Full wwPDB NMR Structure Validation Report (i)

Jun 5, 2023 – 01:17 PM JST

PDB ID	:	6KJN
BMRB ID	:	11490
Title	:	The microtubule-binding domains of yeast cytoplasmic dynein in the high affinity state
Authors	:	Nishida, N.; Komori, Y.; Takarada, O.; Watanabe, A.; Tamura, S.; Kubo, S.; Shimada, I.; Kikkawa, M.
Deposited on	:	2019-07-22

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 (1)) were used in the production of this report:

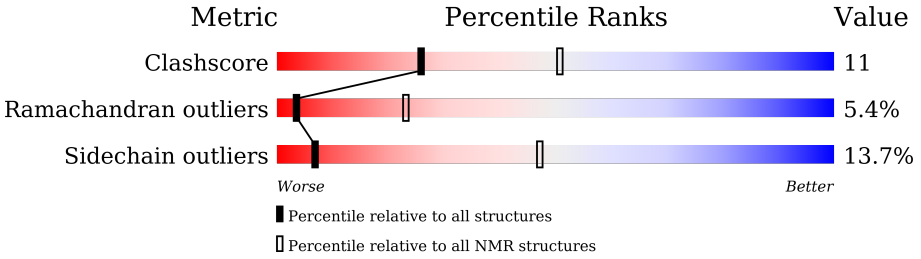
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 70%.

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	141	

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:3101-A:3222 (122)	1.43	6

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 6, 8, 10
2	5, 7, 9

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2294 atoms, of which 1139 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	141	2294	730	1139	202	214	9	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3092	GLY	-	expression tag	UNP P36022
A	3093	SER	-	expression tag	UNP P36022
A	3094	HIS	-	expression tag	UNP P36022
A	3101	CYS	ILE	engineered mutation	UNP P36022
A	3222	CYS	VAL	engineered mutation	UNP P36022

4 Residue-property plots (i)

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: Dynein heavy chain, cytoplasmic

Chain A: 60% 26% • 13%

G3092 S3093 H3094 M3095 K3096 S3097 I3098 Q3099 D3100 C3101 E3102 P3103 V3112 I3115 M3126 G3132 V3133 K3134 I3135 V3136 M3137 I3143 Q3147 I3158 F3163 Y3170 D3171 H3175 M3176 K3177 P3178 Q3179 I3180 Y3183 M3184 E3185 F3188 L3189 F3194 T3195 I3199 S3203 K3204 A3205 C3206

L3209 W3212 V3213 Q3216 F3219 L3223 E3224 N3225 V3226 D3227 P3228 L3229 R3230 Q3231 E3232

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Dynein heavy chain, cytoplasmic

Chain A: 58% 24% • 13%

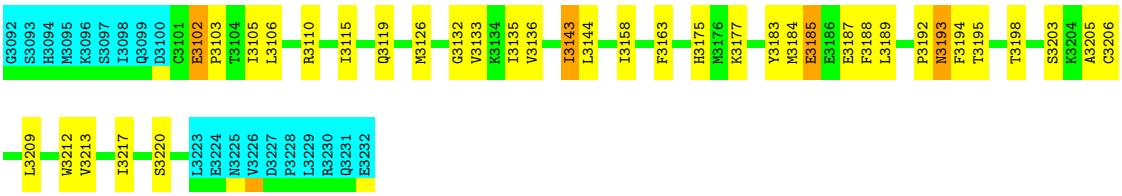
G3092 S3093 H3094 M3095 K3096 S3097 I3098 Q3099 D3100 C3101 E3102 P3103 A3108 Q3109 R3110 K3113 N3114 I3115 G3132 I3135 V3136 I3143 L3144 Q3147 N3150 F3157 I3158 F3163 V3168 H3169 Y3170 D3171 L3174 H3175 M3176 K3177 P3178 L3189 F3194 T3195 Y3196 E3197 T3198 I3199 A3202 S3203

K3204 A3205 C3206 L3209 Y3210 Q3211 W3212 V3213 L3223 E3224 N3225 V3226 D3227 P3228 L3229 R3230 Q3231 E3232

4.2.2 Score per residue for model 2

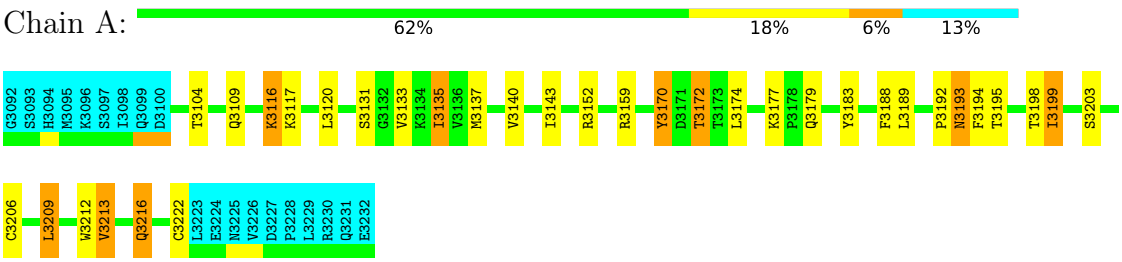
• Molecule 1: Dynein heavy chain, cytoplasmic

Chain A: 60% 23% • 13%



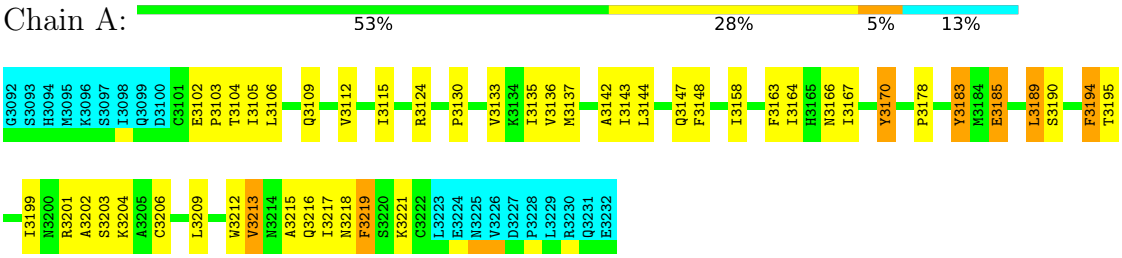
4.2.3 Score per residue for model 3

- Molecule 1: Dynein heavy chain, cytoplasmic



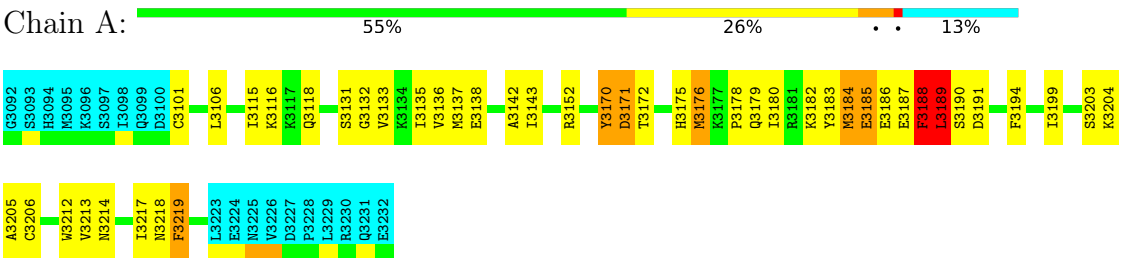
4.2.4 Score per residue for model 4

- Molecule 1: Dynein heavy chain, cytoplasmic



4.2.5 Score per residue for model 5

- Molecule 1: Dynein heavy chain, cytoplasmic



4.2.6 Score per residue for model 6 (medoid)

• Molecule 1: Dynein heavy chain, cytoplasmic

Chain A: 65% 18% • 13%

G3092 S3093 H3094 M3095 K3096 S3097 I3098 Q3099 D3100 T3104 I3105 L3106 R3110 I3115 Q3119 M3126 G3132 V3136 A3142 I3143 Q3147 N3150 I3158 F3163 Y3170 D3171 T3172 M3176 K3177 Y3183 M3184 E3185 F3188 F3194 I3199 A3205 L3209 Q3216 I3217

N3218 F3219 S3220 K3221 C3222 L3223 E3224 N3225 V3226 D3227 P3228 L3229 R3230 Q3231 E3232

4.2.7 Score per residue for model 7

• Molecule 1: Dynein heavy chain, cytoplasmic

Chain A: 51% 27% 9% 13%

G3092 S3093 H3094 M3095 K3096 S3097 I3098 Q3099 D3100 C3101 E3102 P3103 T3104 I3105 A3108 V3112 K3113 N3114 I3115 I3123 M3126 P3130 S3131 G3132 V3133 K3134 I3135 V3136 M3137 C3141 A3142 I3143 L3144 Q3147 R3159 F3163 I3167 D3171 H3175 P3178 Q3179 I3180 R3181 K3182 Y3183 M3184 E3185

E3186 E3187 F3188 L3189 P3192 N3193 F3194 A3202 S3203 K3204 A3205 C3206 G3207 P3208 L3209 W3212 V3213 Q3216 F3219 S3220 K3221 C3222 L3223 E3224 N3225 V3226 D3227 P3228 L3229 R3230 Q3231 E3232

4.2.8 Score per residue for model 8

• Molecule 1: Dynein heavy chain, cytoplasmic

Chain A: 51% 28% 8% 13%

G3092 S3093 H3094 M3095 K3096 S3097 I3098 Q3099 D3100 C3101 E3102 P3103 Q3109 V3112 I3115 R3124 S3125 M3126 G3132 V3133 K3134 I3135 V3136 M3137 C3141 A3142 I3143 Y3146 Q3147 W3151 Q3155 I3158 R3159 K3160 F3163 I3167 L3174 H3175 M3176 K3177 P3178 R3181 K3182 Y3183 M3184 E3185

L3189 S3190 D3191 P3192 N3193 F3194 T3195 T3198 I3199 A3202 S3203 K3204 A3205 C3206 G3207 P3208 L3209 W3212 V3213 N3214 A3215 Q3216 I3217 N3218 F3219 L3223 E3224 N3225 V3226 D3227 P3228 L3229 R3230 Q3231 E3232

4.2.9 Score per residue for model 9

• Molecule 1: Dynein heavy chain, cytoplasmic

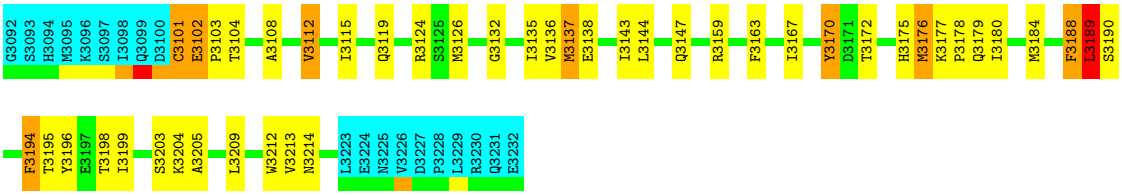
Chain A: 57% 20% 9% 13%

G3092 S3093 H3094 M3095 K3096 S3097 I3098 Q3099 D3100 C3101 E3102 L3106 I3115 K3116 I3123 M3126 G3132 V3133 K3134 I3135 V3136 A3142 I3143 I3158 R3159 F3163 I3167 Y3170 D3171 T3172 T3173 I3180 Y3183 M3184 E3185 E3186 E3187 F3188 L3189 S3190 D3191 P3192 N3193 F3194 T3195 Y3196 I3199

4.2.10 Score per residue for model 10

- Molecule 1: Dynein heavy chain, cytoplasmic

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	

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	1398
Number of shifts mapped to atoms	1398
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	70%

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

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	1003	994	994	22±7
All	All	10030	9940	9940	225

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3115:ILE:HD11	1:A:3164:ILE:HD11	0.92	1.37	4	1
1:A:3212:TRP:CZ3	1:A:3213:VAL:HG13	0.80	2.11	1	1
1:A:3142:ALA:HB1	1:A:3180:ILE:HD12	0.80	1.54	9	2
1:A:3185:GLU:O	1:A:3189:LEU:HD12	0.79	1.78	5	1
1:A:3115:ILE:HG21	1:A:3205:ALA:HA	0.77	1.56	8	2
1:A:3189:LEU:HD13	1:A:3190:SER:N	0.75	1.96	5	1
1:A:3105:ILE:HD11	1:A:3219:PHE:HB2	0.69	1.65	4	2
1:A:3132:GLY:O	1:A:3136:VAL:HG23	0.68	1.89	7	8
1:A:3115:ILE:CD1	1:A:3164:ILE:HD11	0.67	2.19	4	1
1:A:3133:VAL:HG22	1:A:3206:CYS:SG	0.67	2.29	8	5
1:A:3209:LEU:O	1:A:3213:VAL:HG12	0.67	1.90	9	2
1:A:3163:PHE:CZ	1:A:3167:ILE:HD11	0.66	2.25	9	2
1:A:3158:ILE:HG22	1:A:3163:PHE:CE1	0.65	2.26	1	5
1:A:3135:ILE:HD12	1:A:3194:PHE:CD1	0.65	2.26	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3142:ALA:HB1	1:A:3180:ILE:CD1	0.65	2.21	9	2
1:A:3194:PHE:CE2	1:A:3199:ILE:HD11	0.65	2.27	10	4
1:A:3123:ILE:HD12	1:A:3133:VAL:HG11	0.64	1.69	9	1
1:A:3105:ILE:HD11	1:A:3219:PHE:CB	0.64	2.22	6	1
1:A:3194:PHE:CE1	1:A:3199:ILE:HD11	0.63	2.29	5	2
1:A:3167:ILE:HD13	1:A:3209:LEU:HD11	0.63	1.70	7	4
1:A:3163:PHE:CE1	1:A:3167:ILE:HD11	0.62	2.29	4	3
1:A:3189:LEU:O	1:A:3189:LEU:HD22	0.62	1.95	5	1
1:A:3204:LYS:O	1:A:3205:ALA:HB2	0.62	1.94	1	2
1:A:3137:MET:N	1:A:3137:MET:SD	0.61	2.74	10	4
1:A:3192:PRO:O	1:A:3193:ASN:CB	0.60	2.49	2	2
1:A:3130:PRO:HB2	1:A:3202:ALA:HB1	0.60	1.74	4	1
1:A:3189:LEU:HD13	1:A:3189:LEU:C	0.59	2.18	2	1
1:A:3218:ASN:O	1:A:3219:PHE:CB	0.59	2.50	5	2
1:A:3189:LEU:HD22	1:A:3189:LEU:C	0.59	2.18	5	1
1:A:3184:MET:O	1:A:3186:GLU:N	0.58	2.36	5	1
1:A:3101:CYS:O	1:A:3104:THR:N	0.58	2.37	10	1
1:A:3212:TRP:CZ3	1:A:3213:VAL:HG23	0.58	2.33	3	3
1:A:3218:ASN:O	1:A:3219:PHE:HB2	0.58	1.99	4	1
1:A:3115:ILE:HD13	1:A:3205:ALA:HA	0.57	1.76	7	2
1:A:3130:PRO:CB	1:A:3202:ALA:HB1	0.57	2.29	4	1
1:A:3204:LYS:O	1:A:3205:ALA:CB	0.57	2.52	1	2
1:A:3108:ALA:HB1	1:A:3212:TRP:HA	0.57	1.77	7	2
1:A:3105:ILE:O	1:A:3105:ILE:CG2	0.56	2.53	2	1
1:A:3142:ALA:HB1	1:A:3183:TYR:CE1	0.55	2.37	4	1
1:A:3159:ARG:O	1:A:3160:LYS:HB3	0.55	2.01	8	1
1:A:3185:GLU:O	1:A:3186:GLU:HB2	0.55	2.02	7	1
1:A:3185:GLU:HA	1:A:3189:LEU:HD23	0.55	1.76	9	1
1:A:3142:ALA:HB3	1:A:3180:ILE:HD11	0.55	1.79	7	1
1:A:3105:ILE:O	1:A:3105:ILE:HG22	0.55	2.02	2	1
1:A:3189:LEU:C	1:A:3189:LEU:HD13	0.54	2.23	1	1
1:A:3212:TRP:CE3	1:A:3213:VAL:HG23	0.54	2.37	8	3
1:A:3102:GLU:N	1:A:3103:PRO:CD	0.54	2.71	1	4
1:A:3131:SER:O	1:A:3135:ILE:HG13	0.54	2.03	5	2
1:A:3143:ILE:HD13	1:A:3212:TRP:CH2	0.53	2.38	7	1
1:A:3212:TRP:CE3	1:A:3213:VAL:HG13	0.53	2.39	1	1
1:A:3142:ALA:HB1	1:A:3183:TYR:CE2	0.53	2.39	6	1
1:A:3159:ARG:O	1:A:3160:LYS:CB	0.53	2.57	8	1
1:A:3180:ILE:HG22	1:A:3181:ARG:N	0.52	2.20	7	1
1:A:3135:ILE:HD12	1:A:3194:PHE:HD1	0.52	1.65	1	1
1:A:3184:MET:HB2	1:A:3217:ILE:HD11	0.52	1.82	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3189:LEU:HD23	1:A:3190:SER:N	0.51	2.20	10	3
1:A:3123:ILE:HD11	1:A:3203:SER:OG	0.51	2.05	7	1
1:A:3102:GLU:CB	1:A:3103:PRO:CD	0.51	2.88	10	1
1:A:3185:GLU:O	1:A:3186:GLU:CB	0.51	2.59	7	1
1:A:3143:ILE:HD11	1:A:3216:GLN:HG2	0.51	1.83	7	1
1:A:3170:TYR:N	1:A:3170:TYR:CD1	0.50	2.78	3	1
1:A:3170:TYR:O	1:A:3171:ASP:C	0.49	2.50	5	2
1:A:3109:GLN:OE1	1:A:3168:VAL:HG13	0.49	2.08	1	1
1:A:3195:THR:HG23	1:A:3198:THR:H	0.49	1.66	3	4
1:A:3140:VAL:CG2	1:A:3209:LEU:HD12	0.49	2.38	3	1
1:A:3184:MET:O	1:A:3188:PHE:CB	0.48	2.61	10	1
1:A:3210:TYR:CD2	1:A:3210:TYR:C	0.48	2.86	1	1
1:A:3105:ILE:HD11	1:A:3219:PHE:CG	0.48	2.42	7	1
1:A:3184:MET:O	1:A:3188:PHE:N	0.48	2.46	7	1
1:A:3185:GLU:O	1:A:3189:LEU:HB3	0.48	2.09	8	1
1:A:3101:CYS:O	1:A:3103:PRO:N	0.48	2.47	10	1
1:A:3213:VAL:HG13	1:A:3214:ASN:N	0.48	2.24	10	1
1:A:3102:GLU:CB	1:A:3103:PRO:HD3	0.48	2.39	4	1
1:A:3191:ASP:O	1:A:3191:ASP:OD1	0.48	2.31	5	1
1:A:3170:TYR:CE2	1:A:3172:THR:HG22	0.48	2.43	10	1
1:A:3133:VAL:O	1:A:3136:VAL:HG12	0.48	2.08	4	1
1:A:3170:TYR:CD1	1:A:3170:TYR:O	0.48	2.67	3	1
1:A:3189:LEU:HD23	1:A:3189:LEU:H	0.48	1.69	7	1
1:A:3188:PHE:O	1:A:3191:ASP:CG	0.47	2.52	5	1
1:A:3116:LYS:HA	1:A:3120:LEU:HD23	0.47	1.86	3	1
1:A:3101:CYS:O	1:A:3102:GLU:C	0.47	2.52	10	1
1:A:3130:PRO:HG2	1:A:3202:ALA:HB1	0.47	1.87	7	1
1:A:3113:LYS:O	1:A:3114:ASN:C	0.47	2.52	7	1
1:A:3176:MET:O	1:A:3177:LYS:C	0.47	2.52	10	1
1:A:3213:VAL:HG13	1:A:3214:ASN:H	0.47	1.70	9	1
1:A:3143:ILE:HG22	1:A:3144:LEU:N	0.47	2.25	1	1
1:A:3115:ILE:CG2	1:A:3205:ALA:HB1	0.47	2.40	10	3
1:A:3133:VAL:HG23	1:A:3202:ALA:HB1	0.46	1.87	8	2
1:A:3115:ILE:HG22	1:A:3205:ALA:HA	0.46	1.85	2	4
1:A:3123:ILE:HD13	1:A:3126:MET:SD	0.46	2.50	9	1
1:A:3194:PHE:CD2	1:A:3199:ILE:HD11	0.46	2.46	9	1
1:A:3115:ILE:HG21	1:A:3205:ALA:CA	0.46	2.37	8	2
1:A:3188:PHE:CE1	1:A:3194:PHE:CZ	0.45	3.03	10	1
1:A:3143:ILE:HD11	1:A:3216:GLN:CB	0.45	2.41	6	1
1:A:3194:PHE:CD1	1:A:3199:ILE:HD11	0.45	2.46	1	2
1:A:3143:ILE:HD13	1:A:3213:VAL:HG23	0.45	1.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3143:ILE:HG21	1:A:3212:TRP:CH2	0.45	2.46	1	1
1:A:3105:ILE:HD11	1:A:3219:PHE:CD1	0.45	2.47	7	1
1:A:3183:TYR:O	1:A:3184:MET:O	0.45	2.34	5	1
1:A:3112:VAL:CG2	1:A:3209:LEU:HD22	0.45	2.42	7	1
1:A:3108:ALA:O	1:A:3112:VAL:HG13	0.45	2.12	10	1
1:A:3115:ILE:HD12	1:A:3119:GLN:OE1	0.45	2.11	10	1
1:A:3196:TYR:HA	1:A:3210:TYR:CD2	0.45	2.46	1	1
1:A:3199:ILE:O	1:A:3202:ALA:HB3	0.45	2.12	1	1
1:A:3183:TYR:O	1:A:3185:GLU:N	0.44	2.50	9	1
1:A:3206:CYS:O	1:A:3209:LEU:N	0.44	2.50	7	1
1:A:3112:VAL:HG12	1:A:3164:ILE:HD12	0.44	1.89	4	1
1:A:3143:ILE:CG2	1:A:3144:LEU:N	0.44	2.81	1	4
1:A:3115:ILE:HG22	1:A:3205:ALA:CB	0.44	2.43	9	1
1:A:3170:TYR:O	1:A:3172:THR:N	0.44	2.50	5	1
1:A:3183:TYR:O	1:A:3184:MET:C	0.44	2.56	7	2
1:A:3195:THR:HG23	1:A:3198:THR:OG1	0.44	2.13	8	1
1:A:3194:PHE:CE2	1:A:3210:TYR:CD1	0.44	3.06	9	1
1:A:3209:LEU:HD13	1:A:3212:TRP:CE3	0.43	2.48	9	1
1:A:3180:ILE:O	1:A:3183:TYR:N	0.43	2.51	9	2
1:A:3143:ILE:HD11	1:A:3216:GLN:CG	0.43	2.44	7	1
1:A:3135:ILE:HD12	1:A:3194:PHE:CG	0.43	2.48	9	1
1:A:3144:LEU:HD11	1:A:3166:ASN:OD1	0.43	2.14	4	1
1:A:3113:LYS:HE2	1:A:3168:VAL:HG11	0.42	1.92	1	1
1:A:3170:TYR:N	1:A:3170:TYR:HD1	0.42	2.11	3	1
1:A:3189:LEU:HD23	1:A:3189:LEU:N	0.42	2.29	7	1
1:A:3178:PRO:C	1:A:3180:ILE:H	0.42	2.17	10	1
1:A:3143:ILE:HG21	1:A:3212:TRP:HH2	0.42	1.74	1	1
1:A:3170:TYR:O	1:A:3170:TYR:CG	0.42	2.71	4	2
1:A:3199:ILE:O	1:A:3206:CYS:SG	0.42	2.76	4	1
1:A:3176:MET:O	1:A:3177:LYS:CB	0.42	2.68	8	1
1:A:3219:PHE:N	1:A:3219:PHE:CD1	0.42	2.86	8	1
1:A:3146:TYR:O	1:A:3147:GLN:C	0.42	2.58	8	1
1:A:3189:LEU:HD23	1:A:3190:SER:H	0.42	1.75	8	1
1:A:3158:ILE:HG22	1:A:3163:PHE:CD1	0.41	2.50	6	2
1:A:3215:ALA:O	1:A:3218:ASN:O	0.41	2.38	4	1
1:A:3206:CYS:O	1:A:3207:GLY:C	0.41	2.59	8	2
1:A:3215:ALA:O	1:A:3219:PHE:HB2	0.41	2.15	8	1
1:A:3115:ILE:HG22	1:A:3205:ALA:CA	0.41	2.46	9	1
1:A:3204:LYS:O	1:A:3204:LYS:CG	0.41	2.69	1	1
1:A:3188:PHE:O	1:A:3190:SER:N	0.41	2.53	5	1
1:A:3155:GLN:HA	1:A:3158:ILE:HG13	0.41	1.92	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3214:ASN:O	1:A:3217:ILE:HB	0.41	2.15	5	1
1:A:3170:TYR:CE1	1:A:3172:THR:HG22	0.41	2.51	6	1
1:A:3219:PHE:C	1:A:3221:LYS:H	0.41	2.18	6	2
1:A:3141:CYS:SG	1:A:3142:ALA:N	0.41	2.92	7	1
1:A:3189:LEU:C	1:A:3189:LEU:CD1	0.41	2.89	2	1
1:A:3109:GLN:O	1:A:3112:VAL:HG22	0.41	2.16	8	1
1:A:3114:ASN:O	1:A:3115:ILE:C	0.41	2.59	1	1
1:A:3190:SER:O	1:A:3192:PRO:HD3	0.41	2.15	8	1
1:A:3143:ILE:HD11	1:A:3216:GLN:CD	0.41	2.36	7	1
1:A:3188:PHE:O	1:A:3188:PHE:CD2	0.40	2.73	10	1
1:A:3184:MET:O	1:A:3185:GLU:C	0.40	2.58	5	1
1:A:3189:LEU:C	1:A:3189:LEU:CD2	0.40	2.86	5	1
1:A:3172:THR:HG22	1:A:3216:GLN:OE1	0.40	2.17	3	1
1:A:3196:TYR:CD2	1:A:3196:TYR:O	0.40	2.74	9	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	122/141 (87%)	104±5 (85±4%)	12±4 (10±3%)	7±2 (5±1%)	3	23
All	All	1220/1410 (87%)	1037 (85%)	117 (10%)	66 (5%)	3	23

All 31 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	3147	GLN	6
1	A	3178	PRO	5
1	A	3185	GLU	5
1	A	3188	PHE	5
1	A	3171	ASP	3
1	A	3176	MET	3
1	A	3175	HIS	3
1	A	3184	MET	3

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Mol	Chain	Res	Type	Models (Total)
1	A	3174	LEU	2
1	A	3205	ALA	2
1	A	3177	LYS	2
1	A	3193	ASN	2
1	A	3220	SER	2
1	A	3219	PHE	2
1	A	3189	LEU	2
1	A	3180	ILE	2
1	A	3192	PRO	2
1	A	3102	GLU	2
1	A	3204	LYS	1
1	A	3116	LYS	1
1	A	3117	LYS	1
1	A	3170	TYR	1
1	A	3114	ASN	1
1	A	3186	GLU	1
1	A	3160	LYS	1
1	A	3207	GLY	1
1	A	3173	THR	1
1	A	3187	GLU	1
1	A	3203	SER	1
1	A	3101	CYS	1
1	A	3179	GLN	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	112/130 (86%)	97±3 (86±2%)	15±3 (14±2%)	7 47
All	All	1120/1300 (86%)	967 (86%)	153 (14%)	7 47

All 59 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	3143	ILE	8
1	A	3203	SER	8

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Mol	Chain	Res	Type	Models (Total)
1	A	3209	LEU	7
1	A	3189	LEU	6
1	A	3170	TYR	5
1	A	3106	LEU	5
1	A	3126	MET	5
1	A	3183	TYR	5
1	A	3176	MET	4
1	A	3213	VAL	4
1	A	3104	THR	4
1	A	3137	MET	4
1	A	3159	ARG	4
1	A	3216	GLN	4
1	A	3194	PHE	4
1	A	3204	LYS	4
1	A	3188	PHE	4
1	A	3110	ARG	3
1	A	3175	HIS	3
1	A	3185	GLU	3
1	A	3124	ARG	3
1	A	3217	ILE	3
1	A	3150	ASN	2
1	A	3102	GLU	2
1	A	3119	GLN	2
1	A	3187	GLU	2
1	A	3109	GLN	2
1	A	3152	ARG	2
1	A	3179	GLN	2
1	A	3195	THR	2
1	A	3116	LYS	2
1	A	3138	GLU	2
1	A	3177	LYS	2
1	A	3219	PHE	2
1	A	3112	VAL	2
1	A	3141	CYS	2
1	A	3158	ILE	2
1	A	3212	TRP	2
1	A	3113	LYS	1
1	A	3157	PHE	1
1	A	3206	CYS	1
1	A	3135	ILE	1
1	A	3172	THR	1
1	A	3174	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	3199	ILE	1
1	A	3222	CYS	1
1	A	3148	PHE	1
1	A	3201	ARG	1
1	A	3221	LYS	1
1	A	3101	CYS	1
1	A	3118	GLN	1
1	A	3182	LYS	1
1	A	3171	ASP	1
1	A	3151	TRP	1
1	A	3181	ARG	1
1	A	3115	ILE	1
1	A	3173	THR	1
1	A	3191	ASP	1
1	A	3196	TYR	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 70% for the well-defined parts and 70% 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 (i)

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	1398
Number of shifts mapped to atoms	1398
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	130	2.58 ± 0.19	Should be applied
$^{13}C_{\beta}$	125	2.83 ± 0.06	Should be applied
$^{13}C'$	0	—	None (insufficient data)
^{15}N	121	1.16 ± 0.16	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 70%, i.e. 1219 atoms were assigned a chemical shift out of a possible 1735. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	444/602 (74%)	224/242 (93%)	112/244 (46%)	108/116 (93%)
Sidechain	717/983 (73%)	479/635 (75%)	238/304 (78%)	0/44 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	58/150 (39%)	30/74 (41%)	26/71 (37%)	2/5 (40%)
Overall	1219/1735 (70%)	733/951 (77%)	376/619 (61%)	110/165 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 1398 atoms were assigned a chemical shift out of a possible 1993. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	506/696 (73%)	255/280 (91%)	130/282 (46%)	121/134 (90%)
Sidechain	834/1140 (73%)	555/735 (76%)	279/354 (79%)	0/51 (0%)
Aromatic	58/157 (37%)	30/78 (38%)	26/73 (36%)	2/6 (33%)
Overall	1398/1993 (70%)	840/1093 (77%)	435/709 (61%)	123/191 (64%)

7.1.4 Statistically unusual chemical shifts (i)

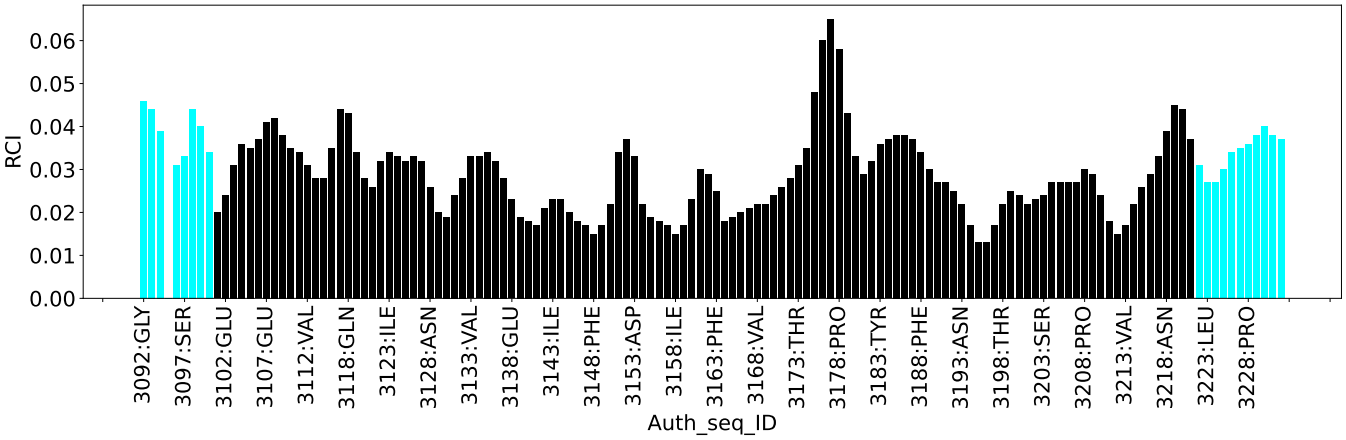
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	3129	PRO	HG2	-0.07	0.41 – 3.45	-6.6
1	A	3216	GLN	HG2	0.66	1.01 – 3.62	-6.3
1	A	3151	TRP	CZ3	111.93	113.48 – 129.28	-6.0
1	A	3167	ILE	HG21	-0.78	-0.56 – 2.11	-5.8
1	A	3167	ILE	HG22	-0.78	-0.56 – 2.11	-5.8
1	A	3167	ILE	HG23	-0.78	-0.56 – 2.11	-5.8

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.00
0.01
0.02
0.03
0.04
0.05
0.06
3092:GLY
3097:SER
3102:GLU
3107:GLU
3112:VAL
3118:GLN
3123:ILE
3128:ASN
3133:VAL
3138:GLU
3143:ILE
3148:PHE
3153:ASP
3158:ILE
3163:PHE
3168:VAL
3173:THR
3178:PRO
3183:TYR
3188:PHE
3193:ASN
3198:THR
3203:SER
3208:PRO
3213:VAL
3218:ASN
3223:LEU
3228:PRO
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	1535
Intra-residue (|i-j|=0)	324
Sequential (|i-j|=1)	369
Medium range (|i-j|>1 and |i-j|<5)	423
Long range (|i-j|≥5)	419
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	141
Number of unmapped restraints	0
Number of restraints per residue	11.9
Number of long range restraints per residue[1]	3.0

[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 (i)

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 (i)

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)	40.1	0.2
0.2-0.5 (Medium)	38.7	0.5
>0.5 (Large)	6.5	1.22

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	10.2	9.8
10.0-20.0 (Medium)	0.8	16.2
>20.0 (Large)	None	None

9 Distance violation analysis (i)

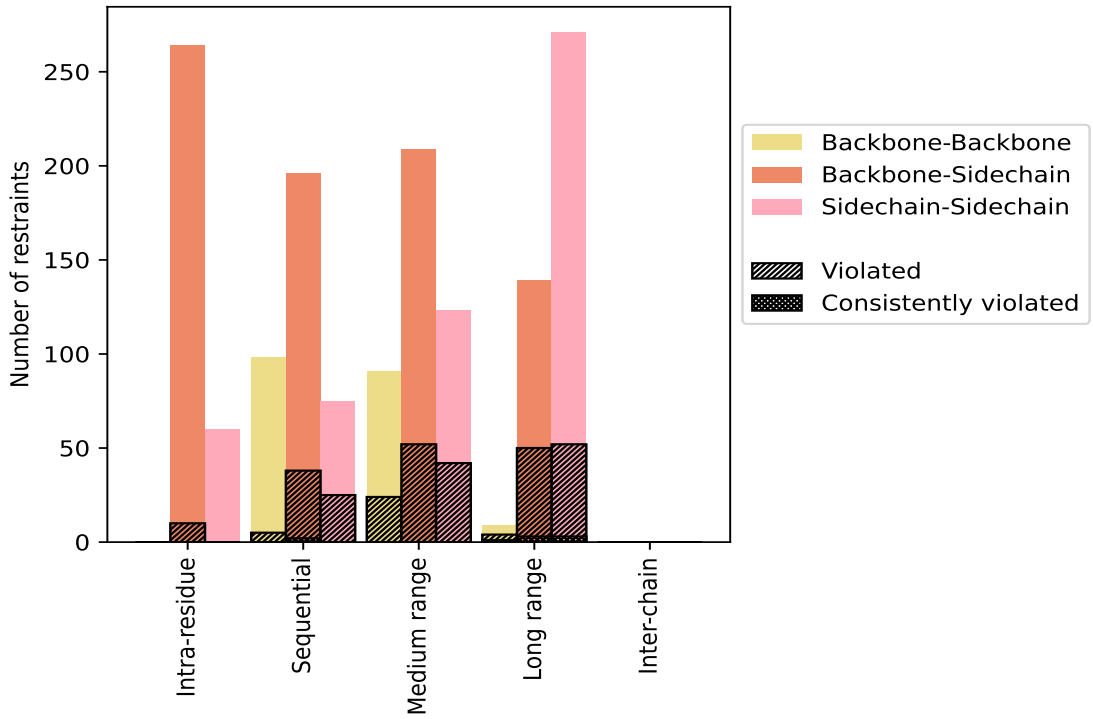
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	324	21.1	10	3.1	0.7	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	264	17.2	10	3.8	0.7	0	0.0	0.0
Sidechain-Sidechain	60	3.9	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	369	24.0	68	18.4	4.4	2	0.5	0.1
Backbone-Backbone	98	6.4	5	5.1	0.3	0	0.0	0.0
Backbone-Sidechain	196	12.8	38	19.4	2.5	2	1.0	0.1
Sidechain-Sidechain	75	4.9	25	33.3	1.6	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	423	27.6	118	27.9	7.7	0	0.0	0.0
Backbone-Backbone	91	5.9	24	26.4	1.6	0	0.0	0.0
Backbone-Sidechain	209	13.6	52	24.9	3.4	0	0.0	0.0
Sidechain-Sidechain	123	8.0	42	34.1	2.7	0	0.0	0.0
Long range (|i-j|≥5)	419	27.3	106	25.3	6.9	7	1.7	0.5
Backbone-Backbone	9	0.6	4	44.4	0.3	1	11.1	0.1
Backbone-Sidechain	139	9.1	50	36.0	3.3	3	2.2	0.2
Sidechain-Sidechain	271	17.7	52	19.2	3.4	3	1.1	0.2
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	1535	100.0	302	19.7	19.7	9	0.6	0.6
Backbone-Backbone	198	12.9	33	16.7	2.1	1	0.5	0.1
Backbone-Sidechain	808	52.6	150	18.6	9.8	5	0.6	0.3
Sidechain-Sidechain	529	34.5	119	22.5	7.8	3	0.6	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 (i)



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 (i)

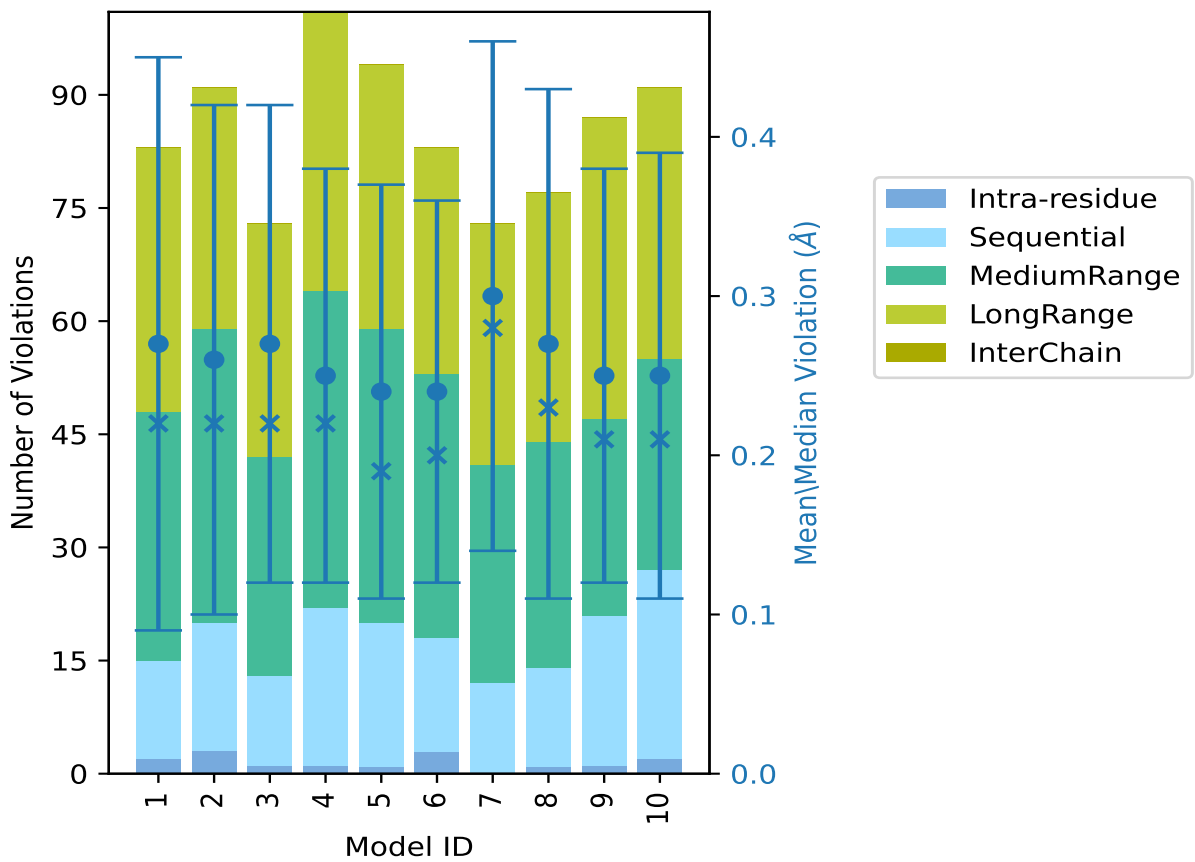
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	2	13	33	35	0	83	0.27	1.22	0.18	0.22
2	3	17	39	32	0	91	0.26	0.94	0.16	0.22
3	1	12	29	31	0	73	0.27	1.03	0.15	0.22
4	1	21	42	37	0	101	0.25	0.8	0.13	0.22
5	1	19	39	35	0	94	0.24	0.65	0.13	0.19
6	3	15	35	30	0	83	0.24	0.63	0.12	0.2
7	0	12	29	32	0	73	0.3	0.72	0.16	0.28
8	1	13	30	33	0	77	0.27	0.87	0.16	0.23
9	1	20	26	40	0	87	0.25	0.6	0.13	0.21
10	2	25	28	36	0	91	0.25	0.87	0.14	0.21

[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 (i)



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, 1233(IR:314, SQ:301, MR:305, LR:313, 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]	%
7	28	42	37	0	114	1	10.0
1	19	27	21	0	68	2	20.0
2	8	16	16	0	42	3	30.0
0	4	10	8	0	22	4	40.0

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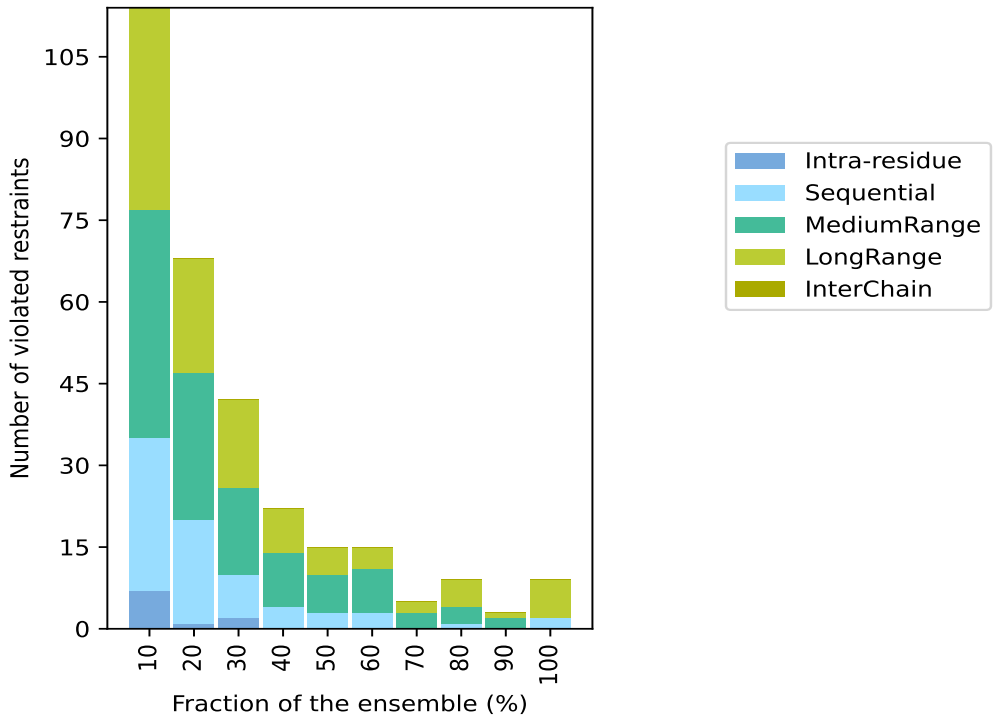
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	3	7	5	0	15	5	50.0
0	3	8	4	0	15	6	60.0
0	0	3	2	0	5	7	70.0
0	1	3	5	0	9	8	80.0
0	0	2	1	0	3	9	90.0
0	2	0	7	0	9	10	100.0

[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

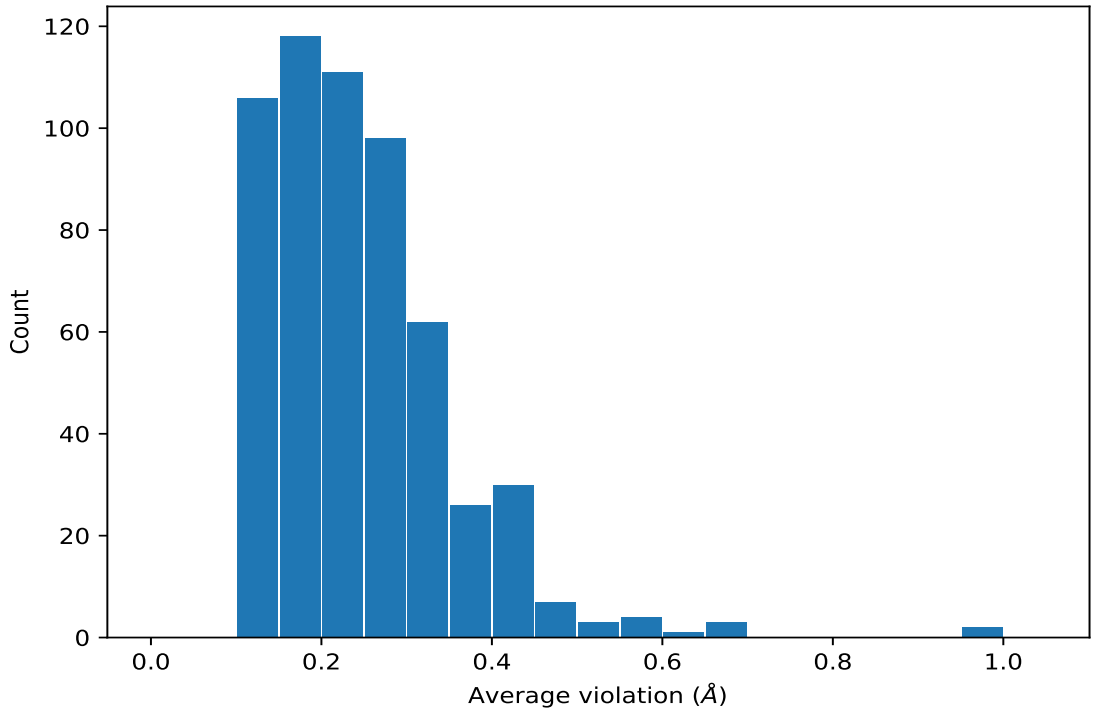
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,735)	1:A:3134:LYS:HA	1:A:3151:TRP:HE1	10	0.58	0.11	0.58
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG21	10	0.42	0.09	0.42
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG22	10	0.42	0.09	0.42
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG23	10	0.42	0.09	0.42
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD11	10	0.35	0.12	0.37
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD12	10	0.35	0.12	0.37
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD13	10	0.35	0.12	0.37
(1,929)	1:A:3115:ILE:HG21	1:A:3207:GLY:H	10	0.33	0.1	0.3
(1,929)	1:A:3115:ILE:HG22	1:A:3207:GLY:H	10	0.33	0.1	0.3
(1,929)	1:A:3115:ILE:HG23	1:A:3207:GLY:H	10	0.33	0.1	0.3
(1,953)	1:A:3143:ILE:HG21	1:A:3212:TRP:HE1	10	0.32	0.11	0.32
(1,953)	1:A:3143:ILE:HG22	1:A:3212:TRP:HE1	10	0.32	0.11	0.32
(1,953)	1:A:3143:ILE:HG23	1:A:3212:TRP:HE1	10	0.32	0.11	0.32
(1,252)	1:A:3140:VAL:HA	1:A:3167:ILE:HA	10	0.31	0.12	0.26
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG2	10	0.25	0.05	0.22
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG3	10	0.25	0.05	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG21	10	0.24	0.03	0.24
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG22	10	0.24	0.03	0.24
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG23	10	0.24	0.03	0.24
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD11	10	0.24	0.08	0.22
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD12	10	0.24	0.08	0.22
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD13	10	0.24	0.08	0.22
(1,991)	1:A:3167:ILE:HA	1:A:3212:TRP:HZ3	9	0.4	0.14	0.35
(1,745)	1:A:3149:SER:HA	1:A:3153:ASP:H	9	0.33	0.07	0.31
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG21	9	0.19	0.06	0.17
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG22	9	0.19	0.06	0.17
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG23	9	0.19	0.06	0.17
(1,436)	1:A:3136:VAL:HG21	1:A:3137:MET:HG3	8	0.65	0.13	0.6
(1,436)	1:A:3136:VAL:HG22	1:A:3137:MET:HG3	8	0.65	0.13	0.6
(1,436)	1:A:3136:VAL:HG23	1:A:3137:MET:HG3	8	0.65	0.13	0.6
(1,961)	1:A:3105:ILE:HG21	1:A:3216:GLN:H	8	0.39	0.15	0.4
(1,961)	1:A:3105:ILE:HG22	1:A:3216:GLN:H	8	0.39	0.15	0.4
(1,961)	1:A:3105:ILE:HG23	1:A:3216:GLN:H	8	0.39	0.15	0.4
(1,950)	1:A:3109:GLN:HG3	1:A:3212:TRP:HE1	8	0.39	0.16	0.32
(1,246)	1:A:3136:VAL:HA	1:A:3210:TYR:HA	8	0.28	0.16	0.26
(1,351)	1:A:3206:CYS:HA	1:A:3209:LEU:HG	8	0.28	0.07	0.29
(1,883)	1:A:3195:THR:HB	1:A:3197:GLU:H	8	0.27	0.15	0.21
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD1	8	0.26	0.09	0.24
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD2	8	0.26	0.09	0.24
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD1	8	0.26	0.09	0.24
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD2	8	0.26	0.09	0.24
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE1	8	0.24	0.04	0.24
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE2	8	0.24	0.04	0.24
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE1	8	0.24	0.04	0.24
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE2	8	0.24	0.04	0.24
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE1	8	0.24	0.04	0.24
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE2	8	0.24	0.04	0.24
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG21	8	0.2	0.07	0.22
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG22	8	0.2	0.07	0.22
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG23	8	0.2	0.07	0.22
(1,1084)	1:A:3144:LEU:HD11	1:A:3212:TRP:HZ2	7	0.29	0.12	0.24
(1,1084)	1:A:3144:LEU:HD12	1:A:3212:TRP:HZ2	7	0.29	0.12	0.24
(1,1084)	1:A:3144:LEU:HD13	1:A:3212:TRP:HZ2	7	0.29	0.12	0.24
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG2	7	0.22	0.05	0.23
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG3	7	0.22	0.05	0.23
(1,673)	1:A:3126:MET:HE1	1:A:3133:VAL:H	7	0.16	0.03	0.17
(1,673)	1:A:3126:MET:HE2	1:A:3133:VAL:H	7	0.16	0.03	0.17
(1,673)	1:A:3126:MET:HE3	1:A:3133:VAL:H	7	0.16	0.03	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,720)	1:A:3140:VAL:HA	1:A:3144:LEU:H	7	0.14	0.04	0.14
(1,932)	1:A:3207:GLY:HA3	1:A:3209:LEU:H	7	0.14	0.02	0.13
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD11	6	0.46	0.08	0.47
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD12	6	0.46	0.08	0.47
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD13	6	0.46	0.08	0.47
(1,25)	1:A:3098:ILE:HD11	1:A:3099:GLN:HA	6	0.43	0.38	0.24
(1,25)	1:A:3098:ILE:HD12	1:A:3099:GLN:HA	6	0.43	0.38	0.24
(1,25)	1:A:3098:ILE:HD13	1:A:3099:GLN:HA	6	0.43	0.38	0.24
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD11	6	0.42	0.17	0.38
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD12	6	0.42	0.17	0.38
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD13	6	0.42	0.17	0.38
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD21	6	0.42	0.17	0.38
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD22	6	0.42	0.17	0.38
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD23	6	0.42	0.17	0.38
(1,345)	1:A:3205:ALA:HB1	1:A:3209:LEU:HB2	6	0.39	0.14	0.38
(1,345)	1:A:3205:ALA:HB2	1:A:3209:LEU:HB2	6	0.39	0.14	0.38
(1,345)	1:A:3205:ALA:HB3	1:A:3209:LEU:HB2	6	0.39	0.14	0.38
(1,1096)	1:A:3099:GLN:HB2	1:A:3101:CYS:H	6	0.31	0.19	0.19
(1,1096)	1:A:3099:GLN:HB3	1:A:3101:CYS:H	6	0.31	0.19	0.19
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG21	6	0.3	0.03	0.31
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG22	6	0.3	0.03	0.31
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG23	6	0.3	0.03	0.31
(1,501)	1:A:3115:ILE:HG21	1:A:3119:GLN:HG2	6	0.3	0.09	0.3
(1,501)	1:A:3115:ILE:HG22	1:A:3119:GLN:HG2	6	0.3	0.09	0.3
(1,501)	1:A:3115:ILE:HG23	1:A:3119:GLN:HG2	6	0.3	0.09	0.3
(1,765)	1:A:3158:ILE:HA	1:A:3160:LYS:H	6	0.28	0.07	0.28
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG11	6	0.25	0.04	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG12	6	0.25	0.04	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG13	6	0.25	0.04	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG21	6	0.25	0.04	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG22	6	0.25	0.04	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG23	6	0.25	0.04	0.24
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG21	6	0.25	0.13	0.22
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG22	6	0.25	0.13	0.22
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG23	6	0.25	0.13	0.22
(1,626)	1:A:3112:VAL:HA	1:A:3115:ILE:H	6	0.24	0.19	0.16
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG21	6	0.23	0.06	0.24
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG22	6	0.23	0.06	0.24
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG23	6	0.23	0.06	0.24
(1,994)	1:A:3108:ALA:HB1	1:A:3212:TRP:HE3	6	0.21	0.09	0.17
(1,994)	1:A:3108:ALA:HB2	1:A:3212:TRP:HE3	6	0.21	0.09	0.17
(1,994)	1:A:3108:ALA:HB3	1:A:3212:TRP:HE3	6	0.21	0.09	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG21	6	0.19	0.03	0.19
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG22	6	0.19	0.03	0.19
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG23	6	0.19	0.03	0.19
(1,934)	1:A:3208:PRO:HG2	1:A:3209:LEU:H	6	0.17	0.02	0.18
(1,934)	1:A:3208:PRO:HG3	1:A:3209:LEU:H	6	0.17	0.02	0.18
(1,1222)	1:A:3130:PRO:HG2	1:A:3132:GLY:HA3	5	0.46	0.07	0.49
(1,1222)	1:A:3130:PRO:HG3	1:A:3132:GLY:HA3	5	0.46	0.07	0.49
(1,837)	1:A:3179:GLN:H	1:A:3182:LYS:H	5	0.37	0.12	0.41
(1,859)	1:A:3185:GLU:HA	1:A:3189:LEU:H	5	0.28	0.19	0.17
(1,867)	1:A:3193:ASN:H	1:A:3195:THR:H	5	0.27	0.06	0.29
(1,808)	1:A:3143:ILE:HG21	1:A:3170:TYR:H	5	0.26	0.12	0.22
(1,808)	1:A:3143:ILE:HG22	1:A:3170:TYR:H	5	0.26	0.12	0.22
(1,808)	1:A:3143:ILE:HG23	1:A:3170:TYR:H	5	0.26	0.12	0.22
(1,888)	1:A:3197:GLU:H	1:A:3210:TYR:HD1	5	0.25	0.16	0.17
(1,888)	1:A:3197:GLU:H	1:A:3210:TYR:HD2	5	0.25	0.16	0.17
(1,482)	1:A:3208:PRO:HA	1:A:3211:GLN:HG2	5	0.25	0.1	0.18
(1,611)	1:A:3111:GLY:H	1:A:3113:LYS:HG3	5	0.21	0.06	0.19
(1,219)	1:A:3112:VAL:HG11	1:A:3212:TRP:HD1	5	0.2	0.05	0.23
(1,219)	1:A:3112:VAL:HG12	1:A:3212:TRP:HD1	5	0.2	0.05	0.23
(1,219)	1:A:3112:VAL:HG13	1:A:3212:TRP:HD1	5	0.2	0.05	0.23
(1,49)	1:A:3115:ILE:HD11	1:A:3205:ALA:HA	5	0.18	0.05	0.19
(1,49)	1:A:3115:ILE:HD12	1:A:3205:ALA:HA	5	0.18	0.05	0.19
(1,49)	1:A:3115:ILE:HD13	1:A:3205:ALA:HA	5	0.18	0.05	0.19
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD11	5	0.18	0.07	0.18
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD12	5	0.18	0.07	0.18
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD13	5	0.18	0.07	0.18
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD11	5	0.18	0.07	0.18
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD12	5	0.18	0.07	0.18
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD13	5	0.18	0.07	0.18
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD11	5	0.17	0.06	0.15
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD12	5	0.17	0.06	0.15
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD13	5	0.17	0.06	0.15
(1,747)	1:A:3153:ASP:H	1:A:3154:ILE:HG13	5	0.15	0.03	0.15
(1,1493)	1:A:3214:ASN:HB2	1:A:3217:ILE:HB	5	0.15	0.04	0.13
(1,1493)	1:A:3214:ASN:HB3	1:A:3217:ILE:HB	5	0.15	0.04	0.13
(1,410)	1:A:3209:LEU:HD11	1:A:3210:TYR:HA	5	0.13	0.01	0.13
(1,410)	1:A:3209:LEU:HD12	1:A:3210:TYR:HA	5	0.13	0.01	0.13
(1,410)	1:A:3209:LEU:HD13	1:A:3210:TYR:HA	5	0.13	0.01	0.13
(1,434)	1:A:3136:VAL:HG21	1:A:3137:MET:HG2	4	0.43	0.13	0.44
(1,434)	1:A:3136:VAL:HG22	1:A:3137:MET:HG2	4	0.43	0.13	0.44
(1,434)	1:A:3136:VAL:HG23	1:A:3137:MET:HG2	4	0.43	0.13	0.44
(1,437)	1:A:3134:LYS:HA	1:A:3137:MET:HG3	4	0.43	0.12	0.46

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG21	4	0.37	0.16	0.34
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG22	4	0.37	0.16	0.34
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG23	4	0.37	0.16	0.34
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG21	4	0.37	0.16	0.34
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG22	4	0.37	0.16	0.34
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG23	4	0.37	0.16	0.34
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG21	4	0.37	0.16	0.34
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG22	4	0.37	0.16	0.34
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG23	4	0.37	0.16	0.34
(1,343)	1:A:3185:GLU:HA	1:A:3189:LEU:HB2	4	0.31	0.14	0.24
(1,1094)	1:A:3098:ILE:HD11	1:A:3099:GLN:HB2	4	0.3	0.14	0.29
(1,1094)	1:A:3098:ILE:HD11	1:A:3099:GLN:HB3	4	0.3	0.14	0.29
(1,1094)	1:A:3098:ILE:HD12	1:A:3099:GLN:HB2	4	0.3	0.14	0.29
(1,1094)	1:A:3098:ILE:HD12	1:A:3099:GLN:HB3	4	0.3	0.14	0.29
(1,1094)	1:A:3098:ILE:HD13	1:A:3099:GLN:HB2	4	0.3	0.14	0.29
(1,1094)	1:A:3098:ILE:HD13	1:A:3099:GLN:HB3	4	0.3	0.14	0.29
(1,159)	1:A:3167:ILE:HG21	1:A:3170:TYR:HB2	4	0.28	0.11	0.25
(1,159)	1:A:3167:ILE:HG22	1:A:3170:TYR:HB2	4	0.28	0.11	0.25
(1,159)	1:A:3167:ILE:HG23	1:A:3170:TYR:HB2	4	0.28	0.11	0.25
(1,1177)	1:A:3123:ILE:HB	1:A:3126:MET:HG2	4	0.26	0.19	0.16
(1,1177)	1:A:3123:ILE:HB	1:A:3126:MET:HG3	4	0.26	0.19	0.16
(1,1382)	1:A:3170:TYR:HB2	1:A:3212:TRP:HH2	4	0.25	0.13	0.21
(1,1382)	1:A:3170:TYR:HB3	1:A:3212:TRP:HH2	4	0.25	0.13	0.21
(1,50)	1:A:3115:ILE:HD11	1:A:3209:LEU:H	4	0.25	0.06	0.26
(1,50)	1:A:3115:ILE:HD12	1:A:3209:LEU:H	4	0.25	0.06	0.26
(1,50)	1:A:3115:ILE:HD13	1:A:3209:LEU:H	4	0.25	0.06	0.26
(1,872)	1:A:3192:PRO:HB3	1:A:3194:PHE:H	4	0.25	0.07	0.24
(1,76)	1:A:3135:ILE:HG21	1:A:3193:ASN:HB2	4	0.24	0.06	0.25
(1,76)	1:A:3135:ILE:HG21	1:A:3193:ASN:HB3	4	0.24	0.06	0.25
(1,76)	1:A:3135:ILE:HG22	1:A:3193:ASN:HB2	4	0.24	0.06	0.25
(1,76)	1:A:3135:ILE:HG22	1:A:3193:ASN:HB3	4	0.24	0.06	0.25
(1,76)	1:A:3135:ILE:HG23	1:A:3193:ASN:HB2	4	0.24	0.06	0.25
(1,76)	1:A:3135:ILE:HG23	1:A:3193:ASN:HB3	4	0.24	0.06	0.25
(1,1001)	1:A:3183:TYR:HE1	1:A:3187:GLU:HB2	4	0.22	0.05	0.2
(1,1001)	1:A:3183:TYR:HE1	1:A:3187:GLU:HB3	4	0.22	0.05	0.2
(1,1001)	1:A:3183:TYR:HE2	1:A:3187:GLU:HB2	4	0.22	0.05	0.2
(1,1001)	1:A:3183:TYR:HE2	1:A:3187:GLU:HB3	4	0.22	0.05	0.2
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG21	4	0.2	0.1	0.16
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG22	4	0.2	0.1	0.16
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG23	4	0.2	0.1	0.16
(1,1150)	1:A:3119:GLN:HB2	1:A:3205:ALA:HA	4	0.2	0.07	0.18
(1,1150)	1:A:3119:GLN:HB3	1:A:3205:ALA:HA	4	0.2	0.07	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,617)	1:A:3111:GLY:H	1:A:3113:LYS:H	4	0.19	0.09	0.14
(1,1236)	1:A:3133:VAL:HG11	1:A:3202:ALA:H	4	0.18	0.06	0.19
(1,1236)	1:A:3133:VAL:HG12	1:A:3202:ALA:H	4	0.18	0.06	0.19
(1,1236)	1:A:3133:VAL:HG13	1:A:3202:ALA:H	4	0.18	0.06	0.19
(1,1236)	1:A:3133:VAL:HG21	1:A:3202:ALA:H	4	0.18	0.06	0.19
(1,1236)	1:A:3133:VAL:HG22	1:A:3202:ALA:H	4	0.18	0.06	0.19
(1,1236)	1:A:3133:VAL:HG23	1:A:3202:ALA:H	4	0.18	0.06	0.19
(1,712)	1:A:3152:ARG:H	1:A:3154:ILE:H	4	0.17	0.01	0.18
(1,764)	1:A:3159:ARG:H	1:A:3163:PHE:HD1	4	0.17	0.03	0.16
(1,764)	1:A:3159:ARG:H	1:A:3163:PHE:HD2	4	0.17	0.03	0.16
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG21	4	0.17	0.01	0.17
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG22	4	0.17	0.01	0.17
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG23	4	0.17	0.01	0.17
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD11	4	0.16	0.02	0.16
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD12	4	0.16	0.02	0.16
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD13	4	0.16	0.02	0.16
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD11	4	0.16	0.02	0.16
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD12	4	0.16	0.02	0.16
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD13	4	0.16	0.02	0.16
(1,1442)	1:A:3195:THR:HG21	1:A:3197:GLU:HG2	4	0.13	0.02	0.14
(1,1442)	1:A:3195:THR:HG21	1:A:3197:GLU:HG3	4	0.13	0.02	0.14
(1,1442)	1:A:3195:THR:HG22	1:A:3197:GLU:HG2	4	0.13	0.02	0.14
(1,1442)	1:A:3195:THR:HG22	1:A:3197:GLU:HG3	4	0.13	0.02	0.14
(1,1442)	1:A:3195:THR:HG23	1:A:3197:GLU:HG2	4	0.13	0.02	0.14
(1,1442)	1:A:3195:THR:HG23	1:A:3197:GLU:HG3	4	0.13	0.02	0.14
(1,928)	1:A:3207:GLY:H	1:A:3208:PRO:HG2	4	0.13	0.02	0.12
(1,928)	1:A:3207:GLY:H	1:A:3208:PRO:HG3	4	0.13	0.02	0.12
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD11	3	0.43	0.19	0.48
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD12	3	0.43	0.19	0.48
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD13	3	0.43	0.19	0.48
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD21	3	0.43	0.19	0.48
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD22	3	0.43	0.19	0.48
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD23	3	0.43	0.19	0.48
(1,842)	1:A:3185:GLU:H	1:A:3217:ILE:HD11	3	0.38	0.07	0.34
(1,842)	1:A:3185:GLU:H	1:A:3217:ILE:HD12	3	0.38	0.07	0.34
(1,842)	1:A:3185:GLU:H	1:A:3217:ILE:HD13	3	0.38	0.07	0.34
(1,1392)	1:A:3178:PRO:HB2	1:A:3181:ARG:H	3	0.34	0.26	0.16
(1,1392)	1:A:3178:PRO:HB3	1:A:3181:ARG:H	3	0.34	0.26	0.16
(1,182)	1:A:3195:THR:HG21	1:A:3199:ILE:HB	3	0.32	0.11	0.39
(1,182)	1:A:3195:THR:HG22	1:A:3199:ILE:HB	3	0.32	0.11	0.39
(1,182)	1:A:3195:THR:HG23	1:A:3199:ILE:HB	3	0.32	0.11	0.39
(1,815)	1:A:3173:THR:H	1:A:3173:THR:HG21	3	0.32	0.02	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,815)	1:A:3173:THR:H	1:A:3173:THR:HG22	3	0.32	0.02	0.32
(1,815)	1:A:3173:THR:H	1:A:3173:THR:HG23	3	0.32	0.02	0.32
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG11	3	0.32	0.08	0.33
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG12	3	0.32	0.08	0.33
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG13	3	0.32	0.08	0.33
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG21	3	0.32	0.08	0.33
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG22	3	0.32	0.08	0.33
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG23	3	0.32	0.08	0.33
(1,1439)	1:A:3192:PRO:HB2	1:A:3194:PHE:H	3	0.31	0.04	0.34
(1,1439)	1:A:3192:PRO:HB3	1:A:3194:PHE:H	3	0.31	0.04	0.34
(1,1000)	1:A:3183:TYR:HE1	1:A:3187:GLU:HG2	3	0.29	0.09	0.35
(1,1000)	1:A:3183:TYR:HE2	1:A:3187:GLU:HG2	3	0.29	0.09	0.35
(1,755)	1:A:3155:GLN:HG2	1:A:3157:PHE:H	3	0.29	0.19	0.18
(1,755)	1:A:3155:GLN:HG3	1:A:3157:PHE:H	3	0.29	0.19	0.18
(1,1391)	1:A:3178:PRO:HB2	1:A:3180:ILE:H	3	0.29	0.05	0.26
(1,1391)	1:A:3178:PRO:HB3	1:A:3180:ILE:H	3	0.29	0.05	0.26
(1,48)	1:A:3112:VAL:HA	1:A:3115:ILE:HD11	3	0.27	0.13	0.25
(1,48)	1:A:3112:VAL:HA	1:A:3115:ILE:HD12	3	0.27	0.13	0.25
(1,48)	1:A:3112:VAL:HA	1:A:3115:ILE:HD13	3	0.27	0.13	0.25
(1,231)	1:A:3140:VAL:HG11	1:A:3212:TRP:HH2	3	0.27	0.04	0.28
(1,231)	1:A:3140:VAL:HG12	1:A:3212:TRP:HH2	3	0.27	0.04	0.28
(1,231)	1:A:3140:VAL:HG13	1:A:3212:TRP:HH2	3	0.27	0.04	0.28
(1,853)	1:A:3185:GLU:HA	1:A:3188:PHE:H	3	0.27	0.1	0.24
(1,951)	1:A:3108:ALA:HB1	1:A:3212:TRP:HE1	3	0.26	0.11	0.24
(1,951)	1:A:3108:ALA:HB2	1:A:3212:TRP:HE1	3	0.26	0.11	0.24
(1,951)	1:A:3108:ALA:HB3	1:A:3212:TRP:HE1	3	0.26	0.11	0.24
(1,79)	1:A:3135:ILE:HG21	1:A:3194:PHE:HA	3	0.25	0.06	0.21
(1,79)	1:A:3135:ILE:HG22	1:A:3194:PHE:HA	3	0.25	0.06	0.21
(1,79)	1:A:3135:ILE:HG23	1:A:3194:PHE:HA	3	0.25	0.06	0.21
(1,1069)	1:A:3105:ILE:HG21	1:A:3212:TRP:HD1	3	0.25	0.07	0.2
(1,1069)	1:A:3105:ILE:HG22	1:A:3212:TRP:HD1	3	0.25	0.07	0.2
(1,1069)	1:A:3105:ILE:HG23	1:A:3212:TRP:HD1	3	0.25	0.07	0.2
(1,548)	1:A:3152:ARG:HA	1:A:3152:ARG:HD2	3	0.24	0.04	0.24
(1,548)	1:A:3152:ARG:HA	1:A:3152:ARG:HD3	3	0.24	0.04	0.24
(1,1424)	1:A:3188:PHE:HB2	1:A:3190:SER:H	3	0.24	0.16	0.13
(1,1424)	1:A:3188:PHE:HB3	1:A:3190:SER:H	3	0.24	0.16	0.13
(1,412)	1:A:3136:VAL:HG11	1:A:3210:TYR:HB3	3	0.23	0.05	0.2
(1,412)	1:A:3136:VAL:HG12	1:A:3210:TYR:HB3	3	0.23	0.05	0.2
(1,412)	1:A:3136:VAL:HG13	1:A:3210:TYR:HB3	3	0.23	0.05	0.2
(1,697)	1:A:3139:ALA:H	1:A:3184:MET:HE1	3	0.23	0.1	0.18
(1,697)	1:A:3139:ALA:H	1:A:3184:MET:HE2	3	0.23	0.1	0.18
(1,697)	1:A:3139:ALA:H	1:A:3184:MET:HE3	3	0.23	0.1	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,342)	1:A:3185:GLU:HA	1:A:3189:LEU:HB3	3	0.22	0.08	0.2
(1,1414)	1:A:3185:GLU:HG2	1:A:3217:ILE:HG21	3	0.22	0.05	0.21
(1,1414)	1:A:3185:GLU:HG2	1:A:3217:ILE:HG22	3	0.22	0.05	0.21
(1,1414)	1:A:3185:GLU:HG2	1:A:3217:ILE:HG23	3	0.22	0.05	0.21
(1,1414)	1:A:3185:GLU:HG3	1:A:3217:ILE:HG21	3	0.22	0.05	0.21
(1,1414)	1:A:3185:GLU:HG3	1:A:3217:ILE:HG22	3	0.22	0.05	0.21
(1,1414)	1:A:3185:GLU:HG3	1:A:3217:ILE:HG23	3	0.22	0.05	0.21
(1,200)	1:A:3181:ARG:HD2	1:A:3217:ILE:HA	3	0.21	0.06	0.2
(1,200)	1:A:3181:ARG:HD3	1:A:3217:ILE:HA	3	0.21	0.06	0.2
(1,327)	1:A:3189:LEU:HD11	1:A:3190:SER:HB2	3	0.21	0.02	0.2
(1,327)	1:A:3189:LEU:HD12	1:A:3190:SER:HB2	3	0.21	0.02	0.2
(1,327)	1:A:3189:LEU:HD13	1:A:3190:SER:HB2	3	0.21	0.02	0.2
(1,956)	1:A:3213:VAL:HB	1:A:3214:ASN:H	3	0.21	0.05	0.21
(1,117)	1:A:3158:ILE:HD11	1:A:3163:PHE:HE1	3	0.19	0.06	0.17
(1,117)	1:A:3158:ILE:HD11	1:A:3163:PHE:HE2	3	0.19	0.06	0.17
(1,117)	1:A:3158:ILE:HD12	1:A:3163:PHE:HE1	3	0.19	0.06	0.17
(1,117)	1:A:3158:ILE:HD12	1:A:3163:PHE:HE2	3	0.19	0.06	0.17
(1,117)	1:A:3158:ILE:HD13	1:A:3163:PHE:HE1	3	0.19	0.06	0.17
(1,117)	1:A:3158:ILE:HD13	1:A:3163:PHE:HE2	3	0.19	0.06	0.17
(1,1450)	1:A:3197:GLU:HG2	1:A:3199:ILE:H	3	0.19	0.08	0.16
(1,1450)	1:A:3197:GLU:HG3	1:A:3199:ILE:H	3	0.19	0.08	0.16
(1,549)	1:A:3120:LEU:HG	1:A:3163:PHE:HB3	3	0.19	0.03	0.17
(1,307)	1:A:3200:ASN:HB3	1:A:3207:GLY:HA2	3	0.18	0.01	0.18
(1,829)	1:A:3179:GLN:H	1:A:3180:ILE:HA	3	0.18	0.05	0.16
(1,1516)	1:A:3224:GLU:HA	1:A:3225:ASN:HB2	3	0.18	0.04	0.19
(1,1516)	1:A:3224:GLU:HA	1:A:3225:ASN:HB3	3	0.18	0.04	0.19
(1,1327)	1:A:3144:LEU:HD11	1:A:3170:TYR:H	3	0.18	0.04	0.15
(1,1327)	1:A:3144:LEU:HD12	1:A:3170:TYR:H	3	0.18	0.04	0.15
(1,1327)	1:A:3144:LEU:HD13	1:A:3170:TYR:H	3	0.18	0.04	0.15
(1,1327)	1:A:3144:LEU:HD21	1:A:3170:TYR:H	3	0.18	0.04	0.15
(1,1327)	1:A:3144:LEU:HD22	1:A:3170:TYR:H	3	0.18	0.04	0.15
(1,1327)	1:A:3144:LEU:HD23	1:A:3170:TYR:H	3	0.18	0.04	0.15
(1,1405)	1:A:3184:MET:HB2	1:A:3185:GLU:H	3	0.17	0.05	0.15
(1,1405)	1:A:3184:MET:HB3	1:A:3185:GLU:H	3	0.17	0.05	0.15
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG11	3	0.17	0.06	0.13
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG12	3	0.17	0.06	0.13
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG13	3	0.17	0.06	0.13
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG21	3	0.17	0.06	0.13
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG22	3	0.17	0.06	0.13
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG23	3	0.17	0.06	0.13
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG11	3	0.17	0.06	0.13
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG12	3	0.17	0.06	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG13	3	0.17	0.06	0.13
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG21	3	0.17	0.06	0.13
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG22	3	0.17	0.06	0.13
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG23	3	0.17	0.06	0.13
(1,287)	1:A:3132:GLY:HA3	1:A:3202:ALA:HA	3	0.16	0.02	0.16
(1,791)	1:A:3164:ILE:HG21	1:A:3167:ILE:H	3	0.16	0.01	0.15
(1,791)	1:A:3164:ILE:HG22	1:A:3167:ILE:H	3	0.16	0.01	0.15
(1,791)	1:A:3164:ILE:HG23	1:A:3167:ILE:H	3	0.16	0.01	0.15
(1,1056)	1:A:3196:TYR:HE1	1:A:3199:ILE:HG21	3	0.15	0.05	0.12
(1,1056)	1:A:3196:TYR:HE1	1:A:3199:ILE:HG22	3	0.15	0.05	0.12
(1,1056)	1:A:3196:TYR:HE1	1:A:3199:ILE:HG23	3	0.15	0.05	0.12
(1,1056)	1:A:3196:TYR:HE2	1:A:3199:ILE:HG21	3	0.15	0.05	0.12
(1,1056)	1:A:3196:TYR:HE2	1:A:3199:ILE:HG22	3	0.15	0.05	0.12
(1,1056)	1:A:3196:TYR:HE2	1:A:3199:ILE:HG23	3	0.15	0.05	0.12
(1,1118)	1:A:3106:LEU:HD11	1:A:3109:GLN:HG2	3	0.15	0.03	0.13
(1,1118)	1:A:3106:LEU:HD12	1:A:3109:GLN:HG2	3	0.15	0.03	0.13
(1,1118)	1:A:3106:LEU:HD13	1:A:3109:GLN:HG2	3	0.15	0.03	0.13
(1,1118)	1:A:3106:LEU:HD21	1:A:3109:GLN:HG2	3	0.15	0.03	0.13
(1,1118)	1:A:3106:LEU:HD22	1:A:3109:GLN:HG2	3	0.15	0.03	0.13
(1,1118)	1:A:3106:LEU:HD23	1:A:3109:GLN:HG2	3	0.15	0.03	0.13
(1,1399)	1:A:3181:ARG:HB2	1:A:3217:ILE:HD11	3	0.14	0.01	0.15
(1,1399)	1:A:3181:ARG:HB2	1:A:3217:ILE:HD12	3	0.14	0.01	0.15
(1,1399)	1:A:3181:ARG:HB2	1:A:3217:ILE:HD13	3	0.14	0.01	0.15
(1,1399)	1:A:3181:ARG:HB3	1:A:3217:ILE:HD11	3	0.14	0.01	0.15
(1,1399)	1:A:3181:ARG:HB3	1:A:3217:ILE:HD12	3	0.14	0.01	0.15
(1,1399)	1:A:3181:ARG:HB3	1:A:3217:ILE:HD13	3	0.14	0.01	0.15
(1,1199)	1:A:3126:MET:HE1	1:A:3203:SER:HB2	3	0.14	0.02	0.14
(1,1199)	1:A:3126:MET:HE1	1:A:3203:SER:HB3	3	0.14	0.02	0.14
(1,1199)	1:A:3126:MET:HE2	1:A:3203:SER:HB2	3	0.14	0.02	0.14
(1,1199)	1:A:3126:MET:HE2	1:A:3203:SER:HB3	3	0.14	0.02	0.14
(1,1199)	1:A:3126:MET:HE3	1:A:3203:SER:HB2	3	0.14	0.02	0.14
(1,1199)	1:A:3126:MET:HE3	1:A:3203:SER:HB3	3	0.14	0.02	0.14
(1,1344)	1:A:3152:ARG:HB3	1:A:3153:ASP:HB2	3	0.14	0.04	0.12
(1,1344)	1:A:3152:ARG:HB3	1:A:3153:ASP:HB3	3	0.14	0.04	0.12
(1,429)	1:A:3137:MET:HA	1:A:3140:VAL:HB	3	0.13	0.02	0.13
(1,1436)	1:A:3191:ASP:HB2	1:A:3193:ASN:H	2	0.98	0.05	0.98
(1,1436)	1:A:3191:ASP:HB3	1:A:3193:ASN:H	2	0.98	0.05	0.98
(1,757)	1:A:3158:ILE:H	1:A:3160:LYS:H	2	0.64	0.12	0.64
(1,16)	1:A:3136:VAL:HA	1:A:3137:MET:HE1	2	0.55	0.01	0.55
(1,16)	1:A:3136:VAL:HA	1:A:3137:MET:HE2	2	0.55	0.01	0.55
(1,16)	1:A:3136:VAL:HA	1:A:3137:MET:HE3	2	0.55	0.01	0.55
(1,846)	1:A:3184:MET:HA	1:A:3186:GLU:H	2	0.52	0.2	0.52

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1519)	1:A:3225:ASN:HB2	1:A:3227:ASP:H	2	0.5	0.1	0.5
(1,1519)	1:A:3225:ASN:HB3	1:A:3227:ASP:H	2	0.5	0.1	0.5
(1,1497)	1:A:3216:GLN:HA	1:A:3219:PHE:HB2	2	0.46	0.34	0.46
(1,1497)	1:A:3216:GLN:HA	1:A:3219:PHE:HB3	2	0.46	0.34	0.46
(1,457)	1:A:3214:ASN:HB2	1:A:3217:ILE:HG21	2	0.44	0.2	0.44
(1,457)	1:A:3214:ASN:HB2	1:A:3217:ILE:HG22	2	0.44	0.2	0.44
(1,457)	1:A:3214:ASN:HB2	1:A:3217:ILE:HG23	2	0.44	0.2	0.44
(1,845)	1:A:3185:GLU:H	1:A:3186:GLU:H	2	0.43	0.26	0.43
(1,77)	1:A:3132:GLY:HA2	1:A:3135:ILE:HG21	2	0.42	0.02	0.42
(1,77)	1:A:3132:GLY:HA2	1:A:3135:ILE:HG22	2	0.42	0.02	0.42
(1,77)	1:A:3132:GLY:HA2	1:A:3135:ILE:HG23	2	0.42	0.02	0.42
(1,372)	1:A:3189:LEU:HD11	1:A:3190:SER:HB3	2	0.37	0.07	0.37
(1,372)	1:A:3189:LEU:HD12	1:A:3190:SER:HB3	2	0.37	0.07	0.37
(1,372)	1:A:3189:LEU:HD13	1:A:3190:SER:HB3	2	0.37	0.07	0.37
(1,328)	1:A:3106:LEU:HD21	1:A:3109:GLN:HG3	2	0.36	0.13	0.36
(1,328)	1:A:3106:LEU:HD22	1:A:3109:GLN:HG3	2	0.36	0.13	0.36
(1,328)	1:A:3106:LEU:HD23	1:A:3109:GLN:HG3	2	0.36	0.13	0.36
(1,1428)	1:A:3189:LEU:HD11	1:A:3190:SER:HB2	2	0.35	0.21	0.35
(1,1428)	1:A:3189:LEU:HD11	1:A:3190:SER:HB3	2	0.35	0.21	0.35
(1,1428)	1:A:3189:LEU:HD12	1:A:3190:SER:HB2	2	0.35	0.21	0.35
(1,1428)	1:A:3189:LEU:HD12	1:A:3190:SER:HB3	2	0.35	0.21	0.35
(1,1428)	1:A:3189:LEU:HD13	1:A:3190:SER:HB2	2	0.35	0.21	0.35
(1,1428)	1:A:3189:LEU:HD13	1:A:3190:SER:HB3	2	0.35	0.21	0.35
(1,1428)	1:A:3189:LEU:HD21	1:A:3190:SER:HB2	2	0.35	0.21	0.35
(1,1428)	1:A:3189:LEU:HD21	1:A:3190:SER:HB3	2	0.35	0.21	0.35
(1,1428)	1:A:3189:LEU:HD22	1:A:3190:SER:HB2	2	0.35	0.21	0.35
(1,1428)	1:A:3189:LEU:HD22	1:A:3190:SER:HB3	2	0.35	0.21	0.35
(1,1428)	1:A:3189:LEU:HD23	1:A:3190:SER:HB2	2	0.35	0.21	0.35
(1,1428)	1:A:3189:LEU:HD23	1:A:3190:SER:HB3	2	0.35	0.21	0.35
(1,861)	1:A:3187:GLU:HB2	1:A:3189:LEU:H	2	0.34	0.09	0.34
(1,861)	1:A:3187:GLU:HB3	1:A:3189:LEU:H	2	0.34	0.09	0.34
(1,1091)	1:A:3098:ILE:HG21	1:A:3099:GLN:HB2	2	0.34	0.04	0.34
(1,1091)	1:A:3098:ILE:HG21	1:A:3099:GLN:HB3	2	0.34	0.04	0.34
(1,1091)	1:A:3098:ILE:HG22	1:A:3099:GLN:HB2	2	0.34	0.04	0.34
(1,1091)	1:A:3098:ILE:HG22	1:A:3099:GLN:HB3	2	0.34	0.04	0.34
(1,1091)	1:A:3098:ILE:HG23	1:A:3099:GLN:HB2	2	0.34	0.04	0.34
(1,1091)	1:A:3098:ILE:HG23	1:A:3099:GLN:HB3	2	0.34	0.04	0.34
(1,32)	1:A:3105:ILE:HD11	1:A:3215:ALA:HB1	2	0.32	0.08	0.32
(1,32)	1:A:3105:ILE:HD11	1:A:3215:ALA:HB2	2	0.32	0.08	0.32
(1,32)	1:A:3105:ILE:HD11	1:A:3215:ALA:HB3	2	0.32	0.08	0.32
(1,32)	1:A:3105:ILE:HD12	1:A:3215:ALA:HB1	2	0.32	0.08	0.32
(1,32)	1:A:3105:ILE:HD12	1:A:3215:ALA:HB2	2	0.32	0.08	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,32)	1:A:3105:ILE:HD12	1:A:3215:ALA:HB3	2	0.32	0.08	0.32
(1,32)	1:A:3105:ILE:HD13	1:A:3215:ALA:HB1	2	0.32	0.08	0.32
(1,32)	1:A:3105:ILE:HD13	1:A:3215:ALA:HB2	2	0.32	0.08	0.32
(1,32)	1:A:3105:ILE:HD13	1:A:3215:ALA:HB3	2	0.32	0.08	0.32
(1,176)	1:A:3143:ILE:HA	1:A:3180:ILE:HG21	2	0.32	0.18	0.32
(1,176)	1:A:3143:ILE:HA	1:A:3180:ILE:HG22	2	0.32	0.18	0.32
(1,176)	1:A:3143:ILE:HA	1:A:3180:ILE:HG23	2	0.32	0.18	0.32
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD11	2	0.3	0.06	0.3
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD12	2	0.3	0.06	0.3
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD13	2	0.3	0.06	0.3
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD21	2	0.3	0.06	0.3
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD22	2	0.3	0.06	0.3
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD23	2	0.3	0.06	0.3
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD11	2	0.3	0.06	0.3
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD12	2	0.3	0.06	0.3
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD13	2	0.3	0.06	0.3
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD21	2	0.3	0.06	0.3
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD22	2	0.3	0.06	0.3
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD23	2	0.3	0.06	0.3
(1,1100)	1:A:3101:CYS:HB2	1:A:3104:THR:HG21	2	0.3	0.1	0.3
(1,1100)	1:A:3101:CYS:HB2	1:A:3104:THR:HG22	2	0.3	0.1	0.3
(1,1100)	1:A:3101:CYS:HB2	1:A:3104:THR:HG23	2	0.3	0.1	0.3
(1,1100)	1:A:3101:CYS:HB3	1:A:3104:THR:HG21	2	0.3	0.1	0.3
(1,1100)	1:A:3101:CYS:HB3	1:A:3104:THR:HG22	2	0.3	0.1	0.3
(1,1100)	1:A:3101:CYS:HB3	1:A:3104:THR:HG23	2	0.3	0.1	0.3
(1,624)	1:A:3113:LYS:H	1:A:3115:ILE:H	2	0.28	0.14	0.28
(1,526)	1:A:3110:ARG:HA	1:A:3113:LYS:HB2	2	0.28	0.14	0.28
(1,974)	1:A:3224:GLU:H	1:A:3225:ASN:HA	2	0.25	0.05	0.25
(1,1432)	1:A:3190:SER:H	1:A:3191:ASP:HB2	2	0.25	0.07	0.25
(1,1432)	1:A:3190:SER:H	1:A:3191:ASP:HB3	2	0.25	0.07	0.25
(1,863)	1:A:3188:PHE:HA	1:A:3190:SER:H	2	0.24	0.12	0.24
(1,1410)	1:A:3185:GLU:H	1:A:3187:GLU:HG2	2	0.24	0.03	0.24
(1,1410)	1:A:3185:GLU:H	1:A:3187:GLU:HG3	2	0.24	0.03	0.24
(1,588)	1:A:3098:ILE:HD11	1:A:3099:GLN:H	2	0.23	0.02	0.23
(1,588)	1:A:3098:ILE:HD12	1:A:3099:GLN:H	2	0.23	0.02	0.23
(1,588)	1:A:3098:ILE:HD13	1:A:3099:GLN:H	2	0.23	0.02	0.23
(1,440)	1:A:3184:MET:HA	1:A:3217:ILE:HD11	2	0.22	0.08	0.22
(1,440)	1:A:3184:MET:HA	1:A:3217:ILE:HD12	2	0.22	0.08	0.22
(1,440)	1:A:3184:MET:HA	1:A:3217:ILE:HD13	2	0.22	0.08	0.22
(1,856)	1:A:3187:GLU:HB2	1:A:3188:PHE:H	2	0.22	0.03	0.22
(1,856)	1:A:3187:GLU:HB3	1:A:3188:PHE:H	2	0.22	0.03	0.22
(1,1419)	1:A:3187:GLU:HG2	1:A:3188:PHE:H	2	0.22	0.04	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1419)	1:A:3187:GLU:HG3	1:A:3188:PHE:H	2	0.22	0.04	0.22
(1,1506)	1:A:3218:ASN:HB2	1:A:3221:LYS:HG2	2	0.22	0.02	0.22
(1,1506)	1:A:3218:ASN:HB2	1:A:3221:LYS:HG3	2	0.22	0.02	0.22
(1,1506)	1:A:3218:ASN:HB3	1:A:3221:LYS:HG2	2	0.22	0.02	0.22
(1,1506)	1:A:3218:ASN:HB3	1:A:3221:LYS:HG3	2	0.22	0.02	0.22
(1,1038)	1:A:3142:ALA:HB1	1:A:3183:TYR:HD1	2	0.22	0.02	0.22
(1,1038)	1:A:3142:ALA:HB1	1:A:3183:TYR:HD2	2	0.22	0.02	0.22
(1,1038)	1:A:3142:ALA:HB2	1:A:3183:TYR:HD1	2	0.22	0.02	0.22
(1,1038)	1:A:3142:ALA:HB2	1:A:3183:TYR:HD2	2	0.22	0.02	0.22
(1,1038)	1:A:3142:ALA:HB3	1:A:3183:TYR:HD1	2	0.22	0.02	0.22
(1,1038)	1:A:3142:ALA:HB3	1:A:3183:TYR:HD2	2	0.22	0.02	0.22
(1,442)	1:A:3184:MET:HG2	1:A:3217:ILE:HD11	2	0.21	0.02	0.21
(1,442)	1:A:3184:MET:HG2	1:A:3217:ILE:HD12	2	0.21	0.02	0.21
(1,442)	1:A:3184:MET:HG2	1:A:3217:ILE:HD13	2	0.21	0.02	0.21
(1,638)	1:A:3119:GLN:H	1:A:3205:ALA:HB1	2	0.21	0.09	0.21
(1,638)	1:A:3119:GLN:H	1:A:3205:ALA:HB2	2	0.21	0.09	0.21
(1,638)	1:A:3119:GLN:H	1:A:3205:ALA:HB3	2	0.21	0.09	0.21
(1,876)	1:A:3135:ILE:HD11	1:A:3195:THR:H	2	0.2	0.03	0.2
(1,876)	1:A:3135:ILE:HD12	1:A:3195:THR:H	2	0.2	0.03	0.2
(1,876)	1:A:3135:ILE:HD13	1:A:3195:THR:H	2	0.2	0.03	0.2
(1,1023)	1:A:3163:PHE:HD1	1:A:3209:LEU:HD21	2	0.2	0.0	0.2
(1,1023)	1:A:3163:PHE:HD1	1:A:3209:LEU:HD22	2	0.2	0.0	0.2
(1,1023)	1:A:3163:PHE:HD1	1:A:3209:LEU:HD23	2	0.2	0.0	0.2
(1,1023)	1:A:3163:PHE:HD2	1:A:3209:LEU:HD21	2	0.2	0.0	0.2
(1,1023)	1:A:3163:PHE:HD2	1:A:3209:LEU:HD22	2	0.2	0.0	0.2
(1,1023)	1:A:3163:PHE:HD2	1:A:3209:LEU:HD23	2	0.2	0.0	0.2
(1,1438)	1:A:3192:PRO:HB2	1:A:3193:ASN:H	2	0.2	0.06	0.2
(1,1438)	1:A:3192:PRO:HB3	1:A:3193:ASN:H	2	0.2	0.06	0.2
(1,91)	1:A:3143:ILE:HD11	1:A:3212:TRP:HZ2	2	0.2	0.05	0.2
(1,91)	1:A:3143:ILE:HD12	1:A:3212:TRP:HZ2	2	0.2	0.05	0.2
(1,91)	1:A:3143:ILE:HD13	1:A:3212:TRP:HZ2	2	0.2	0.05	0.2
(1,946)	1:A:3170:TYR:HE1	1:A:3212:TRP:HE1	2	0.2	0.09	0.2
(1,946)	1:A:3170:TYR:HE2	1:A:3212:TRP:HE1	2	0.2	0.09	0.2
(1,438)	1:A:3096:LYS:HA	1:A:3096:LYS:HE2	2	0.19	0.0	0.19
(1,438)	1:A:3096:LYS:HA	1:A:3096:LYS:HE3	2	0.19	0.0	0.19
(1,12)	1:A:3137:MET:HE1	1:A:3209:LEU:HG	2	0.18	0.05	0.18
(1,12)	1:A:3137:MET:HE2	1:A:3209:LEU:HG	2	0.18	0.05	0.18
(1,12)	1:A:3137:MET:HE3	1:A:3209:LEU:HG	2	0.18	0.05	0.18
(1,162)	1:A:3163:PHE:HD1	1:A:3167:ILE:HG21	2	0.18	0.02	0.18
(1,162)	1:A:3163:PHE:HD1	1:A:3167:ILE:HG22	2	0.18	0.02	0.18
(1,162)	1:A:3163:PHE:HD1	1:A:3167:ILE:HG23	2	0.18	0.02	0.18
(1,162)	1:A:3163:PHE:HD2	1:A:3167:ILE:HG21	2	0.18	0.02	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,162)	1:A:3163:PHE:HD2	1:A:3167:ILE:HG22	2	0.18	0.02	0.18
(1,162)	1:A:3163:PHE:HD2	1:A:3167:ILE:HG23	2	0.18	0.02	0.18
(1,935)	1:A:3115:ILE:HG21	1:A:3209:LEU:H	2	0.18	0.03	0.18
(1,935)	1:A:3115:ILE:HG22	1:A:3209:LEU:H	2	0.18	0.03	0.18
(1,935)	1:A:3115:ILE:HG23	1:A:3209:LEU:H	2	0.18	0.03	0.18
(1,721)	1:A:3144:LEU:H	1:A:3180:ILE:HD11	2	0.18	0.06	0.18
(1,721)	1:A:3144:LEU:H	1:A:3180:ILE:HD12	2	0.18	0.06	0.18
(1,721)	1:A:3144:LEU:H	1:A:3180:ILE:HD13	2	0.18	0.06	0.18
(1,259)	1:A:3109:GLN:HG3	1:A:3168:VAL:HA	2	0.17	0.06	0.17
(1,648)	1:A:3122:GLU:H	1:A:3123:ILE:HD11	2	0.17	0.0	0.17
(1,648)	1:A:3122:GLU:H	1:A:3123:ILE:HD12	2	0.17	0.0	0.17
(1,648)	1:A:3122:GLU:H	1:A:3123:ILE:HD13	2	0.17	0.0	0.17
(1,446)	1:A:3128:ASN:HA	1:A:3129:PRO:HB3	2	0.17	0.04	0.17
(1,480)	1:A:3203:SER:HB2	1:A:3206:CYS:HB3	2	0.17	0.05	0.17
(1,511)	1:A:3124:ARG:HA	1:A:3155:GLN:HG2	2	0.17	0.05	0.17
(1,511)	1:A:3124:ARG:HA	1:A:3155:GLN:HG3	2	0.17	0.05	0.17
(1,978)	1:A:3223:LEU:HA	1:A:3225:ASN:H	2	0.17	0.05	0.17
(1,731)	1:A:3150:ASN:H	1:A:3152:ARG:HB3	2	0.16	0.05	0.16
(1,1043)	1:A:3135:ILE:HG21	1:A:3194:PHE:HD1	2	0.16	0.05	0.16
(1,1043)	1:A:3135:ILE:HG21	1:A:3194:PHE:HD2	2	0.16	0.05	0.16
(1,1043)	1:A:3135:ILE:HG22	1:A:3194:PHE:HD1	2	0.16	0.05	0.16
(1,1043)	1:A:3135:ILE:HG22	1:A:3194:PHE:HD2	2	0.16	0.05	0.16
(1,1043)	1:A:3135:ILE:HG23	1:A:3194:PHE:HD1	2	0.16	0.05	0.16
(1,1043)	1:A:3135:ILE:HG23	1:A:3194:PHE:HD2	2	0.16	0.05	0.16
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG11	2	0.16	0.05	0.16
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG12	2	0.16	0.05	0.16
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG13	2	0.16	0.05	0.16
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG21	2	0.16	0.05	0.16
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG22	2	0.16	0.05	0.16
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG23	2	0.16	0.05	0.16
(1,847)	1:A:3187:GLU:H	1:A:3189:LEU:H	2	0.15	0.01	0.15
(1,1298)	1:A:3140:VAL:HG11	1:A:3212:TRP:HE3	2	0.15	0.0	0.15
(1,1298)	1:A:3140:VAL:HG12	1:A:3212:TRP:HE3	2	0.15	0.0	0.15
(1,1298)	1:A:3140:VAL:HG13	1:A:3212:TRP:HE3	2	0.15	0.0	0.15
(1,1298)	1:A:3140:VAL:HG21	1:A:3212:TRP:HE3	2	0.15	0.0	0.15
(1,1298)	1:A:3140:VAL:HG22	1:A:3212:TRP:HE3	2	0.15	0.0	0.15
(1,1298)	1:A:3140:VAL:HG23	1:A:3212:TRP:HE3	2	0.15	0.0	0.15
(1,868)	1:A:3192:PRO:HB3	1:A:3193:ASN:H	2	0.15	0.0	0.15
(1,870)	1:A:3193:ASN:H	1:A:3195:THR:HG21	2	0.15	0.0	0.15
(1,870)	1:A:3193:ASN:H	1:A:3195:THR:HG22	2	0.15	0.0	0.15
(1,870)	1:A:3193:ASN:H	1:A:3195:THR:HG23	2	0.15	0.0	0.15
(1,1129)	1:A:3112:VAL:HG11	1:A:3164:ILE:HA	2	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1129)	1:A:3112:VAL:HG12	1:A:3164:ILE:HA	2	0.14	0.01	0.14
(1,1129)	1:A:3112:VAL:HG13	1:A:3164:ILE:HA	2	0.14	0.01	0.14
(1,1129)	1:A:3112:VAL:HG21	1:A:3164:ILE:HA	2	0.14	0.01	0.14
(1,1129)	1:A:3112:VAL:HG22	1:A:3164:ILE:HA	2	0.14	0.01	0.14
(1,1129)	1:A:3112:VAL:HG23	1:A:3164:ILE:HA	2	0.14	0.01	0.14
(1,1525)	1:A:3227:ASP:HB2	1:A:3228:PRO:HG2	2	0.14	0.01	0.14
(1,1525)	1:A:3227:ASP:HB2	1:A:3228:PRO:HG3	2	0.14	0.01	0.14
(1,1525)	1:A:3227:ASP:HB3	1:A:3228:PRO:HG2	2	0.14	0.01	0.14
(1,1525)	1:A:3227:ASP:HB3	1:A:3228:PRO:HG3	2	0.14	0.01	0.14
(1,1490)	1:A:3214:ASN:HA	1:A:3217:ILE:HG12	2	0.14	0.01	0.14
(1,1490)	1:A:3214:ASN:HA	1:A:3217:ILE:HG13	2	0.14	0.01	0.14
(1,561)	1:A:3217:ILE:HG21	1:A:3221:LYS:HE2	2	0.13	0.0	0.13
(1,561)	1:A:3217:ILE:HG21	1:A:3221:LYS:HE3	2	0.13	0.0	0.13
(1,561)	1:A:3217:ILE:HG22	1:A:3221:LYS:HE2	2	0.13	0.0	0.13
(1,561)	1:A:3217:ILE:HG22	1:A:3221:LYS:HE3	2	0.13	0.0	0.13
(1,561)	1:A:3217:ILE:HG23	1:A:3221:LYS:HE2	2	0.13	0.0	0.13
(1,561)	1:A:3217:ILE:HG23	1:A:3221:LYS:HE3	2	0.13	0.0	0.13
(1,613)	1:A:3112:VAL:H	1:A:3212:TRP:HB3	2	0.13	0.0	0.13
(1,1119)	1:A:3106:LEU:HD11	1:A:3109:GLN:HG3	2	0.13	0.01	0.13
(1,1119)	1:A:3106:LEU:HD12	1:A:3109:GLN:HG3	2	0.13	0.01	0.13
(1,1119)	1:A:3106:LEU:HD13	1:A:3109:GLN:HG3	2	0.13	0.01	0.13
(1,1119)	1:A:3106:LEU:HD21	1:A:3109:GLN:HG3	2	0.13	0.01	0.13
(1,1119)	1:A:3106:LEU:HD22	1:A:3109:GLN:HG3	2	0.13	0.01	0.13
(1,1119)	1:A:3106:LEU:HD23	1:A:3109:GLN:HG3	2	0.13	0.01	0.13
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG11	2	0.13	0.02	0.13
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG12	2	0.13	0.02	0.13
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG13	2	0.13	0.02	0.13
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG21	2	0.13	0.02	0.13
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG22	2	0.13	0.02	0.13
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG23	2	0.13	0.02	0.13
(1,409)	1:A:3210:TYR:HA	1:A:3213:VAL:HG21	2	0.12	0.01	0.12
(1,409)	1:A:3210:TYR:HA	1:A:3213:VAL:HG22	2	0.12	0.01	0.12
(1,409)	1:A:3210:TYR:HA	1:A:3213:VAL:HG23	2	0.12	0.01	0.12
(1,579)	1:A:3109:GLN:H	1:A:3110:ARG:HG2	2	0.12	0.01	0.12
(1,579)	1:A:3109:GLN:H	1:A:3110:ARG:HG3	2	0.12	0.01	0.12
(1,608)	1:A:3109:GLN:HG3	1:A:3110:ARG:H	2	0.12	0.01	0.12
(1,695)	1:A:3139:ALA:H	1:A:3154:ILE:HD11	2	0.12	0.02	0.12
(1,695)	1:A:3139:ALA:H	1:A:3154:ILE:HD12	2	0.12	0.02	0.12
(1,695)	1:A:3139:ALA:H	1:A:3154:ILE:HD13	2	0.12	0.02	0.12
(1,322)	1:A:3198:THR:HG21	1:A:3201:ARG:HD2	2	0.12	0.01	0.12
(1,322)	1:A:3198:THR:HG21	1:A:3201:ARG:HD3	2	0.12	0.01	0.12
(1,322)	1:A:3198:THR:HG22	1:A:3201:ARG:HD2	2	0.12	0.01	0.12

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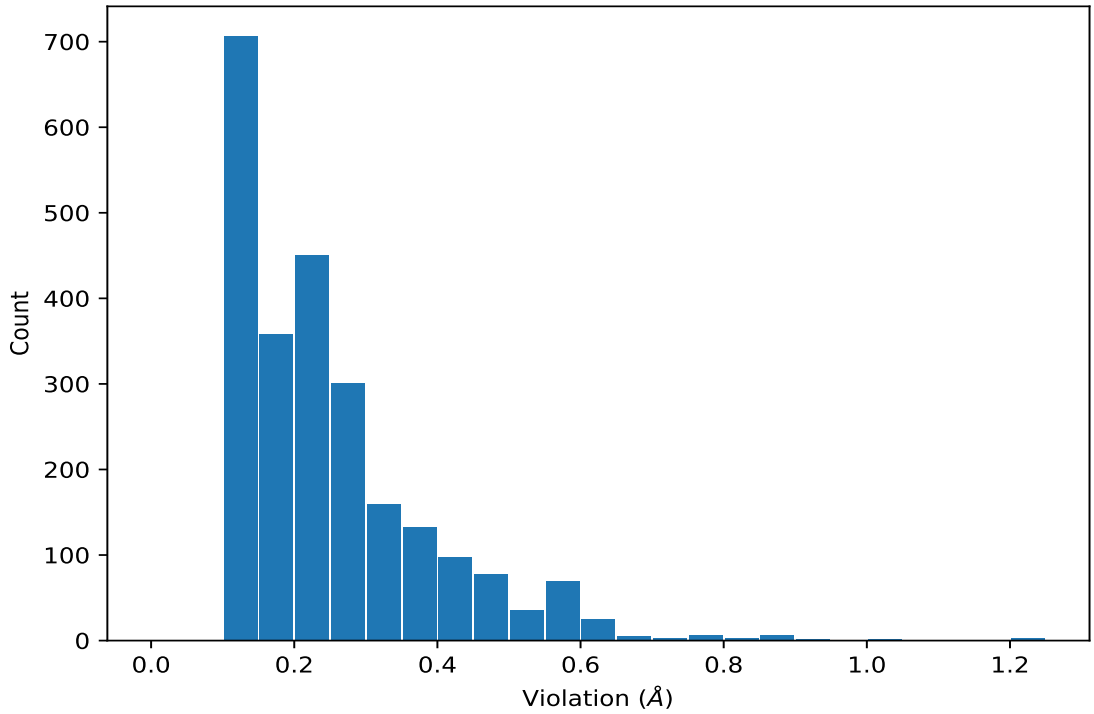
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,322)	1:A:3198:THR:HG22	1:A:3201:ARG:HD3	2	0.12	0.01	0.12
(1,322)	1:A:3198:THR:HG23	1:A:3201:ARG:HD2	2	0.12	0.01	0.12
(1,322)	1:A:3198:THR:HG23	1:A:3201:ARG:HD3	2	0.12	0.01	0.12
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG11	2	0.11	0.0	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG12	2	0.11	0.0	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG13	2	0.11	0.0	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG21	2	0.11	0.0	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG22	2	0.11	0.0	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG23	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)
(1,25)	1:A:3098:ILE:HD11	1:A:3099:GLN:HA	1	1.22
(1,25)	1:A:3098:ILE:HD12	1:A:3099:GLN:HA	1	1.22
(1,25)	1:A:3098:ILE:HD13	1:A:3099:GLN:HA	1	1.22
(1,1436)	1:A:3191:ASP:HB2	1:A:3193:ASN:H	3	1.03
(1,1436)	1:A:3191:ASP:HB3	1:A:3193:ASN:H	3	1.03
(1,1436)	1:A:3191:ASP:HB2	1:A:3193:ASN:H	2	0.94
(1,1436)	1:A:3191:ASP:HB3	1:A:3193:ASN:H	2	0.94
(1,436)	1:A:3136:VAL:HG21	1:A:3137:MET:HG3	8	0.87
(1,436)	1:A:3136:VAL:HG22	1:A:3137:MET:HG3	8	0.87
(1,436)	1:A:3136:VAL:HG23	1:A:3137:MET:HG3	8	0.87
(1,436)	1:A:3136:VAL:HG21	1:A:3137:MET:HG3	10	0.87
(1,436)	1:A:3136:VAL:HG22	1:A:3137:MET:HG3	10	0.87
(1,436)	1:A:3136:VAL:HG23	1:A:3137:MET:HG3	10	0.87
(1,735)	1:A:3134:LYS:HA	1:A:3151:TRP:HE1	1	0.83
(1,1497)	1:A:3216:GLN:HA	1:A:3219:PHE:HB2	4	0.8
(1,1497)	1:A:3216:GLN:HA	1:A:3219:PHE:HB3	4	0.8
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD11	2	0.76
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD12	2	0.76
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD13	2	0.76
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD21	2	0.76
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD22	2	0.76
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD23	2	0.76
(1,757)	1:A:3158:ILE:H	1:A:3160:LYS:H	8	0.75
(1,846)	1:A:3184:MET:HA	1:A:3186:GLU:H	7	0.72
(1,1392)	1:A:3178:PRO:HB2	1:A:3181:ARG:H	10	0.71
(1,1392)	1:A:3178:PRO:HB3	1:A:3181:ARG:H	10	0.71
(1,845)	1:A:3185:GLU:H	1:A:3186:GLU:H	7	0.68
(1,626)	1:A:3112:VAL:HA	1:A:3115:ILE:H	7	0.65
(1,457)	1:A:3214:ASN:HB2	1:A:3217:ILE:HG21	5	0.65
(1,457)	1:A:3214:ASN:HB2	1:A:3217:ILE:HG22	5	0.65
(1,457)	1:A:3214:ASN:HB2	1:A:3217:ILE:HG23	5	0.65
(1,859)	1:A:3185:GLU:HA	1:A:3189:LEU:H	7	0.64
(1,735)	1:A:3134:LYS:HA	1:A:3151:TRP:HE1	8	0.64
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD11	3	0.64
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD12	3	0.64
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD13	3	0.64
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD21	3	0.64
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD22	3	0.64
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD23	3	0.64
(1,883)	1:A:3195:THR:HB	1:A:3197:GLU:H	8	0.63
(1,735)	1:A:3134:LYS:HA	1:A:3151:TRP:HE1	6	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,735)	1:A:3134:LYS:HA	1:A:3151:TRP:HE1	2	0.62
(1,345)	1:A:3205:ALA:HB1	1:A:3209:LEU:HB2	1	0.62
(1,345)	1:A:3205:ALA:HB2	1:A:3209:LEU:HB2	1	0.62
(1,345)	1:A:3205:ALA:HB3	1:A:3209:LEU:HB2	1	0.62
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG21	7	0.61
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG22	7	0.61
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG23	7	0.61
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG21	7	0.61
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG22	7	0.61
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG23	7	0.61
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG21	7	0.61
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG22	7	0.61
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG23	7	0.61
(1,1096)	1:A:3099:GLN:HB2	1:A:3101:CYS:H	10	0.61
(1,1096)	1:A:3099:GLN:HB3	1:A:3101:CYS:H	10	0.61
(1,950)	1:A:3109:GLN:HG3	1:A:3212:TRP:HE1	5	0.6
(1,950)	1:A:3109:GLN:HG3	1:A:3212:TRP:HE1	7	0.6
(1,436)	1:A:3136:VAL:HG21	1:A:3137:MET:HG3	2	0.6
(1,436)	1:A:3136:VAL:HG22	1:A:3137:MET:HG3	2	0.6
(1,436)	1:A:3136:VAL:HG23	1:A:3137:MET:HG3	2	0.6
(1,436)	1:A:3136:VAL:HG21	1:A:3137:MET:HG3	7	0.6
(1,436)	1:A:3136:VAL:HG22	1:A:3137:MET:HG3	7	0.6
(1,436)	1:A:3136:VAL:HG23	1:A:3137:MET:HG3	7	0.6
(1,434)	1:A:3136:VAL:HG21	1:A:3137:MET:HG2	8	0.6
(1,434)	1:A:3136:VAL:HG22	1:A:3137:MET:HG2	8	0.6
(1,434)	1:A:3136:VAL:HG23	1:A:3137:MET:HG2	8	0.6
(1,1519)	1:A:3225:ASN:HB2	1:A:3227:ASP:H	9	0.6
(1,1519)	1:A:3225:ASN:HB3	1:A:3227:ASP:H	9	0.6
(1,991)	1:A:3167:ILE:HA	1:A:3212:TRP:HZ3	1	0.59
(1,991)	1:A:3167:ILE:HA	1:A:3212:TRP:HZ3	3	0.59
(1,735)	1:A:3134:LYS:HA	1:A:3151:TRP:HE1	3	0.59
(1,436)	1:A:3136:VAL:HG21	1:A:3137:MET:HG3	1	0.59
(1,436)	1:A:3136:VAL:HG22	1:A:3137:MET:HG3	1	0.59
(1,436)	1:A:3136:VAL:HG23	1:A:3137:MET:HG3	1	0.59
(1,246)	1:A:3136:VAL:HA	1:A:3210:TYR:HA	2	0.59
(1,1177)	1:A:3123:ILE:HB	1:A:3126:MET:HG2	9	0.59
(1,1177)	1:A:3123:ILE:HB	1:A:3126:MET:HG3	9	0.59
(1,961)	1:A:3105:ILE:HG21	1:A:3216:GLN:H	4	0.58
(1,961)	1:A:3105:ILE:HG22	1:A:3216:GLN:H	4	0.58
(1,961)	1:A:3105:ILE:HG23	1:A:3216:GLN:H	4	0.58
(1,929)	1:A:3115:ILE:HG21	1:A:3207:GLY:H	1	0.58
(1,929)	1:A:3115:ILE:HG22	1:A:3207:GLY:H	1	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:A:3115:ILE:HG23	1:A:3207:GLY:H	1	0.58
(1,735)	1:A:3134:LYS:HA	1:A:3151:TRP:HE1	10	0.58
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG21	1	0.58
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG22	1	0.58
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG23	1	0.58
(1,436)	1:A:3136:VAL:HG21	1:A:3137:MET:HG3	9	0.58
(1,436)	1:A:3136:VAL:HG22	1:A:3137:MET:HG3	9	0.58
(1,436)	1:A:3136:VAL:HG23	1:A:3137:MET:HG3	9	0.58
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD11	1	0.57
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD12	1	0.57
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD13	1	0.57
(1,961)	1:A:3105:ILE:HG21	1:A:3216:GLN:H	6	0.56
(1,961)	1:A:3105:ILE:HG22	1:A:3216:GLN:H	6	0.56
(1,961)	1:A:3105:ILE:HG23	1:A:3216:GLN:H	6	0.56
(1,950)	1:A:3109:GLN:HG3	1:A:3212:TRP:HE1	2	0.56
(1,888)	1:A:3197:GLU:H	1:A:3210:TYR:HD1	2	0.56
(1,888)	1:A:3197:GLU:H	1:A:3210:TYR:HD2	2	0.56
(1,755)	1:A:3155:GLN:HG2	1:A:3157:PHE:H	9	0.56
(1,755)	1:A:3155:GLN:HG3	1:A:3157:PHE:H	9	0.56
(1,1428)	1:A:3189:LEU:HD11	1:A:3190:SER:HB2	9	0.56
(1,1428)	1:A:3189:LEU:HD11	1:A:3190:SER:HB3	9	0.56
(1,1428)	1:A:3189:LEU:HD12	1:A:3190:SER:HB2	9	0.56
(1,1428)	1:A:3189:LEU:HD12	1:A:3190:SER:HB3	9	0.56
(1,1428)	1:A:3189:LEU:HD13	1:A:3190:SER:HB2	9	0.56
(1,1428)	1:A:3189:LEU:HD13	1:A:3190:SER:HB3	9	0.56
(1,1428)	1:A:3189:LEU:HD21	1:A:3190:SER:HB2	9	0.56
(1,1428)	1:A:3189:LEU:HD21	1:A:3190:SER:HB3	9	0.56
(1,1428)	1:A:3189:LEU:HD22	1:A:3190:SER:HB2	9	0.56
(1,1428)	1:A:3189:LEU:HD22	1:A:3190:SER:HB3	9	0.56
(1,1428)	1:A:3189:LEU:HD23	1:A:3190:SER:HB2	9	0.56
(1,1428)	1:A:3189:LEU:HD23	1:A:3190:SER:HB3	9	0.56
(1,437)	1:A:3134:LYS:HA	1:A:3137:MET:HG3	3	0.55
(1,436)	1:A:3136:VAL:HG21	1:A:3137:MET:HG3	5	0.55
(1,436)	1:A:3136:VAL:HG22	1:A:3137:MET:HG3	5	0.55
(1,436)	1:A:3136:VAL:HG23	1:A:3137:MET:HG3	5	0.55
(1,343)	1:A:3185:GLU:HA	1:A:3189:LEU:HB2	10	0.55
(1,16)	1:A:3136:VAL:HA	1:A:3137:MET:HE1	5	0.55
(1,16)	1:A:3136:VAL:HA	1:A:3137:MET:HE2	5	0.55
(1,16)	1:A:3136:VAL:HA	1:A:3137:MET:HE3	5	0.55
(1,1366)	1:A:3159:ARG:HB2	1:A:3160:LYS:H	9	0.55
(1,1366)	1:A:3159:ARG:HB3	1:A:3160:LYS:H	9	0.55
(1,1096)	1:A:3099:GLN:HB2	1:A:3101:CYS:H	4	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1096)	1:A:3099:GLN:HB3	1:A:3101:CYS:H	4	0.55
(1,437)	1:A:3134:LYS:HA	1:A:3137:MET:HG3	4	0.54
(1,436)	1:A:3136:VAL:HG21	1:A:3137:MET:HG3	6	0.54
(1,436)	1:A:3136:VAL:HG22	1:A:3137:MET:HG3	6	0.54
(1,436)	1:A:3136:VAL:HG23	1:A:3137:MET:HG3	6	0.54
(1,16)	1:A:3136:VAL:HA	1:A:3137:MET:HE1	7	0.54
(1,16)	1:A:3136:VAL:HA	1:A:3137:MET:HE2	7	0.54
(1,16)	1:A:3136:VAL:HA	1:A:3137:MET:HE3	7	0.54
(1,1222)	1:A:3130:PRO:HG2	1:A:3132:GLY:HA3	8	0.54
(1,1222)	1:A:3130:PRO:HG3	1:A:3132:GLY:HA3	8	0.54
(1,252)	1:A:3140:VAL:HA	1:A:3167:ILE:HA	2	0.53
(1,25)	1:A:3098:ILE:HD11	1:A:3099:GLN:HA	2	0.53
(1,25)	1:A:3098:ILE:HD12	1:A:3099:GLN:HA	2	0.53
(1,25)	1:A:3098:ILE:HD13	1:A:3099:GLN:HA	2	0.53
(1,1222)	1:A:3130:PRO:HG2	1:A:3132:GLY:HA3	10	0.53
(1,1222)	1:A:3130:PRO:HG3	1:A:3132:GLY:HA3	10	0.53
(1,991)	1:A:3167:ILE:HA	1:A:3212:TRP:HZ3	4	0.52
(1,991)	1:A:3167:ILE:HA	1:A:3212:TRP:HZ3	6	0.52
(1,757)	1:A:3158:ILE:H	1:A:3160:LYS:H	9	0.52
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG21	9	0.52
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG22	9	0.52
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG23	9	0.52
(1,735)	1:A:3134:LYS:HA	1:A:3151:TRP:HE1	7	0.51
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD11	8	0.51
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD12	8	0.51
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD13	8	0.51
(1,953)	1:A:3143:ILE:HG21	1:A:3212:TRP:HE1	8	0.5
(1,953)	1:A:3143:ILE:HG22	1:A:3212:TRP:HE1	8	0.5
(1,953)	1:A:3143:ILE:HG23	1:A:3212:TRP:HE1	8	0.5
(1,735)	1:A:3134:LYS:HA	1:A:3151:TRP:HE1	4	0.5
(1,735)	1:A:3134:LYS:HA	1:A:3151:TRP:HE1	5	0.5
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD11	5	0.5
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD12	5	0.5
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD13	5	0.5
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD11	10	0.5
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD12	10	0.5
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD13	10	0.5
(1,961)	1:A:3105:ILE:HG21	1:A:3216:GLN:H	8	0.49
(1,961)	1:A:3105:ILE:HG22	1:A:3216:GLN:H	8	0.49
(1,961)	1:A:3105:ILE:HG23	1:A:3216:GLN:H	8	0.49
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG21	5	0.49
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG22	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG23	5	0.49
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD11	2	0.49
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD12	2	0.49
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD13	2	0.49
(1,328)	1:A:3106:LEU:HD21	1:A:3109:GLN:HG3	5	0.49
(1,328)	1:A:3106:LEU:HD22	1:A:3109:GLN:HG3	5	0.49
(1,328)	1:A:3106:LEU:HD23	1:A:3109:GLN:HG3	5	0.49
(1,176)	1:A:3143:ILE:HA	1:A:3180:ILE:HG21	7	0.49
(1,176)	1:A:3143:ILE:HA	1:A:3180:ILE:HG22	7	0.49
(1,176)	1:A:3143:ILE:HA	1:A:3180:ILE:HG23	7	0.49
(1,1222)	1:A:3130:PRO:HG2	1:A:3132:GLY:HA3	4	0.49
(1,1222)	1:A:3130:PRO:HG3	1:A:3132:GLY:HA3	4	0.49
(1,1093)	1:A:3098:ILE:HG12	1:A:3099:GLN:HA	10	0.49
(1,1093)	1:A:3098:ILE:HG13	1:A:3099:GLN:HA	10	0.49
(1,837)	1:A:3179:GLN:H	1:A:3182:LYS:H	1	0.48
(1,345)	1:A:3205:ALA:HB1	1:A:3209:LEU:HB2	6	0.48
(1,345)	1:A:3205:ALA:HB2	1:A:3209:LEU:HB2	6	0.48
(1,345)	1:A:3205:ALA:HB3	1:A:3209:LEU:HB2	6	0.48
(1,252)	1:A:3140:VAL:HA	1:A:3167:ILE:HA	5	0.48
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD11	1	0.48
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD12	1	0.48
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD13	1	0.48
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD21	1	0.48
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD22	1	0.48
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD23	1	0.48
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD11	1	0.48
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD12	1	0.48
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD13	1	0.48
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD21	1	0.48
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD22	1	0.48
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD23	1	0.48
(1,842)	1:A:3185:GLU:H	1:A:3217:ILE:HD11	4	0.47
(1,842)	1:A:3185:GLU:H	1:A:3217:ILE:HD12	4	0.47
(1,842)	1:A:3185:GLU:H	1:A:3217:ILE:HD13	4	0.47
(1,837)	1:A:3179:GLN:H	1:A:3182:LYS:H	6	0.47
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG21	6	0.47
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG22	6	0.47
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG23	6	0.47
(1,246)	1:A:3136:VAL:HA	1:A:3210:TYR:HA	7	0.47
(1,310)	1:A:3101:CYS:HA	1:A:3104:THR:HG21	2	0.46
(1,310)	1:A:3101:CYS:HA	1:A:3104:THR:HG22	2	0.46
(1,310)	1:A:3101:CYS:HA	1:A:3104:THR:HG23	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:A:3167:ILE:HG21	1:A:3170:TYR:HB2	3	0.46
(1,159)	1:A:3167:ILE:HG22	1:A:3170:TYR:HB2	3	0.46
(1,159)	1:A:3167:ILE:HG23	1:A:3170:TYR:HB2	3	0.46
(1,1424)	1:A:3188:PHE:HB2	1:A:3190:SER:H	1	0.46
(1,1424)	1:A:3188:PHE:HB3	1:A:3190:SER:H	1	0.46
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD11	6	0.45
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD12	6	0.45
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD13	6	0.45
(1,434)	1:A:3136:VAL:HG21	1:A:3137:MET:HG2	4	0.45
(1,434)	1:A:3136:VAL:HG22	1:A:3137:MET:HG2	4	0.45
(1,434)	1:A:3136:VAL:HG23	1:A:3137:MET:HG2	4	0.45
(1,1429)	1:A:3189:LEU:HD21	1:A:3190:SER:HB3	9	0.45
(1,1429)	1:A:3189:LEU:HD22	1:A:3190:SER:HB3	9	0.45
(1,1429)	1:A:3189:LEU:HD23	1:A:3190:SER:HB3	9	0.45
(1,1412)	1:A:3185:GLU:HA	1:A:3189:LEU:HD11	4	0.45
(1,1412)	1:A:3185:GLU:HA	1:A:3189:LEU:HD12	4	0.45
(1,1412)	1:A:3185:GLU:HA	1:A:3189:LEU:HD13	4	0.45
(1,1412)	1:A:3185:GLU:HA	1:A:3189:LEU:HD21	4	0.45
(1,1412)	1:A:3185:GLU:HA	1:A:3189:LEU:HD22	4	0.45
(1,1412)	1:A:3185:GLU:HA	1:A:3189:LEU:HD23	4	0.45
(1,1382)	1:A:3170:TYR:HB2	1:A:3212:TRP:HH2	3	0.45
(1,1382)	1:A:3170:TYR:HB3	1:A:3212:TRP:HH2	3	0.45
(1,1094)	1:A:3098:ILE:HD11	1:A:3099:GLN:HB2	8	0.45
(1,1094)	1:A:3098:ILE:HD11	1:A:3099:GLN:HB3	8	0.45
(1,1094)	1:A:3098:ILE:HD12	1:A:3099:GLN:HB2	8	0.45
(1,1094)	1:A:3098:ILE:HD12	1:A:3099:GLN:HB3	8	0.45
(1,1094)	1:A:3098:ILE:HD13	1:A:3099:GLN:HB2	8	0.45
(1,1094)	1:A:3098:ILE:HD13	1:A:3099:GLN:HB3	8	0.45
(1,1084)	1:A:3144:LEU:HD11	1:A:3212:TRP:HZ2	1	0.45
(1,1084)	1:A:3144:LEU:HD12	1:A:3212:TRP:HZ2	1	0.45
(1,1084)	1:A:3144:LEU:HD13	1:A:3212:TRP:HZ2	1	0.45
(1,961)	1:A:3105:ILE:HG21	1:A:3216:GLN:H	3	0.44
(1,961)	1:A:3105:ILE:HG22	1:A:3216:GLN:H	3	0.44
(1,961)	1:A:3105:ILE:HG23	1:A:3216:GLN:H	3	0.44
(1,77)	1:A:3132:GLY:HA2	1:A:3135:ILE:HG21	3	0.44
(1,77)	1:A:3132:GLY:HA2	1:A:3135:ILE:HG22	3	0.44
(1,77)	1:A:3132:GLY:HA2	1:A:3135:ILE:HG23	3	0.44
(1,745)	1:A:3149:SER:HA	1:A:3153:ASP:H	4	0.44
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD11	8	0.44
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD12	8	0.44
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD13	8	0.44
(1,501)	1:A:3115:ILE:HG21	1:A:3119:GLN:HG2	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:A:3115:ILE:HG22	1:A:3119:GLN:HG2	5	0.44
(1,501)	1:A:3115:ILE:HG23	1:A:3119:GLN:HG2	5	0.44
(1,48)	1:A:3112:VAL:HA	1:A:3115:ILE:HD11	7	0.44
(1,48)	1:A:3112:VAL:HA	1:A:3115:ILE:HD12	7	0.44
(1,48)	1:A:3112:VAL:HA	1:A:3115:ILE:HD13	7	0.44
(1,372)	1:A:3189:LEU:HD11	1:A:3190:SER:HB3	7	0.44
(1,372)	1:A:3189:LEU:HD12	1:A:3190:SER:HB3	7	0.44
(1,372)	1:A:3189:LEU:HD13	1:A:3190:SER:HB3	7	0.44
(1,252)	1:A:3140:VAL:HA	1:A:3167:ILE:HA	6	0.44
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD11	2	0.44
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD12	2	0.44
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD13	2	0.44
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD11	3	0.44
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD12	3	0.44
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD13	3	0.44
(1,953)	1:A:3143:ILE:HG21	1:A:3212:TRP:HE1	10	0.43
(1,953)	1:A:3143:ILE:HG22	1:A:3212:TRP:HE1	10	0.43
(1,953)	1:A:3143:ILE:HG23	1:A:3212:TRP:HE1	10	0.43
(1,861)	1:A:3187:GLU:HB2	1:A:3189:LEU:H	7	0.43
(1,861)	1:A:3187:GLU:HB3	1:A:3189:LEU:H	7	0.43
(1,808)	1:A:3143:ILE:HG21	1:A:3170:TYR:H	8	0.43
(1,808)	1:A:3143:ILE:HG22	1:A:3170:TYR:H	8	0.43
(1,808)	1:A:3143:ILE:HG23	1:A:3170:TYR:H	8	0.43
(1,74)	1:A:3134:LYS:H	1:A:3135:ILE:HG12	5	0.43
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG21	2	0.43
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG22	2	0.43
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG23	2	0.43
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG21	5	0.43
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG22	5	0.43
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG23	5	0.43
(1,953)	1:A:3143:ILE:HG21	1:A:3212:TRP:HE1	7	0.42
(1,953)	1:A:3143:ILE:HG22	1:A:3212:TRP:HE1	7	0.42
(1,953)	1:A:3143:ILE:HG23	1:A:3212:TRP:HE1	7	0.42
(1,624)	1:A:3113:LYS:H	1:A:3115:ILE:H	7	0.42
(1,526)	1:A:3110:ARG:HA	1:A:3113:LYS:HB2	6	0.42
(1,434)	1:A:3136:VAL:HG21	1:A:3137:MET:HG2	10	0.42
(1,434)	1:A:3136:VAL:HG22	1:A:3137:MET:HG2	10	0.42
(1,434)	1:A:3136:VAL:HG23	1:A:3137:MET:HG2	10	0.42
(1,1094)	1:A:3098:ILE:HD11	1:A:3099:GLN:HB2	9	0.42
(1,1094)	1:A:3098:ILE:HD11	1:A:3099:GLN:HB3	9	0.42
(1,1094)	1:A:3098:ILE:HD12	1:A:3099:GLN:HB2	9	0.42
(1,1094)	1:A:3098:ILE:HD12	1:A:3099:GLN:HB3	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1094)	1:A:3098:ILE:HD13	1:A:3099:GLN:HB2	9	0.42
(1,1094)	1:A:3098:ILE:HD13	1:A:3099:GLN:HB3	9	0.42
(1,1084)	1:A:3144:LEU:HD11	1:A:3212:TRP:HZ2	9	0.42
(1,1084)	1:A:3144:LEU:HD12	1:A:3212:TRP:HZ2	9	0.42
(1,1084)	1:A:3144:LEU:HD13	1:A:3212:TRP:HZ2	9	0.42
(1,853)	1:A:3185:GLU:HA	1:A:3188:PHE:H	5	0.41
(1,848)	1:A:3184:MET:HA	1:A:3187:GLU:H	2	0.41
(1,837)	1:A:3179:GLN:H	1:A:3182:LYS:H	8	0.41
(1,77)	1:A:3132:GLY:HA2	1:A:3135:ILE:HG21	5	0.41
(1,77)	1:A:3132:GLY:HA2	1:A:3135:ILE:HG22	5	0.41
(1,77)	1:A:3132:GLY:HA2	1:A:3135:ILE:HG23	5	0.41
(1,745)	1:A:3149:SER:HA	1:A:3153:ASP:H	1	0.41
(1,734)	1:A:3150:ASN:H	1:A:3153:ASP:HA	8	0.41
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG11	6	0.41
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG12	6	0.41
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG13	6	0.41
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG21	6	0.41
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG22	6	0.41
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG23	6	0.41
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD1	9	0.41
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD2	9	0.41
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD1	9	0.41
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD2	9	0.41
(1,951)	1:A:3108:ALA:HB1	1:A:3212:TRP:HE1	1	0.4
(1,951)	1:A:3108:ALA:HB2	1:A:3212:TRP:HE1	1	0.4
(1,951)	1:A:3108:ALA:HB3	1:A:3212:TRP:HE1	1	0.4
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG21	4	0.4
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG22	4	0.4
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG23	4	0.4
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD11	7	0.4
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD12	7	0.4
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD13	7	0.4
(1,351)	1:A:3206:CYS:HA	1:A:3209:LEU:HG	9	0.4
(1,32)	1:A:3105:ILE:HD11	1:A:3215:ALA:HB1	7	0.4
(1,32)	1:A:3105:ILE:HD11	1:A:3215:ALA:HB2	7	0.4
(1,32)	1:A:3105:ILE:HD11	1:A:3215:ALA:HB3	7	0.4
(1,32)	1:A:3105:ILE:HD12	1:A:3215:ALA:HB1	7	0.4
(1,32)	1:A:3105:ILE:HD12	1:A:3215:ALA:HB2	7	0.4
(1,32)	1:A:3105:ILE:HD12	1:A:3215:ALA:HB3	7	0.4
(1,32)	1:A:3105:ILE:HD13	1:A:3215:ALA:HB1	7	0.4
(1,32)	1:A:3105:ILE:HD13	1:A:3215:ALA:HB2	7	0.4
(1,32)	1:A:3105:ILE:HD13	1:A:3215:ALA:HB3	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:A:3195:THR:HG21	1:A:3199:ILE:HB	6	0.4
(1,182)	1:A:3195:THR:HG22	1:A:3199:ILE:HB	6	0.4
(1,182)	1:A:3195:THR:HG23	1:A:3199:ILE:HB	6	0.4
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG21	3	0.39
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG22	3	0.39
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG23	3	0.39
(1,482)	1:A:3208:PRO:HA	1:A:3211:GLN:HG2	2	0.39
(1,345)	1:A:3205:ALA:HB1	1:A:3209:LEU:HB2	10	0.39
(1,345)	1:A:3205:ALA:HB2	1:A:3209:LEU:HB2	10	0.39
(1,345)	1:A:3205:ALA:HB3	1:A:3209:LEU:HB2	10	0.39
(1,182)	1:A:3195:THR:HG21	1:A:3199:ILE:HB	8	0.39
(1,182)	1:A:3195:THR:HG22	1:A:3199:ILE:HB	8	0.39
(1,182)	1:A:3195:THR:HG23	1:A:3199:ILE:HB	8	0.39
(1,1519)	1:A:3225:ASN:HB2	1:A:3227:ASP:H	1	0.39
(1,1519)	1:A:3225:ASN:HB3	1:A:3227:ASP:H	1	0.39
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD11	9	0.39
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD12	9	0.39
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD13	9	0.39
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD21	9	0.39
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD22	9	0.39
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD23	9	0.39
(1,1222)	1:A:3130:PRO:HG2	1:A:3132:GLY:HA3	6	0.39
(1,1222)	1:A:3130:PRO:HG3	1:A:3132:GLY:HA3	6	0.39
(1,1100)	1:A:3101:CYS:HB2	1:A:3104:THR:HG21	2	0.39
(1,1100)	1:A:3101:CYS:HB2	1:A:3104:THR:HG22	2	0.39
(1,1100)	1:A:3101:CYS:HB2	1:A:3104:THR:HG23	2	0.39
(1,1100)	1:A:3101:CYS:HB3	1:A:3104:THR:HG21	2	0.39
(1,1100)	1:A:3101:CYS:HB3	1:A:3104:THR:HG22	2	0.39
(1,1100)	1:A:3101:CYS:HB3	1:A:3104:THR:HG23	2	0.39
(1,953)	1:A:3143:ILE:HG21	1:A:3212:TRP:HE1	3	0.38
(1,953)	1:A:3143:ILE:HG22	1:A:3212:TRP:HE1	3	0.38
(1,953)	1:A:3143:ILE:HG23	1:A:3212:TRP:HE1	3	0.38
(1,929)	1:A:3115:ILE:HG21	1:A:3207:GLY:H	4	0.38
(1,929)	1:A:3115:ILE:HG22	1:A:3207:GLY:H	4	0.38
(1,929)	1:A:3115:ILE:HG23	1:A:3207:GLY:H	4	0.38
(1,765)	1:A:3158:ILE:HA	1:A:3160:LYS:H	4	0.38
(1,735)	1:A:3134:LYS:HA	1:A:3151:TRP:HE1	9	0.38
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG21	7	0.38
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG22	7	0.38
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG23	7	0.38
(1,345)	1:A:3205:ALA:HB1	1:A:3209:LEU:HB2	9	0.38
(1,345)	1:A:3205:ALA:HB2	1:A:3209:LEU:HB2	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,345)	1:A:3205:ALA:HB3	1:A:3209:LEU:HB2	9	0.38
(1,320)	1:A:3195:THR:HG21	1:A:3196:TYR:HA	8	0.38
(1,320)	1:A:3195:THR:HG22	1:A:3196:TYR:HA	8	0.38
(1,320)	1:A:3195:THR:HG23	1:A:3196:TYR:HA	8	0.38
(1,1522)	1:A:3226:VAL:HG11	1:A:3228:PRO:HD2	4	0.38
(1,1522)	1:A:3226:VAL:HG11	1:A:3228:PRO:HD3	4	0.38
(1,1522)	1:A:3226:VAL:HG12	1:A:3228:PRO:HD2	4	0.38
(1,1522)	1:A:3226:VAL:HG12	1:A:3228:PRO:HD3	4	0.38
(1,1522)	1:A:3226:VAL:HG13	1:A:3228:PRO:HD2	4	0.38
(1,1522)	1:A:3226:VAL:HG13	1:A:3228:PRO:HD3	4	0.38
(1,1522)	1:A:3226:VAL:HG21	1:A:3228:PRO:HD2	4	0.38
(1,1522)	1:A:3226:VAL:HG21	1:A:3228:PRO:HD3	4	0.38
(1,1522)	1:A:3226:VAL:HG22	1:A:3228:PRO:HD2	4	0.38
(1,1522)	1:A:3226:VAL:HG22	1:A:3228:PRO:HD3	4	0.38
(1,1522)	1:A:3226:VAL:HG23	1:A:3228:PRO:HD2	4	0.38
(1,1522)	1:A:3226:VAL:HG23	1:A:3228:PRO:HD3	4	0.38
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD1	3	0.38
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD2	3	0.38
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD1	3	0.38
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD2	3	0.38
(1,1091)	1:A:3098:ILE:HG21	1:A:3099:GLN:HB2	10	0.38
(1,1091)	1:A:3098:ILE:HG21	1:A:3099:GLN:HB3	10	0.38
(1,1091)	1:A:3098:ILE:HG22	1:A:3099:GLN:HB2	10	0.38
(1,1091)	1:A:3098:ILE:HG22	1:A:3099:GLN:HB3	10	0.38
(1,1091)	1:A:3098:ILE:HG23	1:A:3099:GLN:HB2	10	0.38
(1,1091)	1:A:3098:ILE:HG23	1:A:3099:GLN:HB3	10	0.38
(1,961)	1:A:3105:ILE:HG21	1:A:3216:GLN:H	9	0.37
(1,961)	1:A:3105:ILE:HG22	1:A:3216:GLN:H	9	0.37
(1,961)	1:A:3105:ILE:HG23	1:A:3216:GLN:H	9	0.37
(1,745)	1:A:3149:SER:HA	1:A:3153:ASP:H	5	0.37
(1,501)	1:A:3115:ILE:HG21	1:A:3119:GLN:HG2	6	0.37
(1,501)	1:A:3115:ILE:HG22	1:A:3119:GLN:HG2	6	0.37
(1,501)	1:A:3115:ILE:HG23	1:A:3119:GLN:HG2	6	0.37
(1,437)	1:A:3134:LYS:HA	1:A:3137:MET:HG3	8	0.37
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG21	10	0.37
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG22	10	0.37
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG23	10	0.37
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG21	2	0.37
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG22	2	0.37
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG23	2	0.37
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG21	2	0.37
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG22	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG23	2	0.37
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG21	2	0.37
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG22	2	0.37
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG23	2	0.37
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD11	3	0.37
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD12	3	0.37
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD13	3	0.37
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD21	3	0.37
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD22	3	0.37
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD23	3	0.37
(1,1383)	1:A:3171:ASP:HA	1:A:3174:LEU:HB2	3	0.37
(1,1383)	1:A:3171:ASP:HA	1:A:3174:LEU:HB3	3	0.37
(1,1084)	1:A:3144:LEU:HD11	1:A:3212:TRP:HZ2	7	0.37
(1,1084)	1:A:3144:LEU:HD12	1:A:3212:TRP:HZ2	7	0.37
(1,1084)	1:A:3144:LEU:HD13	1:A:3212:TRP:HZ2	7	0.37
(1,1000)	1:A:3183:TYR:HE1	1:A:3187:GLU:HG2	7	0.37
(1,1000)	1:A:3183:TYR:HE2	1:A:3187:GLU:HG2	7	0.37
(1,994)	1:A:3108:ALA:HB1	1:A:3212:TRP:HE3	1	0.36
(1,994)	1:A:3108:ALA:HB2	1:A:3212:TRP:HE3	1	0.36
(1,994)	1:A:3108:ALA:HB3	1:A:3212:TRP:HE3	1	0.36
(1,961)	1:A:3105:ILE:HG21	1:A:3216:GLN:H	7	0.36
(1,961)	1:A:3105:ILE:HG22	1:A:3216:GLN:H	7	0.36
(1,961)	1:A:3105:ILE:HG23	1:A:3216:GLN:H	7	0.36
(1,863)	1:A:3188:PHE:HA	1:A:3190:SER:H	10	0.36
(1,765)	1:A:3158:ILE:HA	1:A:3160:LYS:H	7	0.36
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG21	7	0.36
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG22	7	0.36
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG23	7	0.36
(1,697)	1:A:3139:ALA:H	1:A:3184:MET:HE1	9	0.36
(1,697)	1:A:3139:ALA:H	1:A:3184:MET:HE2	9	0.36
(1,697)	1:A:3139:ALA:H	1:A:3184:MET:HE3	9	0.36
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG2	2	0.36
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG3	2	0.36
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD11	3	0.36
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD12	3	0.36
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD13	3	0.36
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD21	3	0.36
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD22	3	0.36
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD23	3	0.36
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD11	3	0.36
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD12	3	0.36
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD13	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD21	3	0.36
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD22	3	0.36
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD23	3	0.36
(1,1391)	1:A:3178:PRO:HB2	1:A:3180:ILE:H	2	0.36
(1,1391)	1:A:3178:PRO:HB3	1:A:3180:ILE:H	2	0.36
(1,1222)	1:A:3130:PRO:HG2	1:A:3132:GLY:HA3	9	0.36
(1,1222)	1:A:3130:PRO:HG3	1:A:3132:GLY:HA3	9	0.36
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD11	8	0.36
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD12	8	0.36
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD13	8	0.36
(1,991)	1:A:3167:ILE:HA	1:A:3212:TRP:HZ3	2	0.35
(1,953)	1:A:3143:ILE:HG21	1:A:3212:TRP:HE1	4	0.35
(1,953)	1:A:3143:ILE:HG22	1:A:3212:TRP:HE1	4	0.35
(1,953)	1:A:3143:ILE:HG23	1:A:3212:TRP:HE1	4	0.35
(1,808)	1:A:3143:ILE:HG21	1:A:3170:TYR:H	4	0.35
(1,808)	1:A:3143:ILE:HG22	1:A:3170:TYR:H	4	0.35
(1,808)	1:A:3143:ILE:HG23	1:A:3170:TYR:H	4	0.35
(1,745)	1:A:3149:SER:HA	1:A:3153:ASP:H	2	0.35
(1,617)	1:A:3111:GLY:H	1:A:3113:LYS:H	6	0.35
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG21	7	0.35
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG22	7	0.35
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG23	7	0.35
(1,482)	1:A:3208:PRO:HA	1:A:3211:GLN:HG2	4	0.35
(1,194)	1:A:3133:VAL:HA	1:A:3199:ILE:HG21	3	0.35
(1,194)	1:A:3133:VAL:HA	1:A:3199:ILE:HG22	3	0.35
(1,194)	1:A:3133:VAL:HA	1:A:3199:ILE:HG23	3	0.35
(1,1439)	1:A:3192:PRO:HB2	1:A:3194:PHE:H	5	0.35
(1,1439)	1:A:3192:PRO:HB3	1:A:3194:PHE:H	5	0.35
(1,1069)	1:A:3105:ILE:HG21	1:A:3212:TRP:HD1	4	0.35
(1,1069)	1:A:3105:ILE:HG22	1:A:3212:TRP:HD1	4	0.35
(1,1069)	1:A:3105:ILE:HG23	1:A:3212:TRP:HD1	4	0.35
(1,1000)	1:A:3183:TYR:HE1	1:A:3187:GLU:HG2	2	0.35
(1,1000)	1:A:3183:TYR:HE2	1:A:3187:GLU:HG2	2	0.35
(1,950)	1:A:3109:GLN:HG3	1:A:3212:TRP:HE1	9	0.34
(1,929)	1:A:3115:ILE:HG21	1:A:3207:GLY:H	2	0.34
(1,929)	1:A:3115:ILE:HG22	1:A:3207:GLY:H	2	0.34
(1,929)	1:A:3115:ILE:HG23	1:A:3207:GLY:H	2	0.34
(1,929)	1:A:3115:ILE:HG21	1:A:3207:GLY:H	6	0.34
(1,929)	1:A:3115:ILE:HG22	1:A:3207:GLY:H	6	0.34
(1,929)	1:A:3115:ILE:HG23	1:A:3207:GLY:H	6	0.34
(1,883)	1:A:3195:THR:HB	1:A:3197:GLU:H	6	0.34
(1,872)	1:A:3192:PRO:HB3	1:A:3194:PHE:H	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,867)	1:A:3193:ASN:H	1:A:3195:THR:H	7	0.34
(1,842)	1:A:3185:GLU:H	1:A:3217:ILE:HD11	9	0.34
(1,842)	1:A:3185:GLU:H	1:A:3217:ILE:HD12	9	0.34
(1,842)	1:A:3185:GLU:H	1:A:3217:ILE:HD13	9	0.34
(1,815)	1:A:3173:THR:H	1:A:3173:THR:HG21	8	0.34
(1,815)	1:A:3173:THR:H	1:A:3173:THR:HG22	8	0.34
(1,815)	1:A:3173:THR:H	1:A:3173:THR:HG23	8	0.34
(1,79)	1:A:3135:ILE:HG21	1:A:3194:PHE:HA	10	0.34
(1,79)	1:A:3135:ILE:HG22	1:A:3194:PHE:HA	10	0.34
(1,79)	1:A:3135:ILE:HG23	1:A:3194:PHE:HA	10	0.34
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD11	9	0.34
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD12	9	0.34
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD13	9	0.34
(1,1439)	1:A:3192:PRO:HB2	1:A:3194:PHE:H	10	0.34
(1,1439)	1:A:3192:PRO:HB3	1:A:3194:PHE:H	10	0.34
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG11	3	0.34
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG12	3	0.34
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG13	3	0.34
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG21	3	0.34
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG22	3	0.34
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG23	3	0.34
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG21	2	0.33
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG22	2	0.33
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG23	2	0.33
(1,50)	1:A:3115:ILE:HD11	1:A:3209:LEU:H	4	0.33
(1,50)	1:A:3115:ILE:HD12	1:A:3209:LEU:H	4	0.33
(1,50)	1:A:3115:ILE:HD13	1:A:3209:LEU:H	4	0.33
(1,351)	1:A:3206:CYS:HA	1:A:3209:LEU:HG	1	0.33
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG11	10	0.33
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG12	10	0.33
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG13	10	0.33
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG21	10	0.33
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG22	10	0.33
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG23	10	0.33
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG2	5	0.33
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG3	5	0.33
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD11	7	0.33
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD12	7	0.33
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD13	7	0.33
(1,1037)	1:A:3170:TYR:HE1	1:A:3172:THR:HG21	5	0.33
(1,1037)	1:A:3170:TYR:HE1	1:A:3172:THR:HG22	5	0.33
(1,1037)	1:A:3170:TYR:HE1	1:A:3172:THR:HG23	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	1:A:3170:TYR:HE2	1:A:3172:THR:HG21	5	0.33
(1,1037)	1:A:3170:TYR:HE2	1:A:3172:THR:HG22	5	0.33
(1,1037)	1:A:3170:TYR:HE2	1:A:3172:THR:HG23	5	0.33
(1,991)	1:A:3167:ILE:HA	1:A:3212:TRP:HZ3	7	0.32
(1,846)	1:A:3184:MET:HA	1:A:3186:GLU:H	2	0.32
(1,842)	1:A:3185:GLU:H	1:A:3217:ILE:HD11	6	0.32
(1,842)	1:A:3185:GLU:H	1:A:3217:ILE:HD12	6	0.32
(1,842)	1:A:3185:GLU:H	1:A:3217:ILE:HD13	6	0.32
(1,837)	1:A:3179:GLN:H	1:A:3182:LYS:H	4	0.32
(1,815)	1:A:3173:THR:H	1:A:3173:THR:HG21	6	0.32
(1,815)	1:A:3173:THR:H	1:A:3173:THR:HG22	6	0.32
(1,815)	1:A:3173:THR:H	1:A:3173:THR:HG23	6	0.32
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG21	8	0.32
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG22	8	0.32
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG23	8	0.32
(1,342)	1:A:3185:GLU:HA	1:A:3189:LEU:HB3	4	0.32
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD11	6	0.32
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD12	6	0.32
(1,205)	1:A:3214:ASN:HA	1:A:3217:ILE:HD13	6	0.32
(1,1432)	1:A:3190:SER:H	1:A:3191:ASP:HB2	10	0.32
(1,1432)	1:A:3190:SER:H	1:A:3191:ASP:HB3	10	0.32
(1,867)	1:A:3193:ASN:H	1:A:3195:THR:H	6	0.31
(1,859)	1:A:3185:GLU:HA	1:A:3189:LEU:H	4	0.31
(1,745)	1:A:3149:SER:HA	1:A:3153:ASP:H	3	0.31
(1,745)	1:A:3149:SER:HA	1:A:3153:ASP:H	10	0.31
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG21	8	0.31
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG22	8	0.31
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG23	8	0.31
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD11	10	0.31
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD12	10	0.31
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD13	10	0.31
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG21	3	0.31
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG22	3	0.31
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG23	3	0.31
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG21	9	0.31
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG22	9	0.31
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG23	9	0.31
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG21	7	0.31
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG22	7	0.31
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG23	7	0.31
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG21	10	0.31
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG22	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG23	10	0.31
(1,351)	1:A:3206:CYS:HA	1:A:3209:LEU:HG	6	0.31
(1,351)	1:A:3206:CYS:HA	1:A:3209:LEU:HG	10	0.31
(1,231)	1:A:3140:VAL:HG11	1:A:3212:TRP:HH2	2	0.31
(1,231)	1:A:3140:VAL:HG12	1:A:3212:TRP:HH2	2	0.31
(1,231)	1:A:3140:VAL:HG13	1:A:3212:TRP:HH2	2	0.31
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG21	4	0.31
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG22	4	0.31
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG23	4	0.31
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG21	4	0.31
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG22	4	0.31
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG23	4	0.31
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG21	4	0.31
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG22	4	0.31
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG23	4	0.31
(1,1450)	1:A:3197:GLU:HG2	1:A:3199:ILE:H	3	0.31
(1,1450)	1:A:3197:GLU:HG3	1:A:3199:ILE:H	3	0.31
(1,1276)	1:A:3137:MET:HG2	1:A:3140:VAL:HG11	7	0.31
(1,1276)	1:A:3137:MET:HG2	1:A:3140:VAL:HG12	7	0.31
(1,1276)	1:A:3137:MET:HG2	1:A:3140:VAL:HG13	7	0.31
(1,1276)	1:A:3137:MET:HG2	1:A:3140:VAL:HG21	7	0.31
(1,1276)	1:A:3137:MET:HG2	1:A:3140:VAL:HG22	7	0.31
(1,1276)	1:A:3137:MET:HG2	1:A:3140:VAL:HG23	7	0.31
(1,1276)	1:A:3137:MET:HG3	1:A:3140:VAL:HG11	7	0.31
(1,1276)	1:A:3137:MET:HG3	1:A:3140:VAL:HG12	7	0.31
(1,1276)	1:A:3137:MET:HG3	1:A:3140:VAL:HG13	7	0.31
(1,1276)	1:A:3137:MET:HG3	1:A:3140:VAL:HG21	7	0.31
(1,1276)	1:A:3137:MET:HG3	1:A:3140:VAL:HG22	7	0.31
(1,1276)	1:A:3137:MET:HG3	1:A:3140:VAL:HG23	7	0.31
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD11	4	0.31
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD12	4	0.31
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD13	4	0.31
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD11	9	0.31
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD12	9	0.31
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD13	9	0.31
(1,1150)	1:A:3119:GLN:HB2	1:A:3205:ALA:HA	6	0.31
(1,1150)	1:A:3119:GLN:HB3	1:A:3205:ALA:HA	6	0.31
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE1	2	0.31
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE2	2	0.31
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE1	2	0.31
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE2	2	0.31
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE1	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE2	2	0.31
(1,994)	1:A:3108:ALA:HB1	1:A:3212:TRP:HE3	7	0.3
(1,994)	1:A:3108:ALA:HB2	1:A:3212:TRP:HE3	7	0.3
(1,994)	1:A:3108:ALA:HB3	1:A:3212:TRP:HE3	7	0.3
(1,974)	1:A:3224:GLU:H	1:A:3225:ASN:HA	5	0.3
(1,964)	1:A:3218:ASN:H	1:A:3220:SER:H	5	0.3
(1,929)	1:A:3115:ILE:HG21	1:A:3207:GLY:H	7	0.3
(1,929)	1:A:3115:ILE:HG22	1:A:3207:GLY:H	7	0.3
(1,929)	1:A:3115:ILE:HG23	1:A:3207:GLY:H	7	0.3
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG21	9	0.3
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG22	9	0.3
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG23	9	0.3
(1,765)	1:A:3158:ILE:HA	1:A:3160:LYS:H	2	0.3
(1,76)	1:A:3135:ILE:HG21	1:A:3193:ASN:HB2	3	0.3
(1,76)	1:A:3135:ILE:HG21	1:A:3193:ASN:HB3	3	0.3
(1,76)	1:A:3135:ILE:HG22	1:A:3193:ASN:HB2	3	0.3
(1,76)	1:A:3135:ILE:HG22	1:A:3193:ASN:HB3	3	0.3
(1,76)	1:A:3135:ILE:HG23	1:A:3193:ASN:HB2	3	0.3
(1,76)	1:A:3135:ILE:HG23	1:A:3193:ASN:HB3	3	0.3
(1,638)	1:A:3119:GLN:H	1:A:3205:ALA:HB1	1	0.3
(1,638)	1:A:3119:GLN:H	1:A:3205:ALA:HB2	1	0.3
(1,638)	1:A:3119:GLN:H	1:A:3205:ALA:HB3	1	0.3
(1,501)	1:A:3115:ILE:HG21	1:A:3119:GLN:HG2	10	0.3
(1,501)	1:A:3115:ILE:HG22	1:A:3119:GLN:HG2	10	0.3
(1,501)	1:A:3115:ILE:HG23	1:A:3119:GLN:HG2	10	0.3
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG21	4	0.3
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG22	4	0.3
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG23	4	0.3
(1,440)	1:A:3184:MET:HA	1:A:3217:ILE:HD11	5	0.3
(1,440)	1:A:3184:MET:HA	1:A:3217:ILE:HD12	5	0.3
(1,440)	1:A:3184:MET:HA	1:A:3217:ILE:HD13	5	0.3
(1,412)	1:A:3136:VAL:HG11	1:A:3210:TYR:HB3	3	0.3
(1,412)	1:A:3136:VAL:HG12	1:A:3210:TYR:HB3	3	0.3
(1,412)	1:A:3136:VAL:HG13	1:A:3210:TYR:HB3	3	0.3
(1,372)	1:A:3189:LEU:HD11	1:A:3190:SER:HB3	4	0.3
(1,372)	1:A:3189:LEU:HD12	1:A:3190:SER:HB3	4	0.3
(1,372)	1:A:3189:LEU:HD13	1:A:3190:SER:HB3	4	0.3
(1,285)	1:A:3142:ALA:HB1	1:A:3183:TYR:HE1	7	0.3
(1,285)	1:A:3142:ALA:HB1	1:A:3183:TYR:HE2	7	0.3
(1,285)	1:A:3142:ALA:HB2	1:A:3183:TYR:HE1	7	0.3
(1,285)	1:A:3142:ALA:HB2	1:A:3183:TYR:HE2	7	0.3
(1,285)	1:A:3142:ALA:HB3	1:A:3183:TYR:HE1	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	1:A:3142:ALA:HB3	1:A:3183:TYR:HE2	7	0.3
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD11	4	0.3
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD12	4	0.3
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD13	4	0.3
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD21	4	0.3
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD22	4	0.3
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD23	4	0.3
(1,1091)	1:A:3098:ILE:HG21	1:A:3099:GLN:HB2	1	0.3
(1,1091)	1:A:3098:ILE:HG21	1:A:3099:GLN:HB3	1	0.3
(1,1091)	1:A:3098:ILE:HG22	1:A:3099:GLN:HB2	1	0.3
(1,1091)	1:A:3098:ILE:HG22	1:A:3099:GLN:HB3	1	0.3
(1,1091)	1:A:3098:ILE:HG23	1:A:3099:GLN:HB2	1	0.3
(1,1091)	1:A:3098:ILE:HG23	1:A:3099:GLN:HB3	1	0.3
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE1	8	0.3
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE2	8	0.3
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE1	8	0.3
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE2	8	0.3
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE1	8	0.3
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE2	8	0.3
(1,950)	1:A:3109:GLN:HG3	1:A:3212:TRP:HE1	8	0.29
(1,946)	1:A:3170:TYR:HE1	1:A:3212:TRP:HE1	4	0.29
(1,946)	1:A:3170:TYR:HE2	1:A:3212:TRP:HE1	4	0.29
(1,929)	1:A:3115:ILE:HG21	1:A:3207:GLY:H	3	0.29
(1,929)	1:A:3115:ILE:HG22	1:A:3207:GLY:H	3	0.29
(1,929)	1:A:3115:ILE:HG23	1:A:3207:GLY:H	3	0.29
(1,883)	1:A:3195:THR:HB	1:A:3197:GLU:H	3	0.29
(1,872)	1:A:3192:PRO:HB3	1:A:3194:PHE:H	10	0.29
(1,867)	1:A:3193:ASN:H	1:A:3195:THR:H	1	0.29
(1,815)	1:A:3173:THR:H	1:A:3173:THR:HG21	10	0.29
(1,815)	1:A:3173:THR:H	1:A:3173:THR:HG22	10	0.29
(1,815)	1:A:3173:THR:H	1:A:3173:THR:HG23	10	0.29
(1,745)	1:A:3149:SER:HA	1:A:3153:ASP:H	7	0.29
(1,611)	1:A:3111:GLY:H	1:A:3113:LYS:HG3	6	0.29
(1,548)	1:A:3152:ARG:HA	1:A:3152:ARG:HD2	2	0.29
(1,548)	1:A:3152:ARG:HA	1:A:3152:ARG:HD3	2	0.29
(1,501)	1:A:3115:ILE:HG21	1:A:3119:GLN:HG2	2	0.29
(1,501)	1:A:3115:ILE:HG22	1:A:3119:GLN:HG2	2	0.29
(1,501)	1:A:3115:ILE:HG23	1:A:3119:GLN:HG2	2	0.29
(1,252)	1:A:3140:VAL:HA	1:A:3167:ILE:HA	7	0.29
(1,200)	1:A:3181:ARG:HD2	1:A:3217:ILE:HA	8	0.29
(1,200)	1:A:3181:ARG:HD3	1:A:3217:ILE:HA	8	0.29
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD1	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD2	4	0.29
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD1	4	0.29
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD2	4	0.29
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD11	10	0.29
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD12	10	0.29
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD13	10	0.29
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD11	10	0.29
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD12	10	0.29
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD13	10	0.29
(1,1001)	1:A:3183:TYR:HE1	1:A:3187:GLU:HB2	10	0.29
(1,1001)	1:A:3183:TYR:HE1	1:A:3187:GLU:HB3	10	0.29
(1,1001)	1:A:3183:TYR:HE2	1:A:3187:GLU:HB2	10	0.29
(1,1001)	1:A:3183:TYR:HE2	1:A:3187:GLU:HB3	10	0.29
(1,953)	1:A:3143:ILE:HG21	1:A:3212:TRP:HE1	2	0.28
(1,953)	1:A:3143:ILE:HG22	1:A:3212:TRP:HE1	2	0.28
(1,953)	1:A:3143:ILE:HG23	1:A:3212:TRP:HE1	2	0.28
(1,950)	1:A:3109:GLN:HG3	1:A:3212:TRP:HE1	10	0.28
(1,929)	1:A:3115:ILE:HG21	1:A:3207:GLY:H	8	0.28
(1,929)	1:A:3115:ILE:HG22	1:A:3207:GLY:H	8	0.28
(1,929)	1:A:3115:ILE:HG23	1:A:3207:GLY:H	8	0.28
(1,929)	1:A:3115:ILE:HG21	1:A:3207:GLY:H	10	0.28
(1,929)	1:A:3115:ILE:HG22	1:A:3207:GLY:H	10	0.28
(1,929)	1:A:3115:ILE:HG23	1:A:3207:GLY:H	10	0.28
(1,524)	1:A:3138:GLU:HG2	1:A:3154:ILE:HD11	8	0.28
(1,524)	1:A:3138:GLU:HG2	1:A:3154:ILE:HD12	8	0.28
(1,524)	1:A:3138:GLU:HG2	1:A:3154:ILE:HD13	8	0.28
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG2	2	0.28
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG3	2	0.28
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD11	7	0.28
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD12	7	0.28
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD13	7	0.28
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG21	6	0.28
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG22	6	0.28
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG23	6	0.28
(1,345)	1:A:3205:ALA:HB1	1:A:3209:LEU:HB2	5	0.28
(1,345)	1:A:3205:ALA:HB2	1:A:3209:LEU:HB2	5	0.28
(1,345)	1:A:3205:ALA:HB3	1:A:3209:LEU:HB2	5	0.28
(1,272)	1:A:3210:TYR:HA	1:A:3213:VAL:HG11	1	0.28
(1,272)	1:A:3210:TYR:HA	1:A:3213:VAL:HG12	1	0.28
(1,272)	1:A:3210:TYR:HA	1:A:3213:VAL:HG13	1	0.28
(1,231)	1:A:3140:VAL:HG11	1:A:3212:TRP:HH2	6	0.28
(1,231)	1:A:3140:VAL:HG12	1:A:3212:TRP:HH2	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:A:3140:VAL:HG13	1:A:3212:TRP:HH2	6	0.28
(1,1414)	1:A:3185:GLU:HG2	1:A:3217:ILE:HG21	4	0.28
(1,1414)	1:A:3185:GLU:HG2	1:A:3217:ILE:HG22	4	0.28
(1,1414)	1:A:3185:GLU:HG2	1:A:3217:ILE:HG23	4	0.28
(1,1414)	1:A:3185:GLU:HG3	1:A:3217:ILE:HG21	4	0.28
(1,1414)	1:A:3185:GLU:HG3	1:A:3217:ILE:HG22	4	0.28
(1,1414)	1:A:3185:GLU:HG3	1:A:3217:ILE:HG23	4	0.28
(1,1382)	1:A:3170:TYR:HB2	1:A:3212:TRP:HH2	4	0.28
(1,1382)	1:A:3170:TYR:HB3	1:A:3212:TRP:HH2	4	0.28
(1,117)	1:A:3158:ILE:HD11	1:A:3163:PHE:HE1	7	0.28
(1,117)	1:A:3158:ILE:HD11	1:A:3163:PHE:HE2	7	0.28
(1,117)	1:A:3158:ILE:HD12	1:A:3163:PHE:HE1	7	0.28
(1,117)	1:A:3158:ILE:HD12	1:A:3163:PHE:HE2	7	0.28
(1,117)	1:A:3158:ILE:HD13	1:A:3163:PHE:HE1	7	0.28
(1,117)	1:A:3158:ILE:HD13	1:A:3163:PHE:HE2	7	0.28
(1,991)	1:A:3167:ILE:HA	1:A:3212:TRP:HZ3	9	0.27
(1,956)	1:A:3213:VAL:HB	1:A:3214:ASN:H	6	0.27
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG21	7	0.27
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG22	7	0.27
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG23	7	0.27
(1,76)	1:A:3135:ILE:HG21	1:A:3193:ASN:HB2	6	0.27
(1,76)	1:A:3135:ILE:HG21	1:A:3193:ASN:HB3	6	0.27
(1,76)	1:A:3135:ILE:HG22	1:A:3193:ASN:HB2	6	0.27
(1,76)	1:A:3135:ILE:HG22	1:A:3193:ASN:HB3	6	0.27
(1,76)	1:A:3135:ILE:HG23	1:A:3193:ASN:HB2	6	0.27
(1,76)	1:A:3135:ILE:HG23	1:A:3193:ASN:HB3	6	0.27
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG21	10	0.27
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG22	10	0.27
(1,714)	1:A:3142:ALA:H	1:A:3143:ILE:HG23	10	0.27
(1,626)	1:A:3112:VAL:HA	1:A:3115:ILE:H	8	0.27
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG21	6	0.27
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG22	6	0.27
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG23	6	0.27
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG2	6	0.27
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG3	6	0.27
(1,351)	1:A:3206:CYS:HA	1:A:3209:LEU:HG	5	0.27
(1,252)	1:A:3140:VAL:HA	1:A:3167:ILE:HA	3	0.27
(1,246)	1:A:3136:VAL:HA	1:A:3210:TYR:HA	1	0.27
(1,246)	1:A:3136:VAL:HA	1:A:3210:TYR:HA	8	0.27
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG2	4	0.27
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG3	4	0.27
(1,80)	1:A:3135:ILE:HG21	1:A:3194:PHE:HE1	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:A:3135:ILE:HG21	1:A:3194:PHE:HE2	1	0.26
(1,80)	1:A:3135:ILE:HG22	1:A:3194:PHE:HE1	1	0.26
(1,80)	1:A:3135:ILE:HG22	1:A:3194:PHE:HE2	1	0.26
(1,80)	1:A:3135:ILE:HG23	1:A:3194:PHE:HE1	1	0.26
(1,80)	1:A:3135:ILE:HG23	1:A:3194:PHE:HE2	1	0.26
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG21	3	0.26
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG22	3	0.26
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG23	3	0.26
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG21	8	0.26
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG22	8	0.26
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG23	8	0.26
(1,745)	1:A:3149:SER:HA	1:A:3153:ASP:H	9	0.26
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG21	1	0.26
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG22	1	0.26
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG23	1	0.26
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG21	10	0.26
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG22	10	0.26
(1,616)	1:A:3112:VAL:H	1:A:3167:ILE:HG23	10	0.26
(1,611)	1:A:3111:GLY:H	1:A:3113:LYS:HG3	4	0.26
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG2	4	0.26
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG3	4	0.26
(1,506)	1:A:3147:GLN:HA	1:A:3147:GLN:HG3	9	0.26
(1,50)	1:A:3115:ILE:HD11	1:A:3209:LEU:H	1	0.26
(1,50)	1:A:3115:ILE:HD12	1:A:3209:LEU:H	1	0.26
(1,50)	1:A:3115:ILE:HD13	1:A:3209:LEU:H	1	0.26
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG21	3	0.26
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG22	3	0.26
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG23	3	0.26
(1,25)	1:A:3098:ILE:HD11	1:A:3099:GLN:HA	6	0.26
(1,25)	1:A:3098:ILE:HD12	1:A:3099:GLN:HA	6	0.26
(1,25)	1:A:3098:ILE:HD13	1:A:3099:GLN:HA	6	0.26
(1,159)	1:A:3167:ILE:HG21	1:A:3170:TYR:HB2	6	0.26
(1,159)	1:A:3167:ILE:HG22	1:A:3170:TYR:HB2	6	0.26
(1,159)	1:A:3167:ILE:HG23	1:A:3170:TYR:HB2	6	0.26
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG11	2	0.26
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG12	2	0.26
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG13	2	0.26
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG21	2	0.26
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG22	2	0.26
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG23	2	0.26
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG11	2	0.26
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG12	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG13	2	0.26
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG21	2	0.26
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG22	2	0.26
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG23	2	0.26
(1,1438)	1:A:3192:PRO:HB2	1:A:3193:ASN:H	4	0.26
(1,1438)	1:A:3192:PRO:HB3	1:A:3193:ASN:H	4	0.26
(1,1419)	1:A:3187:GLU:HG2	1:A:3188:PHE:H	5	0.26
(1,1419)	1:A:3187:GLU:HG3	1:A:3188:PHE:H	5	0.26
(1,1410)	1:A:3185:GLU:H	1:A:3187:GLU:HG2	5	0.26
(1,1410)	1:A:3185:GLU:H	1:A:3187:GLU:HG3	5	0.26
(1,1391)	1:A:3178:PRO:HB2	1:A:3180:ILE:H	3	0.26
(1,1391)	1:A:3178:PRO:HB3	1:A:3180:ILE:H	3	0.26
(1,1256)	1:A:3136:VAL:H	1:A:3206:CYS:HB2	1	0.26
(1,1256)	1:A:3136:VAL:H	1:A:3206:CYS:HB3	1	0.26
(1,11)	1:A:3123:ILE:HA	1:A:3126:MET:HE1	9	0.26
(1,11)	1:A:3123:ILE:HA	1:A:3126:MET:HE2	9	0.26
(1,11)	1:A:3123:ILE:HA	1:A:3126:MET:HE3	9	0.26
(1,953)	1:A:3143:ILE:HG21	1:A:3212:TRP:HE1	5	0.25
(1,953)	1:A:3143:ILE:HG22	1:A:3212:TRP:HE1	5	0.25
(1,953)	1:A:3143:ILE:HG23	1:A:3212:TRP:HE1	5	0.25
(1,91)	1:A:3143:ILE:HD11	1:A:3212:TRP:HZ2	9	0.25
(1,91)	1:A:3143:ILE:HD12	1:A:3212:TRP:HZ2	9	0.25
(1,91)	1:A:3143:ILE:HD13	1:A:3212:TRP:HZ2	9	0.25
(1,867)	1:A:3193:ASN:H	1:A:3195:THR:H	8	0.25
(1,861)	1:A:3187:GLU:HB2	1:A:3189:LEU:H	5	0.25
(1,861)	1:A:3187:GLU:HB3	1:A:3189:LEU:H	5	0.25
(1,856)	1:A:3187:GLU:HB2	1:A:3188:PHE:H	10	0.25
(1,856)	1:A:3187:GLU:HB3	1:A:3188:PHE:H	10	0.25
(1,829)	1:A:3179:GLN:H	1:A:3180:ILE:HA	2	0.25
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG21	5	0.25
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG22	5	0.25
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG23	5	0.25
(1,765)	1:A:3158:ILE:HA	1:A:3160:LYS:H	10	0.25
(1,588)	1:A:3098:ILE:HD11	1:A:3099:GLN:H	6	0.25
(1,588)	1:A:3098:ILE:HD12	1:A:3099:GLN:H	6	0.25
(1,588)	1:A:3098:ILE:HD13	1:A:3099:GLN:H	6	0.25
(1,50)	1:A:3115:ILE:HD11	1:A:3209:LEU:H	2	0.25
(1,50)	1:A:3115:ILE:HD12	1:A:3209:LEU:H	2	0.25
(1,50)	1:A:3115:ILE:HD13	1:A:3209:LEU:H	2	0.25
(1,49)	1:A:3115:ILE:HD11	1:A:3205:ALA:HA	9	0.25
(1,49)	1:A:3115:ILE:HD12	1:A:3205:ALA:HA	9	0.25
(1,49)	1:A:3115:ILE:HD13	1:A:3205:ALA:HA	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:A:3112:VAL:HA	1:A:3115:ILE:HD11	4	0.25
(1,48)	1:A:3112:VAL:HA	1:A:3115:ILE:HD12	4	0.25
(1,48)	1:A:3112:VAL:HA	1:A:3115:ILE:HD13	4	0.25
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG21	10	0.25
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG22	10	0.25
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG23	10	0.25
(1,437)	1:A:3134:LYS:HA	1:A:3137:MET:HG3	10	0.25
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG21	5	0.25
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG22	5	0.25
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG23	5	0.25
(1,351)	1:A:3206:CYS:HA	1:A:3209:LEU:HG	3	0.25
(1,343)	1:A:3185:GLU:HA	1:A:3189:LEU:HB2	8	0.25
(1,252)	1:A:3140:VAL:HA	1:A:3167:ILE:HA	8	0.25
(1,219)	1:A:3112:VAL:HG11	1:A:3212:TRP:HD1	1	0.25
(1,219)	1:A:3112:VAL:HG12	1:A:3212:TRP:HD1	1	0.25
(1,219)	1:A:3112:VAL:HG13	1:A:3212:TRP:HD1	1	0.25
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG2	3	0.25
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG3	3	0.25
(1,1439)	1:A:3192:PRO:HB2	1:A:3194:PHE:H	4	0.25
(1,1439)	1:A:3192:PRO:HB3	1:A:3194:PHE:H	4	0.25
(1,1391)	1:A:3178:PRO:HB2	1:A:3180:ILE:H	8	0.25
(1,1391)	1:A:3178:PRO:HB3	1:A:3180:ILE:H	8	0.25
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD1	7	0.25
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD2	7	0.25
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD1	7	0.25
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD2	7	0.25
(1,1236)	1:A:3133:VAL:HG11	1:A:3202:ALA:H	1	0.25
(1,1236)	1:A:3133:VAL:HG12	1:A:3202:ALA:H	1	0.25
(1,1236)	1:A:3133:VAL:HG13	1:A:3202:ALA:H	1	0.25
(1,1236)	1:A:3133:VAL:HG21	1:A:3202:ALA:H	1	0.25
(1,1236)	1:A:3133:VAL:HG22	1:A:3202:ALA:H	1	0.25
(1,1236)	1:A:3133:VAL:HG23	1:A:3202:ALA:H	1	0.25
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG11	9	0.25
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG12	9	0.25
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG13	9	0.25
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG21	9	0.25
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG22	9	0.25
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG23	9	0.25
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE1	4	0.25
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE2	4	0.25
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE1	4	0.25
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE2	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE1	4	0.25
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE2	4	0.25
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE1	10	0.25
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE2	10	0.25
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE1	10	0.25
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE2	10	0.25
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE1	10	0.25
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE2	10	0.25
(1,991)	1:A:3167:ILE:HA	1:A:3212:TRP:HZ3	10	0.24
(1,951)	1:A:3108:ALA:HB1	1:A:3212:TRP:HE1	6	0.24
(1,951)	1:A:3108:ALA:HB2	1:A:3212:TRP:HE1	6	0.24
(1,951)	1:A:3108:ALA:HB3	1:A:3212:TRP:HE1	6	0.24
(1,950)	1:A:3109:GLN:HG3	1:A:3212:TRP:HE1	4	0.24
(1,929)	1:A:3115:ILE:HG21	1:A:3207:GLY:H	5	0.24
(1,929)	1:A:3115:ILE:HG22	1:A:3207:GLY:H	5	0.24
(1,929)	1:A:3115:ILE:HG23	1:A:3207:GLY:H	5	0.24
(1,888)	1:A:3197:GLU:H	1:A:3210:TYR:HD1	10	0.24
(1,888)	1:A:3197:GLU:H	1:A:3210:TYR:HD2	10	0.24
(1,883)	1:A:3195:THR:HB	1:A:3197:GLU:H	10	0.24
(1,876)	1:A:3135:ILE:HD11	1:A:3195:THR:H	5	0.24
(1,876)	1:A:3135:ILE:HD12	1:A:3195:THR:H	5	0.24
(1,876)	1:A:3135:ILE:HD13	1:A:3195:THR:H	5	0.24
(1,853)	1:A:3185:GLU:HA	1:A:3188:PHE:H	2	0.24
(1,822)	1:A:3196:TYR:H	1:A:3210:TYR:HD1	2	0.24
(1,822)	1:A:3196:TYR:H	1:A:3210:TYR:HD2	2	0.24
(1,61)	1:A:3180:ILE:HG21	1:A:3181:ARG:HA	8	0.24
(1,61)	1:A:3180:ILE:HG22	1:A:3181:ARG:HA	8	0.24
(1,61)	1:A:3180:ILE:HG23	1:A:3181:ARG:HA	8	0.24
(1,548)	1:A:3152:ARG:HA	1:A:3152:ARG:HD2	4	0.24
(1,548)	1:A:3152:ARG:HA	1:A:3152:ARG:HD3	4	0.24
(1,457)	1:A:3214:ASN:HB2	1:A:3217:ILE:HG21	2	0.24
(1,457)	1:A:3214:ASN:HB2	1:A:3217:ILE:HG22	2	0.24
(1,457)	1:A:3214:ASN:HB2	1:A:3217:ILE:HG23	2	0.24
(1,453)	1:A:3193:ASN:HB2	1:A:3194:PHE:HB2	8	0.24
(1,453)	1:A:3193:ASN:HB3	1:A:3194:PHE:HB2	8	0.24
(1,434)	1:A:3136:VAL:HG21	1:A:3137:MET:HG2	3	0.24
(1,434)	1:A:3136:VAL:HG22	1:A:3137:MET:HG2	3	0.24
(1,434)	1:A:3136:VAL:HG23	1:A:3137:MET:HG2	3	0.24
(1,327)	1:A:3189:LEU:HD11	1:A:3190:SER:HB2	7	0.24
(1,327)	1:A:3189:LEU:HD12	1:A:3190:SER:HB2	7	0.24
(1,327)	1:A:3189:LEU:HD13	1:A:3190:SER:HB2	7	0.24
(1,246)	1:A:3136:VAL:HA	1:A:3210:TYR:HA	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:A:3112:VAL:HG11	1:A:3212:TRP:HD1	4	0.24
(1,219)	1:A:3112:VAL:HG12	1:A:3212:TRP:HD1	4	0.24
(1,219)	1:A:3112:VAL:HG13	1:A:3212:TRP:HD1	4	0.24
(1,159)	1:A:3167:ILE:HG21	1:A:3170:TYR:HB2	1	0.24
(1,159)	1:A:3167:ILE:HG22	1:A:3170:TYR:HB2	1	0.24
(1,159)	1:A:3167:ILE:HG23	1:A:3170:TYR:HB2	1	0.24
(1,1506)	1:A:3218:ASN:HB2	1:A:3221:LYS:HG2	8	0.24
(1,1506)	1:A:3218:ASN:HB2	1:A:3221:LYS:HG3	8	0.24
(1,1506)	1:A:3218:ASN:HB3	1:A:3221:LYS:HG2	8	0.24
(1,1506)	1:A:3218:ASN:HB3	1:A:3221:LYS:HG3	8	0.24
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD11	4	0.24
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD12	4	0.24
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD13	4	0.24
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD21	4	0.24
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD22	4	0.24
(1,1423)	1:A:3188:PHE:HB2	1:A:3189:LEU:HD23	4	0.24
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD11	4	0.24
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD12	4	0.24
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD13	4	0.24
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD21	4	0.24
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD22	4	0.24
(1,1423)	1:A:3188:PHE:HB3	1:A:3189:LEU:HD23	4	0.24
(1,1405)	1:A:3184:MET:HB2	1:A:3185:GLU:H	2	0.24
(1,1405)	1:A:3184:MET:HB3	1:A:3185:GLU:H	2	0.24
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD1	1	0.24
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD2	1	0.24
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD1	1	0.24
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD2	1	0.24
(1,12)	1:A:3137:MET:HE1	1:A:3209:LEU:HG	9	0.24
(1,12)	1:A:3137:MET:HE2	1:A:3209:LEU:HG	9	0.24
(1,12)	1:A:3137:MET:HE3	1:A:3209:LEU:HG	9	0.24
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD11	1	0.24
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD12	1	0.24
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD13	1	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG11	1	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG12	1	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG13	1	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG21	1	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG22	1	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG23	1	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG11	4	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG12	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG13	4	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG21	4	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG22	4	0.24
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG23	4	0.24
(1,1117)	1:A:3106:LEU:HD11	1:A:3109:GLN:HB3	5	0.24
(1,1117)	1:A:3106:LEU:HD12	1:A:3109:GLN:HB3	5	0.24
(1,1117)	1:A:3106:LEU:HD13	1:A:3109:GLN:HB3	5	0.24
(1,1117)	1:A:3106:LEU:HD21	1:A:3109:GLN:HB3	5	0.24
(1,1117)	1:A:3106:LEU:HD22	1:A:3109:GLN:HB3	5	0.24
(1,1117)	1:A:3106:LEU:HD23	1:A:3109:GLN:HB3	5	0.24
(1,1084)	1:A:3144:LEU:HD11	1:A:3212:TRP:HZ2	8	0.24
(1,1084)	1:A:3144:LEU:HD12	1:A:3212:TRP:HZ2	8	0.24
(1,1084)	1:A:3144:LEU:HD13	1:A:3212:TRP:HZ2	8	0.24
(1,1038)	1:A:3142:ALA:HB1	1:A:3183:TYR:HD1	9	0.24
(1,1038)	1:A:3142:ALA:HB1	1:A:3183:TYR:HD2	9	0.24
(1,1038)	1:A:3142:ALA:HB2	1:A:3183:TYR:HD1	9	0.24
(1,1038)	1:A:3142:ALA:HB2	1:A:3183:TYR:HD2	9	0.24
(1,1038)	1:A:3142:ALA:HB3	1:A:3183:TYR:HD1	9	0.24
(1,1038)	1:A:3142:ALA:HB3	1:A:3183:TYR:HD2	9	0.24
(1,991)	1:A:3167:ILE:HA	1:A:3212:TRP:HZ3	5	0.23
(1,929)	1:A:3115:ILE:HG21	1:A:3207:GLY:H	9	0.23
(1,929)	1:A:3115:ILE:HG22	1:A:3207:GLY:H	9	0.23
(1,929)	1:A:3115:ILE:HG23	1:A:3207:GLY:H	9	0.23
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG21	1	0.23
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG22	1	0.23
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG23	1	0.23
(1,76)	1:A:3135:ILE:HG21	1:A:3193:ASN:HB2	1	0.23
(1,76)	1:A:3135:ILE:HG21	1:A:3193:ASN:HB3	1	0.23
(1,76)	1:A:3135:ILE:HG22	1:A:3193:ASN:HB2	1	0.23
(1,76)	1:A:3135:ILE:HG22	1:A:3193:ASN:HB3	1	0.23
(1,76)	1:A:3135:ILE:HG23	1:A:3193:ASN:HB2	1	0.23
(1,76)	1:A:3135:ILE:HG23	1:A:3193:ASN:HB3	1	0.23
(1,721)	1:A:3144:LEU:H	1:A:3180:ILE:HD11	4	0.23
(1,721)	1:A:3144:LEU:H	1:A:3180:ILE:HD12	4	0.23
(1,721)	1:A:3144:LEU:H	1:A:3180:ILE:HD13	4	0.23
(1,720)	1:A:3140:VAL:HA	1:A:3144:LEU:H	1	0.23
(1,549)	1:A:3120:LEU:HG	1:A:3163:PHE:HB3	3	0.23
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG2	5	0.23
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG3	5	0.23
(1,49)	1:A:3115:ILE:HD11	1:A:3205:ALA:HA	10	0.23
(1,49)	1:A:3115:ILE:HD12	1:A:3205:ALA:HA	10	0.23
(1,49)	1:A:3115:ILE:HD13	1:A:3205:ALA:HA	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,472)	1:A:3137:MET:HE1	1:A:3206:CYS:HA	5	0.23
(1,472)	1:A:3137:MET:HE2	1:A:3206:CYS:HA	5	0.23
(1,472)	1:A:3137:MET:HE3	1:A:3206:CYS:HA	5	0.23
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG21	2	0.23
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG22	2	0.23
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG23	2	0.23
(1,442)	1:A:3184:MET:HG2	1:A:3217:ILE:HD11	10	0.23
(1,442)	1:A:3184:MET:HG2	1:A:3217:ILE:HD12	10	0.23
(1,442)	1:A:3184:MET:HG2	1:A:3217:ILE:HD13	10	0.23
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG21	4	0.23
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG22	4	0.23
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG23	4	0.23
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG21	1	0.23
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG22	1	0.23
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG23	1	0.23
(1,343)	1:A:3185:GLU:HA	1:A:3189:LEU:HB2	5	0.23
(1,32)	1:A:3105:ILE:HD11	1:A:3215:ALA:HB1	3	0.23
(1,32)	1:A:3105:ILE:HD11	1:A:3215:ALA:HB2	3	0.23
(1,32)	1:A:3105:ILE:HD11	1:A:3215:ALA:HB3	3	0.23
(1,32)	1:A:3105:ILE:HD12	1:A:3215:ALA:HB1	3	0.23
(1,32)	1:A:3105:ILE:HD12	1:A:3215:ALA:HB2	3	0.23
(1,32)	1:A:3105:ILE:HD12	1:A:3215:ALA:HB3	3	0.23
(1,32)	1:A:3105:ILE:HD13	1:A:3215:ALA:HB1	3	0.23
(1,32)	1:A:3105:ILE:HD13	1:A:3215:ALA:HB2	3	0.23
(1,32)	1:A:3105:ILE:HD13	1:A:3215:ALA:HB3	3	0.23
(1,259)	1:A:3109:GLN:HG3	1:A:3168:VAL:HA	3	0.23
(1,219)	1:A:3112:VAL:HG11	1:A:3212:TRP:HD1	9	0.23
(1,219)	1:A:3112:VAL:HG12	1:A:3212:TRP:HD1	9	0.23
(1,219)	1:A:3112:VAL:HG13	1:A:3212:TRP:HD1	9	0.23
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG2	1	0.23
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG3	1	0.23
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD1	6	0.23
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD2	6	0.23
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD1	6	0.23
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD2	6	0.23
(1,1327)	1:A:3144:LEU:HD11	1:A:3170:TYR:H	8	0.23
(1,1327)	1:A:3144:LEU:HD12	1:A:3170:TYR:H	8	0.23
(1,1327)	1:A:3144:LEU:HD13	1:A:3170:TYR:H	8	0.23
(1,1327)	1:A:3144:LEU:HD21	1:A:3170:TYR:H	8	0.23
(1,1327)	1:A:3144:LEU:HD22	1:A:3170:TYR:H	8	0.23
(1,1327)	1:A:3144:LEU:HD23	1:A:3170:TYR:H	8	0.23
(1,1236)	1:A:3133:VAL:HG11	1:A:3202:ALA:H	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	1:A:3133:VAL:HG12	1:A:3202:ALA:H	4	0.23
(1,1236)	1:A:3133:VAL:HG13	1:A:3202:ALA:H	4	0.23
(1,1236)	1:A:3133:VAL:HG21	1:A:3202:ALA:H	4	0.23
(1,1236)	1:A:3133:VAL:HG22	1:A:3202:ALA:H	4	0.23
(1,1236)	1:A:3133:VAL:HG23	1:A:3202:ALA:H	4	0.23
(1,1202)	1:A:3127:VAL:HB	1:A:3128:ASN:HB2	8	0.23
(1,1202)	1:A:3127:VAL:HB	1:A:3128:ASN:HB3	8	0.23
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG11	5	0.23
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG12	5	0.23
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG13	5	0.23
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG21	5	0.23
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG22	5	0.23
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG23	5	0.23
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE1	7	0.23
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE2	7	0.23
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE1	7	0.23
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE2	7	0.23
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE1	7	0.23
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE2	7	0.23
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE1	9	0.23
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE2	9	0.23
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE1	9	0.23
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE2	9	0.23
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE1	9	0.23
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE2	9	0.23
(1,983)	1:A:3226:VAL:H	1:A:3227:ASP:H	1	0.22
(1,978)	1:A:3223:LEU:HA	1:A:3225:ASN:H	9	0.22
(1,961)	1:A:3105:ILE:HG21	1:A:3216:GLN:H	2	0.22
(1,961)	1:A:3105:ILE:HG22	1:A:3216:GLN:H	2	0.22
(1,961)	1:A:3105:ILE:HG23	1:A:3216:GLN:H	2	0.22
(1,950)	1:A:3109:GLN:HG3	1:A:3212:TRP:HE1	3	0.22
(1,913)	1:A:3201:ARG:HA	1:A:3203:SER:H	1	0.22
(1,808)	1:A:3143:ILE:HG21	1:A:3170:TYR:H	2	0.22
(1,808)	1:A:3143:ILE:HG22	1:A:3170:TYR:H	2	0.22
(1,808)	1:A:3143:ILE:HG23	1:A:3170:TYR:H	2	0.22
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG21	2	0.22
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG22	2	0.22
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG23	2	0.22
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG21	4	0.22
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG22	4	0.22
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG23	4	0.22
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG21	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG22	6	0.22
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG23	6	0.22
(1,765)	1:A:3158:ILE:HA	1:A:3160:LYS:H	5	0.22
(1,764)	1:A:3159:ARG:H	1:A:3163:PHE:HD1	3	0.22
(1,764)	1:A:3159:ARG:H	1:A:3163:PHE:HD2	3	0.22
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD11	3	0.22
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD12	3	0.22
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD13	3	0.22
(1,511)	1:A:3124:ARG:HA	1:A:3155:GLN:HG2	8	0.22
(1,511)	1:A:3124:ARG:HA	1:A:3155:GLN:HG3	8	0.22
(1,509)	1:A:3155:GLN:HG2	1:A:3158:ILE:HD11	8	0.22
(1,509)	1:A:3155:GLN:HG2	1:A:3158:ILE:HD12	8	0.22
(1,509)	1:A:3155:GLN:HG2	1:A:3158:ILE:HD13	8	0.22
(1,509)	1:A:3155:GLN:HG3	1:A:3158:ILE:HD11	8	0.22
(1,509)	1:A:3155:GLN:HG3	1:A:3158:ILE:HD12	8	0.22
(1,509)	1:A:3155:GLN:HG3	1:A:3158:ILE:HD13	8	0.22
(1,501)	1:A:3115:ILE:HG21	1:A:3119:GLN:HG2	9	0.22
(1,501)	1:A:3115:ILE:HG22	1:A:3119:GLN:HG2	9	0.22
(1,501)	1:A:3115:ILE:HG23	1:A:3119:GLN:HG2	9	0.22
(1,480)	1:A:3203:SER:HB2	1:A:3206:CYS:HB3	1	0.22
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG21	1	0.22
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG22	1	0.22
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG23	1	0.22
(1,328)	1:A:3106:LEU:HD21	1:A:3109:GLN:HG3	4	0.22
(1,328)	1:A:3106:LEU:HD22	1:A:3109:GLN:HG3	4	0.22
(1,328)	1:A:3106:LEU:HD23	1:A:3109:GLN:HG3	4	0.22
(1,252)	1:A:3140:VAL:HA	1:A:3167:ILE:HA	4	0.22
(1,236)	1:A:3108:ALA:HB1	1:A:3212:TRP:HB3	1	0.22
(1,236)	1:A:3108:ALA:HB2	1:A:3212:TRP:HB3	1	0.22
(1,236)	1:A:3108:ALA:HB3	1:A:3212:TRP:HB3	1	0.22
(1,231)	1:A:3140:VAL:HG11	1:A:3212:TRP:HH2	5	0.22
(1,231)	1:A:3140:VAL:HG12	1:A:3212:TRP:HH2	5	0.22
(1,231)	1:A:3140:VAL:HG13	1:A:3212:TRP:HH2	5	0.22
(1,210)	1:A:3217:ILE:HG21	1:A:3221:LYS:HD2	8	0.22
(1,210)	1:A:3217:ILE:HG21	1:A:3221:LYS:HD3	8	0.22
(1,210)	1:A:3217:ILE:HG22	1:A:3221:LYS:HD2	8	0.22
(1,210)	1:A:3217:ILE:HG22	1:A:3221:LYS:HD3	8	0.22
(1,210)	1:A:3217:ILE:HG23	1:A:3221:LYS:HD2	8	0.22
(1,210)	1:A:3217:ILE:HG23	1:A:3221:LYS:HD3	8	0.22
(1,1516)	1:A:3224:GLU:HA	1:A:3225:ASN:HB2	2	0.22
(1,1516)	1:A:3224:GLU:HA	1:A:3225:ASN:HB3	2	0.22
(1,1493)	1:A:3214:ASN:HB2	1:A:3217:ILE:HB	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1493)	1:A:3214:ASN:HB3	1:A:3217:ILE:HB	4	0.22
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG2	7	0.22
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG3	7	0.22
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD11	10	0.22
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD12	10	0.22
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD13	10	0.22
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD21	10	0.22
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD22	10	0.22
(1,1421)	1:A:3188:PHE:HA	1:A:3189:LEU:HD23	10	0.22
(1,1201)	1:A:3127:VAL:HA	1:A:3128:ASN:HB2	7	0.22
(1,1201)	1:A:3127:VAL:HA	1:A:3128:ASN:HB3	7	0.22
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD11	2	0.22
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD12	2	0.22
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD13	2	0.22
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD11	2	0.22
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD12	2	0.22
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD13	2	0.22
(1,1150)	1:A:3119:GLN:HB2	1:A:3205:ALA:HA	9	0.22
(1,1150)	1:A:3119:GLN:HB3	1:A:3205:ALA:HA	9	0.22
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG11	2	0.22
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG12	2	0.22
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG13	2	0.22
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG21	2	0.22
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG22	2	0.22
(1,1122)	1:A:3109:GLN:HB3	1:A:3112:VAL:HG23	2	0.22
(1,1084)	1:A:3144:LEU:HD11	1:A:3212:TRP:HZ2	3	0.22
(1,1084)	1:A:3144:LEU:HD12	1:A:3212:TRP:HZ2	3	0.22
(1,1084)	1:A:3144:LEU:HD13	1:A:3212:TRP:HZ2	3	0.22
(1,1056)	1:A:3196:TYR:HE1	1:A:3199:ILE:HG21	2	0.22
(1,1056)	1:A:3196:TYR:HE1	1:A:3199:ILE:HG22	2	0.22
(1,1056)	1:A:3196:TYR:HE1	1:A:3199:ILE:HG23	2	0.22
(1,1056)	1:A:3196:TYR:HE2	1:A:3199:ILE:HG21	2	0.22
(1,1056)	1:A:3196:TYR:HE2	1:A:3199:ILE:HG22	2	0.22
(1,1056)	1:A:3196:TYR:HE2	1:A:3199:ILE:HG23	2	0.22
(1,956)	1:A:3213:VAL:HB	1:A:3214:ASN:H	10	0.21
(1,953)	1:A:3143:ILE:HG21	1:A:3212:TRP:HE1	6	0.21
(1,953)	1:A:3143:ILE:HG22	1:A:3212:TRP:HE1	6	0.21
(1,953)	1:A:3143:ILE:HG23	1:A:3212:TRP:HE1	6	0.21
(1,935)	1:A:3115:ILE:HG21	1:A:3209:LEU:H	7	0.21
(1,935)	1:A:3115:ILE:HG22	1:A:3209:LEU:H	7	0.21
(1,935)	1:A:3115:ILE:HG23	1:A:3209:LEU:H	7	0.21
(1,79)	1:A:3135:ILE:HG21	1:A:3194:PHE:HA	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:A:3135:ILE:HG22	1:A:3194:PHE:HA	8	0.21
(1,79)	1:A:3135:ILE:HG23	1:A:3194:PHE:HA	8	0.21
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG21	10	0.21
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG22	10	0.21
(1,780)	1:A:3166:ASN:H	1:A:3167:ILE:HG23	10	0.21
(1,731)	1:A:3150:ASN:H	1:A:3152:ARG:HB3	8	0.21
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG21	6	0.21
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG22	6	0.21
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG23	6	0.21
(1,588)	1:A:3098:ILE:HD11	1:A:3099:GLN:H	2	0.21
(1,588)	1:A:3098:ILE:HD12	1:A:3099:GLN:H	2	0.21
(1,588)	1:A:3098:ILE:HD13	1:A:3099:GLN:H	2	0.21
(1,446)	1:A:3128:ASN:HA	1:A:3129:PRO:HB3	10	0.21
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG21	10	0.21
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG22	10	0.21
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG23	10	0.21
(1,346)	1:A:3140:VAL:HG11	1:A:3209:LEU:HD11	1	0.21
(1,346)	1:A:3140:VAL:HG11	1:A:3209:LEU:HD12	1	0.21
(1,346)	1:A:3140:VAL:HG11	1:A:3209:LEU:HD13	1	0.21
(1,346)	1:A:3140:VAL:HG12	1:A:3209:LEU:HD11	1	0.21
(1,346)	1:A:3140:VAL:HG12	1:A:3209:LEU:HD12	1	0.21
(1,346)	1:A:3140:VAL:HG12	1:A:3209:LEU:HD13	1	0.21
(1,346)	1:A:3140:VAL:HG13	1:A:3209:LEU:HD11	1	0.21
(1,346)	1:A:3140:VAL:HG13	1:A:3209:LEU:HD12	1	0.21
(1,346)	1:A:3140:VAL:HG13	1:A:3209:LEU:HD13	1	0.21
(1,326)	1:A:3106:LEU:HD11	1:A:3109:GLN:HG3	6	0.21
(1,326)	1:A:3106:LEU:HD12	1:A:3109:GLN:HG3	6	0.21
(1,326)	1:A:3106:LEU:HD13	1:A:3109:GLN:HG3	6	0.21
(1,252)	1:A:3140:VAL:HA	1:A:3167:ILE:HA	9	0.21
(1,25)	1:A:3098:ILE:HD11	1:A:3099:GLN:HA	4	0.21
(1,25)	1:A:3098:ILE:HD12	1:A:3099:GLN:HA	4	0.21
(1,25)	1:A:3098:ILE:HD13	1:A:3099:GLN:HA	4	0.21
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG11	6	0.21
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG12	6	0.21
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG13	6	0.21
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG21	6	0.21
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG22	6	0.21
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG23	6	0.21
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG11	9	0.21
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG12	9	0.21
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG13	9	0.21
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG21	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG22	9	0.21
(1,1480)	1:A:3212:TRP:HE1	1:A:3213:VAL:HG23	9	0.21
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG2	6	0.21
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG3	6	0.21
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG2	8	0.21
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG3	8	0.21
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG2	9	0.21
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG3	9	0.21
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG2	10	0.21
(1,1443)	1:A:3196:TYR:HB2	1:A:3211:GLN:HG3	10	0.21
(1,1434)	1:A:3190:SER:HB2	1:A:3191:ASP:HB2	9	0.21
(1,1434)	1:A:3190:SER:HB2	1:A:3191:ASP:HB3	9	0.21
(1,1434)	1:A:3190:SER:HB3	1:A:3191:ASP:HB2	9	0.21
(1,1434)	1:A:3190:SER:HB3	1:A:3191:ASP:HB3	9	0.21
(1,1414)	1:A:3185:GLU:HG2	1:A:3217:ILE:HG21	8	0.21
(1,1414)	1:A:3185:GLU:HG2	1:A:3217:ILE:HG22	8	0.21
(1,1414)	1:A:3185:GLU:HG2	1:A:3217:ILE:HG23	8	0.21
(1,1414)	1:A:3185:GLU:HG3	1:A:3217:ILE:HG21	8	0.21
(1,1414)	1:A:3185:GLU:HG3	1:A:3217:ILE:HG22	8	0.21
(1,1414)	1:A:3185:GLU:HG3	1:A:3217:ILE:HG23	8	0.21
(1,1410)	1:A:3185:GLU:H	1:A:3187:GLU:HG2	7	0.21
(1,1410)	1:A:3185:GLU:H	1:A:3187:GLU:HG3	7	0.21
(1,1354)	1:A:3155:GLN:HG2	1:A:3156:GLN:HG2	9	0.21
(1,1354)	1:A:3155:GLN:HG2	1:A:3156:GLN:HG3	9	0.21
(1,1354)	1:A:3155:GLN:HG3	1:A:3156:GLN:HG2	9	0.21
(1,1354)	1:A:3155:GLN:HG3	1:A:3156:GLN:HG3	9	0.21
(1,1105)	1:A:3104:THR:HG21	1:A:3219:PHE:HB2	5	0.21
(1,1105)	1:A:3104:THR:HG21	1:A:3219:PHE:HB3	5	0.21
(1,1105)	1:A:3104:THR:HG22	1:A:3219:PHE:HB2	5	0.21
(1,1105)	1:A:3104:THR:HG22	1:A:3219:PHE:HB3	5	0.21
(1,1105)	1:A:3104:THR:HG23	1:A:3219:PHE:HB2	5	0.21
(1,1105)	1:A:3104:THR:HG23	1:A:3219:PHE:HB3	5	0.21
(1,1043)	1:A:3135:ILE:HG21	1:A:3194:PHE:HD1	1	0.21
(1,1043)	1:A:3135:ILE:HG21	1:A:3194:PHE:HD2	1	0.21
(1,1043)	1:A:3135:ILE:HG22	1:A:3194:PHE:HD1	1	0.21
(1,1043)	1:A:3135:ILE:HG22	1:A:3194:PHE:HD2	1	0.21
(1,1043)	1:A:3135:ILE:HG23	1:A:3194:PHE:HD1	1	0.21
(1,1043)	1:A:3135:ILE:HG23	1:A:3194:PHE:HD2	1	0.21
(1,1023)	1:A:3163:PHE:HD1	1:A:3209:LEU:HD21	9	0.21
(1,1023)	1:A:3163:PHE:HD1	1:A:3209:LEU:HD22	9	0.21
(1,1023)	1:A:3163:PHE:HD1	1:A:3209:LEU:HD23	9	0.21
(1,1023)	1:A:3163:PHE:HD2	1:A:3209:LEU:HD21	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1023)	1:A:3163:PHE:HD2	1:A:3209:LEU:HD22	9	0.21
(1,1023)	1:A:3163:PHE:HD2	1:A:3209:LEU:HD23	9	0.21
(1,1001)	1:A:3183:TYR:HE1	1:A:3187:GLU:HB2	2	0.21
(1,1001)	1:A:3183:TYR:HE1	1:A:3187:GLU:HB3	2	0.21
(1,1001)	1:A:3183:TYR:HE2	1:A:3187:GLU:HB2	2	0.21
(1,1001)	1:A:3183:TYR:HE2	1:A:3187:GLU:HB3	2	0.21
(1,974)	1:A:3224:GLU:H	1:A:3225:ASN:HA	4	0.2
(1,934)	1:A:3208:PRO:HG2	1:A:3209:LEU:H	9	0.2
(1,934)	1:A:3208:PRO:HG3	1:A:3209:LEU:H	9	0.2
(1,872)	1:A:3192:PRO:HB3	1:A:3194:PHE:H	4	0.2
(1,79)	1:A:3135:ILE:HG21	1:A:3194:PHE:HA	1	0.2
(1,79)	1:A:3135:ILE:HG22	1:A:3194:PHE:HA	1	0.2
(1,79)	1:A:3135:ILE:HG23	1:A:3194:PHE:HA	1	0.2
(1,765)	1:A:3158:ILE:HA	1:A:3160:LYS:H	3	0.2
(1,747)	1:A:3153:ASP:H	1:A:3154:ILE:HG13	2	0.2
(1,745)	1:A:3149:SER:HA	1:A:3153:ASP:H	6	0.2
(1,673)	1:A:3126:MET:HE1	1:A:3133:VAL:H	5	0.2
(1,673)	1:A:3126:MET:HE2	1:A:3133:VAL:H	5	0.2
(1,673)	1:A:3126:MET:HE3	1:A:3133:VAL:H	5	0.2
(1,412)	1:A:3136:VAL:HG11	1:A:3210:TYR:HB3	4	0.2
(1,412)	1:A:3136:VAL:HG12	1:A:3210:TYR:HB3	4	0.2
(1,412)	1:A:3136:VAL:HG13	1:A:3210:TYR:HB3	4	0.2
(1,351)	1:A:3206:CYS:HA	1:A:3209:LEU:HG	2	0.2
(1,343)	1:A:3185:GLU:HA	1:A:3189:LEU:HB2	6	0.2
(1,342)	1:A:3185:GLU:HA	1:A:3189:LEU:HB3	9	0.2
(1,327)	1:A:3189:LEU:HD11	1:A:3190:SER:HB2	4	0.2
(1,327)	1:A:3189:LEU:HD12	1:A:3190:SER:HB2	4	0.2
(1,327)	1:A:3189:LEU:HD13	1:A:3190:SER:HB2	4	0.2
(1,211)	1:A:3181:ARG:HD2	1:A:3217:ILE:HG21	5	0.2
(1,211)	1:A:3181:ARG:HD2	1:A:3217:ILE:HG22	5	0.2
(1,211)	1:A:3181:ARG:HD2	1:A:3217:ILE:HG23	5	0.2
(1,211)	1:A:3181:ARG:HD3	1:A:3217:ILE:HG21	5	0.2
(1,211)	1:A:3181:ARG:HD3	1:A:3217:ILE:HG22	5	0.2
(1,211)	1:A:3181:ARG:HD3	1:A:3217:ILE:HG23	5	0.2
(1,200)	1:A:3181:ARG:HD2	1:A:3217:ILE:HA	2	0.2
(1,200)	1:A:3181:ARG:HD3	1:A:3217:ILE:HA	2	0.2
(1,162)	1:A:3163:PHE:HD1	1:A:3167:ILE:HG21	3	0.2
(1,162)	1:A:3163:PHE:HD1	1:A:3167:ILE:HG22	3	0.2
(1,162)	1:A:3163:PHE:HD1	1:A:3167:ILE:HG23	3	0.2
(1,162)	1:A:3163:PHE:HD2	1:A:3167:ILE:HG21	3	0.2
(1,162)	1:A:3163:PHE:HD2	1:A:3167:ILE:HG22	3	0.2
(1,162)	1:A:3163:PHE:HD2	1:A:3167:ILE:HG23	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1506)	1:A:3218:ASN:HB2	1:A:3221:LYS:HG2	10	0.2
(1,1506)	1:A:3218:ASN:HB2	1:A:3221:LYS:HG3	10	0.2
(1,1506)	1:A:3218:ASN:HB3	1:A:3221:LYS:HG2	10	0.2
(1,1506)	1:A:3218:ASN:HB3	1:A:3221:LYS:HG3	10	0.2
(1,1214)	1:A:3129:PRO:HG2	1:A:3134:LYS:HA	4	0.2
(1,1214)	1:A:3129:PRO:HG3	1:A:3134:LYS:HA	4	0.2
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD11	3	0.2
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD12	3	0.2
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD13	3	0.2
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD11	5	0.2
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD12	5	0.2
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD13	5	0.2
(1,1100)	1:A:3101:CYS:HB2	1:A:3104:THR:HG21	4	0.2
(1,1100)	1:A:3101:CYS:HB2	1:A:3104:THR:HG22	4	0.2
(1,1100)	1:A:3101:CYS:HB2	1:A:3104:THR:HG23	4	0.2
(1,1100)	1:A:3101:CYS:HB3	1:A:3104:THR:HG21	4	0.2
(1,1100)	1:A:3101:CYS:HB3	1:A:3104:THR:HG22	4	0.2
(1,1100)	1:A:3101:CYS:HB3	1:A:3104:THR:HG23	4	0.2
(1,1096)	1:A:3099:GLN:HB2	1:A:3101:CYS:H	7	0.2
(1,1096)	1:A:3099:GLN:HB3	1:A:3101:CYS:H	7	0.2
(1,1069)	1:A:3105:ILE:HG21	1:A:3212:TRP:HD1	7	0.2
(1,1069)	1:A:3105:ILE:HG22	1:A:3212:TRP:HD1	7	0.2
(1,1069)	1:A:3105:ILE:HG23	1:A:3212:TRP:HD1	7	0.2
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE1	3	0.2
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE2	3	0.2
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE1	3	0.2
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE2	3	0.2
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE1	3	0.2
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE2	3	0.2
(1,1023)	1:A:3163:PHE:HD1	1:A:3209:LEU:HD21	6	0.2
(1,1023)	1:A:3163:PHE:HD1	1:A:3209:LEU:HD22	6	0.2
(1,1023)	1:A:3163:PHE:HD1	1:A:3209:LEU:HD23	6	0.2
(1,1023)	1:A:3163:PHE:HD2	1:A:3209:LEU:HD21	6	0.2
(1,1023)	1:A:3163:PHE:HD2	1:A:3209:LEU:HD22	6	0.2
(1,1023)	1:A:3163:PHE:HD2	1:A:3209:LEU:HD23	6	0.2
(1,1001)	1:A:3183:TYR:HE1	1:A:3187:GLU:HB2	3	0.2
(1,1001)	1:A:3183:TYR:HE1	1:A:3187:GLU:HB3	3	0.2
(1,1001)	1:A:3183:TYR:HE2	1:A:3187:GLU:HB2	3	0.2
(1,1001)	1:A:3183:TYR:HE2	1:A:3187:GLU:HB3	3	0.2
(1,994)	1:A:3108:ALA:HB1	1:A:3212:TRP:HE3	2	0.19
(1,994)	1:A:3108:ALA:HB2	1:A:3212:TRP:HE3	2	0.19
(1,994)	1:A:3108:ALA:HB3	1:A:3212:TRP:HE3	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,953)	1:A:3143:ILE:HG21	1:A:3212:TRP:HE1	1	0.19
(1,953)	1:A:3143:ILE:HG22	1:A:3212:TRP:HE1	1	0.19
(1,953)	1:A:3143:ILE:HG23	1:A:3212:TRP:HE1	1	0.19
(1,953)	1:A:3143:ILE:HG21	1:A:3212:TRP:HE1	9	0.19
(1,953)	1:A:3143:ILE:HG22	1:A:3212:TRP:HE1	9	0.19
(1,953)	1:A:3143:ILE:HG23	1:A:3212:TRP:HE1	9	0.19
(1,856)	1:A:3187:GLU:HB2	1:A:3188:PHE:H	5	0.19
(1,856)	1:A:3187:GLU:HB3	1:A:3188:PHE:H	5	0.19
(1,764)	1:A:3159:ARG:H	1:A:3163:PHE:HD1	8	0.19
(1,764)	1:A:3159:ARG:H	1:A:3163:PHE:HD2	8	0.19
(1,611)	1:A:3111:GLY:H	1:A:3113:LYS:HG3	5	0.19
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD11	10	0.19
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD12	10	0.19
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD13	10	0.19
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD11	10	0.19
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD12	10	0.19
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD13	10	0.19
(1,548)	1:A:3152:ARG:HA	1:A:3152:ARG:HD2	6	0.19
(1,548)	1:A:3152:ARG:HA	1:A:3152:ARG:HD3	6	0.19
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG2	3	0.19
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG3	3	0.19
(1,49)	1:A:3115:ILE:HD11	1:A:3205:ALA:HA	6	0.19
(1,49)	1:A:3115:ILE:HD12	1:A:3205:ALA:HA	6	0.19
(1,49)	1:A:3115:ILE:HD13	1:A:3205:ALA:HA	6	0.19
(1,456)	1:A:3214:ASN:HB2	1:A:3217:ILE:HB	5	0.19
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD11	1	0.19
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD12	1	0.19
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD13	1	0.19
(1,442)	1:A:3184:MET:HG2	1:A:3217:ILE:HD11	5	0.19
(1,442)	1:A:3184:MET:HG2	1:A:3217:ILE:HD12	5	0.19
(1,442)	1:A:3184:MET:HG2	1:A:3217:ILE:HD13	5	0.19
(1,438)	1:A:3096:LYS:HA	1:A:3096:LYS:HE2	3	0.19
(1,438)	1:A:3096:LYS:HA	1:A:3096:LYS:HE3	3	0.19
(1,438)	1:A:3096:LYS:HA	1:A:3096:LYS:HE2	6	0.19
(1,438)	1:A:3096:LYS:HA	1:A:3096:LYS:HE3	6	0.19
(1,402)	1:A:3183:TYR:HB2	1:A:3184:MET:HE1	9	0.19
(1,402)	1:A:3183:TYR:HB2	1:A:3184:MET:HE2	9	0.19
(1,402)	1:A:3183:TYR:HB2	1:A:3184:MET:HE3	9	0.19
(1,402)	1:A:3183:TYR:HB3	1:A:3184:MET:HE1	9	0.19
(1,402)	1:A:3183:TYR:HB3	1:A:3184:MET:HE2	9	0.19
(1,402)	1:A:3183:TYR:HB3	1:A:3184:MET:HE3	9	0.19
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG21	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG22	3	0.19
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG23	3	0.19
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG21	4	0.19
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG22	4	0.19
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG23	4	0.19
(1,327)	1:A:3189:LEU:HD11	1:A:3190:SER:HB2	10	0.19
(1,327)	1:A:3189:LEU:HD12	1:A:3190:SER:HB2	10	0.19
(1,327)	1:A:3189:LEU:HD13	1:A:3190:SER:HB2	10	0.19
(1,307)	1:A:3200:ASN:HB3	1:A:3207:GLY:HA2	4	0.19
(1,298)	1:A:3111:GLY:HA2	1:A:3208:PRO:HB2	9	0.19
(1,287)	1:A:3132:GLY:HA3	1:A:3202:ALA:HA	5	0.19
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG21	4	0.19
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG22	4	0.19
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG23	4	0.19
(1,252)	1:A:3140:VAL:HA	1:A:3167:ILE:HA	1	0.19
(1,252)	1:A:3140:VAL:HA	1:A:3167:ILE:HA	10	0.19
(1,1516)	1:A:3224:GLU:HA	1:A:3225:ASN:HB2	5	0.19
(1,1516)	1:A:3224:GLU:HA	1:A:3225:ASN:HB3	5	0.19
(1,1344)	1:A:3152:ARG:HB3	1:A:3153:ASP:HB2	6	0.19
(1,1344)	1:A:3152:ARG:HB3	1:A:3153:ASP:HB3	6	0.19
(1,1118)	1:A:3106:LEU:HD11	1:A:3109:GLN:HG2	4	0.19
(1,1118)	1:A:3106:LEU:HD12	1:A:3109:GLN:HG2	4	0.19
(1,1118)	1:A:3106:LEU:HD13	1:A:3109:GLN:HG2	4	0.19
(1,1118)	1:A:3106:LEU:HD21	1:A:3109:GLN:HG2	4	0.19
(1,1118)	1:A:3106:LEU:HD22	1:A:3109:GLN:HG2	4	0.19
(1,1118)	1:A:3106:LEU:HD23	1:A:3109:GLN:HG2	4	0.19
(1,1084)	1:A:3144:LEU:HD11	1:A:3212:TRP:HZ2	10	0.19
(1,1084)	1:A:3144:LEU:HD12	1:A:3212:TRP:HZ2	10	0.19
(1,1084)	1:A:3144:LEU:HD13	1:A:3212:TRP:HZ2	10	0.19
(1,1069)	1:A:3105:ILE:HG21	1:A:3212:TRP:HD1	1	0.19
(1,1069)	1:A:3105:ILE:HG22	1:A:3212:TRP:HD1	1	0.19
(1,1069)	1:A:3105:ILE:HG23	1:A:3212:TRP:HD1	1	0.19
(1,1039)	1:A:3183:TYR:HD1	1:A:3187:GLU:HG3	9	0.19
(1,1039)	1:A:3183:TYR:HD2	1:A:3187:GLU:HG3	9	0.19
(1,1038)	1:A:3142:ALA:HB1	1:A:3183:TYR:HD1	5	0.19
(1,1038)	1:A:3142:ALA:HB1	1:A:3183:TYR:HD2	5	0.19
(1,1038)	1:A:3142:ALA:HB2	1:A:3183:TYR:HD1	5	0.19
(1,1038)	1:A:3142:ALA:HB2	1:A:3183:TYR:HD2	5	0.19
(1,1038)	1:A:3142:ALA:HB3	1:A:3183:TYR:HD1	5	0.19
(1,1038)	1:A:3142:ALA:HB3	1:A:3183:TYR:HD2	5	0.19
(1,966)	1:A:3218:ASN:HA	1:A:3220:SER:H	8	0.18
(1,934)	1:A:3208:PRO:HG2	1:A:3209:LEU:H	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:A:3208:PRO:HG3	1:A:3209:LEU:H	1	0.18
(1,934)	1:A:3208:PRO:HG2	1:A:3209:LEU:H	6	0.18
(1,934)	1:A:3208:PRO:HG3	1:A:3209:LEU:H	6	0.18
(1,883)	1:A:3195:THR:HB	1:A:3197:GLU:H	1	0.18
(1,883)	1:A:3195:THR:HB	1:A:3197:GLU:H	9	0.18
(1,755)	1:A:3155:GLN:HG2	1:A:3157:PHE:H	7	0.18
(1,755)	1:A:3155:GLN:HG3	1:A:3157:PHE:H	7	0.18
(1,712)	1:A:3152:ARG:H	1:A:3154:ILE:H	4	0.18
(1,712)	1:A:3152:ARG:H	1:A:3154:ILE:H	5	0.18
(1,697)	1:A:3139:ALA:H	1:A:3184:MET:HE1	8	0.18
(1,697)	1:A:3139:ALA:H	1:A:3184:MET:HE2	8	0.18
(1,697)	1:A:3139:ALA:H	1:A:3184:MET:HE3	8	0.18
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD11	4	0.18
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD12	4	0.18
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD13	4	0.18
(1,626)	1:A:3112:VAL:HA	1:A:3115:ILE:H	1	0.18
(1,482)	1:A:3208:PRO:HA	1:A:3211:GLN:HG2	8	0.18
(1,412)	1:A:3136:VAL:HG11	1:A:3210:TYR:HB3	2	0.18
(1,412)	1:A:3136:VAL:HG12	1:A:3210:TYR:HB3	2	0.18
(1,412)	1:A:3136:VAL:HG13	1:A:3210:TYR:HB3	2	0.18
(1,384)	1:A:3205:ALA:HB1	1:A:3208:PRO:HD2	8	0.18
(1,384)	1:A:3205:ALA:HB1	1:A:3208:PRO:HD3	8	0.18
(1,384)	1:A:3205:ALA:HB2	1:A:3208:PRO:HD2	8	0.18
(1,384)	1:A:3205:ALA:HB2	1:A:3208:PRO:HD3	8	0.18
(1,384)	1:A:3205:ALA:HB3	1:A:3208:PRO:HD2	8	0.18
(1,384)	1:A:3205:ALA:HB3	1:A:3208:PRO:HD3	8	0.18
(1,345)	1:A:3205:ALA:HB1	1:A:3209:LEU:HB2	2	0.18
(1,345)	1:A:3205:ALA:HB2	1:A:3209:LEU:HB2	2	0.18
(1,345)	1:A:3205:ALA:HB3	1:A:3209:LEU:HB2	2	0.18
(1,307)	1:A:3200:ASN:HB3	1:A:3207:GLY:HA2	9	0.18
(1,25)	1:A:3098:ILE:HD11	1:A:3099:GLN:HA	5	0.18
(1,25)	1:A:3098:ILE:HD12	1:A:3099:GLN:HA	5	0.18
(1,25)	1:A:3098:ILE:HD13	1:A:3099:GLN:HA	5	0.18
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG21	6	0.18
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG22	6	0.18
(1,173)	1:A:3142:ALA:HB1	1:A:3180:ILE:HG23	6	0.18
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG21	6	0.18
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG22	6	0.18
(1,173)	1:A:3142:ALA:HB2	1:A:3180:ILE:HG23	6	0.18
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG21	6	0.18
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG22	6	0.18
(1,173)	1:A:3142:ALA:HB3	1:A:3180:ILE:HG23	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1441)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG11	10	0.18
(1,1441)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG12	10	0.18
(1,1441)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG13	10	0.18
(1,1441)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG21	10	0.18
(1,1441)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG22	10	0.18
(1,1441)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG23	10	0.18
(1,1432)	1:A:3190:SER:H	1:A:3191:ASP:HB2	4	0.18
(1,1432)	1:A:3190:SER:H	1:A:3191:ASP:HB3	4	0.18
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD11	2	0.18
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD12	2	0.18
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD13	2	0.18
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD21	2	0.18
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD22	2	0.18
(1,1420)	1:A:3188:PHE:H	1:A:3189:LEU:HD23	2	0.18
(1,1419)	1:A:3187:GLU:HG2	1:A:3188:PHE:H	2	0.18
(1,1419)	1:A:3187:GLU:HG3	1:A:3188:PHE:H	2	0.18
(1,132)	1:A:3113:LYS:HA	1:A:3164:ILE:HD11	9	0.18
(1,132)	1:A:3113:LYS:HA	1:A:3164:ILE:HD12	9	0.18
(1,132)	1:A:3113:LYS:HA	1:A:3164:ILE:HD13	9	0.18
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG21	8	0.18
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG22	8	0.18
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG23	8	0.18
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG21	10	0.18
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG22	10	0.18
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG23	10	0.18
(1,1179)	1:A:3123:ILE:HG21	1:A:3137:MET:HG2	1	0.18
(1,1179)	1:A:3123:ILE:HG21	1:A:3137:MET:HG3	1	0.18
(1,1179)	1:A:3123:ILE:HG22	1:A:3137:MET:HG2	1	0.18
(1,1179)	1:A:3123:ILE:HG22	1:A:3137:MET:HG3	1	0.18
(1,1179)	1:A:3123:ILE:HG23	1:A:3137:MET:HG2	1	0.18
(1,1179)	1:A:3123:ILE:HG23	1:A:3137:MET:HG3	1	0.18
(1,1177)	1:A:3123:ILE:HB	1:A:3126:MET:HG2	4	0.18
(1,1177)	1:A:3123:ILE:HB	1:A:3126:MET:HG3	4	0.18
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD11	8	0.18
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD12	8	0.18
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD13	8	0.18
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD11	8	0.18
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD12	8	0.18
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD13	8	0.18
(1,1096)	1:A:3099:GLN:HB2	1:A:3101:CYS:H	6	0.18
(1,1096)	1:A:3099:GLN:HB3	1:A:3101:CYS:H	6	0.18
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE1	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	1:A:3195:THR:HG21	1:A:3210:TYR:HE2	5	0.18
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE1	5	0.18
(1,1066)	1:A:3195:THR:HG22	1:A:3210:TYR:HE2	5	0.18
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE1	5	0.18
(1,1066)	1:A:3195:THR:HG23	1:A:3210:TYR:HE2	5	0.18
(1,975)	1:A:3224:GLU:H	1:A:3224:GLU:HG2	10	0.17
(1,975)	1:A:3224:GLU:H	1:A:3224:GLU:HG3	10	0.17
(1,940)	1:A:3199:ILE:HD11	1:A:3210:TYR:H	3	0.17
(1,940)	1:A:3199:ILE:HD12	1:A:3210:TYR:H	3	0.17
(1,940)	1:A:3199:ILE:HD13	1:A:3210:TYR:H	3	0.17
(1,934)	1:A:3208:PRO:HG2	1:A:3209:LEU:H	10	0.17
(1,934)	1:A:3208:PRO:HG3	1:A:3209:LEU:H	10	0.17
(1,932)	1:A:3207:GLY:HA3	1:A:3209:LEU:H	3	0.17
(1,928)	1:A:3207:GLY:H	1:A:3208:PRO:HG2	3	0.17
(1,928)	1:A:3207:GLY:H	1:A:3208:PRO:HG3	3	0.17
(1,888)	1:A:3197:GLU:H	1:A:3210:TYR:HD1	1	0.17
(1,888)	1:A:3197:GLU:H	1:A:3210:TYR:HD2	1	0.17
(1,888)	1:A:3197:GLU:H	1:A:3210:TYR:HD1	4	0.17
(1,888)	1:A:3197:GLU:H	1:A:3210:TYR:HD2	4	0.17
(1,876)	1:A:3135:ILE:HD11	1:A:3195:THR:H	3	0.17
(1,876)	1:A:3135:ILE:HD12	1:A:3195:THR:H	3	0.17
(1,876)	1:A:3135:ILE:HD13	1:A:3195:THR:H	3	0.17
(1,867)	1:A:3193:ASN:H	1:A:3195:THR:H	9	0.17
(1,859)	1:A:3185:GLU:HA	1:A:3189:LEU:H	6	0.17
(1,859)	1:A:3185:GLU:HA	1:A:3189:LEU:H	9	0.17
(1,845)	1:A:3185:GLU:H	1:A:3186:GLU:H	5	0.17
(1,826)	1:A:3195:THR:HG21	1:A:3196:TYR:H	8	0.17
(1,826)	1:A:3195:THR:HG22	1:A:3196:TYR:H	8	0.17
(1,826)	1:A:3195:THR:HG23	1:A:3196:TYR:H	8	0.17
(1,791)	1:A:3164:ILE:HG21	1:A:3167:ILE:H	2	0.17
(1,791)	1:A:3164:ILE:HG22	1:A:3167:ILE:H	2	0.17
(1,791)	1:A:3164:ILE:HG23	1:A:3167:ILE:H	2	0.17
(1,747)	1:A:3153:ASP:H	1:A:3154:ILE:HG13	5	0.17
(1,712)	1:A:3152:ARG:H	1:A:3154:ILE:H	2	0.17
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG21	5	0.17
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG22	5	0.17
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG23	5	0.17
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG21	7	0.17
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG22	7	0.17
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG23	7	0.17
(1,673)	1:A:3126:MET:HE1	1:A:3133:VAL:H	4	0.17
(1,673)	1:A:3126:MET:HE2	1:A:3133:VAL:H	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:A:3126:MET:HE3	1:A:3133:VAL:H	4	0.17
(1,673)	1:A:3126:MET:HE1	1:A:3133:VAL:H	8	0.17
(1,673)	1:A:3126:MET:HE2	1:A:3133:VAL:H	8	0.17
(1,673)	1:A:3126:MET:HE3	1:A:3133:VAL:H	8	0.17
(1,673)	1:A:3126:MET:HE1	1:A:3133:VAL:H	9	0.17
(1,673)	1:A:3126:MET:HE2	1:A:3133:VAL:H	9	0.17
(1,673)	1:A:3126:MET:HE3	1:A:3133:VAL:H	9	0.17
(1,648)	1:A:3122:GLU:H	1:A:3123:ILE:HD11	1	0.17
(1,648)	1:A:3122:GLU:H	1:A:3123:ILE:HD12	1	0.17
(1,648)	1:A:3122:GLU:H	1:A:3123:ILE:HD13	1	0.17
(1,648)	1:A:3122:GLU:H	1:A:3123:ILE:HD11	7	0.17
(1,648)	1:A:3122:GLU:H	1:A:3123:ILE:HD12	7	0.17
(1,648)	1:A:3122:GLU:H	1:A:3123:ILE:HD13	7	0.17
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD11	8	0.17
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD12	8	0.17
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD13	8	0.17
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD11	8	0.17
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD12	8	0.17
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD13	8	0.17
(1,549)	1:A:3120:LEU:HG	1:A:3163:PHE:HB3	1	0.17
(1,549)	1:A:3120:LEU:HG	1:A:3163:PHE:HB3	10	0.17
(1,497)	1:A:3119:GLN:HA	1:A:3205:ALA:HB1	8	0.17
(1,497)	1:A:3119:GLN:HA	1:A:3205:ALA:HB2	8	0.17
(1,497)	1:A:3119:GLN:HA	1:A:3205:ALA:HB3	8	0.17
(1,467)	1:A:3101:CYS:HB2	1:A:3104:THR:HB	6	0.17
(1,307)	1:A:3200:ASN:HB3	1:A:3207:GLY:HA2	10	0.17
(1,182)	1:A:3195:THR:HG21	1:A:3199:ILE:HB	10	0.17
(1,182)	1:A:3195:THR:HG22	1:A:3199:ILE:HB	10	0.17
(1,182)	1:A:3195:THR:HG23	1:A:3199:ILE:HB	10	0.17
(1,1416)	1:A:3186:GLU:H	1:A:3187:GLU:HG2	2	0.17
(1,1416)	1:A:3186:GLU:H	1:A:3187:GLU:HG3	2	0.17
(1,1397)	1:A:3181:ARG:HA	1:A:3184:MET:HG2	4	0.17
(1,1397)	1:A:3181:ARG:HA	1:A:3184:MET:HG3	4	0.17
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD11	10	0.17
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD12	10	0.17
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD13	10	0.17
(1,1188)	1:A:3125:SER:HB2	1:A:3126:MET:HG2	4	0.17
(1,1188)	1:A:3125:SER:HB2	1:A:3126:MET:HG3	4	0.17
(1,1188)	1:A:3125:SER:HB3	1:A:3126:MET:HG2	4	0.17
(1,1188)	1:A:3125:SER:HB3	1:A:3126:MET:HG3	4	0.17
(1,117)	1:A:3158:ILE:HD11	1:A:3163:PHE:HE1	3	0.17
(1,117)	1:A:3158:ILE:HD11	1:A:3163:PHE:HE2	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:A:3158:ILE:HD12	1:A:3163:PHE:HE1	3	0.17
(1,117)	1:A:3158:ILE:HD12	1:A:3163:PHE:HE2	3	0.17
(1,117)	1:A:3158:ILE:HD13	1:A:3163:PHE:HE1	3	0.17
(1,117)	1:A:3158:ILE:HD13	1:A:3163:PHE:HE2	3	0.17
(1,1096)	1:A:3099:GLN:HB2	1:A:3101:CYS:H	8	0.17
(1,1096)	1:A:3099:GLN:HB3	1:A:3101:CYS:H	8	0.17
(1,1022)	1:A:3163:PHE:HD1	1:A:3164:ILE:HB	3	0.17
(1,1022)	1:A:3163:PHE:HD2	1:A:3164:ILE:HB	3	0.17
(1,952)	1:A:3172:THR:HG21	1:A:3212:TRP:HE1	1	0.16
(1,952)	1:A:3172:THR:HG22	1:A:3212:TRP:HE1	1	0.16
(1,952)	1:A:3172:THR:HG23	1:A:3212:TRP:HE1	1	0.16
(1,932)	1:A:3207:GLY:HA3	1:A:3209:LEU:H	5	0.16
(1,872)	1:A:3192:PRO:HB3	1:A:3194:PHE:H	2	0.16
(1,853)	1:A:3185:GLU:HA	1:A:3188:PHE:H	9	0.16
(1,849)	1:A:3187:GLU:H	1:A:3187:GLU:HG3	2	0.16
(1,847)	1:A:3187:GLU:H	1:A:3189:LEU:H	7	0.16
(1,837)	1:A:3179:GLN:H	1:A:3182:LYS:H	3	0.16
(1,829)	1:A:3179:GLN:H	1:A:3180:ILE:HA	7	0.16
(1,712)	1:A:3152:ARG:H	1:A:3154:ILE:H	10	0.16
(1,611)	1:A:3111:GLY:H	1:A:3113:LYS:HG3	8	0.16
(1,50)	1:A:3115:ILE:HD11	1:A:3209:LEU:H	10	0.16
(1,50)	1:A:3115:ILE:HD12	1:A:3209:LEU:H	10	0.16
(1,50)	1:A:3115:ILE:HD13	1:A:3209:LEU:H	10	0.16
(1,489)	1:A:3109:GLN:HG3	1:A:3168:VAL:HG11	7	0.16
(1,489)	1:A:3109:GLN:HG3	1:A:3168:VAL:HG12	7	0.16
(1,489)	1:A:3109:GLN:HG3	1:A:3168:VAL:HG13	7	0.16
(1,482)	1:A:3208:PRO:HA	1:A:3211:GLN:HG2	1	0.16
(1,482)	1:A:3208:PRO:HA	1:A:3211:GLN:HG2	3	0.16
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG21	8	0.16
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG22	8	0.16
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG23	8	0.16
(1,351)	1:A:3206:CYS:HA	1:A:3209:LEU:HG	4	0.16
(1,334)	1:A:3205:ALA:HB1	1:A:3209:LEU:HD21	1	0.16
(1,334)	1:A:3205:ALA:HB1	1:A:3209:LEU:HD22	1	0.16
(1,334)	1:A:3205:ALA:HB1	1:A:3209:LEU:HD23	1	0.16
(1,334)	1:A:3205:ALA:HB2	1:A:3209:LEU:HD21	1	0.16
(1,334)	1:A:3205:ALA:HB2	1:A:3209:LEU:HD22	1	0.16
(1,334)	1:A:3205:ALA:HB2	1:A:3209:LEU:HD23	1	0.16
(1,334)	1:A:3205:ALA:HB3	1:A:3209:LEU:HD21	1	0.16
(1,334)	1:A:3205:ALA:HB3	1:A:3209:LEU:HD22	1	0.16
(1,334)	1:A:3205:ALA:HB3	1:A:3209:LEU:HD23	1	0.16
(1,287)	1:A:3132:GLY:HA3	1:A:3202:ALA:HA	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:A:3098:ILE:HD11	1:A:3099:GLN:HA	3	0.16
(1,25)	1:A:3098:ILE:HD12	1:A:3099:GLN:HA	3	0.16
(1,25)	1:A:3098:ILE:HD13	1:A:3099:GLN:HA	3	0.16
(1,219)	1:A:3112:VAL:HG11	1:A:3212:TRP:HD1	2	0.16
(1,219)	1:A:3112:VAL:HG12	1:A:3212:TRP:HD1	2	0.16
(1,219)	1:A:3112:VAL:HG13	1:A:3212:TRP:HD1	2	0.16
(1,162)	1:A:3163:PHE:HD1	1:A:3167:ILE:HG21	9	0.16
(1,162)	1:A:3163:PHE:HD1	1:A:3167:ILE:HG22	9	0.16
(1,162)	1:A:3163:PHE:HD1	1:A:3167:ILE:HG23	9	0.16
(1,162)	1:A:3163:PHE:HD2	1:A:3167:ILE:HG21	9	0.16
(1,162)	1:A:3163:PHE:HD2	1:A:3167:ILE:HG22	9	0.16
(1,162)	1:A:3163:PHE:HD2	1:A:3167:ILE:HG23	9	0.16
(1,159)	1:A:3167:ILE:HG21	1:A:3170:TYR:HB2	2	0.16
(1,159)	1:A:3167:ILE:HG22	1:A:3170:TYR:HB2	2	0.16
(1,159)	1:A:3167:ILE:HG23	1:A:3170:TYR:HB2	2	0.16
(1,1450)	1:A:3197:GLU:HG2	1:A:3199:ILE:H	9	0.16
(1,1450)	1:A:3197:GLU:HG3	1:A:3199:ILE:H	9	0.16
(1,1414)	1:A:3185:GLU:HG2	1:A:3217:ILE:HG21	6	0.16
(1,1414)	1:A:3185:GLU:HG2	1:A:3217:ILE:HG22	6	0.16
(1,1414)	1:A:3185:GLU:HG2	1:A:3217:ILE:HG23	6	0.16
(1,1414)	1:A:3185:GLU:HG3	1:A:3217:ILE:HG21	6	0.16
(1,1414)	1:A:3185:GLU:HG3	1:A:3217:ILE:HG22	6	0.16
(1,1414)	1:A:3185:GLU:HG3	1:A:3217:ILE:HG23	6	0.16
(1,1392)	1:A:3178:PRO:HB2	1:A:3181:ARG:H	2	0.16
(1,1392)	1:A:3178:PRO:HB3	1:A:3181:ARG:H	2	0.16
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD1	2	0.16
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD2	2	0.16
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD1	2	0.16
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD2	2	0.16
(1,1291)	1:A:3140:VAL:HA	1:A:3213:VAL:HG11	9	0.16
(1,1291)	1:A:3140:VAL:HA	1:A:3213:VAL:HG12	9	0.16
(1,1291)	1:A:3140:VAL:HA	1:A:3213:VAL:HG13	9	0.16
(1,1291)	1:A:3140:VAL:HA	1:A:3213:VAL:HG21	9	0.16
(1,1291)	1:A:3140:VAL:HA	1:A:3213:VAL:HG22	9	0.16
(1,1291)	1:A:3140:VAL:HA	1:A:3213:VAL:HG23	9	0.16
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG21	7	0.16
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG22	7	0.16
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG23	7	0.16
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG21	9	0.16
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG22	9	0.16
(1,120)	1:A:3144:LEU:HG	1:A:3167:ILE:HG23	9	0.16
(1,1199)	1:A:3126:MET:HE1	1:A:3203:SER:HB2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1199)	1:A:3126:MET:HE1	1:A:3203:SER:HB3	9	0.16
(1,1199)	1:A:3126:MET:HE2	1:A:3203:SER:HB2	9	0.16
(1,1199)	1:A:3126:MET:HE2	1:A:3203:SER:HB3	9	0.16
(1,1199)	1:A:3126:MET:HE3	1:A:3203:SER:HB2	9	0.16
(1,1199)	1:A:3126:MET:HE3	1:A:3203:SER:HB3	9	0.16
(1,1160)	1:A:3120:LEU:HB2	1:A:3163:PHE:HB3	3	0.16
(1,1160)	1:A:3120:LEU:HB3	1:A:3163:PHE:HB3	3	0.16
(1,1094)	1:A:3098:ILE:HD11	1:A:3099:GLN:HB2	4	0.16
(1,1094)	1:A:3098:ILE:HD11	1:A:3099:GLN:HB3	4	0.16
(1,1094)	1:A:3098:ILE:HD12	1:A:3099:GLN:HB2	4	0.16
(1,1094)	1:A:3098:ILE:HD12	1:A:3099:GLN:HB3	4	0.16
(1,1094)	1:A:3098:ILE:HD13	1:A:3099:GLN:HB2	4	0.16
(1,1094)	1:A:3098:ILE:HD13	1:A:3099:GLN:HB3	4	0.16
(1,1001)	1:A:3183:TYR:HE1	1:A:3187:GLU:HB2	8	0.16
(1,1001)	1:A:3183:TYR:HE1	1:A:3187:GLU:HB3	8	0.16
(1,1001)	1:A:3183:TYR:HE2	1:A:3187:GLU:HB2	8	0.16
(1,1001)	1:A:3183:TYR:HE2	1:A:3187:GLU:HB3	8	0.16
(1,1000)	1:A:3183:TYR:HE1	1:A:3187:GLU:HG2	1	0.16
(1,1000)	1:A:3183:TYR:HE2	1:A:3187:GLU:HG2	1	0.16
(1,994)	1:A:3108:ALA:HB1	1:A:3212:TRP:HE3	6	0.15
(1,994)	1:A:3108:ALA:HB2	1:A:3212:TRP:HE3	6	0.15
(1,994)	1:A:3108:ALA:HB3	1:A:3212:TRP:HE3	6	0.15
(1,971)	1:A:3223:LEU:H	1:A:3224:GLU:HB2	9	0.15
(1,971)	1:A:3223:LEU:H	1:A:3224:GLU:HB3	9	0.15
(1,956)	1:A:3213:VAL:HB	1:A:3214:ASN:H	9	0.15
(1,935)	1:A:3115:ILE:HG21	1:A:3209:LEU:H	8	0.15
(1,935)	1:A:3115:ILE:HG22	1:A:3209:LEU:H	8	0.15
(1,935)	1:A:3115:ILE:HG23	1:A:3209:LEU:H	8	0.15
(1,934)	1:A:3208:PRO:HG2	1:A:3209:LEU:H	3	0.15
(1,934)	1:A:3208:PRO:HG3	1:A:3209:LEU:H	3	0.15
(1,934)	1:A:3208:PRO:HG2	1:A:3209:LEU:H	5	0.15
(1,934)	1:A:3208:PRO:HG3	1:A:3209:LEU:H	5	0.15
(1,91)	1:A:3143:ILE:HD11	1:A:3212:TRP:HZ2	5	0.15
(1,91)	1:A:3143:ILE:HD12	1:A:3212:TRP:HZ2	5	0.15
(1,91)	1:A:3143:ILE:HD13	1:A:3212:TRP:HZ2	5	0.15
(1,883)	1:A:3195:THR:HB	1:A:3197:GLU:H	2	0.15
(1,883)	1:A:3195:THR:HB	1:A:3197:GLU:H	7	0.15
(1,870)	1:A:3193:ASN:H	1:A:3195:THR:HG21	7	0.15
(1,870)	1:A:3193:ASN:H	1:A:3195:THR:HG22	7	0.15
(1,870)	1:A:3193:ASN:H	1:A:3195:THR:HG23	7	0.15
(1,868)	1:A:3192:PRO:HB3	1:A:3193:ASN:H	10	0.15
(1,808)	1:A:3143:ILE:HG21	1:A:3170:TYR:H	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,808)	1:A:3143:ILE:HG22	1:A:3170:TYR:H	6	0.15
(1,808)	1:A:3143:ILE:HG23	1:A:3170:TYR:H	6	0.15
(1,791)	1:A:3164:ILE:HG21	1:A:3167:ILE:H	5	0.15
(1,791)	1:A:3164:ILE:HG22	1:A:3167:ILE:H	5	0.15
(1,791)	1:A:3164:ILE:HG23	1:A:3167:ILE:H	5	0.15
(1,791)	1:A:3164:ILE:HG21	1:A:3167:ILE:H	7	0.15
(1,791)	1:A:3164:ILE:HG22	1:A:3167:ILE:H	7	0.15
(1,791)	1:A:3164:ILE:HG23	1:A:3167:ILE:H	7	0.15
(1,747)	1:A:3153:ASP:H	1:A:3154:ILE:HG13	10	0.15
(1,736)	1:A:3129:PRO:HD2	1:A:3151:TRP:HE1	9	0.15
(1,720)	1:A:3140:VAL:HA	1:A:3144:LEU:H	5	0.15
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG21	2	0.15
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG22	2	0.15
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG23	2	0.15
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG21	3	0.15
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG22	3	0.15
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG23	3	0.15
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG21	4	0.15
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG22	4	0.15
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG23	4	0.15
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD11	1	0.15
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD12	1	0.15
(1,671)	1:A:3133:VAL:H	1:A:3199:ILE:HD13	1	0.15
(1,611)	1:A:3111:GLY:H	1:A:3113:LYS:HG3	3	0.15
(1,55)	1:A:3115:ILE:HB	1:A:3118:GLN:HG2	3	0.15
(1,55)	1:A:3115:ILE:HB	1:A:3118:GLN:HG3	3	0.15
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG2	1	0.15
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG3	1	0.15
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG2	10	0.15
(1,518)	1:A:3152:ARG:HA	1:A:3155:GLN:HG3	10	0.15
(1,515)	1:A:3105:ILE:HG21	1:A:3216:GLN:HA	6	0.15
(1,515)	1:A:3105:ILE:HG22	1:A:3216:GLN:HA	6	0.15
(1,515)	1:A:3105:ILE:HG23	1:A:3216:GLN:HA	6	0.15
(1,501)	1:A:3115:ILE:HG21	1:A:3119:GLN:HG2	4	0.15
(1,501)	1:A:3115:ILE:HG22	1:A:3119:GLN:HG2	4	0.15
(1,501)	1:A:3115:ILE:HG23	1:A:3119:GLN:HG2	4	0.15
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD11	10	0.15
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD12	10	0.15
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD13	10	0.15
(1,429)	1:A:3137:MET:HA	1:A:3140:VAL:HB	6	0.15
(1,410)	1:A:3209:LEU:HD11	1:A:3210:TYR:HA	4	0.15
(1,410)	1:A:3209:LEU:HD12	1:A:3210:TYR:HA	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:A:3209:LEU:HD13	1:A:3210:TYR:HA	4	0.15
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG21	8	0.15
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG22	8	0.15
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG23	8	0.15
(1,303)	1:A:3132:GLY:HA2	1:A:3135:ILE:HG12	5	0.15
(1,286)	1:A:3142:ALA:HB1	1:A:3184:MET:H	9	0.15
(1,286)	1:A:3142:ALA:HB2	1:A:3184:MET:H	9	0.15
(1,286)	1:A:3142:ALA:HB3	1:A:3184:MET:H	9	0.15
(1,224)	1:A:3112:VAL:HG21	1:A:3212:TRP:HB3	10	0.15
(1,224)	1:A:3112:VAL:HG22	1:A:3212:TRP:HB3	10	0.15
(1,224)	1:A:3112:VAL:HG23	1:A:3212:TRP:HB3	10	0.15
(1,203)	1:A:3181:ARG:HD2	1:A:3217:ILE:HD11	7	0.15
(1,203)	1:A:3181:ARG:HD2	1:A:3217:ILE:HD12	7	0.15
(1,203)	1:A:3181:ARG:HD2	1:A:3217:ILE:HD13	7	0.15
(1,203)	1:A:3181:ARG:HD3	1:A:3217:ILE:HD11	7	0.15
(1,203)	1:A:3181:ARG:HD3	1:A:3217:ILE:HD12	7	0.15
(1,203)	1:A:3181:ARG:HD3	1:A:3217:ILE:HD13	7	0.15
(1,200)	1:A:3181:ARG:HD2	1:A:3217:ILE:HA	3	0.15
(1,200)	1:A:3181:ARG:HD3	1:A:3217:ILE:HA	3	0.15
(1,1525)	1:A:3227:ASP:HB2	1:A:3228:PRO:HG2	3	0.15
(1,1525)	1:A:3227:ASP:HB2	1:A:3228:PRO:HG3	3	0.15
(1,1525)	1:A:3227:ASP:HB3	1:A:3228:PRO:HG2	3	0.15
(1,1525)	1:A:3227:ASP:HB3	1:A:3228:PRO:HG3	3	0.15
(1,1515)	1:A:3224:GLU:H	1:A:3225:ASN:HB2	5	0.15
(1,1515)	1:A:3224:GLU:H	1:A:3225:ASN:HB3	5	0.15
(1,1493)	1:A:3214:ASN:HB2	1:A:3217:ILE:HB	6	0.15
(1,1493)	1:A:3214:ASN:HB3	1:A:3217:ILE:HB	6	0.15
(1,1442)	1:A:3195:THR:HG21	1:A:3197:GLU:HG2	6	0.15
(1,1442)	1:A:3195:THR:HG21	1:A:3197:GLU:HG3	6	0.15
(1,1442)	1:A:3195:THR:HG22	1:A:3197:GLU:HG2	6	0.15
(1,1442)	1:A:3195:THR:HG22	1:A:3197:GLU:HG3	6	0.15
(1,1442)	1:A:3195:THR:HG23	1:A:3197:GLU:HG2	6	0.15
(1,1442)	1:A:3195:THR:HG23	1:A:3197:GLU:HG3	6	0.15
(1,1442)	1:A:3195:THR:HG21	1:A:3197:GLU:HG2	7	0.15
(1,1442)	1:A:3195:THR:HG21	1:A:3197:GLU:HG3	7	0.15
(1,1442)	1:A:3195:THR:HG22	1:A:3197:GLU:HG2	7	0.15
(1,1442)	1:A:3195:THR:HG22	1:A:3197:GLU:HG3	7	0.15
(1,1442)	1:A:3195:THR:HG23	1:A:3197:GLU:HG2	7	0.15
(1,1442)	1:A:3195:THR:HG23	1:A:3197:GLU:HG3	7	0.15
(1,1438)	1:A:3192:PRO:HB2	1:A:3193:ASN:H	10	0.15
(1,1438)	1:A:3192:PRO:HB3	1:A:3193:ASN:H	10	0.15
(1,1418)	1:A:3187:GLU:H	1:A:3187:GLU:HG2	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1418)	1:A:3187:GLU:H	1:A:3187:GLU:HG3	2	0.15
(1,1405)	1:A:3184:MET:HB2	1:A:3185:GLU:H	6	0.15
(1,1405)	1:A:3184:MET:HB3	1:A:3185:GLU:H	6	0.15
(1,1399)	1:A:3181:ARG:HB2	1:A:3217:ILE:HD11	8	0.15
(1,1399)	1:A:3181:ARG:HB2	1:A:3217:ILE:HD12	8	0.15
(1,1399)	1:A:3181:ARG:HB2	1:A:3217:ILE:HD13	8	0.15
(1,1399)	1:A:3181:ARG:HB3	1:A:3217:ILE:HD11	8	0.15
(1,1399)	1:A:3181:ARG:HB3	1:A:3217:ILE:HD12	8	0.15
(1,1399)	1:A:3181:ARG:HB3	1:A:3217:ILE:HD13	8	0.15
(1,1399)	1:A:3181:ARG:HB2	1:A:3217:ILE:HD11	10	0.15
(1,1399)	1:A:3181:ARG:HB2	1:A:3217:ILE:HD12	10	0.15
(1,1399)	1:A:3181:ARG:HB2	1:A:3217:ILE:HD13	10	0.15
(1,1399)	1:A:3181:ARG:HB3	1:A:3217:ILE:HD11	10	0.15
(1,1399)	1:A:3181:ARG:HB3	1:A:3217:ILE:HD12	10	0.15
(1,1399)	1:A:3181:ARG:HB3	1:A:3217:ILE:HD13	10	0.15
(1,1398)	1:A:3181:ARG:HA	1:A:3217:ILE:HG12	10	0.15
(1,1398)	1:A:3181:ARG:HA	1:A:3217:ILE:HG13	10	0.15
(1,1392)	1:A:3178:PRO:HB2	1:A:3181:ARG:H	1	0.15
(1,1392)	1:A:3178:PRO:HB3	1:A:3181:ARG:H	1	0.15
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD1	5	0.15
(1,1362)	1:A:3158:ILE:HG12	1:A:3163:PHE:HD2	5	0.15
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD1	5	0.15
(1,1362)	1:A:3158:ILE:HG13	1:A:3163:PHE:HD2	5	0.15
(1,1327)	1:A:3144:LEU:HD11	1:A:3170:TYR:H	4	0.15
(1,1327)	1:A:3144:LEU:HD12	1:A:3170:TYR:H	4	0.15
(1,1327)	1:A:3144:LEU:HD13	1:A:3170:TYR:H	4	0.15
(1,1327)	1:A:3144:LEU:HD21	1:A:3170:TYR:H	4	0.15
(1,1327)	1:A:3144:LEU:HD22	1:A:3170:TYR:H	4	0.15
(1,1327)	1:A:3144:LEU:HD23	1:A:3170:TYR:H	4	0.15
(1,1327)	1:A:3144:LEU:HD11	1:A:3170:TYR:H	9	0.15
(1,1327)	1:A:3144:LEU:HD12	1:A:3170:TYR:H	9	0.15
(1,1327)	1:A:3144:LEU:HD13	1:A:3170:TYR:H	9	0.15
(1,1327)	1:A:3144:LEU:HD21	1:A:3170:TYR:H	9	0.15
(1,1327)	1:A:3144:LEU:HD22	1:A:3170:TYR:H	9	0.15
(1,1327)	1:A:3144:LEU:HD23	1:A:3170:TYR:H	9	0.15
(1,1298)	1:A:3140:VAL:HG11	1:A:3212:TRP:HE3	2	0.15
(1,1298)	1:A:3140:VAL:HG12	1:A:3212:TRP:HE3	2	0.15
(1,1298)	1:A:3140:VAL:HG13	1:A:3212:TRP:HE3	2	0.15
(1,1298)	1:A:3140:VAL:HG21	1:A:3212:TRP:HE3	2	0.15
(1,1298)	1:A:3140:VAL:HG22	1:A:3212:TRP:HE3	2	0.15
(1,1298)	1:A:3140:VAL:HG23	1:A:3212:TRP:HE3	2	0.15
(1,1298)	1:A:3140:VAL:HG11	1:A:3212:TRP:HE3	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1298)	1:A:3140:VAL:HG12	1:A:3212:TRP:HE3	5	0.15
(1,1298)	1:A:3140:VAL:HG13	1:A:3212:TRP:HE3	5	0.15
(1,1298)	1:A:3140:VAL:HG21	1:A:3212:TRP:HE3	5	0.15
(1,1298)	1:A:3140:VAL:HG22	1:A:3212:TRP:HE3	5	0.15
(1,1298)	1:A:3140:VAL:HG23	1:A:3212:TRP:HE3	5	0.15
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG11	9	0.15
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG12	9	0.15
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG13	9	0.15
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG21	9	0.15
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG22	9	0.15
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG23	9	0.15
(1,1236)	1:A:3133:VAL:HG11	1:A:3202:ALA:H	2	0.15
(1,1236)	1:A:3133:VAL:HG12	1:A:3202:ALA:H	2	0.15
(1,1236)	1:A:3133:VAL:HG13	1:A:3202:ALA:H	2	0.15
(1,1236)	1:A:3133:VAL:HG21	1:A:3202:ALA:H	2	0.15
(1,1236)	1:A:3133:VAL:HG22	1:A:3202:ALA:H	2	0.15
(1,1236)	1:A:3133:VAL:HG23	1:A:3202:ALA:H	2	0.15
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD11	6	0.15
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD12	6	0.15
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD13	6	0.15
(1,1129)	1:A:3112:VAL:HG11	1:A:3164:ILE:HA	8	0.15
(1,1129)	1:A:3112:VAL:HG12	1:A:3164:ILE:HA	8	0.15
(1,1129)	1:A:3112:VAL:HG13	1:A:3164:ILE:HA	8	0.15
(1,1129)	1:A:3112:VAL:HG21	1:A:3164:ILE:HA	8	0.15
(1,1129)	1:A:3112:VAL:HG22	1:A:3164:ILE:HA	8	0.15
(1,1129)	1:A:3112:VAL:HG23	1:A:3164:ILE:HA	8	0.15
(1,1114)	1:A:3106:LEU:HB2	1:A:3109:GLN:HG2	3	0.15
(1,1114)	1:A:3106:LEU:HB3	1:A:3109:GLN:HG2	3	0.15
(1,1096)	1:A:3099:GLN:HB2	1:A:3101:CYS:H	1	0.15
(1,1096)	1:A:3099:GLN:HB3	1:A:3101:CYS:H	1	0.15
(1,1094)	1:A:3098:ILE:HD11	1:A:3099:GLN:HB2	5	0.15
(1,1094)	1:A:3098:ILE:HD11	1:A:3099:GLN:HB3	5	0.15
(1,1094)	1:A:3098:ILE:HD12	1:A:3099:GLN:HB2	5	0.15
(1,1094)	1:A:3098:ILE:HD12	1:A:3099:GLN:HB3	5	0.15
(1,1094)	1:A:3098:ILE:HD13	1:A:3099:GLN:HB2	5	0.15
(1,1094)	1:A:3098:ILE:HD13	1:A:3099:GLN:HB3	5	0.15
(1,994)	1:A:3108:ALA:HB1	1:A:3212:TRP:HE3	5	0.14
(1,994)	1:A:3108:ALA:HB2	1:A:3212:TRP:HE3	5	0.14
(1,994)	1:A:3108:ALA:HB3	1:A:3212:TRP:HE3	5	0.14
(1,870)	1:A:3193:ASN:H	1:A:3195:THR:HG21	6	0.14
(1,870)	1:A:3193:ASN:H	1:A:3195:THR:HG22	6	0.14
(1,870)	1:A:3193:ASN:H	1:A:3195:THR:HG23	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:A:3192:PRO:HB3	1:A:3193:ASN:H	4	0.14
(1,847)	1:A:3187:GLU:H	1:A:3189:LEU:H	3	0.14
(1,764)	1:A:3159:ARG:H	1:A:3163:PHE:HD1	4	0.14
(1,764)	1:A:3159:ARG:H	1:A:3163:PHE:HD2	4	0.14
(1,764)	1:A:3159:ARG:H	1:A:3163:PHE:HD1	6	0.14
(1,764)	1:A:3159:ARG:H	1:A:3163:PHE:HD2	6	0.14
(1,76)	1:A:3135:ILE:HG21	1:A:3193:ASN:HB2	8	0.14
(1,76)	1:A:3135:ILE:HG21	1:A:3193:ASN:HB3	8	0.14
(1,76)	1:A:3135:ILE:HG22	1:A:3193:ASN:HB2	8	0.14
(1,76)	1:A:3135:ILE:HG22	1:A:3193:ASN:HB3	8	0.14
(1,76)	1:A:3135:ILE:HG23	1:A:3193:ASN:HB2	8	0.14
(1,76)	1:A:3135:ILE:HG23	1:A:3193:ASN:HB3	8	0.14
(1,720)	1:A:3140:VAL:HA	1:A:3144:LEU:H	4	0.14
(1,720)	1:A:3140:VAL:HA	1:A:3144:LEU:H	6	0.14
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG21	9	0.14
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG22	9	0.14
(1,711)	1:A:3141:CYS:H	1:A:3143:ILE:HG23	9	0.14
(1,697)	1:A:3139:ALA:H	1:A:3184:MET:HE1	5	0.14
(1,697)	1:A:3139:ALA:H	1:A:3184:MET:HE2	5	0.14
(1,697)	1:A:3139:ALA:H	1:A:3184:MET:HE3	5	0.14
(1,695)	1:A:3139:ALA:H	1:A:3154:ILE:HD11	5	0.14
(1,695)	1:A:3139:ALA:H	1:A:3154:ILE:HD12	5	0.14
(1,695)	1:A:3139:ALA:H	1:A:3154:ILE:HD13	5	0.14
(1,673)	1:A:3126:MET:HE1	1:A:3133:VAL:H	7	0.14
(1,673)	1:A:3126:MET:HE2	1:A:3133:VAL:H	7	0.14
(1,673)	1:A:3126:MET:HE3	1:A:3133:VAL:H	7	0.14
(1,624)	1:A:3113:LYS:H	1:A:3115:ILE:H	1	0.14
(1,617)	1:A:3111:GLY:H	1:A:3113:LYS:H	2	0.14
(1,617)	1:A:3111:GLY:H	1:A:3113:LYS:H	5	0.14
(1,617)	1:A:3111:GLY:H	1:A:3113:LYS:H	9	0.14
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD11	4	0.14
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD12	4	0.14
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD13	4	0.14
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD11	4	0.14
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD12	4	0.14
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD13	4	0.14
(1,49)	1:A:3115:ILE:HD11	1:A:3205:ALA:HA	5	0.14
(1,49)	1:A:3115:ILE:HD12	1:A:3205:ALA:HA	5	0.14
(1,49)	1:A:3115:ILE:HD13	1:A:3205:ALA:HA	5	0.14
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG21	8	0.14
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG22	8	0.14
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG23	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:A:3184:MET:HA	1:A:3217:ILE:HD11	7	0.14
(1,440)	1:A:3184:MET:HA	1:A:3217:ILE:HD12	7	0.14
(1,440)	1:A:3184:MET:HA	1:A:3217:ILE:HD13	7	0.14
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG21	2	0.14
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG22	2	0.14
(1,374)	1:A:3113:LYS:HB3	1:A:3168:VAL:HG23	2	0.14
(1,339)	1:A:3125:SER:HB2	1:A:3126:MET:HA	4	0.14
(1,339)	1:A:3125:SER:HB3	1:A:3126:MET:HA	4	0.14
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG21	3	0.14
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG22	3	0.14
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG23	3	0.14
(1,246)	1:A:3136:VAL:HA	1:A:3210:TYR:HA	3	0.14
(1,246)	1:A:3136:VAL:HA	1:A:3210:TYR:HA	6	0.14
(1,176)	1:A:3143:ILE:HA	1:A:3180:ILE:HG21	1	0.14
(1,176)	1:A:3143:ILE:HA	1:A:3180:ILE:HG22	1	0.14
(1,176)	1:A:3143:ILE:HA	1:A:3180:ILE:HG23	1	0.14
(1,1490)	1:A:3214:ASN:HA	1:A:3217:ILE:HG12	4	0.14
(1,1490)	1:A:3214:ASN:HA	1:A:3217:ILE:HG13	4	0.14
(1,1428)	1:A:3189:LEU:HD11	1:A:3190:SER:HB2	7	0.14
(1,1428)	1:A:3189:LEU:HD11	1:A:3190:SER:HB3	7	0.14
(1,1428)	1:A:3189:LEU:HD12	1:A:3190:SER:HB2	7	0.14
(1,1428)	1:A:3189:LEU:HD12	1:A:3190:SER:HB3	7	0.14
(1,1428)	1:A:3189:LEU:HD13	1:A:3190:SER:HB2	7	0.14
(1,1428)	1:A:3189:LEU:HD13	1:A:3190:SER:HB3	7	0.14
(1,1428)	1:A:3189:LEU:HD21	1:A:3190:SER:HB2	7	0.14
(1,1428)	1:A:3189:LEU:HD21	1:A:3190:SER:HB3	7	0.14
(1,1428)	1:A:3189:LEU:HD22	1:A:3190:SER:HB2	7	0.14
(1,1428)	1:A:3189:LEU:HD22	1:A:3190:SER:HB3	7	0.14
(1,1428)	1:A:3189:LEU:HD23	1:A:3190:SER:HB2	7	0.14
(1,1428)	1:A:3189:LEU:HD23	1:A:3190:SER:HB3	7	0.14
(1,1382)	1:A:3170:TYR:HB2	1:A:3212:TRP:HH2	1	0.14
(1,1382)	1:A:3170:TYR:HB3	1:A:3212:TRP:HH2	1	0.14
(1,1382)	1:A:3170:TYR:HB2	1:A:3212:TRP:HH2	6	0.14
(1,1382)	1:A:3170:TYR:HB3	1:A:3212:TRP:HH2	6	0.14
(1,1199)	1:A:3126:MET:HE1	1:A:3203:SER:HB2	4	0.14
(1,1199)	1:A:3126:MET:HE1	1:A:3203:SER:HB3	4	0.14
(1,1199)	1:A:3126:MET:HE2	1:A:3203:SER:HB2	4	0.14
(1,1199)	1:A:3126:MET:HE2	1:A:3203:SER:HB3	4	0.14
(1,1199)	1:A:3126:MET:HE3	1:A:3203:SER:HB2	4	0.14
(1,1199)	1:A:3126:MET:HE3	1:A:3203:SER:HB3	4	0.14
(1,1150)	1:A:3119:GLN:HB2	1:A:3205:ALA:HA	10	0.14
(1,1150)	1:A:3119:GLN:HB3	1:A:3205:ALA:HA	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1119)	1:A:3106:LEU:HD11	1:A:3109:GLN:HG3	2	0.14
(1,1119)	1:A:3106:LEU:HD12	1:A:3109:GLN:HG3	2	0.14
(1,1119)	1:A:3106:LEU:HD13	1:A:3109:GLN:HG3	2	0.14
(1,1119)	1:A:3106:LEU:HD21	1:A:3109:GLN:HG3	2	0.14
(1,1119)	1:A:3106:LEU:HD22	1:A:3109:GLN:HG3	2	0.14
(1,1119)	1:A:3106:LEU:HD23	1:A:3109:GLN:HG3	2	0.14
(1,1104)	1:A:3103:PRO:HA	1:A:3106:LEU:HD11	3	0.14
(1,1104)	1:A:3103:PRO:HA	1:A:3106:LEU:HD12	3	0.14
(1,1104)	1:A:3103:PRO:HA	1:A:3106:LEU:HD13	3	0.14
(1,1104)	1:A:3103:PRO:HA	1:A:3106:LEU:HD21	3	0.14
(1,1104)	1:A:3103:PRO:HA	1:A:3106:LEU:HD22	3	0.14
(1,1104)	1:A:3103:PRO:HA	1:A:3106:LEU:HD23	3	0.14
(1,961)	1:A:3105:ILE:HG21	1:A:3216:GLN:H	10	0.13
(1,961)	1:A:3105:ILE:HG22	1:A:3216:GLN:H	10	0.13
(1,961)	1:A:3105:ILE:HG23	1:A:3216:GLN:H	10	0.13
(1,951)	1:A:3108:ALA:HB1	1:A:3212:TRP:HE1	9	0.13
(1,951)	1:A:3108:ALA:HB2	1:A:3212:TRP:HE1	9	0.13
(1,951)	1:A:3108:ALA:HB3	1:A:3212:TRP:HE1	9	0.13
(1,932)	1:A:3207:GLY:HA3	1:A:3209:LEU:H	4	0.13
(1,932)	1:A:3207:GLY:HA3	1:A:3209:LEU:H	6	0.13
(1,932)	1:A:3207:GLY:HA3	1:A:3209:LEU:H	9	0.13
(1,893)	1:A:3199:ILE:H	1:A:3210:TYR:HD1	2	0.13
(1,893)	1:A:3199:ILE:H	1:A:3210:TYR:HD2	2	0.13
(1,888)	1:A:3197:GLU:H	1:A:3210:TYR:HD1	9	0.13
(1,888)	1:A:3197:GLU:H	1:A:3210:TYR:HD2	9	0.13
(1,863)	1:A:3188:PHE:HA	1:A:3190:SER:H	2	0.13
(1,859)	1:A:3185:GLU:HA	1:A:3189:LEU:H	8	0.13
(1,829)	1:A:3179:GLN:H	1:A:3180:ILE:HA	9	0.13
(1,808)	1:A:3143:ILE:HG21	1:A:3170:TYR:H	3	0.13
(1,808)	1:A:3143:ILE:HG22	1:A:3170:TYR:H	3	0.13
(1,808)	1:A:3143:ILE:HG23	1:A:3170:TYR:H	3	0.13
(1,798)	1:A:3168:VAL:H	1:A:3169:HIS:HB2	5	0.13
(1,755)	1:A:3155:GLN:HG2	1:A:3157:PHE:H	1	0.13
(1,755)	1:A:3155:GLN:HG3	1:A:3157:PHE:H	1	0.13
(1,747)	1:A:3153:ASP:H	1:A:3154:ILE:HG13	4	0.13
(1,69)	1:A:3135:ILE:HD11	1:A:3193:ASN:HB2	2	0.13
(1,69)	1:A:3135:ILE:HD11	1:A:3193:ASN:HB3	2	0.13
(1,69)	1:A:3135:ILE:HD12	1:A:3193:ASN:HB2	2	0.13
(1,69)	1:A:3135:ILE:HD12	1:A:3193:ASN:HB3	2	0.13
(1,69)	1:A:3135:ILE:HD13	1:A:3193:ASN:HB2	2	0.13
(1,69)	1:A:3135:ILE:HD13	1:A:3193:ASN:HB3	2	0.13
(1,673)	1:A:3126:MET:HE1	1:A:3133:VAL:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:A:3126:MET:HE2	1:A:3133:VAL:H	6	0.13
(1,673)	1:A:3126:MET:HE3	1:A:3133:VAL:H	6	0.13
(1,626)	1:A:3112:VAL:HA	1:A:3115:ILE:H	4	0.13
(1,613)	1:A:3112:VAL:H	1:A:3212:TRP:HB3	2	0.13
(1,613)	1:A:3112:VAL:H	1:A:3212:TRP:HB3	5	0.13
(1,608)	1:A:3109:GLN:HG3	1:A:3110:ARG:H	6	0.13
(1,592)	1:A:3134:LYS:H	1:A:3134:LYS:HE2	1	0.13
(1,592)	1:A:3134:LYS:H	1:A:3134:LYS:HE3	1	0.13
(1,579)	1:A:3109:GLN:H	1:A:3110:ARG:HG2	10	0.13
(1,579)	1:A:3109:GLN:H	1:A:3110:ARG:HG3	10	0.13
(1,572)	1:A:3105:ILE:HG13	1:A:3219:PHE:HD1	4	0.13
(1,572)	1:A:3105:ILE:HG13	1:A:3219:PHE:HD2	4	0.13
(1,570)	1:A:3204:LYS:HA	1:A:3204:LYS:HG3	5	0.13
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD11	6	0.13
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD12	6	0.13
(1,57)	1:A:3122:GLU:HG2	1:A:3123:ILE:HD13	6	0.13
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD11	6	0.13
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD12	6	0.13
(1,57)	1:A:3122:GLU:HG3	1:A:3123:ILE:HD13	6	0.13
(1,561)	1:A:3217:ILE:HG21	1:A:3221:LYS:HE2	4	0.13
(1,561)	1:A:3217:ILE:HG21	1:A:3221:LYS:HE3	4	0.13
(1,561)	1:A:3217:ILE:HG22	1:A:3221:LYS:HE2	4	0.13
(1,561)	1:A:3217:ILE:HG22	1:A:3221:LYS:HE3	4	0.13
(1,561)	1:A:3217:ILE:HG23	1:A:3221:LYS:HE2	4	0.13
(1,561)	1:A:3217:ILE:HG23	1:A:3221:LYS:HE3	4	0.13
(1,561)	1:A:3217:ILE:HG21	1:A:3221:LYS:HE2	5	0.13
(1,561)	1:A:3217:ILE:HG21	1:A:3221:LYS:HE3	5	0.13
(1,561)	1:A:3217:ILE:HG22	1:A:3221:LYS:HE2	5	0.13
(1,561)	1:A:3217:ILE:HG22	1:A:3221:LYS:HE3	5	0.13
(1,561)	1:A:3217:ILE:HG23	1:A:3221:LYS:HE2	5	0.13
(1,561)	1:A:3217:ILE:HG23	1:A:3221:LYS:HE3	5	0.13
(1,526)	1:A:3110:ARG:HA	1:A:3113:LYS:HB2	2	0.13
(1,492)	1:A:3109:GLN:HG2	1:A:3113:LYS:HE2	1	0.13
(1,492)	1:A:3109:GLN:HG2	1:A:3113:LYS:HE3	1	0.13
(1,48)	1:A:3112:VAL:HA	1:A:3115:ILE:HD11	8	0.13
(1,48)	1:A:3112:VAL:HA	1:A:3115:ILE:HD12	8	0.13
(1,48)	1:A:3112:VAL:HA	1:A:3115:ILE:HD13	8	0.13
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG21	10	0.13
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG22	10	0.13
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG23	10	0.13
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD11	6	0.13
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD12	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD13	6	0.13
(1,446)	1:A:3128:ASN:HA	1:A:3129:PRO:HB3	4	0.13
(1,429)	1:A:3137:MET:HA	1:A:3140:VAL:HB	5	0.13
(1,42)	1:A:3105:ILE:HG21	1:A:3219:PHE:HD1	10	0.13
(1,42)	1:A:3105:ILE:HG21	1:A:3219:PHE:HD2	10	0.13
(1,42)	1:A:3105:ILE:HG22	1:A:3219:PHE:HD1	10	0.13
(1,42)	1:A:3105:ILE:HG22	1:A:3219:PHE:HD2	10	0.13
(1,42)	1:A:3105:ILE:HG23	1:A:3219:PHE:HD1	10	0.13
(1,42)	1:A:3105:ILE:HG23	1:A:3219:PHE:HD2	10	0.13
(1,410)	1:A:3209:LEU:HD11	1:A:3210:TYR:HA	2	0.13
(1,410)	1:A:3209:LEU:HD12	1:A:3210:TYR:HA	2	0.13
(1,410)	1:A:3209:LEU:HD13	1:A:3210:TYR:HA	2	0.13
(1,410)	1:A:3209:LEU:HD11	1:A:3210:TYR:HA	10	0.13
(1,410)	1:A:3209:LEU:HD12	1:A:3210:TYR:HA	10	0.13
(1,410)	1:A:3209:LEU:HD13	1:A:3210:TYR:HA	10	0.13
(1,409)	1:A:3210:TYR:HA	1:A:3213:VAL:HG21	10	0.13
(1,409)	1:A:3210:TYR:HA	1:A:3213:VAL:HG22	10	0.13
(1,409)	1:A:3210:TYR:HA	1:A:3213:VAL:HG23	10	0.13
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG21	7	0.13
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG22	7	0.13
(1,380)	1:A:3192:PRO:HA	1:A:3195:THR:HG23	7	0.13
(1,342)	1:A:3185:GLU:HA	1:A:3189:LEU:HB3	1	0.13
(1,322)	1:A:3198:THR:HG21	1:A:3201:ARG:HD2	7	0.13
(1,322)	1:A:3198:THR:HG21	1:A:3201:ARG:HD3	7	0.13
(1,322)	1:A:3198:THR:HG22	1:A:3201:ARG:HD2	7	0.13
(1,322)	1:A:3198:THR:HG22	1:A:3201:ARG:HD3	7	0.13
(1,322)	1:A:3198:THR:HG23	1:A:3201:ARG:HD2	7	0.13
(1,322)	1:A:3198:THR:HG23	1:A:3201:ARG:HD3	7	0.13
(1,29)	1:A:3098:ILE:HG21	1:A:3099:GLN:HB3	10	0.13
(1,29)	1:A:3098:ILE:HG22	1:A:3099:GLN:HB3	10	0.13
(1,29)	1:A:3098:ILE:HG23	1:A:3099:GLN:HB3	10	0.13
(1,287)	1:A:3132:GLY:HA3	1:A:3202:ALA:HA	4	0.13
(1,267)	1:A:3113:LYS:HA	1:A:3168:VAL:HG21	8	0.13
(1,267)	1:A:3113:LYS:HA	1:A:3168:VAL:HG22	8	0.13
(1,267)	1:A:3113:LYS:HA	1:A:3168:VAL:HG23	8	0.13
(1,246)	1:A:3136:VAL:HA	1:A:3210:TYR:HA	10	0.13
(1,1525)	1:A:3227:ASP:HB2	1:A:3228:PRO:HG2	10	0.13
(1,1525)	1:A:3227:ASP:HB2	1:A:3228:PRO:HG3	10	0.13
(1,1525)	1:A:3227:ASP:HB3	1:A:3228:PRO:HG2	10	0.13
(1,1525)	1:A:3227:ASP:HB3	1:A:3228:PRO:HG3	10	0.13
(1,1516)	1:A:3224:GLU:HA	1:A:3225:ASN:HB2	1	0.13
(1,1516)	1:A:3224:GLU:HA	1:A:3225:ASN:HB3	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1493)	1:A:3214:ASN:HB2	1:A:3217:ILE:HB	7	0.13
(1,1493)	1:A:3214:ASN:HB3	1:A:3217:ILE:HB	7	0.13
(1,1490)	1:A:3214:ASN:HA	1:A:3217:ILE:HG12	7	0.13
(1,1490)	1:A:3214:ASN:HA	1:A:3217:ILE:HG13	7	0.13
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG11	5	0.13
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG12	5	0.13
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG13	5	0.13
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG21	5	0.13
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG22	5	0.13
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG23	5	0.13
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG11	5	0.13
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG12	5	0.13
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG13	5	0.13
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG21	5	0.13
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG22	5	0.13
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG23	5	0.13
(1,1424)	1:A:3188:PHE:HB2	1:A:3190:SER:H	3	0.13
(1,1424)	1:A:3188:PHE:HB3	1:A:3190:SER:H	3	0.13
(1,1403)	1:A:3184:MET:H	1:A:3187:GLU:HG2	9	0.13
(1,1403)	1:A:3184:MET:H	1:A:3187:GLU:HG3	9	0.13
(1,1399)	1:A:3181:ARG:HB2	1:A:3217:ILE:HD11	4	0.13
(1,1399)	1:A:3181:ARG:HB2	1:A:3217:ILE:HD12	4	0.13
(1,1399)	1:A:3181:ARG:HB2	1:A:3217:ILE:HD13	4	0.13
(1,1399)	1:A:3181:ARG:HB3	1:A:3217:ILE:HD11	4	0.13
(1,1399)	1:A:3181:ARG:HB3	1:A:3217:ILE:HD12	4	0.13
(1,1399)	1:A:3181:ARG:HB3	1:A:3217:ILE:HD13	4	0.13
(1,1384)	1:A:3171:ASP:HB2	1:A:3174:LEU:HB2	3	0.13
(1,1384)	1:A:3171:ASP:HB2	1:A:3174:LEU:HB3	3	0.13
(1,1384)	1:A:3171:ASP:HB3	1:A:3174:LEU:HB2	3	0.13
(1,1384)	1:A:3171:ASP:HB3	1:A:3174:LEU:HB3	3	0.13
(1,12)	1:A:3137:MET:HE1	1:A:3209:LEU:HG	5	0.13
(1,12)	1:A:3137:MET:HE2	1:A:3209:LEU:HG	5	0.13
(1,12)	1:A:3137:MET:HE3	1:A:3209:LEU:HG	5	0.13
(1,1177)	1:A:3123:ILE:HB	1:A:3126:MET:HG2	5	0.13
(1,1177)	1:A:3123:ILE:HB	1:A:3126:MET:HG3	5	0.13
(1,1172)	1:A:3122:GLU:H	1:A:3123:ILE:HG12	2	0.13
(1,1172)	1:A:3122:GLU:H	1:A:3123:ILE:HG13	2	0.13
(1,117)	1:A:3158:ILE:HD11	1:A:3163:PHE:HE1	1	0.13
(1,117)	1:A:3158:ILE:HD11	1:A:3163:PHE:HE2	1	0.13
(1,117)	1:A:3158:ILE:HD12	1:A:3163:PHE:HE1	1	0.13
(1,117)	1:A:3158:ILE:HD12	1:A:3163:PHE:HE2	1	0.13
(1,117)	1:A:3158:ILE:HD13	1:A:3163:PHE:HE1	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:A:3158:ILE:HD13	1:A:3163:PHE:HE2	1	0.13
(1,1150)	1:A:3119:GLN:HB2	1:A:3205:ALA:HA	5	0.13
(1,1150)	1:A:3119:GLN:HB3	1:A:3205:ALA:HA	5	0.13
(1,1129)	1:A:3112:VAL:HG11	1:A:3164:ILE:HA	10	0.13
(1,1129)	1:A:3112:VAL:HG12	1:A:3164:ILE:HA	10	0.13
(1,1129)	1:A:3112:VAL:HG13	1:A:3164:ILE:HA	10	0.13
(1,1129)	1:A:3112:VAL:HG21	1:A:3164:ILE:HA	10	0.13
(1,1129)	1:A:3112:VAL:HG22	1:A:3164:ILE:HA	10	0.13
(1,1129)	1:A:3112:VAL:HG23	1:A:3164:ILE:HA	10	0.13
(1,1118)	1:A:3106:LEU:HD11	1:A:3109:GLN:HG2	6	0.13
(1,1118)	1:A:3106:LEU:HD12	1:A:3109:GLN:HG2	6	0.13
(1,1118)	1:A:3106:LEU:HD13	1:A:3109:GLN:HG2	6	0.13
(1,1118)	1:A:3106:LEU:HD21	1:A:3109:GLN:HG2	6	0.13
(1,1118)	1:A:3106:LEU:HD22	1:A:3109:GLN:HG2	6	0.13
(1,1118)	1:A:3106:LEU:HD23	1:A:3109:GLN:HG2	6	0.13
(1,1115)	1:A:3106:LEU:HB2	1:A:3109:GLN:HG3	9	0.13
(1,1115)	1:A:3106:LEU:HB3	1:A:3109:GLN:HG3	9	0.13
(1,994)	1:A:3108:ALA:HB1	1:A:3212:TRP:HE3	9	0.12
(1,994)	1:A:3108:ALA:HB2	1:A:3212:TRP:HE3	9	0.12
(1,994)	1:A:3108:ALA:HB3	1:A:3212:TRP:HE3	9	0.12
(1,978)	1:A:3223:LEU:HA	1:A:3225:ASN:H	10	0.12
(1,932)	1:A:3207:GLY:HA3	1:A:3209:LEU:H	10	0.12
(1,928)	1:A:3207:GLY:H	1:A:3208:PRO:HG2	1	0.12
(1,928)	1:A:3207:GLY:H	1:A:3208:PRO:HG3	1	0.12
(1,902)	1:A:3201:ARG:H	1:A:3203:SER:H	1	0.12
(1,782)	1:A:3164:ILE:HB	1:A:3166:ASN:H	4	0.12
(1,721)	1:A:3144:LEU:H	1:A:3180:ILE:HD11	6	0.12
(1,721)	1:A:3144:LEU:H	1:A:3180:ILE:HD12	6	0.12
(1,721)	1:A:3144:LEU:H	1:A:3180:ILE:HD13	6	0.12
(1,720)	1:A:3140:VAL:HA	1:A:3144:LEU:H	10	0.12
(1,638)	1:A:3119:GLN:H	1:A:3205:ALA:HB1	7	0.12
(1,638)	1:A:3119:GLN:H	1:A:3205:ALA:HB2	7	0.12
(1,638)	1:A:3119:GLN:H	1:A:3205:ALA:HB3	7	0.12
(1,626)	1:A:3112:VAL:HA	1:A:3115:ILE:H	2	0.12
(1,608)	1:A:3109:GLN:HG3	1:A:3110:ARG:H	1	0.12
(1,579)	1:A:3109:GLN:H	1:A:3110:ARG:HG2	8	0.12
(1,579)	1:A:3109:GLN:H	1:A:3110:ARG:HG3	8	0.12
(1,511)	1:A:3124:ARG:HA	1:A:3155:GLN:HG2	9	0.12
(1,511)	1:A:3124:ARG:HA	1:A:3155:GLN:HG3	9	0.12
(1,490)	1:A:3106:LEU:HB2	1:A:3109:GLN:HG3	7	0.12
(1,480)	1:A:3203:SER:HB2	1:A:3206:CYS:HB3	7	0.12
(1,478)	1:A:3195:THR:HA	1:A:3210:TYR:HD1	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:A:3195:THR:HA	1:A:3210:TYR:HD2	3	0.12
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG21	6	0.12
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG22	6	0.12
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG23	6	0.12
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG21	6	0.12
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG22	6	0.12
(1,452)	1:A:3193:ASN:HA	1:A:3198:THR:HG23	6	0.12
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD11	8	0.12
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD12	8	0.12
(1,45)	1:A:3115:ILE:HB	1:A:3164:ILE:HD13	8	0.12
(1,410)	1:A:3209:LEU:HD11	1:A:3210:TYR:HA	5	0.12
(1,410)	1:A:3209:LEU:HD12	1:A:3210:TYR:HA	5	0.12
(1,410)	1:A:3209:LEU:HD13	1:A:3210:TYR:HA	5	0.12
(1,409)	1:A:3210:TYR:HA	1:A:3213:VAL:HG21	6	0.12
(1,409)	1:A:3210:TYR:HA	1:A:3213:VAL:HG22	6	0.12
(1,409)	1:A:3210:TYR:HA	1:A:3213:VAL:HG23	6	0.12
(1,401)	1:A:3180:ILE:HA	1:A:3183:TYR:HA	7	0.12
(1,336)	1:A:3174:LEU:HA	1:A:3174:LEU:HD11	1	0.12
(1,336)	1:A:3174:LEU:HA	1:A:3174:LEU:HD12	1	0.12
(1,336)	1:A:3174:LEU:HA	1:A:3174:LEU:HD13	1	0.12
(1,279)	1:A:3139:ALA:HB1	1:A:3143:ILE:HB	5	0.12
(1,279)	1:A:3139:ALA:HB2	1:A:3143:ILE:HB	5	0.12
(1,279)	1:A:3139:ALA:HB3	1:A:3143:ILE:HB	5	0.12
(1,278)	1:A:3108:ALA:HA	1:A:3212:TRP:HA	10	0.12
(1,219)	1:A:3112:VAL:HG11	1:A:3212:TRP:HD1	5	0.12
(1,219)	1:A:3112:VAL:HG12	1:A:3212:TRP:HD1	5	0.12
(1,219)	1:A:3112:VAL:HG13	1:A:3212:TRP:HD1	5	0.12
(1,189)	1:A:3195:THR:HA	1:A:3199:ILE:HD11	1	0.12
(1,189)	1:A:3195:THR:HA	1:A:3199:ILE:HD12	1	0.12
(1,189)	1:A:3195:THR:HA	1:A:3199:ILE:HD13	1	0.12
(1,1497)	1:A:3216:GLN:HA	1:A:3219:PHE:HB2	5	0.12
(1,1497)	1:A:3216:GLN:HA	1:A:3219:PHE:HB3	5	0.12
(1,1493)	1:A:3214:ASN:HB2	1:A:3217:ILE:HB	2	0.12
(1,1493)	1:A:3214:ASN:HB3	1:A:3217:ILE:HB	2	0.12
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG11	8	0.12
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG12	8	0.12
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG13	8	0.12
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG21	8	0.12
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG22	8	0.12
(1,1475)	1:A:3210:TYR:HB2	1:A:3213:VAL:HG23	8	0.12
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG11	8	0.12
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG12	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG13	8	0.12
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG21	8	0.12
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG22	8	0.12
(1,1475)	1:A:3210:TYR:HB3	1:A:3213:VAL:HG23	8	0.12
(1,1442)	1:A:3195:THR:HG21	1:A:3197:GLU:HG2	10	0.12
(1,1442)	1:A:3195:THR:HG21	1:A:3197:GLU:HG3	10	0.12
(1,1442)	1:A:3195:THR:HG22	1:A:3197:GLU:HG2	10	0.12
(1,1442)	1:A:3195:THR:HG22	1:A:3197:GLU:HG3	10	0.12
(1,1442)	1:A:3195:THR:HG23	1:A:3197:GLU:HG2	10	0.12
(1,1442)	1:A:3195:THR:HG23	1:A:3197:GLU:HG3	10	0.12
(1,1424)	1:A:3188:PHE:HB2	1:A:3190:SER:H	8	0.12
(1,1424)	1:A:3188:PHE:HB3	1:A:3190:SER:H	8	0.12
(1,1405)	1:A:3184:MET:HB2	1:A:3185:GLU:H	9	0.12
(1,1405)	1:A:3184:MET:HB3	1:A:3185:GLU:H	9	0.12
(1,1344)	1:A:3152:ARG:HB3	1:A:3153:ASP:HB2	2	0.12
(1,1344)	1:A:3152:ARG:HB3	1:A:3153:ASP:HB3	2	0.12
(1,1199)	1:A:3126:MET:HE1	1:A:3203:SER:HB2	5	0.12
(1,1199)	1:A:3126:MET:HE1	1:A:3203:SER:HB3	5	0.12
(1,1199)	1:A:3126:MET:HE2	1:A:3203:SER:HB2	5	0.12
(1,1199)	1:A:3126:MET:HE2	1:A:3203:SER:HB3	5	0.12
(1,1199)	1:A:3126:MET:HE3	1:A:3203:SER:HB2	5	0.12
(1,1199)	1:A:3126:MET:HE3	1:A:3203:SER:HB3	5	0.12
(1,1177)	1:A:3123:ILE:HB	1:A:3126:MET:HG2	1	0.12
(1,1177)	1:A:3123:ILE:HB	1:A:3126:MET:HG3	1	0.12
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD11	3	0.12
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD12	3	0.12
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD13	3	0.12
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD11	3	0.12
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD12	3	0.12
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD13	3	0.12
(1,1119)	1:A:3106:LEU:HD11	1:A:3109:GLN:HG3	6	0.12
(1,1119)	1:A:3106:LEU:HD12	1:A:3109:GLN:HG3	6	0.12
(1,1119)	1:A:3106:LEU:HD13	1:A:3109:GLN:HG3	6	0.12
(1,1119)	1:A:3106:LEU:HD21	1:A:3109:GLN:HG3	6	0.12
(1,1119)	1:A:3106:LEU:HD22	1:A:3109:GLN:HG3	6	0.12
(1,1119)	1:A:3106:LEU:HD23	1:A:3109:GLN:HG3	6	0.12
(1,1118)	1:A:3106:LEU:HD11	1:A:3109:GLN:HG2	5	0.12
(1,1118)	1:A:3106:LEU:HD12	1:A:3109:GLN:HG2	5	0.12
(1,1118)	1:A:3106:LEU:HD13	1:A:3109:GLN:HG2	5	0.12
(1,1118)	1:A:3106:LEU:HD21	1:A:3109:GLN:HG2	5	0.12
(1,1118)	1:A:3106:LEU:HD22	1:A:3109:GLN:HG2	5	0.12
(1,1118)	1:A:3106:LEU:HD23	1:A:3109:GLN:HG2	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:A:3196:TYR:HE1	1:A:3199:ILE:HG21	1	0.12
(1,1056)	1:A:3196:TYR:HE1	1:A:3199:ILE:HG22	1	0.12
(1,1056)	1:A:3196:TYR:HE1	1:A:3199:ILE:HG23	1	0.12
(1,1056)	1:A:3196:TYR:HE2	1:A:3199:ILE:HG21	1	0.12
(1,1056)	1:A:3196:TYR:HE2	1:A:3199:ILE:HG22	1	0.12
(1,1056)	1:A:3196:TYR:HE2	1:A:3199:ILE:HG23	1	0.12
(1,1056)	1:A:3196:TYR:HE1	1:A:3199:ILE:HG21	5	0.12
(1,1056)	1:A:3196:TYR:HE1	1:A:3199:ILE:HG22	5	0.12
(1,1056)	1:A:3196:TYR:HE1	1:A:3199:ILE:HG23	5	0.12
(1,1056)	1:A:3196:TYR:HE2	1:A:3199:ILE:HG21	5	0.12
(1,1056)	1:A:3196:TYR:HE2	1:A:3199:ILE:HG22	5	0.12
(1,1056)	1:A:3196:TYR:HE2	1:A:3199:ILE:HG23	5	0.12
(1,946)	1:A:3170:TYR:HE1	1:A:3212:TRP:HE1	8	0.11
(1,946)	1:A:3170:TYR:HE2	1:A:3212:TRP:HE1	8	0.11
(1,932)	1:A:3207:GLY:HA3	1:A:3209:LEU:H	2	0.11
(1,928)	1:A:3207:GLY:H	1:A:3208:PRO:HG2	5	0.11
(1,928)	1:A:3207:GLY:H	1:A:3208:PRO:HG3	5	0.11
(1,928)	1:A:3207:GLY:H	1:A:3208:PRO:HG2	10	0.11
(1,928)	1:A:3207:GLY:H	1:A:3208:PRO:HG3	10	0.11
(1,747)	1:A:3153:ASP:H	1:A:3154:ILE:HG13	9	0.11
(1,743)	1:A:3218:ASN:H	1:A:3219:PHE:H	4	0.11
(1,731)	1:A:3150:ASN:H	1:A:3152:ARG:HB3	6	0.11
(1,720)	1:A:3140:VAL:HA	1:A:3144:LEU:H	2	0.11
(1,720)	1:A:3140:VAL:HA	1:A:3144:LEU:H	7	0.11
(1,695)	1:A:3139:ALA:H	1:A:3154:ILE:HD11	2	0.11
(1,695)	1:A:3139:ALA:H	1:A:3154:ILE:HD12	2	0.11
(1,695)	1:A:3139:ALA:H	1:A:3154:ILE:HD13	2	0.11
(1,673)	1:A:3126:MET:HE1	1:A:3133:VAL:H	10	0.11
(1,673)	1:A:3126:MET:HE2	1:A:3133:VAL:H	10	0.11
(1,673)	1:A:3126:MET:HE3	1:A:3133:VAL:H	10	0.11
(1,672)	1:A:3129:PRO:HB2	1:A:3133:VAL:H	4	0.11
(1,630)	1:A:3115:ILE:H	1:A:3205:ALA:HB1	8	0.11
(1,630)	1:A:3115:ILE:H	1:A:3205:ALA:HB2	8	0.11
(1,630)	1:A:3115:ILE:H	1:A:3205:ALA:HB3	8	0.11
(1,626)	1:A:3112:VAL:HA	1:A:3115:ILE:H	6	0.11
(1,49)	1:A:3115:ILE:HD11	1:A:3205:ALA:HA	2	0.11
(1,49)	1:A:3115:ILE:HD12	1:A:3205:ALA:HA	2	0.11
(1,49)	1:A:3115:ILE:HD13	1:A:3205:ALA:HA	2	0.11
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG21	4	0.11
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG22	4	0.11
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG23	4	0.11
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG21	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG22	8	0.11
(1,459)	1:A:3214:ASN:HB3	1:A:3217:ILE:HG23	8	0.11
(1,43)	1:A:3189:LEU:HD21	1:A:3190:SER:HB2	9	0.11
(1,43)	1:A:3189:LEU:HD22	1:A:3190:SER:HB2	9	0.11
(1,43)	1:A:3189:LEU:HD23	1:A:3190:SER:HB2	9	0.11
(1,429)	1:A:3137:MET:HA	1:A:3140:VAL:HB	2	0.11
(1,427)	1:A:3137:MET:HA	1:A:3158:ILE:HD11	1	0.11
(1,427)	1:A:3137:MET:HA	1:A:3158:ILE:HD12	1	0.11
(1,427)	1:A:3137:MET:HA	1:A:3158:ILE:HD13	1	0.11
(1,410)	1:A:3209:LEU:HD11	1:A:3210:TYR:HA	6	0.11
(1,410)	1:A:3209:LEU:HD12	1:A:3210:TYR:HA	6	0.11
(1,410)	1:A:3209:LEU:HD13	1:A:3210:TYR:HA	6	0.11
(1,375)	1:A:3123:ILE:HA	1:A:3126:MET:HG2	4	0.11
(1,322)	1:A:3198:THR:HG21	1:A:3201:ARG:HD2	5	0.11
(1,322)	1:A:3198:THR:HG21	1:A:3201:ARG:HD3	5	0.11
(1,322)	1:A:3198:THR:HG22	1:A:3201:ARG:HD2	5	0.11
(1,322)	1:A:3198:THR:HG22	1:A:3201:ARG:HD3	5	0.11
(1,322)	1:A:3198:THR:HG23	1:A:3201:ARG:HD2	5	0.11
(1,322)	1:A:3198:THR:HG23	1:A:3201:ARG:HD3	5	0.11
(1,277)	1:A:3107:GLU:HG2	1:A:3108:ALA:HA	5	0.11
(1,277)	1:A:3107:GLU:HG3	1:A:3108:ALA:HA	5	0.11
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG21	9	0.11
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG22	9	0.11
(1,275)	1:A:3194:PHE:HZ	1:A:3213:VAL:HG23	9	0.11
(1,259)	1:A:3109:GLN:HG3	1:A:3168:VAL:HA	7	0.11
(1,1508)	1:A:3219:PHE:HA	1:A:3221:LYS:HG2	10	0.11
(1,1508)	1:A:3219:PHE:HA	1:A:3221:LYS:HG3	10	0.11
(1,1493)	1:A:3214:ASN:HB2	1:A:3217:ILE:HB	9	0.11
(1,1493)	1:A:3214:ASN:HB3	1:A:3217:ILE:HB	9	0.11
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG11	9	0.11
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG12	9	0.11
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG13	9	0.11
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG21	9	0.11
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG22	9	0.11
(1,1482)	1:A:3212:TRP:HZ2	1:A:3213:VAL:HG23	9	0.11
(1,1450)	1:A:3197:GLU:HG2	1:A:3199:ILE:H	1	0.11
(1,1450)	1:A:3197:GLU:HG3	1:A:3199:ILE:H	1	0.11
(1,1442)	1:A:3195:THR:HG21	1:A:3197:GLU:HG2	5	0.11
(1,1442)	1:A:3195:THR:HG21	1:A:3197:GLU:HG3	5	0.11
(1,1442)	1:A:3195:THR:HG22	1:A:3197:GLU:HG2	5	0.11
(1,1442)	1:A:3195:THR:HG22	1:A:3197:GLU:HG3	5	0.11
(1,1442)	1:A:3195:THR:HG23	1:A:3197:GLU:HG2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1442)	1:A:3195:THR:HG23	1:A:3197:GLU:HG3	5	0.11
(1,1393)	1:A:3179:GLN:H	1:A:3180:ILE:HG12	7	0.11
(1,1393)	1:A:3179:GLN:H	1:A:3180:ILE:HG13	7	0.11
(1,1344)	1:A:3152:ARG:HB3	1:A:3153:ASP:HB2	4	0.11
(1,1344)	1:A:3152:ARG:HB3	1:A:3153:ASP:HB3	4	0.11
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG11	10	0.11
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG12	10	0.11
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG13	10	0.11
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG21	10	0.11
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG22	10	0.11
(1,1290)	1:A:3140:VAL:H	1:A:3213:VAL:HG23	10	0.11
(1,1252)	1:A:3135:ILE:H	1:A:3138:GLU:HB2	4	0.11
(1,1252)	1:A:3135:ILE:H	1:A:3138:GLU:HB3	4	0.11
(1,1236)	1:A:3133:VAL:HG11	1:A:3202:ALA:H	5	0.11
(1,1236)	1:A:3133:VAL:HG12	1:A:3202:ALA:H	5	0.11
(1,1236)	1:A:3133:VAL:HG13	1:A:3202:ALA:H	5	0.11
(1,1236)	1:A:3133:VAL:HG21	1:A:3202:ALA:H	5	0.11
(1,1236)	1:A:3133:VAL:HG22	1:A:3202:ALA:H	5	0.11
(1,1236)	1:A:3133:VAL:HG23	1:A:3202:ALA:H	5	0.11
(1,1206)	1:A:3128:ASN:HB2	1:A:3129:PRO:HD2	10	0.11
(1,1206)	1:A:3128:ASN:HB3	1:A:3129:PRO:HD2	10	0.11
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD11	2	0.11
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD12	2	0.11
(1,119)	1:A:3144:LEU:HG	1:A:3167:ILE:HD13	2	0.11
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD11	6	0.11
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD12	6	0.11
(1,1173)	1:A:3122:GLU:HB2	1:A:3123:ILE:HD13	6	0.11
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD11	6	0.11
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD12	6	0.11
(1,1173)	1:A:3122:GLU:HB3	1:A:3123:ILE:HD13	6	0.11
(1,1159)	1:A:3120:LEU:HB2	1:A:3123:ILE:H	4	0.11
(1,1159)	1:A:3120:LEU:HB3	1:A:3123:ILE:H	4	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG11	2	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG12	2	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG13	2	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG21	2	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG22	2	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG23	2	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG11	4	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG12	4	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG13	4	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG21	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG22	4	0.11
(1,1124)	1:A:3110:ARG:H	1:A:3112:VAL:HG23	4	0.11
(1,1084)	1:A:3144:LEU:HD11	1:A:3212:TRP:HZ2	4	0.11
(1,1084)	1:A:3144:LEU:HD12	1:A:3212:TRP:HZ2	4	0.11
(1,1084)	1:A:3144:LEU:HD13	1:A:3212:TRP:HZ2	4	0.11
(1,1043)	1:A:3135:ILE:HG21	1:A:3194:PHE:HD1	9	0.11
(1,1043)	1:A:3135:ILE:HG21	1:A:3194:PHE:HD2	9	0.11
(1,1043)	1:A:3135:ILE:HG22	1:A:3194:PHE:HD1	9	0.11
(1,1043)	1:A:3135:ILE:HG22	1:A:3194:PHE:HD2	9	0.11
(1,1043)	1:A:3135:ILE:HG23	1:A:3194:PHE:HD1	9	0.11
(1,1043)	1:A:3135:ILE:HG23	1:A:3194:PHE:HD2	9	0.11

10 Dihedral-angle violation analysis (i)

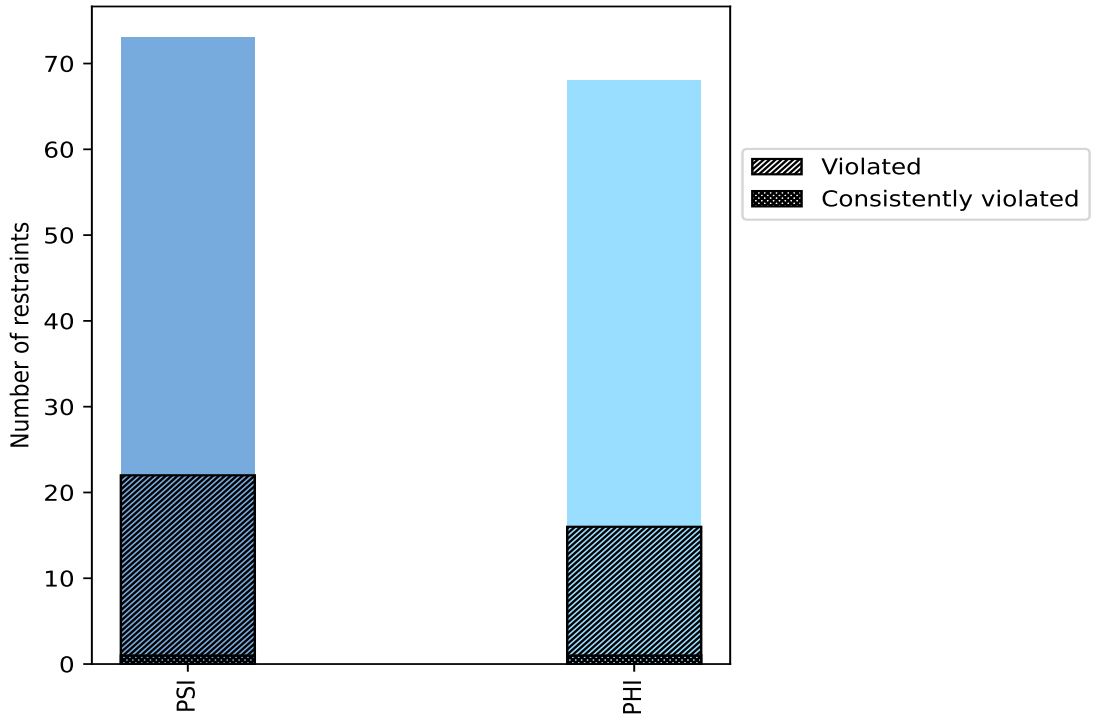
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	73	51.8	22	30.1	15.6	1	1.4	0.7
PHI	68	48.2	16	23.5	11.3	1	1.5	0.7
Total	141	100.0	38	27.0	27.0	2	1.4	1.4

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations (i)



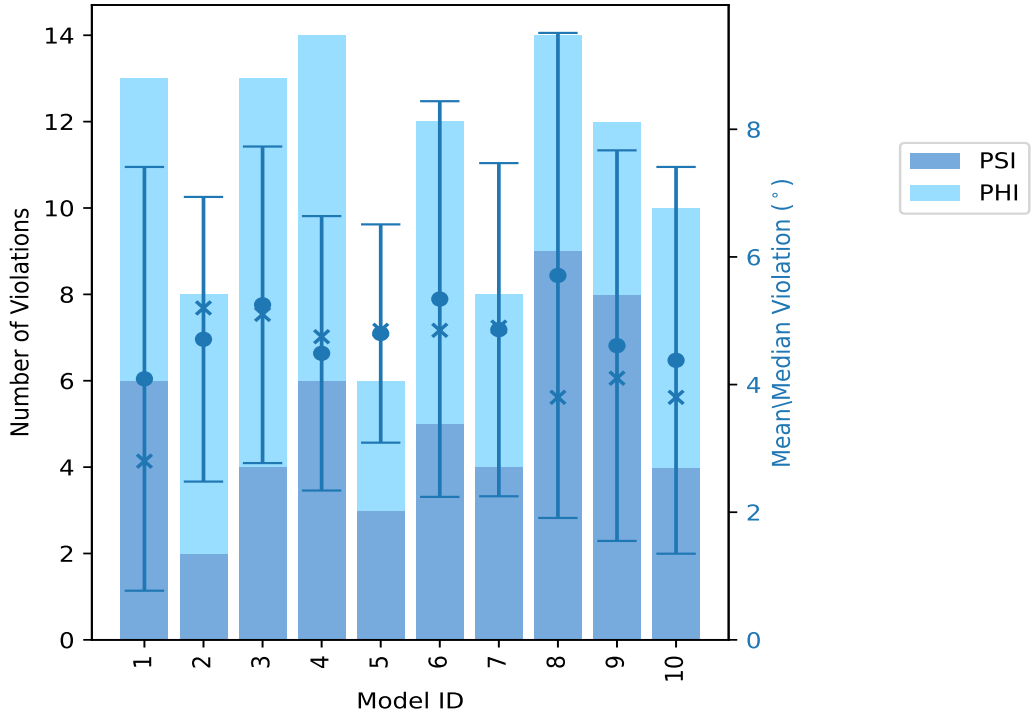
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	6	7	13	4.09	11.5	3.32	2.8
2	2	6	8	4.71	7.6	2.23	5.2
3	4	9	13	5.25	12.5	2.48	5.1
4	6	8	14	4.49	8.3	2.15	4.75
5	3	3	6	4.8	7.0	1.71	4.85
6	5	7	12	5.34	11.5	3.1	4.85
7	4	4	8	4.86	10.5	2.61	4.9
8	9	5	14	5.71	16.2	3.8	3.8
9	8	4	12	4.61	10.6	3.06	4.1
10	4	6	10	4.38	11.6	3.03	3.8

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



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

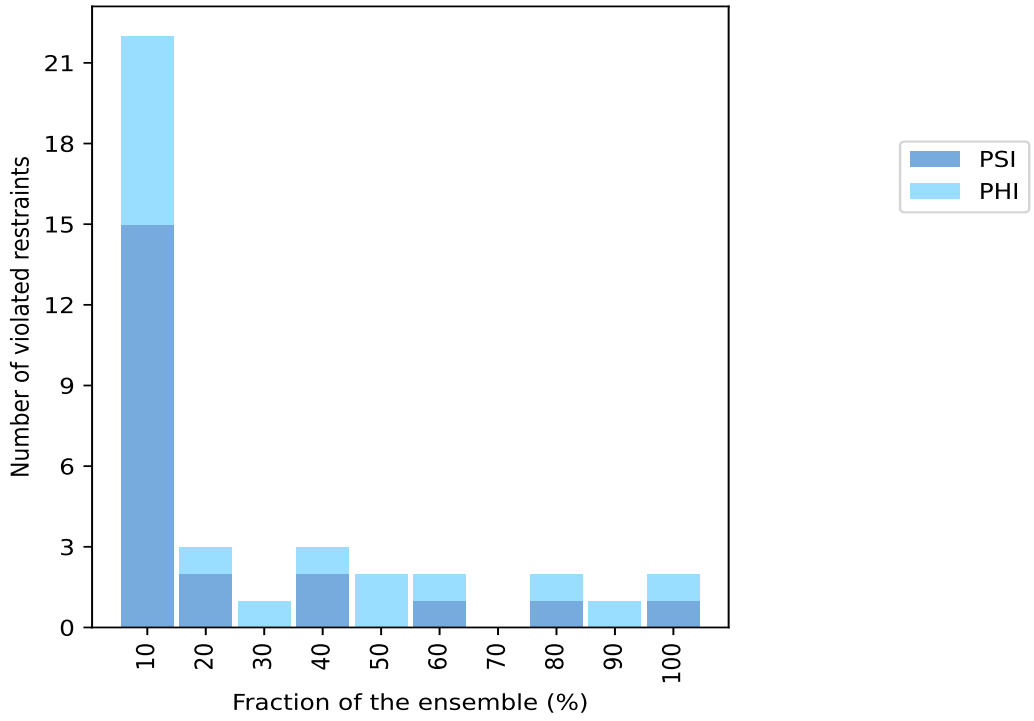
10.3 Dihedral-angle violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
15	7	22	1	10.0
2	1	3	2	20.0
0	1	1	3	30.0
2	1	3	4	40.0
0	2	2	5	50.0
1	1	2	6	60.0
0	0	0	7	70.0
1	1	2	8	80.0
0	1	1	9	90.0
1	1	2	10	100.0

[1] Number of models with violations

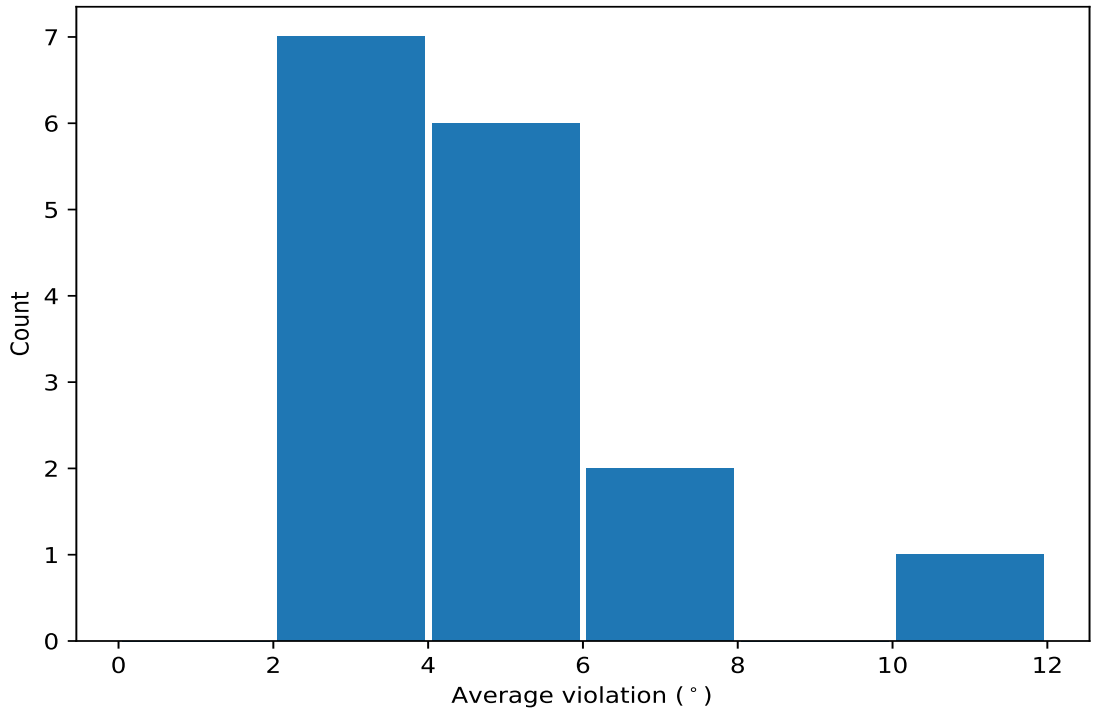
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



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

10.4.1 Histogram : Distribution of mean dihedral-angle violations (i)

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



10.4.2 Table: Most violated dihedral-angle restraints (i)

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Medi
(1,67)	1:A:3151:TRP:N	1:A:3151:TRP:CA	1:A:3151:TRP:C	1:A:3152:ARG:N	10	6.76	2.09	6.55
(1,56)	1:A:3143:ILE:C	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	10	5.44	1.24	5.5
(1,127)	1:A:3216:GLN:C	1:A:3217:ILE:N	1:A:3217:ILE:CA	1:A:3217:ILE:C	9	10.92	2.67	11.5
(1,62)	1:A:3148:PHE:C	1:A:3149:SER:N	1:A:3149:SER:CA	1:A:3149:SER:C	8	5.21	1.39	5.05
(1,57)	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	1:A:3145:GLY:N	8	3.72	2.09	3.2
(1,60)	1:A:3147:GLN:C	1:A:3148:PHE:N	1:A:3148:PHE:CA	1:A:3148:PHE:C	6	5.32	0.89	5.35
(1,105)	1:A:3183:TYR:N	1:A:3183:TYR:CA	1:A:3183:TYR:C	1:A:3184:MET:N	6	3.83	1.41	3.95
(1,98)	1:A:3178:PRO:C	1:A:3179:GLN:N	1:A:3179:GLN:CA	1:A:3179:GLN:C	5	6.18	1.89	7.3
(1,6)	1:A:3103:PRO:C	1:A:3104:THR:N	1:A:3104:THR:CA	1:A:3104:THR:C	5	4.68	1.94	5.1
(1,81)	1:A:3161:ASP:N	1:A:3161:ASP:CA	1:A:3161:ASP:C	1:A:3162:ASP:N	4	4.22	3.31	3.0
(1,5)	1:A:3103:PRO:N	1:A:3103:PRO:CA	1:A:3103:PRO:C	1:A:3104:THR:N	4	4.1	3.12	2.75
(1,92)	1:A:3169:HIS:C	1:A:3170:TYR:N	1:A:3170:TYR:CA	1:A:3170:TYR:C	4	3.4	1.66	3.4
(1,3)	1:A:3097:SER:C	1:A:3098:ILE:N	1:A:3098:ILE:CA	1:A:3098:ILE:C	3	3.9	1.98	5.3

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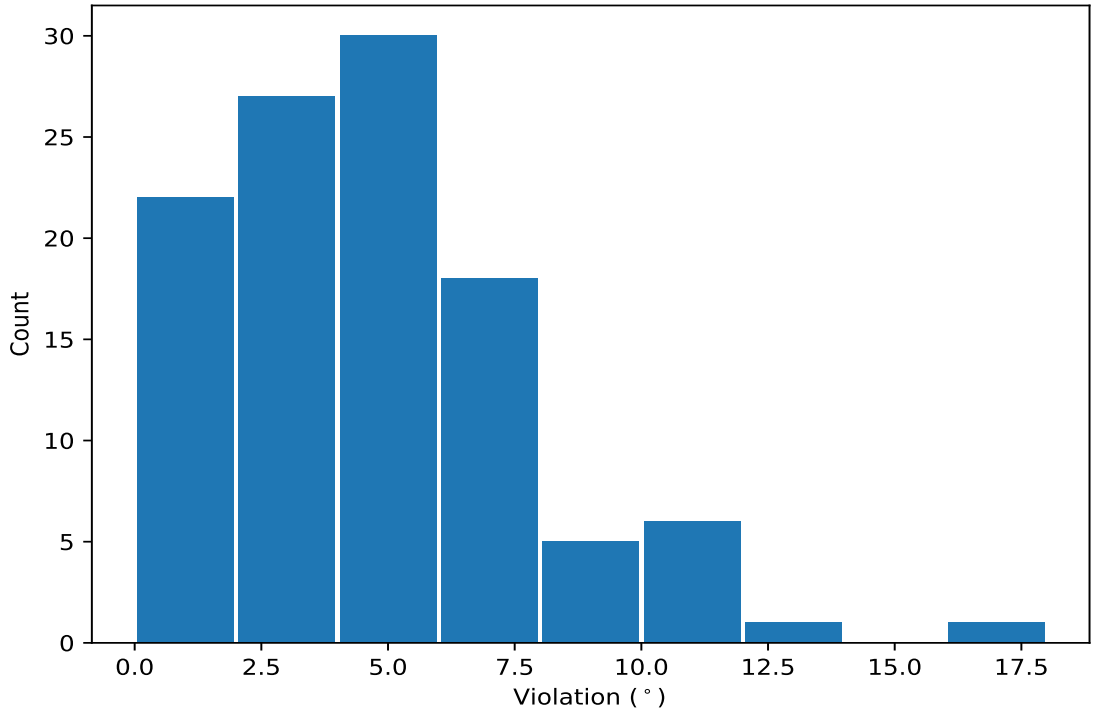
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Medi
(1,93)	1:A:3170:TYR:N	1:A:3170:TYR:CA	1:A:3170:TYR:C	1:A:3171:ASP:N	2	3.65	0.35	3.65
(1,96)	1:A:3173:THR:C	1:A:3174:LEU:N	1:A:3174:LEU:CA	1:A:3174:LEU:C	2	3.5	1.3	3.5
(1,2)	1:A:3097:SER:N	1:A:3097:SER:CA	1:A:3097:SER:C	1:A:3098:ILE:N	2	2.3	0.7	2.3

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints (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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,127)	1:A:3216:GLN:C	1:A:3217:ILE:N	1:A:3217:ILE:CA	1:A:3217:ILE:C	8	16.2
(1,127)	1:A:3216:GLN:C	1:A:3217:ILE:N	1:A:3217:ILE:CA	1:A:3217:ILE:C	3	12.5
(1,127)	1:A:3216:GLN:C	1:A:3217:ILE:N	1:A:3217:ILE:CA	1:A:3217:ILE:C	10	11.6
(1,127)	1:A:3216:GLN:C	1:A:3217:ILE:N	1:A:3217:ILE:CA	1:A:3217:ILE:C	1	11.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,127)	1:A:3216:GLN:C	1:A:3217:ILE:N	1:A:3217:ILE:CA	1:A:3217:ILE:C	6	11.5
(1,67)	1:A:3151:TRP:N	1:A:3151:TRP:CA	1:A:3151:TRP:C	1:A:3152:ARG:N	6	11.2
(1,127)	1:A:3216:GLN:C	1:A:3217:ILE:N	1:A:3217:ILE:CA	1:A:3217:ILE:C	9	10.6
(1,127)	1:A:3216:GLN:C	1:A:3217:ILE:N	1:A:3217:ILE:CA	1:A:3217:ILE:C	7	10.5
(1,81)	1:A:3161:ASP:N	1:A:3161:ASP:CA	1:A:3161:ASP:C	1:A:3162:ASP:N	8	9.8
(1,5)	1:A:3103:PRO:N	1:A:3103:PRO:CA	1:A:3103:PRO:C	1:A:3104:THR:N	9	9.4
(1,67)	1:A:3151:TRP:N	1:A:3151:TRP:CA	1:A:3151:TRP:C	1:A:3152:ARG:N	1	9.3
(1,98)	1:A:3178:PRO:C	1:A:3179:GLN:N	1:A:3179:GLN:CA	1:A:3179:GLN:C	4	8.3
(1,57)	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	1:A:3145:GLY:N	8	8.3
(1,62)	1:A:3148:PHE:C	1:A:3149:SER:N	1:A:3149:SER:CA	1:A:3149:SER:C	4	7.8
(1,56)	1:A:3143:ILE:C	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	8	7.8
(1,127)	1:A:3216:GLN:C	1:A:3217:ILE:N	1:A:3217:ILE:CA	1:A:3217:ILE:C	2	7.6
(1,98)	1:A:3178:PRO:C	1:A:3179:GLN:N	1:A:3179:GLN:CA	1:A:3179:GLN:C	1	7.5
(1,98)	1:A:3178:PRO:C	1:A:3179:GLN:N	1:A:3179:GLN:CA	1:A:3179:GLN:C	6	7.3
(1,67)	1:A:3151:TRP:N	1:A:3151:TRP:CA	1:A:3151:TRP:C	1:A:3152:ARG:N	10	7.2
(1,67)	1:A:3151:TRP:N	1:A:3151:TRP:CA	1:A:3151:TRP:C	1:A:3152:ARG:N	9	7.1
(1,62)	1:A:3148:PHE:C	1:A:3149:SER:N	1:A:3149:SER:CA	1:A:3149:SER:C	5	7.0
(1,61)	1:A:3148:PHE:N	1:A:3148:PHE:CA	1:A:3148:PHE:C	1:A:3149:SER:N	8	7.0
(1,67)	1:A:3151:TRP:N	1:A:3151:TRP:CA	1:A:3151:TRP:C	1:A:3152:ARG:N	2	6.8
(1,60)	1:A:3147:GLN:C	1:A:3148:PHE:N	1:A:3148:PHE:CA	1:A:3148:PHE:C	2	6.7
(1,6)	1:A:3103:PRO:C	1:A:3104:THR:N	1:A:3104:THR:CA	1:A:3104:THR:C	3	6.6
(1,6)	1:A:3103:PRO:C	1:A:3104:THR:N	1:A:3104:THR:CA	1:A:3104:THR:C	8	6.6
(1,67)	1:A:3151:TRP:N	1:A:3151:TRP:CA	1:A:3151:TRP:C	1:A:3152:ARG:N	3	6.3
(1,56)	1:A:3143:ILE:C	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	3	6.3
(1,127)	1:A:3216:GLN:C	1:A:3217:ILE:N	1:A:3217:ILE:CA	1:A:3217:ILE:C	4	6.3
(1,56)	1:A:3143:ILE:C	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	9	6.2
(1,67)	1:A:3151:TRP:N	1:A:3151:TRP:CA	1:A:3151:TRP:C	1:A:3152:ARG:N	5	6.1
(1,60)	1:A:3147:GLN:C	1:A:3148:PHE:N	1:A:3148:PHE:CA	1:A:3148:PHE:C	6	5.9
(1,135)	1:A:3226:VAL:C	1:A:3227:ASP:N	1:A:3227:ASP:CA	1:A:3227:ASP:C	4	5.8
(1,56)	1:A:3143:ILE:C	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	7	5.7
(1,105)	1:A:3183:TYR:N	1:A:3183:TYR:CA	1:A:3183:TYR:C	1:A:3184:MET:N	1	5.7
(1,92)	1:A:3169:HIS:C	1:A:3170:TYR:N	1:A:3170:TYR:CA	1:A:3170:TYR:C	3	5.6
(1,60)	1:A:3147:GLN:C	1:A:3148:PHE:N	1:A:3148:PHE:CA	1:A:3148:PHE:C	4	5.6
(1,56)	1:A:3143:ILE:C	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	4	5.6
(1,67)	1:A:3151:TRP:N	1:A:3151:TRP:CA	1:A:3151:TRP:C	1:A:3152:ARG:N	7	5.5
(1,56)	1:A:3143:ILE:C	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	2	5.4
(1,56)	1:A:3143:ILE:C	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	10	5.3
(1,3)	1:A:3097:SER:C	1:A:3098:ILE:N	1:A:3098:ILE:CA	1:A:3098:ILE:C	3	5.3
(1,3)	1:A:3097:SER:C	1:A:3098:ILE:N	1:A:3098:ILE:CA	1:A:3098:ILE:C	10	5.3
(1,62)	1:A:3148:PHE:C	1:A:3149:SER:N	1:A:3149:SER:CA	1:A:3149:SER:C	9	5.2
(1,1)	1:A:3096:LYS:C	1:A:3097:SER:N	1:A:3097:SER:CA	1:A:3097:SER:C	7	5.2
(1,62)	1:A:3148:PHE:C	1:A:3149:SER:N	1:A:3149:SER:CA	1:A:3149:SER:C	6	5.1
(1,60)	1:A:3147:GLN:C	1:A:3148:PHE:N	1:A:3148:PHE:CA	1:A:3148:PHE:C	3	5.1
(1,6)	1:A:3103:PRO:C	1:A:3104:THR:N	1:A:3104:THR:CA	1:A:3104:THR:C	4	5.1
(1,62)	1:A:3148:PHE:C	1:A:3149:SER:N	1:A:3149:SER:CA	1:A:3149:SER:C	2	5.0
(1,57)	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	1:A:3145:GLY:N	5	5.0
(1,105)	1:A:3183:TYR:N	1:A:3183:TYR:CA	1:A:3183:TYR:C	1:A:3184:MET:N	6	4.9
(1,96)	1:A:3173:THR:C	1:A:3174:LEU:N	1:A:3174:LEU:CA	1:A:3174:LEU:C	1	4.8
(1,56)	1:A:3143:ILE:C	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	6	4.8
(1,60)	1:A:3147:GLN:C	1:A:3148:PHE:N	1:A:3148:PHE:CA	1:A:3148:PHE:C	5	4.7
(1,105)	1:A:3183:TYR:N	1:A:3183:TYR:CA	1:A:3183:TYR:C	1:A:3184:MET:N	7	4.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	1:A:3145:GLY:N	3	4.5
(1,56)	1:A:3143:ILE:C	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	5	4.5
(1,67)	1:A:3151:TRP:N	1:A:3151:TRP:CA	1:A:3151:TRP:C	1:A:3152:ARG:N	4	4.4
(1,92)	1:A:3169:HIS:C	1:A:3170:TYR:N	1:A:3170:TYR:CA	1:A:3170:TYR:C	9	4.2
(1,62)	1:A:3148:PHE:C	1:A:3149:SER:N	1:A:3149:SER:CA	1:A:3149:SER:C	7	4.1
(1,93)	1:A:3170:TYR:N	1:A:3170:TYR:CA	1:A:3170:TYR:C	1:A:3171:ASP:N	9	4.0
(1,98)	1:A:3178:PRO:C	1:A:3179:GLN:N	1:A:3179:GLN:CA	1:A:3179:GLN:C	3	3.9
(1,98)	1:A:3178:PRO:C	1:A:3179:GLN:N	1:A:3179:GLN:CA	1:A:3179:GLN:C	8	3.9
(1,60)	1:A:3147:GLN:C	1:A:3148:PHE:N	1:A:3148:PHE:CA	1:A:3148:PHE:C	10	3.9
(1,62)	1:A:3148:PHE:C	1:A:3149:SER:N	1:A:3149:SER:CA	1:A:3149:SER:C	3	3.8
(1,67)	1:A:3151:TRP:N	1:A:3151:TRP:CA	1:A:3151:TRP:C	1:A:3152:ARG:N	8	3.7
(1,62)	1:A:3148:PHE:C	1:A:3149:SER:N	1:A:3149:SER:CA	1:A:3149:SER:C	10	3.7
(1,6)	1:A:3103:PRO:C	1:A:3104:THR:N	1:A:3104:THR:CA	1:A:3104:THR:C	6	3.6
(1,83)	1:A:3162:ASP:N	1:A:3162:ASP:CA	1:A:3162:ASP:C	1:A:3163:PHE:N	8	3.5
(1,66)	1:A:3150:ASN:C	1:A:3151:TRP:N	1:A:3151:TRP:CA	1:A:3151:TRP:C	8	3.5
(1,57)	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	1:A:3145:GLY:N	4	3.4
(1,93)	1:A:3170:TYR:N	1:A:3170:TYR:CA	1:A:3170:TYR:C	1:A:3171:ASP:N	1	3.3
(1,105)	1:A:3183:TYR:N	1:A:3183:TYR:CA	1:A:3183:TYR:C	1:A:3184:MET:N	8	3.3
(1,5)	1:A:3103:PRO:N	1:A:3103:PRO:CA	1:A:3103:PRO:C	1:A:3104:THR:N	4	3.2
(1,81)	1:A:3161:ASP:N	1:A:3161:ASP:CA	1:A:3161:ASP:C	1:A:3162:ASP:N	6	3.1
(1,105)	1:A:3183:TYR:N	1:A:3183:TYR:CA	1:A:3183:TYR:C	1:A:3184:MET:N	3	3.1
(1,57)	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	1:A:3145:GLY:N	6	3.0
(1,2)	1:A:3097:SER:N	1:A:3097:SER:CA	1:A:3097:SER:C	1:A:3098:ILE:N	3	3.0
(1,81)	1:A:3161:ASP:N	1:A:3161:ASP:CA	1:A:3161:ASP:C	1:A:3162:ASP:N	9	2.9
(1,56)	1:A:3143:ILE:C	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	1	2.8
(1,92)	1:A:3169:HIS:C	1:A:3170:TYR:N	1:A:3170:TYR:CA	1:A:3170:TYR:C	2	2.6
(1,63)	1:A:3149:SER:N	1:A:3149:SER:CA	1:A:3149:SER:C	1:A:3150:ASN:N	8	2.6
(1,57)	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	1:A:3145:GLY:N	2	2.5
(1,104)	1:A:3182:LYS:C	1:A:3183:TYR:N	1:A:3183:TYR:CA	1:A:3183:TYR:C	4	2.5
(1,5)	1:A:3103:PRO:N	1:A:3103:PRO:CA	1:A:3103:PRO:C	1:A:3104:THR:N	10	2.3
(1,96)	1:A:3173:THR:C	1:A:3174:LEU:N	1:A:3174:LEU:CA	1:A:3174:LEU:C	3	2.2
(1,71)	1:A:3154:ILE:N	1:A:3154:ILE:CA	1:A:3154:ILE:C	1:A:3155:GLN:N	8	2.2
(1,137)	1:A:3228:PRO:N	1:A:3228:PRO:CA	1:A:3228:PRO:C	1:A:3229:LEU:N	6	2.1
(1,97)	1:A:3174:LEU:N	1:A:3174:LEU:CA	1:A:3174:LEU:C	1:A:3175:HIS:N	4	1.9
(1,15)	1:A:3109:GLN:N	1:A:3109:GLN:CA	1:A:3109:GLN:C	1:A:3110:ARG:N	7	1.9
(1,130)	1:A:3220:SER:N	1:A:3220:SER:CA	1:A:3220:SER:C	1:A:3221:LYS:N	1	1.9
(1,124)	1:A:3213:VAL:N	1:A:3213:VAL:CA	1:A:3213:VAL:C	1:A:3214:ASN:N	9	1.8
(1,57)	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	1:A:3145:GLY:N	10	1.7
(1,94)	1:A:3171:ASP:C	1:A:3172:THR:N	1:A:3172:THR:CA	1:A:3172:THR:C	6	1.6
(1,78)	1:A:3157:PHE:C	1:A:3158:ILE:N	1:A:3158:ILE:CA	1:A:3158:ILE:C	1	1.6
(1,75)	1:A:3156:GLN:N	1:A:3156:GLN:CA	1:A:3156:GLN:C	1:A:3157:PHE:N	8	1.6
(1,2)	1:A:3097:SER:N	1:A:3097:SER:CA	1:A:3097:SER:C	1:A:3098:ILE:N	4	1.6
(1,79)	1:A:3158:ILE:N	1:A:3158:ILE:CA	1:A:3158:ILE:C	1:A:3159:ARG:N	9	1.5
(1,6)	1:A:3103:PRO:C	1:A:3104:THR:N	1:A:3104:THR:CA	1:A:3104:THR:C	10	1.5
(1,5)	1:A:3103:PRO:N	1:A:3103:PRO:CA	1:A:3103:PRO:C	1:A:3104:THR:N	5	1.5
(1,57)	1:A:3144:LEU:N	1:A:3144:LEU:CA	1:A:3144:LEU:C	1:A:3145:GLY:N	7	1.4
(1,105)	1:A:3183:TYR:N	1:A:3183:TYR:CA	1:A:3183:TYR:C	1:A:3184:MET:N	4	1.4
(1,99)	1:A:3179:GLN:N	1:A:3179:GLN:CA	1:A:3179:GLN:C	1:A:3180:ILE:N	10	1.3
(1,139)	1:A:3229:LEU:N	1:A:3229:LEU:CA	1:A:3229:LEU:C	1:A:3230:ARG:N	9	1.3
(1,111)	1:A:3197:GLU:N	1:A:3197:GLU:CA	1:A:3197:GLU:C	1:A:3198:THR:N	1	1.3
(1,92)	1:A:3169:HIS:C	1:A:3170:TYR:N	1:A:3170:TYR:CA	1:A:3170:TYR:C	1	1.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,140)	1:A:3230:ARG:C	1:A:3231:GLN:N	1:A:3231:GLN:CA	1:A:3231:GLN:C	1	1.2
(1,81)	1:A:3161:ASP:N	1:A:3161:ASP:CA	1:A:3161:ASP:C	1:A:3162:ASP:N	1	1.1
(1,55)	1:A:3143:ILE:N	1:A:3143:ILE:CA	1:A:3143:ILE:C	1:A:3144:LEU:N	9	1.1
(1,3)	1:A:3097:SER:C	1:A:3098:ILE:N	1:A:3098:ILE:CA	1:A:3098:ILE:C	2	1.1