(1,2575)	1:A:246:ASP:HB3	1:A:247:GLU:H	5	0.75
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	5	0.73
(1,2575)	1:A:246:ASP:HB3	1:A:247:GLU:H	6	0.73
(1,3838)	1:A:226:LYS:HG2	1:A:231:LYS:HB2	13	0.71
(1,3838)	1:A:226:LYS:HG3	1:A:231:LYS:HB2	13	0.71
(1,2629)	1:A:239:LEU:HB2	1:A:241:ASP:H	12	0.71
(1,2629)	1:A:239:LEU:HB2	1:A:241:ASP:H	13	0.66
(1,2575)	1:A:246:ASP:HB3	1:A:247:GLU:H	3	0.66
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	19	0.65
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	11	0.64
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	8	0.62
(1,2629)	1:A:239:LEU:HB2	1:A:241:ASP:H	4	0.62
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	10	0.62
(1,2575)	1:A:246:ASP:HB3	1:A:247:GLU:H	8	0.61
(1,2629)	1:A:239:LEU:HB2	1:A:241:ASP:H	1	0.6
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	14	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	3	0.56
(1,3838)	1:A:226:LYS:HG2	1:A:231:LYS:HB2	14	0.55
(1,3838)	1:A:226:LYS:HG3	1:A:231:LYS:HB2	14	0.55
(1,3797)	1:A:140:ILE:HD11	1:A:160:GLN:HG2	13	0.54
(1,3797)	1:A:140:ILE:HD12	1:A:160:GLN:HG2	13	0.54
(1,3797)	1:A:140:ILE:HD13	1:A:160:GLN:HG2	13	0.54
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	1	0.54
(1,2629)	1:A:239:LEU:HB2	1:A:241:ASP:H	7	0.52
(1,2575)	1:A:246:ASP:HB3	1:A:247:GLU:H	13	0.52
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	11	0.5
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	1	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	1	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	1	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	1	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	1	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	1	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	2	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	2	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	2	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	2	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	2	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	2	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	3	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	3	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	3	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	3	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	3	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	3	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	4	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	4	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	4	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	4	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	4	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	4	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	5	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	5	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	5	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	5	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	5	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	5	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	6	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	6	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	6	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	6	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	6	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	7	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	7	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	7	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	7	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	7	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	7	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	8	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	8	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	8	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	8	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	8	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	8	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	9	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	9	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	9	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	9	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	9	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	9	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	10	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	10	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	10	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	10	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	10	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	10	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	11	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	11	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	11	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	11	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	11	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	11	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	12	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	12	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	12	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	12	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	12	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	12	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	13	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	13	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	13	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	13	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	13	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	13	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	14	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	14	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	14	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	14	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	14	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	14	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	15	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	15	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	15	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	15	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	15	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	15	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	16	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	16	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	16	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	16	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	16	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	16	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	17	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	17	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	17	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	17	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	17	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	17	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	18	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	18	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	18	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	18	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	18	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	18	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	19	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	19	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	19	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	19	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	19	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	19	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG22	20	0.49
(1,375)	1:A:150:THR:HG21	1:A:150:THR:HG23	20	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG21	20	0.49
(1,375)	1:A:150:THR:HG22	1:A:150:THR:HG23	20	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG21	20	0.49
(1,375)	1:A:150:THR:HG23	1:A:150:THR:HG22	20	0.49
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	18	0.49
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	12	0.48
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	15	0.47
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	13	0.42
(1,3261)	1:A:55:SER:HB3	1:A:65:VAL:HG21	9	0.41
(1,3261)	1:A:55:SER:HB3	1:A:65:VAL:HG22	9	0.41
(1,3261)	1:A:55:SER:HB3	1:A:65:VAL:HG23	9	0.41
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	8	0.41
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	19	0.4
(1,2629)	1:A:239:LEU:HB2	1:A:241:ASP:H	14	0.38
(1,3837)	1:A:226:LYS:HE2	1:A:231:LYS:HB2	1	0.37
(1,3837)	1:A:226:LYS:HE3	1:A:231:LYS:HB2	1	0.37
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	20	0.37
(1,3798)	1:A:140:ILE:HG12	1:A:160:GLN:HG2	15	0.36
(1,3798)	1:A:140:ILE:HG13	1:A:160:GLN:HG2	15	0.36
(1,3798)	1:A:140:ILE:HG21	1:A:160:GLN:HG2	15	0.36
(1,3798)	1:A:140:ILE:HG22	1:A:160:GLN:HG2	15	0.36
(1,3798)	1:A:140:ILE:HG23	1:A:160:GLN:HG2	15	0.36
(1,3295)	1:A:72:ILE:HG12	1:A:78:ASP:HB3	14	0.36
(1,3295)	1:A:72:ILE:HG13	1:A:78:ASP:HB3	14	0.36
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	19	0.36
(1,3853)	1:A:142:TYR:HD1	1:A:160:GLN:HG2	15	0.35
(1,3853)	1:A:142:TYR:HD2	1:A:160:GLN:HG2	15	0.35
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	2	0.35
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	9	0.35
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	1	0.34
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	6	0.34
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	14	0.33
(1,3295)	1:A:72:ILE:HG12	1:A:78:ASP:HB3	3	0.33
(1,3295)	1:A:72:ILE:HG13	1:A:78:ASP:HB3	3	0.33
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	3	0.31
(1,3261)	1:A:55:SER:HB3	1:A:65:VAL:HG21	19	0.31
(1,3261)	1:A:55:SER:HB3	1:A:65:VAL:HG22	19	0.31
(1,3261)	1:A:55:SER:HB3	1:A:65:VAL:HG23	19	0.31
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	9	0.31
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	9	0.31
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	9	0.31
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	9	0.31
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	9	0.31
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	9	0.31
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	9	0.31
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	5	0.3
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	5	0.3
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	5	0.3
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	5	0.3
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	5	0.3
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	5	0.3
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	5	0.3
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	5	0.3
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	16	0.3
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	16	0.3
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	16	0.3
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	16	0.3
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	16	0.3
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	16	0.3
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	16	0.3
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	16	0.3
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	17	0.3
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	17	0.3
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	17	0.3
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	17	0.3
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	17	0.3
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	17	0.3
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	17	0.3
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	17	0.3
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	11	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	11	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	11	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	11	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	11	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	11	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	11	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	11	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	17	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	17	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	17	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	17	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	17	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	17	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	17	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	19	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	19	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	19	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	19	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	19	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	19	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	19	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	19	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	20	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	20	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	20	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	20	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	20	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	20	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	20	0.29
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	20	0.29
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	6	0.29
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	6	0.29
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	6	0.29
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	6	0.29
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	6	0.29
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	6	0.29
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	6	0.29
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	6	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	4	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	4	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	4	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	4	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	4	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	4	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	4	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	4	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	7	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	7	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	7	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	7	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	7	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	7	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	7	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	13	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	13	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	13	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	13	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	13	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	13	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	13	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	13	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	19	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	19	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	19	0.29
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	19	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	19	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	19	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	19	0.29
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	19	0.29
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	2	0.29
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	2	0.29
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	2	0.29
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	2	0.29
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	2	0.29
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	2	0.29
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	2	0.29
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	2	0.29
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	5	0.29
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	5	0.29
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	5	0.29
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	5	0.29
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	5	0.29
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	5	0.29
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	5	0.29
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	5	0.29
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	8	0.29
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	8	0.29
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	8	0.29
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	8	0.29
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	8	0.29
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	8	0.29
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	8	0.29
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	8	0.29
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	9	0.29
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	9	0.29
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	9	0.29
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	9	0.29
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	9	0.29
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	9	0.29
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	9	0.29
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	12	0.29
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	12	0.29
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	12	0.29
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	12	0.29
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	12	0.29
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	12	0.29
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	12	0.29
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	12	0.29
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	13	0.29
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	13	0.29
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	13	0.29
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	13	0.29
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	13	0.29
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	13	0.29
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	13	0.29
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	13	0.29
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	5	0.29
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	5	0.29
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	5	0.29
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	5	0.29
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	5	0.29
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	5	0.29
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	5	0.29
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	5	0.29
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	20	0.29
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	20	0.29
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	20	0.29
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	20	0.29
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	20	0.29
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	20	0.29
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	20	0.29
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	20	0.29
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	2	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	2	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	2	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	2	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	2	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	2	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	2	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	4	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	4	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	4	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	4	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	4	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	4	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	4	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	4	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	8	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	8	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	8	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	8	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	8	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	8	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	8	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	8	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	12	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	12	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	12	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	12	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	12	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	12	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	12	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	12	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	15	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	15	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	15	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	15	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	15	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	15	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	15	0.28
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	15	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	3	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	3	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	3	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	3	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	3	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	3	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	3	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	11	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	11	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	11	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	11	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	11	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	11	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	11	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	11	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	12	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	12	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	12	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	12	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	12	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	12	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	12	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	12	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	14	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	14	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	14	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	14	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	14	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	14	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	14	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	14	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	16	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	16	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	16	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	16	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	16	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	16	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	16	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	16	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	20	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	20	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	20	0.28
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	20	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	20	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	20	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	20	0.28
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	3	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	3	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	3	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	3	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	3	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	3	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	3	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	3	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	5	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	5	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	5	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	5	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	5	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	5	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	5	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	5	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	6	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	6	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	6	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	6	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	6	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	6	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	6	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	6	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	8	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	8	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	8	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	8	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	8	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	8	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	8	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	8	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	10	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	10	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	10	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	10	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	10	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	10	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	10	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	10	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	14	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	14	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	14	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	14	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	14	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	14	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	14	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	20	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	20	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	20	0.28
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	20	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	20	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	20	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	20	0.28
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	20	0.28
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	6	0.28
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	6	0.28
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	6	0.28
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	6	0.28
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	6	0.28
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	6	0.28
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	6	0.28
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	6	0.28
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	14	0.28
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	14	0.28
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	14	0.28
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	14	0.28
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	14	0.28
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	14	0.28
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	14	0.28
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	14	0.28
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	6	0.28
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	6	0.28
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	6	0.28
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	6	0.28
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	6	0.28
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	6	0.28
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	6	0.28
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	6	0.28
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	11	0.28
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	11	0.28
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	11	0.28
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	11	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	11	0.28
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	11	0.28
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	11	0.28
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	11	0.28
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	14	0.28
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	14	0.28
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	14	0.28
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	14	0.28
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	14	0.28
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	14	0.28
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	14	0.28
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	14	0.28
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	11	0.28
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	11	0.28
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	11	0.28
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	11	0.28
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	11	0.28
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	11	0.28
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	11	0.28
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	11	0.28
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	1	0.27
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	1	0.27
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	1	0.27
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	1	0.27
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	1	0.27
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	1	0.27
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	1	0.27
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	1	0.27
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	14	0.27
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	14	0.27
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	14	0.27
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	14	0.27
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	14	0.27
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	14	0.27
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	14	0.27
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	14	0.27
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	17	0.27
(1,3295)	1:A:72:ILE:HG12	1:A:78:ASP:HB3	17	0.27
(1,3295)	1:A:72:ILE:HG13	1:A:78:ASP:HB3	17	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	1	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	1	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	1	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	1	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	1	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	1	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	1	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	2	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	2	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	2	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	2	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	2	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	2	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	2	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	2	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	5	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	5	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	5	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	5	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	5	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	5	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	5	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	5	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	7	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	7	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	7	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	7	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	7	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	7	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	7	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	7	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	8	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	8	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	8	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	8	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	8	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	8	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	8	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	8	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	9	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	9	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	9	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	9	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	9	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	9	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	9	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	13	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	13	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	13	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	13	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	13	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	13	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	13	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	13	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	19	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	19	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	19	0.27
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	19	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	19	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	19	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	19	0.27
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	19	0.27
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	1	0.27
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	1	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	1	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	1	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	1	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	1	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	1	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	1	0.27
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	3	0.27
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	3	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	3	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	3	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	3	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	3	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	3	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	3	0.27
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	4	0.27
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	4	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	4	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	4	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	4	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	4	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	4	0.27
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	7	0.27
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	7	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	7	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	7	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	7	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	7	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	7	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	7	0.27
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	11	0.27
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	11	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	11	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	11	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	11	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	11	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	11	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	11	0.27
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	15	0.27
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	15	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	15	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	15	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	15	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	15	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	15	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	15	0.27
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	18	0.27
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	18	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	18	0.27
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	18	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	18	0.27
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	18	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	18	0.27
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	18	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	1	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	1	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	1	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	1	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	1	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	1	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	1	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	1	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	9	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	9	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	9	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	9	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	9	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	9	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	9	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	16	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	16	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	16	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	16	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	16	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	16	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	16	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	16	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	18	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	18	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	18	0.27
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	18	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	18	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	18	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	18	0.27
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	18	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	1	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	1	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	1	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	1	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	1	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	1	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	1	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	1	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	4	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	4	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	4	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	4	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	4	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	4	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	4	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	4	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	6	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	6	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	6	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	6	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	6	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	6	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	6	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	10	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	10	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	10	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	10	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	10	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	10	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	10	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	10	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	12	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	12	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	12	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	12	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	12	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	12	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	12	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	12	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	14	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	14	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	14	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	14	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	14	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	14	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	14	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	14	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	15	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	15	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	15	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	15	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	15	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	15	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	15	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	15	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	17	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	17	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	17	0.27
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	17	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	17	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	17	0.27
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	17	0.27
(1,3838)	1:A:226:LYS:HG2	1:A:231:LYS:HB2	12	0.26
(1,3838)	1:A:226:LYS:HG3	1:A:231:LYS:HB2	12	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	3	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	3	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	3	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	3	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	3	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	3	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	3	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	3	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	6	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	6	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	6	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	6	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	6	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	6	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	6	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	6	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	7	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	7	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	7	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	7	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	7	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	7	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	7	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	7	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	9	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	9	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	9	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	9	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	9	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	9	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	9	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	9	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	10	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	10	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	10	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	10	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	10	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	10	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	10	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	13	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	13	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	13	0.26
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	13	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	13	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	13	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	13	0.26
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	13	0.26
(1,3261)	1:A:55:SER:HB3	1:A:65:VAL:HG21	13	0.26
(1,3261)	1:A:55:SER:HB3	1:A:65:VAL:HG22	13	0.26
(1,3261)	1:A:55:SER:HB3	1:A:65:VAL:HG23	13	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	4	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	4	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	4	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	4	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	4	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	4	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	4	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	4	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	10	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	10	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	10	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	10	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	10	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	10	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	10	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	10	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	15	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	15	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	15	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	15	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	15	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	15	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	15	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	15	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	17	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	17	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	17	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	17	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	17	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	17	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	17	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG13	18	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG21	18	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG22	18	0.26
(1,314)	1:A:87:ILE:HG12	1:A:87:ILE:HG23	18	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG12	18	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG21	18	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG22	18	0.26
(1,314)	1:A:87:ILE:HG13	1:A:87:ILE:HG23	18	0.26
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	12	0.26
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	12	0.26
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	12	0.26
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	12	0.26
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	12	0.26
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	12	0.26
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	12	0.26
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	12	0.26
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	10	0.26
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	10	0.26
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	10	0.26
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	10	0.26
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	10	0.26
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	10	0.26
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	10	0.26
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	10	0.26
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	16	0.26
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	16	0.26
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	16	0.26
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	16	0.26
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	16	0.26
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	16	0.26
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	16	0.26
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	16	0.26
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	17	0.26
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	17	0.26
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	17	0.26
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	17	0.26
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	17	0.26
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	17	0.26
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	17	0.26
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	19	0.26
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	19	0.26
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	19	0.26
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	19	0.26
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	19	0.26
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	19	0.26
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	19	0.26
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	19	0.26
(1,18)	1:A:111:ILE:HG12	1:A:111:ILE:HG13	20	0.26
(1,18)	1:A:111:ILE:HG13	1:A:111:ILE:HG12	20	0.26
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG12	20	0.26
(1,18)	1:A:111:ILE:HG21	1:A:111:ILE:HG13	20	0.26
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG12	20	0.26
(1,18)	1:A:111:ILE:HG22	1:A:111:ILE:HG13	20	0.26
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG12	20	0.26
(1,18)	1:A:111:ILE:HG23	1:A:111:ILE:HG13	20	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	2	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	2	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	2	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	2	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	2	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	2	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	2	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	2	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	3	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	3	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	3	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	3	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	3	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	3	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	3	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	3	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	4	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	4	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	4	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	4	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	4	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	4	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	4	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	7	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	7	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	7	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	7	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	7	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	7	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	7	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	7	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	8	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	8	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	8	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	8	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	8	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	8	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	8	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	8	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	10	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	10	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	10	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	10	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	10	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	10	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	10	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	10	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	12	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	12	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	12	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	12	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	12	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	12	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	12	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	12	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	15	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	15	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	15	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	15	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	15	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	15	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	15	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	15	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	17	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	17	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	17	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	17	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	17	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	17	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	17	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	19	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	19	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	19	0.26
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	19	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	19	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	19	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	19	0.26
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	19	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	2	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	2	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	2	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	2	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	2	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	2	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	2	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	2	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	3	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	3	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	3	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	3	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	3	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	3	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	3	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	3	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	5	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	5	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	5	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	5	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	5	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	5	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	5	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	5	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	7	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	7	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	7	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	7	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	7	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	7	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	7	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	8	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	8	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	8	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	8	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	8	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	8	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	8	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	8	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	9	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	9	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	9	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	9	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	9	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	9	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	9	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	9	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	13	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	13	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	13	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	13	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	13	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	13	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	13	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	13	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	18	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	18	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	18	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	18	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	18	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	18	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	18	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	18	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	19	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	19	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	19	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	19	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	19	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	19	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	19	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	20	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	20	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	20	0.26
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	20	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	20	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	20	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	20	0.26
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	20	0.26
(1,3856)	1:A:142:TYR:HA	1:A:137:MET:HG2	20	0.25
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG13	18	0.25
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG21	18	0.25
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG22	18	0.25
(1,367)	1:A:133:ILE:HG12	1:A:133:ILE:HG23	18	0.25
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG12	18	0.25
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG21	18	0.25
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG22	18	0.25
(1,367)	1:A:133:ILE:HG13	1:A:133:ILE:HG23	18	0.25
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	15	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	1	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	1	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	1	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	1	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	1	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	1	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	1	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	1	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	2	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	2	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	2	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	2	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	2	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	2	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	2	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	2	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	11	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	11	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	11	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	11	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	11	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	11	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	11	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	15	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	15	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	15	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	15	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	15	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	15	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	15	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	15	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	16	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	16	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	16	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	16	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	16	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	16	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	16	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	16	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG13	18	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG21	18	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG22	18	0.25
(1,225)	1:A:29:ILE:HG12	1:A:29:ILE:HG23	18	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG12	18	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG21	18	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG22	18	0.25
(1,225)	1:A:29:ILE:HG13	1:A:29:ILE:HG23	18	0.25
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG13	13	0.25
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG21	13	0.25
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG22	13	0.25
(1,156)	1:A:3:ILE:HG12	1:A:3:ILE:HG23	13	0.25
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG12	13	0.25
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG21	13	0.25
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG22	13	0.25
(1,156)	1:A:3:ILE:HG13	1:A:3:ILE:HG23	13	0.25
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG13	16	0.25
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG21	16	0.25
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG22	16	0.25
(1,1096)	1:A:83:ILE:HG12	1:A:83:ILE:HG23	16	0.25
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG12	16	0.25
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG21	16	0.25
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG22	16	0.25
(1,1096)	1:A:83:ILE:HG13	1:A:83:ILE:HG23	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	11	0.24
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	11	0.24
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	11	0.24
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	11	0.24
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	11	0.24
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	11	0.24
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	11	0.24
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	11	0.24
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	11	0.24
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	11	0.24
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	11	0.24
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	11	0.24
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	11	0.24
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	11	0.24
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	11	0.24
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	11	0.24
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	11	0.24
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	11	0.24
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	11	0.24
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	11	0.24
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	11	0.24
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	11	0.24
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	11	0.24
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	11	0.24
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	11	0.24
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	11	0.24
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	11	0.24
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	11	0.24
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	11	0.24
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	11	0.24
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	17	0.24
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	17	0.24
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	17	0.24
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	17	0.24
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	17	0.24
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	17	0.24
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	17	0.24
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	17	0.24
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	17	0.24
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	17	0.24
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	17	0.24
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	17	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	17	0.24
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	17	0.24
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	17	0.24
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	17	0.24
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	17	0.24
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	17	0.24
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	17	0.24
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	17	0.24
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	17	0.24
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	17	0.24
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	17	0.24
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	17	0.24
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	17	0.24
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	17	0.24
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	17	0.24
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	17	0.24
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	17	0.24
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	17	0.24
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG12	20	0.23
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG13	20	0.23
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG21	20	0.23
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG22	20	0.23
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG23	20	0.23
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG12	20	0.23
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG13	20	0.23
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG21	20	0.23
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG22	20	0.23
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG23	20	0.23
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG12	20	0.23
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG13	20	0.23
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG21	20	0.23
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG22	20	0.23
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG23	20	0.23
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	8	0.23
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	14	0.22
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	14	0.22
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	14	0.22
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	14	0.22
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	14	0.22
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	14	0.22
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	14	0.22
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	14	0.22
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	14	0.22
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	14	0.22
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	14	0.22
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	14	0.22
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	14	0.22
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	14	0.22
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	14	0.22
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	14	0.22
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	14	0.22
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	14	0.22
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	14	0.22
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	14	0.22
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	14	0.22
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	14	0.22
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	14	0.22
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	14	0.22
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	14	0.22
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	14	0.22
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	14	0.22
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	14	0.22
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	14	0.22
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	20	0.22
(1,2936)	1:A:67:LYS:HB3	1:A:70:ASP:H	5	0.22
(1,2629)	1:A:239:LEU:HB2	1:A:241:ASP:H	2	0.22
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	13	0.22
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	7	0.21
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	7	0.21
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	7	0.21
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	7	0.21
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	7	0.21
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	7	0.21
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	7	0.21
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	7	0.21
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	7	0.21
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	7	0.21
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	7	0.21
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	7	0.21
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	7	0.21
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	7	0.21
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	7	0.21
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	7	0.21
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	7	0.21
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	7	0.21
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	7	0.21
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	7	0.21
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	7	0.21
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	7	0.21
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	7	0.21
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	7	0.21
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	7	0.21
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	7	0.21
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	7	0.21
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	7	0.21
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	7	0.21
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	13	0.21
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	13	0.21
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	13	0.21
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	13	0.21
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	13	0.21
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	13	0.21
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	13	0.21
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	13	0.21
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	13	0.21
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	13	0.21
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	13	0.21
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	13	0.21
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	13	0.21
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	13	0.21
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	13	0.21
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	13	0.21
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	13	0.21
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	13	0.21
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	13	0.21
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	13	0.21
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	13	0.21
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	13	0.21
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	13	0.21
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	13	0.21
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	13	0.21
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	13	0.21
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	13	0.21
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	13	0.21
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	13	0.21
(1,3798)	1:A:140:ILE:HG12	1:A:160:GLN:HG2	17	0.21
(1,3798)	1:A:140:ILE:HG13	1:A:160:GLN:HG2	17	0.21
(1,3798)	1:A:140:ILE:HG21	1:A:160:GLN:HG2	17	0.21
(1,3798)	1:A:140:ILE:HG22	1:A:160:GLN:HG2	17	0.21
(1,3798)	1:A:140:ILE:HG23	1:A:160:GLN:HG2	17	0.21
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD11	2	0.21
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD12	2	0.21
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD13	2	0.21
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD11	2	0.21
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD12	2	0.21
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD13	2	0.21
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD11	2	0.21
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD12	2	0.21
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD13	2	0.21
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD11	2	0.21
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD12	2	0.21
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD13	2	0.21
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD11	2	0.21
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD12	2	0.21
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD13	2	0.21
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD11	2	0.21
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD12	2	0.21
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD13	2	0.21
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG12	6	0.2
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG13	6	0.2
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG21	6	0.2
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG22	6	0.2
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG23	6	0.2
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG12	6	0.2
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG13	6	0.2
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG21	6	0.2
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG22	6	0.2
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG23	6	0.2
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG12	6	0.2
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG13	6	0.2
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG21	6	0.2
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG22	6	0.2
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG23	6	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	4	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	4	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	4	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	4	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	4	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	4	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	4	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	4	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	4	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	4	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	4	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	4	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	4	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	4	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	4	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	4	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	4	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	4	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	4	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	4	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	4	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	4	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	4	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	4	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	4	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	4	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	4	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	4	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	4	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	5	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	5	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	5	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	5	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	5	0.2
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	5	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	5	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	5	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	5	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	5	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	5	0.2
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	5	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	5	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	5	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	5	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	5	0.2
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	5	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	5	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	5	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	5	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	5	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	5	0.2
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	5	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	5	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	5	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	5	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	5	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	5	0.2
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	5	0.2
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	1	0.2
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG12	14	0.2
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG13	14	0.2
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG21	14	0.2
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG22	14	0.2
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG23	14	0.2
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG12	14	0.2
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG13	14	0.2
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG21	14	0.2
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG22	14	0.2
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG23	14	0.2
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD11	6	0.2
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD12	6	0.2
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD13	6	0.2
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD11	6	0.2
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD12	6	0.2
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD13	6	0.2
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD11	6	0.2
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD12	6	0.2
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD13	6	0.2
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD11	6	0.2
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD12	6	0.2
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD13	6	0.2
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD11	6	0.2
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD12	6	0.2
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD13	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD11	6	0.2
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD12	6	0.2
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD13	6	0.2
(1,3295)	1:A:72:ILE:HG12	1:A:78:ASP:HB3	5	0.2
(1,3295)	1:A:72:ILE:HG13	1:A:78:ASP:HB3	5	0.2
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	3	0.2
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	17	0.2
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG12	13	0.19
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG13	13	0.19
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG21	13	0.19
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG22	13	0.19
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG23	13	0.19
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG12	13	0.19
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG13	13	0.19
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG21	13	0.19
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG22	13	0.19
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG23	13	0.19
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG12	13	0.19
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG13	13	0.19
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG21	13	0.19
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG22	13	0.19
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG23	13	0.19
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	18	0.19
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	18	0.19
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	18	0.19
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	18	0.19
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	18	0.19
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	18	0.19
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	18	0.19
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	18	0.19
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	18	0.19
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	18	0.19
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	18	0.19
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	18	0.19
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	18	0.19
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	18	0.19
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	18	0.19
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	18	0.19
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	18	0.19
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	18	0.19
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	18	0.19
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	18	0.19
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	18	0.19
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	18	0.19
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	18	0.19
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	18	0.19
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	18	0.19
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	18	0.19
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	18	0.19
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	18	0.19
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	18	0.19
(1,3797)	1:A:140:ILE:HD11	1:A:160:GLN:HG2	17	0.19
(1,3797)	1:A:140:ILE:HD12	1:A:160:GLN:HG2	17	0.19
(1,3797)	1:A:140:ILE:HD13	1:A:160:GLN:HG2	17	0.19
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	2	0.19
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	6	0.19
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG12	13	0.19
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG13	13	0.19
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG21	13	0.19
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG22	13	0.19
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG23	13	0.19
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG12	13	0.19
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG13	13	0.19
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG21	13	0.19
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG22	13	0.19
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG23	13	0.19
(1,1095)	1:A:83:ILE:HD11	1:A:83:ILE:HG12	16	0.19
(1,1095)	1:A:83:ILE:HD11	1:A:83:ILE:HG13	16	0.19
(1,1095)	1:A:83:ILE:HD11	1:A:83:ILE:HG21	16	0.19
(1,1095)	1:A:83:ILE:HD11	1:A:83:ILE:HG22	16	0.19
(1,1095)	1:A:83:ILE:HD11	1:A:83:ILE:HG23	16	0.19
(1,1095)	1:A:83:ILE:HD12	1:A:83:ILE:HG12	16	0.19
(1,1095)	1:A:83:ILE:HD12	1:A:83:ILE:HG13	16	0.19
(1,1095)	1:A:83:ILE:HD12	1:A:83:ILE:HG21	16	0.19
(1,1095)	1:A:83:ILE:HD12	1:A:83:ILE:HG22	16	0.19
(1,1095)	1:A:83:ILE:HD12	1:A:83:ILE:HG23	16	0.19
(1,1095)	1:A:83:ILE:HD13	1:A:83:ILE:HG12	16	0.19
(1,1095)	1:A:83:ILE:HD13	1:A:83:ILE:HG13	16	0.19
(1,1095)	1:A:83:ILE:HD13	1:A:83:ILE:HG21	16	0.19
(1,1095)	1:A:83:ILE:HD13	1:A:83:ILE:HG22	16	0.19
(1,1095)	1:A:83:ILE:HD13	1:A:83:ILE:HG23	16	0.19
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	9	0.18
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	9	0.18
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	9	0.18
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	9	0.18
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	9	0.18
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	9	0.18
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	9	0.18
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	9	0.18
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	9	0.18
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	9	0.18
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	9	0.18
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	9	0.18
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	9	0.18
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	9	0.18
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	9	0.18
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	9	0.18
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	9	0.18
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	9	0.18
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	9	0.18
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	9	0.18
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	9	0.18
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	9	0.18
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	9	0.18
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	9	0.18
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	9	0.18
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	9	0.18
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	9	0.18
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	9	0.18
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	9	0.18
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	19	0.18
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	19	0.18
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	19	0.18
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	19	0.18
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	19	0.18
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	19	0.18
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	19	0.18
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	19	0.18
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	19	0.18
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	19	0.18
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	19	0.18
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	19	0.18
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	19	0.18
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	19	0.18
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	19	0.18
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	19	0.18
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	19	0.18
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	19	0.18
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	19	0.18
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	19	0.18
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	19	0.18
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	19	0.18
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	19	0.18
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	19	0.18
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	19	0.18
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	19	0.18
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	19	0.18
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	19	0.18
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	19	0.18
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG12	11	0.18
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG13	11	0.18
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG21	11	0.18
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG22	11	0.18
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG23	11	0.18
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG12	11	0.18
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG13	11	0.18
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG21	11	0.18
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG22	11	0.18
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG23	11	0.18
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD11	12	0.18
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD12	12	0.18
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD13	12	0.18
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD11	12	0.18
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD12	12	0.18
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD13	12	0.18
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD11	12	0.18
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD12	12	0.18
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD13	12	0.18
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD11	12	0.18
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD12	12	0.18
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD13	12	0.18
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD11	12	0.18
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD12	12	0.18
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD13	12	0.18
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD11	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD12	12	0.18
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD13	12	0.18
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	4	0.18
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	15	0.17
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	15	0.17
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	15	0.17
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	15	0.17
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	15	0.17
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	15	0.17
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	15	0.17
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	15	0.17
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	15	0.17
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	15	0.17
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	15	0.17
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	15	0.17
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	15	0.17
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	15	0.17
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	15	0.17
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	15	0.17
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	15	0.17
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	15	0.17
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	15	0.17
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	15	0.17
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	15	0.17
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	15	0.17
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	15	0.17
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	15	0.17
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	15	0.17
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	15	0.17
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	15	0.17
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	15	0.17
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	15	0.17
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	15	0.17
(1,3797)	1:A:140:ILE:HD11	1:A:160:GLN:HG2	7	0.17
(1,3797)	1:A:140:ILE:HD12	1:A:160:GLN:HG2	7	0.17
(1,3797)	1:A:140:ILE:HD13	1:A:160:GLN:HG2	7	0.17
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG12	3	0.17
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG13	3	0.17
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG21	3	0.17
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG22	3	0.17
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG23	3	0.17
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG12	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG13	3	0.17
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG21	3	0.17
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG22	3	0.17
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG23	3	0.17
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD11	18	0.17
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD12	18	0.17
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD13	18	0.17
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD11	18	0.17
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD12	18	0.17
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD13	18	0.17
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD11	18	0.17
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD12	18	0.17
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD13	18	0.17
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD11	18	0.17
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD12	18	0.17
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD13	18	0.17
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD11	18	0.17
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD12	18	0.17
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD13	18	0.17
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD11	18	0.17
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD12	18	0.17
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD13	18	0.17
(1,2580)	1:A:248:LYS:H	1:A:249:PHE:HB3	19	0.17
(1,3797)	1:A:140:ILE:HD11	1:A:160:GLN:HG2	3	0.16
(1,3797)	1:A:140:ILE:HD12	1:A:160:GLN:HG2	3	0.16
(1,3797)	1:A:140:ILE:HD13	1:A:160:GLN:HG2	3	0.16
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	13	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG12	16	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG13	16	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG21	16	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG22	16	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG23	16	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG12	16	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG13	16	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG21	16	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG22	16	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG23	16	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG12	20	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG13	20	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG21	20	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG22	20	0.16
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG23	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG12	20	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG13	20	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG21	20	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG22	20	0.16
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG23	20	0.16
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD11	14	0.16
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD12	14	0.16
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD13	14	0.16
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD11	14	0.16
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD12	14	0.16
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD13	14	0.16
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD11	14	0.16
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD12	14	0.16
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD13	14	0.16
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD11	14	0.16
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD12	14	0.16
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD13	14	0.16
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD11	14	0.16
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD12	14	0.16
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD13	14	0.16
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD11	14	0.16
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD12	14	0.16
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD13	14	0.16
(1,365)	1:A:133:ILE:HD11	1:A:133:ILE:HG12	18	0.15
(1,365)	1:A:133:ILE:HD11	1:A:133:ILE:HG13	18	0.15
(1,365)	1:A:133:ILE:HD11	1:A:133:ILE:HG21	18	0.15
(1,365)	1:A:133:ILE:HD11	1:A:133:ILE:HG22	18	0.15
(1,365)	1:A:133:ILE:HD11	1:A:133:ILE:HG23	18	0.15
(1,365)	1:A:133:ILE:HD12	1:A:133:ILE:HG12	18	0.15
(1,365)	1:A:133:ILE:HD12	1:A:133:ILE:HG13	18	0.15
(1,365)	1:A:133:ILE:HD12	1:A:133:ILE:HG21	18	0.15
(1,365)	1:A:133:ILE:HD12	1:A:133:ILE:HG22	18	0.15
(1,365)	1:A:133:ILE:HD12	1:A:133:ILE:HG23	18	0.15
(1,365)	1:A:133:ILE:HD13	1:A:133:ILE:HG12	18	0.15
(1,365)	1:A:133:ILE:HD13	1:A:133:ILE:HG13	18	0.15
(1,365)	1:A:133:ILE:HD13	1:A:133:ILE:HG21	18	0.15
(1,365)	1:A:133:ILE:HD13	1:A:133:ILE:HG22	18	0.15
(1,365)	1:A:133:ILE:HD13	1:A:133:ILE:HG23	18	0.15
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG12	1	0.15
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG13	1	0.15
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG21	1	0.15
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG22	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG23	1	0.15
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG12	1	0.15
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG13	1	0.15
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG21	1	0.15
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG22	1	0.15
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG23	1	0.15
(1,3320)	1:A:85:LYS:HE2	1:A:47:LEU:HD21	14	0.15
(1,3320)	1:A:85:LYS:HE2	1:A:47:LEU:HD22	14	0.15
(1,3320)	1:A:85:LYS:HE2	1:A:47:LEU:HD23	14	0.15
(1,3320)	1:A:85:LYS:HE3	1:A:47:LEU:HD21	14	0.15
(1,3320)	1:A:85:LYS:HE3	1:A:47:LEU:HD22	14	0.15
(1,3320)	1:A:85:LYS:HE3	1:A:47:LEU:HD23	14	0.15
(1,1047)	1:A:75:PHE:HB3	1:A:75:PHE:H	18	0.15
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG12	11	0.14
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG13	11	0.14
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG21	11	0.14
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG22	11	0.14
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG23	11	0.14
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG12	11	0.14
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG13	11	0.14
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG21	11	0.14
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG22	11	0.14
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG23	11	0.14
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG12	11	0.14
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG13	11	0.14
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG21	11	0.14
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG22	11	0.14
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG23	11	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG12	7	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG13	7	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG21	7	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG22	7	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG23	7	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG12	7	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG13	7	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG21	7	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG22	7	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG23	7	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG12	7	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG13	7	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG21	7	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG22	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG23	7	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG12	18	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG13	18	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG21	18	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG22	18	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG23	18	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG12	18	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG13	18	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG21	18	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG22	18	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG23	18	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG12	18	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG13	18	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG21	18	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG22	18	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG23	18	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG12	19	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG13	19	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG21	19	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG22	19	0.14
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG23	19	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG12	19	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG13	19	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG21	19	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG22	19	0.14
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG23	19	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG12	19	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG13	19	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG21	19	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG22	19	0.14
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG23	19	0.14
(1,3974)	1:A:190:LEU:HD21	1:A:224:ILE:HD11	14	0.14
(1,3974)	1:A:190:LEU:HD21	1:A:224:ILE:HD12	14	0.14
(1,3974)	1:A:190:LEU:HD21	1:A:224:ILE:HD13	14	0.14
(1,3974)	1:A:190:LEU:HD22	1:A:224:ILE:HD11	14	0.14
(1,3974)	1:A:190:LEU:HD22	1:A:224:ILE:HD12	14	0.14
(1,3974)	1:A:190:LEU:HD22	1:A:224:ILE:HD13	14	0.14
(1,3974)	1:A:190:LEU:HD23	1:A:224:ILE:HD11	14	0.14
(1,3974)	1:A:190:LEU:HD23	1:A:224:ILE:HD12	14	0.14
(1,3974)	1:A:190:LEU:HD23	1:A:224:ILE:HD13	14	0.14
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	6	0.14
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	6	0.14
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	6	0.14
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	6	0.14
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	6	0.14
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	6	0.14
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	6	0.14
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	6	0.14
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	6	0.14
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	6	0.14
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	6	0.14
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	6	0.14
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	6	0.14
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	6	0.14
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	6	0.14
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	6	0.14
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	6	0.14
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	6	0.14
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	6	0.14
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	6	0.14
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	6	0.14
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	6	0.14
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	6	0.14
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	6	0.14
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	6	0.14
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	6	0.14
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	6	0.14
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	6	0.14
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	6	0.14
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG12	12	0.14
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG13	12	0.14
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG21	12	0.14
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG22	12	0.14
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG23	12	0.14
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG12	12	0.14
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG13	12	0.14
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG21	12	0.14
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG22	12	0.14
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG23	12	0.14
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD11	8	0.14
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD12	8	0.14
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD13	8	0.14
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD11	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD12	8	0.14
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD13	8	0.14
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD11	8	0.14
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD12	8	0.14
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD13	8	0.14
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD11	8	0.14
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD12	8	0.14
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD13	8	0.14
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD11	8	0.14
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD12	8	0.14
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD13	8	0.14
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD11	8	0.14
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD12	8	0.14
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD13	8	0.14
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD11	13	0.14
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD12	13	0.14
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD13	13	0.14
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD11	13	0.14
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD12	13	0.14
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD13	13	0.14
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD11	13	0.14
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD12	13	0.14
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD13	13	0.14
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD11	13	0.14
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD12	13	0.14
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD13	13	0.14
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD11	13	0.14
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD12	13	0.14
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD13	13	0.14
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD11	13	0.14
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD12	13	0.14
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD13	13	0.14
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD11	16	0.14
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD12	16	0.14
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD13	16	0.14
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD11	16	0.14
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD12	16	0.14
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD13	16	0.14
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD11	16	0.14
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD12	16	0.14
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD13	16	0.14
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD11	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD12	16	0.14
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD13	16	0.14
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD11	16	0.14
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD12	16	0.14
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD13	16	0.14
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD11	16	0.14
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD12	16	0.14
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD13	16	0.14
(1,2936)	1:A:67:LYS:HB3	1:A:70:ASP:H	3	0.14
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	16	0.14
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG12	15	0.13
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG13	15	0.13
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG21	15	0.13
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG22	15	0.13
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG23	15	0.13
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG12	15	0.13
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG13	15	0.13
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG21	15	0.13
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG22	15	0.13
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG23	15	0.13
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG12	15	0.13
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG13	15	0.13
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG21	15	0.13
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG22	15	0.13
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG23	15	0.13
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	12	0.13
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	12	0.13
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	12	0.13
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	12	0.13
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	12	0.13
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	12	0.13
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	12	0.13
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	12	0.13
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	12	0.13
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	12	0.13
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	12	0.13
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	12	0.13
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	12	0.13
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	12	0.13
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	12	0.13
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	12	0.13
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	12	0.13
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	12	0.13
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	12	0.13
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	12	0.13
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	12	0.13
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	12	0.13
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	12	0.13
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	12	0.13
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	12	0.13
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	12	0.13
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	12	0.13
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	12	0.13
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	12	0.13
(1,3365)	1:A:178:LEU:HB3	1:A:207:GLU:H	18	0.13
(1,3320)	1:A:85:LYS:HE2	1:A:47:LEU:HD21	11	0.13
(1,3320)	1:A:85:LYS:HE2	1:A:47:LEU:HD22	11	0.13
(1,3320)	1:A:85:LYS:HE2	1:A:47:LEU:HD23	11	0.13
(1,3320)	1:A:85:LYS:HE3	1:A:47:LEU:HD21	11	0.13
(1,3320)	1:A:85:LYS:HE3	1:A:47:LEU:HD22	11	0.13
(1,3320)	1:A:85:LYS:HE3	1:A:47:LEU:HD23	11	0.13
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD11	1	0.13
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD12	1	0.13
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD13	1	0.13
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD11	1	0.13
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD12	1	0.13
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD13	1	0.13
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD11	1	0.13
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD12	1	0.13
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD13	1	0.13
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD11	1	0.13
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD12	1	0.13
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD13	1	0.13
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD11	1	0.13
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD12	1	0.13
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD13	1	0.13
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD11	1	0.13
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD12	1	0.13
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD13	1	0.13
(1,2713)	1:A:55:SER:HB3	1:A:57:PHE:HE1	9	0.13
(1,2713)	1:A:55:SER:HB3	1:A:57:PHE:HE2	9	0.13
(1,2217)	1:A:67:LYS:HB2	1:A:68:LYS:H	12	0.13
(1,1047)	1:A:75:PHE:HB3	1:A:75:PHE:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1047)	1:A:75:PHE:HB3	1:A:75:PHE:H	16	0.13
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG12	18	0.12
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG13	18	0.12
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG21	18	0.12
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG22	18	0.12
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG23	18	0.12
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG12	18	0.12
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG13	18	0.12
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG21	18	0.12
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG22	18	0.12
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG23	18	0.12
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG12	18	0.12
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG13	18	0.12
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG21	18	0.12
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG22	18	0.12
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG23	18	0.12
(1,3997)	1:A:212:ILE:HG12	1:A:173:ARG:HG2	11	0.12
(1,3997)	1:A:212:ILE:HG12	1:A:173:ARG:HG3	11	0.12
(1,3997)	1:A:212:ILE:HG13	1:A:173:ARG:HG2	11	0.12
(1,3997)	1:A:212:ILE:HG13	1:A:173:ARG:HG3	11	0.12
(1,3997)	1:A:212:ILE:HG21	1:A:173:ARG:HG2	11	0.12
(1,3997)	1:A:212:ILE:HG21	1:A:173:ARG:HG3	11	0.12
(1,3997)	1:A:212:ILE:HG22	1:A:173:ARG:HG2	11	0.12
(1,3997)	1:A:212:ILE:HG22	1:A:173:ARG:HG3	11	0.12
(1,3997)	1:A:212:ILE:HG23	1:A:173:ARG:HG2	11	0.12
(1,3997)	1:A:212:ILE:HG23	1:A:173:ARG:HG3	11	0.12
(1,3990)	1:A:211:LEU:HA	1:A:174:LEU:HA	10	0.12
(1,3847)	1:A:212:ILE:HG12	1:A:173:ARG:HG2	11	0.12
(1,3847)	1:A:212:ILE:HG12	1:A:173:ARG:HG3	11	0.12
(1,3847)	1:A:212:ILE:HG13	1:A:173:ARG:HG2	11	0.12
(1,3847)	1:A:212:ILE:HG13	1:A:173:ARG:HG3	11	0.12
(1,3847)	1:A:212:ILE:HG21	1:A:173:ARG:HG2	11	0.12
(1,3847)	1:A:212:ILE:HG21	1:A:173:ARG:HG3	11	0.12
(1,3847)	1:A:212:ILE:HG22	1:A:173:ARG:HG2	11	0.12
(1,3847)	1:A:212:ILE:HG22	1:A:173:ARG:HG3	11	0.12
(1,3847)	1:A:212:ILE:HG23	1:A:173:ARG:HG2	11	0.12
(1,3847)	1:A:212:ILE:HG23	1:A:173:ARG:HG3	11	0.12
(1,3797)	1:A:140:ILE:HD11	1:A:160:GLN:HG2	14	0.12
(1,3797)	1:A:140:ILE:HD12	1:A:160:GLN:HG2	14	0.12
(1,3797)	1:A:140:ILE:HD13	1:A:160:GLN:HG2	14	0.12
(1,3326)	1:A:20:MET:HG2	1:A:87:ILE:HG12	9	0.12
(1,3326)	1:A:20:MET:HG2	1:A:87:ILE:HG13	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3326)	1:A:20:MET:HG2	1:A:87:ILE:HG21	9	0.12
(1,3326)	1:A:20:MET:HG2	1:A:87:ILE:HG22	9	0.12
(1,3326)	1:A:20:MET:HG2	1:A:87:ILE:HG23	9	0.12
(1,3326)	1:A:20:MET:HG3	1:A:87:ILE:HG12	9	0.12
(1,3326)	1:A:20:MET:HG3	1:A:87:ILE:HG13	9	0.12
(1,3326)	1:A:20:MET:HG3	1:A:87:ILE:HG21	9	0.12
(1,3326)	1:A:20:MET:HG3	1:A:87:ILE:HG22	9	0.12
(1,3326)	1:A:20:MET:HG3	1:A:87:ILE:HG23	9	0.12
(1,3320)	1:A:85:LYS:HE2	1:A:47:LEU:HD21	20	0.12
(1,3320)	1:A:85:LYS:HE2	1:A:47:LEU:HD22	20	0.12
(1,3320)	1:A:85:LYS:HE2	1:A:47:LEU:HD23	20	0.12
(1,3320)	1:A:85:LYS:HE3	1:A:47:LEU:HD21	20	0.12
(1,3320)	1:A:85:LYS:HE3	1:A:47:LEU:HD22	20	0.12
(1,3320)	1:A:85:LYS:HE3	1:A:47:LEU:HD23	20	0.12
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD11	7	0.12
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD12	7	0.12
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD13	7	0.12
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD11	7	0.12
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD12	7	0.12
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD13	7	0.12
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD11	7	0.12
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD12	7	0.12
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD13	7	0.12
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD11	7	0.12
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD12	7	0.12
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD13	7	0.12
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD11	7	0.12
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD12	7	0.12
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD13	7	0.12
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD11	7	0.12
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD12	7	0.12
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD13	7	0.12
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD11	9	0.12
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD12	9	0.12
(1,3311)	1:A:71:LEU:HD11	1:A:83:ILE:HD13	9	0.12
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD11	9	0.12
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD12	9	0.12
(1,3311)	1:A:71:LEU:HD12	1:A:83:ILE:HD13	9	0.12
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD11	9	0.12
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD12	9	0.12
(1,3311)	1:A:71:LEU:HD13	1:A:83:ILE:HD13	9	0.12
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD11	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD12	9	0.12
(1,3311)	1:A:71:LEU:HD21	1:A:83:ILE:HD13	9	0.12
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD11	9	0.12
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD12	9	0.12
(1,3311)	1:A:71:LEU:HD22	1:A:83:ILE:HD13	9	0.12
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD11	9	0.12
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD12	9	0.12
(1,3311)	1:A:71:LEU:HD23	1:A:83:ILE:HD13	9	0.12
(1,2629)	1:A:239:LEU:HB2	1:A:241:ASP:H	20	0.12
(1,1047)	1:A:75:PHE:HB3	1:A:75:PHE:H	11	0.12
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG12	1	0.11
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG13	1	0.11
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG21	1	0.11
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG22	1	0.11
(1,839)	1:A:29:ILE:HD11	1:A:29:ILE:HG23	1	0.11
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG12	1	0.11
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG13	1	0.11
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG21	1	0.11
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG22	1	0.11
(1,839)	1:A:29:ILE:HD12	1:A:29:ILE:HG23	1	0.11
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG12	1	0.11
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG13	1	0.11
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG21	1	0.11
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG22	1	0.11
(1,839)	1:A:29:ILE:HD13	1:A:29:ILE:HG23	1	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG12	1	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG13	1	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG21	1	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG22	1	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG23	1	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG12	1	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG13	1	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG21	1	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG22	1	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG23	1	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG12	1	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG13	1	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG21	1	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG22	1	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG23	1	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG12	11	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG13	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG21	11	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG22	11	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG23	11	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG12	11	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG13	11	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG21	11	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG22	11	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG23	11	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG12	11	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG13	11	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG21	11	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG22	11	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG23	11	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG12	14	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG13	14	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG21	14	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG22	14	0.11
(1,432)	1:A:212:ILE:HD11	1:A:212:ILE:HG23	14	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG12	14	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG13	14	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG21	14	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG22	14	0.11
(1,432)	1:A:212:ILE:HD12	1:A:212:ILE:HG23	14	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG12	14	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG13	14	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG21	14	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG22	14	0.11
(1,432)	1:A:212:ILE:HD13	1:A:212:ILE:HG23	14	0.11
(1,3990)	1:A:211:LEU:HA	1:A:174:LEU:HA	12	0.11
(1,3990)	1:A:211:LEU:HA	1:A:174:LEU:HA	16	0.11
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD11	20	0.11
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD12	20	0.11
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD13	20	0.11
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD21	20	0.11
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD22	20	0.11
(1,3970)	1:A:224:ILE:HG12	1:A:193:LEU:HD23	20	0.11
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD11	20	0.11
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD12	20	0.11
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD13	20	0.11
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD21	20	0.11
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD22	20	0.11
(1,3970)	1:A:224:ILE:HG13	1:A:193:LEU:HD23	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD11	20	0.11
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD12	20	0.11
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD13	20	0.11
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD21	20	0.11
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD22	20	0.11
(1,3970)	1:A:224:ILE:HG21	1:A:193:LEU:HD23	20	0.11
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD11	20	0.11
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD12	20	0.11
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD13	20	0.11
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD21	20	0.11
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD22	20	0.11
(1,3970)	1:A:224:ILE:HG22	1:A:193:LEU:HD23	20	0.11
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD11	20	0.11
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD12	20	0.11
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD13	20	0.11
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD21	20	0.11
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD22	20	0.11
(1,3970)	1:A:224:ILE:HG23	1:A:193:LEU:HD23	20	0.11
(1,3852)	1:A:197:ILE:HG12	1:A:212:ILE:HD11	15	0.11
(1,3852)	1:A:197:ILE:HG12	1:A:212:ILE:HD12	15	0.11
(1,3852)	1:A:197:ILE:HG12	1:A:212:ILE:HD13	15	0.11
(1,3852)	1:A:197:ILE:HG13	1:A:212:ILE:HD11	15	0.11
(1,3852)	1:A:197:ILE:HG13	1:A:212:ILE:HD12	15	0.11
(1,3852)	1:A:197:ILE:HG13	1:A:212:ILE:HD13	15	0.11
(1,3852)	1:A:197:ILE:HG21	1:A:212:ILE:HD11	15	0.11
(1,3852)	1:A:197:ILE:HG21	1:A:212:ILE:HD12	15	0.11
(1,3852)	1:A:197:ILE:HG21	1:A:212:ILE:HD13	15	0.11
(1,3852)	1:A:197:ILE:HG22	1:A:212:ILE:HD11	15	0.11
(1,3852)	1:A:197:ILE:HG22	1:A:212:ILE:HD12	15	0.11
(1,3852)	1:A:197:ILE:HG22	1:A:212:ILE:HD13	15	0.11
(1,3852)	1:A:197:ILE:HG23	1:A:212:ILE:HD11	15	0.11
(1,3852)	1:A:197:ILE:HG23	1:A:212:ILE:HD12	15	0.11
(1,3852)	1:A:197:ILE:HG23	1:A:212:ILE:HD13	15	0.11
(1,3806)	1:A:201:ASP:HB2	1:A:207:GLU:HG2	12	0.11
(1,3806)	1:A:201:ASP:HB2	1:A:207:GLU:HG3	12	0.11
(1,3806)	1:A:201:ASP:HB3	1:A:207:GLU:HG2	12	0.11
(1,3806)	1:A:201:ASP:HB3	1:A:207:GLU:HG3	12	0.11
(1,3806)	1:A:201:ASP:HB2	1:A:207:GLU:HG2	16	0.11
(1,3806)	1:A:201:ASP:HB2	1:A:207:GLU:HG3	16	0.11
(1,3806)	1:A:201:ASP:HB3	1:A:207:GLU:HG2	16	0.11
(1,3806)	1:A:201:ASP:HB3	1:A:207:GLU:HG3	16	0.11
(1,3340)	1:A:93:VAL:HG11	1:A:18:VAL:HG21	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3340)	1:A:93:VAL:HG11	1:A:18:VAL:HG22	20	0.11
(1,3340)	1:A:93:VAL:HG11	1:A:18:VAL:HG23	20	0.11
(1,3340)	1:A:93:VAL:HG12	1:A:18:VAL:HG21	20	0.11
(1,3340)	1:A:93:VAL:HG12	1:A:18:VAL:HG22	20	0.11
(1,3340)	1:A:93:VAL:HG12	1:A:18:VAL:HG23	20	0.11
(1,3340)	1:A:93:VAL:HG13	1:A:18:VAL:HG21	20	0.11
(1,3340)	1:A:93:VAL:HG13	1:A:18:VAL:HG22	20	0.11
(1,3340)	1:A:93:VAL:HG13	1:A:18:VAL:HG23	20	0.11
(1,3340)	1:A:93:VAL:HG21	1:A:18:VAL:HG21	20	0.11
(1,3340)	1:A:93:VAL:HG21	1:A:18:VAL:HG22	20	0.11
(1,3340)	1:A:93:VAL:HG21	1:A:18:VAL:HG23	20	0.11
(1,3340)	1:A:93:VAL:HG22	1:A:18:VAL:HG21	20	0.11
(1,3340)	1:A:93:VAL:HG22	1:A:18:VAL:HG22	20	0.11
(1,3340)	1:A:93:VAL:HG22	1:A:18:VAL:HG23	20	0.11
(1,3340)	1:A:93:VAL:HG23	1:A:18:VAL:HG21	20	0.11
(1,3340)	1:A:93:VAL:HG23	1:A:18:VAL:HG22	20	0.11
(1,3340)	1:A:93:VAL:HG23	1:A:18:VAL:HG23	20	0.11
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG12	10	0.11
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG13	10	0.11
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG21	10	0.11
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG22	10	0.11
(1,3325)	1:A:20:MET:HB2	1:A:87:ILE:HG23	10	0.11
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG12	10	0.11
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG13	10	0.11
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG21	10	0.11
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG22	10	0.11
(1,3325)	1:A:20:MET:HB3	1:A:87:ILE:HG23	10	0.11
(1,256)	1:A:51:LEU:HA	1:A:51:LEU:HD21	20	0.11
(1,256)	1:A:51:LEU:HA	1:A:51:LEU:HD22	20	0.11
(1,256)	1:A:51:LEU:HA	1:A:51:LEU:HD23	20	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found