



Full wwPDB NMR Structure Validation Report ⓘ

Jun 3, 2023 – 04:13 AM EDT

PDB ID : 5VTO
BMRB ID : 30295
Title : Solution Structure of BlsM
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Deposited on : 2017-05-17

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

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

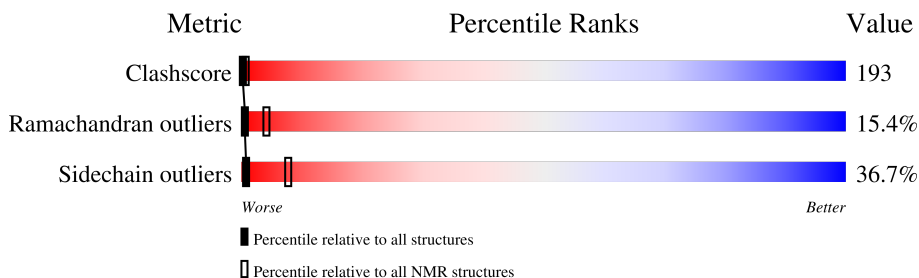
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 39%.

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	163	 60% 29% 6%
1	B	163	 60% 29% 6%

2 Ensemble composition and analysis i

This entry contains 15 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:15-A:168, B:215-B:368 (308)	0.99	1

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, 7, 8, 9, 10, 11, 12, 13, 14, 15
2	5, 6

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5056 atoms, of which 2534 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Blastocidin M.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	163	2528	812	1267	214	232	3	0
1	B	163	2528	812	1267	214	232	3	0

There are 8 discrepancies between the modelled and reference sequences:

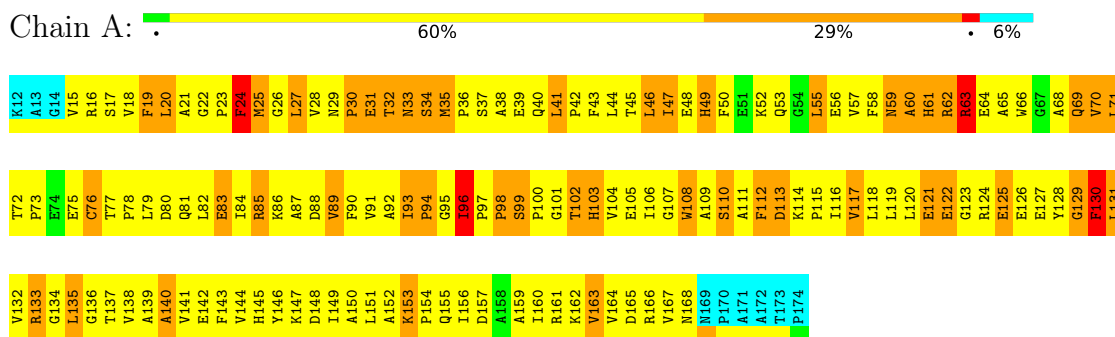
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	LYS	-	expression tag	UNP A0A1B1BCS8
A	13	ALA	-	expression tag	UNP A0A1B1BCS8
A	14	GLY	-	expression tag	UNP A0A1B1BCS8
A	15	VAL	-	expression tag	UNP A0A1B1BCS8
B	212	LYS	-	expression tag	UNP A0A1B1BCS8
B	213	ALA	-	expression tag	UNP A0A1B1BCS8
B	214	GLY	-	expression tag	UNP A0A1B1BCS8
B	215	VAL	-	expression tag	UNP A0A1B1BCS8

4 Residue-property plots i

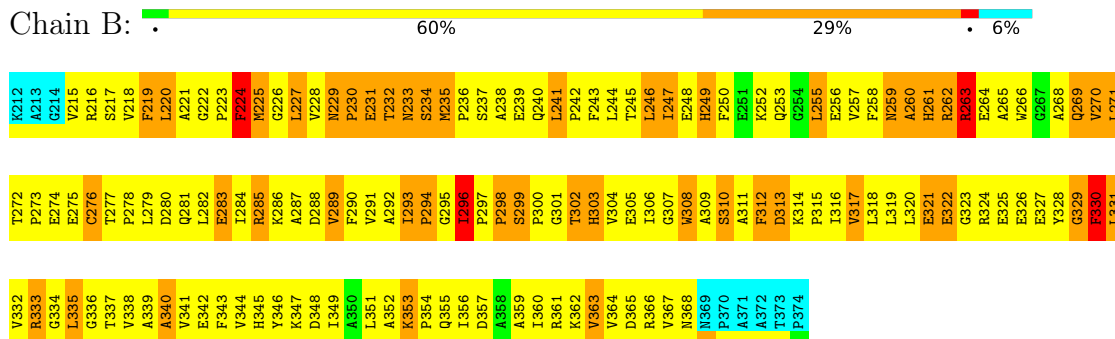
4.1 Average score per residue in the NMR ensemble

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: Blasticidin M



- Molecule 1: Blasticidin M



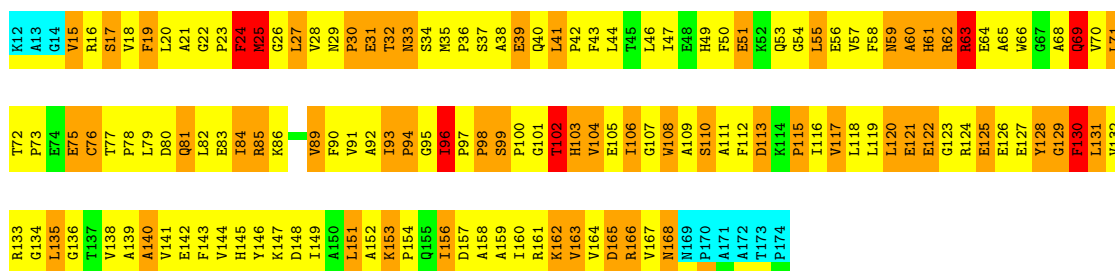
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

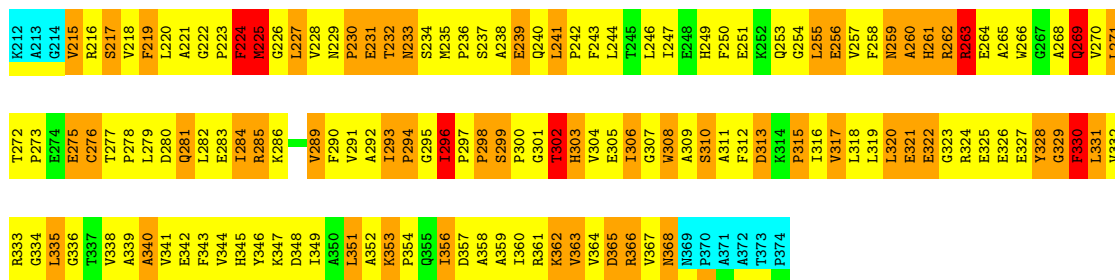
- Molecule 1: Blasticidin M

Chain A: 7% 52% 32% 6%



- Molecule 1: Blasticidin M

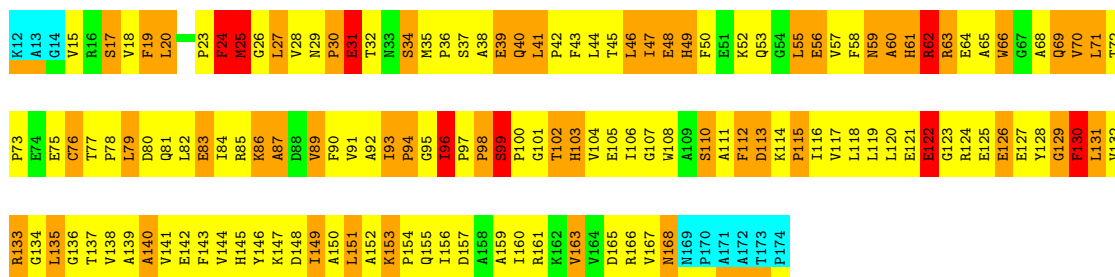
Chain B: 7% 53% 31% 6%



4.2.2 Score per residue for model 2

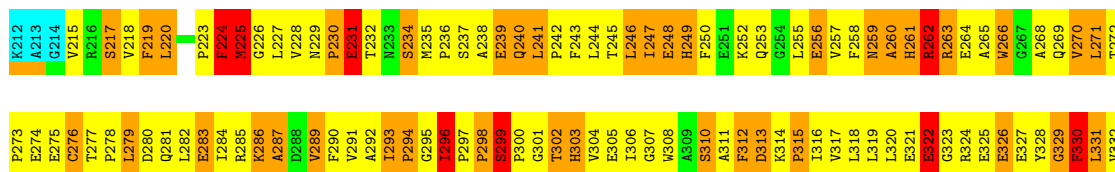
- Molecule 1: Blasticidin M

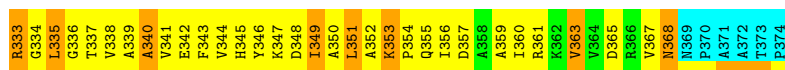
Chain A: 8% 52% 30% 5% 6%



- Molecule 1: Blasticidin M

Chain B: 8% 53% 28% 5% 6%





4.2.3 Score per residue for model 3

- Molecule 1: Blasticidin M

Chain A: 8% 54% 29% 6%



- Molecule 1: Blasticidin M

Chain B: 7% 55% 29% 6%



4.2.4 Score per residue for model 4

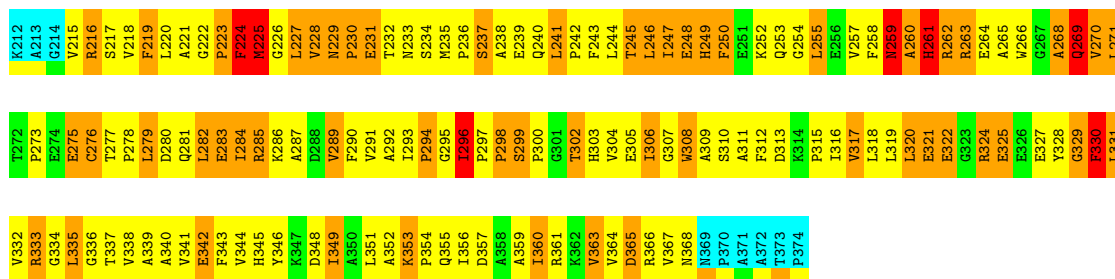
- Molecule 1: Blasticidin M

Chain A: 8% 49% 33% 6%



- Molecule 1: Blasticidin M

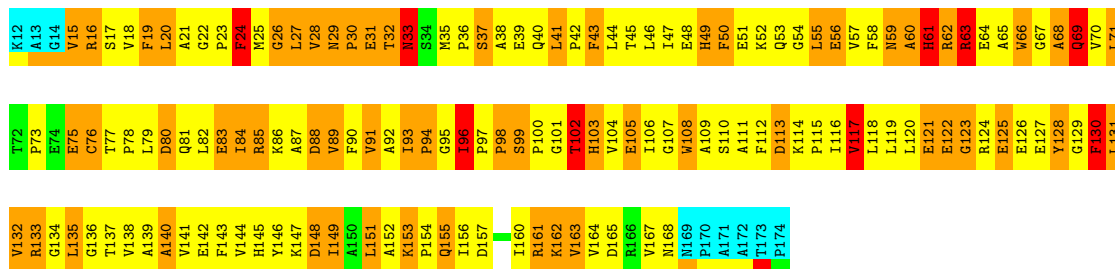
Chain B: 9% 49% 33% 6%



4.2.5 Score per residue for model 5

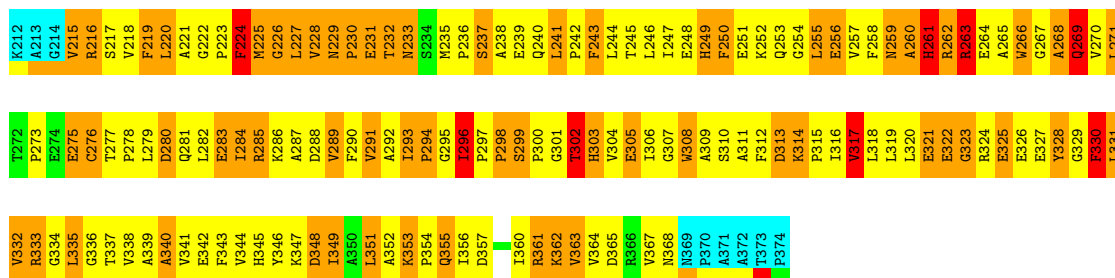
- Molecule 1: Blasticidin M

Chain A: 48% 36% 6% 6%



- Molecule 1: Blasticidin M

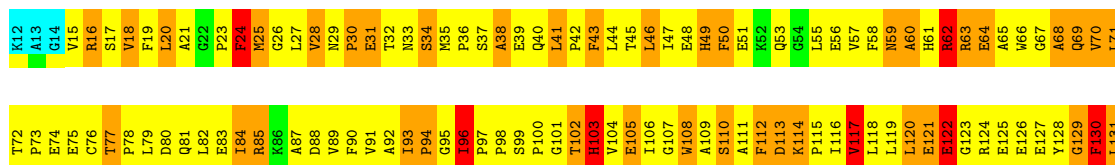
Chain B: 48% 37% 5% 6%



4.2.6 Score per residue for model 6

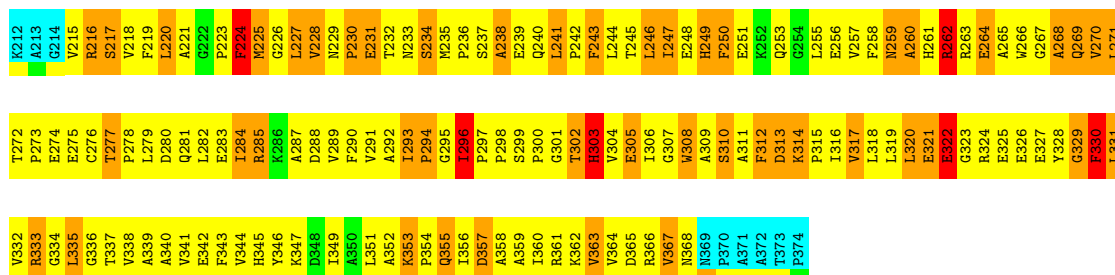
- Molecule 1: Blasticidin M

Chain A: 57% 29% 6%



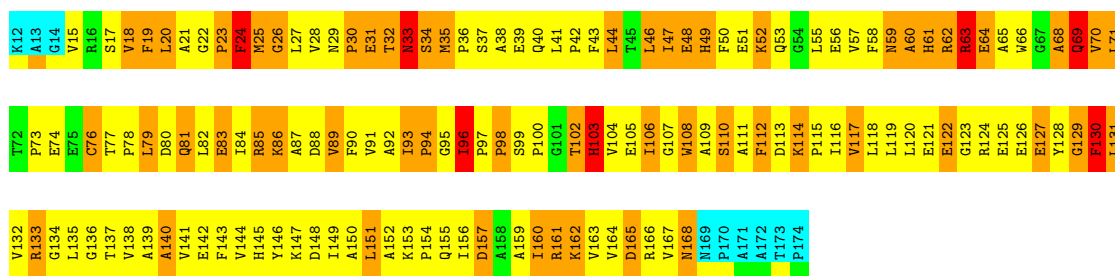


- Molecule 1: Blasticidin M

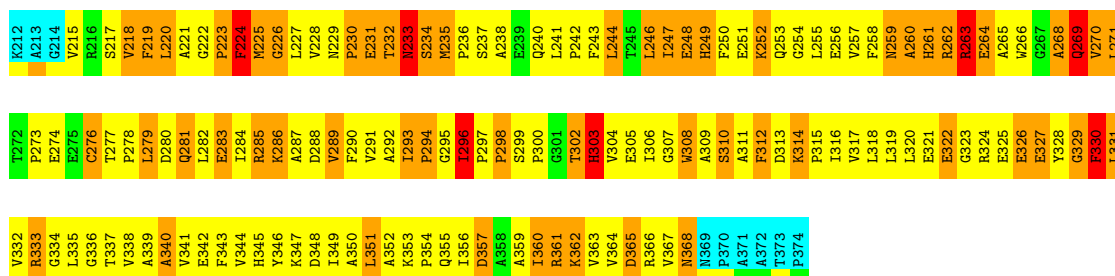


4.2.7 Score per residue for model 7

- Molecule 1: Blasticidin M



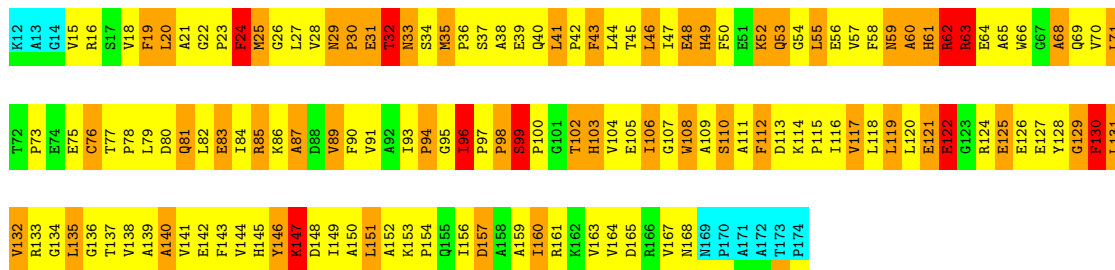
- Molecule 1: Blasticidin M



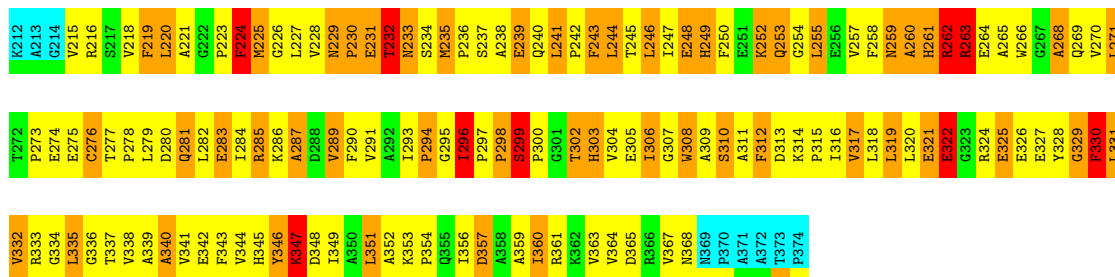
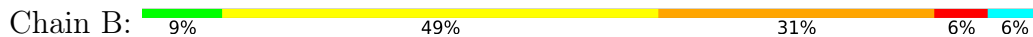
4.2.8 Score per residue for model 8

- Molecule 1: Blasticidin M



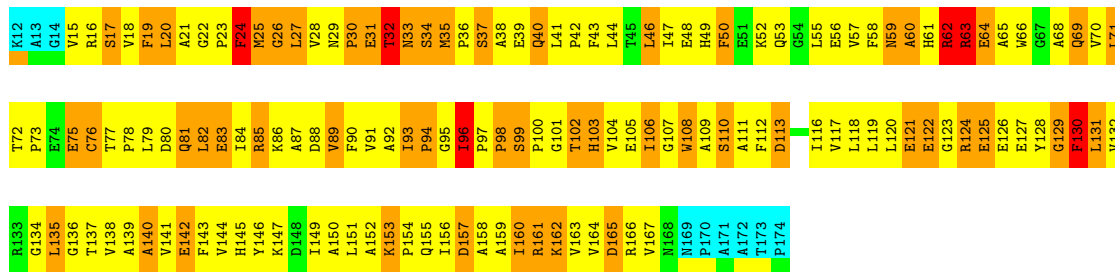
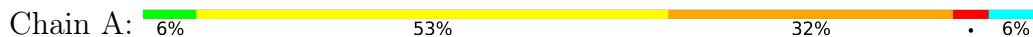


• Molecule 1: Blasticidin M

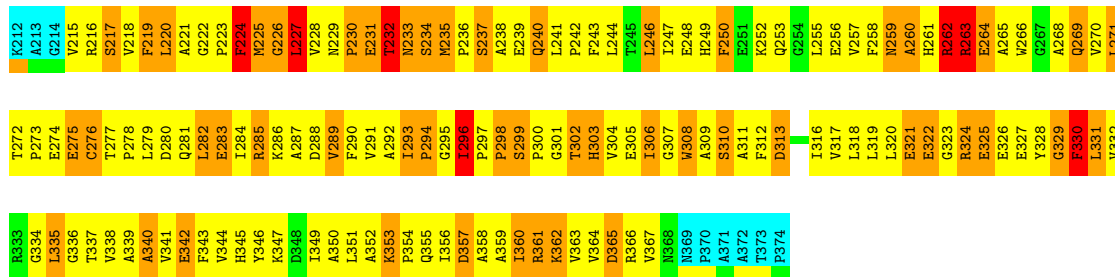


4.2.9 Score per residue for model 9

• Molecule 1: Blasticidin M



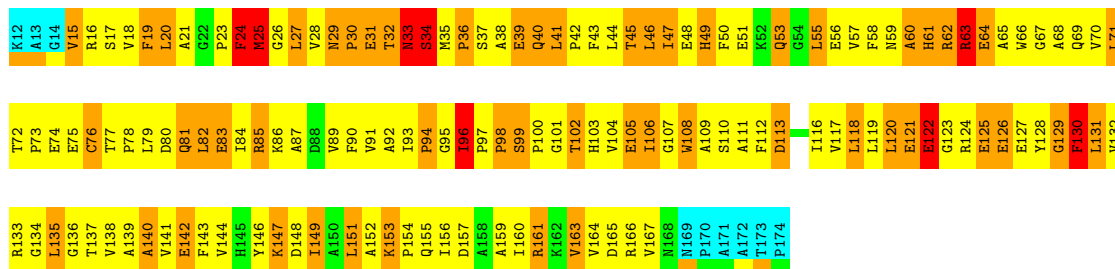
• Molecule 1: Blasticidin M



4.2.10 Score per residue for model 10

• Molecule 1: Blastocidin M

Chain A: 7% 51% 32% 5% 6%



• Molecule 1: Blastocidin M

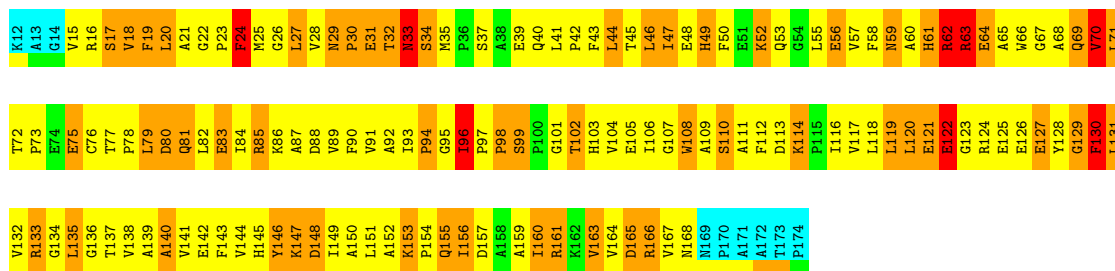
Chain B: 6% 51% 33% 6% 6%



4.2.11 Score per residue for model 11

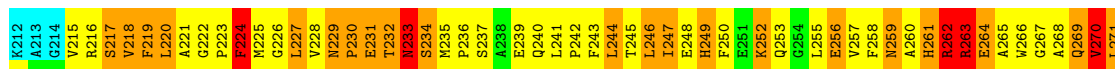
• Molecule 1: Blastocidin M

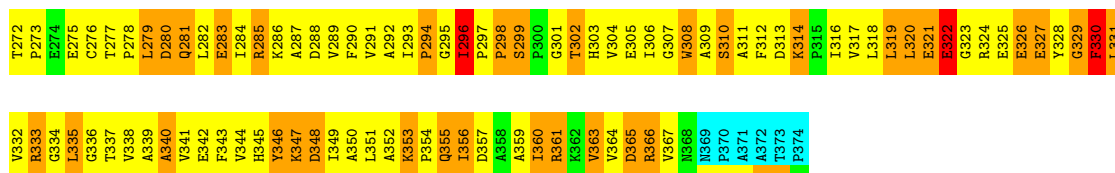
Chain A: 6% 51% 33% 5% 6%



• Molecule 1: Blastocidin M

Chain B: 6% 51% 33% 5% 6%

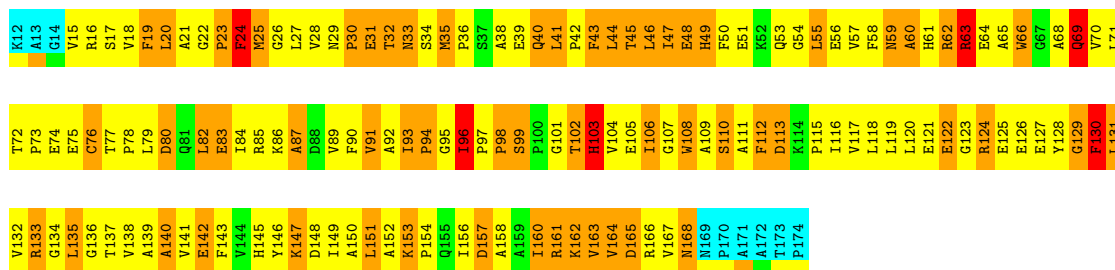




4.2.12 Score per residue for model 12

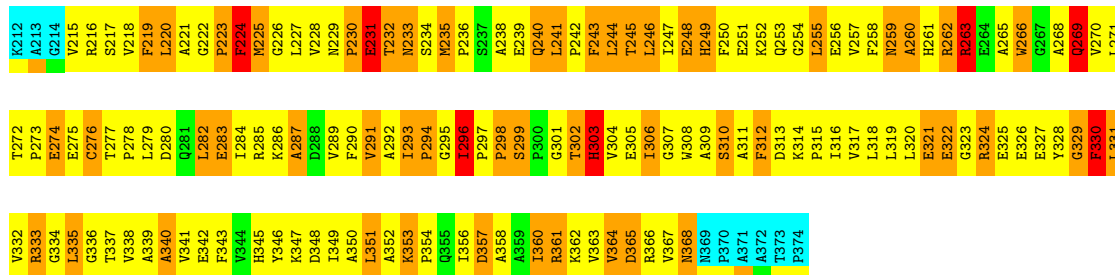
- Molecule 1: Blasticidin M

Chain A: 6% 49% 36% 6%



- Molecule 1: Blasticidin M

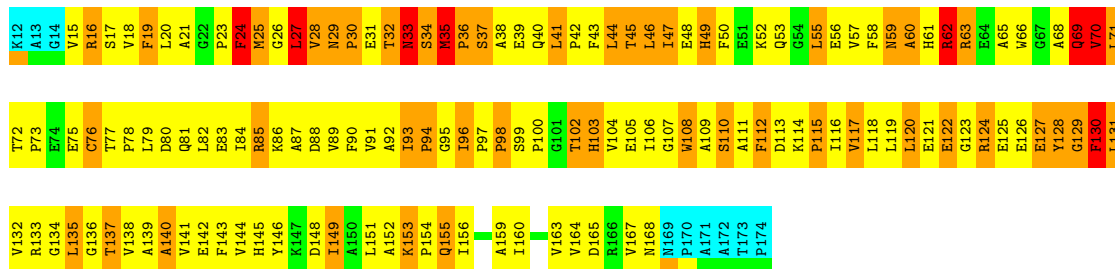
Chain B: 6% 53% 31% 6%



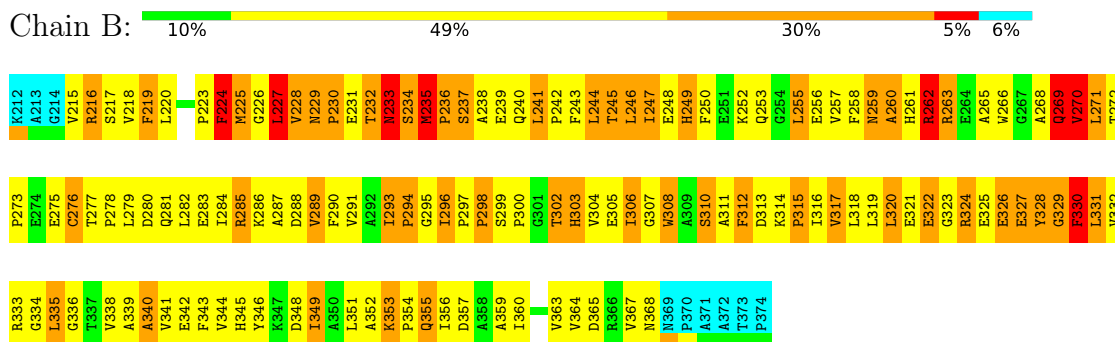
4.2.13 Score per residue for model 13

- Molecule 1: Blasticidin M

Chain A: 9% 52% 29% 6%

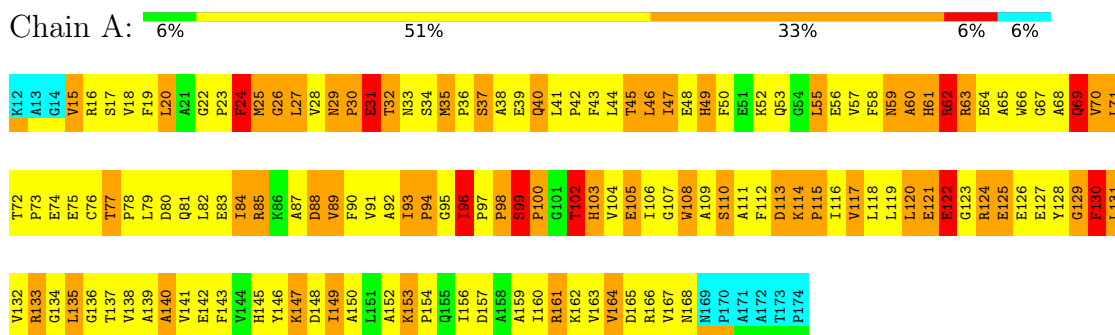


- Molecule 1: Blasticidin M

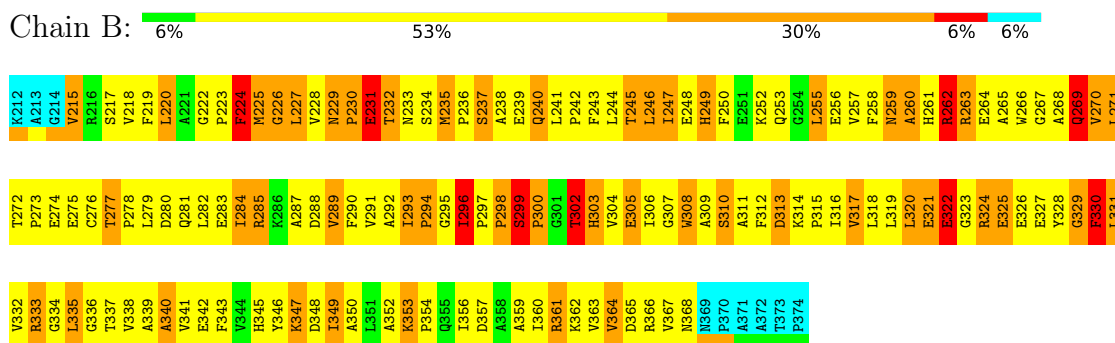


4.2.14 Score per residue for model 14

- Molecule 1: Blasticidin M

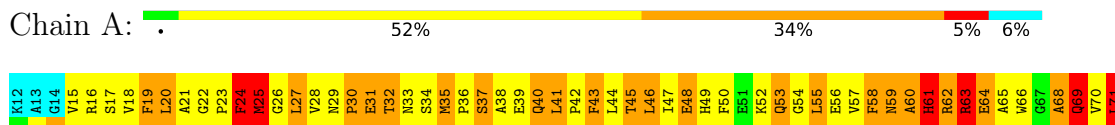


- Molecule 1: Blasticidin M



4.2.15 Score per residue for model 15

- Molecule 1: Blasticidin M



V172 P73 E74 E75 C76 T77 P78 L79 D80 V141 Q81 L82 E83 F143 V144 I84 R85 Y146 K86 A87 D88 V89 F90 V91 A92 P94 P94 Q155 G95 I156 P97 P98 A158 A159 S99 I160 P100 G101 R161 G102 T102 H103 V104 V105 E106 R166 V167 G107 V108 W168 A109 S110 A111 F112 D113 T173 K114 P115 I116 V117 L118 L119 L120 L120 E121 E122 G123 R124 E125 E126 E127 Y128 G129 F130 L131

V132 R133 G134 L135 V215 G136 T217 V138 A139 A140 V141 Q81 L82 E83 F143 V144 I84 R85 Y146 K86 A87 D88 V89 F90 V91 A92 P94 P94 Q155 G95 I156 P97 P98 A158 A159 S99 I160 P100 G101 R161 G102 T102 H103 V104 V105 E106 R166 V167 G107 V108 W168 A109 S110 A111 F112 D113 T173 K114 P115 I116 V117 L118 L119 L120 L120 E121 E122 G123 R124 E125 E126 E127 Y128 G129 F130 L131

• Molecule 1: Blasticidin M

Chain B: . 50% 36% 5% 6%

K212 A213 G214 R216 S217 V218 F219 L220 L220 A221 Q222 G222 P223 F224 A225 K226 G227 L227 V228 N229 P230 E231 E232 T232 N233 S234 P234 M235 P236 S237 A238 E239 Q300 Q301 L241 P242 F243 L244 T245 I246 G307 I247 E248 H249 F250 E251 K252 Q253 G254 L255 E256 F257 F258 N259 A260 H261 R262 R263 E264 A265 V266 G267 A268 Q269 V270 L271

T272 P273 E274 C276 T277 P278 L279 D280 Q281 L282 E283 I284 R285 K286 A287 D288 V289 F290 V291 A292 I293 P294 Q355 I296 P297 P298 S299 I360 R361 K362 V363 V364 D365 R366 V367 N368 A309 S310 A311 F312 D313 K314 P315 I316 V317 L318 L319 L320 L320 E321 E322 G323 R324 E325 E326 E327 Y328 F330 G329 L331

V332 R333 G334 L335 G336 T337 V338 A339 A340 V341 E342 F343 V344 H345 Y346 K347 D348 I349 A350 L351 A352 K353 P354 Q355 I356 D357 A358 A359 I360 R361 K362 V363 V364 D365 R366 V367 N368 A309 S310 A311 F312 D313 K314 P315 I316 V317 L318 L319 L320 L320 E321 E322 G323 R324 E325 E326 E327 Y328 F330 G329 L331

5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1686
Number of shifts mapped to atoms	1686
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	39%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1203	1207	1203	504±23
1	B	1203	1207	1203	503±25
All	All	36090	36210	36090	13898

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 193.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:240:GLN:HB2	1:B:266:TRP:CD2	1.19	1.71	13	2
1:A:70:VAL:O	1:A:71:LEU:O	1.18	1.61	11	12
1:B:270:VAL:O	1:B:271:LEU:O	1.17	1.59	11	12
1:B:224:PHE:O	1:B:227:LEU:HD23	1.16	1.40	14	13
1:B:264:GLU:O	1:B:269:GLN:N	1.16	1.77	14	10
1:A:40:GLN:HB2	1:A:66:TRP:CD2	1.16	1.74	13	2
1:A:64:GLU:O	1:A:69:GLN:N	1.14	1.81	14	12
1:A:24:PHE:O	1:A:27:LEU:HD23	1.14	1.42	12	13
1:B:300:PRO:O	1:B:304:VAL:HG23	1.13	1.43	1	9
1:A:103:HIS:CE1	1:A:128:TYR:HD2	1.12	1.62	3	6
1:B:240:GLN:HG2	1:B:241:LEU:HD13	1.11	1.20	12	1
1:B:360:ILE:O	1:B:364:VAL:HG23	1.10	1.46	9	6
1:A:134:GLY:C	1:B:277:THR:HG21	1.10	1.67	8	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:160:ILE:O	1:A:164:VAL:HG23	1.10	1.47	9	6
1:A:80:ASP:O	1:A:84:ILE:HG12	1.10	1.44	15	13
1:B:228:VAL:HG11	1:B:270:VAL:HB	1.10	1.18	11	2
1:B:331:LEU:O	1:B:335:LEU:HD22	1.10	1.47	10	1
1:A:77:THR:HG21	1:B:334:GLY:C	1.09	1.68	8	13
1:A:100:PRO:O	1:A:104:VAL:HG23	1.09	1.46	1	9
1:B:303:HIS:CE1	1:B:328:TYR:HD2	1.09	1.63	3	6
1:A:131:LEU:O	1:A:135:LEU:HD22	1.09	1.45	10	1
1:B:228:VAL:HG21	1:B:270:VAL:HG21	1.09	1.18	13	11
1:B:280:ASP:O	1:B:284:ILE:HG12	1.09	1.47	15	13
1:A:28:VAL:HG11	1:A:70:VAL:HB	1.09	1.17	11	2
1:A:40:GLN:HB2	1:A:66:TRP:CE2	1.09	1.82	12	2
1:A:28:VAL:HG23	1:A:33:ASN:HB2	1.08	1.25	13	3
1:A:44:LEU:HD23	1:A:44:LEU:N	1.07	1.63	12	4
1:A:95:GLY:N	1:A:128:TYR:OH	1.07	1.87	8	15
1:B:218:VAL:HG11	1:B:250:PHE:CE1	1.06	1.85	1	5
1:B:228:VAL:HG21	1:B:270:VAL:CG2	1.06	1.79	13	13
1:B:240:GLN:HB2	1:B:266:TRP:CE2	1.06	1.84	12	2
1:A:96:ILE:N	1:A:128:TYR:OH	1.06	1.88	8	15
1:A:40:GLN:HG2	1:A:41:LEU:HD13	1.06	1.19	12	1
1:A:130:PHE:CZ	1:B:270:VAL:HG22	1.06	1.85	7	2
1:A:28:VAL:HG11	1:A:70:VAL:HG22	1.05	1.29	1	11
1:B:232:THR:O	1:B:233:ASN:HB2	1.05	1.51	10	7
1:B:240:GLN:HA	1:B:240:GLN:OE1	1.05	1.51	14	1
1:A:28:VAL:HG23	1:A:33:ASN:CB	1.05	1.81	8	3
1:A:28:VAL:HG21	1:A:70:VAL:HG21	1.04	1.24	13	11
1:A:70:VAL:HG22	1:B:330:PHE:CZ	1.04	1.87	7	2
1:A:61:HIS:O	1:A:65:ALA:HB3	1.04	1.52	10	4
1:A:28:VAL:HG21	1:A:70:VAL:CG2	1.04	1.81	5	13
1:B:280:ASP:O	1:B:284:ILE:HG13	1.04	1.51	5	6
1:A:15:VAL:HG11	1:A:18:VAL:HG23	1.04	1.17	14	7
1:A:25:MET:O	1:A:28:VAL:O	1.04	1.76	6	14
1:B:218:VAL:HG21	1:B:250:PHE:CE2	1.04	1.88	7	3
1:B:228:VAL:HG23	1:B:233:ASN:CB	1.04	1.83	8	3
1:A:18:VAL:HG11	1:A:50:PHE:CE1	1.03	1.88	1	5
1:B:295:GLY:N	1:B:328:TYR:OH	1.03	1.90	8	15
1:A:111:ALA:HB3	1:B:311:ALA:HB3	1.03	1.10	6	5
1:B:261:HIS:O	1:B:265:ALA:HB3	1.03	1.53	10	4
1:A:18:VAL:HG21	1:A:50:PHE:CE2	1.03	1.88	15	3
1:A:55:LEU:N	1:A:55:LEU:HD23	1.02	1.69	4	6
1:B:215:VAL:HG11	1:B:218:VAL:HG23	1.02	1.17	14	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:228:VAL:HG11	1:B:270:VAL:HG22	1.02	1.26	1	11
1:B:218:VAL:HG11	1:B:250:PHE:CD2	1.02	1.89	6	2
1:B:218:VAL:HG11	1:B:250:PHE:CZ	1.02	1.88	2	12
1:B:225:MET:O	1:B:228:VAL:O	1.02	1.77	6	14
1:B:296:ILE:N	1:B:328:TYR:OH	1.02	1.91	8	15
1:A:146:TYR:O	1:A:147:LYS:HB2	1.02	1.54	15	3
1:B:303:HIS:CE1	1:B:328:TYR:CD2	1.01	2.48	3	6
1:B:228:VAL:HG23	1:B:233:ASN:HB2	1.01	1.32	13	3
1:B:346:TYR:O	1:B:347:LYS:HB2	1.01	1.55	15	3
1:A:40:GLN:HA	1:A:40:GLN:OE1	1.01	1.53	14	1
1:A:92:ALA:HB3	1:A:118:LEU:HD23	1.01	1.31	5	7
1:B:232:THR:O	1:B:270:VAL:HG21	1.01	1.54	1	4
1:B:292:ALA:HB3	1:B:318:LEU:HD23	1.01	1.32	5	6
1:B:334:GLY:O	1:B:338:VAL:HG22	1.01	1.56	11	15
1:B:284:ILE:HG21	1:B:308:TRP:HB3	1.01	1.31	8	7
1:A:80:ASP:O	1:A:84:ILE:HG13	1.00	1.56	5	6
1:A:134:GLY:O	1:A:138:VAL:HG22	1.00	1.57	11	15
1:B:244:LEU:HD22	1:B:266:TRP:CZ2	1.00	1.91	11	11
1:A:106:ILE:HG12	1:A:118:LEU:HD21	1.00	1.32	6	7
1:B:244:LEU:HD23	1:B:244:LEU:N	1.00	1.67	12	4
1:A:84:ILE:HG21	1:A:108:TRP:HB3	1.00	1.29	7	7
1:B:240:GLN:HG2	1:B:241:LEU:CD1	1.00	1.86	12	1
1:A:104:VAL:CG2	1:B:303:HIS:HB3	1.00	1.86	9	12
1:B:331:LEU:O	1:B:335:LEU:HD23	1.00	1.56	14	1
1:A:103:HIS:CE1	1:A:128:TYR:CD2	0.99	2.49	3	6
1:A:131:LEU:HD21	1:B:308:TRP:CH2	0.99	1.91	12	5
1:A:40:GLN:HA	1:A:66:TRP:CH2	0.99	1.92	12	2
1:B:284:ILE:HD13	1:B:290:PHE:CE1	0.99	1.92	6	6
1:B:228:VAL:HG11	1:B:270:VAL:CB	0.99	1.87	7	2
1:A:18:VAL:HG11	1:A:50:PHE:CE2	0.99	1.92	3	7
1:A:103:HIS:HB3	1:B:304:VAL:CG2	0.99	1.87	9	11
1:B:240:GLN:HA	1:B:266:TRP:CH2	0.99	1.92	12	2
1:B:255:LEU:N	1:B:255:LEU:HD23	0.99	1.70	4	6
1:A:24:PHE:CE2	1:A:70:VAL:HA	0.99	1.92	7	10
1:A:95:GLY:C	1:A:128:TYR:OH	0.99	2.01	8	15
1:B:292:ALA:HB3	1:B:318:LEU:CD2	0.99	1.88	7	9
1:A:28:VAL:HG11	1:A:70:VAL:CB	0.98	1.88	7	2
1:B:244:LEU:CD2	1:B:266:TRP:CZ2	0.98	2.47	9	11
1:A:24:PHE:HA	1:A:27:LEU:HD21	0.98	1.33	11	10
1:A:18:VAL:HG11	1:A:50:PHE:CD2	0.98	1.93	6	2
1:A:112:PHE:CE2	1:B:311:ALA:HB2	0.98	1.92	14	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:261:HIS:HB2	1:B:265:ALA:HB2	0.98	1.36	13	10
1:A:94:PRO:HB3	1:A:128:TYR:CE2	0.98	1.93	12	12
1:B:306:ILE:HG12	1:B:318:LEU:HD21	0.98	1.31	6	7
1:B:236:PRO:O	1:B:239:GLU:HG2	0.97	1.58	10	1
1:A:130:PHE:CD2	1:B:225:MET:HG2	0.97	1.93	11	1
1:B:246:LEU:HD11	1:B:250:PHE:CE1	0.97	1.93	1	2
1:A:92:ALA:HB3	1:A:118:LEU:CD2	0.97	1.88	4	9
1:A:84:ILE:HD13	1:A:90:PHE:CE1	0.97	1.94	6	6
1:A:23:PRO:O	1:A:24:PHE:O	0.97	1.83	9	14
1:A:32:THR:N	1:A:70:VAL:HG11	0.97	1.73	10	6
1:A:107:GLY:O	1:B:308:TRP:CD1	0.97	2.17	15	15
1:B:284:ILE:HD13	1:B:290:PHE:CE2	0.96	1.95	3	3
1:B:224:PHE:CE2	1:B:270:VAL:HA	0.96	1.95	7	10
1:B:295:GLY:C	1:B:328:TYR:OH	0.96	2.03	8	15
1:A:38:ALA:O	1:A:42:PRO:CG	0.96	2.12	13	10
1:B:223:PRO:O	1:B:224:PHE:O	0.96	1.81	7	14
1:A:32:THR:O	1:A:70:VAL:HG21	0.96	1.58	1	4
1:B:254:GLY:C	1:B:255:LEU:HD23	0.96	1.80	4	7
1:B:227:LEU:CD2	1:B:228:VAL:HG12	0.96	1.91	13	3
1:B:320:LEU:HD13	1:B:325:GLU:CB	0.96	1.90	4	14
1:A:44:LEU:HD22	1:A:66:TRP:CZ2	0.96	1.95	11	11
1:B:238:ALA:O	1:B:242:PRO:CG	0.96	2.13	13	10
1:B:351:LEU:HD23	1:B:352:ALA:N	0.96	1.75	7	2
1:A:111:ALA:HB2	1:B:312:PHE:CE2	0.96	1.94	14	5
1:A:40:GLN:CB	1:A:66:TRP:CD2	0.96	2.49	12	1
1:B:294:PRO:HB3	1:B:328:TYR:CE2	0.95	1.96	1	11
1:A:131:LEU:HD23	1:A:135:LEU:CD1	0.95	1.89	8	7
1:A:108:TRP:CH2	1:B:331:LEU:HD21	0.95	1.96	12	5
1:A:32:THR:O	1:A:33:ASN:HB2	0.95	1.53	10	7
1:A:41:LEU:HD13	1:A:41:LEU:H	0.95	1.17	13	2
1:B:280:ASP:O	1:B:284:ILE:CG1	0.95	2.14	6	13
1:B:317:VAL:HG22	1:B:342:GLU:HB2	0.95	1.37	13	7
1:B:218:VAL:HG11	1:B:250:PHE:CE2	0.95	1.97	3	7
1:A:151:LEU:HD23	1:A:152:ALA:N	0.95	1.75	7	1
1:B:276:CYS:O	1:B:280:ASP:HB2	0.95	1.61	15	9
1:B:363:VAL:O	1:B:367:VAL:HG23	0.95	1.61	3	11
1:A:46:LEU:HD11	1:A:50:PHE:CE1	0.95	1.96	1	2
1:A:54:GLY:C	1:A:55:LEU:HD23	0.95	1.81	4	6
1:B:352:ALA:O	1:B:356:ILE:HG22	0.95	1.61	9	5
1:B:264:GLU:OE1	1:B:268:ALA:HB3	0.95	1.60	8	1
1:A:152:ALA:O	1:A:156:ILE:HG22	0.95	1.60	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:241:LEU:HD13	1:B:241:LEU:H	0.95	1.19	13	2
1:A:61:HIS:HB2	1:A:65:ALA:HB2	0.94	1.33	13	9
1:B:225:MET:SD	1:B:230:PRO:HA	0.94	2.02	12	5
1:B:296:ILE:HD12	1:B:328:TYR:CE2	0.94	1.97	6	9
1:A:36:PRO:O	1:A:39:GLU:HG2	0.94	1.62	10	1
1:B:240:GLN:CB	1:B:266:TRP:CD2	0.94	2.49	12	2
1:A:28:VAL:CG2	1:A:70:VAL:HG21	0.94	1.92	5	10
1:A:96:ILE:HD12	1:A:128:TYR:CE2	0.94	1.96	6	8
1:B:331:LEU:HD23	1:B:335:LEU:CD1	0.94	1.93	8	7
1:B:328:TYR:O	1:B:330:PHE:N	0.94	2.00	2	13
1:A:27:LEU:CD2	1:A:28:VAL:HG12	0.94	1.92	13	3
1:A:40:GLN:HG2	1:A:41:LEU:CD1	0.94	1.91	12	1
1:A:103:HIS:CE1	1:A:128:TYR:HD1	0.94	1.81	14	9
1:B:224:PHE:HA	1:B:227:LEU:HD21	0.94	1.35	11	8
1:A:80:ASP:O	1:A:84:ILE:CG1	0.94	2.16	6	13
1:B:303:HIS:CE1	1:B:328:TYR:HD1	0.94	1.80	6	9
1:A:29:ASN:O	1:A:31:GLU:N	0.94	2.01	11	15
1:A:132:VAL:O	1:A:143:PHE:HZ	0.94	1.44	15	15
1:B:332:VAL:O	1:B:343:PHE:HZ	0.94	1.46	15	15
1:A:131:LEU:O	1:A:135:LEU:HD23	0.94	1.63	14	1
1:A:64:GLU:CD	1:A:71:LEU:HD11	0.94	1.84	15	1
1:A:70:VAL:O	1:A:70:VAL:CG1	0.93	2.16	11	7
1:A:128:TYR:O	1:A:130:PHE:N	0.93	2.01	2	13
1:A:25:MET:SD	1:A:30:PRO:HA	0.93	2.02	12	5
1:B:229:ASN:O	1:B:231:GLU:N	0.93	2.00	11	15
1:B:215:VAL:HG21	1:B:360:ILE:HG21	0.93	1.39	15	8
1:A:99:SER:CB	1:A:102:THR:HG1	0.93	1.75	10	1
1:B:228:VAL:CG2	1:B:270:VAL:HG21	0.93	1.94	12	9
1:B:284:ILE:HG22	1:B:312:PHE:CD1	0.93	1.98	5	4
1:B:319:LEU:HG	1:B:356:ILE:HD12	0.93	1.39	8	2
1:A:18:VAL:HG11	1:A:50:PHE:CZ	0.93	1.99	2	12
1:A:102:THR:C	1:A:106:ILE:HD12	0.93	1.83	2	3
1:B:270:VAL:O	1:B:270:VAL:CG1	0.93	2.17	7	6
1:B:303:HIS:CE1	1:B:328:TYR:CD1	0.92	2.57	6	9
1:A:130:PHE:O	1:B:273:PRO:HB3	0.92	1.62	12	13
1:B:294:PRO:HB3	1:B:328:TYR:CZ	0.92	1.98	6	15
1:B:220:LEU:O	1:B:259:ASN:OD1	0.92	1.88	7	6
1:A:117:VAL:HG22	1:A:142:GLU:HB2	0.92	1.40	13	9
1:A:50:PHE:CD2	1:A:55:LEU:HD12	0.92	1.99	1	7
1:A:94:PRO:C	1:A:128:TYR:OH	0.92	2.07	12	15
1:A:134:GLY:O	1:B:277:THR:HG21	0.92	1.64	6	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:278:PRO:O	1:B:282:LEU:HD23	0.92	1.63	1	7
1:A:120:LEU:HD13	1:A:125:GLU:CB	0.92	1.94	4	14
1:A:73:PRO:HB3	1:B:330:PHE:O	0.92	1.65	12	12
1:A:108:TRP:HE1	1:B:310:SER:CB	0.92	1.77	9	12
1:B:219:PHE:O	1:B:291:VAL:O	0.92	1.86	1	12
1:A:84:ILE:HD13	1:A:90:PHE:CE2	0.92	1.99	3	3
1:B:264:GLU:O	1:B:268:ALA:C	0.92	2.08	15	6
1:B:320:LEU:HD13	1:B:325:GLU:HB2	0.92	1.41	14	14
1:A:77:THR:HG21	1:B:334:GLY:O	0.92	1.64	6	7
1:B:321:GLU:O	1:B:323:GLY:N	0.92	2.03	5	9
1:A:110:SER:CB	1:B:308:TRP:HE1	0.91	1.78	9	12
1:B:299:SER:CB	1:B:302:THR:HG1	0.91	1.77	10	1
1:A:15:VAL:HG11	1:A:18:VAL:CG2	0.91	1.95	14	9
1:A:59:ASN:O	1:A:60:ALA:O	0.91	1.88	1	10
1:A:70:VAL:O	1:A:70:VAL:HG13	0.91	1.64	11	2
1:B:270:VAL:O	1:B:270:VAL:HG13	0.91	1.65	11	2
1:A:19:PHE:O	1:A:91:VAL:O	0.91	1.87	1	12
1:A:44:LEU:CD2	1:A:66:TRP:CZ2	0.91	2.54	9	12
1:B:264:GLU:CD	1:B:271:LEU:HD11	0.91	1.85	15	1
1:A:103:HIS:CE1	1:A:128:TYR:CD1	0.91	2.59	6	9
1:B:224:PHE:O	1:B:226:GLY:N	0.91	2.04	9	12
1:B:232:THR:N	1:B:270:VAL:HG11	0.91	1.81	10	6
1:A:104:VAL:HA	1:B:304:VAL:HA	0.91	1.41	10	8
1:A:130:PHE:CE2	1:B:270:VAL:HG22	0.91	2.00	11	2
1:A:104:VAL:HG21	1:B:303:HIS:HB3	0.91	1.38	10	2
1:B:229:ASN:HB2	1:B:232:THR:OG1	0.91	1.66	2	2
1:A:25:MET:HB2	1:B:330:PHE:CD2	0.91	2.01	6	6
1:A:20:LEU:HD13	1:A:47:ILE:CD1	0.91	1.95	11	4
1:A:24:PHE:O	1:A:26:GLY:N	0.91	2.04	15	12
1:A:103:HIS:HB3	1:B:304:VAL:HG22	0.91	1.39	2	6
1:A:119:LEU:HG	1:A:156:ILE:HD12	0.91	1.39	8	2
1:A:94:PRO:HB3	1:A:128:TYR:CZ	0.91	2.00	6	15
1:A:84:ILE:HG22	1:A:112:PHE:CD1	0.91	2.01	5	4
1:A:108:TRP:HE1	1:B:310:SER:HB2	0.90	1.26	14	5
1:A:76:CYS:O	1:A:80:ASP:HB2	0.90	1.66	15	9
1:B:227:LEU:HD11	1:B:235:MET:SD	0.90	2.06	12	5
1:A:15:VAL:CG1	1:A:18:VAL:HG23	0.90	1.96	14	10
1:B:215:VAL:CG1	1:B:218:VAL:HG23	0.90	1.96	14	9
1:B:294:PRO:CB	1:B:328:TYR:CE2	0.90	2.55	11	9
1:A:28:VAL:HG22	1:A:29:ASN:H	0.90	1.25	1	4
1:B:228:VAL:HG22	1:B:229:ASN:H	0.90	1.26	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:VAL:HG11	1:B:331:LEU:CD1	0.90	1.96	6	3
1:A:79:LEU:HD23	1:A:80:ASP:N	0.90	1.82	4	1
1:B:215:VAL:HG11	1:B:218:VAL:CG2	0.90	1.97	14	11
1:B:224:PHE:O	1:B:227:LEU:CD2	0.90	2.20	7	12
1:A:64:GLU:O	1:A:68:ALA:C	0.90	2.11	15	4
1:A:24:PHE:O	1:A:27:LEU:CD2	0.89	2.19	7	11
1:A:66:TRP:CD1	1:A:66:TRP:N	0.89	2.38	12	15
1:A:102:THR:O	1:A:105:GLU:N	0.89	2.04	11	15
1:B:294:PRO:C	1:B:328:TYR:OH	0.89	2.11	12	15
1:A:108:TRP:CD1	1:B:307:GLY:O	0.89	2.25	12	14
1:B:219:PHE:HB2	1:B:287:ALA:CB	0.89	1.97	6	13
1:A:120:LEU:HD13	1:A:125:GLU:HB2	0.89	1.41	14	14
1:A:41:LEU:HD13	1:A:41:LEU:N	0.89	1.78	13	3
1:A:19:PHE:HB2	1:A:87:ALA:CB	0.89	1.97	6	14
1:A:78:PRO:O	1:A:82:LEU:HD23	0.89	1.66	1	8
1:B:218:VAL:O	1:B:257:VAL:HA	0.89	1.68	15	13
1:B:219:PHE:CD1	1:B:259:ASN:HB2	0.89	2.02	1	5
1:A:118:LEU:N	1:A:118:LEU:HD12	0.89	1.82	9	2
1:B:335:LEU:HB3	1:B:341:VAL:HG21	0.89	1.45	13	15
1:A:15:VAL:HG21	1:A:160:ILE:HG21	0.89	1.45	15	9
1:B:241:LEU:HD13	1:B:241:LEU:N	0.89	1.81	13	3
1:B:302:THR:C	1:B:306:ILE:HD12	0.89	1.88	2	3
1:A:41:LEU:N	1:A:41:LEU:CD1	0.89	2.36	13	4
1:A:73:PRO:HG3	1:B:329:GLY:C	0.88	1.88	1	5
1:B:302:THR:O	1:B:305:GLU:N	0.88	2.06	11	15
1:A:27:LEU:HD11	1:A:35:MET:SD	0.88	2.08	12	5
1:A:64:GLU:OE1	1:A:68:ALA:HB3	0.88	1.68	8	1
1:B:303:HIS:HE1	1:B:328:TYR:HD1	0.88	1.06	14	2
1:A:46:LEU:C	1:A:46:LEU:HD13	0.88	1.88	1	2
1:A:18:VAL:O	1:A:57:VAL:HA	0.88	1.68	11	13
1:A:112:PHE:CE1	1:B:311:ALA:HB2	0.88	2.03	1	2
1:B:296:ILE:HB	1:B:324:ARG:HB3	0.88	1.45	7	12
1:A:25:MET:HG2	1:B:330:PHE:CD2	0.88	2.03	11	1
1:B:259:ASN:O	1:B:260:ALA:O	0.88	1.90	1	9
1:B:293:ILE:HG12	1:B:319:LEU:HB2	0.88	1.44	3	9
1:A:131:LEU:CD1	1:B:304:VAL:HG11	0.88	1.97	6	3
1:A:70:VAL:O	1:B:330:PHE:CE1	0.88	2.26	11	1
1:A:94:PRO:CB	1:A:128:TYR:CE2	0.88	2.57	11	9
1:A:61:HIS:O	1:A:65:ALA:CB	0.88	2.21	10	4
1:B:266:TRP:N	1:B:266:TRP:CD1	0.88	2.41	12	12
1:A:163:VAL:O	1:A:167:VAL:HG23	0.88	1.69	3	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:237:SER:O	1:B:241:LEU:HD22	0.88	1.68	4	4
1:A:31:GLU:O	1:A:32:THR:OG1	0.88	1.90	5	6
1:B:231:GLU:O	1:B:232:THR:OG1	0.88	1.92	5	6
1:A:19:PHE:CD1	1:A:59:ASN:HB2	0.88	2.04	1	5
1:A:96:ILE:HD12	1:A:128:TYR:CZ	0.88	2.04	6	13
1:A:28:VAL:HG13	1:A:32:THR:HG22	0.88	1.44	4	1
1:B:241:LEU:N	1:B:241:LEU:CD1	0.88	2.36	13	4
1:B:318:LEU:N	1:B:318:LEU:HD12	0.88	1.83	9	2
1:B:234:SER:CA	1:B:268:ALA:HB1	0.88	1.98	11	1
1:B:250:PHE:CD2	1:B:255:LEU:HD12	0.88	2.04	13	7
1:B:261:HIS:O	1:B:265:ALA:CB	0.87	2.21	10	4
1:B:296:ILE:HA	1:B:297:PRO:C	0.87	1.89	10	15
1:B:298:PRO:HA	1:B:328:TYR:CE1	0.87	2.04	8	7
1:A:96:ILE:HD13	1:A:124:ARG:O	0.87	1.66	9	10
1:A:121:GLU:O	1:A:123:GLY:N	0.87	2.07	5	8
1:B:237:SER:O	1:B:241:LEU:HD13	0.87	1.70	14	10
1:A:37:SER:O	1:A:41:LEU:HD22	0.87	1.68	4	5
1:B:312:PHE:O	1:B:313:ASP:HB3	0.87	1.68	14	6
1:A:135:LEU:HB3	1:A:141:VAL:HG21	0.87	1.46	13	15
1:B:303:HIS:NE2	1:B:328:TYR:CD2	0.87	2.42	2	3
1:A:29:ASN:HB2	1:A:32:THR:OG1	0.87	1.68	2	2
1:B:250:PHE:CD1	1:B:255:LEU:HD12	0.87	2.05	6	8
1:B:265:ALA:HB3	1:B:266:TRP:CD1	0.87	2.04	12	2
1:A:111:ALA:HB2	1:B:312:PHE:CE1	0.87	2.04	1	2
1:A:50:PHE:CD1	1:A:55:LEU:HD12	0.87	2.04	6	8
1:B:228:VAL:HG11	1:B:270:VAL:CG2	0.87	2.00	6	11
1:A:19:PHE:HB2	1:A:87:ALA:HB2	0.87	1.47	8	11
1:B:289:VAL:HG12	1:B:289:VAL:O	0.87	1.70	15	8
1:A:125:GLU:C	1:A:125:GLU:OE2	0.87	2.13	5	3
1:A:20:LEU:O	1:A:59:ASN:OD1	0.87	1.91	7	7
1:A:89:VAL:HG12	1:A:89:VAL:O	0.87	1.68	15	8
1:A:65:ALA:HB3	1:A:66:TRP:CD1	0.87	2.04	12	2
1:B:228:VAL:HG13	1:B:232:THR:HG22	0.86	1.47	4	1
1:B:245:THR:HG23	1:B:249:HIS:CE1	0.86	2.05	5	1
1:A:65:ALA:C	1:A:66:TRP:HD1	0.86	1.73	14	13
1:A:49:HIS:O	1:A:53:GLN:CG	0.86	2.23	11	4
1:B:294:PRO:CB	1:B:328:TYR:CZ	0.86	2.58	15	15
1:B:332:VAL:O	1:B:343:PHE:CZ	0.86	2.29	9	15
1:A:98:PRO:HA	1:A:128:TYR:CE1	0.86	2.05	8	7
1:A:94:PRO:CB	1:A:128:TYR:CZ	0.86	2.58	15	15
1:A:130:PHE:CD2	1:B:225:MET:HB2	0.86	2.06	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:THR:HG22	1:A:33:ASN:H	0.86	1.31	5	3
1:A:103:HIS:HE1	1:A:128:TYR:HD1	0.86	1.04	14	2
1:A:62:ARG:HA	1:A:66:TRP:CE2	0.85	2.06	9	8
1:B:321:GLU:OE2	1:B:324:ARG:HG3	0.85	1.70	4	1
1:A:46:LEU:HA	1:A:49:HIS:CD2	0.85	2.06	5	1
1:B:246:LEU:HA	1:B:249:HIS:CD2	0.85	2.06	5	1
1:A:96:ILE:HA	1:A:97:PRO:C	0.85	1.89	10	15
1:A:92:ALA:HB3	1:A:118:LEU:HD22	0.85	1.48	4	4
1:A:103:HIS:HB3	1:B:304:VAL:HG21	0.85	1.47	10	4
1:B:278:PRO:O	1:B:282:LEU:HG	0.85	1.72	9	3
1:B:235:MET:HG2	1:B:266:TRP:CE3	0.85	2.06	12	2
1:A:136:GLY:HA2	1:A:141:VAL:HB	0.85	1.47	4	15
1:A:131:LEU:O	1:A:135:LEU:CD2	0.85	2.25	10	2
1:A:35:MET:HG2	1:A:66:TRP:CE3	0.85	2.06	12	2
1:A:34:SER:CA	1:A:68:ALA:HB1	0.85	2.01	11	1
1:A:24:PHE:CA	1:A:27:LEU:CD2	0.85	2.54	12	15
1:A:32:THR:O	1:A:70:VAL:HB	0.85	1.72	2	4
1:B:240:GLN:HB2	1:B:266:TRP:CE3	0.85	2.06	13	1
1:B:246:LEU:C	1:B:246:LEU:HD13	0.85	1.91	1	2
1:B:265:ALA:C	1:B:266:TRP:HD1	0.85	1.75	14	13
1:A:78:PRO:O	1:A:82:LEU:HD13	0.85	1.71	13	2
1:B:219:PHE:CE1	1:B:290:PHE:CE1	0.85	2.65	9	5
1:A:103:HIS:NE2	1:A:128:TYR:CD2	0.85	2.45	2	2
1:B:296:ILE:HD12	1:B:328:TYR:CE1	0.85	2.07	3	5
1:A:32:THR:O	1:A:70:VAL:CB	0.85	2.24	14	5
1:A:96:ILE:HB	1:A:124:ARG:HB3	0.85	1.49	7	11
1:B:279:LEU:HD23	1:B:280:ASP:N	0.85	1.85	4	1
1:B:235:MET:CB	1:B:269:GLN:OE1	0.85	2.24	8	1
1:B:232:THR:O	1:B:270:VAL:HB	0.84	1.72	2	4
1:A:78:PRO:O	1:A:82:LEU:HG	0.84	1.72	9	3
1:B:232:THR:O	1:B:270:VAL:CB	0.84	2.25	14	5
1:A:112:PHE:O	1:A:113:ASP:HB2	0.84	1.73	15	8
1:B:296:ILE:HD12	1:B:328:TYR:CZ	0.84	2.08	6	13
1:B:353:LYS:O	1:B:356:ILE:HG22	0.84	1.72	12	12
1:A:119:LEU:HD22	1:A:146:TYR:CE1	0.84	2.07	8	2
1:B:336:GLY:HA2	1:B:341:VAL:HB	0.84	1.46	4	15
1:A:111:ALA:O	1:B:312:PHE:CD1	0.84	2.29	7	5
1:B:233:ASN:ND2	1:B:268:ALA:O	0.84	2.10	4	1
1:A:35:MET:CB	1:A:69:GLN:OE1	0.84	2.25	8	1
1:A:19:PHE:CE1	1:A:90:PHE:CE1	0.84	2.66	9	5
1:A:120:LEU:HD22	1:A:125:GLU:HB2	0.84	1.49	12	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:VAL:O	1:A:143:PHE:CZ	0.84	2.31	8	15
1:A:104:VAL:HG22	1:B:304:VAL:N	0.84	1.88	10	5
1:B:228:VAL:CG1	1:B:270:VAL:HB	0.84	2.02	11	2
1:B:224:PHE:HA	1:B:227:LEU:CD2	0.84	2.01	13	11
1:B:220:LEU:HD13	1:B:247:ILE:CD1	0.84	2.01	11	4
1:A:40:GLN:HB2	1:A:66:TRP:CE3	0.84	2.07	13	1
1:A:104:VAL:CG2	1:B:303:HIS:CB	0.84	2.56	9	2
1:B:320:LEU:HD13	1:B:325:GLU:CG	0.84	2.02	9	14
1:B:249:HIS:CE1	1:B:250:PHE:CD1	0.84	2.66	6	2
1:B:224:PHE:CA	1:B:227:LEU:CD2	0.83	2.56	12	14
1:A:112:PHE:CD1	1:B:311:ALA:O	0.83	2.31	12	5
1:B:278:PRO:O	1:B:282:LEU:HD13	0.83	1.73	13	2
1:B:291:VAL:HA	1:B:317:VAL:O	0.83	1.72	2	15
1:A:131:LEU:HD22	1:B:304:VAL:HG11	0.83	1.48	1	12
1:B:220:LEU:O	1:B:259:ASN:HB3	0.83	1.73	13	3
1:A:28:VAL:CG2	1:A:33:ASN:HB2	0.83	2.03	13	2
1:A:19:PHE:C	1:A:19:PHE:CD2	0.83	2.52	4	7
1:A:40:GLN:NE2	1:A:44:LEU:HD11	0.83	1.89	1	1
1:B:279:LEU:O	1:B:283:GLU:OE1	0.83	1.96	4	4
1:B:249:HIS:O	1:B:253:GLN:CG	0.83	2.27	11	3
1:A:116:ILE:O	1:A:163:VAL:HG21	0.83	1.72	11	4
1:A:116:ILE:HG23	1:A:118:LEU:HD11	0.83	1.50	9	2
1:A:24:PHE:HA	1:A:27:LEU:CD2	0.83	2.03	12	13
1:A:96:ILE:HD12	1:A:128:TYR:CE1	0.83	2.08	4	5
1:A:24:PHE:CA	1:A:27:LEU:HD22	0.83	2.02	3	8
1:A:129:GLY:C	1:B:273:PRO:HG3	0.83	1.93	1	7
1:A:112:PHE:O	1:A:113:ASP:HB3	0.83	1.72	14	4
1:A:28:VAL:HG21	1:A:69:GLN:O	0.83	1.72	11	1
1:B:227:LEU:HD11	1:B:235:MET:HG3	0.83	1.49	1	4
1:B:218:VAL:HG21	1:B:250:PHE:CE1	0.83	2.09	2	5
1:A:24:PHE:CE1	1:A:61:HIS:CE1	0.83	2.67	6	6
1:B:258:PHE:O	1:B:259:ASN:HB3	0.83	1.73	7	10
1:B:309:ALA:HB3	1:B:316:ILE:HD11	0.83	1.50	11	10
1:A:23:PRO:O	1:A:26:GLY:N	0.83	2.11	11	8
1:B:223:PRO:O	1:B:226:GLY:N	0.83	2.11	11	8
1:A:85:ARG:HD2	1:A:112:PHE:CE1	0.83	2.09	8	9
1:A:112:PHE:CD2	1:B:311:ALA:HB2	0.83	2.08	11	5
1:B:299:SER:HB2	1:B:302:THR:OG1	0.83	1.72	9	8
1:A:69:GLN:NE2	1:A:70:VAL:HG23	0.83	1.88	14	1
1:A:93:ILE:HG22	1:A:93:ILE:O	0.82	1.74	9	8
1:A:28:VAL:CG1	1:A:70:VAL:HB	0.82	2.02	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:O	1:A:59:ASN:HB3	0.82	1.75	13	3
1:B:219:PHE:HB2	1:B:287:ALA:HB2	0.82	1.50	8	10
1:A:60:ALA:O	1:A:61:HIS:ND1	0.82	2.12	4	5
1:B:260:ALA:O	1:B:261:HIS:ND1	0.82	2.12	4	5
1:B:283:GLU:OE1	1:B:283:GLU:N	0.82	2.12	4	1
1:A:58:PHE:O	1:A:59:ASN:HB3	0.82	1.73	7	10
1:A:93:ILE:HG12	1:A:119:LEU:HB2	0.82	1.50	3	9
1:B:243:PHE:O	1:B:247:ILE:HD13	0.82	1.73	5	9
1:B:230:PRO:O	1:B:231:GLU:HB2	0.82	1.71	14	9
1:A:116:ILE:HG21	1:A:141:VAL:HG22	0.82	1.51	9	4
1:B:240:GLN:HA	1:B:266:TRP:CZ2	0.82	2.08	13	2
1:A:104:VAL:HG11	1:B:331:LEU:HD22	0.82	1.51	1	12
1:B:228:VAL:HG11	1:B:270:VAL:CG1	0.82	2.03	7	3
1:A:55:LEU:N	1:A:55:LEU:CD2	0.82	2.40	4	3
1:B:277:THR:HB	1:B:278:PRO:CD	0.82	2.05	14	9
1:B:221:ALA:HB2	1:B:259:ASN:ND2	0.82	1.88	3	1
1:B:292:ALA:HB3	1:B:318:LEU:HD22	0.82	1.51	4	4
1:B:232:THR:HG22	1:B:233:ASN:H	0.82	1.32	5	3
1:B:297:PRO:O	1:B:299:SER:N	0.82	2.13	12	15
1:B:296:ILE:HD13	1:B:324:ARG:O	0.82	1.74	9	10
1:B:331:LEU:O	1:B:335:LEU:CD2	0.82	2.27	10	2
1:A:111:ALA:HB2	1:B:312:PHE:CD1	0.82	2.09	1	2
1:A:94:PRO:HB3	1:A:128:TYR:CE1	0.82	2.08	9	10
1:B:270:VAL:HG12	1:B:270:VAL:O	0.82	1.73	1	4
1:A:61:HIS:O	1:A:64:GLU:N	0.82	2.12	4	5
1:A:79:LEU:O	1:A:83:GLU:OE1	0.82	1.96	4	4
1:B:233:ASN:CG	1:B:268:ALA:O	0.82	2.17	4	1
1:A:130:PHE:CE1	1:B:270:VAL:O	0.82	2.33	11	1
1:B:262:ARG:HA	1:B:266:TRP:CE2	0.82	2.09	14	9
1:A:121:GLU:OE2	1:A:124:ARG:HG3	0.82	1.74	4	1
1:B:231:GLU:O	1:B:232:THR:HB	0.82	1.74	9	3
1:A:27:LEU:HD11	1:A:35:MET:HG3	0.82	1.49	1	4
1:A:28:VAL:HG11	1:A:70:VAL:CG2	0.82	2.05	6	12
1:B:247:ILE:HG13	1:B:257:VAL:HG11	0.82	1.52	5	5
1:A:104:VAL:N	1:B:304:VAL:HG22	0.82	1.89	10	6
1:A:111:ALA:HB2	1:B:312:PHE:CD2	0.82	2.09	10	5
1:B:219:PHE:CE2	1:B:290:PHE:CE2	0.82	2.68	7	1
1:A:19:PHE:CZ	1:A:90:PHE:CE1	0.81	2.68	4	5
1:A:21:ALA:HB2	1:A:59:ASN:ND2	0.81	1.90	3	1
1:B:219:PHE:CZ	1:B:290:PHE:CE1	0.81	2.68	4	5
1:A:106:ILE:CG1	1:A:118:LEU:HD21	0.81	2.05	12	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ARG:HD2	1:A:66:TRP:CH2	0.81	2.09	6	1
1:B:364:VAL:O	1:B:368:ASN:HB3	0.81	1.75	8	1
1:B:219:PHE:C	1:B:219:PHE:CD2	0.81	2.54	4	7
1:A:25:MET:O	1:A:28:VAL:HG12	0.81	1.75	5	2
1:A:131:LEU:HD22	1:B:304:VAL:CG1	0.81	2.05	1	4
1:B:219:PHE:CZ	1:B:290:PHE:CZ	0.81	2.68	4	4
1:B:229:ASN:CB	1:B:232:THR:OG1	0.81	2.29	12	4
1:A:103:HIS:CB	1:B:304:VAL:CG2	0.81	2.59	9	2
1:B:227:LEU:HD12	1:B:235:MET:HA	0.81	1.53	11	1
1:A:104:VAL:CG1	1:B:331:LEU:HD22	0.81	2.05	1	4
1:A:37:SER:O	1:A:40:GLN:HG3	0.81	1.74	15	2
1:B:215:VAL:HG21	1:B:360:ILE:CG2	0.81	2.05	15	9
1:A:24:PHE:N	1:A:27:LEU:HD22	0.81	1.90	3	9
1:A:139:ALA:O	1:A:141:VAL:HG23	0.81	1.74	11	6
1:A:153:LYS:O	1:A:156:ILE:HG22	0.81	1.75	13	13
1:A:164:VAL:O	1:A:168:ASN:HB3	0.81	1.73	8	1
1:A:104:VAL:HG22	1:B:303:HIS:HB3	0.81	1.51	4	4
1:B:320:LEU:HD22	1:B:325:GLU:HB2	0.81	1.52	12	8
1:B:316:ILE:O	1:B:363:VAL:HG21	0.81	1.76	11	4
1:A:83:GLU:OE1	1:A:83:GLU:N	0.81	2.14	4	1
1:A:20:LEU:HD13	1:A:47:ILE:HD11	0.81	1.52	11	5
1:B:342:GLU:OE2	1:B:359:ALA:HB1	0.81	1.75	13	2
1:A:37:SER:O	1:A:41:LEU:HD13	0.81	1.76	14	9
1:B:312:PHE:O	1:B:313:ASP:HB2	0.81	1.72	15	7
1:A:50:PHE:HD2	1:A:55:LEU:HD12	0.81	1.34	1	6
1:B:224:PHE:CA	1:B:227:LEU:HD22	0.81	2.06	3	8
1:A:108:TRP:NE1	1:B:307:GLY:O	0.80	2.13	13	12
1:A:84:ILE:HD11	1:A:105:GLU:HG3	0.80	1.53	6	2
1:A:18:VAL:HG13	1:A:91:VAL:CG1	0.80	2.06	12	1
1:A:32:THR:O	1:A:70:VAL:CG2	0.80	2.28	15	4
1:A:91:VAL:HA	1:A:117:VAL:O	0.80	1.74	2	15
1:A:47:ILE:HG13	1:A:57:VAL:HG11	0.80	1.53	5	6
1:B:319:LEU:HD21	1:B:352:ALA:HB1	0.80	1.53	11	3
1:A:45:THR:HG23	1:A:49:HIS:CE1	0.80	2.10	5	1
1:B:250:PHE:O	1:B:255:LEU:N	0.80	2.15	5	10
1:A:27:LEU:HD12	1:A:35:MET:HA	0.80	1.53	11	1
1:A:75:GLU:OE1	1:A:79:LEU:HD11	0.80	1.76	13	1
1:A:19:PHE:CZ	1:A:90:PHE:CZ	0.80	2.69	4	4
1:A:49:HIS:CE1	1:A:50:PHE:CD1	0.80	2.69	6	2
1:B:261:HIS:O	1:B:264:GLU:N	0.80	2.14	4	5
1:A:33:ASN:ND2	1:A:68:ALA:O	0.80	2.14	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:245:THR:CG2	1:B:249:HIS:CE1	0.80	2.64	5	1
1:A:70:VAL:HG22	1:B:330:PHE:CE2	0.80	2.12	11	2
1:A:39:GLU:C	1:A:42:PRO:HD2	0.80	1.97	13	11
1:A:44:LEU:O	1:A:48:GLU:HB2	0.80	1.77	6	8
1:B:306:ILE:CG1	1:B:318:LEU:HD21	0.80	2.06	12	6
1:A:85:ARG:HD2	1:A:112:PHE:CE2	0.80	2.12	2	3
1:A:85:ARG:HB3	1:A:112:PHE:CE1	0.80	2.12	13	8
1:A:33:ASN:CG	1:A:68:ALA:O	0.80	2.19	4	1
1:A:97:PRO:O	1:A:99:SER:N	0.80	2.15	12	15
1:B:239:GLU:C	1:B:242:PRO:HD2	0.80	1.97	13	10
1:A:18:VAL:HG21	1:A:50:PHE:CE1	0.80	2.12	12	6
1:A:62:ARG:O	1:A:64:GLU:N	0.80	2.15	14	9
1:A:131:LEU:HD23	1:A:135:LEU:HD12	0.80	1.53	4	6
1:A:43:PHE:O	1:A:47:ILE:HD13	0.80	1.77	1	10
1:A:70:VAL:HG12	1:A:70:VAL:O	0.80	1.77	8	5
1:A:112:PHE:CD1	1:B:311:ALA:HB2	0.80	2.12	1	2
1:A:120:LEU:HD13	1:A:125:GLU:CG	0.80	2.06	9	14
1:B:243:PHE:O	1:B:247:ILE:CG1	0.80	2.30	14	2
1:A:84:ILE:HD11	1:A:105:GLU:CG	0.80	2.07	6	2
1:A:40:GLN:HA	1:A:66:TRP:CZ2	0.80	2.12	13	2
1:A:77:THR:OG1	1:B:334:GLY:HA3	0.79	1.76	8	9
1:B:273:PRO:O	1:B:278:PRO:HD2	0.79	1.77	13	8
1:B:284:ILE:HD11	1:B:305:GLU:CG	0.79	2.06	6	2
1:B:228:VAL:HG21	1:B:269:GLN:O	0.79	1.75	11	1
1:A:103:HIS:HE1	1:A:128:TYR:CD1	0.79	1.95	8	8
1:B:219:PHE:CE1	1:B:290:PHE:CZ	0.79	2.70	3	5
1:A:120:LEU:HD22	1:A:125:GLU:CB	0.79	2.08	12	5
1:B:224:PHE:CE2	1:B:261:HIS:CE1	0.79	2.71	4	2
1:A:111:ALA:CB	1:B:311:ALA:HB3	0.79	2.03	6	1
1:A:99:SER:HB2	1:A:102:THR:OG1	0.79	1.75	9	9
1:B:303:HIS:HE1	1:B:328:TYR:CD1	0.79	1.95	8	8
1:B:339:ALA:O	1:B:341:VAL:HG23	0.79	1.78	11	6
1:B:237:SER:O	1:B:240:GLN:HG3	0.79	1.77	15	2
1:A:158:ALA:O	1:A:162:LYS:HG3	0.79	1.78	9	1
1:A:79:LEU:O	1:A:83:GLU:HB2	0.79	1.76	6	9
1:B:293:ILE:HG22	1:B:293:ILE:O	0.79	1.77	13	8
1:A:25:MET:HE2	1:A:26:GLY:H	0.79	1.38	2	2
1:B:294:PRO:HB3	1:B:328:TYR:CE1	0.79	2.13	9	10
1:A:65:ALA:HB3	1:A:66:TRP:NE1	0.79	1.92	12	1
1:B:240:GLN:CB	1:B:266:TRP:CE3	0.79	2.66	12	2
1:A:81:GLN:HB2	1:A:108:TRP:CZ2	0.79	2.12	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:218:VAL:CG1	1:B:291:VAL:HB	0.79	2.08	5	3
1:A:30:PRO:O	1:A:31:GLU:HB2	0.79	1.75	14	9
1:A:58:PHE:O	1:A:59:ASN:CB	0.79	2.31	12	12
1:B:219:PHE:CE1	1:B:290:PHE:CE2	0.79	2.70	3	4
1:B:298:PRO:HA	1:B:328:TYR:CE2	0.79	2.13	15	5
1:A:60:ALA:O	1:A:61:HIS:CD2	0.79	2.36	6	2
1:A:60:ALA:O	1:A:61:HIS:HB2	0.79	1.75	11	1
1:A:134:GLY:HA3	1:B:277:THR:OG1	0.79	1.78	8	11
1:A:160:ILE:O	1:A:163:VAL:HG12	0.79	1.78	9	3
1:A:134:GLY:O	1:A:137:THR:HG22	0.79	1.78	5	11
1:A:38:ALA:O	1:A:42:PRO:HG3	0.79	1.77	4	4
1:A:27:LEU:HD23	1:A:28:VAL:HG12	0.79	1.54	13	2
1:A:131:LEU:C	1:A:135:LEU:HD22	0.79	1.98	10	1
1:B:218:VAL:HG13	1:B:291:VAL:CG1	0.79	2.06	12	1
1:A:96:ILE:HD13	1:A:128:TYR:CE1	0.79	2.12	15	1
1:B:224:PHE:N	1:B:227:LEU:HD22	0.79	1.92	3	9
1:B:320:LEU:HD12	1:B:345:HIS:CE1	0.79	2.12	2	4
1:A:98:PRO:HA	1:A:128:TYR:CE2	0.79	2.13	15	5
1:A:43:PHE:CZ	1:A:93:ILE:HG21	0.79	2.13	13	1
1:B:228:VAL:HG22	1:B:232:THR:OG1	0.79	1.78	14	1
1:A:107:GLY:O	1:B:308:TRP:NE1	0.78	2.16	7	11
1:B:285:ARG:HB3	1:B:312:PHE:CD1	0.78	2.13	3	4
1:B:275:GLU:O	1:B:279:LEU:HD12	0.78	1.77	8	4
1:A:50:PHE:O	1:A:55:LEU:N	0.78	2.14	5	10
1:B:281:GLN:HB2	1:B:308:TRP:CH2	0.78	2.13	5	5
1:B:225:MET:O	1:B:228:VAL:HG12	0.78	1.77	5	2
1:A:43:PHE:O	1:A:47:ILE:CG1	0.78	2.30	14	2
1:A:19:PHE:CE2	1:A:90:PHE:CE2	0.78	2.71	7	1
1:A:40:GLN:HG2	1:A:66:TRP:CD1	0.78	2.14	8	3
1:A:66:TRP:N	1:A:66:TRP:HD1	0.78	1.77	11	1
1:A:40:GLN:CB	1:A:66:TRP:CE3	0.78	2.67	12	2
1:A:15:VAL:O	1:A:55:LEU:HD22	0.78	1.77	4	8
1:B:296:ILE:HD13	1:B:328:TYR:CE1	0.78	2.12	15	2
1:B:240:GLN:OE1	1:B:240:GLN:CA	0.78	2.31	14	2
1:B:316:ILE:HG23	1:B:318:LEU:HD11	0.78	1.52	9	2
1:A:28:VAL:HG11	1:A:70:VAL:CG1	0.78	2.07	7	2
1:B:215:VAL:HG22	1:B:289:VAL:HG21	0.78	1.53	7	4
1:B:348:ASP:O	1:B:351:LEU:CD2	0.78	2.31	7	1
1:A:35:MET:N	1:A:36:PRO:HD3	0.78	1.94	10	1
1:A:19:PHE:O	1:A:91:VAL:HG13	0.78	1.76	12	1
1:B:219:PHE:O	1:B:291:VAL:HG13	0.78	1.75	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ALA:HB3	1:A:116:ILE:HD11	0.78	1.53	11	11
1:B:285:ARG:HB3	1:B:312:PHE:CE1	0.78	2.14	13	8
1:A:75:GLU:O	1:A:79:LEU:HD12	0.78	1.77	8	4
1:B:245:THR:HG22	1:B:249:HIS:NE2	0.78	1.92	5	1
1:A:18:VAL:CG1	1:A:91:VAL:HB	0.78	2.08	5	3
1:A:29:ASN:CB	1:A:32:THR:OG1	0.78	2.31	12	4
1:B:296:ILE:CD1	1:B:328:TYR:CD1	0.78	2.66	7	6
1:B:243:PHE:O	1:B:247:ILE:HG12	0.78	1.78	14	2
1:B:285:ARG:CD	1:B:312:PHE:CE1	0.78	2.67	5	6
1:A:92:ALA:HB1	1:A:102:THR:HG22	0.78	1.54	15	8
1:B:229:ASN:HB2	1:B:232:THR:HG21	0.78	1.54	4	1
1:B:224:PHE:CE1	1:B:276:CYS:SG	0.78	2.76	5	3
1:B:294:PRO:O	1:B:299:SER:HB3	0.78	1.79	10	2
1:B:243:PHE:CZ	1:B:293:ILE:HG21	0.78	2.12	13	1
1:B:224:PHE:CE1	1:B:261:HIS:CE1	0.78	2.72	6	6
1:B:308:TRP:O	1:B:312:PHE:HB2	0.78	1.79	9	14
1:A:111:ALA:CB	1:B:312:PHE:CD2	0.78	2.67	11	7
1:B:262:ARG:O	1:B:264:GLU:N	0.78	2.16	4	9
1:B:325:GLU:C	1:B:325:GLU:OE2	0.78	2.22	5	3
1:B:258:PHE:O	1:B:259:ASN:HB2	0.78	1.78	15	3
1:A:120:LEU:HD12	1:A:145:HIS:NE2	0.78	1.94	7	7
1:A:85:ARG:CD	1:A:112:PHE:CE1	0.78	2.67	5	6
1:A:58:PHE:O	1:A:59:ASN:HB2	0.78	1.79	15	3
1:A:94:PRO:CB	1:A:128:TYR:CE1	0.78	2.67	15	6
1:B:277:THR:CB	1:B:278:PRO:CD	0.78	2.62	14	9
1:B:360:ILE:O	1:B:363:VAL:HG12	0.78	1.79	9	3
1:B:294:PRO:CB	1:B:328:TYR:CE1	0.77	2.68	15	6
1:A:112:PHE:CD2	1:B:311:ALA:O	0.77	2.37	2	2
1:B:292:ALA:HB1	1:B:302:THR:HG22	0.77	1.54	15	7
1:B:238:ALA:O	1:B:242:PRO:HG3	0.77	1.78	4	4
1:A:43:PHE:HZ	1:A:93:ILE:HG21	0.77	1.39	13	1
1:A:28:VAL:HG22	1:A:32:THR:OG1	0.77	1.79	14	1
1:A:46:LEU:HD12	1:A:47:ILE:HD12	0.77	1.56	1	2
1:B:321:GLU:HB3	1:B:324:ARG:CG	0.77	2.10	9	6
1:B:215:VAL:HG12	1:B:255:LEU:HD22	0.77	1.56	3	3
1:B:262:ARG:HD2	1:B:266:TRP:CH2	0.77	2.14	6	1
1:B:316:ILE:HG21	1:B:341:VAL:HG22	0.77	1.55	9	5
1:A:27:LEU:HD12	1:A:35:MET:HB3	0.77	1.57	10	1
1:B:305:GLU:N	1:B:305:GLU:OE2	0.77	2.17	10	1
1:B:232:THR:O	1:B:270:VAL:CG2	0.77	2.32	1	4
1:A:19:PHE:CD1	1:A:19:PHE:C	0.77	2.56	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:HIS:CD2	1:A:65:ALA:HB2	0.77	2.15	2	3
1:B:321:GLU:O	1:B:322:GLU:O	0.77	2.02	4	5
1:A:47:ILE:HG23	1:A:57:VAL:HG21	0.77	1.56	5	6
1:B:237:SER:C	1:B:241:LEU:HD22	0.77	2.00	5	3
1:B:247:ILE:HG23	1:B:257:VAL:HG21	0.77	1.55	5	6
1:A:130:PHE:CE1	1:B:271:LEU:O	0.77	2.36	5	4
1:B:266:TRP:N	1:B:266:TRP:HD1	0.77	1.76	11	3
1:B:269:GLN:NE2	1:B:270:VAL:HG23	0.77	1.94	14	1
1:A:73:PRO:O	1:A:78:PRO:HD2	0.77	1.79	13	10
1:B:320:LEU:HD22	1:B:325:GLU:CB	0.77	2.10	12	5
1:A:148:ASP:O	1:A:151:LEU:CD2	0.77	2.33	7	1
1:B:227:LEU:HD23	1:B:228:VAL:HG12	0.77	1.52	13	2
1:B:281:GLN:HB2	1:B:308:TRP:CZ2	0.77	2.15	10	4
1:B:321:GLU:OE1	1:B:346:TYR:CZ	0.77	2.38	1	1
1:B:331:LEU:C	1:B:335:LEU:HD22	0.77	2.00	10	1
1:A:40:GLN:OE1	1:A:40:GLN:CA	0.77	2.33	14	1
1:A:38:ALA:O	1:A:42:PRO:CD	0.77	2.32	8	12
1:A:81:GLN:HB2	1:A:108:TRP:CH2	0.77	2.15	5	7
1:B:215:VAL:O	1:B:255:LEU:HD22	0.77	1.78	4	9
1:B:334:GLY:O	1:B:337:THR:HG22	0.77	1.79	5	11
1:A:43:PHE:O	1:A:47:ILE:HG12	0.77	1.78	14	2
1:B:240:GLN:NE2	1:B:244:LEU:HD11	0.77	1.93	1	1
1:A:15:VAL:HG21	1:A:160:ILE:CG2	0.77	2.10	15	10
1:B:219:PHE:CD1	1:B:219:PHE:C	0.77	2.57	15	5
1:B:319:LEU:HD22	1:B:346:TYR:CE1	0.77	2.13	8	2
1:B:358:ALA:O	1:B:362:LYS:HG3	0.77	1.80	9	1
1:A:25:MET:HB3	1:B:330:PHE:CD1	0.77	2.15	4	2
1:B:258:PHE:O	1:B:259:ASN:CB	0.77	2.33	12	11
1:A:121:GLU:O	1:A:122:GLU:O	0.77	2.01	4	5
1:A:105:GLU:N	1:A:105:GLU:OE2	0.77	2.18	10	1
1:A:44:LEU:N	1:A:44:LEU:CD2	0.77	2.39	12	1
1:A:62:ARG:O	1:A:65:ALA:N	0.77	2.18	6	12
1:B:230:PRO:O	1:B:231:GLU:CB	0.77	2.33	9	13
1:B:296:ILE:CD1	1:B:328:TYR:CE1	0.77	2.67	4	6
1:B:218:VAL:HG21	1:B:250:PHE:CZ	0.77	2.14	7	3
1:A:28:VAL:HG22	1:A:29:ASN:N	0.76	1.95	1	4
1:A:99:SER:O	1:A:103:HIS:HB2	0.76	1.79	11	6
1:A:19:PHE:CE1	1:A:90:PHE:CZ	0.76	2.73	13	5
1:B:285:ARG:HD2	1:B:312:PHE:CE1	0.76	2.14	8	9
1:A:24:PHE:CE1	1:A:76:CYS:SG	0.76	2.78	5	3
1:A:131:LEU:HD11	1:B:304:VAL:HG11	0.76	1.55	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:PRO:O	1:A:31:GLU:CB	0.76	2.33	9	14
1:A:77:THR:HB	1:A:78:PRO:CD	0.76	2.10	14	11
1:B:235:MET:N	1:B:236:PRO:HD3	0.76	1.94	10	1
1:A:19:PHE:CE1	1:A:90:PHE:CE2	0.76	2.73	3	4
1:B:240:GLN:OE1	1:B:243:PHE:HB2	0.76	1.81	3	2
1:B:284:ILE:HD11	1:B:305:GLU:HG3	0.76	1.55	6	2
1:B:319:LEU:HD22	1:B:352:ALA:HB1	0.76	1.57	9	1
1:B:243:PHE:HZ	1:B:293:ILE:HG21	0.76	1.38	13	1
1:B:285:ARG:HD2	1:B:312:PHE:CE2	0.76	2.15	2	3
1:A:96:ILE:CD1	1:A:128:TYR:CE1	0.76	2.68	4	6
1:B:306:ILE:HG12	1:B:318:LEU:HD11	0.76	1.54	7	3
1:A:111:ALA:HB3	1:B:311:ALA:CB	0.76	2.03	6	1
1:B:228:VAL:HG11	1:B:270:VAL:HG11	0.76	1.56	7	1
1:A:134:GLY:HA3	1:B:277:THR:CB	0.76	2.11	8	14
1:B:240:GLN:O	1:B:244:LEU:HG	0.76	1.80	12	13
1:A:119:LEU:HD11	1:A:156:ILE:HD12	0.76	1.56	3	3
1:A:130:PHE:CZ	1:B:270:VAL:HG13	0.76	2.15	9	3
1:B:351:LEU:C	1:B:351:LEU:HD23	0.76	2.01	4	1
1:B:364:VAL:O	1:B:368:ASN:CB	0.76	2.34	8	2
1:A:108:TRP:NE1	1:B:310:SER:CB	0.76	2.48	9	6
1:A:116:ILE:O	1:A:117:VAL:HG23	0.76	1.80	10	10
1:A:45:THR:CG2	1:A:49:HIS:CE1	0.76	2.69	5	1
1:B:228:VAL:HG21	1:B:270:VAL:HG22	0.76	1.58	9	2
1:A:103:HIS:NE2	1:A:132:VAL:HG23	0.76	1.96	14	3
1:A:44:LEU:HD13	1:A:62:ARG:HG2	0.76	1.58	12	1
1:B:300:PRO:O	1:B:304:VAL:CG2	0.76	2.31	1	5
1:B:312:PHE:O	1:B:313:ASP:CB	0.76	2.34	6	15
1:A:19:PHE:CE2	1:A:59:ASN:HB2	0.76	2.16	3	3
1:A:39:GLU:O	1:A:42:PRO:HG2	0.76	1.79	9	5
1:A:23:PRO:C	1:A:27:LEU:HD22	0.76	2.02	9	3
1:B:231:GLU:O	1:B:232:THR:CB	0.76	2.31	11	5
1:A:25:MET:HB3	1:B:330:PHE:CD2	0.76	2.15	15	1
1:B:220:LEU:HA	1:B:291:VAL:O	0.76	1.80	1	12
1:A:112:PHE:CD2	1:B:311:ALA:CB	0.76	2.69	11	6
1:A:120:LEU:HD12	1:A:145:HIS:CD2	0.76	2.16	7	3
1:A:43:PHE:O	1:A:47:ILE:HB	0.75	1.81	5	13
1:B:299:SER:O	1:B:303:HIS:HB2	0.75	1.82	11	5
1:B:264:GLU:HB3	1:B:271:LEU:HD21	0.75	1.57	7	6
1:B:220:LEU:H	1:B:259:ASN:CG	0.75	1.84	7	1
1:B:260:ALA:O	1:B:261:HIS:HB2	0.75	1.80	11	1
1:A:120:LEU:HD12	1:A:145:HIS:CE1	0.75	2.16	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:262:ARG:O	1:B:265:ALA:N	0.75	2.19	7	13
1:B:260:ALA:C	1:B:261:HIS:CG	0.75	2.60	15	9
1:B:281:GLN:HG2	1:B:282:LEU:CD1	0.75	2.11	10	2
1:A:45:THR:HG22	1:A:49:HIS:NE2	0.75	1.96	5	1
1:B:245:THR:O	1:B:249:HIS:CD2	0.75	2.39	5	1
1:B:228:VAL:CG2	1:B:233:ASN:HB2	0.75	2.09	13	2
1:A:129:GLY:O	1:B:273:PRO:HG3	0.75	1.81	1	6
1:B:224:PHE:CA	1:B:227:LEU:HD21	0.75	2.11	11	4
1:A:71:LEU:O	1:B:330:PHE:CE1	0.75	2.40	5	4
1:B:368:ASN:O	1:B:368:ASN:OD1	0.75	2.04	6	1
1:A:18:VAL:HG21	1:A:50:PHE:CZ	0.75	2.15	7	3
1:A:18:VAL:HG11	1:A:50:PHE:CD1	0.75	2.16	7	1
1:A:31:GLU:O	1:A:32:THR:CB	0.75	2.34	11	6
1:A:95:GLY:O	1:A:96:ILE:O	0.75	2.05	14	14
1:B:228:VAL:HG22	1:B:229:ASN:N	0.75	1.95	1	5
1:B:331:LEU:HD23	1:B:335:LEU:HD12	0.75	1.56	4	6
1:A:149:ILE:O	1:A:153:LYS:HG3	0.75	1.80	8	4
1:A:72:THR:O	1:A:76:CYS:SG	0.75	2.45	11	2
1:B:227:LEU:HB2	1:B:235:MET:SD	0.75	2.22	10	1
1:B:296:ILE:CD1	1:B:328:TYR:CE2	0.75	2.70	12	9
1:B:269:GLN:O	1:B:271:LEU:N	0.75	2.19	2	4
1:A:47:ILE:HD13	1:A:47:ILE:N	0.75	1.97	14	2
1:A:24:PHE:CE1	1:A:61:HIS:ND1	0.75	2.55	5	3
1:B:244:LEU:N	1:B:244:LEU:CD2	0.75	2.42	12	3
1:A:40:GLN:OE1	1:A:43:PHE:HB2	0.75	1.81	3	2
1:A:27:LEU:HB2	1:A:35:MET:SD	0.75	2.21	10	1
1:B:239:GLU:OE2	1:B:239:GLU:N	0.75	2.20	10	1
1:A:24:PHE:CE2	1:A:70:VAL:CA	0.75	2.69	14	6
1:A:121:GLU:OE1	1:A:146:TYR:CZ	0.75	2.39	1	1
1:A:134:GLY:N	1:B:273:PRO:HB3	0.75	1.97	2	9
1:B:227:LEU:HD23	1:B:228:VAL:H	0.75	1.41	3	6
1:A:60:ALA:C	1:A:61:HIS:ND1	0.75	2.41	2	5
1:B:284:ILE:HG21	1:B:308:TRP:CB	0.75	2.12	2	5
1:A:60:ALA:C	1:A:61:HIS:CG	0.75	2.60	4	9
1:A:37:SER:C	1:A:41:LEU:HD22	0.75	2.01	5	2
1:B:276:CYS:O	1:B:280:ASP:OD2	0.75	2.05	5	6
1:B:320:LEU:HD12	1:B:345:HIS:NE2	0.75	1.97	7	6
1:B:220:LEU:HD13	1:B:247:ILE:HD11	0.75	1.59	9	5
1:B:303:HIS:NE2	1:B:332:VAL:HG23	0.75	1.97	14	3
1:A:82:LEU:N	1:A:82:LEU:HD23	0.75	1.96	12	3
1:A:140:ALA:HB3	1:A:167:VAL:HG22	0.75	1.57	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:THR:HB	1:A:78:PRO:HD3	0.74	1.59	9	12
1:A:151:LEU:C	1:A:151:LEU:HD23	0.74	2.02	4	1
1:B:261:HIS:HB3	1:B:271:LEU:HD11	0.74	1.58	4	3
1:A:29:ASN:HB2	1:A:32:THR:HG21	0.74	1.56	4	1
1:A:104:VAL:HG13	1:B:307:GLY:HA3	0.74	1.56	6	4
1:A:106:ILE:HG12	1:A:118:LEU:HD11	0.74	1.57	7	3
1:A:130:PHE:CD1	1:B:225:MET:HB3	0.74	2.16	4	1
1:B:220:LEU:HD12	1:B:247:ILE:HD11	0.74	1.60	4	2
1:A:35:MET:HG2	1:A:66:TRP:CD2	0.74	2.17	13	1
1:A:77:THR:CB	1:A:78:PRO:CD	0.74	2.65	14	11
1:B:227:LEU:CD1	1:B:235:MET:SD	0.74	2.76	8	4
1:A:135:LEU:HB3	1:A:141:VAL:HG11	0.74	1.59	10	3
1:A:73:PRO:HB3	1:B:334:GLY:H	0.74	1.42	14	3
1:A:32:THR:O	1:A:70:VAL:HG11	0.74	1.81	12	3
1:B:243:PHE:O	1:B:247:ILE:HB	0.74	1.81	5	12
1:B:296:ILE:HA	1:B:297:PRO:O	0.74	1.81	2	10
1:B:349:ILE:O	1:B:353:LYS:HG3	0.74	1.82	8	4
1:B:228:VAL:HG21	1:B:269:GLN:OE1	0.74	1.81	7	1
1:A:106:ILE:HG21	1:A:135:LEU:CD2	0.74	2.13	10	1
1:A:121:GLU:O	1:A:122:GLU:C	0.74	2.26	13	15
1:B:218:VAL:HG13	1:B:291:VAL:HB	0.74	1.60	1	3
1:A:119:LEU:HD21	1:A:152:ALA:HB1	0.74	1.57	11	3
1:A:151:LEU:O	1:A:154:PRO:HD2	0.74	1.83	5	6
1:A:24:PHE:CE2	1:A:61:HIS:CE1	0.74	2.75	4	2
1:B:272:THR:O	1:B:276:CYS:SG	0.74	2.45	11	3
1:A:130:PHE:CZ	1:B:270:VAL:HG12	0.74	2.17	13	1
1:A:112:PHE:O	1:A:113:ASP:CB	0.74	2.35	6	14
1:B:260:ALA:C	1:B:261:HIS:ND1	0.74	2.41	2	5
1:A:95:GLY:CA	1:A:128:TYR:OH	0.74	2.35	8	5
1:A:61:HIS:CB	1:A:65:ALA:HB2	0.74	2.12	13	4
1:A:41:LEU:H	1:A:41:LEU:CD1	0.74	1.94	13	1
1:B:319:LEU:O	1:B:346:TYR:CE2	0.74	2.39	1	2
1:A:111:ALA:O	1:B:312:PHE:CD2	0.74	2.40	2	2
1:B:281:GLN:HB3	1:B:308:TRP:CZ2	0.74	2.18	4	1
1:A:20:LEU:O	1:A:59:ASN:HB2	0.74	1.82	7	1
1:A:96:ILE:HG21	1:A:127:GLU:OE2	0.74	1.81	14	1
1:B:285:ARG:CD	1:B:312:PHE:CE2	0.74	2.71	4	3
1:B:290:PHE:CB	1:B:315:PRO:O	0.74	2.36	2	9
1:A:69:GLN:O	1:A:71:LEU:N	0.74	2.20	2	3
1:B:320:LEU:HD13	1:B:325:GLU:CD	0.74	2.01	5	4
1:A:104:VAL:HG11	1:B:331:LEU:HD11	0.74	1.58	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:235:MET:HG2	1:B:266:TRP:CD2	0.74	2.17	13	1
1:B:295:GLY:O	1:B:296:ILE:O	0.74	2.06	14	14
1:A:50:PHE:CD1	1:A:55:LEU:HB2	0.74	2.18	2	5
1:A:28:VAL:HG21	1:A:69:GLN:OE1	0.74	1.83	7	1
1:A:69:GLN:OE1	1:A:69:GLN:HA	0.74	1.83	9	1
1:B:306:ILE:HG21	1:B:335:LEU:CD2	0.74	2.12	10	1
1:B:347:LYS:H	1:B:347:LYS:HD3	0.74	1.42	10	1
1:B:265:ALA:HB3	1:B:266:TRP:NE1	0.74	1.97	12	1
1:A:77:THR:CB	1:B:334:GLY:HA3	0.73	2.13	1	12
1:B:279:LEU:O	1:B:283:GLU:HB2	0.73	1.82	6	9
1:B:321:GLU:O	1:B:322:GLU:C	0.73	2.25	13	15
1:A:96:ILE:CD1	1:A:128:TYR:CD1	0.73	2.71	7	6
1:B:244:LEU:O	1:B:248:GLU:HB2	0.73	1.83	10	8
1:A:140:ALA:CB	1:A:167:VAL:HG22	0.73	2.13	11	5
1:B:260:ALA:O	1:B:261:HIS:CD2	0.73	2.41	6	2
1:A:164:VAL:O	1:A:168:ASN:CB	0.73	2.35	8	2
1:A:49:HIS:O	1:A:53:GLN:HB3	0.73	1.83	10	1
1:B:225:MET:HE3	1:B:301:GLY:H	0.73	1.42	15	1
1:A:121:GLU:HB3	1:A:124:ARG:CG	0.73	2.13	9	6
1:B:224:PHE:O	1:B:225:MET:C	0.73	2.26	14	14
1:B:240:GLN:HG2	1:B:266:TRP:CD1	0.73	2.17	8	3
1:A:20:LEU:O	1:A:59:ASN:CB	0.73	2.36	7	3
1:A:117:VAL:C	1:A:118:LEU:HD12	0.73	2.02	9	1
1:B:261:HIS:O	1:B:262:ARG:O	0.73	2.06	11	1
1:A:70:VAL:HG12	1:B:330:PHE:CZ	0.73	2.18	13	1
1:B:264:GLU:OE2	1:B:271:LEU:HD21	0.73	1.83	14	1
1:B:277:THR:HB	1:B:278:PRO:HD3	0.73	1.59	9	12
1:A:142:GLU:CG	1:A:159:ALA:HB1	0.73	2.13	8	5
1:B:329:GLY:O	1:B:331:LEU:N	0.73	2.22	5	2
1:A:124:ARG:O	1:A:127:GLU:N	0.73	2.22	11	8
1:B:285:ARG:HB3	1:B:312:PHE:CE2	0.73	2.18	6	4
1:A:24:PHE:CA	1:A:27:LEU:HD21	0.73	2.12	11	4
1:A:18:VAL:CG1	1:A:50:PHE:CE2	0.73	2.72	3	2
1:B:216:ARG:O	1:B:256:GLU:HG3	0.73	1.83	6	1
1:B:218:VAL:CG2	1:B:250:PHE:CE2	0.73	2.72	7	2
1:A:49:HIS:O	1:A:53:GLN:HG3	0.73	1.83	11	2
1:B:325:GLU:CD	1:B:326:GLU:N	0.73	2.41	12	7
1:B:320:LEU:HD12	1:B:345:HIS:CD2	0.73	2.19	7	3
1:A:39:GLU:OE2	1:A:39:GLU:N	0.73	2.20	10	1
1:B:296:ILE:HG13	1:B:297:PRO:HA	0.73	1.59	12	5
1:B:247:ILE:HD13	1:B:247:ILE:N	0.73	1.97	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:THR:O	1:A:49:HIS:CD2	0.73	2.41	5	1
1:A:107:GLY:HA3	1:B:304:VAL:HG13	0.73	1.59	6	4
1:A:129:GLY:O	1:A:131:LEU:N	0.73	2.21	5	2
1:A:18:VAL:HG13	1:A:91:VAL:HB	0.73	1.59	1	3
1:A:19:PHE:CD2	1:A:59:ASN:HB2	0.73	2.19	2	2
1:B:224:PHE:CE1	1:B:270:VAL:HA	0.73	2.19	10	5
1:A:134:GLY:O	1:A:138:VAL:HG13	0.73	1.81	7	4
1:B:239:GLU:O	1:B:242:PRO:HG2	0.73	1.84	9	4
1:A:131:LEU:HD23	1:A:135:LEU:HD11	0.73	1.61	8	1
1:B:340:ALA:HB3	1:B:367:VAL:HG22	0.73	1.58	11	1
1:A:108:TRP:HE1	1:B:310:SER:HB3	0.73	1.40	1	5
1:B:218:VAL:CG1	1:B:250:PHE:CE1	0.73	2.71	13	4
1:A:84:ILE:HG21	1:A:108:TRP:CB	0.73	2.12	7	5
1:A:130:PHE:CE2	1:B:271:LEU:O	0.73	2.42	4	3
1:B:294:PRO:HB2	1:B:328:TYR:CE2	0.73	2.18	11	4
1:A:20:LEU:H	1:A:59:ASN:CG	0.73	1.86	7	1
1:A:44:LEU:HD13	1:A:62:ARG:CG	0.73	2.13	12	1
1:A:20:LEU:HA	1:A:91:VAL:O	0.73	1.83	1	12
1:A:108:TRP:O	1:A:112:PHE:HB2	0.73	1.82	9	13
1:B:219:PHE:CE2	1:B:290:PHE:CZ	0.73	2.77	4	5
1:A:20:LEU:HD12	1:A:47:ILE:HD11	0.73	1.61	4	2
1:B:260:ALA:O	1:B:265:ALA:HB2	0.73	1.84	12	2
1:A:76:CYS:O	1:A:80:ASP:CG	0.73	2.27	10	8
1:B:272:THR:O	1:B:275:GLU:N	0.73	2.22	14	7
1:B:225:MET:HE2	1:B:226:GLY:H	0.73	1.44	2	2
1:A:119:LEU:O	1:A:146:TYR:CE1	0.73	2.41	6	1
1:B:264:GLU:O	1:B:269:GLN:OE1	0.73	2.07	11	1
1:B:324:ARG:O	1:B:327:GLU:N	0.72	2.22	11	9
1:A:61:HIS:HB3	1:A:71:LEU:HD11	0.72	1.60	4	3
1:A:102:THR:O	1:A:104:VAL:N	0.72	2.21	9	2
1:B:334:GLY:O	1:B:338:VAL:HG13	0.72	1.83	7	5
1:B:223:PRO:C	1:B:227:LEU:HD22	0.72	2.02	7	3
1:A:76:CYS:O	1:A:80:ASP:OD1	0.72	2.06	8	1
1:A:29:ASN:HB3	1:A:32:THR:OG1	0.72	1.83	15	3
1:A:53:GLN:O	1:A:53:GLN:CD	0.72	2.28	15	1
1:A:62:ARG:O	1:A:66:TRP:CD1	0.72	2.43	11	6
1:A:110:SER:CB	1:B:308:TRP:NE1	0.72	2.51	9	5
1:B:225:MET:CA	1:B:228:VAL:HG12	0.72	2.13	3	4
1:A:19:PHE:CB	1:A:87:ALA:CB	0.72	2.67	8	9
1:B:224:PHE:O	1:B:227:LEU:HG	0.72	1.84	5	1
1:B:324:ARG:O	1:B:328:TYR:CD2	0.72	2.41	5	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:227:LEU:HD12	1:B:235:MET:HB3	0.72	1.62	10	1
1:B:250:PHE:HD1	1:B:255:LEU:HD12	0.72	1.45	14	7
1:A:24:PHE:CE1	1:A:70:VAL:HA	0.72	2.19	13	5
1:A:67:GLY:O	1:A:68:ALA:HB2	0.72	1.83	5	2
1:B:319:LEU:O	1:B:346:TYR:CE1	0.72	2.41	6	1
1:A:96:ILE:CD1	1:A:128:TYR:CE2	0.72	2.71	1	9
1:B:250:PHE:CD1	1:B:255:LEU:HB2	0.72	2.19	2	5
1:B:219:PHE:CE2	1:B:290:PHE:CE1	0.72	2.78	6	5
1:A:31:GLU:O	1:A:32:THR:HB	0.72	1.84	9	2
1:A:72:THR:HB	1:A:73:PRO:HD2	0.72	1.60	11	1
1:A:107:GLY:O	1:A:110:SER:HB2	0.72	1.84	5	5
1:B:321:GLU:HG2	1:B:346:TYR:OH	0.72	1.85	6	2
1:A:32:THR:H	1:A:70:VAL:HG11	0.72	1.43	10	2
1:A:71:LEU:O	1:B:330:PHE:HE1	0.72	1.67	6	6
1:A:70:VAL:O	1:B:330:PHE:HE1	0.72	1.67	11	1
1:B:349:ILE:O	1:B:353:LYS:HG2	0.72	1.85	12	1
1:B:285:ARG:HB3	1:B:312:PHE:CD2	0.72	2.19	2	3
1:B:260:ALA:O	1:B:265:ALA:CB	0.72	2.37	12	2
1:A:25:MET:CA	1:A:28:VAL:HG12	0.72	2.14	3	4
1:B:303:HIS:O	1:B:306:ILE:N	0.72	2.23	4	10
1:B:319:LEU:HD11	1:B:356:ILE:HD12	0.72	1.59	3	3
1:B:341:VAL:CG1	1:B:343:PHE:CE2	0.72	2.73	6	3
1:A:28:VAL:HB	1:A:70:VAL:HG21	0.72	1.61	11	1
1:A:130:PHE:CG	1:B:225:MET:HE3	0.72	2.18	1	1
1:B:244:LEU:HD22	1:B:266:TRP:CH2	0.72	2.20	9	4
1:A:68:ALA:O	1:A:69:GLN:CB	0.72	2.37	9	5
1:B:302:THR:O	1:B:304:VAL:N	0.72	2.22	9	2
1:B:295:GLY:CA	1:B:328:TYR:OH	0.72	2.38	8	6
1:A:30:PRO:O	1:A:31:GLU:CG	0.72	2.37	4	1
1:B:331:LEU:HD23	1:B:335:LEU:HD11	0.72	1.62	8	2
1:A:64:GLU:HB3	1:A:71:LEU:HD21	0.72	1.62	7	6
1:A:107:GLY:HA2	1:A:110:SER:OG	0.72	1.84	14	4
1:A:110:SER:HB2	1:B:308:TRP:HE1	0.72	1.43	9	4
1:B:282:LEU:HD13	1:B:285:ARG:HE	0.72	1.45	7	1
1:A:60:ALA:O	1:A:65:ALA:HB2	0.72	1.85	12	2
1:B:244:LEU:HD13	1:B:262:ARG:HG2	0.72	1.59	12	1
1:A:142:GLU:OE2	1:A:159:ALA:HB1	0.72	1.84	13	2
1:A:23:PRO:CA	1:A:99:SER:CB	0.72	2.67	13	2
1:B:245:THR:CG2	1:B:249:HIS:NE2	0.72	2.53	5	1
1:B:263:ARG:CZ	1:B:263:ARG:HB3	0.72	2.13	5	1
1:A:56:GLU:O	1:A:58:PHE:CE2	0.72	2.43	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:CE2	1:A:90:PHE:CE1	0.72	2.78	6	6
1:B:324:ARG:O	1:B:328:TYR:CD1	0.72	2.43	2	5
1:B:244:LEU:HD13	1:B:262:ARG:CG	0.72	2.15	12	1
1:B:301:GLY:O	1:B:305:GLU:HG2	0.72	1.84	15	1
1:B:273:PRO:O	1:B:278:PRO:CD	0.71	2.38	2	11
1:B:296:ILE:CD1	1:B:328:TYR:CD2	0.71	2.73	12	8
1:B:316:ILE:O	1:B:317:VAL:HG23	0.71	1.84	11	9
1:A:103:HIS:HE1	1:A:128:TYR:CD2	0.71	2.03	3	5
1:A:106:ILE:CG2	1:A:135:LEU:HD22	0.71	2.15	15	7
1:A:28:VAL:HG11	1:A:70:VAL:HG21	0.71	1.60	4	2
1:A:15:VAL:HG22	1:A:89:VAL:HG21	0.71	1.59	7	4
1:A:28:VAL:HG11	1:A:70:VAL:HG11	0.71	1.62	7	1
1:B:220:LEU:O	1:B:259:ASN:CG	0.71	2.27	7	2
1:B:220:LEU:O	1:B:259:ASN:HB2	0.71	1.85	7	1
1:A:17:SER:O	1:A:88:ASP:HB3	0.71	1.85	9	1
1:A:126:GLU:O	1:B:231:GLU:OE2	0.71	2.08	11	1
1:B:229:ASN:HB3	1:B:232:THR:OG1	0.71	1.85	15	3
1:A:96:ILE:HA	1:A:97:PRO:O	0.71	1.84	2	11
1:B:307:GLY:O	1:B:310:SER:HB2	0.71	1.86	5	5
1:B:303:HIS:CE1	1:B:328:TYR:CE2	0.71	2.78	2	3
1:B:249:HIS:O	1:B:253:GLN:HG2	0.71	1.84	7	5
1:A:20:LEU:O	1:A:59:ASN:CG	0.71	2.27	7	2
1:B:249:HIS:O	1:B:253:GLN:HB3	0.71	1.85	10	1
1:B:284:ILE:HG22	1:B:312:PHE:CD2	0.71	2.20	1	2
1:A:72:THR:O	1:A:75:GLU:N	0.71	2.23	14	6
1:A:89:VAL:O	1:A:89:VAL:CG1	0.71	2.37	15	7
1:A:120:LEU:HD13	1:A:125:GLU:CD	0.71	2.06	5	5
1:B:218:VAL:HG21	1:B:250:PHE:HE2	0.71	1.43	8	1
1:A:100:PRO:O	1:A:104:VAL:CG2	0.71	2.34	1	4
1:A:96:ILE:H	1:A:124:ARG:HB3	0.71	1.45	8	11
1:A:108:TRP:CD1	1:B:307:GLY:C	0.71	2.64	12	6
1:A:111:ALA:CA	1:B:312:PHE:CD1	0.71	2.73	3	6
1:B:224:PHE:CE1	1:B:261:HIS:ND1	0.71	2.59	5	3
1:A:27:LEU:HD23	1:A:28:VAL:H	0.71	1.44	3	5
1:A:76:CYS:O	1:A:80:ASP:CB	0.71	2.38	6	12
1:B:219:PHE:CE2	1:B:259:ASN:HB2	0.71	2.19	3	3
1:B:302:THR:O	1:B:305:GLU:HB2	0.71	1.86	5	10
1:B:225:MET:HE2	1:B:225:MET:HA	0.71	1.61	5	2
1:B:281:GLN:HG2	1:B:282:LEU:HD13	0.71	1.61	10	1
1:A:35:MET:SD	1:A:35:MET:C	0.71	2.68	15	1
1:B:299:SER:N	1:B:328:TYR:HE2	0.71	1.83	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:ILE:HG22	1:A:112:PHE:CD2	0.71	2.21	1	1
1:A:111:ALA:CB	1:B:312:PHE:CD1	0.71	2.73	1	8
1:A:19:PHE:CD1	1:A:90:PHE:CE2	0.71	2.79	10	3
1:B:294:PRO:HB2	1:B:328:TYR:CE1	0.71	2.21	15	3
1:A:25:MET:CB	1:B:330:PHE:CD2	0.71	2.74	6	4
1:A:85:ARG:HB3	1:A:112:PHE:CD1	0.71	2.21	3	5
1:B:241:LEU:CD1	1:B:241:LEU:N	0.71	2.53	12	7
1:B:289:VAL:O	1:B:289:VAL:CG1	0.71	2.39	15	7
1:A:24:PHE:N	1:A:27:LEU:CD2	0.71	2.54	4	3
1:B:228:VAL:CG1	1:B:270:VAL:HG21	0.71	2.15	7	3
1:B:282:LEU:N	1:B:282:LEU:HD23	0.71	2.00	12	3
1:B:275:GLU:O	1:B:279:LEU:HB2	0.71	1.86	10	3
1:A:75:GLU:C	1:A:79:LEU:HD12	0.71	2.06	14	1
1:B:329:GLY:HA2	1:B:333:ARG:HD3	0.71	1.62	14	1
1:A:25:MET:HE3	1:A:101:GLY:H	0.71	1.46	15	1
1:A:85:ARG:NE	1:A:112:PHE:CZ	0.71	2.59	15	1
1:A:94:PRO:HB2	1:A:128:TYR:CE1	0.71	2.21	15	3
1:B:219:PHE:CD2	1:B:290:PHE:CE1	0.71	2.79	6	1
1:B:220:LEU:O	1:B:259:ASN:CB	0.71	2.39	7	3
1:B:331:LEU:O	1:B:335:LEU:HD13	0.71	1.85	7	2
1:A:81:GLN:HA	1:A:84:ILE:CG1	0.71	2.16	13	3
1:A:41:LEU:CD1	1:A:41:LEU:N	0.71	2.54	12	7
1:A:50:PHE:HD1	1:A:55:LEU:HD12	0.71	1.44	14	6
1:A:101:GLY:O	1:A:105:GLU:HG2	0.71	1.85	15	2
1:B:226:GLY:O	1:B:228:VAL:N	0.71	2.23	10	6
1:A:40:GLN:O	1:A:44:LEU:HG	0.70	1.84	12	14
1:B:232:THR:O	1:B:270:VAL:HG11	0.70	1.86	12	3
1:A:50:PHE:HD1	1:A:55:LEU:HB2	0.70	1.46	11	5
1:A:106:ILE:HG22	1:A:135:LEU:HD22	0.70	1.63	6	3
1:A:92:ALA:HB3	1:A:118:LEU:HD21	0.70	1.63	7	1
1:A:131:LEU:O	1:A:135:LEU:HD13	0.70	1.85	7	2
1:B:292:ALA:HB3	1:B:318:LEU:HD21	0.70	1.63	7	1
1:B:258:PHE:N	1:B:258:PHE:CD2	0.70	2.59	15	1
1:B:289:VAL:CG2	1:B:364:VAL:CG2	0.70	2.69	13	4
1:A:76:CYS:O	1:A:80:ASP:OD2	0.70	2.09	5	7
1:A:84:ILE:HD13	1:A:90:PHE:HE1	0.70	1.43	15	2
1:B:272:THR:HB	1:B:273:PRO:HD2	0.70	1.60	11	1
1:A:130:PHE:CD2	1:B:225:MET:HB3	0.70	2.22	15	1
1:B:256:GLU:O	1:B:258:PHE:CE2	0.70	2.44	15	1
1:A:19:PHE:CE2	1:A:90:PHE:CZ	0.70	2.79	4	5
1:A:24:PHE:C	1:A:27:LEU:HD23	0.70	2.07	12	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:HIS:O	1:A:106:ILE:N	0.70	2.24	4	9
1:B:227:LEU:HD23	1:B:228:VAL:N	0.70	2.02	3	7
1:B:238:ALA:O	1:B:242:PRO:CD	0.70	2.39	8	13
1:A:85:ARG:HB3	1:A:112:PHE:CD2	0.70	2.21	2	4
1:A:124:ARG:O	1:A:128:TYR:CD2	0.70	2.44	5	8
1:A:134:GLY:CA	1:B:277:THR:HG21	0.70	2.16	8	2
1:A:104:VAL:HG22	1:B:303:HIS:C	0.70	2.07	11	5
1:B:317:VAL:C	1:B:318:LEU:HD12	0.70	2.06	9	1
1:A:84:ILE:HD12	1:A:90:PHE:CE1	0.70	2.21	12	1
1:A:93:ILE:CG1	1:A:119:LEU:HB2	0.70	2.16	12	7
1:A:130:PHE:N	1:B:273:PRO:HG3	0.70	2.01	5	3
1:B:223:PRO:O	1:B:224:PHE:C	0.70	2.29	5	15
1:B:281:GLN:HG2	1:B:282:LEU:HD22	0.70	1.61	7	3
1:A:110:SER:HB2	1:B:308:TRP:NE1	0.70	2.01	9	8
1:A:146:TYR:O	1:A:147:LYS:CB	0.70	2.38	8	4
1:B:268:ALA:O	1:B:269:GLN:CB	0.70	2.39	9	4
1:B:219:PHE:CB	1:B:287:ALA:CB	0.70	2.69	8	9
1:A:119:LEU:HD22	1:A:152:ALA:HB1	0.70	1.63	9	1
1:A:94:PRO:O	1:A:99:SER:HB3	0.70	1.86	10	2
1:A:60:ALA:O	1:A:65:ALA:CB	0.70	2.39	12	2
1:A:24:PHE:O	1:A:25:MET:C	0.70	2.29	7	14
1:B:224:PHE:CE2	1:B:270:VAL:CA	0.70	2.75	7	6
1:A:15:VAL:HB	1:A:55:LEU:HD22	0.70	1.63	2	4
1:A:73:PRO:HB3	1:B:334:GLY:CA	0.70	2.17	2	4
1:A:16:ARG:O	1:A:56:GLU:HG3	0.70	1.86	6	1
1:B:353:LYS:HG2	1:B:354:PRO:N	0.70	2.02	9	1
1:A:81:GLN:HG2	1:A:82:LEU:HD13	0.70	1.62	10	1
1:A:125:GLU:CD	1:A:125:GLU:N	0.70	2.45	15	1
1:A:119:LEU:O	1:A:146:TYR:CE2	0.70	2.44	1	2
1:A:32:THR:HG22	1:A:33:ASN:N	0.70	2.00	5	1
1:B:218:VAL:HG11	1:B:250:PHE:CD1	0.70	2.21	7	1
1:A:98:PRO:HA	1:A:128:TYR:CD1	0.70	2.21	8	2
1:B:325:GLU:CD	1:B:325:GLU:N	0.70	2.44	15	1
1:A:85:ARG:CD	1:A:112:PHE:CE2	0.70	2.73	4	3
1:B:261:HIS:O	1:B:262:ARG:C	0.70	2.29	8	11
1:A:35:MET:HB2	1:A:69:GLN:HG2	0.70	1.62	2	2
1:A:15:VAL:HG12	1:A:55:LEU:HD22	0.70	1.64	3	3
1:A:27:LEU:CD1	1:A:35:MET:SD	0.70	2.79	8	4
1:A:116:ILE:CG2	1:A:141:VAL:HG22	0.70	2.17	9	5
1:A:153:LYS:HG2	1:A:154:PRO:N	0.70	2.01	9	1
1:A:61:HIS:O	1:A:62:ARG:O	0.70	2.08	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:ARG:HD3	1:A:124:ARG:N	0.70	2.01	15	1
1:B:246:LEU:HD13	1:B:246:LEU:O	0.70	1.87	5	2
1:B:340:ALA:CB	1:B:367:VAL:HG22	0.70	2.16	11	4
1:B:292:ALA:HB1	1:B:302:THR:CG2	0.70	2.17	14	8
1:A:19:PHE:CD2	1:A:90:PHE:CE1	0.70	2.79	6	3
1:A:40:GLN:CG	1:A:41:LEU:CD1	0.70	2.68	12	1
1:B:229:ASN:OD1	1:B:229:ASN:C	0.70	2.29	13	1
1:A:90:PHE:CB	1:A:115:PRO:O	0.70	2.39	2	9
1:A:146:TYR:O	1:A:146:TYR:CG	0.70	2.45	10	8
1:A:168:ASN:O	1:A:168:ASN:ND2	0.70	2.24	14	3
1:B:219:PHE:CE2	1:B:259:ASN:CB	0.70	2.75	5	5
1:B:223:PRO:CA	1:B:299:SER:CB	0.70	2.69	13	2
1:A:141:VAL:CG1	1:A:143:PHE:CE2	0.70	2.75	6	3
1:B:319:LEU:O	1:B:346:TYR:HE1	0.70	1.68	6	1
1:A:144:VAL:HG13	1:A:155:GLN:HB3	0.70	1.64	11	1
1:A:131:LEU:CD2	1:B:308:TRP:CH2	0.70	2.74	12	1
1:B:282:LEU:HB3	1:B:286:LYS:HE2	0.70	1.63	13	1
1:A:90:PHE:CE1	1:A:106:ILE:HA	0.70	2.21	2	3
1:B:296:ILE:H	1:B:324:ARG:HB3	0.70	1.47	8	11
1:A:29:ASN:C	1:A:29:ASN:ND2	0.70	2.45	5	1
1:A:46:LEU:CA	1:A:49:HIS:CD2	0.70	2.75	5	1
1:B:229:ASN:H	1:B:233:ASN:HB2	0.70	1.47	7	6
1:B:249:HIS:O	1:B:253:GLN:HG3	0.70	1.87	11	2
1:A:105:GLU:OE2	1:A:105:GLU:CA	0.70	2.40	10	1
1:B:234:SER:HA	1:B:268:ALA:HB1	0.70	1.62	11	1
1:A:96:ILE:CD1	1:A:128:TYR:CD2	0.69	2.74	12	8
1:B:276:CYS:O	1:B:280:ASP:CB	0.69	2.40	6	13
1:A:32:THR:O	1:A:33:ASN:CB	0.69	2.38	10	4
1:A:125:GLU:CD	1:A:126:GLU:N	0.69	2.45	12	6
1:B:256:GLU:CA	1:B:256:GLU:OE2	0.69	2.39	11	1
1:B:324:ARG:N	1:B:324:ARG:CD	0.69	2.55	14	4
1:A:135:LEU:CB	1:A:141:VAL:HG21	0.69	2.17	12	4
1:A:73:PRO:HB3	1:B:334:GLY:N	0.69	2.01	14	5
1:B:219:PHE:CD1	1:B:290:PHE:CE2	0.69	2.80	2	3
1:A:111:ALA:O	1:B:312:PHE:CE1	0.69	2.46	3	5
1:A:25:MET:HE1	1:A:101:GLY:H	0.69	1.47	10	1
1:B:346:TYR:CG	1:B:346:TYR:O	0.69	2.44	10	1
1:B:235:MET:SD	1:B:235:MET:C	0.69	2.71	15	1
1:A:47:ILE:HG13	1:A:57:VAL:HG21	0.69	1.63	11	5
1:B:225:MET:HA	1:B:228:VAL:HG12	0.69	1.64	3	4
1:A:130:PHE:CD2	1:B:225:MET:CB	0.69	2.75	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:PHE:N	1:A:58:PHE:CD2	0.69	2.60	15	1
1:A:64:GLU:OE1	1:A:71:LEU:HD11	0.69	1.88	15	1
1:A:73:PRO:O	1:A:78:PRO:CD	0.69	2.39	2	11
1:B:309:ALA:CB	1:B:316:ILE:HD11	0.69	2.16	11	6
1:B:344:VAL:HG21	1:B:356:ILE:HA	0.69	1.65	7	5
1:B:215:VAL:HB	1:B:255:LEU:HD22	0.69	1.64	2	4
1:B:250:PHE:HD1	1:B:255:LEU:HB2	0.69	1.46	10	5
1:B:282:LEU:O	1:B:286:LYS:HB3	0.69	1.87	2	3
1:B:234:SER:HB2	1:B:268:ALA:O	0.69	1.88	3	1
1:B:276:CYS:O	1:B:280:ASP:OD1	0.69	2.10	8	1
1:A:129:GLY:HA2	1:A:133:ARG:HD3	0.69	1.62	14	1
1:A:65:ALA:C	1:A:66:TRP:CD1	0.69	2.66	1	14
1:B:290:PHE:CE1	1:B:306:ILE:HA	0.69	2.22	7	3
1:B:307:GLY:HA2	1:B:310:SER:OG	0.69	1.87	14	6
1:A:98:PRO:HB3	1:A:103:HIS:CE1	0.69	2.22	7	5
1:A:168:ASN:O	1:A:168:ASN:OD1	0.69	2.09	6	1
1:B:228:VAL:HG23	1:B:233:ASN:HB3	0.69	1.64	10	2
1:B:281:GLN:HA	1:B:284:ILE:CG1	0.69	2.17	13	3
1:A:99:SER:N	1:A:128:TYR:HE2	0.69	1.85	15	1
1:A:68:ALA:O	1:A:69:GLN:O	0.69	2.09	14	5
1:B:224:PHE:C	1:B:227:LEU:HD23	0.69	2.08	15	7
1:B:250:PHE:HD2	1:B:255:LEU:HD12	0.69	1.47	9	6
1:B:276:CYS:O	1:B:280:ASP:CG	0.69	2.31	10	8
1:A:107:GLY:C	1:B:308:TRP:CD1	0.69	2.66	12	7
1:B:241:LEU:O	1:B:244:LEU:N	0.69	2.26	6	10
1:A:102:THR:O	1:A:105:GLU:HB2	0.69	1.86	5	7
1:A:15:VAL:CG1	1:A:18:VAL:CG2	0.69	2.71	4	3
1:A:79:LEU:HD23	1:A:79:LEU:C	0.69	2.06	4	1
1:A:81:GLN:HB3	1:A:108:TRP:CZ2	0.69	2.23	4	1
1:A:92:ALA:HB1	1:A:102:THR:CG2	0.69	2.17	14	8
1:A:63:ARG:CZ	1:A:63:ARG:HB3	0.69	2.16	5	1
1:B:229:ASN:C	1:B:229:ASN:ND2	0.69	2.46	5	1
1:B:267:GLY:O	1:B:268:ALA:HB2	0.69	1.87	5	2
1:A:117:VAL:HG13	1:A:142:GLU:HB2	0.69	1.64	6	2
1:B:220:LEU:H	1:B:259:ASN:ND2	0.69	1.84	7	1
1:B:329:GLY:O	1:B:333:ARG:HB2	0.69	1.86	13	3
1:B:261:HIS:CD2	1:B:265:ALA:HB2	0.69	2.23	15	3
1:B:279:LEU:HD23	1:B:279:LEU:C	0.69	2.07	4	1
1:A:109:ALA:CB	1:A:116:ILE:HD11	0.69	2.17	11	6
1:B:219:PHE:CD1	1:B:259:ASN:CB	0.69	2.75	1	2
1:B:301:GLY:O	1:B:305:GLU:HG3	0.69	1.87	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:335:LEU:HB3	1:B:341:VAL:HG11	0.69	1.63	10	4
1:A:82:LEU:O	1:A:86:LYS:HB3	0.69	1.87	2	3
1:A:25:MET:HB2	1:B:330:PHE:CE2	0.69	2.22	3	2
1:A:112:PHE:CE1	1:B:311:ALA:O	0.69	2.46	3	5
1:A:134:GLY:N	1:B:273:PRO:CB	0.69	2.56	3	4
1:A:24:PHE:O	1:A:27:LEU:HG	0.69	1.86	5	1
1:B:235:MET:SD	1:B:236:PRO:HD2	0.69	2.28	8	1
1:B:246:LEU:HD12	1:B:349:ILE:HG23	0.69	1.63	10	3
1:A:81:GLN:HG2	1:A:82:LEU:CD1	0.69	2.17	10	1
1:B:228:VAL:CG2	1:B:232:THR:O	0.69	2.40	10	1
1:B:324:ARG:HD3	1:B:324:ARG:N	0.69	2.01	15	1
1:A:81:GLN:HG2	1:A:82:LEU:HD22	0.69	1.65	7	3
1:A:131:LEU:CD2	1:B:304:VAL:HG11	0.69	2.17	13	5
1:A:26:GLY:O	1:A:28:VAL:N	0.69	2.26	10	6
1:A:93:ILE:O	1:A:93:ILE:CG2	0.69	2.41	12	5
1:B:284:ILE:O	1:B:314:LYS:HG2	0.69	1.88	7	2
1:B:346:TYR:O	1:B:347:LYS:CB	0.69	2.40	8	4
1:A:78:PRO:O	1:A:82:LEU:HD22	0.69	1.88	4	1
1:B:228:VAL:HG11	1:B:270:VAL:HG21	0.69	1.63	4	2
1:B:230:PRO:O	1:B:231:GLU:CG	0.69	2.41	4	1
1:A:94:PRO:HB2	1:A:128:TYR:CE2	0.69	2.22	11	5
1:B:291:VAL:HG22	1:B:317:VAL:O	0.69	1.88	9	1
1:A:136:GLY:CA	1:A:141:VAL:HB	0.69	2.18	12	7
1:A:29:ASN:O	1:A:32:THR:OG1	0.69	2.10	14	4
1:B:217:SER:O	1:B:288:ASP:HB3	0.69	1.87	9	1
1:A:149:ILE:O	1:A:153:LYS:HG2	0.69	1.88	12	1
1:A:23:PRO:HB2	1:A:27:LEU:HB3	0.68	1.65	3	4
1:A:89:VAL:CG2	1:A:164:VAL:CG2	0.68	2.71	13	5
1:B:243:PHE:O	1:B:247:ILE:CD1	0.68	2.41	4	5
1:A:129:GLY:HA2	1:A:133:ARG:HB2	0.68	1.63	15	9
1:B:236:PRO:O	1:B:239:GLU:HB3	0.68	1.87	8	7
1:A:34:SER:HB2	1:A:68:ALA:O	0.68	1.88	3	1
1:B:229:ASN:OD1	1:B:233:ASN:ND2	0.68	2.26	3	1
1:B:306:ILE:CG2	1:B:335:LEU:HD22	0.68	2.17	8	5
1:B:306:ILE:HG22	1:B:335:LEU:HD13	0.68	1.65	11	2
1:A:119:LEU:O	1:A:146:TYR:HE1	0.68	1.69	6	1
1:B:322:GLU:HA	1:B:325:GLU:OE2	0.68	1.88	10	2
1:B:331:LEU:HD23	1:B:335:LEU:HD21	0.68	1.65	14	1
1:A:23:PRO:HA	1:A:99:SER:CB	0.68	2.18	12	9
1:A:108:TRP:CD1	1:B:311:ALA:HB2	0.68	2.22	2	8
1:A:24:PHE:CE1	1:A:69:GLN:OE1	0.68	2.46	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:275:GLU:O	1:B:279:LEU:CD1	0.68	2.41	8	2
1:A:28:VAL:HB	1:A:70:VAL:CG2	0.68	2.18	11	1
1:A:40:GLN:HB3	1:A:66:TRP:CE3	0.68	2.23	12	1
1:B:277:THR:HB	1:B:278:PRO:HD2	0.68	1.62	14	1
1:B:253:GLN:O	1:B:253:GLN:CD	0.68	2.30	15	1
1:A:61:HIS:O	1:A:62:ARG:C	0.68	2.31	8	11
1:B:293:ILE:CG1	1:B:319:LEU:HB2	0.68	2.18	12	8
1:B:335:LEU:HA	1:B:338:VAL:HG22	0.68	1.65	15	9
1:B:219:PHE:CD2	1:B:259:ASN:HB2	0.68	2.23	2	2
1:A:96:ILE:N	1:A:128:TYR:CZ	0.68	2.60	8	3
1:B:310:SER:OG	1:B:335:LEU:HD21	0.68	1.88	5	4
1:B:222:GLY:N	1:B:261:HIS:CE1	0.68	2.61	9	1
1:B:244:LEU:O	1:B:248:GLU:OE2	0.68	2.12	12	1
1:A:82:LEU:HB3	1:A:86:LYS:HE2	0.68	1.65	13	1
1:B:265:ALA:C	1:B:266:TRP:CD1	0.68	2.66	1	15
1:A:130:PHE:CE1	1:B:224:PHE:HB3	0.68	2.24	2	2
1:B:259:ASN:N	1:B:283:GLU:HG2	0.68	2.03	2	1
1:B:223:PRO:C	1:B:227:LEU:HD23	0.68	2.09	11	2
1:A:45:THR:CG2	1:A:49:HIS:NE2	0.68	2.56	5	1
1:A:28:VAL:HG21	1:A:70:VAL:HG22	0.68	1.65	9	2
1:B:323:GLY:O	1:B:326:GLU:HB2	0.68	1.89	6	2
1:A:90:PHE:HE1	1:A:106:ILE:HG13	0.68	1.49	7	2
1:B:215:VAL:CG2	1:B:360:ILE:CG2	0.68	2.70	15	3
1:A:46:LEU:HD12	1:A:149:ILE:HG23	0.68	1.64	10	3
1:A:75:GLU:O	1:A:79:LEU:HB2	0.68	1.88	10	3
1:B:217:SER:OG	1:B:256:GLU:OE2	0.68	2.07	1	1
1:A:69:GLN:O	1:A:70:VAL:C	0.68	2.32	2	6
1:A:104:VAL:O	1:A:108:TRP:HB2	0.68	1.87	3	7
1:B:218:VAL:CG1	1:B:250:PHE:CE2	0.68	2.75	3	2
1:B:353:LYS:CB	1:B:354:PRO:CD	0.68	2.71	13	6
1:B:224:PHE:N	1:B:227:LEU:CD2	0.68	2.56	4	4
1:B:261:HIS:CB	1:B:265:ALA:HB2	0.68	2.15	13	4
1:A:44:LEU:HD13	1:A:66:TRP:CH2	0.68	2.23	6	2
1:A:161:ARG:O	1:A:165:ASP:OD1	0.68	2.12	12	1
1:B:259:ASN:O	1:B:260:ALA:C	0.68	2.32	15	7
1:B:266:TRP:CD1	1:B:266:TRP:N	0.68	2.55	1	3
1:B:323:GLY:N	1:B:325:GLU:OE1	0.68	2.26	11	4
1:A:59:ASN:N	1:A:83:GLU:HG2	0.68	2.03	2	1
1:A:96:ILE:HG13	1:A:97:PRO:HA	0.68	1.64	12	6
1:A:25:MET:O	1:A:28:VAL:N	0.68	2.27	14	2
1:B:240:GLN:CA	1:B:266:TRP:CH2	0.68	2.74	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ASN:OD1	1:A:29:ASN:C	0.68	2.32	13	1
1:A:23:PRO:O	1:A:24:PHE:C	0.68	2.31	5	15
1:B:247:ILE:CG1	1:B:257:VAL:HG11	0.68	2.17	13	6
1:A:142:GLU:HG2	1:A:159:ALA:HB1	0.68	1.64	8	4
1:B:279:LEU:O	1:B:283:GLU:OE2	0.68	2.12	5	1
1:A:103:HIS:C	1:B:304:VAL:HG22	0.68	2.09	9	4
1:A:104:VAL:HG11	1:B:331:LEU:CD2	0.68	2.19	13	4
1:A:40:GLN:CG	1:A:41:LEU:HD13	0.68	2.10	12	1
1:A:53:GLN:HA	1:A:53:GLN:OE1	0.68	1.88	12	1
1:B:259:ASN:O	1:B:261:HIS:N	0.68	2.27	12	2
1:A:76:CYS:SG	1:A:80:ASP:OD2	0.68	2.49	14	1
1:A:24:PHE:HD2	1:B:330:PHE:CZ	0.68	2.07	1	2
1:B:228:VAL:CG2	1:B:270:VAL:CG2	0.68	2.67	13	9
1:B:298:PRO:O	1:B:299:SER:C	0.68	2.32	1	11
1:B:325:GLU:HA	1:B:328:TYR:CD2	0.68	2.24	5	9
1:B:229:ASN:ND2	1:B:232:THR:HB	0.68	2.03	5	1
1:A:130:PHE:CZ	1:B:270:VAL:CG2	0.68	2.73	7	2
1:B:228:VAL:HB	1:B:270:VAL:HG21	0.68	1.66	11	2
1:A:85:ARG:CG	1:A:112:PHE:HE1	0.68	2.02	11	3
1:A:134:GLY:H	1:B:273:PRO:HB3	0.68	1.49	7	7
1:A:41:LEU:O	1:A:44:LEU:N	0.68	2.27	6	10
1:B:296:ILE:N	1:B:328:TYR:CZ	0.68	2.61	8	4
1:B:342:GLU:CG	1:B:359:ALA:HB1	0.68	2.18	8	5
1:A:76:CYS:SG	1:A:77:THR:N	0.68	2.66	7	3
1:B:235:MET:N	1:B:236:PRO:CD	0.68	2.57	10	1
1:B:361:ARG:O	1:B:365:ASP:OD1	0.68	2.11	12	2
1:A:64:GLU:OE2	1:A:71:LEU:HD21	0.68	1.88	14	1
1:A:28:VAL:CG2	1:A:70:VAL:CG2	0.68	2.65	5	9
1:A:77:THR:HG21	1:B:334:GLY:CA	0.68	2.19	8	3
1:A:49:HIS:O	1:A:53:GLN:HG2	0.68	1.88	7	5
1:B:347:LYS:O	1:B:348:ASP:O	0.68	2.10	3	1
1:B:346:TYR:CD2	1:B:346:TYR:O	0.68	2.47	6	3
1:A:104:VAL:HG22	1:B:307:GLY:H	0.68	1.49	5	1
1:B:244:LEU:HD13	1:B:266:TRP:CH2	0.68	2.24	6	2
1:B:316:ILE:CG2	1:B:318:LEU:HD11	0.68	2.19	9	2
1:A:20:LEU:H	1:A:59:ASN:ND2	0.68	1.87	7	1
1:A:35:MET:CG	1:A:66:TRP:CE3	0.68	2.76	13	2
1:A:75:GLU:OE1	1:A:79:LEU:CD1	0.68	2.42	13	1
1:B:218:VAL:HG22	1:B:289:VAL:CG1	0.67	2.19	9	8
1:B:268:ALA:O	1:B:269:GLN:O	0.67	2.13	12	4
1:A:27:LEU:HD12	1:A:36:PRO:HD2	0.67	1.65	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:GLU:HA	1:A:128:TYR:CD1	0.67	2.23	2	6
1:A:70:VAL:HG13	1:B:330:PHE:CZ	0.67	2.23	9	3
1:A:25:MET:HE2	1:A:25:MET:HA	0.67	1.63	5	2
1:A:98:PRO:CD	1:B:230:PRO:HG3	0.67	2.18	8	1
1:B:267:GLY:O	1:B:268:ALA:HB3	0.67	1.89	11	1
1:A:18:VAL:HG22	1:A:89:VAL:CG1	0.67	2.19	12	8
1:B:247:ILE:HG13	1:B:257:VAL:HG21	0.67	1.66	11	3
1:B:302:THR:O	1:B:303:HIS:C	0.67	2.33	6	15
1:A:23:PRO:HB3	1:A:99:SER:HA	0.67	1.65	10	3
1:B:325:GLU:HA	1:B:328:TYR:CD1	0.67	2.22	2	6
1:A:130:PHE:HE1	1:B:271:LEU:O	0.67	1.71	11	6
1:A:59:ASN:OD1	1:A:60:ALA:N	0.67	2.26	10	4
1:B:229:ASN:CB	1:B:232:THR:O	0.67	2.43	7	5
1:B:284:ILE:HD12	1:B:305:GLU:O	0.67	1.90	7	1
1:A:30:PRO:HG3	1:B:298:PRO:CD	0.67	2.18	8	1
1:B:232:THR:H	1:B:270:VAL:HG11	0.67	1.50	10	1
1:B:240:GLN:CG	1:B:241:LEU:CD1	0.67	2.71	12	1
1:A:43:PHE:O	1:A:47:ILE:CD1	0.67	2.43	4	7
1:A:81:GLN:CB	1:A:108:TRP:CH2	0.67	2.78	1	4
1:A:110:SER:HB3	1:B:308:TRP:HE1	0.67	1.48	1	5
1:A:112:PHE:CD1	1:B:311:ALA:CB	0.67	2.78	1	5
1:A:144:VAL:HG21	1:A:156:ILE:HA	0.67	1.64	7	6
1:B:273:PRO:O	1:B:278:PRO:HD3	0.67	1.89	10	10
1:A:152:ALA:O	1:A:156:ILE:HB	0.67	1.89	14	8
1:B:246:LEU:CA	1:B:249:HIS:CD2	0.67	2.76	5	1
1:A:28:VAL:HG23	1:A:33:ASN:HB3	0.67	1.66	10	2
1:A:35:MET:SD	1:A:36:PRO:HD2	0.67	2.30	8	1
1:B:322:GLU:HG3	1:B:346:TYR:O	0.67	1.90	15	2
1:B:223:PRO:HB2	1:B:227:LEU:HB3	0.67	1.66	3	4
1:B:321:GLU:N	1:B:325:GLU:HB3	0.67	2.05	11	5
1:A:108:TRP:NE1	1:B:310:SER:HB2	0.67	2.02	9	7
1:A:149:ILE:O	1:A:151:LEU:N	0.67	2.28	12	5
1:B:227:LEU:HG	1:B:228:VAL:N	0.67	2.02	14	8
1:B:215:VAL:CG1	1:B:218:VAL:CG2	0.67	2.72	4	4
1:A:29:ASN:ND2	1:A:32:THR:HB	0.67	2.04	5	1
1:A:19:PHE:CD1	1:A:83:GLU:HB3	0.67	2.24	7	3
1:B:224:PHE:HE1	1:B:270:VAL:H	0.67	1.32	10	1
1:A:59:ASN:O	1:A:60:ALA:C	0.67	2.33	15	8
1:A:19:PHE:CE2	1:A:59:ASN:CB	0.67	2.77	3	5
1:A:29:ASN:H	1:A:33:ASN:HB2	0.67	1.48	8	6
1:A:110:SER:OG	1:A:135:LEU:HD21	0.67	1.89	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:318:LEU:N	1:B:318:LEU:CD1	0.67	2.58	9	2
1:B:298:PRO:HA	1:B:328:TYR:CD1	0.67	2.23	8	2
1:A:124:ARG:N	1:A:124:ARG:CD	0.67	2.56	14	4
1:B:286:LYS:HG2	1:B:287:ALA:N	0.67	2.05	15	1
1:A:108:TRP:O	1:A:112:PHE:CD1	0.67	2.48	4	2
1:B:262:ARG:O	1:B:266:TRP:CD1	0.67	2.47	11	7
1:B:284:ILE:HD12	1:B:308:TRP:HB3	0.67	1.66	1	4
1:A:47:ILE:CG1	1:A:57:VAL:HG11	0.67	2.19	13	6
1:A:103:HIS:NE2	1:A:128:TYR:HD2	0.67	1.80	2	4
1:A:106:ILE:CG2	1:A:135:LEU:CD2	0.67	2.73	7	2
1:A:111:ALA:CB	1:B:308:TRP:O	0.67	2.42	12	5
1:B:285:ARG:O	1:B:314:LYS:HE2	0.67	1.90	14	4
1:B:306:ILE:CG2	1:B:335:LEU:CD2	0.67	2.72	7	2
1:B:349:ILE:O	1:B:351:LEU:N	0.67	2.27	12	4
1:B:229:ASN:HB3	1:B:232:THR:O	0.67	1.88	9	4
1:A:24:PHE:HE1	1:A:70:VAL:H	0.67	1.31	10	1
1:B:342:GLU:CD	1:B:359:ALA:HB1	0.67	2.10	14	3
1:B:275:GLU:C	1:B:279:LEU:HD12	0.67	2.09	14	1
1:A:18:VAL:CG1	1:A:50:PHE:CE1	0.67	2.77	9	4
1:A:135:LEU:HA	1:A:138:VAL:HG22	0.67	1.67	7	8
1:B:223:PRO:HA	1:B:299:SER:CB	0.67	2.20	6	9
1:A:111:ALA:CA	1:B:312:PHE:CD2	0.67	2.77	2	2
1:A:157:ASP:O	1:A:161:ARG:HG2	0.67	1.88	14	2
1:B:219:PHE:CZ	1:B:305:GLU:OE1	0.67	2.47	4	1
1:B:291:VAL:O	1:B:291:VAL:HG12	0.67	1.90	5	2
1:A:18:VAL:CG2	1:A:50:PHE:CE2	0.67	2.75	7	3
1:A:40:GLN:NE2	1:A:66:TRP:CG	0.67	2.63	7	1
1:B:290:PHE:HE1	1:B:306:ILE:HG13	0.67	1.49	7	2
1:B:271:LEU:HD12	1:B:276:CYS:SG	0.67	2.30	10	1
1:A:130:PHE:HE1	1:B:270:VAL:O	0.67	1.72	11	1
1:B:291:VAL:HG23	1:B:317:VAL:O	0.67	1.89	12	1
1:B:276:CYS:SG	1:B:280:ASP:OD2	0.67	2.50	14	1
1:A:85:ARG:HB3	1:A:112:PHE:CE2	0.67	2.25	6	5
1:B:340:ALA:CB	1:B:367:VAL:HG21	0.67	2.20	8	6
1:A:104:VAL:HG11	1:B:331:LEU:CG	0.67	2.20	6	3
1:B:303:HIS:HE1	1:B:328:TYR:CD2	0.67	2.03	3	4
1:A:96:ILE:HD12	1:A:128:TYR:CD2	0.67	2.25	10	2
1:A:74:GLU:O	1:A:78:PRO:CG	0.67	2.43	15	2
1:A:35:MET:N	1:A:36:PRO:CD	0.67	2.57	10	1
1:A:65:ALA:CB	1:A:66:TRP:CD1	0.67	2.77	12	2
1:A:161:ARG:O	1:A:165:ASP:OD2	0.67	2.13	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LEU:CG	1:B:304:VAL:HG11	0.67	2.20	6	3
1:A:35:MET:SD	1:A:69:GLN:OE1	0.67	2.53	4	2
1:B:240:GLN:CG	1:B:266:TRP:NE1	0.67	2.58	8	4
1:A:149:ILE:HD13	1:A:152:ALA:HB3	0.67	1.66	5	1
1:B:240:GLN:NE2	1:B:266:TRP:CD1	0.67	2.63	10	1
1:B:325:GLU:OE1	1:B:326:GLU:N	0.67	2.28	10	2
1:A:129:GLY:O	1:A:133:ARG:HB2	0.67	1.89	14	3
1:B:235:MET:CG	1:B:266:TRP:CE3	0.67	2.78	13	2
1:B:265:ALA:CB	1:B:266:TRP:CD1	0.67	2.78	12	2
1:A:121:GLU:N	1:A:125:GLU:HB3	0.67	2.05	11	5
1:B:312:PHE:O	1:B:313:ASP:CG	0.67	2.33	5	1
1:A:24:PHE:HD2	1:B:330:PHE:CE2	0.67	2.08	6	1
1:A:29:ASN:CB	1:A:32:THR:O	0.67	2.43	7	5
1:B:228:VAL:CG2	1:B:233:ASN:CB	0.67	2.70	8	3
1:A:27:LEU:HD21	1:A:28:VAL:HG12	0.67	1.67	13	2
1:A:33:ASN:O	1:A:34:SER:HB3	0.67	1.88	10	1
1:A:31:GLU:OE2	1:B:326:GLU:O	0.67	2.13	11	1
1:A:40:GLN:CA	1:A:66:TRP:CH2	0.67	2.74	12	2
1:B:219:PHE:CD2	1:B:259:ASN:ND2	0.67	2.63	15	1
1:A:140:ALA:CB	1:A:167:VAL:HG21	0.66	2.21	8	6
1:B:240:GLN:OE1	1:B:241:LEU:CD1	0.66	2.43	1	2
1:A:101:GLY:O	1:A:105:GLU:CG	0.66	2.43	2	1
1:B:223:PRO:O	1:B:227:LEU:HD23	0.66	1.89	2	2
1:B:352:ALA:O	1:B:356:ILE:HB	0.66	1.90	14	10
1:B:338:VAL:HG23	1:B:339:ALA:N	0.66	2.05	3	8
1:B:285:ARG:CG	1:B:312:PHE:HE1	0.66	2.02	11	3
1:A:123:GLY:O	1:A:126:GLU:HB2	0.66	1.90	6	2
1:A:19:PHE:CZ	1:A:90:PHE:CE2	0.66	2.83	7	1
1:B:219:PHE:CD1	1:B:283:GLU:HB3	0.66	2.25	7	3
1:B:259:ASN:CA	1:B:283:GLU:HG2	0.66	2.19	8	1
1:A:64:GLU:CD	1:A:64:GLU:H	0.66	1.91	9	1
1:A:129:GLY:O	1:A:130:PHE:C	0.66	2.34	10	15
1:A:111:ALA:HA	1:B:312:PHE:CD1	0.66	2.25	3	6
1:B:285:ARG:HB2	1:B:312:PHE:CE2	0.66	2.25	7	2
1:B:247:ILE:O	1:B:251:GLU:OE1	0.66	2.13	6	1
1:A:24:PHE:HE2	1:A:70:VAL:HA	0.66	1.41	7	3
1:A:20:LEU:CD1	1:A:47:ILE:HD11	0.66	2.19	9	2
1:A:59:ASN:O	1:A:61:HIS:N	0.66	2.28	12	2
1:A:19:PHE:CD2	1:A:59:ASN:CG	0.66	2.69	15	1
1:B:241:LEU:HA	1:B:244:LEU:HG	0.66	1.67	14	10
1:A:85:ARG:HB2	1:A:112:PHE:CE2	0.66	2.25	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:PHE:HD1	1:B:311:ALA:HB1	0.66	1.50	6	4
1:B:344:VAL:HG13	1:B:355:GLN:HG2	0.66	1.64	15	4
1:A:61:HIS:HB2	1:A:65:ALA:CB	0.66	2.18	13	4
1:B:269:GLN:CG	1:B:270:VAL:H	0.66	2.03	8	2
1:A:64:GLU:O	1:A:69:GLN:OE1	0.66	2.12	11	1
1:A:46:LEU:C	1:A:46:LEU:CD1	0.66	2.63	1	2
1:B:339:ALA:O	1:B:341:VAL:N	0.66	2.28	1	13
1:B:235:MET:SD	1:B:269:GLN:OE1	0.66	2.53	6	2
1:A:19:PHE:CB	1:A:87:ALA:HB2	0.66	2.19	8	1
1:A:122:GLU:HG3	1:A:146:TYR:O	0.66	1.90	15	2
1:A:91:VAL:HG23	1:A:117:VAL:O	0.66	1.90	12	1
1:B:253:GLN:HA	1:B:253:GLN:OE1	0.66	1.89	12	1
1:A:121:GLU:HG2	1:A:146:TYR:OH	0.66	1.90	6	2
1:B:228:VAL:CG2	1:B:229:ASN:N	0.66	2.58	10	4
1:B:228:VAL:CG1	1:B:270:VAL:CG2	0.66	2.74	9	5
1:B:244:LEU:N	1:B:244:LEU:HD23	0.66	2.06	6	4
1:B:304:VAL:O	1:B:308:TRP:HB2	0.66	1.90	3	7
1:A:67:GLY:O	1:A:68:ALA:CB	0.66	2.44	5	2
1:B:316:ILE:CG2	1:B:341:VAL:HG22	0.66	2.20	8	5
1:B:319:LEU:HD22	1:B:346:TYR:HB3	0.66	1.66	6	1
1:B:229:ASN:OD1	1:B:230:PRO:N	0.66	2.27	13	1
1:A:125:GLU:N	1:A:125:GLU:OE1	0.66	2.28	15	1
1:A:98:PRO:O	1:A:99:SER:C	0.66	2.33	1	11
1:A:141:VAL:HG12	1:A:143:PHE:CE2	0.66	2.26	9	3
1:A:108:TRP:NE1	1:B:307:GLY:CA	0.66	2.58	12	4
1:A:22:GLY:N	1:A:61:HIS:CE1	0.66	2.63	9	1
1:B:234:SER:OG	1:B:236:PRO:CD	0.66	2.44	10	1
1:A:27:LEU:HD23	1:A:28:VAL:N	0.66	2.04	3	6
1:A:44:LEU:N	1:A:44:LEU:HD23	0.66	2.05	6	5
1:A:124:ARG:O	1:A:128:TYR:CD1	0.66	2.49	2	5
1:B:280:ASP:OD2	1:B:280:ASP:C	0.66	2.34	2	1
1:B:329:GLY:HA2	1:B:333:ARG:HB2	0.66	1.66	15	9
1:A:153:LYS:CB	1:A:154:PRO:CD	0.66	2.73	13	4
1:A:82:LEU:HD13	1:A:85:ARG:HE	0.66	1.49	7	1
1:B:219:PHE:CB	1:B:287:ALA:HB2	0.66	2.21	8	1
1:B:228:VAL:HB	1:B:270:VAL:CG2	0.66	2.21	11	1
1:A:108:TRP:CH2	1:B:331:LEU:CD2	0.66	2.77	12	1
1:A:120:LEU:HB2	1:A:144:VAL:O	0.66	1.91	15	1
1:B:331:LEU:O	1:B:335:LEU:HB2	0.66	1.91	9	10
1:A:116:ILE:HG22	1:A:141:VAL:HG13	0.66	1.67	11	3
1:A:40:GLN:CG	1:A:66:TRP:NE1	0.66	2.58	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:225:MET:O	1:B:228:VAL:N	0.66	2.29	14	2
1:A:28:VAL:HG23	1:A:33:ASN:N	0.66	2.05	8	2
1:B:227:LEU:HD21	1:B:228:VAL:HG12	0.66	1.68	13	2
1:A:23:PRO:CB	1:A:99:SER:HB3	0.66	2.21	13	2
1:A:90:PHE:O	1:A:116:ILE:HA	0.66	1.91	12	1
1:B:291:VAL:HG21	1:B:356:ILE:HD11	0.66	1.68	12	1
1:A:132:VAL:HG13	1:A:143:PHE:CE2	0.66	2.26	15	1
1:B:299:SER:N	1:B:328:TYR:CE2	0.66	2.64	15	1
1:A:41:LEU:HA	1:A:44:LEU:HG	0.66	1.67	14	10
1:A:146:TYR:O	1:A:146:TYR:CD1	0.66	2.48	14	3
1:B:262:ARG:HA	1:B:266:TRP:NE1	0.66	2.06	7	13
1:A:34:SER:O	1:A:35:MET:C	0.66	2.34	13	5
1:A:112:PHE:CD1	1:B:311:ALA:CA	0.66	2.79	12	6
1:A:106:ILE:HG22	1:A:135:LEU:HD13	0.66	1.67	11	2
1:B:284:ILE:HD12	1:B:290:PHE:CE1	0.66	2.26	12	1
1:B:331:LEU:HD23	1:B:335:LEU:CD2	0.66	2.20	14	1
1:A:139:ALA:O	1:A:141:VAL:N	0.66	2.29	12	13
1:A:153:LYS:N	1:A:154:PRO:HD2	0.66	2.06	15	10
1:A:70:VAL:O	1:A:70:VAL:HG12	0.66	1.90	7	5
1:A:112:PHE:O	1:A:113:ASP:CG	0.66	2.35	5	1
1:A:157:ASP:C	1:A:157:ASP:OD1	0.66	2.35	6	1
1:A:84:ILE:HD12	1:A:105:GLU:O	0.66	1.91	7	1
1:B:344:VAL:HG13	1:B:355:GLN:HB3	0.66	1.67	11	1
1:B:223:PRO:CB	1:B:299:SER:HB3	0.66	2.21	13	2
1:B:296:ILE:HG21	1:B:327:GLU:OE2	0.66	1.91	14	1
1:A:19:PHE:CD2	1:A:59:ASN:ND2	0.66	2.62	15	1
1:A:130:PHE:CD1	1:B:225:MET:HB2	0.65	2.26	1	1
1:A:131:LEU:HD23	1:A:135:LEU:HD13	0.65	1.68	2	1
1:A:138:VAL:HG23	1:A:139:ALA:N	0.65	2.06	3	9
1:B:283:GLU:OE2	1:B:286:LYS:HE3	0.65	1.90	4	1
1:A:75:GLU:O	1:A:79:LEU:CD1	0.65	2.43	8	1
1:A:122:GLU:HA	1:A:125:GLU:OE2	0.65	1.91	10	2
1:A:34:SER:HA	1:A:68:ALA:HB1	0.65	1.66	11	1
1:A:104:VAL:HG23	1:B:303:HIS:HB3	0.65	1.68	11	3
1:A:91:VAL:HG21	1:A:156:ILE:HD11	0.65	1.68	12	1
1:B:244:LEU:HD23	1:B:244:LEU:H	0.65	1.51	12	1
1:A:29:ASN:OD1	1:A:30:PRO:N	0.65	2.29	13	1
1:A:80:ASP:OD2	1:A:84:ILE:HD11	0.65	1.90	2	1
1:A:101:GLY:HA2	1:B:331:LEU:HD23	0.65	1.66	5	2
1:A:112:PHE:CD1	1:B:311:ALA:HB1	0.65	2.26	6	6
1:A:101:GLY:O	1:A:105:GLU:CD	0.65	2.34	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:LEU:HB3	1:A:125:GLU:HG2	0.65	1.69	7	2
1:B:259:ASN:OD1	1:B:260:ALA:N	0.65	2.30	10	4
1:A:118:LEU:N	1:A:118:LEU:CD1	0.65	2.56	9	2
1:A:15:VAL:CG2	1:A:160:ILE:CG2	0.65	2.73	15	4
1:B:225:MET:HE1	1:B:301:GLY:H	0.65	1.49	10	1
1:A:44:LEU:HD22	1:A:66:TRP:CH2	0.65	2.26	9	4
1:A:142:GLU:OE1	1:A:144:VAL:HG23	0.65	1.91	1	1
1:B:360:ILE:O	1:B:364:VAL:HB	0.65	1.90	8	2
1:A:19:PHE:CD2	1:A:19:PHE:O	0.65	2.49	4	3
1:B:219:PHE:CD1	1:B:283:GLU:O	0.65	2.49	5	2
1:A:84:ILE:CD1	1:A:90:PHE:CE1	0.65	2.79	12	2
1:B:317:VAL:HG13	1:B:342:GLU:HB2	0.65	1.66	6	2
1:A:64:GLU:CB	1:A:71:LEU:HD21	0.65	2.20	9	5
1:A:119:LEU:CD2	1:A:152:ALA:HB1	0.65	2.22	9	2
1:A:28:VAL:CG2	1:A:32:THR:O	0.65	2.43	10	1
1:B:305:GLU:OE2	1:B:305:GLU:CA	0.65	2.41	10	1
1:A:138:VAL:HG11	1:B:281:GLN:OE1	0.65	1.90	14	1
1:A:38:ALA:O	1:A:42:PRO:HG2	0.65	1.92	13	4
1:A:62:ARG:O	1:A:63:ARG:C	0.65	2.35	14	15
1:A:73:PRO:HG3	1:B:330:PHE:N	0.65	2.07	4	3
1:A:101:GLY:O	1:A:105:GLU:HG3	0.65	1.91	1	3
1:B:293:ILE:O	1:B:293:ILE:CG2	0.65	2.44	12	7
1:A:24:PHE:CE2	1:A:70:VAL:N	0.65	2.65	14	4
1:A:36:PRO:O	1:A:39:GLU:HB3	0.65	1.92	8	7
1:B:223:PRO:HB3	1:B:299:SER:HA	0.65	1.68	10	3
1:B:229:ASN:O	1:B:232:THR:OG1	0.65	2.14	14	3
1:B:342:GLU:HG2	1:B:359:ALA:HB1	0.65	1.68	8	4
1:B:283:GLU:N	1:B:283:GLU:CD	0.65	2.50	4	2
1:B:301:GLY:O	1:B:305:GLU:CD	0.65	2.35	5	2
1:B:219:PHE:CE1	1:B:283:GLU:HB2	0.65	2.27	14	1
1:A:125:GLU:HA	1:A:128:TYR:CD2	0.65	2.25	5	9
1:A:103:HIS:CE1	1:A:128:TYR:CE2	0.65	2.85	9	3
1:B:219:PHE:CE2	1:B:259:ASN:ND2	0.65	2.64	2	1
1:A:24:PHE:CE1	1:A:70:VAL:CA	0.65	2.80	13	4
1:A:117:VAL:HG11	1:A:160:ILE:HG13	0.65	1.68	7	7
1:A:120:LEU:CD1	1:A:125:GLU:OE2	0.65	2.44	4	1
1:B:317:VAL:HG11	1:B:360:ILE:HG13	0.65	1.68	7	6
1:A:58:PHE:CD1	1:A:83:GLU:OE1	0.65	2.49	8	1
1:A:28:VAL:CG2	1:A:69:GLN:O	0.65	2.45	11	1
1:A:31:GLU:CD	1:A:31:GLU:O	0.65	2.34	14	1
1:A:131:LEU:HD23	1:A:135:LEU:HD21	0.65	1.66	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:303:HIS:HE1	1:B:328:TYR:HD2	0.65	1.33	15	1
1:A:73:PRO:O	1:A:77:THR:HB	0.65	1.91	3	10
1:A:142:GLU:CD	1:A:159:ALA:HB1	0.65	2.12	13	4
1:A:156:ILE:O	1:A:160:ILE:HG13	0.65	1.91	6	8
1:A:99:SER:CB	1:A:102:THR:OG1	0.65	2.45	5	6
1:B:349:ILE:HD13	1:B:352:ALA:HB3	0.65	1.67	5	1
1:A:82:LEU:O	1:A:86:LYS:CG	0.65	2.44	8	1
1:B:320:LEU:HD13	1:B:325:GLU:HG3	0.65	1.68	9	2
1:A:125:GLU:OE1	1:A:126:GLU:HB2	0.65	1.92	10	1
1:B:319:LEU:HB3	1:B:346:TYR:CD2	0.65	2.26	1	6
1:B:329:GLY:O	1:B:330:PHE:C	0.65	2.33	10	15
1:B:342:GLU:OE1	1:B:344:VAL:HG23	0.65	1.92	1	1
1:A:28:VAL:HG13	1:A:29:ASN:N	0.65	2.05	2	5
1:B:280:ASP:OD2	1:B:284:ILE:HD11	0.65	1.92	2	1
1:A:29:ASN:OD1	1:A:33:ASN:ND2	0.65	2.29	3	1
1:A:111:ALA:HB1	1:B:312:PHE:CD1	0.65	2.26	6	6
1:A:147:LYS:O	1:A:148:ASP:O	0.65	2.14	3	1
1:B:356:ILE:O	1:B:360:ILE:CG1	0.65	2.45	11	8
1:A:49:HIS:CE1	1:A:157:ASP:OD1	0.65	2.50	10	2
1:B:233:ASN:O	1:B:234:SER:HB3	0.65	1.90	10	1
1:A:67:GLY:O	1:A:68:ALA:HB3	0.65	1.92	11	1
1:B:320:LEU:O	1:B:346:TYR:HD2	0.65	1.74	15	1
1:A:62:ARG:HA	1:A:66:TRP:NE1	0.65	2.06	10	12
1:A:107:GLY:CA	1:B:308:TRP:NE1	0.65	2.59	12	7
1:B:241:LEU:CB	1:B:242:PRO:CD	0.65	2.74	7	11
1:A:131:LEU:HG	1:B:304:VAL:CB	0.65	2.22	6	3
1:A:23:PRO:C	1:A:27:LEU:HD23	0.65	2.12	11	2
1:B:290:PHE:HZ	1:B:305:GLU:HB3	0.65	1.52	11	5
1:A:19:PHE:CE1	1:A:59:ASN:CB	0.65	2.80	6	1
1:B:284:ILE:CD1	1:B:290:PHE:CE1	0.65	2.80	12	2
1:A:46:LEU:HD23	1:A:50:PHE:CE1	0.65	2.27	7	1
1:A:166:ARG:HG3	1:A:167:VAL:N	0.65	2.07	1	1
1:B:262:ARG:O	1:B:263:ARG:C	0.65	2.35	7	15
1:B:336:GLY:HA3	1:B:343:PHE:CE1	0.65	2.27	8	5
1:B:351:LEU:C	1:B:354:PRO:HD2	0.65	2.12	2	10
1:B:353:LYS:N	1:B:354:PRO:HD2	0.65	2.07	15	10
1:A:84:ILE:O	1:A:114:LYS:HG2	0.65	1.92	7	2
1:B:227:LEU:HD12	1:B:236:PRO:HD2	0.65	1.68	8	6
1:B:270:VAL:O	1:B:270:VAL:HG12	0.65	1.91	6	5
1:A:120:LEU:O	1:A:146:TYR:HD1	0.65	1.75	3	3
1:A:83:GLU:N	1:A:83:GLU:CD	0.65	2.51	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:TYR:CD2	1:A:146:TYR:O	0.65	2.50	6	3
1:B:325:GLU:HG2	1:B:345:HIS:CE1	0.65	2.27	6	2
1:B:348:ASP:O	1:B:351:LEU:HD23	0.65	1.92	7	1
1:A:35:MET:CG	1:A:69:GLN:OE1	0.65	2.45	8	1
1:A:56:GLU:CA	1:A:56:GLU:OE2	0.65	2.43	11	1
1:B:247:ILE:HG12	1:B:257:VAL:HG11	0.65	1.68	13	1
1:B:231:GLU:CD	1:B:231:GLU:O	0.65	2.35	14	1
1:B:215:VAL:HG13	1:B:289:VAL:HB	0.65	1.69	2	3
1:A:122:GLU:HA	1:A:145:HIS:ND1	0.65	2.07	15	4
1:B:318:LEU:CD1	1:B:332:VAL:HG22	0.65	2.21	8	2
1:A:34:SER:OG	1:A:36:PRO:CD	0.65	2.45	10	1
1:B:299:SER:OG	1:B:302:THR:OG1	0.65	2.10	10	2
1:B:296:ILE:HB	1:B:324:ARG:CG	0.65	2.22	15	4
1:A:16:ARG:O	1:A:16:ARG:NH1	0.65	2.30	12	1
1:A:25:MET:SD	1:B:330:PHE:HD2	0.65	2.14	14	1
1:A:108:TRP:NE1	1:B:310:SER:HB3	0.64	2.07	1	4
1:B:346:TYR:O	1:B:346:TYR:CD1	0.64	2.50	14	3
1:B:290:PHE:HB3	1:B:315:PRO:O	0.64	1.91	2	9
1:B:219:PHE:CZ	1:B:290:PHE:CE2	0.64	2.85	7	2
1:B:284:ILE:CG2	1:B:312:PHE:CD1	0.64	2.80	5	1
1:A:18:VAL:HG21	1:A:50:PHE:HE2	0.64	1.43	8	2
1:A:96:ILE:HB	1:A:124:ARG:CG	0.64	2.22	15	3
1:A:142:GLU:HA	1:A:142:GLU:OE1	0.64	1.90	15	1
1:A:24:PHE:CD2	1:B:330:PHE:CZ	0.64	2.84	1	2
1:A:95:GLY:O	1:A:96:ILE:C	0.64	2.36	5	15
1:A:108:TRP:O	1:B:311:ALA:CB	0.64	2.45	12	5
1:B:235:MET:HB2	1:B:269:GLN:HG2	0.64	1.67	2	2
1:B:249:HIS:CE1	1:B:250:PHE:CE1	0.64	2.86	6	2
1:B:357:ASP:O	1:B:361:ARG:HG2	0.64	1.91	14	2
1:B:306:ILE:CG2	1:B:335:LEU:HD13	0.64	2.22	11	2
1:B:320:LEU:CD1	1:B:325:GLU:OE2	0.64	2.45	4	1
1:A:25:MET:SD	1:A:30:PRO:CA	0.64	2.85	5	1
1:A:162:LYS:HG2	1:A:163:VAL:N	0.64	2.07	7	2
1:B:228:VAL:HG23	1:B:233:ASN:N	0.64	2.07	8	2
1:A:136:GLY:HA3	1:A:143:PHE:CE1	0.64	2.27	9	5
1:A:68:ALA:O	1:A:69:GLN:HB2	0.64	1.92	2	1
1:B:320:LEU:O	1:B:346:TYR:CD1	0.64	2.50	8	3
1:A:40:GLN:OE1	1:A:65:ALA:CB	0.64	2.46	4	1
1:B:219:PHE:CE1	1:B:259:ASN:OD1	0.64	2.50	4	1
1:A:147:LYS:H	1:A:147:LYS:HD3	0.64	1.51	10	1
1:B:275:GLU:O	1:B:279:LEU:CD2	0.64	2.45	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:MET:HA	1:A:28:VAL:HG12	0.64	1.66	3	4
1:B:244:LEU:HD21	1:B:266:TRP:CZ2	0.64	2.27	4	4
1:A:82:LEU:HG	1:A:85:ARG:NH1	0.64	2.07	3	1
1:A:111:ALA:HB1	1:B:312:PHE:HD1	0.64	1.51	6	5
1:A:125:GLU:HG3	1:A:126:GLU:N	0.64	2.08	8	5
1:B:224:PHE:CA	1:B:227:LEU:HD23	0.64	2.22	5	4
1:B:224:PHE:CE1	1:B:269:GLN:OE1	0.64	2.51	6	1
1:A:66:TRP:HA	1:A:69:GLN:CG	0.64	2.23	12	1
1:A:84:ILE:HD12	1:A:108:TRP:HB3	0.64	1.67	1	4
1:B:295:GLY:O	1:B:296:ILE:C	0.64	2.36	9	15
1:A:44:LEU:HD21	1:A:66:TRP:CZ2	0.64	2.28	4	4
1:B:303:HIS:NE2	1:B:328:TYR:HD2	0.64	1.83	2	4
1:A:130:PHE:CE2	1:B:225:MET:HB2	0.64	2.28	6	2
1:B:245:THR:HG22	1:B:246:LEU:N	0.64	2.07	12	7
1:B:316:ILE:HG22	1:B:341:VAL:HG13	0.64	1.68	11	4
1:A:24:PHE:CA	1:A:27:LEU:HD23	0.64	2.23	5	4
1:A:27:LEU:HG	1:A:28:VAL:N	0.64	2.06	14	7
1:B:357:ASP:C	1:B:357:ASP:OD1	0.64	2.35	6	1
1:A:120:LEU:HD13	1:A:125:GLU:OE2	0.64	1.93	7	3
1:B:229:ASN:N	1:B:233:ASN:HB2	0.64	2.07	7	4
1:A:125:GLU:OE1	1:A:126:GLU:N	0.64	2.31	10	2
1:A:32:THR:O	1:A:70:VAL:CG1	0.64	2.45	12	2
1:B:342:GLU:OE2	1:B:359:ALA:CB	0.64	2.45	13	1
1:A:34:SER:O	1:A:69:GLN:NE2	0.64	2.31	14	1
1:A:131:LEU:HD23	1:A:135:LEU:CD2	0.64	2.23	14	1
1:A:28:VAL:CG1	1:A:70:VAL:CG2	0.64	2.75	9	5
1:A:41:LEU:HB2	1:A:42:PRO:HD3	0.64	1.70	12	8
1:A:85:ARG:O	1:A:114:LYS:HE2	0.64	1.91	14	3
1:B:349:ILE:C	1:B:351:LEU:H	0.64	1.95	12	5
1:B:224:PHE:CE1	1:B:270:VAL:CA	0.64	2.80	13	4
1:A:20:LEU:HD13	1:A:47:ILE:HD12	0.64	1.69	11	3
1:A:104:VAL:HG22	1:B:303:HIS:CB	0.64	2.21	9	1
1:B:234:SER:O	1:B:269:GLN:NE2	0.64	2.31	14	1
1:A:117:VAL:HG22	1:A:142:GLU:HB3	0.64	1.69	1	2
1:B:220:LEU:HG	1:B:247:ILE:HD11	0.64	1.68	6	2
1:B:246:LEU:HD12	1:B:247:ILE:HD12	0.64	1.68	1	2
1:B:336:GLY:CA	1:B:341:VAL:HB	0.64	2.21	12	9
1:A:85:ARG:HB2	1:A:112:PHE:CE1	0.64	2.27	2	1
1:A:94:PRO:HA	1:A:99:SER:OG	0.64	1.93	4	2
1:A:125:GLU:CG	1:A:126:GLU:N	0.64	2.61	5	11
1:A:149:ILE:C	1:A:151:LEU:H	0.64	1.94	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:TYR:HB3	1:A:132:VAL:HB	0.64	1.70	8	5
1:A:79:LEU:O	1:A:83:GLU:OE2	0.64	2.15	5	1
1:A:116:ILE:CG2	1:A:118:LEU:HD11	0.64	2.21	9	2
1:B:284:ILE:HD13	1:B:290:PHE:HE1	0.64	1.53	15	3
1:B:302:THR:O	1:B:306:ILE:HD12	0.64	1.92	6	1
1:B:325:GLU:CD	1:B:325:GLU:C	0.64	2.57	14	5
1:A:84:ILE:CG2	1:A:108:TRP:HB3	0.64	2.18	7	3
1:A:33:ASN:O	1:A:34:SER:CB	0.64	2.46	9	2
1:B:264:GLU:CD	1:B:264:GLU:H	0.64	1.93	9	1
1:A:35:MET:O	1:A:39:GLU:CG	0.64	2.45	10	1
1:A:35:MET:O	1:A:39:GLU:HG3	0.64	1.92	10	1
1:B:264:GLU:O	1:B:269:GLN:CA	0.64	2.45	14	1
1:A:146:TYR:HB2	1:A:152:ALA:HB2	0.64	1.69	9	9
1:A:160:ILE:O	1:A:164:VAL:HB	0.64	1.92	8	3
1:B:221:ALA:HB2	1:B:259:ASN:OD1	0.64	1.93	8	2
1:B:317:VAL:HG22	1:B:342:GLU:HB3	0.64	1.68	1	2
1:B:320:LEU:HB3	1:B:325:GLU:CB	0.64	2.23	11	8
1:B:325:GLU:CG	1:B:326:GLU:N	0.64	2.61	5	12
1:B:356:ILE:O	1:B:360:ILE:HG13	0.64	1.92	6	9
1:A:123:GLY:N	1:A:125:GLU:OE2	0.64	2.30	15	2
1:A:104:VAL:CG1	1:B:307:GLY:HA3	0.64	2.22	3	2
1:B:234:SER:O	1:B:235:MET:C	0.64	2.36	13	5
1:B:246:LEU:HD21	1:B:356:ILE:HG21	0.64	1.70	12	3
1:B:296:ILE:HD13	1:B:327:GLU:HB2	0.64	1.69	6	2
1:A:28:VAL:CG2	1:A:33:ASN:CB	0.64	2.69	8	3
1:A:40:GLN:NE2	1:A:66:TRP:CD1	0.64	2.66	10	1
1:A:19:PHE:CE1	1:A:83:GLU:HB2	0.64	2.28	14	1
1:A:71:LEU:HD23	1:A:71:LEU:N	0.64	2.08	5	2
1:A:73:PRO:HG3	1:B:329:GLY:O	0.64	1.91	1	4
1:B:361:ARG:O	1:B:365:ASP:OD2	0.64	2.15	1	1
1:A:77:THR:O	1:A:81:GLN:HB3	0.64	1.91	3	1
1:A:107:GLY:C	1:B:308:TRP:NE1	0.64	2.51	7	5
1:A:156:ILE:O	1:A:160:ILE:HB	0.64	1.93	9	8
1:B:215:VAL:CG1	1:B:255:LEU:HD22	0.64	2.22	3	2
1:B:289:VAL:HG23	1:B:364:VAL:CG2	0.64	2.23	13	3
1:A:83:GLU:OE2	1:A:86:LYS:HE3	0.64	1.92	4	2
1:A:49:HIS:CE1	1:A:153:LYS:CE	0.64	2.81	5	1
1:B:291:VAL:O	1:B:291:VAL:CG1	0.64	2.46	5	1
1:B:342:GLU:OE1	1:B:342:GLU:HA	0.64	1.90	15	2
1:A:40:GLN:CB	1:A:66:TRP:CE2	0.64	2.74	12	2
1:A:112:PHE:HD2	1:B:311:ALA:CA	0.64	2.06	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:THR:O	1:A:103:HIS:C	0.64	2.36	6	15
1:A:132:VAL:O	1:A:143:PHE:CE2	0.64	2.50	11	2
1:B:319:LEU:O	1:B:346:TYR:HE2	0.64	1.75	1	2
1:B:335:LEU:CB	1:B:341:VAL:HG21	0.64	2.23	12	5
1:B:357:ASP:O	1:B:361:ARG:HG3	0.64	1.93	9	9
1:A:23:PRO:HG2	1:A:27:LEU:HB3	0.64	1.68	15	6
1:A:89:VAL:HG23	1:A:164:VAL:CG2	0.64	2.21	13	3
1:B:320:LEU:HB2	1:B:345:HIS:HA	0.64	1.69	8	6
1:B:356:ILE:O	1:B:360:ILE:HB	0.64	1.93	9	8
1:A:156:ILE:O	1:A:160:ILE:CG1	0.64	2.46	10	8
1:B:261:HIS:HB2	1:B:265:ALA:CB	0.64	2.21	13	4
1:B:296:ILE:HB	1:B:324:ARG:CB	0.64	2.23	15	10
1:A:40:GLN:OE1	1:A:66:TRP:HA	0.64	1.92	7	1
1:A:59:ASN:CA	1:A:83:GLU:HG2	0.64	2.23	8	1
1:B:319:LEU:CD2	1:B:352:ALA:HB1	0.64	2.22	9	2
1:A:18:VAL:HG13	1:A:91:VAL:HG11	0.64	1.69	12	1
1:B:244:LEU:O	1:B:248:GLU:CD	0.64	2.36	12	1
1:B:266:TRP:HA	1:B:269:GLN:HG2	0.64	1.70	13	2
1:A:28:VAL:CG2	1:A:29:ASN:H	0.63	2.05	1	2
1:A:40:GLN:OE1	1:A:41:LEU:CD1	0.63	2.46	1	2
1:A:119:LEU:HD21	1:A:156:ILE:HB	0.63	1.70	1	2
1:B:255:LEU:N	1:B:255:LEU:CD2	0.63	2.41	4	4
1:B:284:ILE:HD13	1:B:290:PHE:HE2	0.63	1.51	3	4
1:B:249:HIS:ND1	1:B:253:GLN:HG2	0.63	2.08	3	2
1:A:28:VAL:CG1	1:A:70:VAL:HG21	0.63	2.23	9	3
1:B:224:PHE:N	1:B:227:LEU:HD23	0.63	2.09	5	2
1:B:219:PHE:CE1	1:B:284:ILE:HG12	0.63	2.28	5	1
1:A:25:MET:CE	1:B:330:PHE:CD2	0.63	2.81	12	2
1:B:229:ASN:H	1:B:233:ASN:CB	0.63	2.06	7	3
1:A:69:GLN:CG	1:A:70:VAL:H	0.63	2.06	8	3
1:A:35:MET:CE	1:A:61:HIS:CD2	0.63	2.81	9	1
1:A:70:VAL:HA	1:B:330:PHE:HZ	0.63	1.54	13	3
1:B:240:GLN:CA	1:B:266:TRP:CZ3	0.63	2.82	12	1
1:B:285:ARG:O	1:B:314:LYS:HE3	0.63	1.94	15	2
1:A:24:PHE:HD2	1:B:330:PHE:CE1	0.63	2.11	1	1
1:B:271:LEU:HD23	1:B:271:LEU:N	0.63	2.08	1	2
1:B:273:PRO:O	1:B:277:THR:HB	0.63	1.93	15	11
1:B:335:LEU:HA	1:B:338:VAL:CG2	0.63	2.22	11	13
1:A:19:PHE:CE2	1:A:59:ASN:ND2	0.63	2.66	2	1
1:B:226:GLY:O	1:B:228:VAL:O	0.63	2.17	5	3
1:A:152:ALA:O	1:A:156:ILE:CB	0.63	2.46	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:298:PRO:HB3	1:B:303:HIS:CE1	0.63	2.28	7	4
1:A:20:LEU:HD22	1:A:47:ILE:HD11	0.63	1.69	10	1
1:A:77:THR:HB	1:A:78:PRO:HD2	0.63	1.70	14	1
1:B:271:LEU:HD12	1:B:275:GLU:OE2	0.63	1.94	15	1
1:B:275:GLU:O	1:B:279:LEU:HD23	0.63	1.92	15	1
1:A:107:GLY:HA3	1:B:304:VAL:HG12	0.63	1.70	1	2
1:A:104:VAL:CB	1:B:331:LEU:HG	0.63	2.22	6	3
1:A:44:LEU:O	1:A:48:GLU:CD	0.63	2.36	12	1
1:A:73:PRO:O	1:A:78:PRO:HD3	0.63	1.92	10	10
1:A:153:LYS:O	1:A:157:ASP:HB2	0.63	1.94	1	1
1:B:269:GLN:O	1:B:270:VAL:C	0.63	2.37	2	6
1:A:24:PHE:CE1	1:A:70:VAL:N	0.63	2.67	3	3
1:B:223:PRO:HG2	1:B:227:LEU:HB3	0.63	1.69	8	7
1:B:320:LEU:O	1:B:346:TYR:HD1	0.63	1.77	3	3
1:B:346:TYR:O	1:B:347:LYS:HG2	0.63	1.94	3	1
1:A:96:ILE:HB	1:A:124:ARG:CB	0.63	2.23	15	8
1:B:223:PRO:HA	1:B:299:SER:HB3	0.63	1.71	8	4
1:A:119:LEU:HD22	1:A:146:TYR:HB3	0.63	1.69	6	1
1:A:148:ASP:O	1:A:151:LEU:HD23	0.63	1.93	7	1
1:B:224:PHE:HE2	1:B:270:VAL:HA	0.63	1.47	7	2
1:A:131:LEU:HD21	1:B:308:TRP:CZ2	0.63	2.27	8	2
1:A:142:GLU:OE1	1:A:159:ALA:HB1	0.63	1.94	9	1
1:A:90:PHE:CD2	1:A:116:ILE:HG12	0.63	2.28	15	1
1:A:15:VAL:O	1:A:55:LEU:CD2	0.63	2.47	5	8
1:A:82:LEU:O	1:A:86:LYS:HB2	0.63	1.94	5	6
1:A:123:GLY:N	1:A:125:GLU:OE1	0.63	2.31	13	4
1:B:325:GLU:HG3	1:B:326:GLU:N	0.63	2.09	8	5
1:B:342:GLU:CD	1:B:363:VAL:HG23	0.63	2.13	4	1
1:A:117:VAL:CG2	1:A:163:VAL:HG21	0.63	2.23	13	1
1:B:296:ILE:HD13	1:B:328:TYR:CE2	0.63	2.29	11	5
1:A:17:SER:HB3	1:A:58:PHE:CD2	0.63	2.29	2	1
1:A:49:HIS:CE1	1:A:50:PHE:CE1	0.63	2.86	6	2
1:B:331:LEU:HD23	1:B:335:LEU:HD13	0.63	1.71	2	1
1:A:149:ILE:O	1:A:153:LYS:CG	0.63	2.47	6	3
1:B:232:THR:HG22	1:B:233:ASN:N	0.63	2.07	5	2
1:B:235:MET:H	1:B:269:GLN:HG3	0.63	1.54	5	1
1:B:332:VAL:HG12	1:B:343:PHE:CZ	0.63	2.29	6	1
1:A:50:PHE:HD2	1:A:55:LEU:HB2	0.63	1.54	8	3
1:B:240:GLN:NE2	1:B:266:TRP:CG	0.63	2.67	7	1
1:B:218:VAL:HG13	1:B:291:VAL:HG11	0.63	1.69	12	1
1:A:30:PRO:CB	1:B:327:GLU:OE1	0.63	2.47	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:227:LEU:HD11	1:B:235:MET:CG	0.63	2.24	12	4
1:B:306:ILE:HG23	1:B:335:LEU:HD22	0.63	1.70	8	6
1:B:320:LEU:N	1:B:320:LEU:HD23	0.63	2.08	14	6
1:A:111:ALA:CA	1:B:312:PHE:HD2	0.63	2.07	13	2
1:B:246:LEU:O	1:B:249:HIS:N	0.63	2.31	6	5
1:A:112:PHE:CD1	1:B:311:ALA:HA	0.63	2.28	12	6
1:B:228:VAL:CG1	1:B:270:VAL:HG22	0.63	2.23	6	4
1:A:144:VAL:HG13	1:A:155:GLN:HG2	0.63	1.71	15	4
1:A:117:VAL:HG13	1:A:142:GLU:CB	0.63	2.23	6	2
1:A:130:PHE:CD2	1:B:225:MET:HE2	0.63	2.28	8	3
1:A:148:ASP:OD1	1:A:150:ALA:HB3	0.63	1.94	7	1
1:A:71:LEU:HD12	1:A:76:CYS:SG	0.63	2.33	10	1
1:A:112:PHE:CE2	1:B:311:ALA:CB	0.63	2.78	14	2
1:B:219:PHE:CE1	1:B:259:ASN:CG	0.63	2.72	6	3
1:A:49:HIS:CE1	1:A:50:PHE:CG	0.63	2.87	2	1
1:A:50:PHE:HB3	1:A:55:LEU:O	0.63	1.94	4	9
1:B:217:SER:HB3	1:B:258:PHE:CD2	0.63	2.29	2	1
1:B:245:THR:O	1:B:248:GLU:CB	0.63	2.47	11	4
1:B:306:ILE:HG22	1:B:335:LEU:HD21	0.63	1.71	7	2
1:B:328:TYR:HB3	1:B:332:VAL:HB	0.63	1.69	8	4
1:B:360:ILE:O	1:B:364:VAL:CG2	0.63	2.38	9	5
1:A:19:PHE:CD1	1:A:83:GLU:O	0.63	2.52	5	2
1:A:35:MET:HB2	1:A:69:GLN:CD	0.63	2.14	6	2
1:A:125:GLU:HG2	1:A:145:HIS:CE1	0.63	2.29	6	3
1:A:125:GLU:CD	1:A:125:GLU:C	0.63	2.57	14	5
1:A:44:LEU:O	1:A:48:GLU:OE2	0.63	2.16	12	1
1:A:66:TRP:HA	1:A:69:GLN:HG2	0.63	1.69	13	2
1:A:19:PHE:CE1	1:A:59:ASN:CG	0.63	2.72	6	3
1:A:24:PHE:C	1:A:27:LEU:CD2	0.63	2.66	7	8
1:A:23:PRO:O	1:A:27:LEU:HD23	0.63	1.94	2	2
1:A:84:ILE:HD13	1:A:90:PHE:HE2	0.63	1.51	3	4
1:A:111:ALA:HA	1:B:312:PHE:CD2	0.63	2.29	2	2
1:B:301:GLY:O	1:B:305:GLU:CG	0.63	2.47	2	1
1:A:43:PHE:CZ	1:A:93:ILE:HD12	0.63	2.29	3	2
1:B:352:ALA:O	1:B:356:ILE:CB	0.63	2.47	14	4
1:A:19:PHE:CE1	1:A:84:ILE:HG12	0.63	2.29	5	1
1:A:120:LEU:HD13	1:A:125:GLU:HG3	0.63	1.70	9	2
1:A:81:GLN:HA	1:A:84:ILE:HG13	0.63	1.69	13	3
1:A:99:SER:N	1:A:128:TYR:CE2	0.63	2.67	15	1
1:B:224:PHE:CE2	1:B:270:VAL:N	0.62	2.67	2	6
1:B:238:ALA:O	1:B:242:PRO:HG2	0.62	1.94	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:241:LEU:N	1:B:242:PRO:CD	0.62	2.62	13	3
1:A:157:ASP:O	1:A:161:ARG:CG	0.62	2.47	2	4
1:B:260:ALA:O	1:B:261:HIS:CG	0.62	2.52	15	6
1:B:240:GLN:OE1	1:B:265:ALA:CB	0.62	2.47	4	1
1:B:218:VAL:CG1	1:B:218:VAL:O	0.62	2.48	7	1
1:A:142:GLU:OE2	1:A:144:VAL:HG23	0.62	1.94	13	1
1:B:368:ASN:O	1:B:368:ASN:ND2	0.62	2.32	14	1
1:A:75:GLU:O	1:A:79:LEU:HD23	0.62	1.94	15	1
1:A:103:HIS:HE1	1:A:128:TYR:HD2	0.62	1.33	15	1
1:B:320:LEU:HB2	1:B:344:VAL:O	0.62	1.93	15	1
1:A:21:ALA:HB2	1:A:59:ASN:OD1	0.62	1.93	1	2
1:B:228:VAL:CG2	1:B:229:ASN:H	0.62	2.07	1	2
1:A:90:PHE:HB3	1:A:115:PRO:O	0.62	1.95	2	9
1:B:349:ILE:C	1:B:351:LEU:N	0.62	2.53	12	8
1:B:357:ASP:O	1:B:361:ARG:CG	0.62	2.47	2	5
1:A:82:LEU:N	1:A:82:LEU:HD22	0.62	2.08	5	1
1:A:90:PHE:HZ	1:A:105:GLU:HB3	0.62	1.53	11	4
1:B:308:TRP:O	1:B:312:PHE:CD2	0.62	2.52	9	3
1:B:274:GLU:O	1:B:278:PRO:CG	0.62	2.46	15	2
1:B:362:LYS:HG2	1:B:363:VAL:N	0.62	2.08	7	2
1:A:84:ILE:O	1:A:114:LYS:HD2	0.62	1.94	13	1
1:B:307:GLY:O	1:B:310:SER:OG	0.62	2.17	15	1
1:A:112:PHE:CD2	1:B:311:ALA:HA	0.62	2.29	13	2
1:B:225:MET:HE2	1:B:225:MET:N	0.62	2.09	4	3
1:A:62:ARG:CD	1:A:66:TRP:CZ2	0.62	2.83	6	1
1:B:296:ILE:HD13	1:B:328:TYR:CD1	0.62	2.29	7	3
1:A:27:LEU:HD11	1:A:35:MET:CG	0.62	2.24	13	3
1:A:41:LEU:N	1:A:42:PRO:CD	0.62	2.62	13	3
1:B:249:HIS:CE1	1:B:250:PHE:CG	0.62	2.87	2	1
1:B:278:PRO:O	1:B:282:LEU:HD22	0.62	1.93	4	1
1:B:295:GLY:HA2	1:B:324:ARG:CD	0.62	2.25	5	1
1:B:258:PHE:CD1	1:B:283:GLU:OE1	0.62	2.52	8	1
1:A:130:PHE:CD2	1:B:225:MET:CG	0.62	2.79	11	1
1:A:86:LYS:HG2	1:A:87:ALA:N	0.62	2.08	15	1
1:B:363:VAL:CG1	1:B:364:VAL:N	0.62	2.63	4	6
1:B:219:PHE:CE2	1:B:259:ASN:CG	0.62	2.73	5	2
1:B:299:SER:CB	1:B:302:THR:OG1	0.62	2.48	10	6
1:A:85:ARG:HB2	1:A:112:PHE:CD2	0.62	2.29	3	2
1:A:82:LEU:CD1	1:A:82:LEU:N	0.62	2.62	4	3
1:B:220:LEU:CD1	1:B:247:ILE:HD11	0.62	2.24	9	3
1:B:322:GLU:HA	1:B:345:HIS:ND1	0.62	2.10	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:233:ASN:O	1:B:234:SER:CB	0.62	2.47	9	2
1:B:235:MET:CE	1:B:261:HIS:CD2	0.62	2.82	9	1
1:B:235:MET:O	1:B:239:GLU:CG	0.62	2.47	10	1
1:B:260:ALA:O	1:B:261:HIS:CB	0.62	2.48	11	3
1:A:47:ILE:HG12	1:A:57:VAL:HG11	0.62	1.71	13	1
1:A:82:LEU:O	1:A:86:LYS:CB	0.62	2.47	2	6
1:A:131:LEU:O	1:A:135:LEU:HB2	0.62	1.94	7	11
1:B:358:ALA:O	1:B:362:LYS:HB2	0.62	1.95	1	1
1:A:24:PHE:HE2	1:A:70:VAL:H	0.62	1.36	15	4
1:B:224:PHE:HE2	1:B:270:VAL:N	0.62	1.92	5	4
1:A:112:PHE:HD1	1:B:311:ALA:CB	0.62	2.06	6	5
1:B:276:CYS:SG	1:B:277:THR:N	0.62	2.71	7	3
1:A:98:PRO:CG	1:B:230:PRO:HG3	0.62	2.25	8	2
1:A:44:LEU:HD23	1:A:44:LEU:H	0.62	1.50	12	1
1:A:24:PHE:CZ	1:A:61:HIS:ND1	0.62	2.67	15	2
1:B:316:ILE:O	1:B:317:VAL:CG2	0.62	2.48	11	8
1:A:28:VAL:CB	1:A:70:VAL:CG2	0.62	2.78	11	3
1:B:325:GLU:OE1	1:B:345:HIS:NE2	0.62	2.33	5	1
1:B:220:LEU:HD13	1:B:221:ALA:H	0.62	1.53	6	1
1:A:29:ASN:N	1:A:33:ASN:HB2	0.62	2.09	7	4
1:A:61:HIS:C	1:A:64:GLU:OE1	0.62	2.38	11	1
1:A:53:GLN:CD	1:A:53:GLN:C	0.62	2.58	15	1
1:B:219:PHE:CE1	1:B:259:ASN:CB	0.62	2.83	6	2
1:B:286:LYS:O	1:B:287:ALA:O	0.62	2.17	3	2
1:A:32:THR:HG23	1:A:33:ASN:N	0.62	2.10	3	2
1:B:229:ASN:N	1:B:229:ASN:HD22	0.62	1.92	3	1
1:A:132:VAL:HG12	1:A:143:PHE:CZ	0.62	2.30	6	1
1:B:290:PHE:O	1:B:316:ILE:HA	0.62	1.94	12	1
1:B:219:PHE:CD2	1:B:259:ASN:CG	0.62	2.73	15	1
1:A:60:ALA:O	1:A:61:HIS:CG	0.62	2.53	6	6
1:A:120:LEU:HD13	1:A:125:GLU:OE1	0.62	1.95	6	2
1:B:317:VAL:HG13	1:B:342:GLU:CB	0.62	2.24	6	2
1:B:250:PHE:HD2	1:B:255:LEU:HB2	0.62	1.54	8	3
1:B:235:MET:O	1:B:239:GLU:HG3	0.62	1.94	10	1
1:A:40:GLN:CA	1:A:66:TRP:CZ3	0.62	2.82	12	1
1:B:243:PHE:N	1:B:243:PHE:CD2	0.62	2.67	1	2
1:B:281:GLN:CB	1:B:308:TRP:CH2	0.62	2.82	1	4
1:A:80:ASP:OD2	1:A:80:ASP:C	0.62	2.34	2	1
1:A:138:VAL:HG23	1:A:139:ALA:H	0.62	1.54	9	9
1:B:228:VAL:HG13	1:B:229:ASN:N	0.62	2.09	2	5
1:B:285:ARG:CB	1:B:312:PHE:CE1	0.62	2.83	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:CE1	1:A:59:ASN:OD1	0.62	2.53	4	1
1:B:282:LEU:N	1:B:282:LEU:CD1	0.62	2.62	13	2
1:A:84:ILE:CG2	1:A:112:PHE:CD1	0.62	2.82	5	1
1:A:138:VAL:HB	1:B:281:GLN:HE22	0.62	1.54	7	1
1:B:284:ILE:O	1:B:314:LYS:HG3	0.62	1.95	8	3
1:A:60:ALA:O	1:A:61:HIS:CB	0.62	2.45	11	3
1:B:228:VAL:HG13	1:B:232:THR:C	0.62	2.15	11	1
1:B:229:ASN:N	1:B:232:THR:OG1	0.62	2.33	14	1
1:B:224:PHE:C	1:B:227:LEU:CD2	0.61	2.68	7	7
1:A:41:LEU:CB	1:A:42:PRO:CD	0.61	2.78	7	11
1:A:46:LEU:HD21	1:A:156:ILE:HG21	0.61	1.70	3	3
1:A:48:GLU:O	1:A:52:LYS:HB2	0.61	1.95	8	5
1:A:82:LEU:N	1:A:82:LEU:HD13	0.61	2.10	4	1
1:A:91:VAL:O	1:A:91:VAL:HG12	0.61	1.94	5	1
1:B:336:GLY:HA3	1:B:343:PHE:CE2	0.61	2.30	5	1
1:A:25:MET:HE3	1:B:330:PHE:CD2	0.61	2.29	7	2
1:B:325:GLU:OE1	1:B:326:GLU:HB2	0.61	1.95	10	1
1:A:29:ASN:OD1	1:A:33:ASN:OD1	0.61	2.17	11	1
1:B:266:TRP:HA	1:B:269:GLN:CG	0.61	2.24	12	1
1:B:240:GLN:HG2	1:B:244:LEU:HD22	0.61	1.70	13	1
1:B:244:LEU:N	1:B:244:LEU:HD13	0.61	2.10	13	1
1:B:285:ARG:NE	1:B:312:PHE:CZ	0.61	2.68	15	1
1:A:19:PHE:CD1	1:A:59:ASN:CB	0.61	2.82	1	3
1:A:77:THR:OG1	1:B:330:PHE:O	0.61	2.18	10	4
1:B:282:LEU:O	1:B:286:LYS:CB	0.61	2.48	2	6
1:B:319:LEU:HD21	1:B:356:ILE:HB	0.61	1.71	1	2
1:A:46:LEU:O	1:A:49:HIS:ND1	0.61	2.26	6	2
1:B:224:PHE:HE2	1:B:270:VAL:H	0.61	1.36	15	4
1:A:119:LEU:CD1	1:A:156:ILE:HD12	0.61	2.24	3	1
1:B:223:PRO:HB3	1:B:294:PRO:O	0.61	1.95	3	2
1:A:130:PHE:HZ	1:B:270:VAL:HA	0.61	1.54	12	4
1:B:282:LEU:O	1:B:286:LYS:CG	0.61	2.48	8	1
1:A:130:PHE:HD2	1:B:225:MET:HG2	0.61	1.54	11	1
1:A:93:ILE:O	1:A:94:PRO:O	0.61	2.18	5	13
1:B:215:VAL:O	1:B:255:LEU:CD2	0.61	2.48	10	8
1:A:98:PRO:O	1:A:100:PRO:N	0.61	2.34	8	5
1:A:112:PHE:CD2	1:B:311:ALA:CA	0.61	2.82	13	2
1:A:149:ILE:C	1:A:151:LEU:N	0.61	2.53	12	8
1:B:248:GLU:O	1:B:252:LYS:HB2	0.61	1.95	15	5
1:A:91:VAL:O	1:A:91:VAL:CG1	0.61	2.48	5	1
1:A:69:GLN:O	1:A:70:VAL:HB	0.61	1.95	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:332:VAL:HG12	1:B:343:PHE:CE2	0.61	2.31	11	2
1:A:18:VAL:CG1	1:A:18:VAL:O	0.61	2.48	7	1
1:B:224:PHE:CE1	1:B:261:HIS:CD2	0.61	2.89	9	1
1:B:274:GLU:O	1:B:274:GLU:CG	0.61	2.48	10	1
1:B:216:ARG:O	1:B:216:ARG:NH1	0.61	2.33	12	1
1:A:69:GLN:CD	1:A:70:VAL:HG23	0.61	2.14	14	1
1:A:90:PHE:HB3	1:A:116:ILE:HA	0.61	1.71	10	7
1:A:120:LEU:HB2	1:A:145:HIS:HA	0.61	1.72	11	8
1:B:277:THR:N	1:B:278:PRO:HD2	0.61	2.11	1	6
1:B:366:ARG:HG3	1:B:367:VAL:N	0.61	2.10	1	1
1:A:134:GLY:O	1:A:138:VAL:CG2	0.61	2.42	10	5
1:B:285:ARG:HB2	1:B:312:PHE:CE1	0.61	2.31	2	1
1:B:221:ALA:HB1	1:B:305:GLU:OE1	0.61	1.95	3	1
1:B:224:PHE:CZ	1:B:269:GLN:HG3	0.61	2.30	6	3
1:B:352:ALA:O	1:B:356:ILE:CG2	0.61	2.48	14	2
1:B:308:TRP:O	1:B:312:PHE:CD1	0.61	2.53	4	1
1:B:282:LEU:N	1:B:282:LEU:HD22	0.61	2.11	5	1
1:A:29:ASN:HB3	1:A:32:THR:O	0.61	1.95	9	4
1:A:73:PRO:CB	1:B:330:PHE:O	0.61	2.48	10	5
1:A:130:PHE:CD2	1:B:225:MET:CE	0.61	2.83	12	2
1:B:281:GLN:N	1:B:308:TRP:CZ3	0.61	2.68	7	2
1:B:360:ILE:O	1:B:364:VAL:CB	0.61	2.47	8	1
1:B:249:HIS:CE1	1:B:357:ASP:OD1	0.61	2.53	11	2
1:B:296:ILE:HD13	1:B:328:TYR:CD2	0.61	2.30	12	5
1:B:353:LYS:O	1:B:357:ASP:HB2	0.61	1.95	1	2
1:A:94:PRO:C	1:A:99:SER:OG	0.61	2.39	4	2
1:B:260:ALA:C	1:B:261:HIS:HD1	0.61	1.98	2	1
1:B:294:PRO:HA	1:B:299:SER:OG	0.61	1.95	4	2
1:B:341:VAL:HG12	1:B:343:PHE:CE2	0.61	2.30	6	3
1:A:108:TRP:O	1:A:112:PHE:CD2	0.61	2.54	9	4
1:B:240:GLN:CB	1:B:266:TRP:CE2	0.61	2.76	12	2
1:A:24:PHE:CD1	1:A:70:VAL:HA	0.61	2.30	13	1
1:A:96:ILE:HG12	1:A:127:GLU:OE2	0.61	1.96	1	1
1:B:250:PHE:HB3	1:B:255:LEU:O	0.61	1.95	4	9
1:B:294:PRO:C	1:B:299:SER:OG	0.61	2.39	4	2
1:A:23:PRO:HG2	1:A:27:LEU:CB	0.61	2.25	3	2
1:A:152:ALA:O	1:A:156:ILE:CG2	0.61	2.48	14	2
1:A:103:HIS:HB3	1:B:304:VAL:HG23	0.61	1.72	15	4
1:B:224:PHE:CE1	1:B:269:GLN:NE2	0.61	2.68	7	3
1:B:356:ILE:O	1:B:360:ILE:HD12	0.61	1.96	8	2
1:B:269:GLN:OE1	1:B:269:GLN:HA	0.61	1.94	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:PHE:CE1	1:B:270:VAL:HG13	0.61	2.30	11	1
1:B:234:SER:CB	1:B:268:ALA:HB1	0.61	2.26	11	1
1:A:47:ILE:N	1:A:47:ILE:CD1	0.61	2.63	14	1
1:B:225:MET:HE2	1:B:226:GLY:N	0.61	2.10	15	1
1:A:43:PHE:N	1:A:43:PHE:CD2	0.61	2.67	1	4
1:A:46:LEU:HD11	1:A:50:PHE:CD1	0.61	2.31	1	1
1:A:46:LEU:HD13	1:A:46:LEU:O	0.61	1.95	5	2
1:B:316:ILE:CG2	1:B:341:VAL:HG13	0.61	2.25	10	9
1:B:246:LEU:O	1:B:249:HIS:ND1	0.61	2.32	2	2
1:B:274:GLU:O	1:B:278:PRO:HG3	0.61	1.95	7	3
1:B:319:LEU:CG	1:B:356:ILE:HD12	0.61	2.21	8	5
1:A:92:ALA:CB	1:A:118:LEU:HD23	0.61	2.18	5	1
1:A:156:ILE:O	1:A:160:ILE:CB	0.61	2.48	11	4
1:B:235:MET:HB2	1:B:269:GLN:CD	0.61	2.16	6	2
1:A:56:GLU:HB3	1:A:58:PHE:HE2	0.61	1.55	7	3
1:A:75:GLU:O	1:A:79:LEU:HG	0.61	1.95	12	2
1:B:320:LEU:O	1:B:346:TYR:CD2	0.61	2.53	15	2
1:B:284:ILE:O	1:B:314:LYS:HD2	0.61	1.95	13	1
1:A:106:ILE:HG23	1:A:135:LEU:HD22	0.61	1.71	9	6
1:B:317:VAL:HG22	1:B:342:GLU:CB	0.61	2.19	13	6
1:B:353:LYS:HB2	1:B:354:PRO:HD3	0.61	1.70	10	8
1:A:120:LEU:O	1:A:146:TYR:CD1	0.61	2.53	8	3
1:B:271:LEU:HB2	1:B:276:CYS:SG	0.61	2.35	4	2
1:A:96:ILE:HD13	1:A:127:GLU:HB2	0.61	1.71	6	2
1:A:40:GLN:HG3	1:A:65:ALA:O	0.61	1.96	6	1
1:A:58:PHE:C	1:A:59:ASN:HD22	0.61	1.99	7	2
1:A:62:ARG:HB3	1:A:62:ARG:NH1	0.61	2.10	9	1
1:B:224:PHE:HD2	1:B:270:VAL:HG23	0.61	1.55	11	1
1:A:135:LEU:HA	1:A:138:VAL:CG2	0.61	2.25	11	12
1:B:316:ILE:HG21	1:B:341:VAL:HG13	0.61	1.73	5	5
1:A:71:LEU:O	1:B:330:PHE:CE2	0.61	2.53	4	4
1:A:107:GLY:HA2	1:A:135:LEU:HD11	0.61	1.73	3	1
1:B:225:MET:HG3	1:B:226:GLY:N	0.61	2.11	3	2
1:B:240:GLN:OE1	1:B:240:GLN:O	0.61	2.19	3	1
1:B:219:PHE:CD2	1:B:219:PHE:O	0.61	2.54	4	3
1:B:267:GLY:O	1:B:268:ALA:CB	0.61	2.49	5	2
1:A:84:ILE:HG13	1:A:108:TRP:CE3	0.61	2.31	8	3
1:B:351:LEU:HD23	1:B:352:ALA:H	0.61	1.56	7	1
1:B:220:LEU:HD13	1:B:247:ILE:HD12	0.61	1.73	8	3
1:B:269:GLN:OE1	1:B:270:VAL:HG23	0.61	1.95	10	1
1:B:294:PRO:HB3	1:B:328:TYR:CD2	0.61	2.29	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:224:PHE:CD1	1:B:270:VAL:HA	0.61	2.30	13	1
1:A:71:LEU:O	1:B:330:PHE:HE2	0.61	1.79	9	4
1:A:41:LEU:HB2	1:A:42:PRO:CD	0.61	2.26	2	8
1:B:294:PRO:O	1:B:299:SER:OG	0.61	2.19	4	3
1:B:224:PHE:CE1	1:B:270:VAL:N	0.61	2.69	3	3
1:B:347:LYS:O	1:B:351:LEU:HB2	0.61	1.96	15	2
1:B:306:ILE:O	1:B:309:ALA:N	0.61	2.33	10	3
1:A:112:PHE:CE1	1:B:311:ALA:HA	0.61	2.31	6	2
1:A:120:LEU:HD12	1:A:145:HIS:HE2	0.61	1.54	6	2
1:A:118:LEU:CD1	1:A:132:VAL:HG22	0.61	2.26	8	2
1:A:160:ILE:O	1:A:164:VAL:CB	0.61	2.49	8	1
1:B:269:GLN:CD	1:B:270:VAL:HG23	0.61	2.16	14	1
1:A:110:SER:HB3	1:B:308:TRP:NE1	0.60	2.10	1	5
1:A:151:LEU:C	1:A:154:PRO:HD2	0.60	2.17	8	10
1:B:261:HIS:ND1	1:B:261:HIS:N	0.60	2.49	7	5
1:A:46:LEU:O	1:A:49:HIS:N	0.60	2.33	6	5
1:A:80:ASP:OD1	1:A:105:GLU:CD	0.60	2.40	2	2
1:A:23:PRO:HB3	1:A:94:PRO:O	0.60	1.95	3	2
1:A:25:MET:HB3	1:B:330:PHE:CE1	0.60	2.31	4	1
1:B:259:ASN:OD1	1:B:280:ASP:OD1	0.60	2.19	14	2
1:A:56:GLU:HB3	1:A:58:PHE:CE2	0.60	2.30	7	3
1:A:46:LEU:HD21	1:A:153:LYS:HA	0.60	1.72	12	2
1:B:247:ILE:HG13	1:B:257:VAL:CG2	0.60	2.26	13	2
1:A:90:PHE:CE2	1:A:106:ILE:HA	0.60	2.31	15	2
1:A:93:ILE:HG13	1:A:119:LEU:HB2	0.60	1.73	12	1
1:B:275:GLU:OE1	1:B:279:LEU:HD11	0.60	1.95	13	1
1:B:264:GLU:OE1	1:B:271:LEU:HD11	0.60	1.95	15	1
1:A:106:ILE:HG22	1:A:107:GLY:N	0.60	2.12	1	5
1:A:130:PHE:HE2	1:B:271:LEU:O	0.60	1.79	9	4
1:B:346:TYR:HB2	1:B:352:ALA:HB2	0.60	1.70	9	9
1:A:49:HIS:ND1	1:A:53:GLN:HG2	0.60	2.10	3	2
1:A:59:ASN:OD1	1:A:105:GLU:OE1	0.60	2.18	4	1
1:B:319:LEU:HB3	1:B:346:TYR:CD1	0.60	2.31	4	3
1:B:240:GLN:NE2	1:B:266:TRP:HE1	0.60	1.93	6	1
1:A:74:GLU:O	1:A:78:PRO:HG3	0.60	1.94	7	2
1:A:30:PRO:HG3	1:B:298:PRO:CG	0.60	2.26	8	1
1:A:98:PRO:CD	1:B:230:PRO:CG	0.60	2.80	8	1
1:B:275:GLU:O	1:B:279:LEU:CG	0.60	2.49	15	3
1:B:266:TRP:HD1	1:B:266:TRP:N	0.60	1.89	9	1
1:A:70:VAL:HG13	1:B:330:PHE:CE1	0.60	2.31	11	1
1:A:94:PRO:HB3	1:A:128:TYR:CD2	0.60	2.31	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:256:GLU:OE2	1:B:257:VAL:N	0.60	2.34	11	1
1:B:232:THR:O	1:B:270:VAL:CG1	0.60	2.50	12	2
1:B:256:GLU:O	1:B:258:PHE:HE2	0.60	1.79	15	1
1:B:246:LEU:C	1:B:246:LEU:CD1	0.60	2.66	5	2
1:B:319:LEU:HD22	1:B:346:TYR:CD2	0.60	2.31	2	1
1:A:104:VAL:O	1:A:108:TRP:CB	0.60	2.49	3	2
1:B:232:THR:O	1:B:233:ASN:CB	0.60	2.49	9	4
1:A:116:ILE:O	1:A:117:VAL:CG2	0.60	2.49	15	9
1:A:74:GLU:O	1:A:74:GLU:CG	0.60	2.49	10	1
1:A:130:PHE:O	1:B:273:PRO:HA	0.60	1.96	14	3
1:A:25:MET:HG3	1:B:330:PHE:CD2	0.60	2.31	14	1
1:A:157:ASP:O	1:A:161:ARG:HG3	0.60	1.97	9	7
1:B:308:TRP:O	1:B:312:PHE:CB	0.60	2.49	9	5
1:A:25:MET:O	1:A:26:GLY:C	0.60	2.40	14	2
1:A:25:MET:HE1	1:A:31:GLU:H	0.60	1.56	5	1
1:A:99:SER:HB3	1:A:102:THR:OG1	0.60	1.96	5	1
1:A:120:LEU:CD2	1:A:125:GLU:HB2	0.60	2.23	12	3
1:A:148:ASP:OD1	1:A:150:ALA:N	0.60	2.35	14	2
1:A:66:TRP:HD1	1:A:66:TRP:N	0.60	1.88	9	1
1:B:240:GLN:N	1:B:266:TRP:CZ3	0.60	2.69	13	2
1:A:56:GLU:O	1:A:58:PHE:HE2	0.60	1.78	15	1
1:A:23:PRO:HG3	1:A:94:PRO:O	0.60	1.97	7	3
1:A:130:PHE:CZ	1:B:224:PHE:HD2	0.60	2.14	6	3
1:B:280:ASP:OD1	1:B:305:GLU:CD	0.60	2.39	2	2
1:A:96:ILE:CD1	1:A:127:GLU:HB2	0.60	2.26	15	5
1:A:160:ILE:O	1:A:164:VAL:CG2	0.60	2.38	9	3
1:A:136:GLY:HA3	1:A:143:PHE:CE2	0.60	2.31	5	3
1:B:320:LEU:HB3	1:B:325:GLU:HG2	0.60	1.73	7	2
1:A:120:LEU:CB	1:A:145:HIS:CD2	0.60	2.84	6	2
1:B:320:LEU:CB	1:B:345:HIS:CD2	0.60	2.84	6	2
1:B:281:GLN:HA	1:B:308:TRP:CE3	0.60	2.31	7	1
1:A:84:ILE:O	1:A:114:LYS:HG3	0.60	1.95	8	1
1:A:91:VAL:HG22	1:A:117:VAL:O	0.60	1.96	9	1
1:B:290:PHE:HE2	1:B:306:ILE:HA	0.60	1.57	12	1
1:A:53:GLN:HA	1:A:53:GLN:NE2	0.60	2.10	14	1
1:A:130:PHE:CE1	1:B:224:PHE:HD2	0.60	2.15	1	1
1:A:45:THR:HG22	1:A:46:LEU:N	0.60	2.12	12	8
1:A:119:LEU:O	1:A:121:GLU:OE2	0.60	2.19	3	2
1:B:223:PRO:HG2	1:B:227:LEU:CB	0.60	2.27	3	2
1:B:319:LEU:CD1	1:B:356:ILE:HD12	0.60	2.25	3	1
1:A:29:ASN:H	1:A:33:ASN:CB	0.60	2.10	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:GLU:CG	1:A:124:ARG:HB2	0.60	2.27	7	1
1:A:44:LEU:O	1:A:48:GLU:HB3	0.60	1.97	8	1
1:B:340:ALA:HB1	1:B:363:VAL:CG2	0.60	2.26	8	1
1:A:33:ASN:O	1:A:34:SER:HB2	0.60	1.95	9	1
1:B:320:LEU:HB3	1:B:325:GLU:HG3	0.60	1.74	13	4
1:B:258:PHE:CE1	1:B:286:LYS:HB3	0.60	2.32	13	1
1:A:153:LYS:HB2	1:A:154:PRO:HD3	0.60	1.73	10	9
1:B:220:LEU:HD11	1:B:250:PHE:HE2	0.60	1.55	2	1
1:B:281:GLN:HA	1:B:284:ILE:HG13	0.60	1.71	13	6
1:B:325:GLU:CA	1:B:328:TYR:HD1	0.60	2.09	2	6
1:A:19:PHE:CZ	1:A:105:GLU:OE1	0.60	2.54	4	1
1:A:23:PRO:HA	1:A:99:SER:HB3	0.60	1.73	8	4
1:A:130:PHE:CE2	1:B:224:PHE:HD2	0.60	2.15	7	2
1:A:30:PRO:CG	1:B:298:PRO:CD	0.60	2.79	8	1
1:B:234:SER:HA	1:B:269:GLN:OE1	0.60	1.97	10	1
1:A:40:GLN:HG2	1:A:44:LEU:HD22	0.60	1.72	13	1
1:A:121:GLU:HB3	1:A:124:ARG:HG2	0.60	1.72	13	1
1:B:241:LEU:HB2	1:B:242:PRO:CD	0.60	2.27	5	8
1:B:285:ARG:CB	1:B:312:PHE:CE2	0.60	2.84	2	4
1:B:304:VAL:O	1:B:308:TRP:CB	0.60	2.50	3	2
1:A:39:GLU:O	1:A:42:PRO:CG	0.60	2.49	9	4
1:B:225:MET:SD	1:B:230:PRO:CA	0.60	2.89	5	1
1:B:316:ILE:HB	1:B:340:ALA:O	0.60	1.97	5	2
1:B:321:GLU:C	1:B:323:GLY:N	0.60	2.54	5	2
1:A:69:GLN:HG3	1:A:70:VAL:N	0.60	2.10	6	2
1:B:356:ILE:O	1:B:360:ILE:CB	0.60	2.49	11	4
1:A:130:PHE:O	1:B:277:THR:OG1	0.60	2.20	15	4
1:B:264:GLU:CB	1:B:271:LEU:HD21	0.60	2.27	9	5
1:B:368:ASN:C	1:B:368:ASN:ND2	0.60	2.55	7	1
1:B:228:VAL:CG2	1:B:269:GLN:O	0.60	2.48	11	1
1:A:65:ALA:CB	1:A:66:TRP:NE1	0.60	2.64	12	1
1:B:275:GLU:O	1:B:279:LEU:HG	0.60	1.96	12	2
1:A:44:LEU:N	1:A:44:LEU:HD13	0.60	2.12	13	1
1:A:99:SER:OG	1:A:102:THR:OG1	0.60	2.10	10	3
1:A:111:ALA:CB	1:B:312:PHE:HD1	0.60	2.09	6	5
1:B:240:GLN:OE1	1:B:266:TRP:HA	0.60	1.97	7	1
1:A:27:LEU:HD12	1:A:36:PRO:CD	0.60	2.27	8	1
1:A:27:LEU:CD2	1:A:28:VAL:HG23	0.60	2.27	9	1
1:A:96:ILE:HB	1:A:124:ARG:HG3	0.60	1.74	12	3
1:B:342:GLU:OE2	1:B:344:VAL:HG23	0.60	1.96	13	1
1:B:247:ILE:N	1:B:247:ILE:CD1	0.60	2.64	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:ILE:HD11	1:A:105:GLU:OE1	0.60	1.97	15	1
1:A:114:LYS:N	1:A:114:LYS:CD	0.60	2.65	15	1
1:B:290:PHE:CD2	1:B:316:ILE:HG12	0.60	2.31	15	1
1:A:116:ILE:CG2	1:A:141:VAL:HG13	0.60	2.26	5	11
1:A:120:LEU:N	1:A:120:LEU:HD23	0.60	2.12	14	6
1:A:121:GLU:CB	1:A:124:ARG:HB2	0.60	2.27	14	6
1:B:336:GLY:HA3	1:B:343:PHE:CZ	0.60	2.32	11	5
1:B:298:PRO:O	1:B:300:PRO:N	0.60	2.35	14	5
1:B:235:MET:CG	1:B:269:GLN:OE1	0.60	2.50	8	1
1:B:274:GLU:C	1:B:275:GLU:OE1	0.60	2.40	10	1
1:A:93:ILE:CG1	1:A:119:LEU:CB	0.60	2.79	12	2
1:A:87:ALA:O	1:A:114:LYS:HD3	0.60	1.96	13	1
1:B:281:GLN:OE1	1:B:308:TRP:CZ2	0.60	2.55	13	1
1:A:29:ASN:N	1:A:32:THR:OG1	0.60	2.35	14	1
1:B:324:ARG:HD3	1:B:324:ARG:H	0.60	1.57	14	1
1:A:23:PRO:O	1:A:100:PRO:HD2	0.59	1.96	1	1
1:A:77:THR:N	1:A:78:PRO:HD2	0.59	2.12	2	7
1:B:328:TYR:HB3	1:B:332:VAL:CG2	0.59	2.27	7	5
1:A:86:LYS:O	1:A:87:ALA:O	0.59	2.19	3	1
1:B:232:THR:HG23	1:B:233:ASN:N	0.59	2.12	3	2
1:B:281:GLN:O	1:B:285:ARG:HD3	0.59	1.97	5	2
1:B:322:GLU:CD	1:B:346:TYR:O	0.59	2.40	6	1
1:B:262:ARG:HG3	1:B:262:ARG:NH1	0.59	2.11	7	1
1:A:161:ARG:O	1:A:165:ASP:CG	0.59	2.41	8	1
1:B:283:GLU:CA	1:B:283:GLU:OE2	0.59	2.48	8	1
1:A:24:PHE:CE1	1:A:61:HIS:CD2	0.59	2.90	9	1
1:A:39:GLU:HG3	1:A:66:TRP:CZ3	0.59	2.32	12	1
1:A:23:PRO:CB	1:A:99:SER:CB	0.59	2.80	13	1
1:B:323:GLY:C	1:B:325:GLU:OE2	0.59	2.40	15	1
1:A:122:GLU:CA	1:A:125:GLU:OE1	0.59	2.50	13	2
1:A:163:VAL:CG1	1:A:164:VAL:N	0.59	2.65	4	8
1:A:19:PHE:CE2	1:A:59:ASN:CG	0.59	2.76	5	2
1:A:27:LEU:HD12	1:A:39:GLU:OE2	0.59	1.97	3	1
1:B:360:ILE:HG22	1:B:361:ARG:N	0.59	2.12	9	5
1:A:81:GLN:HB3	1:A:108:TRP:CH2	0.59	2.32	4	1
1:B:259:ASN:OD1	1:B:305:GLU:OE1	0.59	2.19	4	1
1:A:69:GLN:HG3	1:A:70:VAL:H	0.59	1.55	9	3
1:B:348:ASP:OD1	1:B:350:ALA:N	0.59	2.35	14	2
1:A:36:PRO:HG2	1:A:39:GLU:CB	0.59	2.27	8	1
1:B:236:PRO:HG2	1:B:239:GLU:CB	0.59	2.27	8	1
1:B:240:GLN:CG	1:B:266:TRP:CD1	0.59	2.84	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:299:SER:HB3	1:B:302:THR:HB	0.59	1.73	14	1
1:A:75:GLU:O	1:A:79:LEU:CD2	0.59	2.50	15	1
1:A:61:HIS:ND1	1:A:61:HIS:N	0.59	2.49	7	6
1:B:240:GLN:HG3	1:B:241:LEU:HD13	0.59	1.73	5	2
1:B:220:LEU:N	1:B:259:ASN:ND2	0.59	2.49	7	1
1:B:228:VAL:HG13	1:B:233:ASN:N	0.59	2.11	11	1
1:A:44:LEU:CD1	1:A:62:ARG:HB3	0.59	2.27	12	1
1:B:235:MET:CB	1:B:269:GLN:HG2	0.59	2.27	12	1
1:B:342:GLU:OE1	1:B:362:LYS:CE	0.59	2.50	14	1
1:A:119:LEU:HB3	1:A:146:TYR:CD2	0.59	2.32	1	5
1:B:351:LEU:O	1:B:354:PRO:HD2	0.59	1.97	5	4
1:A:121:GLU:OE2	1:A:121:GLU:N	0.59	2.36	3	1
1:B:277:THR:O	1:B:281:GLN:HB3	0.59	1.98	3	1
1:A:24:PHE:N	1:A:27:LEU:HD23	0.59	2.11	5	2
1:A:77:THR:CB	1:A:78:PRO:HD3	0.59	2.27	11	8
1:A:49:HIS:CE1	1:A:153:LYS:HE3	0.59	2.31	5	1
1:B:240:GLN:O	1:B:244:LEU:CD2	0.59	2.51	10	5
1:B:306:ILE:HG22	1:B:335:LEU:HD22	0.59	1.73	15	3
1:A:81:GLN:N	1:A:108:TRP:CZ3	0.59	2.71	7	2
1:B:220:LEU:N	1:B:259:ASN:CG	0.59	2.54	7	1
1:B:250:PHE:CD2	1:B:255:LEU:HB2	0.59	2.32	15	3
1:B:361:ARG:O	1:B:365:ASP:CG	0.59	2.41	8	1
1:A:61:HIS:CD2	1:A:61:HIS:H	0.59	2.14	10	1
1:B:240:GLN:HB3	1:B:266:TRP:CE3	0.59	2.32	12	1
1:A:142:GLU:CG	1:A:163:VAL:HB	0.59	2.27	15	1
1:A:42:PRO:HB3	1:A:149:ILE:HG13	0.59	1.75	15	4
1:A:20:LEU:HD11	1:A:50:PHE:HE2	0.59	1.58	2	1
1:B:249:HIS:ND1	1:B:250:PHE:N	0.59	2.50	2	1
1:A:106:ILE:CG2	1:A:135:LEU:HD13	0.59	2.28	11	2
1:A:17:SER:OG	1:A:88:ASP:OD2	0.59	2.20	5	1
1:B:258:PHE:C	1:B:259:ASN:HD22	0.59	2.00	7	1
1:A:108:TRP:CD1	1:A:112:PHE:CE2	0.59	2.91	10	1
1:B:215:VAL:HG13	1:B:218:VAL:HG23	0.59	1.74	12	1
1:A:40:GLN:HG3	1:A:66:TRP:NE1	0.59	2.12	1	3
1:A:96:ILE:HD13	1:A:128:TYR:CE2	0.59	2.32	13	4
1:A:106:ILE:O	1:A:109:ALA:N	0.59	2.35	10	4
1:B:242:PRO:HB3	1:B:349:ILE:HG13	0.59	1.73	15	5
1:A:60:ALA:C	1:A:61:HIS:HD1	0.59	1.99	2	1
1:B:223:PRO:HA	1:B:299:SER:HB2	0.59	1.74	9	4
1:A:59:ASN:N	1:A:83:GLU:OE2	0.59	2.36	7	1
1:B:217:SER:OG	1:B:256:GLU:HB2	0.59	1.98	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ARG:O	1:A:16:ARG:HD3	0.59	1.97	8	1
1:A:103:HIS:CE1	1:A:132:VAL:HG23	0.59	2.32	14	2
1:B:321:GLU:HB3	1:B:324:ARG:HG2	0.59	1.73	13	2
1:B:321:GLU:C	1:B:321:GLU:OE1	0.59	2.40	9	1
1:B:235:MET:SD	1:B:265:ALA:HA	0.59	2.38	11	1
1:B:235:MET:HB3	1:B:269:GLN:HG2	0.59	1.74	12	1
1:B:220:LEU:HD22	1:B:221:ALA:N	0.59	2.12	1	1
1:B:241:LEU:HB2	1:B:242:PRO:HD3	0.59	1.75	12	10
1:B:353:LYS:HB2	1:B:354:PRO:CD	0.59	2.28	13	7
1:B:286:LYS:O	1:B:287:ALA:C	0.59	2.41	15	5
1:A:25:MET:HG3	1:A:26:GLY:N	0.59	2.11	3	2
1:B:320:LEU:CD2	1:B:325:GLU:HB2	0.59	2.28	5	3
1:B:342:GLU:OE1	1:B:362:LYS:NZ	0.59	2.35	14	2
1:B:269:GLN:CG	1:B:270:VAL:N	0.59	2.63	8	2
1:B:296:ILE:HB	1:B:324:ARG:HG3	0.59	1.73	12	3
1:A:17:SER:OG	1:A:56:GLU:OE2	0.59	2.10	1	1
1:A:20:LEU:HG	1:A:47:ILE:HD11	0.59	1.73	6	3
1:A:116:ILE:HG21	1:A:141:VAL:HG13	0.59	1.73	5	5
1:A:140:ALA:HB1	1:A:167:VAL:HG21	0.59	1.73	10	3
1:B:340:ALA:HB1	1:B:367:VAL:HG21	0.59	1.73	10	4
1:A:102:THR:O	1:A:106:ILE:HD12	0.59	1.98	6	2
1:B:229:ASN:CA	1:B:232:THR:OG1	0.59	2.51	14	3
1:A:160:ILE:HG22	1:A:161:ARG:N	0.59	2.12	9	4
1:B:221:ALA:CB	1:B:305:GLU:OE1	0.59	2.50	12	4
1:B:224:PHE:CZ	1:B:271:LEU:HG	0.59	2.32	5	2
1:A:40:GLN:NE2	1:A:66:TRP:HE1	0.59	1.95	6	1
1:A:36:PRO:HG2	1:A:39:GLU:HB3	0.59	1.75	8	1
1:A:69:GLN:CG	1:A:70:VAL:N	0.59	2.66	8	2
1:B:261:HIS:CD2	1:B:261:HIS:H	0.59	2.15	10	1
1:A:24:PHE:O	1:A:27:LEU:N	0.59	2.36	3	7
1:A:24:PHE:C	1:A:26:GLY:N	0.59	2.55	10	9
1:A:90:PHE:HB2	1:A:115:PRO:O	0.59	1.98	1	2
1:A:121:GLU:OE1	1:A:146:TYR:CE2	0.59	2.55	1	2
1:B:293:ILE:HG12	1:B:319:LEU:CB	0.59	2.28	12	4
1:A:125:GLU:CA	1:A:128:TYR:HD1	0.59	2.10	2	6
1:A:89:VAL:HG23	1:A:164:VAL:HG23	0.59	1.74	3	1
1:A:146:TYR:O	1:A:147:LYS:HB3	0.59	1.97	3	2
1:A:107:GLY:H	1:B:304:VAL:HG22	0.59	1.58	5	1
1:A:20:LEU:HD13	1:A:21:ALA:H	0.59	1.56	6	1
1:A:124:ARG:HB3	1:A:128:TYR:HE2	0.59	1.57	14	3
1:A:151:LEU:HD23	1:A:151:LEU:C	0.59	2.17	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:227:LEU:O	1:B:233:ASN:OD1	0.59	2.20	9	1
1:A:69:GLN:OE1	1:A:70:VAL:HG23	0.59	1.98	10	1
1:B:261:HIS:C	1:B:264:GLU:OE1	0.59	2.41	11	1
1:A:35:MET:CB	1:A:69:GLN:HG2	0.59	2.28	12	1
1:B:286:LYS:CG	1:B:287:ALA:N	0.59	2.65	15	1
1:A:23:PRO:CB	1:A:27:LEU:HB3	0.59	2.26	3	3
1:A:25:MET:HE3	1:B:330:PHE:CG	0.59	2.33	1	1
1:A:28:VAL:CG2	1:A:29:ASN:N	0.59	2.65	10	4
1:A:43:PHE:N	1:A:43:PHE:HD2	0.59	1.96	1	2
1:B:290:PHE:HB2	1:B:315:PRO:O	0.59	1.97	1	2
1:B:296:ILE:HG12	1:B:327:GLU:OE2	0.59	1.97	1	1
1:B:342:GLU:HG3	1:B:359:ALA:O	0.59	1.98	6	3
1:A:23:PRO:HA	1:A:102:THR:OG1	0.59	1.98	8	4
1:B:245:THR:HG21	1:B:349:ILE:HG21	0.59	1.75	3	3
1:A:80:ASP:CG	1:A:105:GLU:OE2	0.59	2.41	4	1
1:B:312:PHE:C	1:B:313:ASP:OD1	0.59	2.42	5	1
1:A:101:GLY:O	1:A:105:GLU:OE2	0.59	2.20	6	1
1:A:140:ALA:HB1	1:A:163:VAL:CG2	0.59	2.28	8	1
1:B:219:PHE:CD1	1:B:290:PHE:CE1	0.59	2.91	9	2
1:B:258:PHE:CE1	1:B:286:LYS:HG2	0.59	2.33	9	1
1:A:124:ARG:HD3	1:A:124:ARG:H	0.59	1.58	14	1
1:A:86:LYS:CG	1:A:87:ALA:N	0.59	2.66	15	1
1:B:314:LYS:N	1:B:314:LYS:CD	0.59	2.65	15	1
1:B:241:LEU:O	1:B:244:LEU:HG	0.58	1.98	7	5
1:B:282:LEU:O	1:B:286:LYS:HB2	0.58	1.98	12	5
1:B:366:ARG:HG3	1:B:367:VAL:HG23	0.58	1.73	1	1
1:B:219:PHE:O	1:B:291:VAL:HB	0.58	1.98	7	5
1:A:71:LEU:HB2	1:A:76:CYS:SG	0.58	2.37	4	2
1:B:224:PHE:CZ	1:B:261:HIS:ND1	0.58	2.71	15	2
1:B:279:LEU:C	1:B:279:LEU:CD2	0.58	2.71	4	1
1:B:269:GLN:O	1:B:270:VAL:HB	0.58	1.96	6	2
1:B:228:VAL:CG1	1:B:270:VAL:HG11	0.58	2.28	7	1
1:A:28:VAL:CG2	1:A:32:THR:C	0.58	2.71	8	1
1:A:80:ASP:OD2	1:A:105:GLU:CD	0.58	2.42	8	2
1:A:27:LEU:O	1:A:33:ASN:OD1	0.58	2.20	9	1
1:A:34:SER:HA	1:A:69:GLN:OE1	0.58	1.98	10	1
1:B:240:GLN:O	1:B:244:LEU:CG	0.58	2.51	12	3
1:A:35:MET:HG3	1:A:35:MET:O	0.58	1.97	15	1
1:B:223:PRO:CB	1:B:227:LEU:HB3	0.58	2.27	3	2
1:B:236:PRO:O	1:B:239:GLU:HB2	0.58	1.99	9	2
1:B:316:ILE:HB	1:B:341:VAL:HG22	0.58	1.74	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:321:GLU:O	1:B:324:ARG:HG2	0.58	1.98	4	2
1:A:116:ILE:HB	1:A:140:ALA:O	0.58	1.99	10	2
1:B:349:ILE:O	1:B:353:LYS:CG	0.58	2.50	6	3
1:A:62:ARG:NH1	1:A:62:ARG:HG3	0.58	2.10	7	1
1:B:246:LEU:HD23	1:B:250:PHE:CE1	0.58	2.33	7	1
1:A:25:MET:HE2	1:B:330:PHE:CD2	0.58	2.32	8	2
1:B:347:LYS:HD3	1:B:347:LYS:N	0.58	2.14	10	1
1:A:35:MET:N	1:A:68:ALA:HA	0.58	2.13	11	1
1:B:244:LEU:CD1	1:B:262:ARG:HB3	0.58	2.28	12	1
1:A:17:SER:HA	1:A:56:GLU:N	0.58	2.13	5	10
1:A:19:PHE:O	1:A:19:PHE:HD2	0.58	1.81	4	3
1:A:117:VAL:HG22	1:A:142:GLU:CB	0.58	2.28	14	5
1:A:117:VAL:HG12	1:A:117:VAL:O	0.58	1.99	1	1
1:A:130:PHE:O	1:B:273:PRO:CB	0.58	2.51	10	6
1:A:86:LYS:O	1:A:87:ALA:C	0.58	2.41	15	5
1:B:281:GLN:HB3	1:B:308:TRP:CH2	0.58	2.33	4	1
1:A:148:ASP:OD1	1:A:151:LEU:HD11	0.58	1.98	5	1
1:A:47:ILE:O	1:A:51:GLU:OE1	0.58	2.21	6	1
1:A:20:LEU:N	1:A:59:ASN:ND2	0.58	2.51	7	1
1:B:321:GLU:OE1	1:B:346:TYR:HE2	0.58	1.81	7	1
1:A:147:LYS:O	1:A:148:ASP:HB2	0.58	1.97	8	1
1:A:27:LEU:CD1	1:A:35:MET:HB3	0.58	2.27	10	1
1:A:64:GLU:O	1:A:69:GLN:CG	0.58	2.51	11	1
1:A:70:VAL:O	1:B:330:PHE:CZ	0.58	2.56	11	1
1:B:293:ILE:CG1	1:B:319:LEU:CB	0.58	2.81	12	2
1:A:130:PHE:HD2	1:B:225:MET:SD	0.58	2.20	14	1
1:A:120:LEU:HB3	1:A:125:GLU:CB	0.58	2.28	11	8
1:B:289:VAL:CG1	1:B:289:VAL:O	0.58	2.52	9	2
1:A:26:GLY:O	1:A:28:VAL:O	0.58	2.20	5	2
1:A:45:THR:O	1:A:48:GLU:CB	0.58	2.50	11	3
1:A:103:HIS:O	1:B:304:VAL:HG13	0.58	1.99	2	1
1:B:338:VAL:HG23	1:B:339:ALA:H	0.58	1.58	3	9
1:A:109:ALA:HB3	1:A:116:ILE:CD1	0.58	2.28	3	2
1:B:285:ARG:CB	1:B:312:PHE:CD1	0.58	2.87	3	1
1:B:261:HIS:O	1:B:264:GLU:HG3	0.58	1.97	4	1
1:B:225:MET:O	1:B:226:GLY:C	0.58	2.41	14	2
1:B:218:VAL:CG1	1:B:250:PHE:CD2	0.58	2.77	6	1
1:B:348:ASP:OD1	1:B:350:ALA:HB3	0.58	1.99	7	1
1:A:23:PRO:CA	1:A:99:SER:HB3	0.58	2.28	12	3
1:B:262:ARG:HB3	1:B:262:ARG:NH1	0.58	2.13	9	1
1:A:56:GLU:OE2	1:A:56:GLU:HA	0.58	1.98	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:261:HIS:O	1:B:264:GLU:OE1	0.58	2.21	11	1
1:A:125:GLU:HG3	1:A:145:HIS:CD2	0.58	2.33	13	1
1:B:287:ALA:O	1:B:314:LYS:HD3	0.58	1.98	13	1
1:B:224:PHE:O	1:B:227:LEU:N	0.58	2.36	8	6
1:B:240:GLN:CD	1:B:241:LEU:CD1	0.58	2.72	2	1
1:A:58:PHE:CD2	1:A:83:GLU:OE2	0.58	2.56	3	2
1:A:153:LYS:HB3	1:A:154:PRO:HD3	0.58	1.75	4	1
1:A:59:ASN:OD1	1:A:80:ASP:OD1	0.58	2.21	14	2
1:B:271:LEU:O	1:B:276:CYS:HB2	0.58	1.98	12	1
1:B:293:ILE:HG13	1:B:319:LEU:HB2	0.58	1.75	12	1
1:A:132:VAL:O	1:A:135:LEU:HB2	0.58	1.99	14	1
1:A:25:MET:HE2	1:A:26:GLY:N	0.58	2.12	15	1
1:A:116:ILE:CG2	1:A:117:VAL:N	0.58	2.66	15	9
1:A:24:PHE:HE1	1:A:70:VAL:CA	0.58	2.12	3	1
1:A:146:TYR:O	1:A:147:LYS:HG2	0.58	1.99	3	1
1:A:40:GLN:O	1:A:44:LEU:CD2	0.58	2.51	10	6
1:A:125:GLU:OE1	1:A:145:HIS:NE2	0.58	2.36	5	1
1:B:228:VAL:HG22	1:B:232:THR:O	0.58	1.98	5	2
1:B:240:GLN:HG3	1:B:265:ALA:O	0.58	1.98	6	1
1:B:296:ILE:HD12	1:B:328:TYR:CD2	0.58	2.31	10	2
1:A:81:GLN:HA	1:A:108:TRP:CE3	0.58	2.34	7	1
1:B:275:GLU:OE1	1:B:279:LEU:CD1	0.58	2.51	13	1
1:A:35:MET:SD	1:A:36:PRO:O	0.58	2.62	15	1
1:A:120:LEU:O	1:A:146:TYR:HD2	0.58	1.81	15	1
1:A:22:GLY:O	1:A:102:THR:OG1	0.58	2.21	5	5
1:A:94:PRO:C	1:A:128:TYR:HH	0.58	2.00	12	4
1:A:25:MET:CE	1:A:31:GLU:H	0.58	2.12	5	2
1:B:296:ILE:CD1	1:B:327:GLU:HB2	0.58	2.29	15	5
1:A:19:PHE:O	1:A:91:VAL:HB	0.58	1.98	7	5
1:B:332:VAL:HG13	1:B:343:PHE:CE2	0.58	2.33	15	2
1:B:342:GLU:HG2	1:B:363:VAL:HG23	0.58	1.75	6	1
1:B:216:ARG:O	1:B:216:ARG:HD3	0.58	1.99	8	1
1:A:134:GLY:N	1:B:273:PRO:HB2	0.58	2.13	11	2
1:A:71:LEU:O	1:A:76:CYS:HB2	0.58	1.99	12	1
1:B:253:GLN:HA	1:B:253:GLN:NE2	0.58	2.14	14	2
1:A:85:ARG:HB3	1:A:112:PHE:CG	0.58	2.33	15	1
1:A:20:LEU:HD22	1:A:21:ALA:N	0.58	2.13	1	1
1:A:23:PRO:HA	1:A:99:SER:HB2	0.58	1.75	9	4
1:A:24:PHE:CD2	1:B:330:PHE:CE1	0.58	2.91	1	1
1:A:142:GLU:HG3	1:A:159:ALA:HB1	0.58	1.75	13	2
1:A:112:PHE:CE2	1:B:311:ALA:O	0.58	2.56	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:PHE:HD1	1:B:225:MET:SD	0.58	2.22	2	1
1:A:111:ALA:HA	1:B:312:PHE:CE1	0.58	2.33	6	3
1:A:121:GLU:C	1:A:123:GLY:N	0.58	2.56	5	2
1:B:324:ARG:O	1:B:328:TYR:HD2	0.58	1.80	5	6
1:B:262:ARG:CD	1:B:266:TRP:CZ2	0.58	2.87	6	1
1:A:61:HIS:HB3	1:A:65:ALA:HB2	0.58	1.74	9	1
1:A:121:GLU:C	1:A:121:GLU:OE1	0.58	2.42	9	1
1:A:146:TYR:CB	1:A:152:ALA:HB2	0.58	2.29	14	2
1:B:239:GLU:OE2	1:B:239:GLU:CA	0.58	2.52	10	1
1:A:22:GLY:C	1:A:102:THR:OG1	0.58	2.42	14	3
1:A:28:VAL:HG13	1:A:33:ASN:N	0.58	2.13	11	1
1:A:29:ASN:HB2	1:A:33:ASN:OD1	0.58	1.99	11	1
1:B:346:TYR:OH	1:B:349:ILE:HD11	0.58	1.99	11	1
1:B:296:ILE:HG12	1:B:327:GLU:CD	0.58	2.18	15	1
1:A:158:ALA:O	1:A:162:LYS:HB2	0.58	1.99	1	1
1:A:102:THR:O	1:A:105:GLU:CB	0.58	2.52	15	5
1:A:81:GLN:HG3	1:A:82:LEU:HD13	0.58	1.76	4	1
1:B:256:GLU:HB3	1:B:258:PHE:CE2	0.58	2.34	7	4
1:B:217:SER:HB3	1:B:256:GLU:HB2	0.58	1.74	6	2
1:B:283:GLU:OE2	1:B:283:GLU:HA	0.58	1.97	8	1
1:B:312:PHE:O	1:B:313:ASP:OD1	0.58	2.21	9	1
1:A:29:ASN:CA	1:A:32:THR:OG1	0.58	2.52	14	2
1:B:265:ALA:CB	1:B:266:TRP:NE1	0.58	2.67	12	1
1:A:79:LEU:O	1:A:83:GLU:CG	0.58	2.52	14	1
1:A:99:SER:HB3	1:A:102:THR:HB	0.58	1.74	14	1
1:B:298:PRO:HA	1:B:328:TYR:CD2	0.58	2.33	15	1
1:B:332:VAL:O	1:B:343:PHE:CE2	0.58	2.56	11	2
1:B:285:ARG:HB2	1:B:312:PHE:CD2	0.58	2.34	3	2
1:B:262:ARG:C	1:B:264:GLU:N	0.58	2.55	14	3
1:B:224:PHE:CD1	1:B:269:GLN:NE2	0.58	2.71	7	1
1:B:334:GLY:O	1:B:338:VAL:CG2	0.58	2.45	10	4
1:B:355:GLN:HA	1:B:355:GLN:OE1	0.58	1.97	10	1
1:A:24:PHE:HD2	1:A:70:VAL:HG23	0.58	1.59	11	1
1:B:346:TYR:O	1:B:347:LYS:HG3	0.58	1.99	11	1
1:A:20:LEU:HD13	1:A:43:PHE:CD1	0.58	2.34	14	1
1:B:342:GLU:CG	1:B:363:VAL:HB	0.58	2.29	15	1
1:A:93:ILE:HG12	1:A:119:LEU:CB	0.57	2.28	12	4
1:B:259:ASN:HA	1:B:283:GLU:OE1	0.57	1.99	13	2
1:A:40:GLN:CD	1:A:41:LEU:CD1	0.57	2.72	2	1
1:B:217:SER:HA	1:B:256:GLU:N	0.57	2.13	5	8
1:A:36:PRO:O	1:A:39:GLU:HB2	0.57	1.99	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:320:LEU:CD1	1:B:325:GLU:HB2	0.57	2.29	5	8
1:A:121:GLU:O	1:A:124:ARG:HG2	0.57	1.99	4	2
1:B:353:LYS:HB3	1:B:354:PRO:HD3	0.57	1.76	4	1
1:A:81:GLN:O	1:A:85:ARG:HD3	0.57	1.99	5	2
1:A:40:GLN:CG	1:A:66:TRP:CD1	0.57	2.86	11	2
1:B:224:PHE:HE1	1:B:270:VAL:N	0.57	1.96	10	1
1:B:225:MET:N	1:B:225:MET:HE3	0.57	2.14	10	1
1:A:28:VAL:HG13	1:A:32:THR:C	0.57	2.19	11	1
1:A:90:PHE:HE2	1:A:106:ILE:HA	0.57	1.59	12	1
1:A:58:PHE:CE1	1:A:86:LYS:HB3	0.57	2.34	13	1
1:B:325:GLU:CA	1:B:328:TYR:HD2	0.57	2.11	13	7
1:B:335:LEU:HD23	1:B:341:VAL:CG2	0.57	2.29	9	3
1:A:79:LEU:C	1:A:79:LEU:CD2	0.57	2.71	4	1
1:A:46:LEU:HA	1:A:49:HIS:NE2	0.57	2.14	5	1
1:B:292:ALA:CB	1:B:318:LEU:HD23	0.57	2.21	5	1
1:B:275:GLU:OE1	1:B:275:GLU:N	0.57	2.36	10	1
1:B:321:GLU:O	1:B:321:GLU:OE2	0.57	2.21	12	1
1:A:107:GLY:CA	1:A:110:SER:OG	0.57	2.51	14	2
1:B:325:GLU:OE2	1:B:326:GLU:N	0.57	2.34	15	1
1:B:243:PHE:N	1:B:243:PHE:HD2	0.57	1.97	1	2
1:A:49:HIS:ND1	1:A:50:PHE:N	0.57	2.51	2	1
1:B:325:GLU:CA	1:B:328:TYR:CD1	0.57	2.87	2	2
1:A:130:PHE:CZ	1:B:224:PHE:HD1	0.57	2.18	3	1
1:B:221:ALA:HB2	1:B:259:ASN:HD21	0.57	1.60	3	1
1:B:279:LEU:O	1:B:283:GLU:CG	0.57	2.51	14	2
1:B:282:LEU:HG	1:B:285:ARG:NH1	0.57	2.14	3	1
1:B:321:GLU:N	1:B:321:GLU:OE2	0.57	2.37	3	1
1:B:235:MET:CB	1:B:269:GLN:CD	0.57	2.73	6	2
1:B:277:THR:CB	1:B:278:PRO:HD3	0.57	2.29	11	8
1:A:142:GLU:HG2	1:A:163:VAL:HG23	0.57	1.75	6	1
1:A:20:LEU:N	1:A:59:ASN:CG	0.57	2.57	7	1
1:A:18:VAL:HG22	1:A:89:VAL:HG11	0.57	1.75	12	3
1:B:227:LEU:HD12	1:B:236:PRO:CD	0.57	2.29	8	1
1:B:235:MET:HB3	1:B:269:GLN:OE1	0.57	1.98	8	1
1:B:244:LEU:O	1:B:248:GLU:HB3	0.57	1.99	8	1
1:A:63:ARG:O	1:A:66:TRP:N	0.57	2.32	11	1
1:B:281:GLN:CA	1:B:284:ILE:HG12	0.57	2.29	13	1
1:A:64:GLU:O	1:A:69:GLN:CA	0.57	2.52	14	1
1:B:325:GLU:N	1:B:325:GLU:OE1	0.57	2.38	15	1
1:A:111:ALA:O	1:B:312:PHE:CE2	0.57	2.56	2	1
1:B:309:ALA:HB3	1:B:316:ILE:CD1	0.57	2.29	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:TRP:O	1:A:112:PHE:CB	0.57	2.53	9	5
1:A:131:LEU:HA	1:B:277:THR:OG1	0.57	1.98	14	4
1:B:249:HIS:CE1	1:B:353:LYS:HE3	0.57	2.35	5	1
1:B:301:GLY:O	1:B:305:GLU:OE2	0.57	2.22	6	1
1:A:19:PHE:HB3	1:A:87:ALA:CB	0.57	2.29	8	1
1:A:108:TRP:CZ2	1:B:331:LEU:HD21	0.57	2.33	8	1
1:B:219:PHE:HB3	1:B:287:ALA:CB	0.57	2.29	8	1
1:A:34:SER:C	1:A:36:PRO:HD3	0.57	2.19	10	1
1:B:322:GLU:CA	1:B:325:GLU:OE2	0.57	2.52	10	1
1:B:239:GLU:HG3	1:B:266:TRP:CZ3	0.57	2.34	12	1
1:B:223:PRO:CB	1:B:299:SER:CB	0.57	2.82	13	1
1:A:19:PHE:CD1	1:A:90:PHE:CE1	0.57	2.92	9	2
1:A:121:GLU:HB3	1:A:124:ARG:HB2	0.57	1.74	14	4
1:A:136:GLY:HA3	1:A:143:PHE:CZ	0.57	2.34	11	6
1:B:240:GLN:HG3	1:B:266:TRP:CD1	0.57	2.33	1	1
1:B:359:ALA:O	1:B:363:VAL:HB	0.57	2.00	4	3
1:A:19:PHE:CE2	1:A:84:ILE:HD13	0.57	2.35	2	1
1:A:106:ILE:HG22	1:A:135:LEU:HD21	0.57	1.74	7	2
1:B:250:PHE:CD1	1:B:255:LEU:CD1	0.57	2.87	12	5
1:B:321:GLU:HB2	1:B:324:ARG:HB2	0.57	1.73	2	2
1:B:223:PRO:HA	1:B:302:THR:OG1	0.57	2.00	7	3
1:B:302:THR:O	1:B:305:GLU:CB	0.57	2.52	5	5
1:A:119:LEU:HB3	1:A:146:TYR:CD1	0.57	2.35	9	3
1:B:247:ILE:CD1	1:B:247:ILE:N	0.57	2.66	4	2
1:B:299:SER:HB3	1:B:302:THR:OG1	0.57	1.98	5	1
1:A:25:MET:H	1:B:330:PHE:HE2	0.57	1.42	6	3
1:A:84:ILE:CG2	1:A:109:ALA:N	0.57	2.67	7	3
1:B:268:ALA:O	1:B:269:GLN:HB3	0.57	2.00	9	2
1:B:280:ASP:OD2	1:B:305:GLU:CD	0.57	2.42	8	1
1:B:348:ASP:O	1:B:351:LEU:N	0.57	2.36	11	3
1:A:39:GLU:OE2	1:A:39:GLU:CA	0.57	2.53	10	1
1:B:332:VAL:O	1:B:335:LEU:HB2	0.57	1.99	14	1
1:B:342:GLU:OE2	1:B:359:ALA:O	0.57	2.23	15	1
1:A:120:LEU:HB3	1:A:125:GLU:HG3	0.57	1.77	13	4
1:B:223:PRO:HG3	1:B:294:PRO:O	0.57	2.00	7	3
1:B:246:LEU:HD11	1:B:250:PHE:CD1	0.57	2.33	1	1
1:A:120:LEU:CD1	1:A:125:GLU:HB2	0.57	2.28	5	9
1:A:98:PRO:HB3	1:B:300:PRO:HB3	0.57	1.76	5	1
1:A:148:ASP:OD1	1:A:148:ASP:N	0.57	2.38	5	1
1:B:216:ARG:CD	1:B:216:ARG:O	0.57	2.53	5	1
1:A:94:PRO:CG	1:A:121:GLU:OE2	0.57	2.53	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:PHE:HD2	1:B:225:MET:HB2	0.57	1.58	13	2
1:B:321:GLU:CG	1:B:324:ARG:HB2	0.57	2.28	7	1
1:A:73:PRO:HA	1:B:330:PHE:O	0.57	2.00	10	3
1:B:240:GLN:CG	1:B:244:LEU:CD2	0.57	2.82	13	1
1:A:77:THR:HG1	1:B:334:GLY:HA3	0.57	1.58	10	2
1:A:121:GLU:HB3	1:A:124:ARG:HG3	0.57	1.74	2	3
1:B:293:ILE:O	1:B:294:PRO:O	0.57	2.21	3	13
1:A:26:GLY:C	1:A:28:VAL:N	0.57	2.56	9	5
1:A:96:ILE:HD13	1:A:128:TYR:CD1	0.57	2.34	7	4
1:A:28:VAL:HG22	1:A:32:THR:O	0.57	1.99	5	2
1:B:351:LEU:HD23	1:B:351:LEU:C	0.57	2.19	7	1
1:B:228:VAL:CG2	1:B:232:THR:C	0.57	2.73	8	1
1:A:25:MET:HE2	1:B:330:PHE:CD1	0.57	2.33	9	1
1:B:244:LEU:N	1:B:244:LEU:CD1	0.57	2.67	13	1
1:B:284:ILE:O	1:B:314:LYS:CD	0.57	2.52	13	1
1:B:219:PHE:CE1	1:B:283:GLU:CB	0.57	2.88	14	1
1:A:134:GLY:CA	1:B:273:PRO:CB	0.57	2.82	3	2
1:B:284:ILE:HG13	1:B:308:TRP:CE3	0.57	2.35	8	4
1:A:46:LEU:CD1	1:A:153:LYS:HG3	0.57	2.30	3	1
1:A:49:HIS:CE1	1:A:53:GLN:HG3	0.57	2.35	9	4
1:A:135:LEU:HD23	1:A:141:VAL:CG2	0.57	2.29	9	3
1:A:147:LYS:O	1:A:147:LYS:HG3	0.57	2.00	3	1
1:B:245:THR:C	1:B:249:HIS:NE2	0.57	2.57	5	1
1:A:108:TRP:NE1	1:B:307:GLY:C	0.57	2.58	13	4
1:A:89:VAL:CG1	1:A:89:VAL:O	0.57	2.53	9	1
1:B:317:VAL:CG2	1:B:363:VAL:HG21	0.57	2.30	13	1
1:B:350:ALA:O	1:B:354:PRO:CD	0.57	2.53	14	2
1:B:316:ILE:CG2	1:B:317:VAL:N	0.57	2.68	11	11
1:B:317:VAL:HG12	1:B:317:VAL:O	0.57	1.99	1	1
1:A:17:SER:HB3	1:A:56:GLU:HB3	0.57	1.75	2	3
1:A:73:PRO:CB	1:B:334:GLY:CA	0.57	2.83	3	2
1:B:323:GLY:N	1:B:325:GLU:OE2	0.57	2.37	2	2
1:A:40:GLN:OE1	1:A:40:GLN:O	0.57	2.22	3	1
1:B:289:VAL:HG23	1:B:364:VAL:HG23	0.57	1.75	3	1
1:B:319:LEU:O	1:B:321:GLU:OE2	0.57	2.23	3	2
1:B:282:LEU:N	1:B:282:LEU:HD13	0.57	2.15	4	1
1:A:30:PRO:O	1:A:31:GLU:HB3	0.57	2.00	7	3
1:B:223:PRO:CA	1:B:299:SER:HB3	0.57	2.29	12	2
1:A:40:GLN:CG	1:A:44:LEU:CD2	0.57	2.83	13	1
1:B:307:GLY:CA	1:B:310:SER:OG	0.57	2.53	15	2
1:B:321:GLU:HB3	1:B:324:ARG:HG3	0.57	1.77	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:MET:HE2	1:A:25:MET:N	0.57	2.15	2	3
1:A:21:ALA:CB	1:A:105:GLU:OE1	0.57	2.53	12	4
1:A:125:GLU:HA	1:A:128:TYR:HD1	0.57	1.59	9	3
1:A:24:PHE:CZ	1:A:71:LEU:HG	0.57	2.35	5	1
1:A:104:VAL:HG23	1:B:303:HIS:C	0.57	2.19	5	1
1:B:320:LEU:HB2	1:B:345:HIS:CD2	0.57	2.35	6	2
1:A:41:LEU:HA	1:A:44:LEU:CG	0.57	2.30	14	3
1:B:227:LEU:CD2	1:B:228:VAL:HG23	0.57	2.30	9	1
1:A:155:GLN:HA	1:A:155:GLN:OE1	0.57	1.99	10	1
1:B:235:MET:N	1:B:268:ALA:HA	0.57	2.14	11	1
1:A:81:GLN:CA	1:A:84:ILE:HG12	0.57	2.30	13	1
1:A:117:VAL:HG22	1:A:163:VAL:HG21	0.57	1.77	13	1
1:A:99:SER:HG	1:A:102:THR:CB	0.57	2.13	15	1
1:A:123:GLY:N	1:A:125:GLU:CD	0.57	2.58	15	1
1:A:85:ARG:CB	1:A:112:PHE:CE2	0.56	2.87	2	3
1:A:27:LEU:HD11	1:A:35:MET:HB2	0.56	1.77	3	2
1:A:32:THR:CG2	1:A:33:ASN:N	0.56	2.67	3	3
1:A:89:VAL:CG2	1:A:164:VAL:HG23	0.56	2.30	3	1
1:B:310:SER:OG	1:B:335:LEU:CD2	0.56	2.53	5	3
1:A:142:GLU:OE1	1:A:162:LYS:NZ	0.56	2.37	14	2
1:B:219:PHE:CE1	1:B:283:GLU:C	0.56	2.78	14	2
1:A:111:ALA:O	1:B:311:ALA:O	0.56	2.22	6	1
1:A:24:PHE:CE1	1:A:69:GLN:NE2	0.56	2.73	7	3
1:A:25:MET:HB2	1:B:330:PHE:HD2	0.56	1.60	13	2
1:A:59:ASN:ND2	1:A:83:GLU:HG2	0.56	2.15	15	1
1:A:153:LYS:N	1:A:154:PRO:CD	0.56	2.68	15	10
1:A:61:HIS:CD2	1:A:65:ALA:CB	0.56	2.87	2	2
1:A:131:LEU:HD23	1:B:301:GLY:HA2	0.56	1.76	5	2
1:B:320:LEU:CD1	1:B:325:GLU:CG	0.56	2.82	4	2
1:B:246:LEU:HA	1:B:249:HIS:NE2	0.56	2.14	5	1
1:B:310:SER:OG	1:B:335:LEU:CG	0.56	2.53	5	1
1:A:111:ALA:HB1	1:B:308:TRP:O	0.56	2.00	12	2
1:B:292:ALA:HB3	1:B:318:LEU:HG	0.56	1.77	6	1
1:B:320:LEU:HD13	1:B:325:GLU:OE2	0.56	1.99	7	2
1:B:218:VAL:HG22	1:B:289:VAL:HG11	0.56	1.77	12	3
1:A:24:PHE:HE1	1:A:70:VAL:N	0.56	1.99	10	1
1:B:250:PHE:HD1	1:B:255:LEU:CB	0.56	2.12	10	3
1:B:229:ASN:OD1	1:B:233:ASN:OD1	0.56	2.23	11	1
1:B:256:GLU:OE2	1:B:256:GLU:HA	0.56	1.99	11	1
1:A:46:LEU:CD2	1:A:156:ILE:HG21	0.56	2.30	12	2
1:A:120:LEU:O	1:A:146:TYR:CD2	0.56	2.58	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LEU:O	1:A:135:LEU:HD12	0.56	2.00	15	1
1:A:148:ASP:O	1:A:151:LEU:N	0.56	2.35	11	4
1:B:263:ARG:O	1:B:266:TRP:N	0.56	2.33	11	2
1:B:346:TYR:O	1:B:346:TYR:CG	0.56	2.58	1	7
1:A:15:VAL:HG13	1:A:89:VAL:HB	0.56	1.76	2	3
1:A:17:SER:HB3	1:A:58:PHE:CE2	0.56	2.35	15	2
1:A:24:PHE:HE2	1:A:70:VAL:N	0.56	1.97	15	4
1:A:111:ALA:HB2	1:B:308:TRP:CD1	0.56	2.35	7	7
1:A:142:GLU:HG3	1:A:159:ALA:O	0.56	2.00	6	2
1:A:21:ALA:HB1	1:A:105:GLU:OE1	0.56	2.00	3	1
1:A:125:GLU:HG3	1:A:126:GLU:H	0.56	1.60	3	3
1:A:16:ARG:CD	1:A:16:ARG:O	0.56	2.53	5	1
1:A:103:HIS:C	1:B:304:VAL:HG23	0.56	2.21	5	1
1:B:301:GLY:O	1:B:305:GLU:OE1	0.56	2.24	5	2
1:A:144:VAL:CG1	1:A:155:GLN:HB3	0.56	2.30	11	2
1:A:50:PHE:CD2	1:A:55:LEU:HB2	0.56	2.33	15	3
1:B:320:LEU:HD12	1:B:345:HIS:HE2	0.56	1.58	7	1
1:A:83:GLU:CA	1:A:83:GLU:OE2	0.56	2.54	8	1
1:B:228:VAL:O	1:B:229:ASN:C	0.56	2.43	11	3
1:A:135:LEU:CB	1:A:141:VAL:HG11	0.56	2.29	10	1
1:A:35:MET:SD	1:A:65:ALA:HA	0.56	2.40	11	1
1:A:61:HIS:O	1:A:64:GLU:OE1	0.56	2.22	11	1
1:B:222:GLY:C	1:B:302:THR:OG1	0.56	2.44	14	3
1:B:227:LEU:HD12	1:B:235:MET:CA	0.56	2.27	11	1
1:A:112:PHE:CG	1:B:311:ALA:O	0.56	2.59	12	1
1:B:325:GLU:HG3	1:B:345:HIS:CD2	0.56	2.35	13	1
1:A:49:HIS:HB3	1:A:153:LYS:NZ	0.56	2.16	14	1
1:B:220:LEU:HD23	1:B:291:VAL:O	0.56	1.98	14	1
1:A:123:GLY:C	1:A:125:GLU:OE2	0.56	2.44	15	1
1:B:290:PHE:HB3	1:B:316:ILE:HA	0.56	1.76	10	6
1:B:258:PHE:CD1	1:B:286:LYS:HD2	0.56	2.35	2	1
1:B:229:ASN:CB	1:B:232:THR:HG21	0.56	2.27	4	1
1:B:219:PHE:HD1	1:B:283:GLU:O	0.56	1.84	5	2
1:B:348:ASP:OD1	1:B:348:ASP:N	0.56	2.37	5	1
1:A:28:VAL:HG23	1:A:32:THR:C	0.56	2.21	8	2
1:A:116:ILE:HG23	1:A:118:LEU:CD1	0.56	2.29	9	1
1:B:220:LEU:HD22	1:B:247:ILE:HD11	0.56	1.76	10	1
1:A:146:TYR:O	1:A:147:LYS:HG3	0.56	2.00	11	1
1:A:146:TYR:OH	1:A:149:ILE:HD11	0.56	2.00	11	1
1:A:40:GLN:N	1:A:66:TRP:CZ3	0.56	2.74	13	2
1:B:290:PHE:CE2	1:B:306:ILE:HA	0.56	2.35	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:ALA:HA	1:B:312:PHE:CE2	0.56	2.36	13	1
1:A:93:ILE:H	1:A:102:THR:HG21	0.56	1.61	15	1
1:B:275:GLU:C	1:B:279:LEU:HD23	0.56	2.20	15	1
1:A:17:SER:CB	1:A:58:PHE:CD2	0.56	2.89	2	1
1:A:46:LEU:C	1:A:48:GLU:N	0.56	2.59	10	5
1:A:128:TYR:HB3	1:A:132:VAL:CG2	0.56	2.30	7	4
1:B:219:PHE:CE2	1:B:284:ILE:HD13	0.56	2.36	2	1
1:A:85:ARG:CB	1:A:112:PHE:CE1	0.56	2.89	9	4
1:B:296:ILE:HD12	1:B:328:TYR:CD1	0.56	2.34	9	3
1:B:285:ARG:CD	1:B:312:PHE:CZ	0.56	2.88	5	3
1:A:95:GLY:HA2	1:A:124:ARG:CD	0.56	2.30	5	1
1:A:18:VAL:CG1	1:A:50:PHE:CD2	0.56	2.82	6	1
1:B:342:GLU:OE1	1:B:359:ALA:HB1	0.56	2.01	9	1
1:A:85:ARG:O	1:A:114:LYS:HE3	0.56	2.01	13	2
1:B:253:GLN:CD	1:B:253:GLN:C	0.56	2.63	15	1
1:A:35:MET:HG2	1:A:36:PRO:HD2	0.56	1.77	1	1
1:A:125:GLU:CA	1:A:128:TYR:HD2	0.56	2.14	5	7
1:B:223:PRO:O	1:B:300:PRO:HD2	0.56	2.00	1	1
1:A:46:LEU:O	1:A:48:GLU:N	0.56	2.38	2	5
1:A:85:ARG:CD	1:A:112:PHE:CZ	0.56	2.89	5	4
1:B:246:LEU:C	1:B:248:GLU:N	0.56	2.59	10	5
1:B:284:ILE:CG2	1:B:308:TRP:HB3	0.56	2.20	8	4
1:A:21:ALA:HB2	1:A:59:ASN:HD21	0.56	1.58	3	1
1:A:35:MET:CB	1:A:69:GLN:CD	0.56	2.74	6	2
1:B:283:GLU:OE2	1:B:286:LYS:CE	0.56	2.53	4	1
1:B:303:HIS:NE2	1:B:328:TYR:HD1	0.56	1.98	10	3
1:B:269:GLN:HG3	1:B:270:VAL:N	0.56	2.15	6	2
1:A:156:ILE:O	1:A:160:ILE:HD12	0.56	2.00	8	1
1:B:346:TYR:CB	1:B:352:ALA:HB2	0.56	2.31	14	2
1:A:122:GLU:CA	1:A:125:GLU:OE2	0.56	2.53	10	1
1:B:227:LEU:CD1	1:B:235:MET:HB3	0.56	2.30	10	1
1:B:241:LEU:HA	1:B:244:LEU:CG	0.56	2.30	14	2
1:A:75:GLU:CA	1:A:79:LEU:HD12	0.56	2.30	14	1
1:A:40:GLN:HG3	1:A:66:TRP:CD1	0.56	2.35	1	1
1:A:81:GLN:CG	1:A:82:LEU:HD22	0.56	2.30	1	1
1:B:296:ILE:HG13	1:B:298:PRO:HD3	0.56	1.77	3	6
1:B:240:GLN:CG	1:B:266:TRP:HE1	0.56	2.14	14	3
1:A:19:PHE:CE1	1:A:83:GLU:C	0.56	2.79	14	2
1:A:90:PHE:HE2	1:A:106:ILE:HG13	0.56	1.60	8	1
1:B:347:LYS:O	1:B:348:ASP:HB2	0.56	2.00	8	1
1:A:24:PHE:CE1	1:A:69:GLN:CD	0.56	2.78	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:264:GLU:O	1:B:269:GLN:CG	0.56	2.54	11	1
1:A:20:LEU:HD23	1:A:91:VAL:O	0.56	2.01	14	1
1:A:142:GLU:OE1	1:A:162:LYS:CE	0.56	2.53	14	1
1:A:41:LEU:O	1:A:44:LEU:HG	0.56	2.00	7	5
1:A:130:PHE:CZ	1:B:224:PHE:CD2	0.56	2.94	6	3
1:B:240:GLN:HG3	1:B:266:TRP:NE1	0.56	2.16	1	3
1:B:246:LEU:O	1:B:248:GLU:N	0.56	2.38	2	5
1:B:229:ASN:CG	1:B:233:ASN:CG	0.56	2.64	3	1
1:B:239:GLU:O	1:B:242:PRO:CG	0.56	2.53	9	3
1:B:317:VAL:HG11	1:B:360:ILE:CG1	0.56	2.30	7	2
1:A:120:LEU:HB2	1:A:145:HIS:CD2	0.56	2.35	6	2
1:A:107:GLY:C	1:B:308:TRP:HE1	0.56	2.01	7	2
1:B:224:PHE:CE1	1:B:269:GLN:CD	0.56	2.80	10	1
1:B:246:LEU:CD2	1:B:356:ILE:HG21	0.56	2.30	12	1
1:B:240:GLN:CG	1:B:244:LEU:HD22	0.56	2.30	13	1
1:A:70:VAL:C	1:A:71:LEU:O	0.56	2.45	9	10
1:A:96:ILE:HG12	1:A:127:GLU:CB	0.56	2.31	4	7
1:A:96:ILE:HD13	1:A:128:TYR:CD2	0.56	2.35	14	5
1:A:134:GLY:CA	1:B:273:PRO:HB3	0.56	2.30	2	4
1:A:45:THR:HG21	1:A:149:ILE:HG21	0.56	1.77	3	2
1:A:142:GLU:OE1	1:A:166:ARG:NH1	0.56	2.39	3	1
1:A:19:PHE:CD2	1:A:20:LEU:N	0.56	2.74	14	3
1:A:32:THR:CG2	1:A:33:ASN:H	0.56	2.11	5	1
1:B:228:VAL:CB	1:B:270:VAL:CG2	0.56	2.84	11	4
1:B:295:GLY:C	1:B:324:ARG:HD3	0.56	2.22	5	1
1:B:227:LEU:HD21	1:B:228:VAL:HG23	0.56	1.78	9	1
1:A:40:GLN:CG	1:A:44:LEU:HD22	0.56	2.30	13	1
1:A:81:GLN:OE1	1:A:108:TRP:CZ2	0.56	2.58	13	1
1:A:98:PRO:HG3	1:B:225:MET:SD	0.56	2.41	14	1
1:A:150:ALA:O	1:A:154:PRO:CD	0.56	2.54	14	2
1:B:253:GLN:O	1:B:253:GLN:OE1	0.56	2.24	15	1
1:A:166:ARG:HG3	1:A:167:VAL:HG23	0.56	1.78	1	1
1:B:226:GLY:C	1:B:228:VAL:N	0.56	2.59	5	6
1:A:80:ASP:OD1	1:A:105:GLU:OE2	0.56	2.24	4	2
1:A:96:ILE:CD1	1:A:124:ARG:O	0.56	2.54	4	1
1:B:215:VAL:O	1:B:215:VAL:HG12	0.56	2.01	4	3
1:A:25:MET:HA	1:A:25:MET:CE	0.56	2.30	5	1
1:B:324:ARG:C	1:B:328:TYR:CD2	0.56	2.80	5	7
1:B:240:GLN:NE2	1:B:266:TRP:NE1	0.56	2.54	6	1
1:A:58:PHE:CE1	1:A:86:LYS:HG2	0.56	2.36	9	1
1:B:323:GLY:N	1:B:325:GLU:CD	0.56	2.59	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:ILE:HD13	1:A:135:LEU:HD23	0.55	1.76	1	1
1:A:121:GLU:C	1:A:125:GLU:OE1	0.55	2.45	15	3
1:A:112:PHE:HD2	1:B:311:ALA:CB	0.55	2.14	13	2
1:B:243:PHE:CZ	1:B:293:ILE:HD12	0.55	2.35	3	1
1:B:320:LEU:O	1:B:346:TYR:HB2	0.55	2.01	3	4
1:A:130:PHE:CE1	1:B:225:MET:HB3	0.55	2.36	4	1
1:A:125:GLU:HG2	1:A:145:HIS:NE2	0.55	2.14	8	3
1:B:225:MET:HA	1:B:225:MET:CE	0.55	2.26	5	1
1:B:269:GLN:HG3	1:B:270:VAL:H	0.55	1.61	9	3
1:A:95:GLY:HA2	1:A:121:GLU:OE1	0.55	2.01	10	1
1:A:24:PHE:HD1	1:B:330:PHE:CE2	0.55	2.19	13	2
1:A:96:ILE:CB	1:A:124:ARG:HG3	0.55	2.31	12	2
1:A:98:PRO:HA	1:A:128:TYR:CD2	0.55	2.36	15	1
1:A:20:LEU:O	1:A:59:ASN:ND2	0.55	2.30	14	2
1:A:147:LYS:O	1:A:151:LEU:HB2	0.55	2.01	15	2
1:B:232:THR:CG2	1:B:233:ASN:N	0.55	2.70	3	2
1:A:142:GLU:CA	1:A:142:GLU:OE1	0.55	2.54	4	1
1:B:229:ASN:CB	1:B:232:THR:CG2	0.55	2.83	4	1
1:A:130:PHE:CE2	1:B:224:PHE:HB3	0.55	2.37	14	2
1:B:237:SER:HA	1:B:240:GLN:CG	0.55	2.31	15	2
1:B:316:ILE:C	1:B:317:VAL:CG2	0.55	2.74	5	2
1:A:24:PHE:CD2	1:B:330:PHE:CE2	0.55	2.94	6	1
1:A:124:ARG:HB3	1:A:128:TYR:CE2	0.55	2.35	14	2
1:B:321:GLU:CG	1:B:346:TYR:OH	0.55	2.53	6	1
1:A:153:LYS:HB2	1:A:154:PRO:CD	0.55	2.30	13	4
1:B:228:VAL:HA	1:B:233:ASN:CB	0.55	2.32	8	3
1:B:234:SER:C	1:B:236:PRO:HD3	0.55	2.21	10	1
1:A:64:GLU:O	1:A:69:GLN:HG2	0.55	1.99	11	1
1:A:64:GLU:CB	1:A:69:GLN:HG3	0.55	2.32	11	1
1:A:35:MET:HB3	1:A:69:GLN:HG2	0.55	1.76	12	1
1:A:112:PHE:HD2	1:B:311:ALA:HB1	0.55	1.61	13	1
1:A:96:ILE:HG12	1:A:127:GLU:CD	0.55	2.21	15	1
1:A:62:ARG:C	1:A:64:GLU:N	0.55	2.54	14	4
1:B:224:PHE:C	1:B:226:GLY:N	0.55	2.60	15	8
1:A:28:VAL:CG1	1:A:70:VAL:HG22	0.55	2.26	8	5
1:A:47:ILE:CD1	1:A:47:ILE:N	0.55	2.69	4	2
1:B:224:PHE:CZ	1:B:261:HIS:CE1	0.55	2.95	4	1
1:A:124:ARG:O	1:A:128:TYR:HD2	0.55	1.84	5	7
1:B:344:VAL:CG2	1:B:359:ALA:HB3	0.55	2.32	6	1
1:A:50:PHE:CD2	1:A:55:LEU:CD1	0.55	2.89	7	4
1:A:34:SER:CB	1:A:68:ALA:HB1	0.55	2.30	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:MET:CE	1:A:31:GLU:OE2	0.55	2.55	3	1
1:A:104:VAL:HG11	1:B:331:LEU:HG	0.55	1.78	6	2
1:B:240:GLN:OE1	1:B:265:ALA:HB1	0.55	2.02	4	1
1:A:28:VAL:CG2	1:A:69:GLN:OE1	0.55	2.54	7	1
1:A:103:HIS:CB	1:B:304:VAL:HG22	0.55	2.30	9	1
1:A:124:ARG:HG2	1:A:124:ARG:HH11	0.55	1.62	15	1
1:B:227:LEU:CD2	1:B:228:VAL:N	0.55	2.69	3	3
1:B:246:LEU:CD1	1:B:250:PHE:CD1	0.55	2.89	1	1
1:B:270:VAL:C	1:B:271:LEU:O	0.55	2.45	13	10
1:B:321:GLU:HB3	1:B:324:ARG:HB2	0.55	1.77	12	5
1:A:45:THR:O	1:A:48:GLU:HB2	0.55	2.02	5	2
1:B:340:ALA:CB	1:B:367:VAL:CG2	0.55	2.84	14	3
1:B:227:LEU:HD12	1:B:239:GLU:OE2	0.55	2.02	3	1
1:B:279:LEU:O	1:B:283:GLU:HG2	0.55	2.01	3	1
1:B:346:TYR:O	1:B:347:LYS:HB3	0.55	2.01	3	2
1:B:222:GLY:C	1:B:224:PHE:H	0.55	2.05	4	4
1:A:19:PHE:O	1:A:91:VAL:HG12	0.55	2.01	5	1
1:B:332:VAL:CG1	1:B:343:PHE:CE2	0.55	2.90	6	1
1:A:138:VAL:HB	1:B:281:GLN:NE2	0.55	2.16	7	1
1:A:75:GLU:O	1:A:79:LEU:CG	0.55	2.53	15	3
1:A:31:GLU:O	1:A:31:GLU:CG	0.55	2.54	11	2
1:B:281:GLN:O	1:B:285:ARG:HG2	0.55	2.00	10	2
1:A:98:PRO:HD3	1:B:230:PRO:HB3	0.55	1.78	11	1
1:B:234:SER:C	1:B:268:ALA:HB1	0.55	2.22	11	1
1:A:18:VAL:CG1	1:A:91:VAL:CG1	0.55	2.84	12	1
1:A:81:GLN:OE1	1:B:338:VAL:HG11	0.55	2.02	14	1
1:B:320:LEU:O	1:B:345:HIS:HA	0.55	2.01	1	2
1:B:353:LYS:N	1:B:354:PRO:CD	0.55	2.69	15	10
1:A:40:GLN:HG3	1:A:41:LEU:HD13	0.55	1.78	5	2
1:A:49:HIS:CE1	1:A:53:GLN:CG	0.55	2.90	3	3
1:A:73:PRO:CB	1:B:334:GLY:N	0.55	2.70	11	3
1:A:79:LEU:O	1:A:83:GLU:HG2	0.55	2.02	3	1
1:A:111:ALA:CB	1:B:312:PHE:CE2	0.55	2.81	11	3
1:A:35:MET:O	1:A:35:MET:HE2	0.55	2.02	10	1
1:B:289:VAL:HG13	1:B:290:PHE:N	0.55	2.17	10	1
1:A:112:PHE:CE2	1:B:311:ALA:HA	0.55	2.37	13	1
1:B:259:ASN:OD1	1:B:283:GLU:HB3	0.55	2.02	15	1
1:A:129:GLY:O	1:B:273:PRO:CG	0.55	2.55	1	2
1:B:316:ILE:HD13	1:B:335:LEU:HD23	0.55	1.77	1	1
1:A:111:ALA:HB1	1:B:312:PHE:CD2	0.55	2.36	2	2
1:A:81:GLN:O	1:A:85:ARG:HG2	0.55	2.01	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:278:PRO:O	1:B:281:GLN:HG3	0.55	2.01	4	2
1:A:95:GLY:C	1:A:124:ARG:HD3	0.55	2.22	5	1
1:B:226:GLY:O	1:B:227:LEU:C	0.55	2.44	10	5
1:B:218:VAL:O	1:B:218:VAL:HG12	0.55	2.02	7	1
1:B:219:PHE:HA	1:B:258:PHE:O	0.55	2.01	7	2
1:B:228:VAL:HG23	1:B:232:THR:C	0.55	2.22	8	2
1:A:50:PHE:HD1	1:A:55:LEU:CB	0.55	2.15	10	3
1:B:355:GLN:NE2	1:B:355:GLN:HA	0.55	2.17	13	1
1:B:285:ARG:HB3	1:B:312:PHE:CG	0.55	2.36	15	1
1:A:39:GLU:O	1:A:42:PRO:HD2	0.55	2.01	14	9
1:A:43:PHE:O	1:A:47:ILE:CB	0.55	2.55	4	3
1:A:73:PRO:HB3	1:B:329:GLY:O	0.55	2.00	11	2
1:B:225:MET:HA	1:B:228:VAL:CG1	0.55	2.31	3	4
1:B:349:ILE:O	1:B:353:LYS:HD3	0.55	2.02	1	1
1:A:94:PRO:O	1:A:99:SER:OG	0.55	2.25	4	3
1:A:140:ALA:CB	1:A:167:VAL:CG2	0.55	2.85	14	4
1:B:276:CYS:HA	1:B:279:LEU:CD2	0.55	2.32	2	1
1:A:131:LEU:HG	1:B:304:VAL:HG11	0.55	1.79	3	2
1:A:78:PRO:O	1:A:81:GLN:HG3	0.55	2.02	4	2
1:A:168:ASN:C	1:A:168:ASN:ND2	0.55	2.59	7	1
1:B:250:PHE:HD2	1:B:255:LEU:CB	0.55	2.15	7	3
1:B:241:LEU:CA	1:B:244:LEU:HG	0.55	2.32	14	7
1:B:281:GLN:CG	1:B:282:LEU:HD22	0.55	2.32	1	1
1:A:98:PRO:HB2	1:B:300:PRO:HB3	0.55	1.79	2	2
1:A:111:ALA:CB	1:B:312:PHE:HD2	0.55	2.14	13	3
1:A:23:PRO:O	1:A:99:SER:HB2	0.55	2.02	13	2
1:A:40:GLN:O	1:A:43:PHE:HB2	0.55	2.02	11	3
1:B:245:THR:O	1:B:248:GLU:HB3	0.55	2.00	11	3
1:B:258:PHE:CD2	1:B:283:GLU:OE2	0.55	2.59	3	2
1:B:249:HIS:CE1	1:B:353:LYS:CE	0.55	2.89	5	1
1:B:353:LYS:CB	1:B:354:PRO:HD3	0.55	2.32	5	5
1:A:18:VAL:HG11	1:A:50:PHE:CG	0.55	2.36	7	2
1:A:50:PHE:HD2	1:A:55:LEU:CB	0.55	2.14	8	3
1:A:131:LEU:O	1:A:135:LEU:CD1	0.55	2.54	10	2
1:A:65:ALA:HB1	1:A:69:GLN:NE2	0.55	2.17	8	1
1:A:27:LEU:HD21	1:A:28:VAL:HG23	0.55	1.78	9	1
1:A:132:VAL:HG12	1:A:143:PHE:CE2	0.55	2.36	11	1
1:A:100:PRO:HB3	1:B:298:PRO:HB2	0.55	1.77	14	1
1:B:306:ILE:HG22	1:B:307:GLY:N	0.55	2.15	1	5
1:A:121:GLU:HB2	1:A:124:ARG:HB2	0.55	1.77	2	3
1:B:217:SER:HB3	1:B:256:GLU:HB3	0.55	1.78	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:302:THR:HA	1:B:305:GLU:HG3	0.55	1.79	15	2
1:A:77:THR:HG22	1:B:338:VAL:HG11	0.55	1.78	14	2
1:B:342:GLU:OE1	1:B:363:VAL:HG23	0.55	2.02	4	2
1:A:24:PHE:CD1	1:A:76:CYS:SG	0.55	3.00	5	1
1:A:26:GLY:O	1:A:27:LEU:C	0.55	2.46	10	4
1:A:90:PHE:O	1:A:117:VAL:HG23	0.55	2.02	5	1
1:B:219:PHE:CZ	1:B:259:ASN:HB2	0.55	2.37	5	2
1:B:220:LEU:HD11	1:B:243:PHE:CE1	0.55	2.37	5	1
1:B:224:PHE:O	1:B:227:LEU:CG	0.55	2.54	5	1
1:B:285:ARG:N	1:B:312:PHE:CE1	0.55	2.75	5	2
1:B:348:ASP:OD1	1:B:351:LEU:HD11	0.55	2.02	5	1
1:B:284:ILE:CG2	1:B:309:ALA:N	0.55	2.70	7	3
1:A:119:LEU:HD22	1:A:146:TYR:CD1	0.55	2.36	8	1
1:A:125:GLU:CD	1:A:145:HIS:HE2	0.55	2.06	9	1
1:B:314:LYS:HA	1:B:314:LYS:HZ3	0.55	1.61	11	1
1:A:142:GLU:OE2	1:A:159:ALA:CB	0.55	2.53	13	2
1:A:25:MET:HA	1:A:28:VAL:CG1	0.54	2.32	3	4
1:A:103:HIS:CE1	1:A:128:TYR:CE1	0.54	2.94	13	5
1:A:121:GLU:OE1	1:A:121:GLU:HA	0.54	2.02	1	1
1:B:321:GLU:C	1:B:325:GLU:OE1	0.54	2.45	15	3
1:A:125:GLU:CA	1:A:128:TYR:CD1	0.54	2.88	2	3
1:A:29:ASN:N	1:A:29:ASN:HD22	0.54	1.98	3	1
1:B:227:LEU:HD11	1:B:235:MET:HB2	0.54	1.78	3	2
1:B:230:PRO:O	1:B:231:GLU:HB3	0.54	2.02	7	2
1:A:18:VAL:CG1	1:A:91:VAL:HG11	0.54	2.32	12	1
1:A:121:GLU:O	1:A:121:GLU:OE2	0.54	2.25	12	1
1:B:281:GLN:HG2	1:B:308:TRP:CE2	0.54	2.38	15	1
1:B:296:ILE:HG12	1:B:327:GLU:CB	0.54	2.31	4	7
1:B:219:PHE:CZ	1:B:259:ASN:CB	0.54	2.90	5	1
1:A:37:SER:O	1:A:39:GLU:N	0.54	2.40	6	1
1:A:59:ASN:HA	1:A:83:GLU:HG2	0.54	1.78	8	1
1:A:85:ARG:CB	1:A:112:PHE:HE1	0.54	2.15	9	3
1:A:27:LEU:HB2	1:A:35:MET:CB	0.54	2.33	10	1
1:A:111:ALA:HB2	1:B:312:PHE:HE2	0.54	1.60	11	2
1:A:84:ILE:O	1:A:114:LYS:CD	0.54	2.56	13	1
1:B:355:GLN:HA	1:B:355:GLN:HE21	0.54	1.62	13	1
1:A:24:PHE:HB3	1:B:330:PHE:CE2	0.54	2.36	14	1
1:A:69:GLN:HG2	1:A:70:VAL:HG23	0.54	1.79	1	1
1:A:119:LEU:O	1:A:146:TYR:HE2	0.54	1.83	1	2
1:A:149:ILE:HA	1:A:152:ALA:HB3	0.54	1.79	7	3
1:B:222:GLY:O	1:B:302:THR:OG1	0.54	2.25	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:239:GLU:O	1:B:243:PHE:CD2	0.54	2.61	9	2
1:B:321:GLU:O	1:B:324:ARG:N	0.54	2.40	1	2
1:B:268:ALA:O	1:B:269:GLN:HB2	0.54	2.01	2	1
1:B:245:THR:HG21	1:B:349:ILE:CG2	0.54	2.32	8	2
1:A:45:THR:C	1:A:49:HIS:NE2	0.54	2.60	5	1
1:B:219:PHE:CD1	1:B:284:ILE:HA	0.54	2.38	5	1
1:B:265:ALA:HA	1:B:269:GLN:NE2	0.54	2.16	6	1
1:B:228:VAL:CG2	1:B:269:GLN:OE1	0.54	2.53	7	1
1:A:96:ILE:N	1:A:124:ARG:HB3	0.54	2.16	8	1
1:A:34:SER:C	1:A:68:ALA:HB1	0.54	2.22	11	1
1:A:35:MET:HB3	1:A:68:ALA:HA	0.54	1.80	11	1
1:B:235:MET:HB3	1:B:268:ALA:HA	0.54	1.80	11	1
1:B:240:GLN:CG	1:B:241:LEU:HD13	0.54	2.14	12	1
1:B:325:GLU:OE1	1:B:326:GLU:OE1	0.54	2.25	12	1
1:A:131:LEU:CD2	1:B:304:VAL:CG1	0.54	2.85	13	1
1:B:303:HIS:CE1	1:B:332:VAL:HG23	0.54	2.36	14	1
1:A:75:GLU:C	1:A:79:LEU:HD23	0.54	2.22	15	1
1:B:284:ILE:HD11	1:B:305:GLU:OE1	0.54	2.02	15	1
1:B:293:ILE:H	1:B:302:THR:HG21	0.54	1.61	15	1
1:A:19:PHE:O	1:A:19:PHE:CD2	0.54	2.61	1	1
1:A:96:ILE:CA	1:A:97:PRO:C	0.54	2.75	1	8
1:A:96:ILE:HG13	1:A:98:PRO:HD3	0.54	1.79	7	7
1:B:218:VAL:HG22	1:B:289:VAL:HG12	0.54	1.79	1	2
1:B:303:HIS:CE1	1:B:328:TYR:CE1	0.54	2.96	13	5
1:B:325:GLU:HG3	1:B:326:GLU:H	0.54	1.62	3	3
1:A:124:ARG:C	1:A:128:TYR:CD2	0.54	2.81	5	7
1:B:219:PHE:CD2	1:B:220:LEU:N	0.54	2.76	14	3
1:B:325:GLU:CA	1:B:328:TYR:CD2	0.54	2.90	13	3
1:A:69:GLN:O	1:A:70:VAL:CB	0.54	2.54	6	1
1:A:48:GLU:OE2	1:A:52:LYS:HE2	0.54	2.02	11	1
1:B:264:GLU:CB	1:B:269:GLN:HG3	0.54	2.33	11	1
1:B:228:VAL:HG22	1:B:232:THR:CB	0.54	2.32	14	1
1:A:81:GLN:HG2	1:A:108:TRP:CE2	0.54	2.37	15	1
1:A:130:PHE:HE1	1:B:224:PHE:HB3	0.54	1.60	2	1
1:B:223:PRO:C	1:B:225:MET:CE	0.54	2.76	2	1
1:A:15:VAL:CG1	1:A:55:LEU:HD22	0.54	2.31	3	2
1:A:20:LEU:HD11	1:A:43:PHE:CE1	0.54	2.38	5	1
1:B:236:PRO:HG2	1:B:239:GLU:HB3	0.54	1.79	8	1
1:A:64:GLU:HB2	1:A:69:GLN:OE1	0.54	2.03	9	1
1:B:228:VAL:CG1	1:B:232:THR:C	0.54	2.75	11	1
1:B:229:ASN:HB2	1:B:233:ASN:OD1	0.54	2.03	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:ALA:O	1:A:153:LYS:C	0.54	2.45	6	2
1:B:321:GLU:CB	1:B:324:ARG:HB2	0.54	2.33	14	5
1:A:19:PHE:HA	1:A:58:PHE:O	0.54	2.03	7	3
1:A:81:GLN:O	1:A:84:ILE:HB	0.54	2.03	6	3
1:B:332:VAL:HG13	1:B:343:PHE:CE1	0.54	2.38	5	3
1:B:346:TYR:O	1:B:347:LYS:CG	0.54	2.55	3	2
1:A:46:LEU:CD1	1:A:149:ILE:HG23	0.54	2.33	10	3
1:A:134:GLY:O	1:A:137:THR:CG2	0.54	2.54	11	7
1:A:110:SER:OG	1:A:135:LEU:CD2	0.54	2.55	5	2
1:A:117:VAL:HG11	1:A:160:ILE:CG1	0.54	2.32	7	3
1:B:279:LEU:O	1:B:283:GLU:CB	0.54	2.56	5	2
1:B:325:GLU:HG2	1:B:345:HIS:NE2	0.54	2.17	14	3
1:A:19:PHE:CE1	1:A:59:ASN:HB2	0.54	2.38	12	2
1:B:321:GLU:HG2	1:B:346:TYR:CZ	0.54	2.38	6	1
1:B:324:ARG:HB3	1:B:328:TYR:CE2	0.54	2.38	14	2
1:A:35:MET:HB3	1:A:69:GLN:OE1	0.54	2.00	8	1
1:B:325:GLU:OE2	1:B:345:HIS:NE2	0.54	2.40	8	1
1:B:261:HIS:HB3	1:B:265:ALA:HB2	0.54	1.79	9	1
1:B:224:PHE:CD2	1:B:270:VAL:HG23	0.54	2.37	11	1
1:A:15:VAL:HG13	1:A:18:VAL:HG23	0.54	1.76	12	1
1:B:296:ILE:CB	1:B:324:ARG:HG3	0.54	2.31	12	2
1:A:28:VAL:CG2	1:A:32:THR:CB	0.54	2.86	14	1
1:A:33:ASN:HB2	1:A:69:GLN:OE1	0.54	2.02	1	1
1:A:41:LEU:CA	1:A:44:LEU:HG	0.54	2.33	11	7
1:B:217:SER:HB3	1:B:258:PHE:CE2	0.54	2.37	15	2
1:B:306:ILE:HG12	1:B:318:LEU:CD2	0.54	2.32	2	6
1:A:120:LEU:O	1:A:146:TYR:HB2	0.54	2.02	3	4
1:B:249:HIS:CE1	1:B:253:GLN:CG	0.54	2.90	3	3
1:A:40:GLN:CG	1:A:66:TRP:HE1	0.54	2.15	14	2
1:B:215:VAL:HG12	1:B:255:LEU:HB3	0.54	1.79	4	1
1:A:103:HIS:O	1:B:304:VAL:HG22	0.54	2.03	9	2
1:B:224:PHE:CD1	1:B:276:CYS:SG	0.54	3.01	5	2
1:B:251:GLU:OE2	1:B:256:GLU:HG3	0.54	2.02	5	1
1:B:344:VAL:CG1	1:B:355:GLN:HB3	0.54	2.33	6	2
1:B:261:HIS:C	1:B:265:ALA:HB2	0.54	2.23	12	2
1:B:280:ASP:O	1:B:284:ILE:CD1	0.54	2.55	13	2
1:A:148:ASP:HB3	1:A:151:LEU:HD12	0.54	1.80	13	1
1:B:244:LEU:O	1:B:247:ILE:HG22	0.54	2.03	13	1
1:B:220:LEU:HD13	1:B:243:PHE:CD1	0.54	2.37	14	1
1:A:46:LEU:CD1	1:A:50:PHE:CD1	0.54	2.91	1	1
1:A:134:GLY:HA3	1:B:277:THR:HG1	0.54	1.61	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:LYS:O	1:A:148:ASP:OD1	0.54	2.26	1	1
1:B:235:MET:HG2	1:B:236:PRO:HD2	0.54	1.78	1	1
1:A:23:PRO:C	1:A:25:MET:CE	0.54	2.76	2	1
1:A:111:ALA:HB1	1:B:312:PHE:HD2	0.54	1.61	13	2
1:B:335:LEU:HD23	1:B:341:VAL:HG21	0.54	1.80	9	3
1:A:16:ARG:CD	1:A:16:ARG:N	0.54	2.70	4	1
1:A:16:ARG:O	1:A:54:GLY:O	0.54	2.26	4	1
1:A:112:PHE:C	1:A:113:ASP:OD1	0.54	2.46	5	2
1:B:313:ASP:OD1	1:B:313:ASP:N	0.54	2.39	5	1
1:B:285:ARG:CG	1:B:312:PHE:HE2	0.54	2.16	6	1
1:A:130:PHE:HD1	1:B:225:MET:CG	0.54	2.16	10	2
1:B:235:MET:O	1:B:235:MET:HG2	0.54	2.03	10	1
1:A:156:ILE:HG22	1:A:157:ASP:OD1	0.54	2.02	11	1
1:B:248:GLU:OE2	1:B:252:LYS:HE2	0.54	2.03	11	1
1:A:23:PRO:O	1:A:99:SER:CB	0.54	2.56	13	1
1:A:44:LEU:N	1:A:44:LEU:CD1	0.54	2.68	13	1
1:A:124:ARG:CD	1:A:124:ARG:H	0.54	2.14	14	1
1:B:249:HIS:HB3	1:B:353:LYS:NZ	0.54	2.16	14	1
1:A:53:GLN:HG3	1:A:55:LEU:HD21	0.54	1.79	15	1
1:A:142:GLU:OE1	1:A:143:PHE:N	0.54	2.40	1	2
1:A:159:ALA:O	1:A:163:VAL:HB	0.54	2.03	1	2
1:B:223:PRO:O	1:B:226:GLY:CA	0.54	2.56	10	2
1:B:249:HIS:CE1	1:B:253:GLN:HG3	0.54	2.37	13	4
1:A:19:PHE:CD2	1:A:91:VAL:O	0.54	2.61	4	1
1:A:132:VAL:CG1	1:A:143:PHE:CE2	0.54	2.91	6	1
1:B:316:ILE:CG2	1:B:318:LEU:CD1	0.54	2.85	9	2
1:A:28:VAL:HA	1:A:33:ASN:CB	0.54	2.31	8	3
1:B:239:GLU:C	1:B:239:GLU:CD	0.54	2.65	8	1
1:A:103:HIS:NE2	1:A:128:TYR:CE2	0.54	2.76	9	1
1:B:290:PHE:CD2	1:B:309:ALA:HB2	0.54	2.37	9	2
1:A:40:GLN:O	1:A:44:LEU:CG	0.54	2.55	12	2
1:B:225:MET:CB	1:B:230:PRO:HA	0.54	2.33	10	2
1:B:299:SER:HB2	1:B:302:THR:HG1	0.54	1.61	10	1
1:A:73:PRO:HB2	1:B:334:GLY:N	0.54	2.18	11	1
1:B:324:ARG:N	1:B:324:ARG:HD2	0.54	2.17	12	2
1:A:100:PRO:CG	1:B:298:PRO:HB2	0.54	2.33	13	1
1:B:324:ARG:CD	1:B:324:ARG:H	0.54	2.13	14	1
1:B:269:GLN:HG2	1:B:270:VAL:HG23	0.54	1.78	1	1
1:B:303:HIS:NE2	1:B:328:TYR:CE2	0.54	2.75	2	2
1:A:28:VAL:HG22	1:A:33:ASN:CB	0.54	2.33	5	2
1:B:228:VAL:HG22	1:B:233:ASN:CB	0.54	2.32	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:CE1	1:A:90:PHE:HE1	0.54	2.21	4	1
1:B:256:GLU:HB3	1:B:258:PHE:HE2	0.54	1.61	7	3
1:A:75:GLU:OE1	1:A:75:GLU:N	0.54	2.41	10	1
1:A:98:PRO:CD	1:B:230:PRO:HB3	0.54	2.33	11	1
1:A:98:PRO:HB2	1:B:300:PRO:CG	0.54	2.33	13	1
1:A:49:HIS:CB	1:A:153:LYS:NZ	0.54	2.71	14	1
1:A:53:GLN:O	1:A:53:GLN:OE1	0.54	2.26	15	1
1:A:142:GLU:HG2	1:A:163:VAL:CB	0.54	2.33	15	1
1:B:233:ASN:HB2	1:B:269:GLN:OE1	0.53	2.03	1	1
1:B:285:ARG:CB	1:B:312:PHE:CD2	0.53	2.91	2	1
1:B:240:GLN:O	1:B:243:PHE:HB2	0.53	2.03	11	3
1:B:319:LEU:HB3	1:B:346:TYR:CE1	0.53	2.38	11	2
1:B:320:LEU:CD1	1:B:325:GLU:CD	0.53	2.77	4	1
1:A:37:SER:HA	1:A:40:GLN:CG	0.53	2.32	15	2
1:A:125:GLU:OE2	1:A:125:GLU:O	0.53	2.25	5	1
1:B:228:VAL:CG1	1:B:270:VAL:CB	0.53	2.76	11	2
1:B:259:ASN:HA	1:B:283:GLU:HG2	0.53	1.79	8	1
1:A:130:PHE:CZ	1:B:270:VAL:CG1	0.53	2.90	9	1
1:A:130:PHE:CD1	1:B:225:MET:HE2	0.53	2.38	9	1
1:A:18:VAL:HG12	1:A:57:VAL:HG22	0.53	1.78	11	1
1:B:264:GLU:O	1:B:269:GLN:HG2	0.53	2.03	11	1
1:A:125:GLU:OE1	1:A:126:GLU:OE1	0.53	2.26	12	1
1:B:249:HIS:CB	1:B:353:LYS:NZ	0.53	2.71	14	1
1:A:59:ASN:OD1	1:A:83:GLU:HB3	0.53	2.03	15	1
1:A:85:ARG:HD2	1:A:112:PHE:CZ	0.53	2.38	2	4
1:A:94:PRO:CA	1:A:99:SER:OG	0.53	2.56	4	2
1:A:24:PHE:CZ	1:A:69:GLN:HG3	0.53	2.38	6	2
1:B:282:LEU:O	1:B:286:LYS:HG3	0.53	2.03	10	4
1:A:61:HIS:O	1:A:64:GLU:CB	0.53	2.56	4	1
1:A:120:LEU:CD1	1:A:125:GLU:CG	0.53	2.85	4	1
1:A:120:LEU:CD1	1:A:143:PHE:HB3	0.53	2.32	4	2
1:B:259:ASN:ND2	1:B:280:ASP:OD2	0.53	2.40	5	1
1:A:112:PHE:HD1	1:B:311:ALA:CA	0.53	2.16	6	3
1:B:227:LEU:HD13	1:B:235:MET:HG3	0.53	1.79	11	1
1:B:284:ILE:O	1:B:314:LYS:CG	0.53	2.56	13	1
1:B:271:LEU:N	1:B:271:LEU:HD22	0.53	2.18	14	1
1:A:104:VAL:HG12	1:B:307:GLY:HA3	0.53	1.79	1	2
1:B:352:ALA:O	1:B:353:LYS:C	0.53	2.47	1	2
1:B:364:VAL:O	1:B:368:ASN:HB2	0.53	2.04	1	1
1:A:50:PHE:CD1	1:A:55:LEU:CD1	0.53	2.90	10	6
1:A:102:THR:HA	1:A:105:GLU:HG3	0.53	1.79	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:TRP:O	1:B:311:ALA:HB1	0.53	2.03	6	3
1:A:42:PRO:O	1:A:45:THR:HB	0.53	2.04	8	2
1:A:72:THR:C	1:A:76:CYS:SG	0.53	2.87	6	1
1:B:269:GLN:O	1:B:270:VAL:CB	0.53	2.56	6	1
1:B:331:LEU:O	1:B:335:LEU:CD1	0.53	2.57	10	2
1:B:344:VAL:HG12	1:B:344:VAL:O	0.53	2.01	9	2
1:A:36:PRO:O	1:A:39:GLU:N	0.53	2.37	10	1
1:B:246:LEU:HD21	1:B:353:LYS:HA	0.53	1.79	11	2
1:A:28:VAL:HG22	1:A:32:THR:CB	0.53	2.32	14	1
1:A:19:PHE:HD2	1:A:59:ASN:ND2	0.53	2.01	15	1
1:A:27:LEU:CD2	1:A:28:VAL:N	0.53	2.71	3	3
1:A:106:ILE:HG12	1:A:118:LEU:CD2	0.53	2.32	2	6
1:A:29:ASN:CG	1:A:33:ASN:CG	0.53	2.66	3	1
1:B:264:GLU:OE2	1:B:271:LEU:CD1	0.53	2.56	3	1
1:A:62:ARG:CD	1:A:66:TRP:CH2	0.53	2.90	6	1
1:A:144:VAL:CG2	1:A:159:ALA:HB3	0.53	2.32	6	1
1:B:335:LEU:O	1:B:339:ALA:O	0.53	2.27	11	5
1:A:107:GLY:O	1:A:110:SER:N	0.53	2.42	7	3
1:A:108:TRP:HE1	1:B:307:GLY:C	0.53	2.07	13	2
1:A:141:VAL:HG12	1:A:143:PHE:CE1	0.53	2.38	13	3
1:B:219:PHE:HD2	1:B:291:VAL:H	0.53	1.45	7	1
1:B:250:PHE:CD2	1:B:255:LEU:CD1	0.53	2.89	7	3
1:B:259:ASN:N	1:B:283:GLU:OE2	0.53	2.42	7	1
1:A:28:VAL:HG23	1:A:33:ASN:CA	0.53	2.33	8	1
1:A:28:VAL:O	1:A:29:ASN:C	0.53	2.44	11	2
1:A:47:ILE:HG13	1:A:57:VAL:CG2	0.53	2.33	13	2
1:A:45:THR:O	1:A:48:GLU:HB3	0.53	2.04	3	3
1:B:224:PHE:HE1	1:B:270:VAL:CA	0.53	2.16	3	2
1:B:242:PRO:O	1:B:245:THR:HB	0.53	2.03	8	3
1:A:33:ASN:OD1	1:A:68:ALA:O	0.53	2.25	4	1
1:A:41:LEU:O	1:A:44:LEU:HB2	0.53	2.03	4	2
1:B:275:GLU:O	1:B:279:LEU:HB3	0.53	2.03	4	1
1:B:294:PRO:C	1:B:328:TYR:HH	0.53	2.07	4	2
1:A:40:GLN:NE2	1:A:65:ALA:O	0.53	2.42	10	2
1:B:316:ILE:O	1:B:317:VAL:HG22	0.53	2.03	6	2
1:A:80:ASP:HB3	1:A:108:TRP:HZ3	0.53	1.64	6	1
1:A:122:GLU:OE1	1:A:146:TYR:O	0.53	2.27	6	1
1:A:81:GLN:HE22	1:B:311:ALA:HA	0.53	1.63	8	1
1:A:64:GLU:N	1:A:64:GLU:OE2	0.53	2.42	10	2
1:B:264:GLU:OE2	1:B:264:GLU:N	0.53	2.40	9	1
1:A:74:GLU:C	1:A:75:GLU:OE1	0.53	2.46	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:325:GLU:OE2	1:B:345:HIS:HD2	0.53	1.86	11	2
1:A:132:VAL:O	1:A:143:PHE:CE1	0.53	2.61	12	1
1:A:71:LEU:HD12	1:A:75:GLU:OE2	0.53	2.04	15	1
1:B:259:ASN:HA	1:B:283:GLU:CD	0.53	2.24	13	2
1:A:58:PHE:CD1	1:A:86:LYS:HD2	0.53	2.38	2	1
1:A:59:ASN:ND2	1:A:80:ASP:HA	0.53	2.19	2	1
1:B:215:VAL:O	1:B:255:LEU:HD23	0.53	2.04	10	3
1:B:344:VAL:HG13	1:B:355:GLN:CG	0.53	2.33	15	3
1:A:85:ARG:CB	1:A:112:PHE:CD1	0.53	2.92	3	1
1:B:225:MET:HE2	1:B:225:MET:CA	0.53	2.34	5	3
1:B:281:GLN:CA	1:B:308:TRP:CZ3	0.53	2.91	7	1
1:A:25:MET:CE	1:B:330:PHE:HB3	0.53	2.34	8	2
1:A:89:VAL:HG13	1:A:90:PHE:N	0.53	2.17	10	1
1:B:236:PRO:O	1:B:239:GLU:N	0.53	2.36	10	1
1:B:228:VAL:CG2	1:B:232:THR:CB	0.53	2.86	14	1
1:B:246:LEU:CD1	1:B:250:PHE:CE1	0.53	2.82	1	1
1:B:281:GLN:O	1:B:284:ILE:HB	0.53	2.03	6	3
1:B:342:GLU:OE1	1:B:366:ARG:NH1	0.53	2.42	3	1
1:B:222:GLY:O	1:B:224:PHE:N	0.53	2.42	4	3
1:B:312:PHE:C	1:B:313:ASP:CG	0.53	2.66	5	1
1:B:342:GLU:HB3	1:B:359:ALA:HB1	0.53	1.80	11	2
1:B:223:PRO:HB3	1:B:299:SER:CA	0.53	2.34	10	1
1:B:308:TRP:CD1	1:B:312:PHE:CE2	0.53	2.96	10	1
1:A:27:LEU:HD12	1:A:35:MET:CA	0.53	2.30	11	1
1:B:355:GLN:NE2	1:B:355:GLN:CA	0.53	2.70	11	2
1:B:218:VAL:CG1	1:B:291:VAL:HG11	0.53	2.34	12	1
1:A:21:ALA:O	1:A:102:THR:HG23	0.53	2.04	15	1
1:A:29:ASN:HB3	1:A:32:THR:CB	0.53	2.34	15	1
1:B:331:LEU:O	1:B:335:LEU:HD12	0.53	2.03	15	1
1:A:130:PHE:CE1	1:B:224:PHE:CD2	0.53	2.97	1	1
1:B:239:GLU:O	1:B:242:PRO:HD2	0.53	2.02	13	10
1:B:303:HIS:N	1:B:306:ILE:HD12	0.53	2.18	2	1
1:B:225:MET:CE	1:B:231:GLU:OE2	0.53	2.57	3	1
1:B:313:ASP:OD1	1:B:313:ASP:O	0.53	2.26	3	2
1:B:331:LEU:CD1	1:B:335:LEU:CD1	0.53	2.86	3	2
1:A:19:PHE:HD1	1:A:83:GLU:O	0.53	1.86	5	2
1:A:35:MET:HE3	1:A:39:GLU:HG2	0.53	1.79	6	1
1:A:40:GLN:NE2	1:A:66:TRP:NE1	0.53	2.57	6	1
1:A:29:ASN:HB2	1:A:32:THR:O	0.53	2.03	10	2
1:A:130:PHE:HE2	1:B:224:PHE:HB3	0.53	1.63	14	1
1:B:275:GLU:CA	1:B:279:LEU:HD12	0.53	2.34	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:269:GLN:HG2	1:B:270:VAL:N	0.53	2.18	1	1
1:B:285:ARG:O	1:B:314:LYS:CE	0.53	2.57	15	3
1:B:296:ILE:N	1:B:324:ARG:HB3	0.53	2.16	8	3
1:A:50:PHE:O	1:A:55:LEU:HG	0.53	2.03	5	2
1:A:70:VAL:O	1:A:71:LEU:C	0.53	2.47	4	2
1:B:216:ARG:CD	1:B:216:ARG:N	0.53	2.71	4	1
1:A:85:ARG:CB	1:A:85:ARG:HH11	0.53	2.17	5	1
1:A:93:ILE:HD11	1:A:119:LEU:HD12	0.53	1.81	5	1
1:A:113:ASP:OD1	1:A:113:ASP:N	0.53	2.41	5	1
1:A:116:ILE:O	1:A:117:VAL:HG22	0.53	2.03	6	2
1:B:295:GLY:HA2	1:B:324:ARG:HD2	0.53	1.80	5	1
1:A:35:MET:O	1:A:35:MET:CG	0.53	2.56	15	2
1:B:335:LEU:CB	1:B:341:VAL:HG11	0.53	2.32	10	1
1:B:306:ILE:CG2	1:B:335:LEU:CD1	0.53	2.87	14	1
1:B:219:PHE:CE1	1:B:259:ASN:HB2	0.53	2.39	12	3
1:A:35:MET:HB3	1:A:69:GLN:NE2	0.53	2.19	3	3
1:A:116:ILE:HB	1:A:141:VAL:HG22	0.53	1.80	3	3
1:B:334:GLY:O	1:B:337:THR:CG2	0.53	2.56	11	7
1:A:24:PHE:O	1:A:27:LEU:CG	0.53	2.57	5	1
1:A:59:ASN:ND2	1:A:80:ASP:OD2	0.53	2.41	5	1
1:A:112:PHE:C	1:A:113:ASP:CG	0.53	2.66	5	1
1:A:74:GLU:O	1:A:78:PRO:HG2	0.53	2.04	6	2
1:A:96:ILE:HD12	1:A:128:TYR:CD1	0.53	2.36	7	2
1:B:290:PHE:HE2	1:B:306:ILE:HG13	0.53	1.64	8	1
1:A:144:VAL:HG12	1:A:144:VAL:O	0.53	2.02	9	2
1:A:27:LEU:HD13	1:A:35:MET:HG3	0.53	1.79	11	1
1:A:104:VAL:CG1	1:B:331:LEU:CD2	0.53	2.86	13	1
1:B:325:GLU:CD	1:B:326:GLU:H	0.53	2.07	15	2
1:A:130:PHE:CD2	1:B:225:MET:HE3	0.52	2.39	12	2
1:A:119:LEU:HD22	1:A:146:TYR:CD2	0.52	2.39	2	1
1:B:293:ILE:HG23	1:B:321:GLU:OE1	0.52	2.04	3	1
1:B:331:LEU:HD12	1:B:335:LEU:CD1	0.52	2.35	3	1
1:A:22:GLY:C	1:A:24:PHE:H	0.52	2.06	7	4
1:A:19:PHE:CD1	1:A:84:ILE:HA	0.52	2.39	5	1
1:A:130:PHE:CA	1:B:273:PRO:HG3	0.52	2.34	5	3
1:A:73:PRO:CA	1:B:330:PHE:O	0.52	2.57	10	3
1:A:108:TRP:CD1	1:A:112:PHE:HE2	0.52	2.23	10	1
1:A:147:LYS:HD3	1:A:147:LYS:N	0.52	2.19	10	1
1:B:224:PHE:CD2	1:B:270:VAL:CG2	0.52	2.92	11	1
1:B:240:GLN:CA	1:B:266:TRP:CZ2	0.52	2.89	13	1
1:B:355:GLN:HE21	1:B:355:GLN:CA	0.52	2.15	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:321:GLU:OE1	1:B:346:TYR:CE2	0.52	2.62	1	2
1:B:349:ILE:HA	1:B:352:ALA:HB3	0.52	1.80	7	3
1:A:59:ASN:N	1:A:83:GLU:HB3	0.52	2.19	4	1
1:A:82:LEU:HB2	1:A:83:GLU:OE1	0.52	2.03	4	1
1:A:16:ARG:O	1:A:16:ARG:HD2	0.52	2.05	5	1
1:A:153:LYS:CB	1:A:154:PRO:HD3	0.52	2.34	5	4
1:B:324:ARG:HB3	1:B:328:TYR:HE2	0.52	1.63	14	3
1:B:228:VAL:HG21	1:B:270:VAL:HB	0.52	1.81	7	1
1:A:68:ALA:O	1:A:69:GLN:HB3	0.52	2.01	9	2
1:A:142:GLU:HA	1:A:142:GLU:OE2	0.52	2.04	9	1
1:B:219:PHE:CD1	1:B:219:PHE:O	0.52	2.61	15	3
1:B:218:VAL:CG1	1:B:291:VAL:CG1	0.52	2.85	12	1
1:A:77:THR:OG1	1:B:331:LEU:HA	0.52	2.04	11	5
1:B:227:LEU:CG	1:B:228:VAL:N	0.52	2.72	7	5
1:B:243:PHE:O	1:B:247:ILE:CB	0.52	2.56	5	3
1:B:296:ILE:CA	1:B:297:PRO:C	0.52	2.75	1	10
1:A:23:PRO:O	1:A:26:GLY:CA	0.52	2.57	10	2
1:A:24:PHE:HB3	1:B:330:PHE:CE1	0.52	2.40	2	2
1:B:280:ASP:OD1	1:B:305:GLU:OE2	0.52	2.27	12	3
1:B:324:ARG:O	1:B:328:TYR:HD1	0.52	1.85	2	3
1:A:132:VAL:HG12	1:A:133:ARG:N	0.52	2.20	3	3
1:B:272:THR:C	1:B:276:CYS:SG	0.52	2.87	6	2
1:A:37:SER:O	1:A:41:LEU:CD2	0.52	2.52	4	2
1:A:61:HIS:O	1:A:64:GLU:HG3	0.52	2.03	4	1
1:B:277:THR:O	1:B:280:ASP:HB2	0.52	2.04	4	2
1:A:96:ILE:N	1:A:124:ARG:HD3	0.52	2.19	11	2
1:A:110:SER:OG	1:A:135:LEU:CG	0.52	2.58	5	1
1:A:116:ILE:C	1:A:117:VAL:CG2	0.52	2.77	6	3
1:B:246:LEU:O	1:B:249:HIS:HD2	0.52	1.88	11	2
1:A:104:VAL:CG1	1:B:331:LEU:HG	0.52	2.33	6	1
1:A:77:THR:HG21	1:B:335:LEU:N	0.52	2.19	8	1
1:A:90:PHE:HD2	1:A:116:ILE:HG12	0.52	1.65	15	2
1:A:104:VAL:HA	1:B:304:VAL:CA	0.52	2.27	10	1
1:A:135:LEU:HB3	1:A:141:VAL:CG1	0.52	2.34	10	1
1:A:44:LEU:HD13	1:A:66:TRP:CZ3	0.52	2.39	11	1
1:A:114:LYS:HZ3	1:A:114:LYS:HA	0.52	1.64	11	1
1:B:239:GLU:OE2	1:B:243:PHE:CZ	0.52	2.62	13	1
1:A:142:GLU:HG2	1:A:163:VAL:HG21	0.52	1.81	15	1
1:A:149:ILE:O	1:A:153:LYS:HD3	0.52	2.04	1	1
1:B:229:ASN:HB2	1:B:232:THR:CB	0.52	2.35	2	1
1:A:107:GLY:HA3	1:B:304:VAL:CG1	0.52	2.35	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ASN:CB	1:A:32:THR:CG2	0.52	2.88	4	1
1:B:320:LEU:CD1	1:B:343:PHE:HB3	0.52	2.33	4	2
1:B:319:LEU:HD21	1:B:356:ILE:HD12	0.52	1.82	5	1
1:A:120:LEU:CD1	1:A:145:HIS:NE2	0.52	2.70	7	3
1:B:262:ARG:CD	1:B:266:TRP:CH2	0.52	2.90	6	1
1:B:280:ASP:HB3	1:B:308:TRP:HZ3	0.52	1.65	6	1
1:B:250:PHE:HD2	1:B:255:LEU:CD1	0.52	2.17	15	3
1:A:24:PHE:CD2	1:A:70:VAL:CG2	0.52	2.92	11	1
1:B:233:ASN:HD22	1:B:234:SER:N	0.52	2.03	13	1
1:B:265:ALA:O	1:B:269:GLN:HG3	0.52	2.04	2	1
1:B:223:PRO:O	1:B:299:SER:HB2	0.52	2.03	13	2
1:A:40:GLN:OE1	1:A:65:ALA:HB1	0.52	2.05	4	1
1:A:153:LYS:HB3	1:A:154:PRO:CD	0.52	2.34	4	1
1:B:216:ARG:O	1:B:216:ARG:HD2	0.52	2.04	5	1
1:A:121:GLU:OE1	1:A:146:TYR:HE2	0.52	1.87	7	1
1:B:321:GLU:N	1:B:321:GLU:CD	0.52	2.62	7	1
1:A:83:GLU:OE2	1:A:83:GLU:HA	0.52	2.05	8	1
1:A:23:PRO:HB3	1:A:99:SER:CA	0.52	2.33	10	1
1:A:89:VAL:CG1	1:A:90:PHE:N	0.52	2.72	10	1
1:B:225:MET:N	1:B:225:MET:CE	0.52	2.73	10	1
1:B:320:LEU:CB	1:B:325:GLU:HB2	0.52	2.34	11	2
1:A:82:LEU:N	1:A:82:LEU:HD12	0.52	2.20	13	1
1:A:21:ALA:O	1:A:102:THR:CG2	0.52	2.58	15	1
1:A:18:VAL:HG22	1:A:89:VAL:HG12	0.52	1.82	1	2
1:B:296:ILE:HG12	1:B:327:GLU:HB3	0.52	1.81	7	5
1:B:322:GLU:CA	1:B:325:GLU:OE1	0.52	2.58	13	2
1:B:306:ILE:HG22	1:B:335:LEU:CD2	0.52	2.33	7	2
1:B:264:GLU:OE2	1:B:271:LEU:HD13	0.52	2.03	3	1
1:B:291:VAL:HG11	1:B:356:ILE:HD11	0.52	1.81	3	2
1:B:237:SER:O	1:B:241:LEU:CD2	0.52	2.51	4	1
1:B:320:LEU:HD11	1:B:343:PHE:HB3	0.52	1.82	9	2
1:B:325:GLU:HA	1:B:328:TYR:HD1	0.52	1.62	9	2
1:B:295:GLY:HA2	1:B:321:GLU:OE1	0.52	2.04	10	2
1:A:65:ALA:HA	1:A:69:GLN:NE2	0.52	2.19	6	1
1:A:116:ILE:CG2	1:A:118:LEU:CD1	0.52	2.87	9	2
1:A:62:ARG:CB	1:A:62:ARG:CZ	0.52	2.88	9	1
1:B:325:GLU:OE2	1:B:345:HIS:CD2	0.52	2.63	11	2
1:B:342:GLU:HB2	1:B:363:VAL:HG21	0.52	1.82	13	1
1:A:107:GLY:O	1:A:110:SER:OG	0.52	2.28	15	2
1:B:319:LEU:O	1:B:346:TYR:CD2	0.52	2.63	1	1
1:A:49:HIS:HE1	1:A:50:PHE:CE2	0.52	2.23	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:CYS:HA	1:A:79:LEU:CD2	0.52	2.34	2	1
1:A:93:ILE:HG23	1:A:121:GLU:OE1	0.52	2.04	3	1
1:A:40:GLN:HG2	1:A:66:TRP:NE1	0.52	2.19	14	2
1:B:246:LEU:CD1	1:B:349:ILE:HG23	0.52	2.35	10	3
1:A:125:GLU:CA	1:A:128:TYR:CD2	0.52	2.92	5	3
1:A:125:GLU:OE2	1:A:145:HIS:NE2	0.52	2.42	8	1
1:B:342:GLU:HA	1:B:342:GLU:OE2	0.52	2.05	9	1
1:A:125:GLU:OE1	1:A:125:GLU:N	0.52	2.42	11	1
1:A:111:ALA:O	1:B:312:PHE:CG	0.52	2.62	12	1
1:A:130:PHE:CZ	1:B:270:VAL:HA	0.52	2.39	12	1
1:A:155:GLN:HA	1:A:155:GLN:NE2	0.52	2.20	13	1
1:B:219:PHE:HD1	1:B:291:VAL:N	0.52	2.02	13	1
1:B:240:GLN:HG2	1:B:244:LEU:CD2	0.52	2.35	13	1
1:B:285:ARG:HB3	1:B:312:PHE:HE1	0.52	1.63	13	1
1:A:19:PHE:CE1	1:A:83:GLU:CB	0.52	2.92	14	1
1:A:41:LEU:CB	1:A:42:PRO:HD3	0.52	2.35	11	6
1:A:103:HIS:O	1:A:106:ILE:HB	0.52	2.04	1	4
1:B:217:SER:CB	1:B:258:PHE:CD2	0.52	2.92	2	1
1:B:323:GLY:O	1:B:326:GLU:HB3	0.52	2.05	5	3
1:B:216:ARG:O	1:B:254:GLY:O	0.52	2.28	4	1
1:B:247:ILE:HG13	1:B:257:VAL:CG1	0.52	2.35	7	3
1:B:293:ILE:HD11	1:B:319:LEU:HD12	0.52	1.80	5	1
1:A:18:VAL:O	1:A:18:VAL:HG12	0.52	2.05	7	1
1:A:134:GLY:HA3	1:B:277:THR:CG2	0.52	2.35	8	2
1:A:19:PHE:CD1	1:A:19:PHE:O	0.52	2.62	15	2
1:A:26:GLY:C	1:A:28:VAL:H	0.52	2.08	9	1
1:B:223:PRO:HB3	1:B:299:SER:CB	0.52	2.35	10	2
1:B:303:HIS:NE2	1:B:328:TYR:CD1	0.52	2.77	10	1
1:B:316:ILE:HD13	1:B:335:LEU:CD2	0.52	2.34	12	3
1:B:259:ASN:ND2	1:B:280:ASP:HA	0.52	2.19	2	1
1:B:224:PHE:CE2	1:B:261:HIS:ND1	0.52	2.78	4	2
1:A:120:LEU:HB3	1:A:145:HIS:ND1	0.52	2.20	4	1
1:A:120:LEU:HD11	1:A:143:PHE:HB3	0.52	1.81	4	2
1:B:282:LEU:HB2	1:B:283:GLU:OE1	0.52	2.05	4	1
1:B:224:PHE:CD2	1:B:270:VAL:HA	0.52	2.39	7	1
1:B:255:LEU:HD23	1:B:255:LEU:N	0.52	2.19	8	3
1:B:289:VAL:O	1:B:289:VAL:HG12	0.52	2.05	9	1
1:A:25:MET:CB	1:A:30:PRO:HA	0.52	2.35	10	2
1:A:55:LEU:HD23	1:A:55:LEU:N	0.52	2.19	12	2
1:B:259:ASN:ND2	1:B:283:GLU:HG2	0.52	2.19	15	1
1:B:342:GLU:HG2	1:B:363:VAL:HG21	0.52	1.81	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:CG	1:A:28:VAL:N	0.52	2.73	7	6
1:A:49:HIS:CD2	1:A:53:GLN:HG3	0.52	2.40	1	1
1:A:25:MET:SD	1:B:330:PHE:HD1	0.52	2.27	2	1
1:A:85:ARG:HB2	1:A:112:PHE:CD1	0.52	2.39	2	1
1:B:324:ARG:C	1:B:328:TYR:CD1	0.52	2.83	2	3
1:A:64:GLU:OE2	1:A:71:LEU:HD13	0.52	2.05	3	1
1:B:289:VAL:CG2	1:B:364:VAL:HG23	0.52	2.34	3	2
1:A:83:GLU:OE2	1:A:86:LYS:CE	0.52	2.58	4	1
1:A:142:GLU:CD	1:A:163:VAL:HG23	0.52	2.25	4	1
1:B:261:HIS:O	1:B:264:GLU:CB	0.52	2.57	4	1
1:B:270:VAL:O	1:B:271:LEU:C	0.52	2.40	11	3
1:B:293:ILE:HD11	1:B:319:LEU:CD1	0.52	2.35	4	2
1:B:353:LYS:HB3	1:B:354:PRO:CD	0.52	2.34	4	1
1:B:284:ILE:HG22	1:B:312:PHE:CE1	0.52	2.39	5	1
1:A:58:PHE:O	1:A:59:ASN:ND2	0.52	2.44	15	2
1:B:262:ARG:HG3	1:B:262:ARG:HH11	0.52	1.65	7	1
1:B:280:ASP:HB3	1:B:305:GLU:CD	0.52	2.25	7	1
1:B:245:THR:HG23	1:B:353:LYS:NZ	0.52	2.19	8	1
1:B:219:PHE:CD2	1:B:283:GLU:HB3	0.52	2.40	10	1
1:A:35:MET:N	1:A:68:ALA:CA	0.52	2.73	11	1
1:B:282:LEU:N	1:B:282:LEU:HD12	0.52	2.20	13	1
1:A:79:LEU:C	1:A:79:LEU:HD12	0.52	2.25	15	1
1:A:81:GLN:HG2	1:A:108:TRP:CZ2	0.52	2.40	15	1
1:B:253:GLN:HG3	1:B:255:LEU:HD21	0.52	1.81	15	1
1:A:127:GLU:OE1	1:B:230:PRO:CB	0.51	2.58	1	1
1:A:69:GLN:C	1:A:71:LEU:N	0.51	2.63	4	2
1:A:131:LEU:HG	1:B:304:VAL:CG1	0.51	2.34	6	3
1:B:346:TYR:C	1:B:346:TYR:CD2	0.51	2.83	4	1
1:B:217:SER:OG	1:B:288:ASP:OD2	0.51	2.28	5	1
1:B:218:VAL:HG11	1:B:250:PHE:CG	0.51	2.39	6	2
1:B:265:ALA:CA	1:B:269:GLN:NE2	0.51	2.72	6	1
1:B:320:LEU:HD13	1:B:325:GLU:OE1	0.51	2.06	8	2
1:B:228:VAL:HG23	1:B:233:ASN:CA	0.51	2.35	8	1
1:A:85:ARG:CD	1:A:112:PHE:HE1	0.51	2.18	10	3
1:A:131:LEU:O	1:A:135:LEU:CG	0.51	2.57	10	2
1:A:30:PRO:HB3	1:B:298:PRO:HD3	0.51	1.81	11	1
1:B:241:LEU:N	1:B:242:PRO:HD2	0.51	2.19	4	7
1:B:278:PRO:O	1:B:282:LEU:CD2	0.51	2.59	15	4
1:A:102:THR:C	1:A:106:ILE:CD1	0.51	2.72	2	1
1:A:104:VAL:HG13	1:B:303:HIS:O	0.51	2.06	2	2
1:B:249:HIS:HE1	1:B:250:PHE:CE2	0.51	2.23	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:VAL:HG12	1:A:55:LEU:HB3	0.51	1.82	4	1
1:A:46:LEU:O	1:A:49:HIS:HD2	0.51	1.88	5	2
1:A:85:ARG:N	1:A:112:PHE:CE1	0.51	2.78	5	2
1:B:225:MET:O	1:B:228:VAL:C	0.51	2.48	14	2
1:A:121:GLU:CG	1:A:146:TYR:OH	0.51	2.59	6	1
1:A:135:LEU:O	1:A:139:ALA:O	0.51	2.28	9	5
1:A:49:HIS:ND1	1:A:49:HIS:C	0.51	2.63	8	2
1:B:219:PHE:HB3	1:B:287:ALA:HB1	0.51	1.81	8	1
1:A:79:LEU:O	1:A:83:GLU:CD	0.51	2.49	9	2
1:B:218:VAL:HG12	1:B:257:VAL:HG22	0.51	1.82	11	1
1:B:227:LEU:CD1	1:B:235:MET:CB	0.51	2.88	11	1
1:A:46:LEU:HG	1:A:153:LYS:HG3	0.51	1.81	13	1
1:A:81:GLN:HG2	1:A:82:LEU:CD2	0.51	2.35	1	1
1:B:258:PHE:CE1	1:B:286:LYS:HD2	0.51	2.41	2	1
1:A:99:SER:OG	1:A:102:THR:HB	0.51	2.05	3	2
1:A:24:PHE:HE1	1:A:61:HIS:ND1	0.51	2.04	6	2
1:A:35:MET:H	1:A:69:GLN:HG3	0.51	1.63	5	1
1:A:101:GLY:O	1:A:105:GLU:OE1	0.51	2.27	5	2
1:A:39:GLU:O	1:A:42:PRO:CD	0.51	2.59	9	6
1:A:80:ASP:HB3	1:A:108:TRP:CZ3	0.51	2.40	6	1
1:A:105:GLU:O	1:A:108:TRP:HB2	0.51	2.04	6	1
1:A:122:GLU:CD	1:A:146:TYR:O	0.51	2.48	6	1
1:A:50:PHE:HD2	1:A:55:LEU:CD1	0.51	2.18	7	3
1:B:228:VAL:CB	1:B:270:VAL:HG21	0.51	2.36	7	1
1:B:235:MET:SD	1:B:239:GLU:HG2	0.51	2.46	8	1
1:A:75:GLU:O	1:A:79:LEU:CB	0.51	2.58	13	1
1:B:276:CYS:O	1:B:280:ASP:HB3	0.51	2.05	2	1
1:A:99:SER:OG	1:A:102:THR:CB	0.51	2.58	3	2
1:A:146:TYR:O	1:A:147:LYS:CG	0.51	2.59	3	2
1:B:220:LEU:O	1:B:259:ASN:ND2	0.51	2.44	3	1
1:B:294:PRO:HG2	1:B:320:LEU:HA	0.51	1.81	12	3
1:A:121:GLU:HG2	1:A:146:TYR:CZ	0.51	2.40	6	1
1:A:24:PHE:CD1	1:A:69:GLN:NE2	0.51	2.78	7	1
1:A:80:ASP:HB3	1:A:105:GLU:CD	0.51	2.26	7	1
1:A:116:ILE:C	1:A:117:VAL:HG23	0.51	2.25	7	6
1:A:111:ALA:HA	1:B:281:GLN:HE22	0.51	1.65	8	1
1:A:25:MET:CG	1:B:330:PHE:HD1	0.51	2.18	9	2
1:B:222:GLY:N	1:B:261:HIS:HE1	0.51	2.03	9	1
1:B:233:ASN:O	1:B:234:SER:HB2	0.51	2.05	9	1
1:B:243:PHE:CD2	1:B:243:PHE:N	0.51	2.79	9	1
1:A:25:MET:SD	1:A:100:PRO:HB2	0.51	2.46	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:HD13	1:A:35:MET:CG	0.51	2.35	11	1
1:B:219:PHE:O	1:B:291:VAL:CG1	0.51	2.55	12	1
1:B:223:PRO:HB3	1:B:299:SER:HB2	0.51	1.82	15	1
1:B:229:ASN:HB3	1:B:232:THR:CB	0.51	2.35	15	1
1:A:119:LEU:O	1:A:146:TYR:CD2	0.51	2.63	1	1
1:B:342:GLU:HG3	1:B:359:ALA:HB1	0.51	1.83	1	2
1:A:29:ASN:CB	1:A:32:THR:HG21	0.51	2.32	4	2
1:A:49:HIS:O	1:A:53:GLN:HB2	0.51	2.06	2	1
1:A:119:LEU:O	1:A:146:TYR:CD1	0.51	2.64	11	2
1:B:234:SER:O	1:B:234:SER:OG	0.51	2.29	11	2
1:A:112:PHE:O	1:A:113:ASP:OD1	0.51	2.27	9	1
1:A:130:PHE:HA	1:B:273:PRO:HD3	0.51	1.82	10	1
1:B:347:LYS:N	1:B:347:LYS:CD	0.51	2.73	10	1
1:B:268:ALA:O	1:B:269:GLN:C	0.51	2.48	14	2
1:A:148:ASP:OD1	1:A:148:ASP:C	0.51	2.49	14	1
1:B:261:HIS:CG	1:B:265:ALA:HB2	0.51	2.41	15	1
1:A:59:ASN:HA	1:A:83:GLU:CD	0.51	2.26	1	2
1:A:96:ILE:HG12	1:A:127:GLU:HB3	0.51	1.83	1	5
1:A:25:MET:N	1:A:25:MET:CE	0.51	2.74	10	2
1:A:124:ARG:O	1:A:128:TYR:HD1	0.51	1.89	15	4
1:A:119:LEU:CG	1:A:156:ILE:HD12	0.51	2.24	8	2
1:B:307:GLY:HA2	1:B:335:LEU:HD11	0.51	1.81	3	1
1:A:24:PHE:CZ	1:A:61:HIS:CE1	0.51	2.98	4	1
1:B:296:ILE:CD1	1:B:324:ARG:O	0.51	2.57	4	1
1:A:31:GLU:C	1:A:32:THR:OG1	0.51	2.47	6	1
1:A:62:ARG:CG	1:A:63:ARG:H	0.51	2.18	13	2
1:A:28:VAL:CG1	1:A:70:VAL:HG11	0.51	2.34	7	1
1:B:229:ASN:HB2	1:B:232:THR:O	0.51	2.04	10	3
1:B:294:PRO:CG	1:B:321:GLU:OE2	0.51	2.58	7	1
1:A:104:VAL:HG22	1:B:304:VAL:HA	0.51	1.82	8	1
1:B:246:LEU:O	1:B:249:HIS:CD2	0.51	2.63	8	2
1:A:102:THR:C	1:A:104:VAL:N	0.51	2.63	9	1
1:B:240:GLN:NE2	1:B:265:ALA:O	0.51	2.44	10	3
1:B:285:ARG:CB	1:B:312:PHE:HE1	0.51	2.18	9	3
1:A:58:PHE:HB3	1:A:83:GLU:HG2	0.51	1.82	13	2
1:B:235:MET:N	1:B:268:ALA:CA	0.51	2.74	11	1
1:A:19:PHE:CD1	1:A:90:PHE:CD2	0.51	2.99	13	1
1:A:40:GLN:HG2	1:A:44:LEU:CD2	0.51	2.35	13	1
1:A:68:ALA:O	1:A:69:GLN:C	0.51	2.48	14	1
1:A:122:GLU:OE1	1:A:147:LYS:HG3	0.51	2.05	14	1
1:B:235:MET:HG3	1:B:235:MET:O	0.51	2.05	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:342:GLU:HG2	1:B:363:VAL:CB	0.51	2.36	15	1
1:A:25:MET:HB2	1:B:330:PHE:CD1	0.51	2.40	1	1
1:B:303:HIS:O	1:B:306:ILE:HB	0.51	2.05	1	4
1:A:19:PHE:CD2	1:A:83:GLU:HB3	0.51	2.41	10	2
1:B:245:THR:O	1:B:248:GLU:HB2	0.51	2.06	2	3
1:B:294:PRO:CA	1:B:299:SER:OG	0.51	2.58	4	2
1:A:19:PHE:CZ	1:A:59:ASN:ND2	0.51	2.79	3	1
1:A:29:ASN:OD1	1:A:33:ASN:CG	0.51	2.49	3	1
1:A:45:THR:HG21	1:A:149:ILE:CG2	0.51	2.36	8	2
1:B:284:ILE:CD1	1:B:290:PHE:CE2	0.51	2.85	3	1
1:A:15:VAL:O	1:A:15:VAL:HG12	0.51	2.05	12	3
1:A:29:ASN:HB2	1:A:33:ASN:ND2	0.51	2.20	6	1
1:B:219:PHE:CE1	1:B:283:GLU:HB3	0.51	2.41	12	2
1:A:38:ALA:O	1:A:42:PRO:HD3	0.51	2.04	8	2
1:A:35:MET:O	1:A:35:MET:HG2	0.51	2.06	10	1
1:A:116:ILE:HD13	1:A:135:LEU:CD2	0.51	2.36	12	3
1:A:120:LEU:O	1:A:145:HIS:HA	0.51	2.06	1	1
1:A:121:GLU:C	1:A:125:GLU:OE2	0.51	2.49	2	1
1:B:353:LYS:CB	1:B:353:LYS:NZ	0.51	2.74	2	1
1:B:319:LEU:HD23	1:B:344:VAL:CG1	0.51	2.35	3	1
1:B:263:ARG:CG	1:B:264:GLU:N	0.51	2.73	6	1
1:A:65:ALA:HA	1:A:69:GLN:CG	0.51	2.36	7	1
1:B:265:ALA:HA	1:B:269:GLN:CG	0.51	2.36	7	2
1:B:273:PRO:C	1:B:275:GLU:H	0.51	2.09	8	3
1:A:61:HIS:HB3	1:A:65:ALA:CB	0.51	2.35	9	1
1:A:106:ILE:CG2	1:A:135:LEU:CD1	0.51	2.88	14	1
1:A:96:ILE:HD11	1:A:127:GLU:HB2	0.51	1.83	15	1
1:A:47:ILE:HA	1:A:57:VAL:HG21	0.51	1.83	2	2
1:A:144:VAL:HG13	1:A:155:GLN:CG	0.51	2.35	4	3
1:B:285:ARG:HD2	1:B:312:PHE:CZ	0.51	2.40	8	4
1:A:138:VAL:CG2	1:A:139:ALA:N	0.51	2.74	3	3
1:B:282:LEU:N	1:B:282:LEU:CD2	0.51	2.72	12	4
1:B:240:GLN:CD	1:B:266:TRP:CD1	0.51	2.85	10	2
1:B:320:LEU:HB3	1:B:325:GLU:CG	0.51	2.36	11	4
1:A:130:PHE:HB3	1:B:225:MET:CE	0.51	2.36	8	2
1:B:228:VAL:CG2	1:B:270:VAL:HG22	0.51	2.34	9	1
1:B:331:LEU:O	1:B:335:LEU:CG	0.51	2.59	10	2
1:B:256:GLU:OE2	1:B:256:GLU:C	0.51	2.49	11	1
1:B:328:TYR:O	1:B:329:GLY:C	0.51	2.49	11	1
1:B:355:GLN:NE2	1:B:355:GLN:N	0.51	2.59	11	1
1:A:40:GLN:CA	1:A:66:TRP:CZ2	0.51	2.93	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:322:GLU:OE1	1:B:347:LYS:HG3	0.51	2.06	14	1
1:A:142:GLU:OE2	1:A:159:ALA:CA	0.51	2.59	15	1
1:A:152:ALA:C	1:A:154:PRO:HD2	0.51	2.26	1	1
1:B:342:GLU:OE1	1:B:343:PHE:N	0.51	2.44	1	2
1:A:31:GLU:HA	1:A:31:GLU:OE2	0.51	2.06	2	1
1:A:130:PHE:CZ	1:B:224:PHE:CD1	0.51	2.99	3	1
1:A:151:LEU:C	1:A:151:LEU:CD2	0.51	2.75	4	1
1:A:63:ARG:CG	1:A:64:GLU:N	0.51	2.74	6	1
1:A:40:GLN:HG3	1:A:44:LEU:HD21	0.51	1.82	9	2
1:B:329:GLY:O	1:B:332:VAL:N	0.51	2.45	10	1
1:A:124:ARG:N	1:A:124:ARG:HD2	0.51	2.21	12	2
1:A:147:LYS:O	1:A:148:ASP:CG	0.50	2.49	1	1
1:A:164:VAL:O	1:A:168:ASN:HB2	0.50	2.06	1	1
1:A:23:PRO:HB3	1:A:99:SER:HB3	0.50	1.81	2	2
1:A:25:MET:CB	1:B:330:PHE:CE2	0.50	2.93	3	3
1:B:259:ASN:N	1:B:283:GLU:HB3	0.50	2.21	4	1
1:A:24:PHE:CD2	1:A:70:VAL:HG23	0.50	2.41	11	2
1:A:62:ARG:HG3	1:A:62:ARG:HH11	0.50	1.66	7	1
1:B:281:GLN:HG2	1:B:282:LEU:N	0.50	2.21	10	2
1:B:228:VAL:CG2	1:B:233:ASN:HB3	0.50	2.34	8	1
1:B:333:ARG:HA	1:B:343:PHE:CZ	0.50	2.41	8	3
1:A:130:PHE:HD1	1:B:225:MET:HG3	0.50	1.66	9	1
1:A:89:VAL:HG21	1:A:160:ILE:HG23	0.50	1.83	13	1
1:A:49:HIS:CE1	1:A:53:GLN:CD	0.50	2.85	1	1
1:A:73:PRO:C	1:A:75:GLU:H	0.50	2.09	8	4
1:B:307:GLY:O	1:B:310:SER:N	0.50	2.44	8	4
1:A:119:LEU:HB3	1:A:146:TYR:CE1	0.50	2.41	3	2
1:B:235:MET:HB3	1:B:269:GLN:NE2	0.50	2.21	4	3
1:B:240:GLN:HG2	1:B:266:TRP:NE1	0.50	2.21	14	3
1:A:19:PHE:CZ	1:A:59:ASN:CB	0.50	2.94	5	1
1:A:94:PRO:HG2	1:A:120:LEU:HA	0.50	1.84	12	3
1:A:92:ALA:HB3	1:A:118:LEU:HG	0.50	1.81	6	1
1:B:228:VAL:HG21	1:B:270:VAL:HG23	0.50	1.79	6	1
1:B:262:ARG:CG	1:B:263:ARG:H	0.50	2.19	13	2
1:B:322:GLU:OE1	1:B:346:TYR:O	0.50	2.29	6	1
1:A:84:ILE:HG21	1:A:108:TRP:C	0.50	2.27	7	2
1:A:39:GLU:C	1:A:39:GLU:CD	0.50	2.70	8	1
1:A:125:GLU:HG2	1:A:145:HIS:CD2	0.50	2.41	8	2
1:B:332:VAL:O	1:B:343:PHE:CE1	0.50	2.64	12	1
1:B:247:ILE:CG1	1:B:257:VAL:HG21	0.50	2.36	13	1
1:B:278:PRO:O	1:B:282:LEU:CG	0.50	2.60	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:324:ARG:HG2	1:B:324:ARG:HH11	0.50	1.65	15	1
1:A:130:PHE:CD1	1:B:225:MET:HE3	0.50	2.40	1	1
1:B:249:HIS:HE1	1:B:250:PHE:CD2	0.50	2.24	2	1
1:A:135:LEU:HD23	1:A:141:VAL:HG21	0.50	1.81	9	3
1:A:73:PRO:HG3	1:B:330:PHE:CA	0.50	2.37	5	4
1:A:146:TYR:C	1:A:146:TYR:CD2	0.50	2.85	4	1
1:B:219:PHE:O	1:B:219:PHE:HD2	0.50	1.86	4	2
1:A:17:SER:HB3	1:A:56:GLU:HB2	0.50	1.83	6	2
1:A:19:PHE:HD2	1:A:91:VAL:H	0.50	1.50	7	1
1:A:119:LEU:HB3	1:A:146:TYR:CE2	0.50	2.40	15	2
1:B:341:VAL:HG12	1:B:343:PHE:CE1	0.50	2.40	13	3
1:A:129:GLY:O	1:A:132:VAL:N	0.50	2.45	10	1
1:B:223:PRO:O	1:B:299:SER:CB	0.50	2.60	13	1
1:B:281:GLN:HA	1:B:284:ILE:HG12	0.50	1.83	13	1
1:A:71:LEU:N	1:A:71:LEU:HD22	0.50	2.20	14	1
1:A:142:GLU:OE2	1:A:159:ALA:O	0.50	2.29	15	1
1:A:142:GLU:HG2	1:A:163:VAL:CG2	0.50	2.36	15	1
1:B:220:LEU:HD11	1:B:250:PHE:CE2	0.50	2.40	2	1
1:B:319:LEU:CD2	1:B:346:TYR:HB3	0.50	2.37	2	1
1:A:19:PHE:CZ	1:A:59:ASN:HB2	0.50	2.41	5	1
1:B:219:PHE:HE1	1:B:284:ILE:N	0.50	2.05	5	2
1:B:275:GLU:OE2	1:B:279:LEU:HD11	0.50	2.06	5	1
1:A:65:ALA:HA	1:A:69:GLN:HE21	0.50	1.67	6	1
1:A:85:ARG:HB2	1:A:114:LYS:HE2	0.50	1.84	6	1
1:B:316:ILE:C	1:B:317:VAL:HG23	0.50	2.27	7	3
1:A:98:PRO:O	1:B:300:PRO:HB3	0.50	2.06	8	1
1:A:47:ILE:N	1:A:47:ILE:HD12	0.50	2.22	9	2
1:A:63:ARG:CA	1:A:63:ARG:HH11	0.50	2.20	9	1
1:A:89:VAL:O	1:A:89:VAL:HG12	0.50	2.06	9	1
1:A:28:VAL:CG1	1:A:70:VAL:CB	0.50	2.75	11	1
1:A:29:ASN:CB	1:A:33:ASN:OD1	0.50	2.59	11	1
1:B:227:LEU:HD13	1:B:235:MET:CG	0.50	2.36	11	1
1:B:250:PHE:CB	1:B:257:VAL:CG2	0.50	2.89	11	1
1:B:245:THR:CG2	1:B:246:LEU:N	0.50	2.74	12	1
1:A:19:PHE:HD1	1:A:91:VAL:N	0.50	2.05	13	1
1:A:123:GLY:CA	1:A:125:GLU:OE2	0.50	2.60	15	1
1:A:30:PRO:CG	1:B:327:GLU:OE1	0.50	2.60	1	1
1:A:133:ARG:HA	1:A:143:PHE:CZ	0.50	2.41	8	3
1:B:241:LEU:HD12	1:B:244:LEU:HD11	0.50	1.82	11	2
1:B:276:CYS:SG	1:B:280:ASP:OD1	0.50	2.61	1	2
1:B:309:ALA:HA	1:B:312:PHE:HB2	0.50	1.84	4	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:347:LYS:O	1:B:348:ASP:OD1	0.50	2.29	1	1
1:A:50:PHE:CB	1:A:57:VAL:CG2	0.50	2.89	11	2
1:A:61:HIS:CG	1:A:65:ALA:HB2	0.50	2.42	15	2
1:B:321:GLU:C	1:B:325:GLU:OE2	0.50	2.49	2	1
1:A:120:LEU:HB3	1:A:145:HIS:CE1	0.50	2.42	9	2
1:A:25:MET:O	1:A:28:VAL:CG1	0.50	2.57	5	1
1:A:77:THR:CG2	1:A:78:PRO:HD3	0.50	2.36	14	2
1:A:19:PHE:CE1	1:A:83:GLU:HB3	0.50	2.41	7	2
1:A:46:LEU:O	1:A:49:HIS:CD2	0.50	2.64	8	3
1:B:295:GLY:HA2	1:B:324:ARG:HH11	0.50	1.67	7	1
1:A:22:GLY:N	1:A:61:HIS:HE1	0.50	2.02	9	1
1:B:234:SER:O	1:B:235:MET:O	0.50	2.29	9	1
1:B:225:MET:SD	1:B:300:PRO:HB2	0.50	2.47	15	2
1:A:20:LEU:HG	1:A:91:VAL:HG12	0.50	1.83	11	1
1:A:70:VAL:CG2	1:B:330:PHE:CZ	0.50	2.88	11	1
1:B:299:SER:O	1:B:303:HIS:CB	0.50	2.59	11	1
1:B:262:ARG:O	1:B:266:TRP:HD1	0.50	1.89	12	1
1:A:23:PRO:CA	1:A:99:SER:HB2	0.50	2.37	13	2
1:A:98:PRO:CG	1:B:225:MET:SD	0.50	3.00	14	1
1:B:219:PHE:HD2	1:B:259:ASN:ND2	0.50	2.03	15	1
1:A:59:ASN:HA	1:A:83:GLU:OE1	0.50	2.06	1	2
1:A:124:ARG:O	1:A:126:GLU:N	0.50	2.45	1	2
1:B:313:ASP:OD1	1:B:313:ASP:C	0.50	2.49	3	1
1:A:25:MET:HG3	1:A:30:PRO:HA	0.50	1.83	6	1
1:A:90:PHE:CD2	1:A:109:ALA:HB2	0.50	2.41	9	2
1:B:325:GLU:CD	1:B:345:HIS:HE2	0.50	2.10	9	1
1:B:285:ARG:CD	1:B:312:PHE:HE1	0.50	2.20	10	2
1:A:85:ARG:HA	1:A:114:LYS:CD	0.50	2.37	11	1
1:A:24:PHE:HD1	1:B:330:PHE:CZ	0.50	2.24	13	1
1:A:81:GLN:HB2	1:A:108:TRP:CZ3	0.50	2.42	13	1
1:A:87:ALA:O	1:A:114:LYS:CD	0.50	2.60	13	1
1:A:104:VAL:CB	1:B:331:LEU:HD22	0.50	2.36	13	1
1:B:228:VAL:CA	1:B:233:ASN:HB2	0.50	2.37	13	1
1:B:246:LEU:HG	1:B:353:LYS:HG3	0.50	1.83	13	1
1:B:317:VAL:HG22	1:B:363:VAL:HG21	0.50	1.83	13	1
1:A:76:CYS:SG	1:A:80:ASP:OD1	0.50	2.58	15	2
1:A:15:VAL:O	1:A:55:LEU:HD23	0.50	2.07	10	3
1:A:111:ALA:CA	1:B:312:PHE:HD1	0.50	2.19	6	4
1:A:131:LEU:HD11	1:B:308:TRP:CZ2	0.50	2.42	3	1
1:B:229:ASN:N	1:B:229:ASN:ND2	0.50	2.60	3	1
1:A:153:LYS:O	1:A:157:ASP:OD2	0.50	2.30	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:THR:HG22	1:A:78:PRO:N	0.50	2.22	6	5
1:A:40:GLN:NE2	1:A:44:LEU:HD21	0.50	2.22	6	1
1:A:85:ARG:CG	1:A:112:PHE:HE2	0.50	2.19	6	1
1:A:34:SER:O	1:A:34:SER:OG	0.50	2.30	11	2
1:B:239:GLU:HG3	1:B:240:GLN:N	0.50	2.20	8	1
1:A:65:ALA:HB2	1:A:69:GLN:HG3	0.50	1.83	10	1
1:A:125:GLU:HG2	1:A:126:GLU:N	0.50	2.18	10	1
1:A:19:PHE:O	1:A:91:VAL:CG1	0.50	2.55	12	1
1:A:44:LEU:O	1:A:47:ILE:HG22	0.50	2.06	13	1
1:A:48:GLU:C	1:A:52:LYS:HE2	0.50	2.26	14	1
1:B:219:PHE:HE1	1:B:283:GLU:C	0.50	2.10	14	1
1:B:246:LEU:CD1	1:B:349:ILE:HD12	0.50	2.36	15	1
1:B:241:LEU:CB	1:B:242:PRO:HD3	0.50	2.37	3	6
1:B:321:GLU:OE1	1:B:321:GLU:HA	0.50	2.06	1	1
1:A:49:HIS:O	1:A:53:GLN:CB	0.50	2.59	2	2
1:A:49:HIS:HE1	1:A:50:PHE:CD2	0.50	2.24	2	1
1:B:219:PHE:CE1	1:B:290:PHE:HE1	0.50	2.22	4	2
1:B:245:THR:O	1:B:249:HIS:NE2	0.50	2.43	5	1
1:B:220:LEU:CB	1:B:259:ASN:OD1	0.50	2.59	7	1
1:B:224:PHE:CZ	1:B:261:HIS:CD2	0.50	3.00	7	1
1:B:227:LEU:HB2	1:B:235:MET:CB	0.50	2.37	10	1
1:B:289:VAL:CG1	1:B:290:PHE:N	0.50	2.72	10	1
1:B:285:ARG:HA	1:B:314:LYS:CD	0.50	2.37	11	1
1:A:23:PRO:HB3	1:A:99:SER:HB2	0.50	1.83	15	1
1:A:59:ASN:C	1:A:60:ALA:O	0.50	2.49	1	3
1:A:127:GLU:OE1	1:B:230:PRO:CG	0.50	2.60	1	1
1:A:124:ARG:C	1:A:128:TYR:CD1	0.50	2.85	2	3
1:B:228:VAL:CG2	1:B:234:SER:H	0.50	2.20	2	1
1:B:241:LEU:O	1:B:244:LEU:HB2	0.50	2.06	4	2
1:A:130:PHE:CZ	1:B:271:LEU:O	0.50	2.64	5	1
1:B:220:LEU:CD1	1:B:221:ALA:N	0.50	2.75	6	2
1:B:239:GLU:O	1:B:242:PRO:CD	0.50	2.60	9	4
1:B:274:GLU:O	1:B:278:PRO:HG2	0.50	2.06	6	2
1:B:282:LEU:HD13	1:B:285:ARG:NE	0.50	2.20	7	1
1:B:319:LEU:HD22	1:B:346:TYR:CD1	0.50	2.41	8	1
1:A:59:ASN:OD1	1:A:59:ASN:C	0.50	2.50	10	1
1:A:56:GLU:OE2	1:A:57:VAL:N	0.50	2.45	11	1
1:B:281:GLN:O	1:B:284:ILE:N	0.50	2.44	11	1
1:A:167:VAL:HG12	1:A:167:VAL:O	0.50	2.07	12	1
1:A:25:MET:SD	1:B:330:PHE:CD2	0.50	3.00	14	1
1:A:99:SER:O	1:A:99:SER:OG	0.50	2.30	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LYS:N	1:A:114:LYS:HD2	0.50	2.21	15	1
1:A:96:ILE:CA	1:A:97:PRO:O	0.49	2.60	2	3
1:A:151:LEU:O	1:A:154:PRO:HG2	0.49	2.07	8	5
1:B:219:PHE:O	1:B:219:PHE:CD2	0.49	2.65	1	1
1:B:240:GLN:OE1	1:B:241:LEU:HD13	0.49	2.06	1	1
1:B:352:ALA:C	1:B:354:PRO:HD2	0.49	2.28	1	1
1:A:47:ILE:HG13	1:A:57:VAL:CG1	0.49	2.31	5	4
1:B:342:GLU:HG2	1:B:363:VAL:CG2	0.49	2.37	15	2
1:B:221:ALA:CB	1:B:259:ASN:ND2	0.49	2.71	3	1
1:A:130:PHE:HD1	1:B:273:PRO:HD3	0.49	1.66	15	2
1:B:277:THR:HG22	1:B:278:PRO:N	0.49	2.21	6	5
1:A:81:GLN:CG	1:A:112:PHE:CZ	0.49	2.94	6	1
1:A:81:GLN:CA	1:A:108:TRP:CZ3	0.49	2.95	7	1
1:B:247:ILE:N	1:B:247:ILE:HD12	0.49	2.21	9	2
1:A:106:ILE:HG21	1:A:135:LEU:HD21	0.49	1.84	10	1
1:B:265:ALA:HB2	1:B:269:GLN:HG3	0.49	1.84	10	1
1:A:155:GLN:NE2	1:A:155:GLN:CA	0.49	2.75	13	2
1:A:18:VAL:HG21	1:A:50:PHE:HE1	0.49	1.61	12	1
1:A:80:ASP:CG	1:A:105:GLU:CD	0.49	2.70	13	1
1:A:85:ARG:HB3	1:A:112:PHE:HE1	0.49	1.59	13	1
1:B:299:SER:N	1:B:328:TYR:HE1	0.49	2.05	14	1
1:B:221:ALA:O	1:B:302:THR:CG2	0.49	2.60	15	1
1:B:259:ASN:OD1	1:B:283:GLU:CB	0.49	2.60	15	1
1:B:281:GLN:CG	1:B:308:TRP:CZ2	0.49	2.94	15	1
1:A:64:GLU:OE2	1:A:71:LEU:HD22	0.49	2.08	1	1
1:B:216:ARG:O	1:B:256:GLU:CD	0.49	2.51	1	1
1:A:85:ARG:CB	1:A:112:PHE:CD2	0.49	2.94	2	1
1:B:296:ILE:CA	1:B:297:PRO:O	0.49	2.57	2	2
1:A:91:VAL:HG11	1:A:156:ILE:HD11	0.49	1.84	3	1
1:B:360:ILE:CG2	1:B:361:ARG:N	0.49	2.73	3	1
1:A:134:GLY:C	1:A:137:THR:HG22	0.49	2.27	11	7
1:B:334:GLY:C	1:B:337:THR:HG22	0.49	2.27	14	6
1:A:120:LEU:HB3	1:A:125:GLU:CG	0.49	2.37	11	4
1:A:39:GLU:HG3	1:A:40:GLN:N	0.49	2.22	8	1
1:A:63:ARG:HH11	1:A:63:ARG:HA	0.49	1.67	9	1
1:B:226:GLY:C	1:B:228:VAL:H	0.49	2.10	9	2
1:B:216:ARG:HB3	1:B:288:ASP:OD1	0.49	2.06	13	1
1:B:280:ASP:CG	1:B:305:GLU:CD	0.49	2.70	13	1
1:A:134:GLY:HA3	1:B:277:THR:HG21	0.49	1.84	15	1
1:B:347:LYS:O	1:B:351:LEU:CB	0.49	2.60	15	1
1:A:29:ASN:O	1:A:30:PRO:C	0.49	2.51	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ILE:O	1:A:94:PRO:C	0.49	2.49	5	9
1:A:142:GLU:OE1	1:A:142:GLU:HA	0.49	2.08	4	1
1:A:125:GLU:OE2	1:A:126:GLU:N	0.49	2.45	5	1
1:A:130:PHE:CD1	1:B:273:PRO:HD3	0.49	2.42	15	2
1:B:296:ILE:N	1:B:324:ARG:HD3	0.49	2.23	11	2
1:B:227:LEU:CG	1:B:235:MET:HB3	0.49	2.38	10	1
1:A:28:VAL:CG1	1:A:32:THR:C	0.49	2.79	11	1
1:A:62:ARG:C	1:A:64:GLU:OE1	0.49	2.51	11	1
1:A:19:PHE:HE1	1:A:83:GLU:C	0.49	2.10	14	1
1:A:121:GLU:O	1:A:124:ARG:N	0.49	2.44	1	1
1:B:223:PRO:HB3	1:B:299:SER:HB3	0.49	1.83	2	2
1:B:229:ASN:OD1	1:B:233:ASN:CG	0.49	2.50	3	1
1:B:319:LEU:O	1:B:346:TYR:CD1	0.49	2.65	11	3
1:A:30:PRO:C	1:A:31:GLU:HG2	0.49	2.27	4	1
1:B:320:LEU:HB3	1:B:345:HIS:CE1	0.49	2.43	9	2
1:B:231:GLU:C	1:B:232:THR:OG1	0.49	2.51	6	2
1:A:104:VAL:HG22	1:B:304:VAL:CA	0.49	2.37	8	1
1:B:271:LEU:HB2	1:B:276:CYS:HB3	0.49	1.83	9	1
1:A:125:GLU:OE2	1:A:145:HIS:HD2	0.49	1.91	11	1
1:A:125:GLU:CD	1:A:126:GLU:H	0.49	2.10	15	2
1:A:142:GLU:HB2	1:A:163:VAL:HG21	0.49	1.84	13	1
1:B:247:ILE:CG1	1:B:257:VAL:CG1	0.49	2.88	13	1
1:A:122:GLU:N	1:A:125:GLU:OE1	0.49	2.46	13	2
1:B:281:GLN:HG2	1:B:282:LEU:CD2	0.49	2.36	1	1
1:A:58:PHE:CE1	1:A:86:LYS:HD2	0.49	2.42	2	1
1:B:293:ILE:CG2	1:B:321:GLU:OE1	0.49	2.61	3	1
1:B:230:PRO:C	1:B:231:GLU:HG2	0.49	2.28	4	1
1:B:233:ASN:OD1	1:B:268:ALA:O	0.49	2.30	4	1
1:B:280:ASP:O	1:B:284:ILE:CB	0.49	2.59	6	1
1:A:44:LEU:O	1:A:48:GLU:CB	0.49	2.60	8	2
1:A:134:GLY:CA	1:B:277:THR:CG2	0.49	2.91	8	1
1:A:125:GLU:HB3	1:A:145:HIS:HE1	0.49	1.68	9	1
1:B:224:PHE:O	1:B:228:VAL:HG12	0.49	2.08	10	1
1:A:46:LEU:CD1	1:A:149:ILE:HD12	0.49	2.38	14	2
1:A:155:GLN:CA	1:A:155:GLN:HE21	0.49	2.20	13	1
1:B:221:ALA:O	1:B:302:THR:HG23	0.49	2.07	15	1
1:B:241:LEU:HA	1:B:244:LEU:CD1	0.49	2.38	1	3
1:B:295:GLY:HA2	1:B:324:ARG:NH1	0.49	2.22	1	1
1:A:111:ALA:HB1	1:B:312:PHE:HB2	0.49	1.85	2	4
1:B:299:SER:OG	1:B:302:THR:HB	0.49	2.07	3	2
1:B:338:VAL:CG2	1:B:339:ALA:N	0.49	2.75	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:281:GLN:HG3	1:B:282:LEU:HD13	0.49	1.83	4	1
1:B:351:LEU:C	1:B:351:LEU:CD2	0.49	2.74	4	1
1:B:258:PHE:O	1:B:259:ASN:ND2	0.49	2.43	15	2
1:B:325:GLU:HG2	1:B:326:GLU:N	0.49	2.19	10	1
1:A:35:MET:H	1:A:68:ALA:CA	0.49	2.20	11	1
1:B:316:ILE:HG22	1:B:317:VAL:N	0.49	2.22	11	2
1:A:23:PRO:HG3	1:A:95:GLY:HA3	0.49	1.84	13	1
1:B:279:LEU:HD12	1:B:280:ASP:N	0.49	2.23	15	1
1:B:314:LYS:CD	1:B:314:LYS:H	0.49	2.20	15	1
1:A:20:LEU:HD22	1:A:21:ALA:H	0.49	1.68	1	1
1:B:259:ASN:C	1:B:260:ALA:O	0.49	2.51	1	5
1:A:29:ASN:HB2	1:A:32:THR:CB	0.49	2.38	2	1
1:B:261:HIS:CD2	1:B:265:ALA:CB	0.49	2.95	2	1
1:A:119:LEU:HD23	1:A:144:VAL:CG1	0.49	2.38	3	1
1:A:129:GLY:O	1:A:133:ARG:CB	0.49	2.59	14	3
1:B:285:ARG:CD	1:B:312:PHE:HE2	0.49	2.21	6	2
1:A:51:GLU:OE2	1:A:56:GLU:HG3	0.49	2.07	5	1
1:A:82:LEU:N	1:A:82:LEU:CD2	0.49	2.75	5	3
1:B:321:GLU:OE1	1:B:324:ARG:HG2	0.49	2.08	6	1
1:A:39:GLU:HA	1:A:42:PRO:HG2	0.49	1.84	15	3
1:B:290:PHE:HD2	1:B:316:ILE:HG12	0.49	1.65	15	2
1:B:244:LEU:HD13	1:B:266:TRP:CZ3	0.49	2.42	11	1
1:B:262:ARG:O	1:B:264:GLU:OE1	0.49	2.31	11	1
1:B:292:ALA:O	1:B:318:LEU:HA	0.49	2.08	11	1
1:A:116:ILE:HG22	1:A:141:VAL:HA	0.49	1.83	12	1
1:B:285:ARG:HB3	1:B:312:PHE:CZ	0.49	2.42	12	2
1:A:47:ILE:CG1	1:A:57:VAL:CG1	0.49	2.91	13	1
1:B:307:GLY:C	1:B:310:SER:OG	0.49	2.50	15	1
1:B:293:ILE:O	1:B:293:ILE:HG22	0.49	2.06	7	3
1:B:227:LEU:CD1	1:B:235:MET:HG3	0.49	2.37	12	3
1:B:250:PHE:O	1:B:255:LEU:HG	0.49	2.08	5	2
1:B:220:LEU:HD13	1:B:221:ALA:N	0.49	2.21	6	1
1:B:265:ALA:HA	1:B:269:GLN:HE21	0.49	1.68	6	1
1:A:95:GLY:HA2	1:A:124:ARG:HH11	0.49	1.68	7	1
1:B:331:LEU:O	1:B:335:LEU:CB	0.49	2.61	14	2
1:B:264:GLU:HB2	1:B:269:GLN:OE1	0.49	2.07	9	1
1:A:40:GLN:C	1:A:42:PRO:HD2	0.49	2.28	13	1
1:B:317:VAL:CG2	1:B:342:GLU:HB2	0.49	2.37	15	1
1:B:281:GLN:HB2	1:B:308:TRP:CZ3	0.49	2.42	13	2
1:A:133:ARG:HB3	1:B:273:PRO:CG	0.49	2.38	3	1
1:A:20:LEU:HB2	1:A:57:VAL:CG1	0.49	2.38	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:HIS:NE2	1:A:153:LYS:HG2	0.49	2.22	5	1
1:B:219:PHE:CE1	1:B:284:ILE:N	0.49	2.80	14	2
1:B:219:PHE:CD2	1:B:219:PHE:C	0.49	2.85	6	1
1:B:265:ALA:HB1	1:B:269:GLN:HE22	0.49	1.68	6	1
1:B:306:ILE:C	1:B:308:TRP:N	0.49	2.65	10	2
1:A:17:SER:CB	1:A:56:GLU:HB2	0.49	2.38	7	2
1:A:100:PRO:HB3	1:B:298:PRO:O	0.49	2.07	8	1
1:A:130:PHE:CD1	1:B:225:MET:HG3	0.49	2.43	10	2
1:B:235:MET:H	1:B:268:ALA:CA	0.49	2.21	11	1
1:B:277:THR:CG2	1:B:278:PRO:HD3	0.49	2.38	14	1
1:A:61:HIS:CD2	1:A:71:LEU:HD11	0.49	2.42	1	1
1:B:224:PHE:HE2	1:B:270:VAL:CA	0.49	2.20	1	2
1:A:108:TRP:CD1	1:B:311:ALA:CB	0.49	2.96	2	1
1:B:231:GLU:OE2	1:B:231:GLU:HA	0.49	2.07	2	2
1:A:93:ILE:CG2	1:A:121:GLU:OE1	0.49	2.61	3	1
1:B:285:ARG:HA	1:B:314:LYS:HG3	0.49	1.83	3	1
1:B:218:VAL:HG23	1:B:255:LEU:HB3	0.49	1.85	5	2
1:B:290:PHE:O	1:B:317:VAL:HG23	0.49	2.08	5	1
1:B:347:LYS:HG3	1:B:348:ASP:OD1	0.49	2.07	5	1
1:A:121:GLU:N	1:A:121:GLU:CD	0.49	2.64	7	1
1:A:19:PHE:HB3	1:A:87:ALA:HB1	0.49	1.83	8	1
1:B:231:GLU:O	1:B:231:GLU:CG	0.49	2.58	9	2
1:A:24:PHE:C	1:A:26:GLY:H	0.49	2.11	10	1
1:A:130:PHE:O	1:B:273:PRO:CA	0.49	2.61	10	3
1:B:259:ASN:OD1	1:B:259:ASN:C	0.49	2.50	10	1
1:A:128:TYR:O	1:A:129:GLY:C	0.49	2.51	11	1
1:A:61:HIS:C	1:A:65:ALA:HB2	0.49	2.28	12	2
1:B:340:ALA:HB2	1:B:367:VAL:HG21	0.49	1.85	12	1
1:B:342:GLU:OE2	1:B:344:VAL:CG2	0.49	2.61	13	1
1:A:94:PRO:O	1:A:99:SER:CB	0.49	2.61	15	1
1:A:102:THR:HA	1:A:105:GLU:CG	0.49	2.37	15	1
1:A:41:LEU:N	1:A:42:PRO:HD2	0.48	2.23	4	8
1:A:85:ARG:CD	1:A:112:PHE:HE2	0.48	2.21	6	2
1:A:27:LEU:CD1	1:A:35:MET:HG3	0.48	2.37	4	3
1:B:280:ASP:CG	1:B:305:GLU:OE2	0.48	2.51	4	1
1:B:285:ARG:N	1:B:312:PHE:HE1	0.48	2.05	5	1
1:B:316:ILE:C	1:B:317:VAL:HG22	0.48	2.29	5	1
1:B:237:SER:O	1:B:239:GLU:N	0.48	2.46	6	1
1:B:301:GLY:O	1:B:305:GLU:HB2	0.48	2.07	6	1
1:B:320:LEU:CD1	1:B:345:HIS:NE2	0.48	2.73	7	3
1:A:134:GLY:CA	1:B:273:PRO:HB2	0.48	2.37	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:285:ARG:HA	1:B:314:LYS:HD2	0.48	1.85	11	1
1:A:44:LEU:HD13	1:A:62:ARG:CB	0.48	2.37	12	1
1:A:84:ILE:O	1:A:114:LYS:CG	0.48	2.61	13	1
1:A:142:GLU:OE2	1:A:144:VAL:CG2	0.48	2.61	13	1
1:B:327:GLU:OE1	1:B:327:GLU:N	0.48	2.46	13	1
1:A:124:ARG:HG2	1:A:124:ARG:NH1	0.48	2.23	15	1
1:B:274:GLU:N	1:B:274:GLU:CD	0.48	2.66	15	1
1:A:41:LEU:HA	1:A:44:LEU:CD1	0.48	2.38	14	2
1:A:109:ALA:HA	1:A:112:PHE:HB2	0.48	1.84	10	6
1:A:142:GLU:HG2	1:A:159:ALA:CB	0.48	2.37	8	2
1:A:157:ASP:OD2	1:A:157:ASP:C	0.48	2.51	3	1
1:A:77:THR:O	1:A:80:ASP:HB2	0.48	2.07	4	2
1:A:29:ASN:C	1:A:29:ASN:HD22	0.48	2.09	5	1
1:B:219:PHE:HD2	1:B:220:LEU:N	0.48	2.06	5	1
1:B:223:PRO:HA	1:B:299:SER:OG	0.48	2.08	6	3
1:B:229:ASN:C	1:B:229:ASN:HD22	0.48	2.09	5	1
1:B:259:ASN:ND2	1:B:280:ASP:CG	0.48	2.66	5	1
1:B:321:GLU:OE2	1:B:346:TYR:OH	0.48	2.28	5	1
1:B:357:ASP:OD1	1:B:358:ALA:N	0.48	2.45	12	2
1:A:120:LEU:CD1	1:A:125:GLU:HG3	0.48	2.38	10	2
1:A:25:MET:N	1:A:25:MET:HE3	0.48	2.23	10	1
1:A:62:ARG:CA	1:A:66:TRP:CE2	0.48	2.91	10	1
1:A:81:GLN:O	1:A:84:ILE:N	0.48	2.45	11	1
1:B:314:LYS:HZ3	1:B:314:LYS:CA	0.48	2.20	11	1
1:A:21:ALA:HA	1:A:59:ASN:OD1	0.48	2.08	13	2
1:B:235:MET:HB2	1:B:269:GLN:CB	0.48	2.38	12	1
1:B:265:ALA:O	1:B:269:GLN:HB3	0.48	2.08	12	1
1:A:96:ILE:CG1	1:A:127:GLU:HB2	0.48	2.38	15	1
1:A:119:LEU:CD2	1:A:144:VAL:HG11	0.48	2.38	15	1
1:B:279:LEU:HD12	1:B:279:LEU:C	0.48	2.28	15	1
1:A:130:PHE:HE1	1:B:225:MET:H	0.48	1.50	1	2
1:B:349:ILE:O	1:B:353:LYS:CD	0.48	2.61	5	3
1:A:50:PHE:HD1	1:A:55:LEU:CD1	0.48	2.19	14	5
1:A:83:GLU:N	1:A:83:GLU:OE2	0.48	2.46	2	1
1:B:285:ARG:CB	1:B:312:PHE:CZ	0.48	2.96	7	3
1:A:131:LEU:HD12	1:A:135:LEU:CD1	0.48	2.37	3	1
1:A:132:VAL:HG13	1:A:143:PHE:CE1	0.48	2.43	5	2
1:B:246:LEU:CD1	1:B:353:LYS:HG3	0.48	2.38	3	1
1:B:261:HIS:O	1:B:264:GLU:CG	0.48	2.61	4	1
1:A:100:PRO:O	1:A:104:VAL:HB	0.48	2.08	6	1
1:A:28:VAL:CG2	1:A:33:ASN:HB3	0.48	2.34	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:244:LEU:O	1:B:248:GLU:CB	0.48	2.61	8	1
1:B:224:PHE:HE1	1:B:261:HIS:CD2	0.48	2.23	9	1
1:B:320:LEU:CD1	1:B:325:GLU:HG3	0.48	2.38	10	2
1:A:27:LEU:HD23	1:A:27:LEU:N	0.48	2.24	10	1
1:B:294:PRO:O	1:B:299:SER:CB	0.48	2.61	15	2
1:A:28:VAL:HA	1:A:33:ASN:HB3	0.48	1.83	11	1
1:B:319:LEU:HD21	1:B:352:ALA:CB	0.48	2.35	11	1
1:A:28:VAL:CA	1:A:33:ASN:HB2	0.48	2.38	13	1
1:B:223:PRO:CA	1:B:299:SER:HB2	0.48	2.38	13	2
1:A:25:MET:O	1:A:28:VAL:C	0.48	2.48	14	1
1:B:231:GLU:O	1:B:231:GLU:OE2	0.48	2.31	14	1
1:A:25:MET:CE	1:A:101:GLY:H	0.48	2.20	15	1
1:A:149:ILE:O	1:A:153:LYS:CD	0.48	2.61	1	3
1:B:269:GLN:C	1:B:271:LEU:N	0.48	2.65	4	2
1:B:347:LYS:O	1:B:347:LYS:HG3	0.48	2.08	3	1
1:A:99:SER:O	1:A:103:HIS:ND1	0.48	2.46	15	2
1:A:100:PRO:HB3	1:B:298:PRO:HB3	0.48	1.84	5	1
1:A:104:VAL:HG22	1:B:307:GLY:N	0.48	2.21	5	1
1:B:219:PHE:O	1:B:291:VAL:HG12	0.48	2.07	5	1
1:A:101:GLY:O	1:A:105:GLU:HB2	0.48	2.08	6	1
1:B:239:GLU:HA	1:B:242:PRO:HG2	0.48	1.86	13	4
1:B:264:GLU:HB3	1:B:271:LEU:CD2	0.48	2.38	8	2
1:A:131:LEU:HD13	1:B:304:VAL:HG11	0.48	1.83	15	2
1:B:313:ASP:OD2	1:B:313:ASP:C	0.48	2.52	10	1
1:A:80:ASP:O	1:A:84:ILE:CD1	0.48	2.61	13	2
1:A:16:ARG:HB3	1:A:88:ASP:OD1	0.48	2.08	13	1
1:A:39:GLU:OE2	1:A:43:PHE:CZ	0.48	2.66	13	1
1:A:25:MET:CE	1:A:26:GLY:H	0.48	2.21	15	1
1:B:274:GLU:N	1:B:274:GLU:OE2	0.48	2.47	15	1
1:B:229:ASN:HB2	1:B:232:THR:HB	0.48	1.85	1	1
1:B:293:ILE:O	1:B:294:PRO:C	0.48	2.52	3	11
1:A:65:ALA:O	1:A:69:GLN:HG3	0.48	2.08	2	1
1:A:79:LEU:O	1:A:83:GLU:CB	0.48	2.60	5	2
1:A:20:LEU:CB	1:A:59:ASN:OD1	0.48	2.61	7	1
1:B:240:GLN:HG3	1:B:244:LEU:HD21	0.48	1.86	9	1
1:B:241:LEU:HD12	1:B:244:LEU:CD1	0.48	2.38	11	1
1:A:94:PRO:CA	1:A:128:TYR:CZ	0.48	2.96	12	1
1:A:65:ALA:HA	1:A:69:GLN:CB	0.48	2.38	14	1
1:A:79:LEU:O	1:A:83:GLU:HG3	0.48	2.08	14	1
1:B:296:ILE:HG12	1:B:327:GLU:HB2	0.48	1.86	15	1
1:B:296:ILE:CG1	1:B:327:GLU:HB2	0.48	2.39	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:GLN:HG2	1:A:70:VAL:N	0.48	2.21	1	1
1:B:323:GLY:H	1:B:325:GLU:CD	0.48	2.12	2	5
1:A:49:HIS:HE1	1:A:50:PHE:CZ	0.48	2.27	2	1
1:B:218:VAL:CG2	1:B:250:PHE:CE1	0.48	2.92	2	2
1:B:285:ARG:HB2	1:B:312:PHE:CD1	0.48	2.43	2	1
1:B:302:THR:C	1:B:304:VAL:N	0.48	2.64	9	2
1:A:85:ARG:HA	1:A:114:LYS:HG3	0.48	1.84	3	2
1:A:21:ALA:HB2	1:A:105:GLU:OE1	0.48	2.08	4	1
1:A:22:GLY:O	1:A:24:PHE:N	0.48	2.47	4	2
1:B:219:PHE:CE1	1:B:305:GLU:OE1	0.48	2.67	4	1
1:A:147:LYS:HG3	1:A:148:ASP:OD1	0.48	2.08	5	1
1:B:249:HIS:NE2	1:B:250:PHE:CE1	0.48	2.81	8	1
1:B:261:HIS:HB3	1:B:265:ALA:CB	0.48	2.39	9	1
1:B:265:ALA:HB2	1:B:269:GLN:NE2	0.48	2.24	9	1
1:A:116:ILE:HG22	1:A:117:VAL:N	0.48	2.23	15	2
1:B:249:HIS:HE1	1:B:357:ASP:OD1	0.48	1.89	11	1
1:A:112:PHE:HB2	1:B:311:ALA:HB1	0.48	1.86	12	1
1:A:37:SER:OG	1:A:38:ALA:N	0.48	2.47	13	1
1:B:348:ASP:HB3	1:B:351:LEU:HD12	0.48	1.85	13	1
1:A:25:MET:C	1:A:28:VAL:O	0.48	2.51	14	1
1:A:64:GLU:OE1	1:A:71:LEU:CD1	0.48	2.59	15	1
1:B:219:PHE:CD2	1:B:291:VAL:O	0.48	2.66	4	1
1:A:19:PHE:HE1	1:A:84:ILE:N	0.48	2.06	5	2
1:B:292:ALA:CB	1:B:318:LEU:CD2	0.48	2.79	7	1
1:A:28:VAL:O	1:A:30:PRO:HD3	0.48	2.07	9	1
1:A:73:PRO:HD3	1:B:330:PHE:HA	0.48	1.86	10	2
1:A:106:ILE:O	1:A:108:TRP:N	0.48	2.46	10	1
1:A:27:LEU:HG	1:A:28:VAL:HG23	0.48	1.85	11	1
1:A:130:PHE:CZ	1:B:270:VAL:O	0.48	2.67	11	1
1:B:239:GLU:CG	1:B:266:TRP:HZ3	0.48	2.22	12	1
1:A:35:MET:HB3	1:A:66:TRP:HB3	0.48	1.85	13	1
1:B:223:PRO:HG3	1:B:295:GLY:HA3	0.48	1.85	13	1
1:B:240:GLN:C	1:B:242:PRO:HD2	0.48	2.28	13	1
1:A:56:GLU:HB3	1:A:58:PHE:CE1	0.48	2.44	14	1
1:A:78:PRO:O	1:A:82:LEU:CG	0.48	2.61	15	1
1:B:299:SER:O	1:B:299:SER:OG	0.48	2.30	15	1
1:A:28:VAL:CG2	1:A:34:SER:H	0.48	2.22	2	1
1:A:85:ARG:O	1:A:114:LYS:CE	0.48	2.62	15	3
1:A:153:LYS:CB	1:A:153:LYS:NZ	0.48	2.76	2	1
1:B:250:PHE:HD1	1:B:255:LEU:CD1	0.48	2.19	14	5
1:A:131:LEU:HD11	1:B:308:TRP:CH2	0.48	2.44	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:HIS:CE1	1:A:153:LYS:HG2	0.48	2.43	5	1
1:A:20:LEU:HD13	1:A:21:ALA:N	0.48	2.23	6	1
1:A:35:MET:HB2	1:A:69:GLN:CG	0.48	2.39	6	1
1:B:280:ASP:HB3	1:B:308:TRP:CZ3	0.48	2.43	6	1
1:A:28:VAL:HG21	1:A:70:VAL:HB	0.48	1.86	7	1
1:A:142:GLU:HG2	1:A:159:ALA:O	0.48	2.09	7	1
1:A:148:ASP:OD1	1:A:150:ALA:CB	0.48	2.61	7	1
1:B:321:GLU:HG2	1:B:324:ARG:HB2	0.48	1.86	7	1
1:A:31:GLU:OE1	1:A:73:PRO:HD3	0.48	2.08	8	1
1:B:325:GLU:HG2	1:B:345:HIS:CD2	0.48	2.44	8	2
1:B:216:ARG:O	1:B:216:ARG:HG3	0.48	2.08	9	1
1:A:106:ILE:CG2	1:A:135:LEU:HG	0.48	2.38	10	1
1:A:64:GLU:CA	1:A:69:GLN:HG3	0.48	2.38	11	1
1:A:101:GLY:C	1:A:105:GLU:OE2	0.48	2.52	11	1
1:B:258:PHE:HB3	1:B:283:GLU:HG2	0.48	1.85	13	2
1:A:140:ALA:HB2	1:A:167:VAL:HG21	0.48	1.86	12	1
1:B:237:SER:O	1:B:241:LEU:CD1	0.48	2.55	14	1
1:A:96:ILE:HD11	1:A:127:GLU:CB	0.48	2.37	15	1
1:B:218:VAL:HB	1:B:257:VAL:HG22	0.48	1.83	15	1
1:B:302:THR:HA	1:B:305:GLU:CG	0.48	2.38	15	1
1:A:121:GLU:H	1:A:125:GLU:HB3	0.48	1.69	11	4
1:B:285:ARG:O	1:B:314:LYS:NZ	0.48	2.44	2	2
1:B:302:THR:HB	1:B:306:ILE:CD1	0.48	2.38	2	1
1:A:25:MET:HE1	1:A:31:GLU:OE2	0.48	2.09	3	1
1:B:223:PRO:CG	1:B:227:LEU:HB3	0.48	2.39	3	4
1:A:65:ALA:HA	1:A:69:GLN:HA	0.48	1.86	4	1
1:A:120:LEU:CD1	1:A:125:GLU:CD	0.48	2.82	4	1
1:A:36:PRO:O	1:A:40:GLN:HG2	0.48	2.09	7	2
1:A:37:SER:C	1:A:39:GLU:N	0.48	2.67	6	3
1:A:49:HIS:NE2	1:A:50:PHE:CE1	0.48	2.82	8	1
1:A:117:VAL:HG13	1:A:142:GLU:HB3	0.48	1.86	8	1
1:B:321:GLU:HA	1:B:346:TYR:HB2	0.48	1.85	8	1
1:A:62:ARG:HB3	1:A:62:ARG:CZ	0.48	2.38	9	1
1:B:236:PRO:O	1:B:239:GLU:CG	0.48	2.49	10	1
1:A:96:ILE:HB	1:A:124:ARG:HG2	0.48	1.84	11	1
1:B:281:GLN:HG2	1:B:308:TRP:CZ2	0.48	2.44	15	1
1:A:16:ARG:HD2	1:A:56:GLU:OE1	0.48	2.08	1	1
1:A:124:ARG:O	1:A:125:GLU:C	0.48	2.52	6	4
1:B:320:LEU:N	1:B:344:VAL:O	0.48	2.47	15	6
1:A:112:PHE:CD2	1:B:311:ALA:HB1	0.48	2.44	13	2
1:A:23:PRO:CG	1:A:27:LEU:HB3	0.48	2.38	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:249:HIS:CE1	1:B:353:LYS:HG2	0.48	2.44	5	1
1:B:249:HIS:CD2	1:B:249:HIS:H	0.48	2.25	5	1
1:A:91:VAL:HG12	1:A:91:VAL:O	0.48	2.08	6	1
1:A:130:PHE:CE2	1:B:224:PHE:CD2	0.48	3.00	6	1
1:A:34:SER:C	1:A:36:PRO:CD	0.48	2.83	10	1
1:B:224:PHE:O	1:B:228:VAL:CG1	0.48	2.62	10	1
1:B:306:ILE:CG2	1:B:335:LEU:HG	0.48	2.39	10	1
1:B:356:ILE:HG22	1:B:357:ASP:OD1	0.48	2.09	11	1
1:A:35:MET:HB2	1:A:69:GLN:CB	0.48	2.39	12	1
1:A:85:ARG:HB3	1:A:112:PHE:CZ	0.48	2.42	12	2
1:A:53:GLN:HG3	1:A:55:LEU:CD2	0.48	2.39	15	1
1:B:223:PRO:HB2	1:B:227:LEU:H	0.47	1.69	13	2
1:A:102:THR:HB	1:A:106:ILE:CD1	0.47	2.38	2	1
1:A:106:ILE:HG22	1:A:135:LEU:CD2	0.47	2.36	15	2
1:B:229:ASN:O	1:B:230:PRO:C	0.47	2.51	14	9
1:A:64:GLU:OE2	1:A:71:LEU:CD1	0.47	2.62	3	1
1:B:219:PHE:HZ	1:B:305:GLU:OE1	0.47	1.87	4	2
1:A:103:HIS:NE2	1:A:128:TYR:HD1	0.47	2.05	10	3
1:A:123:GLY:O	1:A:126:GLU:HB3	0.47	2.09	5	2
1:B:220:LEU:HB2	1:B:257:VAL:CG1	0.47	2.39	11	2
1:B:228:VAL:HG22	1:B:233:ASN:HB3	0.47	1.85	5	1
1:B:240:GLN:NE2	1:B:244:LEU:HD21	0.47	2.24	6	1
1:A:17:SER:OG	1:A:56:GLU:HB2	0.47	2.08	7	1
1:A:107:GLY:CA	1:B:308:TRP:HE1	0.47	2.21	7	3
1:A:62:ARG:HB3	1:A:66:TRP:CZ2	0.47	2.44	8	1
1:A:135:LEU:HB3	1:A:141:VAL:CG2	0.47	2.35	12	2
1:A:142:GLU:OE2	1:A:143:PHE:N	0.47	2.46	10	1
1:A:73:PRO:HD3	1:B:330:PHE:CD1	0.47	2.44	15	1
1:A:79:LEU:HD12	1:A:80:ASP:N	0.47	2.23	15	1
1:A:125:GLU:HG3	1:A:145:HIS:CE1	0.47	2.44	15	1
1:A:29:ASN:HB2	1:A:32:THR:HB	0.47	1.86	1	1
1:A:121:GLU:HB3	1:A:124:ARG:CB	0.47	2.39	9	2
1:B:229:ASN:N	1:B:232:THR:CG2	0.47	2.78	4	1
1:B:230:PRO:C	1:B:231:GLU:CG	0.47	2.83	4	1
1:A:28:VAL:HG22	1:A:33:ASN:HB3	0.47	1.85	5	1
1:A:89:VAL:CG2	1:A:164:VAL:HG22	0.47	2.38	8	2
1:A:80:ASP:O	1:A:84:ILE:CB	0.47	2.61	6	1
1:B:245:THR:HG23	1:B:353:LYS:HE3	0.47	1.85	10	1
1:A:99:SER:O	1:A:103:HIS:CB	0.47	2.58	11	1
1:B:228:VAL:HG13	1:B:233:ASN:HB2	0.47	1.85	11	1
1:A:110:SER:OG	1:A:139:ALA:HB3	0.47	2.09	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LEU:HD22	1:B:304:VAL:CB	0.47	2.39	13	1
1:B:299:SER:N	1:B:328:TYR:CE1	0.47	2.83	14	1
1:A:59:ASN:OD1	1:A:83:GLU:CB	0.47	2.61	15	1
1:A:119:LEU:CD2	1:A:146:TYR:HB3	0.47	2.38	2	1
1:B:284:ILE:HD11	1:B:305:GLU:HB3	0.47	1.87	2	2
1:A:19:PHE:HD2	1:A:20:LEU:N	0.47	2.07	5	1
1:A:85:ARG:N	1:A:112:PHE:HE1	0.47	2.07	5	1
1:B:291:VAL:HG12	1:B:291:VAL:O	0.47	2.08	6	1
1:A:33:ASN:CG	1:A:34:SER:H	0.47	2.13	7	1
1:A:49:HIS:NE2	1:A:157:ASP:OD1	0.47	2.47	9	1
1:A:125:GLU:CD	1:A:145:HIS:NE2	0.47	2.68	9	1
1:B:249:HIS:NE2	1:B:357:ASP:OD1	0.47	2.48	9	1
1:A:125:GLU:OE2	1:A:145:HIS:CD2	0.47	2.68	11	1
1:B:225:MET:HE1	1:B:231:GLU:N	0.47	2.24	11	1
1:A:28:VAL:HG21	1:A:32:THR:O	0.47	2.09	12	1
1:A:70:VAL:HA	1:B:330:PHE:CZ	0.47	2.40	13	2
1:A:46:LEU:HD13	1:A:149:ILE:HD12	0.47	1.85	14	1
1:A:112:PHE:HE2	1:B:311:ALA:HB2	0.47	1.54	14	1
1:B:280:ASP:CB	1:B:308:TRP:HZ3	0.47	2.23	14	1
1:B:237:SER:HA	1:B:240:GLN:CD	0.47	2.29	15	1
1:B:253:GLN:HG3	1:B:255:LEU:CD2	0.47	2.39	15	1
1:A:20:LEU:CD1	1:A:50:PHE:CE2	0.47	2.97	2	1
1:A:46:LEU:O	1:A:47:ILE:C	0.47	2.52	2	4
1:A:75:GLU:O	1:A:78:PRO:HG2	0.47	2.09	2	1
1:B:241:LEU:N	1:B:241:LEU:HD13	0.47	2.23	2	2
1:A:29:ASN:HB2	1:A:32:THR:HG22	0.47	1.85	3	1
1:A:47:ILE:HD13	1:A:47:ILE:H	0.47	1.69	14	2
1:A:19:PHE:C	1:A:19:PHE:HD2	0.47	2.13	5	1
1:B:220:LEU:CD1	1:B:221:ALA:H	0.47	2.22	6	1
1:B:300:PRO:O	1:B:304:VAL:HB	0.47	2.09	6	1
1:B:325:GLU:OE2	1:B:326:GLU:HG3	0.47	2.09	6	1
1:A:31:GLU:HA	1:A:70:VAL:CG1	0.47	2.39	10	1
1:A:30:PRO:HB3	1:B:298:PRO:CD	0.47	2.38	11	1
1:A:50:PHE:HB3	1:A:57:VAL:CG2	0.47	2.39	11	1
1:A:92:ALA:O	1:A:118:LEU:HA	0.47	2.09	11	1
1:B:329:GLY:HA2	1:B:333:ARG:CD	0.47	2.39	13	1
1:A:24:PHE:HB3	1:B:330:PHE:HE2	0.47	1.68	14	1
1:A:18:VAL:HB	1:A:57:VAL:HG22	0.47	1.84	15	1
1:B:285:ARG:CB	1:B:312:PHE:HE2	0.47	2.23	6	2
1:B:353:LYS:O	1:B:357:ASP:CB	0.47	2.62	1	1
1:B:220:LEU:CD1	1:B:250:PHE:CE2	0.47	2.97	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:285:ARG:HB2	1:B:312:PHE:CZ	0.47	2.44	2	2
1:A:24:PHE:HA	1:A:27:LEU:HD22	0.47	1.74	3	2
1:A:130:PHE:CE2	1:B:225:MET:CB	0.47	2.98	3	1
1:A:130:PHE:HE2	1:B:225:MET:H	0.47	1.53	6	3
1:B:229:ASN:HB2	1:B:232:THR:HG22	0.47	1.85	3	1
1:A:20:LEU:CD1	1:A:21:ALA:N	0.47	2.77	6	2
1:A:82:LEU:O	1:A:86:LYS:CD	0.47	2.63	8	1
1:A:28:VAL:O	1:A:30:PRO:CD	0.47	2.63	9	1
1:A:27:LEU:CG	1:A:35:MET:HB3	0.47	2.40	10	1
1:A:45:THR:HG23	1:A:153:LYS:HE3	0.47	1.86	10	1
1:B:247:ILE:HA	1:B:257:VAL:HG21	0.47	1.87	11	1
1:A:65:ALA:HB3	1:A:66:TRP:HE1	0.47	1.67	12	1
1:B:244:LEU:HD13	1:B:262:ARG:CB	0.47	2.40	12	1
1:B:228:VAL:HG22	1:B:229:ASN:O	0.47	2.09	13	1
1:B:220:LEU:HD22	1:B:221:ALA:H	0.47	1.69	1	1
1:A:85:ARG:CB	1:A:112:PHE:CZ	0.47	2.97	2	3
1:B:249:HIS:O	1:B:253:GLN:CB	0.47	2.62	2	2
1:B:325:GLU:O	1:B:328:TYR:HB2	0.47	2.09	15	3
1:A:35:MET:HG3	1:A:36:PRO:N	0.47	2.24	3	2
1:A:82:LEU:O	1:A:86:LYS:HG3	0.47	2.09	10	5
1:A:113:ASP:C	1:A:113:ASP:OD1	0.47	2.53	3	1
1:B:299:SER:OG	1:B:302:THR:CB	0.47	2.62	3	2
1:A:121:GLU:OE1	1:A:124:ARG:HG2	0.47	2.09	6	1
1:B:272:THR:C	1:B:276:CYS:HG	0.47	2.12	6	1
1:A:35:MET:SD	1:A:39:GLU:HG2	0.47	2.50	8	1
1:A:104:VAL:HA	1:B:304:VAL:HG22	0.47	1.86	8	1
1:A:125:GLU:HB3	1:A:145:HIS:CE1	0.47	2.44	9	1
1:B:321:GLU:HB3	1:B:324:ARG:CB	0.47	2.39	9	1
1:A:61:HIS:CD2	1:A:61:HIS:N	0.47	2.77	10	1
1:B:219:PHE:CE2	1:B:305:GLU:OE1	0.47	2.67	13	1
1:B:239:GLU:OE2	1:B:243:PHE:HZ	0.47	1.92	13	1
1:A:25:MET:SD	1:B:298:PRO:HG3	0.47	2.50	14	1
1:A:33:ASN:C	1:A:69:GLN:HE21	0.47	2.13	14	1
1:A:140:ALA:HB3	1:A:167:VAL:CG2	0.47	2.40	14	1
1:B:248:GLU:C	1:B:252:LYS:HE2	0.47	2.30	14	1
1:A:122:GLU:HA	1:A:145:HIS:CE1	0.47	2.44	15	1
1:B:219:PHE:HD1	1:B:259:ASN:HB2	0.47	1.65	1	1
1:B:240:GLN:HG2	1:B:244:LEU:HD21	0.47	1.86	1	1
1:B:249:HIS:CD2	1:B:253:GLN:HG3	0.47	2.45	1	1
1:B:277:THR:N	1:B:278:PRO:CD	0.47	2.77	1	3
1:A:107:GLY:O	1:B:308:TRP:HD1	0.47	1.79	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:265:ALA:C	1:B:269:GLN:HG3	0.47	2.30	2	1
1:A:30:PRO:C	1:A:31:GLU:CG	0.47	2.81	4	1
1:A:35:MET:CG	1:A:36:PRO:HD2	0.47	2.38	4	1
1:B:239:GLU:OE2	1:B:239:GLU:HA	0.47	2.10	4	1
1:B:281:GLN:HG2	1:B:308:TRP:CH2	0.47	2.44	4	1
1:A:83:GLU:CD	1:A:83:GLU:N	0.47	2.68	5	1
1:B:284:ILE:CG2	1:B:312:PHE:CE1	0.47	2.98	5	1
1:B:285:ARG:CB	1:B:285:ARG:HH11	0.47	2.22	5	1
1:A:24:PHE:CD2	1:A:70:VAL:HA	0.47	2.41	7	1
1:A:159:ALA:O	1:A:163:VAL:HG12	0.47	2.10	7	1
1:A:65:ALA:CB	1:A:69:GLN:NE2	0.47	2.78	8	1
1:A:77:THR:CG2	1:B:334:GLY:C	0.47	2.62	8	1
1:A:77:THR:CG2	1:B:334:GLY:HA3	0.47	2.38	8	1
1:B:325:GLU:C	1:B:325:GLU:OE1	0.47	2.53	8	1
1:A:104:VAL:HG22	1:B:303:HIS:O	0.47	2.08	9	1
1:B:279:LEU:O	1:B:283:GLU:CD	0.47	2.53	14	2
1:B:235:MET:O	1:B:235:MET:CG	0.47	2.62	15	2
1:B:308:TRP:CD1	1:B:312:PHE:HE2	0.47	2.28	10	1
1:B:335:LEU:HB3	1:B:341:VAL:CG1	0.47	2.37	10	1
1:A:25:MET:CG	1:B:330:PHE:CD2	0.47	2.90	11	2
1:A:72:THR:CB	1:A:73:PRO:HD2	0.47	2.36	11	1
1:A:39:GLU:CG	1:A:66:TRP:HZ3	0.47	2.22	12	1
1:A:28:VAL:HG22	1:A:29:ASN:O	0.47	2.09	13	1
1:A:96:ILE:HG12	1:A:127:GLU:HB2	0.47	1.87	15	2
1:B:265:ALA:HA	1:B:269:GLN:CB	0.47	2.39	14	1
1:B:225:MET:HE3	1:B:301:GLY:N	0.47	2.21	15	1
1:B:277:THR:O	1:B:281:GLN:HB2	0.47	2.10	15	1
1:B:264:GLU:OE2	1:B:271:LEU:HD22	0.47	2.09	1	1
1:A:24:PHE:C	1:A:25:MET:HE2	0.47	2.30	2	1
1:B:224:PHE:HA	1:B:227:LEU:HD22	0.47	1.73	13	2
1:B:235:MET:HG3	1:B:236:PRO:N	0.47	2.21	8	2
1:A:93:ILE:HD11	1:A:119:LEU:CD1	0.47	2.39	4	2
1:A:19:PHE:CE1	1:A:84:ILE:N	0.47	2.83	14	2
1:B:225:MET:CE	1:B:231:GLU:H	0.47	2.22	5	1
1:B:244:LEU:O	1:B:248:GLU:CG	0.47	2.63	5	1
1:A:81:GLN:HE22	1:B:338:VAL:HB	0.47	1.70	7	1
1:A:28:VAL:CG2	1:A:70:VAL:HG22	0.47	2.39	9	1
1:A:65:ALA:HB2	1:A:69:GLN:NE2	0.47	2.25	9	1
1:A:142:GLU:HB3	1:A:159:ALA:HB1	0.47	1.86	11	1
1:B:289:VAL:HG11	1:B:360:ILE:HG12	0.47	1.85	11	1
1:B:316:ILE:HG22	1:B:341:VAL:HA	0.47	1.86	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:THR:CG2	1:B:334:GLY:O	0.47	2.56	13	1
1:A:80:ASP:CB	1:A:108:TRP:HZ3	0.47	2.22	14	1
1:B:224:PHE:CE2	1:B:269:GLN:OE1	0.47	2.68	14	1
1:A:34:SER:O	1:A:36:PRO:HD3	0.47	2.10	15	1
1:A:114:LYS:CD	1:A:114:LYS:H	0.47	2.21	15	1
1:A:123:GLY:H	1:A:125:GLU:CD	0.47	2.13	15	5
1:A:85:ARG:HB2	1:A:112:PHE:CZ	0.47	2.45	2	2
1:A:130:PHE:CD1	1:B:225:MET:SD	0.47	3.07	2	1
1:B:223:PRO:C	1:B:225:MET:HE2	0.47	2.30	2	1
1:A:24:PHE:CE2	1:A:61:HIS:ND1	0.47	2.83	4	2
1:A:96:ILE:HB	1:A:124:ARG:HD3	0.47	1.86	3	2
1:A:130:PHE:CE2	1:B:224:PHE:HD1	0.47	2.28	12	3
1:A:131:LEU:CD1	1:A:135:LEU:HD12	0.47	2.39	5	2
1:B:310:SER:CB	1:B:335:LEU:HD21	0.47	2.40	3	1
1:B:225:MET:O	1:B:228:VAL:CG1	0.47	2.58	5	1
1:A:121:GLU:HA	1:A:146:TYR:HB2	0.47	1.87	8	2
1:B:226:GLY:CA	1:B:300:PRO:HD2	0.47	2.39	8	1
1:A:16:ARG:NH1	1:A:16:ARG:HG2	0.47	2.24	9	1
1:B:253:GLN:HG2	1:B:255:LEU:HD11	0.47	1.87	10	1
1:B:228:VAL:HA	1:B:233:ASN:HB3	0.47	1.86	11	1
1:A:59:ASN:CG	1:A:60:ALA:H	0.47	2.11	13	2
1:B:228:VAL:HG21	1:B:232:THR:O	0.47	2.09	12	1
1:B:275:GLU:O	1:B:279:LEU:CB	0.47	2.63	13	1
1:A:40:GLN:HE21	1:A:66:TRP:HE1	0.47	1.53	14	1
1:A:57:VAL:O	1:A:57:VAL:HG12	0.47	2.09	14	1
1:A:131:LEU:HD13	1:B:304:VAL:CG1	0.47	2.40	15	1
1:B:264:GLU:OE1	1:B:271:LEU:CD1	0.47	2.63	15	1
1:A:73:PRO:CG	1:B:329:GLY:O	0.47	2.62	1	1
1:A:73:PRO:HD3	1:B:330:PHE:HD2	0.47	1.69	1	1
1:B:284:ILE:HD12	1:B:308:TRP:CB	0.47	2.39	5	3
1:B:324:ARG:O	1:B:325:GLU:C	0.47	2.53	6	5
1:A:29:ASN:HB2	1:A:32:THR:CG2	0.47	2.34	4	1
1:B:320:LEU:HB3	1:B:345:HIS:ND1	0.47	2.24	4	1
1:B:342:GLU:CD	1:B:363:VAL:CG2	0.47	2.82	4	1
1:A:84:ILE:HG22	1:A:112:PHE:CE1	0.47	2.45	5	1
1:A:125:GLU:C	1:A:125:GLU:CD	0.47	2.69	5	1
1:B:228:VAL:HG13	1:B:233:ASN:HB3	0.47	1.86	7	1
1:B:262:ARG:HH11	1:B:262:ARG:CG	0.47	2.23	7	1
1:A:40:GLN:HA	1:A:40:GLN:NE2	0.47	2.24	8	1
1:B:262:ARG:CB	1:B:262:ARG:CZ	0.47	2.92	9	1
1:B:263:ARG:HD3	1:B:263:ARG:N	0.47	2.25	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ASN:HD22	1:A:34:SER:N	0.47	2.08	13	1
1:B:229:ASN:ND2	1:B:232:THR:O	0.47	2.48	13	1
1:A:77:THR:O	1:A:81:GLN:HG2	0.47	2.09	14	1
1:B:294:PRO:HB2	1:B:328:TYR:CZ	0.47	2.37	15	1
1:B:228:VAL:CG1	1:B:229:ASN:N	0.46	2.78	2	2
1:B:259:ASN:H	1:B:283:GLU:HG2	0.46	1.69	2	1
1:A:103:HIS:C	1:B:304:VAL:CG2	0.46	2.83	5	1
1:A:19:PHE:CD2	1:A:19:PHE:C	0.46	2.88	6	1
1:A:157:ASP:OD1	1:A:158:ALA:N	0.46	2.48	12	2
1:B:262:ARG:CG	1:B:263:ARG:N	0.46	2.79	13	2
1:A:120:LEU:CB	1:A:125:GLU:HB2	0.46	2.40	11	2
1:B:248:GLU:HB3	1:B:252:LYS:CE	0.46	2.40	14	1
1:B:366:ARG:O	1:B:366:ARG:HG2	0.46	2.10	14	1
1:B:235:MET:SD	1:B:236:PRO:O	0.46	2.72	15	1
1:B:342:GLU:OE2	1:B:359:ALA:CA	0.46	2.62	15	1
1:A:124:ARG:C	1:A:126:GLU:N	0.46	2.66	1	2
1:A:125:GLU:O	1:A:128:TYR:HB2	0.46	2.10	3	3
1:A:40:GLN:OE1	1:A:43:PHE:CB	0.46	2.61	3	1
1:B:302:THR:O	1:B:305:GLU:CA	0.46	2.62	5	2
1:A:19:PHE:CE2	1:A:91:VAL:O	0.46	2.69	4	1
1:A:24:PHE:CD2	1:B:330:PHE:HE2	0.46	2.28	5	1
1:A:49:HIS:CD2	1:A:49:HIS:H	0.46	2.25	5	1
1:A:116:ILE:C	1:A:117:VAL:HG22	0.46	2.31	5	1
1:A:127:GLU:O	1:A:128:TYR:C	0.46	2.52	7	3
1:B:228:VAL:HG13	1:B:233:ASN:CB	0.46	2.41	11	2
1:B:280:ASP:CG	1:B:305:GLU:OE1	0.46	2.54	7	1
1:B:327:GLU:O	1:B:328:TYR:C	0.46	2.54	8	3
1:A:125:GLU:CG	1:A:145:HIS:NE2	0.46	2.79	8	1
1:B:316:ILE:HG23	1:B:318:LEU:CD1	0.46	2.32	9	1
1:A:23:PRO:HB3	1:A:99:SER:CB	0.46	2.40	10	2
1:A:58:PHE:HB3	1:A:83:GLU:HG3	0.46	1.87	10	1
1:A:119:LEU:O	1:A:120:LEU:C	0.46	2.54	8	7
1:A:153:LYS:O	1:A:157:ASP:CB	0.46	2.63	1	1
1:A:56:GLU:OE2	1:A:58:PHE:CZ	0.46	2.69	12	2
1:A:49:HIS:ND1	1:A:49:HIS:O	0.46	2.48	14	3
1:A:118:LEU:O	1:A:144:VAL:HB	0.46	2.10	3	1
1:A:78:PRO:O	1:A:82:LEU:CD2	0.46	2.64	15	2
1:B:325:GLU:OE2	1:B:325:GLU:O	0.46	2.32	5	1
1:B:218:VAL:O	1:B:218:VAL:CG1	0.46	2.63	6	1
1:A:108:TRP:HE1	1:B:307:GLY:CA	0.46	2.24	7	3
1:B:298:PRO:O	1:B:300:PRO:HD3	0.46	2.10	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:MET:HE3	1:A:61:HIS:CD2	0.46	2.46	9	1
1:A:63:ARG:O	1:A:63:ARG:NH1	0.46	2.48	9	1
1:B:225:MET:CA	1:B:230:PRO:HA	0.46	2.41	10	1
1:A:85:ARG:HA	1:A:114:LYS:HD2	0.46	1.86	11	1
1:B:234:SER:O	1:B:236:PRO:HD3	0.46	2.09	15	1
1:B:275:GLU:C	1:B:279:LEU:CD2	0.46	2.84	15	1
1:B:249:HIS:HE1	1:B:250:PHE:CZ	0.46	2.27	2	1
1:A:120:LEU:HB2	1:A:145:HIS:CA	0.46	2.40	4	1
1:B:229:ASN:H	1:B:232:THR:CG2	0.46	2.23	4	1
1:B:285:ARG:HD3	1:B:312:PHE:CZ	0.46	2.45	5	2
1:A:35:MET:SD	1:A:69:GLN:CD	0.46	2.94	6	1
1:A:106:ILE:C	1:A:108:TRP:N	0.46	2.68	6	2
1:B:305:GLU:O	1:B:308:TRP:HB2	0.46	2.11	6	2
1:A:97:PRO:CB	1:A:98:PRO:HD2	0.46	2.40	8	1
1:A:104:VAL:CA	1:B:304:VAL:HG22	0.46	2.41	8	1
1:A:106:ILE:O	1:A:107:GLY:C	0.46	2.54	10	1
1:B:239:GLU:N	1:B:239:GLU:CD	0.46	2.64	10	1
1:B:314:LYS:N	1:B:314:LYS:HD2	0.46	2.25	15	1
1:B:325:GLU:HA	1:B:328:TYR:HD2	0.46	1.70	14	3
1:A:50:PHE:HB3	1:A:57:VAL:HG23	0.46	1.88	15	3
1:B:319:LEU:HD22	1:B:346:TYR:CG	0.46	2.45	2	1
1:A:93:ILE:O	1:A:93:ILE:HG22	0.46	2.10	4	3
1:A:160:ILE:CG2	1:A:161:ARG:N	0.46	2.76	3	3
1:A:163:VAL:HG12	1:A:164:VAL:N	0.46	2.25	3	3
1:B:363:VAL:HG12	1:B:364:VAL:N	0.46	2.25	11	3
1:B:281:GLN:CG	1:B:308:TRP:CH2	0.46	2.99	4	1
1:A:62:ARG:CG	1:A:63:ARG:N	0.46	2.78	13	2
1:B:237:SER:C	1:B:239:GLU:N	0.46	2.68	8	4
1:B:285:ARG:HB2	1:B:314:LYS:HE2	0.46	1.86	6	1
1:B:219:PHE:CZ	1:B:221:ALA:HB2	0.46	2.46	7	3
1:A:19:PHE:CB	1:A:87:ALA:HB1	0.46	2.41	8	2
1:A:131:LEU:CD2	1:B:308:TRP:CZ2	0.46	2.98	12	2
1:B:233:ASN:C	1:B:233:ASN:ND2	0.46	2.69	9	1
1:B:263:ARG:CA	1:B:263:ARG:HH11	0.46	2.24	9	1
1:B:227:LEU:HD23	1:B:227:LEU:N	0.46	2.26	10	1
1:B:335:LEU:HB3	1:B:341:VAL:CG2	0.46	2.40	10	1
1:B:342:GLU:OE2	1:B:343:PHE:N	0.46	2.49	10	1
1:B:277:THR:O	1:B:281:GLN:HG2	0.46	2.10	14	1
1:B:216:ARG:HD2	1:B:256:GLU:OE1	0.46	2.11	1	1
1:B:351:LEU:O	1:B:354:PRO:HG2	0.46	2.11	1	3
1:A:103:HIS:N	1:A:106:ILE:HD12	0.46	2.22	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:246:LEU:O	1:B:247:ILE:C	0.46	2.53	2	3
1:B:329:GLY:O	1:B:333:ARG:CB	0.46	2.63	14	4
1:B:258:PHE:CG	1:B:283:GLU:OE2	0.46	2.69	3	1
1:A:131:LEU:CD2	1:A:135:LEU:CD1	0.46	2.85	4	1
1:B:235:MET:CG	1:B:236:PRO:HD2	0.46	2.41	4	1
1:B:271:LEU:N	1:B:271:LEU:CD2	0.46	2.74	5	2
1:B:275:GLU:OE2	1:B:279:LEU:CD1	0.46	2.64	5	1
1:A:153:LYS:O	1:A:156:ILE:CG2	0.46	2.64	9	2
1:B:225:MET:HG3	1:B:230:PRO:HA	0.46	1.86	6	1
1:B:265:ALA:HB1	1:B:269:GLN:NE2	0.46	2.26	6	2
1:B:265:ALA:CB	1:B:269:GLN:NE2	0.46	2.79	6	1
1:A:62:ARG:NH1	1:A:62:ARG:CG	0.46	2.77	7	1
1:B:269:GLN:OE1	1:B:270:VAL:N	0.46	2.48	7	1
1:B:296:ILE:CD1	1:B:328:TYR:CG	0.46	2.98	7	1
1:B:365:ASP:HA	1:B:368:ASN:ND2	0.46	2.25	7	1
1:B:249:HIS:NE2	1:B:250:PHE:CZ	0.46	2.84	8	1
1:B:282:LEU:O	1:B:286:LYS:CD	0.46	2.63	8	1
1:A:19:PHE:CD1	1:A:90:PHE:CD1	0.46	3.04	9	1
1:A:141:VAL:HG12	1:A:141:VAL:O	0.46	2.10	9	1
1:A:81:GLN:HG2	1:A:82:LEU:N	0.46	2.25	10	1
1:B:306:ILE:O	1:B:308:TRP:N	0.46	2.48	10	1
1:A:40:GLN:CG	1:A:41:LEU:N	0.46	2.78	12	1
1:B:296:ILE:HD11	1:B:327:GLU:HB2	0.46	1.87	15	1
1:A:77:THR:N	1:A:78:PRO:CD	0.46	2.79	1	2
1:B:319:LEU:O	1:B:320:LEU:C	0.46	2.54	8	6
1:A:39:GLU:OE2	1:A:43:PHE:HE2	0.46	1.94	2	1
1:A:121:GLU:CB	1:A:124:ARG:HG3	0.46	2.41	2	1
1:B:284:ILE:HD13	1:B:290:PHE:CZ	0.46	2.44	3	1
1:B:217:SER:CB	1:B:256:GLU:HB2	0.46	2.41	7	2
1:B:237:SER:O	1:B:241:LEU:HB2	0.46	2.11	7	1
1:B:348:ASP:OD1	1:B:350:ALA:CB	0.46	2.63	7	1
1:B:226:GLY:HA3	1:B:299:SER:HA	0.46	1.88	8	1
1:B:263:ARG:HH11	1:B:263:ARG:HA	0.46	1.70	9	1
1:B:234:SER:OG	1:B:236:PRO:HD2	0.46	2.11	10	1
1:B:283:GLU:OE1	1:B:286:LYS:NZ	0.46	2.49	10	1
1:B:250:PHE:HB3	1:B:257:VAL:CG2	0.46	2.41	11	1
1:B:296:ILE:CD1	1:B:327:GLU:HB3	0.46	2.41	11	1
1:B:247:ILE:O	1:B:257:VAL:HG21	0.46	2.10	12	1
1:B:235:MET:HB3	1:B:266:TRP:HB3	0.46	1.87	13	1
1:B:233:ASN:C	1:B:269:GLN:HE21	0.46	2.14	14	1
1:B:347:LYS:O	1:B:348:ASP:CG	0.46	2.54	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:ILE:HD11	1:A:105:GLU:HB3	0.46	1.88	2	1
1:A:120:LEU:N	1:A:144:VAL:O	0.46	2.48	15	6
1:B:340:ALA:HB2	1:B:367:VAL:HG22	0.46	1.87	2	1
1:B:229:ASN:HB3	1:B:233:ASN:HB2	0.46	1.87	5	1
1:B:261:HIS:CD2	1:B:261:HIS:N	0.46	2.79	10	1
1:B:256:GLU:OE2	1:B:258:PHE:CZ	0.46	2.69	12	1
1:A:44:LEU:HA	1:A:47:ILE:HB	0.46	1.87	13	1
1:B:250:PHE:HB3	1:B:257:VAL:HG23	0.46	1.88	15	2
1:A:39:GLU:O	1:A:43:PHE:CD2	0.46	2.69	9	2
1:A:131:LEU:CD1	1:A:135:LEU:CD1	0.46	2.94	3	3
1:B:318:LEU:O	1:B:344:VAL:HB	0.46	2.11	3	1
1:B:332:VAL:HG12	1:B:333:ARG:N	0.46	2.25	8	3
1:B:280:ASP:C	1:B:284:ILE:HG13	0.46	2.30	4	1
1:B:259:ASN:HD21	1:B:280:ASP:CG	0.46	2.15	5	1
1:A:25:MET:HG3	1:B:330:PHE:HD1	0.46	1.70	9	1
1:A:69:GLN:OE1	1:A:69:GLN:CA	0.46	2.60	9	1
1:B:235:MET:O	1:B:235:MET:HE2	0.46	2.11	10	1
1:B:263:ARG:CD	1:B:263:ARG:H	0.46	2.23	10	1
1:B:344:VAL:HG22	1:B:359:ALA:CB	0.46	2.40	10	1
1:A:49:HIS:HE1	1:A:157:ASP:OD1	0.46	1.93	11	1
1:B:235:MET:SD	1:B:265:ALA:CA	0.46	3.03	11	1
1:A:47:ILE:HG23	1:A:57:VAL:CG2	0.46	2.38	12	1
1:A:48:GLU:C	1:A:50:PHE:N	0.46	2.69	12	1
1:A:108:TRP:NE1	1:B:307:GLY:HA2	0.46	2.25	12	1
1:B:240:GLN:N	1:B:266:TRP:CH2	0.46	2.83	13	1
1:A:77:THR:CG2	1:A:78:PRO:CD	0.46	2.94	14	1
1:A:130:PHE:CD2	1:B:225:MET:SD	0.46	3.07	14	1
1:B:224:PHE:C	1:B:225:MET:HE2	0.46	2.31	2	1
1:A:95:GLY:N	1:A:128:TYR:CZ	0.46	2.80	8	2
1:A:96:ILE:HD13	1:A:124:ARG:C	0.46	2.29	4	1
1:B:233:ASN:CG	1:B:233:ASN:O	0.46	2.52	4	1
1:B:247:ILE:HD13	1:B:247:ILE:H	0.46	1.70	4	1
1:A:100:PRO:HB3	1:B:303:HIS:CE1	0.46	2.46	5	1
1:B:232:THR:CG2	1:B:233:ASN:H	0.46	2.15	5	1
1:A:40:GLN:HE21	1:A:44:LEU:HD21	0.46	1.71	6	1
1:A:65:ALA:CA	1:A:69:GLN:NE2	0.46	2.79	6	1
1:B:353:LYS:O	1:B:356:ILE:CG2	0.46	2.64	6	2
1:B:240:GLN:HA	1:B:240:GLN:NE2	0.46	2.25	8	1
1:B:262:ARG:HB3	1:B:266:TRP:CZ2	0.46	2.46	8	1
1:B:306:ILE:HG21	1:B:335:LEU:HD21	0.46	1.84	10	1
1:A:62:ARG:O	1:A:66:TRP:HD1	0.46	1.94	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:237:SER:OG	1:B:238:ALA:N	0.46	2.49	13	1
1:A:84:ILE:HD12	1:A:108:TRP:CB	0.45	2.41	5	2
1:A:50:PHE:CD2	1:A:57:VAL:HG22	0.45	2.46	2	1
1:A:56:GLU:OE2	1:A:58:PHE:CE2	0.45	2.69	2	1
1:A:58:PHE:CG	1:A:83:GLU:OE2	0.45	2.69	3	1
1:A:111:ALA:C	1:B:312:PHE:CD1	0.45	2.89	12	3
1:B:328:TYR:CB	1:B:332:VAL:HB	0.45	2.40	3	2
1:B:222:GLY:C	1:B:224:PHE:N	0.45	2.68	4	1
1:B:342:GLU:OE1	1:B:342:GLU:CA	0.45	2.63	4	1
1:A:23:PRO:HA	1:A:99:SER:OG	0.45	2.10	13	3
1:A:45:THR:O	1:A:49:HIS:NE2	0.45	2.47	5	1
1:A:59:ASN:ND2	1:A:80:ASP:CG	0.45	2.69	5	1
1:B:236:PRO:O	1:B:240:GLN:HG2	0.45	2.11	7	2
1:A:28:VAL:HG21	1:A:70:VAL:HG23	0.45	1.81	6	1
1:A:28:VAL:HG13	1:A:33:ASN:HB3	0.45	1.88	7	2
1:A:90:PHE:CE2	1:A:106:ILE:HG13	0.45	2.46	8	1
1:A:24:PHE:HE1	1:A:61:HIS:CD2	0.45	2.29	9	1
1:A:121:GLU:OE1	1:A:121:GLU:CA	0.45	2.63	9	1
1:A:25:MET:CA	1:A:30:PRO:HA	0.45	2.41	10	1
1:B:220:LEU:HD13	1:B:247:ILE:HG13	0.45	1.87	10	1
1:B:320:LEU:CB	1:B:325:GLU:CB	0.45	2.92	11	3
1:A:25:MET:HE1	1:A:31:GLU:N	0.45	2.26	11	1
1:B:325:GLU:OE1	1:B:325:GLU:N	0.45	2.49	11	1
1:A:53:GLN:NE2	1:A:53:GLN:HA	0.45	2.26	13	1
1:A:24:PHE:CE2	1:A:69:GLN:OE1	0.45	2.69	14	1
1:A:130:PHE:CD2	1:B:225:MET:HG3	0.45	2.46	14	1
1:A:23:PRO:HB2	1:A:27:LEU:H	0.45	1.69	1	3
1:B:219:PHE:HE2	1:B:292:ALA:HB2	0.45	1.70	1	1
1:B:233:ASN:O	1:B:233:ASN:CG	0.45	2.53	1	1
1:A:133:ARG:HB3	1:B:273:PRO:HG2	0.45	1.88	3	1
1:A:135:LEU:C	1:A:137:THR:N	0.45	2.69	15	2
1:A:18:VAL:CG1	1:A:91:VAL:CB	0.45	2.91	5	1
1:A:95:GLY:HA2	1:A:124:ARG:HD2	0.45	1.87	5	1
1:B:258:PHE:HB3	1:B:283:GLU:HG3	0.45	1.87	10	2
1:A:77:THR:CG2	1:B:334:GLY:CA	0.45	2.93	8	1
1:B:235:MET:HB2	1:B:269:GLN:OE1	0.45	2.08	8	1
1:B:280:ASP:CB	1:B:305:GLU:OE1	0.45	2.65	8	1
1:A:61:HIS:O	1:A:66:TRP:NE1	0.45	2.49	9	1
1:B:365:ASP:OD2	1:B:365:ASP:C	0.45	2.55	9	1
1:B:225:MET:HE3	1:B:226:GLY:H	0.45	1.71	10	1
1:B:262:ARG:CA	1:B:266:TRP:CE2	0.45	2.96	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:282:LEU:CD1	1:B:282:LEU:N	0.45	2.79	10	1
1:A:112:PHE:CD1	1:B:311:ALA:C	0.45	2.89	12	1
1:B:294:PRO:CA	1:B:328:TYR:CZ	0.45	2.99	12	1
1:A:129:GLY:HA2	1:A:133:ARG:CD	0.45	2.41	13	1
1:A:40:GLN:HG2	1:A:66:TRP:HE1	0.45	1.70	14	1
1:B:277:THR:CG2	1:B:278:PRO:CD	0.45	2.94	14	1
1:A:103:HIS:HA	1:A:106:ILE:HB	0.45	1.88	9	2
1:B:319:LEU:HB3	1:B:346:TYR:CE2	0.45	2.46	7	3
1:B:353:LYS:O	1:B:357:ASP:OD2	0.45	2.33	5	2
1:B:219:PHE:C	1:B:219:PHE:HD2	0.45	2.14	5	1
1:A:35:MET:SD	1:A:69:GLN:NE2	0.45	2.88	7	2
1:A:62:ARG:HD2	1:A:66:TRP:CZ2	0.45	2.42	6	1
1:A:144:VAL:CG2	1:A:159:ALA:CB	0.45	2.93	6	1
1:B:285:ARG:HB3	1:B:312:PHE:HE2	0.45	1.67	6	1
1:B:227:LEU:CD2	1:B:228:VAL:H	0.45	2.21	7	1
1:B:233:ASN:CG	1:B:234:SER:H	0.45	2.15	7	1
1:B:237:SER:C	1:B:239:GLU:H	0.45	2.15	8	1
1:B:296:ILE:HG22	1:B:324:ARG:HH11	0.45	1.71	8	1
1:A:144:VAL:HG22	1:A:159:ALA:CB	0.45	2.41	10	1
1:A:27:LEU:CD1	1:A:35:MET:CB	0.45	2.94	11	1
1:B:262:ARG:CD	1:B:262:ARG:H	0.45	2.24	14	1
1:B:319:LEU:CD2	1:B:346:TYR:CD2	0.45	2.99	2	1
1:B:229:ASN:N	1:B:232:THR:HG22	0.45	2.27	4	1
1:A:44:LEU:O	1:A:48:GLU:CG	0.45	2.65	5	1
1:B:235:MET:H	1:B:269:GLN:CG	0.45	2.23	5	1
1:B:325:GLU:CD	1:B:345:HIS:NE2	0.45	2.70	9	1
1:B:299:SER:OG	1:B:299:SER:O	0.45	2.29	10	1
1:B:306:ILE:O	1:B:307:GLY:C	0.45	2.54	10	1
1:A:23:PRO:HB3	1:A:99:SER:OG	0.45	2.11	14	1
1:A:50:PHE:CB	1:A:57:VAL:HG23	0.45	2.41	14	1
1:A:99:SER:N	1:A:128:TYR:HE1	0.45	2.08	14	1
1:A:147:LYS:O	1:A:151:LEU:CB	0.45	2.65	15	1
1:B:249:HIS:O	1:B:253:GLN:HB2	0.45	2.12	2	1
1:A:142:GLU:OE2	1:A:162:LYS:HD2	0.45	2.12	3	1
1:B:249:HIS:ND1	1:B:249:HIS:O	0.45	2.50	13	3
1:B:293:ILE:HD13	1:B:346:TYR:CE1	0.45	2.47	4	1
1:A:31:GLU:O	1:A:31:GLU:CD	0.45	2.54	5	1
1:B:225:MET:HE1	1:B:231:GLU:H	0.45	1.71	5	1
1:B:229:ASN:ND2	1:B:229:ASN:O	0.45	2.46	5	1
1:B:246:LEU:CA	1:B:249:HIS:NE2	0.45	2.79	5	1
1:A:18:VAL:O	1:A:18:VAL:CG1	0.45	2.64	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:GLU:OE2	1:A:126:GLU:HG3	0.45	2.11	6	1
1:A:151:LEU:HD23	1:A:152:ALA:H	0.45	1.61	7	1
1:B:282:LEU:HB3	1:B:286:LYS:NZ	0.45	2.26	7	1
1:A:80:ASP:CB	1:A:105:GLU:OE1	0.45	2.64	8	1
1:B:280:ASP:OD2	1:B:305:GLU:OE1	0.45	2.34	8	1
1:B:282:LEU:HB3	1:B:286:LYS:HD2	0.45	1.88	8	1
1:A:81:GLN:HG3	1:A:112:PHE:HZ	0.45	1.71	11	2
1:A:25:MET:HG3	1:B:330:PHE:CD1	0.45	2.47	10	1
1:B:234:SER:C	1:B:236:PRO:CD	0.45	2.85	10	1
1:A:96:ILE:CD1	1:A:127:GLU:HB3	0.45	2.42	11	1
1:A:148:ASP:C	1:A:150:ALA:N	0.45	2.69	11	1
1:B:244:LEU:HA	1:B:247:ILE:HB	0.45	1.87	13	1
1:B:279:LEU:O	1:B:283:GLU:HG3	0.45	2.11	14	1
1:A:25:MET:CA	1:A:28:VAL:CG1	0.45	2.95	15	2
1:A:30:PRO:HB3	1:B:327:GLU:OE1	0.45	2.11	1	1
1:B:282:LEU:CD2	1:B:282:LEU:N	0.45	2.80	15	2
1:B:295:GLY:CA	1:B:324:ARG:NH1	0.45	2.80	1	1
1:A:96:ILE:CG2	1:A:124:ARG:HD3	0.45	2.42	3	2
1:B:249:HIS:NE2	1:B:353:LYS:HG2	0.45	2.25	5	1
1:A:25:MET:HE2	1:B:330:PHE:CG	0.45	2.46	8	1
1:A:130:PHE:CD1	1:B:225:MET:CG	0.45	2.99	10	1
1:A:47:ILE:O	1:A:50:PHE:HB2	0.45	2.12	12	1
1:A:71:LEU:O	1:A:72:THR:C	0.45	2.55	12	1
1:B:323:GLY:CA	1:B:325:GLU:OE2	0.45	2.65	15	1
1:A:18:VAL:HG13	1:A:91:VAL:CB	0.45	2.39	1	1
1:A:130:PHE:HD2	1:B:273:PRO:HD3	0.45	1.71	1	1
1:A:157:ASP:OD2	1:A:157:ASP:O	0.45	2.35	3	1
1:B:249:HIS:HA	1:B:252:LYS:HB2	0.45	1.88	5	1
1:A:133:ARG:CG	1:A:133:ARG:NH1	0.45	2.79	6	1
1:B:344:VAL:CG2	1:B:359:ALA:CB	0.45	2.95	6	1
1:A:58:PHE:C	1:A:59:ASN:ND2	0.45	2.70	7	1
1:A:26:GLY:CA	1:A:100:PRO:HD2	0.45	2.41	8	1
1:B:284:ILE:HB	1:B:312:PHE:CE1	0.45	2.46	9	1
1:A:25:MET:HE3	1:A:26:GLY:H	0.45	1.72	10	1
1:B:296:ILE:CG1	1:B:327:GLU:HB3	0.45	2.41	11	1
1:A:44:LEU:CD1	1:A:62:ARG:HG2	0.45	2.38	12	1
1:A:47:ILE:O	1:A:57:VAL:HG21	0.45	2.12	12	1
1:B:357:ASP:OD1	1:B:357:ASP:C	0.45	2.55	12	1
1:A:23:PRO:C	1:A:99:SER:HB2	0.45	2.31	13	1
1:B:223:PRO:C	1:B:299:SER:HB2	0.45	2.32	13	1
1:B:257:VAL:O	1:B:257:VAL:HG12	0.45	2.12	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:HIS:CD2	1:A:71:LEU:CD1	0.45	3.00	1	1
1:A:17:SER:HB3	1:A:58:PHE:HD2	0.45	1.69	2	1
1:B:291:VAL:CG1	1:B:356:ILE:HD11	0.45	2.42	3	1
1:B:303:HIS:O	1:B:304:VAL:C	0.45	2.55	5	3
1:A:49:HIS:HA	1:A:52:LYS:HB2	0.45	1.87	5	2
1:A:75:GLU:OE2	1:A:79:LEU:CD1	0.45	2.64	5	1
1:A:35:MET:CE	1:A:39:GLU:HG2	0.45	2.41	6	1
1:A:84:ILE:HG21	1:A:109:ALA:N	0.45	2.27	8	3
1:A:131:LEU:O	1:A:135:LEU:CB	0.45	2.64	14	2
1:A:95:GLY:C	1:A:128:TYR:HH	0.45	2.11	8	1
1:A:35:MET:O	1:A:35:MET:CE	0.45	2.64	10	1
1:A:127:GLU:OE1	1:A:127:GLU:N	0.45	2.50	13	1
1:A:77:THR:O	1:A:81:GLN:HB2	0.45	2.11	15	1
1:A:90:PHE:CZ	1:A:105:GLU:C	0.45	2.90	15	1
1:A:94:PRO:HB2	1:A:128:TYR:CZ	0.45	2.38	15	1
1:A:107:GLY:CA	1:B:304:VAL:HG12	0.45	2.42	1	1
1:B:225:MET:CA	1:B:228:VAL:CG1	0.45	2.94	15	2
1:B:349:ILE:O	1:B:352:ALA:N	0.45	2.50	2	1
1:A:91:VAL:CG1	1:A:156:ILE:HD11	0.45	2.41	3	1
1:A:110:SER:CB	1:A:135:LEU:HD21	0.45	2.42	3	1
1:A:46:LEU:CA	1:A:49:HIS:NE2	0.45	2.80	5	1
1:A:75:GLU:OE2	1:A:79:LEU:HD11	0.45	2.12	5	1
1:A:96:ILE:HG13	1:A:98:PRO:CD	0.45	2.42	12	2
1:A:130:PHE:CE2	1:B:270:VAL:CG2	0.45	2.96	7	1
1:A:120:LEU:CB	1:A:125:GLU:CB	0.45	2.95	11	3
1:A:64:GLU:HA	1:A:69:GLN:CD	0.45	2.32	11	1
1:A:133:ARG:HE	1:B:273:PRO:HG3	0.45	1.72	11	1
1:B:227:LEU:CD1	1:B:235:MET:CG	0.45	2.95	11	1
1:A:44:LEU:HD13	1:A:62:ARG:HB3	0.45	1.88	12	1
1:B:239:GLU:CG	1:B:266:TRP:CZ3	0.45	3.00	12	1
1:A:62:ARG:CD	1:A:62:ARG:H	0.45	2.24	14	1
1:A:29:ASN:N	1:A:29:ASN:ND2	0.45	2.63	3	1
1:A:35:MET:HB3	1:A:69:GLN:CD	0.45	2.32	3	2
1:B:249:HIS:ND1	1:B:253:GLN:CG	0.45	2.79	3	1
1:A:16:ARG:N	1:A:16:ARG:HD3	0.45	2.28	4	1
1:B:229:ASN:HB2	1:B:233:ASN:ND2	0.45	2.26	6	1
1:A:19:PHE:CZ	1:A:21:ALA:HB2	0.45	2.47	7	3
1:A:28:VAL:HG13	1:A:33:ASN:CB	0.45	2.41	11	2
1:A:37:SER:O	1:A:41:LEU:HB2	0.45	2.12	7	1
1:B:321:GLU:HG3	1:B:324:ARG:HD2	0.45	1.87	7	1
1:A:65:ALA:CB	1:A:69:GLN:HE21	0.45	2.25	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:235:MET:HG3	1:B:236:PRO:HD2	0.45	1.89	9	1
1:B:325:GLU:HB3	1:B:345:HIS:HE1	0.45	1.72	9	1
1:B:223:PRO:O	1:B:227:LEU:CD2	0.45	2.65	10	1
1:B:291:VAL:HG21	1:B:360:ILE:HD11	0.45	1.87	10	1
1:B:301:GLY:C	1:B:305:GLU:OE2	0.45	2.55	11	1
1:A:74:GLU:N	1:A:74:GLU:CD	0.45	2.70	15	1
1:A:19:PHE:HE2	1:A:92:ALA:HB2	0.44	1.71	1	1
1:A:40:GLN:OE1	1:A:41:LEU:HD13	0.44	2.10	1	1
1:A:125:GLU:HA	1:A:128:TYR:HD2	0.44	1.72	8	4
1:B:346:TYR:CD1	1:B:346:TYR:C	0.44	2.90	2	1
1:A:49:HIS:ND1	1:A:53:GLN:CG	0.44	2.80	3	1
1:A:20:LEU:HD12	1:A:47:ILE:CD1	0.44	2.39	4	1
1:A:84:ILE:HD11	1:A:105:GLU:CB	0.44	2.41	4	1
1:A:29:ASN:HB3	1:A:33:ASN:HB2	0.44	1.88	5	1
1:A:121:GLU:OE2	1:A:146:TYR:OH	0.44	2.27	5	1
1:B:302:THR:C	1:B:306:ILE:CD1	0.44	2.82	6	1
1:A:62:ARG:HH11	1:A:62:ARG:CG	0.44	2.23	7	1
1:A:82:LEU:HB3	1:A:86:LYS:NZ	0.44	2.28	7	1
1:A:63:ARG:NH1	1:A:63:ARG:CG	0.44	2.80	9	1
1:A:70:VAL:CG1	1:B:330:PHE:CZ	0.44	2.96	9	1
1:A:165:ASP:OD2	1:A:165:ASP:C	0.44	2.55	9	1
1:A:82:LEU:O	1:A:86:LYS:HE2	0.44	2.12	10	1
1:B:224:PHE:C	1:B:226:GLY:H	0.44	2.14	10	1
1:A:62:ARG:O	1:A:64:GLU:OE1	0.44	2.34	11	1
1:B:260:ALA:O	1:B:265:ALA:HB1	0.44	2.12	12	1
1:A:51:GLU:O	1:A:51:GLU:OE1	0.44	2.36	1	1
1:A:111:ALA:CB	1:B:312:PHE:CE1	0.44	2.92	1	1
1:A:18:VAL:CG2	1:A:50:PHE:CE1	0.44	2.96	12	3
1:A:25:MET:HB2	1:A:30:PRO:HA	0.44	1.88	2	1
1:A:102:THR:O	1:A:105:GLU:CA	0.44	2.64	5	5
1:B:344:VAL:HG13	1:B:355:GLN:HG3	0.44	1.89	3	1
1:B:346:TYR:C	1:B:347:LYS:HG2	0.44	2.32	3	1
1:A:41:LEU:N	1:A:41:LEU:HD13	0.44	2.28	8	2
1:A:61:HIS:O	1:A:64:GLU:CG	0.44	2.66	4	1
1:A:94:PRO:HA	1:A:99:SER:HG	0.44	1.70	4	1
1:A:73:PRO:HG3	1:B:330:PHE:HA	0.44	1.89	5	2
1:B:219:PHE:CD1	1:B:283:GLU:C	0.44	2.90	5	1
1:B:289:VAL:CG2	1:B:364:VAL:HG22	0.44	2.42	8	2
1:B:217:SER:HB2	1:B:258:PHE:CD2	0.44	2.48	6	1
1:B:220:LEU:HD11	1:B:243:PHE:CE2	0.44	2.47	6	1
1:B:246:LEU:HD11	1:B:353:LYS:N	0.44	2.27	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:PRO:HB2	1:A:121:GLU:OE2	0.44	2.13	7	1
1:B:258:PHE:C	1:B:259:ASN:ND2	0.44	2.69	7	1
1:B:259:ASN:CG	1:B:260:ALA:N	0.44	2.71	7	3
1:A:28:VAL:CA	1:A:33:ASN:CB	0.44	2.95	13	2
1:A:134:GLY:C	1:B:277:THR:CG2	0.44	2.62	8	1
1:B:228:VAL:CA	1:B:233:ASN:CB	0.44	2.95	13	2
1:B:342:GLU:OE1	1:B:363:VAL:HB	0.44	2.12	8	1
1:A:27:LEU:CD1	1:A:35:MET:CG	0.44	2.95	11	1
1:B:263:ARG:O	1:B:264:GLU:C	0.44	2.55	11	1
1:A:65:ALA:O	1:A:69:GLN:HB3	0.44	2.13	12	1
1:B:224:PHE:HE1	1:B:271:LEU:N	0.44	2.10	13	1
1:B:320:LEU:N	1:B:320:LEU:CD2	0.44	2.79	14	1
1:A:17:SER:HB3	1:A:58:PHE:HE2	0.44	1.72	15	1
1:A:33:ASN:O	1:A:33:ASN:CG	0.44	2.54	1	1
1:A:82:LEU:HD13	1:A:82:LEU:H	0.44	1.72	4	1
1:B:220:LEU:HD12	1:B:247:ILE:CD1	0.44	2.37	4	1
1:B:320:LEU:HB2	1:B:345:HIS:CA	0.44	2.42	4	1
1:A:104:VAL:CG2	1:B:303:HIS:C	0.44	2.85	5	1
1:B:244:LEU:CD1	1:B:266:TRP:CH2	0.44	2.97	6	1
1:A:134:GLY:O	1:A:138:VAL:CG1	0.44	2.61	7	1
1:B:280:ASP:HB3	1:B:305:GLU:OE1	0.44	2.12	8	1
1:A:33:ASN:C	1:A:33:ASN:ND2	0.44	2.70	9	1
1:B:228:VAL:CG2	1:B:234:SER:N	0.44	2.80	10	1
1:B:231:GLU:HA	1:B:270:VAL:CG1	0.44	2.41	10	1
1:A:28:VAL:HG13	1:A:33:ASN:HB2	0.44	1.88	11	1
1:A:129:GLY:O	1:B:273:PRO:HB3	0.44	2.11	11	1
1:B:235:MET:H	1:B:268:ALA:HA	0.44	1.72	11	1
1:B:318:LEU:CD1	1:B:332:VAL:HG13	0.44	2.42	12	1
1:A:24:PHE:CD1	1:B:330:PHE:CZ	0.44	3.05	13	1
1:A:95:GLY:HA2	1:A:124:ARG:NH1	0.44	2.27	1	1
1:B:275:GLU:O	1:B:278:PRO:HG2	0.44	2.12	2	1
1:B:321:GLU:CB	1:B:324:ARG:HG3	0.44	2.42	2	1
1:A:18:VAL:HG13	1:A:91:VAL:HG21	0.44	1.89	3	1
1:B:279:LEU:HA	1:B:283:GLU:OE2	0.44	2.12	5	1
1:B:224:PHE:HE1	1:B:261:HIS:ND1	0.44	2.11	6	1
1:B:294:PRO:HB2	1:B:321:GLU:OE2	0.44	2.13	7	1
1:B:228:VAL:O	1:B:230:PRO:HD3	0.44	2.12	9	1
1:B:325:GLU:HB3	1:B:345:HIS:CE1	0.44	2.47	9	1
1:B:367:VAL:HG12	1:B:367:VAL:O	0.44	2.11	12	2
1:A:113:ASP:OD2	1:A:113:ASP:C	0.44	2.55	10	1
1:B:262:ARG:C	1:B:264:GLU:OE1	0.44	2.55	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:264:GLU:HA	1:B:269:GLN:CD	0.44	2.33	11	1
1:B:355:GLN:N	1:B:355:GLN:HE21	0.44	2.10	11	1
1:A:33:ASN:CA	1:A:69:GLN:OE1	0.44	2.65	12	1
1:A:24:PHE:CE1	1:A:61:HIS:HD2	0.44	2.30	14	1
1:B:250:PHE:CB	1:B:257:VAL:HG23	0.44	2.42	14	1
1:B:350:ALA:O	1:B:354:PRO:HD3	0.44	2.12	14	1
1:A:106:ILE:HG12	1:A:118:LEU:CD1	0.44	2.42	15	1
1:B:296:ILE:HD11	1:B:327:GLU:CB	0.44	2.42	15	1
1:B:314:LYS:H	1:B:314:LYS:HD3	0.44	1.72	15	1
1:B:361:ARG:CZ	1:B:361:ARG:CB	0.44	2.96	15	1
1:B:289:VAL:HG21	1:B:364:VAL:CG2	0.44	2.42	1	1
1:B:240:GLN:OE1	1:B:243:PHE:CB	0.44	2.62	3	1
1:A:39:GLU:OE2	1:A:39:GLU:HA	0.44	2.11	4	1
1:A:137:THR:HG23	1:A:138:VAL:N	0.44	2.28	4	1
1:B:233:ASN:OD1	1:B:233:ASN:O	0.44	2.34	4	1
1:A:64:GLU:HB3	1:A:71:LEU:CD2	0.44	2.37	15	2
1:A:121:GLU:HG3	1:A:124:ARG:HD2	0.44	1.89	7	1
1:B:333:ARG:C	1:B:335:LEU:N	0.44	2.70	7	3
1:A:26:GLY:HA3	1:A:99:SER:HA	0.44	1.88	8	1
1:A:45:THR:HG23	1:A:153:LYS:NZ	0.44	2.28	8	1
1:A:80:ASP:HB3	1:A:105:GLU:OE1	0.44	2.13	8	1
1:B:259:ASN:CG	1:B:260:ALA:H	0.44	2.15	8	1
1:A:63:ARG:HH11	1:A:63:ARG:CG	0.44	2.26	9	1
1:A:71:LEU:HB2	1:A:76:CYS:HB3	0.44	1.89	9	1
1:A:84:ILE:HB	1:A:112:PHE:CE1	0.44	2.47	9	1
1:A:44:LEU:CD1	1:A:62:ARG:CB	0.44	2.95	12	1
1:A:43:PHE:N	1:A:43:PHE:CD1	0.44	2.84	13	1
1:B:306:ILE:HG12	1:B:318:LEU:CD1	0.44	2.42	14	1
1:A:89:VAL:CG1	1:A:91:VAL:HG23	0.44	2.43	15	1
1:A:117:VAL:CG2	1:A:142:GLU:HB2	0.44	2.41	15	1
1:A:89:VAL:HG21	1:A:164:VAL:CG2	0.44	2.43	1	2
1:A:108:TRP:CD1	1:A:112:PHE:HE1	0.44	2.31	1	1
1:A:35:MET:SD	1:A:39:GLU:HB3	0.44	2.52	3	1
1:B:229:ASN:HB3	1:B:232:THR:HB	0.44	1.89	4	1
1:B:299:SER:O	1:B:303:HIS:ND1	0.44	2.51	15	2
1:B:353:LYS:HD3	1:B:354:PRO:HD3	0.44	1.88	5	1
1:B:219:PHE:CD1	1:B:290:PHE:CD1	0.44	3.06	9	1
1:B:353:LYS:HD2	1:B:354:PRO:HD3	0.44	1.88	9	1
1:A:147:LYS:N	1:A:147:LYS:CD	0.44	2.79	10	1
1:A:63:ARG:O	1:A:64:GLU:C	0.44	2.56	11	1
1:B:271:LEU:O	1:B:272:THR:C	0.44	2.54	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:THR:OG1	1:A:75:GLU:HG3	0.44	2.13	14	1
1:B:282:LEU:HD22	1:B:282:LEU:N	0.44	2.27	1	1
1:A:49:HIS:CE1	1:A:50:PHE:CD2	0.44	3.05	2	1
1:B:303:HIS:N	1:B:306:ILE:CD1	0.44	2.81	2	1
1:B:317:VAL:CG2	1:B:363:VAL:HG11	0.44	2.43	14	2
1:A:151:LEU:HD23	1:A:151:LEU:O	0.44	2.13	4	1
1:B:218:VAL:HB	1:B:250:PHE:CE1	0.44	2.48	5	1
1:B:310:SER:OG	1:B:335:LEU:HD11	0.44	2.13	5	1
1:B:235:MET:CB	1:B:269:GLN:NE2	0.44	2.81	6	1
1:B:296:ILE:CD1	1:B:327:GLU:CB	0.44	2.96	6	1
1:B:284:ILE:HG21	1:B:308:TRP:C	0.44	2.32	7	1
1:A:16:ARG:O	1:A:16:ARG:HG3	0.44	2.11	9	1
1:A:84:ILE:HB	1:A:112:PHE:CZ	0.44	2.48	9	1
1:A:20:LEU:HD13	1:A:47:ILE:HG13	0.44	1.90	10	1
1:A:117:VAL:HG21	1:A:160:ILE:HA	0.44	1.90	13	1
1:B:259:ASN:CA	1:B:283:GLU:CD	0.44	2.85	13	1
1:A:28:VAL:CG2	1:A:32:THR:HB	0.44	2.43	14	1
1:A:37:SER:O	1:A:41:LEU:CD1	0.44	2.60	14	1
1:B:225:MET:CE	1:B:226:GLY:H	0.44	2.22	15	1
1:B:264:GLU:CD	1:B:271:LEU:CD1	0.44	2.75	15	1
1:A:108:TRP:CD1	1:A:112:PHE:CE1	0.44	3.06	1	1
1:B:284:ILE:CG2	1:B:312:PHE:CD2	0.44	2.98	1	1
1:B:308:TRP:CD1	1:B:312:PHE:CE1	0.44	3.06	1	1
1:B:324:ARG:C	1:B:326:GLU:N	0.44	2.69	6	2
1:B:217:SER:HB3	1:B:258:PHE:HD2	0.44	1.69	2	1
1:A:41:LEU:O	1:A:44:LEU:CB	0.44	2.66	4	1
1:B:250:PHE:CE1	1:B:255:LEU:HD12	0.44	2.47	4	1
1:A:59:ASN:HD21	1:A:80:ASP:CG	0.44	2.16	5	1
1:A:88:ASP:OD2	1:A:88:ASP:N	0.44	2.51	5	1
1:A:131:LEU:HG	1:B:304:VAL:CG2	0.44	2.42	6	1
1:A:25:MET:HE2	1:B:330:PHE:CE2	0.44	2.48	7	1
1:A:30:PRO:HG3	1:B:298:PRO:HD2	0.44	1.86	8	1
1:B:235:MET:SD	1:B:239:GLU:CG	0.44	3.06	8	1
1:A:130:PHE:O	1:B:273:PRO:HG3	0.44	2.13	9	1
1:B:225:MET:O	1:B:230:PRO:HD3	0.44	2.13	10	1
1:B:225:MET:CE	1:B:301:GLY:H	0.44	2.23	10	2
1:B:220:LEU:HG	1:B:291:VAL:HG12	0.44	1.89	11	1
1:B:229:ASN:CB	1:B:233:ASN:OD1	0.44	2.65	11	1
1:B:268:ALA:N	1:B:269:GLN:OE1	0.44	2.51	11	1
1:A:136:GLY:N	1:A:141:VAL:HB	0.44	2.27	12	1
1:B:324:ARG:N	1:B:324:ARG:HD3	0.44	2.27	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:SER:N	1:A:128:TYR:CE1	0.44	2.86	14	1
1:A:19:PHE:CE2	1:A:59:ASN:OD1	0.44	2.71	15	1
1:A:150:ALA:O	1:A:154:PRO:HG3	0.44	2.12	15	1
1:B:296:ILE:N	1:B:324:ARG:HD2	0.44	2.28	1	1
1:B:240:GLN:CD	1:B:241:LEU:HD13	0.44	2.32	2	1
1:B:338:VAL:CG2	1:B:339:ALA:H	0.44	2.26	3	1
1:A:18:VAL:HB	1:A:50:PHE:CE1	0.44	2.48	5	1
1:A:130:PHE:HE2	1:B:224:PHE:CG	0.44	2.30	5	1
1:B:219:PHE:CE2	1:B:259:ASN:HB3	0.44	2.47	5	1
1:A:133:ARG:CG	1:A:133:ARG:HH11	0.44	2.26	6	1
1:B:333:ARG:CG	1:B:333:ARG:NH1	0.44	2.80	6	1
1:A:148:ASP:O	1:A:150:ALA:N	0.44	2.50	11	1
1:A:63:ARG:HA	1:A:63:ARG:CZ	0.44	2.43	12	1
1:B:296:ILE:HG13	1:B:297:PRO:CA	0.44	2.39	12	2
1:B:225:MET:C	1:B:228:VAL:O	0.44	2.51	14	1
1:A:49:HIS:NE2	1:A:53:GLN:HG3	0.43	2.28	1	1
1:B:348:ASP:O	1:B:349:ILE:C	0.43	2.56	1	1
1:A:64:GLU:C	1:A:66:TRP:N	0.43	2.70	8	3
1:A:146:TYR:CD1	1:A:146:TYR:C	0.43	2.89	2	1
1:A:59:ASN:CG	1:A:60:ALA:N	0.43	2.71	8	4
1:A:61:HIS:O	1:A:64:GLU:CA	0.43	2.66	4	1
1:A:85:ARG:HD3	1:A:112:PHE:CZ	0.43	2.48	5	2
1:A:77:THR:HG22	1:A:78:PRO:CD	0.43	2.42	14	2
1:A:122:GLU:OE2	1:A:145:HIS:CD2	0.43	2.71	5	1
1:A:125:GLU:HG2	1:A:145:HIS:HE2	0.43	1.72	5	1
1:A:161:ARG:O	1:A:161:ARG:HG3	0.43	2.11	5	1
1:B:322:GLU:OE2	1:B:345:HIS:CD2	0.43	2.71	5	1
1:A:96:ILE:CD1	1:A:128:TYR:CG	0.43	3.01	7	1
1:A:23:PRO:HD2	1:A:27:LEU:HD13	0.43	1.89	9	1
1:B:216:ARG:NH1	1:B:216:ARG:HG2	0.43	2.28	9	1
1:B:222:GLY:H	1:B:261:HIS:CE1	0.43	2.26	9	1
1:A:25:MET:O	1:A:30:PRO:HD3	0.43	2.13	10	1
1:A:39:GLU:N	1:A:39:GLU:CD	0.43	2.66	10	1
1:B:296:ILE:HB	1:B:324:ARG:HG2	0.43	1.89	11	1
1:B:225:MET:C	1:B:225:MET:SD	0.43	2.95	13	1
1:A:166:ARG:O	1:A:166:ARG:HG2	0.43	2.12	14	1
1:B:342:GLU:OE2	1:B:362:LYS:HE2	0.43	2.13	14	1
1:B:264:GLU:HG2	1:B:268:ALA:O	0.43	2.14	15	1
1:A:25:MET:H	1:B:330:PHE:HE1	0.43	1.56	1	2
1:A:69:GLN:O	1:A:71:LEU:HD23	0.43	2.14	2	1
1:A:24:PHE:CE2	1:A:76:CYS:SG	0.43	3.11	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:CD1	1:A:83:GLU:C	0.43	2.92	5	1
1:A:25:MET:HB2	1:B:330:PHE:CG	0.43	2.49	5	1
1:A:25:MET:HE2	1:A:25:MET:CA	0.43	2.43	15	2
1:A:125:GLU:CG	1:A:145:HIS:HE2	0.43	2.26	5	1
1:A:130:PHE:HA	1:B:273:PRO:HG3	0.43	1.90	5	1
1:B:231:GLU:O	1:B:231:GLU:CD	0.43	2.56	5	1
1:A:81:GLN:HG3	1:A:112:PHE:CZ	0.43	2.48	6	1
1:B:235:MET:SD	1:B:269:GLN:CD	0.43	2.96	6	1
1:B:325:GLU:OE1	1:B:325:GLU:C	0.43	2.56	6	1
1:A:98:PRO:HD2	1:B:230:PRO:HG3	0.43	1.89	8	1
1:A:153:LYS:O	1:A:156:ILE:HG23	0.43	2.13	9	1
1:A:40:GLN:N	1:A:66:TRP:CH2	0.43	2.86	13	1
1:B:287:ALA:O	1:B:314:LYS:CD	0.43	2.66	13	1
1:B:314:LYS:O	1:B:315:PRO:C	0.43	2.57	13	1
1:B:340:ALA:HB3	1:B:367:VAL:CG2	0.43	2.42	14	1
1:B:324:ARG:HG2	1:B:324:ARG:NH1	0.43	2.27	15	1
1:A:85:ARG:CB	1:A:112:PHE:HE2	0.43	2.26	1	2
1:A:104:VAL:HG21	1:B:331:LEU:HG	0.43	1.90	3	2
1:B:296:ILE:HB	1:B:324:ARG:HD3	0.43	1.90	3	2
1:A:22:GLY:C	1:A:24:PHE:N	0.43	2.71	4	2
1:A:17:SER:HB3	1:A:56:GLU:CB	0.43	2.43	5	1
1:B:324:ARG:C	1:B:328:TYR:CE2	0.43	2.92	5	1
1:B:235:MET:SD	1:B:269:GLN:NE2	0.43	2.91	6	2
1:A:142:GLU:OE1	1:A:163:VAL:HB	0.43	2.13	8	1
1:B:264:GLU:CB	1:B:271:LEU:CD2	0.43	2.96	8	1
1:A:108:TRP:O	1:A:112:PHE:HD2	0.43	1.93	9	1
1:B:229:ASN:O	1:B:232:THR:N	0.43	2.52	10	3
1:B:334:GLY:HA2	1:B:337:THR:HG22	0.43	1.90	10	1
1:A:33:ASN:OD1	1:A:33:ASN:N	0.43	2.51	12	1
1:A:137:THR:HG21	1:B:274:GLU:OE1	0.43	2.12	12	1
1:A:135:LEU:O	1:A:137:THR:N	0.43	2.51	15	1
1:B:355:GLN:O	1:B:355:GLN:HG3	0.43	2.13	15	1
1:A:24:PHE:HE2	1:A:70:VAL:CA	0.43	2.27	6	2
1:A:140:ALA:HB2	1:A:167:VAL:HG22	0.43	1.90	2	1
1:B:296:ILE:HD13	1:B:324:ARG:C	0.43	2.33	4	1
1:A:18:VAL:HG23	1:A:55:LEU:HB3	0.43	1.90	5	1
1:A:98:PRO:CB	1:A:103:HIS:CE1	0.43	3.00	5	2
1:B:218:VAL:CB	1:B:250:PHE:CE1	0.43	3.01	5	1
1:A:120:LEU:CD1	1:A:145:HIS:HE2	0.43	2.24	7	1
1:A:140:ALA:HB1	1:A:163:VAL:HG22	0.43	1.89	8	1
1:B:342:GLU:HG2	1:B:359:ALA:CB	0.43	2.42	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:240:GLN:HG2	1:B:241:LEU:N	0.43	2.28	9	1
1:A:19:PHE:CE1	1:A:90:PHE:HE2	0.43	2.28	10	1
1:B:259:ASN:O	1:B:260:ALA:HB3	0.43	2.13	11	1
1:B:348:ASP:C	1:B:350:ALA:N	0.43	2.71	11	1
1:A:118:LEU:CD1	1:A:132:VAL:HG13	0.43	2.43	12	1
1:B:296:ILE:HG13	1:B:298:PRO:CD	0.43	2.42	12	2
1:B:219:PHE:CD1	1:B:290:PHE:CD2	0.43	3.06	13	1
1:B:224:PHE:CE1	1:B:261:HIS:HD2	0.43	2.30	14	1
1:A:73:PRO:HD3	1:B:330:PHE:HD1	0.43	1.73	15	1
1:B:303:HIS:HA	1:B:306:ILE:HB	0.43	1.89	9	2
1:B:225:MET:HE3	1:B:300:PRO:HG2	0.43	1.91	4	1
1:B:331:LEU:CD2	1:B:335:LEU:CD1	0.43	2.86	4	1
1:B:218:VAL:CG1	1:B:291:VAL:CB	0.43	2.91	5	1
1:B:295:GLY:CA	1:B:321:GLU:OE1	0.43	2.66	5	1
1:A:94:PRO:CB	1:A:121:GLU:OE2	0.43	2.66	7	1
1:B:325:GLU:CG	1:B:345:HIS:NE2	0.43	2.81	8	1
1:A:53:GLN:HG2	1:A:55:LEU:HD11	0.43	1.90	10	1
1:B:244:LEU:CD2	1:B:244:LEU:N	0.43	2.77	11	1
1:B:264:GLU:CA	1:B:269:GLN:HG3	0.43	2.43	11	1
1:B:353:LYS:HG2	1:B:353:LYS:H	0.43	1.33	12	1
1:A:59:ASN:CA	1:A:83:GLU:CD	0.43	2.87	13	1
1:B:223:PRO:CB	1:B:299:SER:HB2	0.43	2.43	15	1
1:A:35:MET:CB	1:A:69:GLN:NE2	0.43	2.81	6	1
1:B:333:ARG:NH1	1:B:333:ARG:HG2	0.43	2.28	6	1
1:A:108:TRP:CE2	1:B:310:SER:CB	0.43	3.01	9	1
1:A:99:SER:OG	1:A:99:SER:O	0.43	2.28	10	1
1:A:103:HIS:NE2	1:A:128:TYR:CD1	0.43	2.85	10	1
1:B:282:LEU:C	1:B:286:LYS:HE2	0.43	2.34	10	1
1:B:244:LEU:CD1	1:B:262:ARG:CB	0.43	2.96	12	1
1:A:28:VAL:CB	1:A:33:ASN:CB	0.43	2.97	13	1
1:A:114:LYS:O	1:A:115:PRO:C	0.43	2.57	13	1
1:B:215:VAL:CG2	1:B:360:ILE:HG21	0.43	2.44	13	1
1:B:342:GLU:OE1	1:B:362:LYS:HE2	0.43	2.13	14	1
1:B:322:GLU:HA	1:B:345:HIS:CE1	0.43	2.49	15	1
1:A:148:ASP:O	1:A:149:ILE:C	0.43	2.57	1	2
1:B:217:SER:CB	1:B:258:PHE:CE2	0.43	3.01	2	1
1:B:261:HIS:O	1:B:264:GLU:OE2	0.43	2.36	2	1
1:A:110:SER:HB2	1:A:135:LEU:HD21	0.43	1.91	3	1
1:A:64:GLU:HB3	1:A:71:LEU:HD22	0.43	1.89	4	1
1:A:109:ALA:CA	1:A:112:PHE:HB2	0.43	2.44	10	2
1:B:293:ILE:CD1	1:B:319:LEU:HB2	0.43	2.43	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:VAL:CB	1:A:50:PHE:CE1	0.43	3.02	5	1
1:A:156:ILE:CG2	1:A:157:ASP:N	0.43	2.82	7	2
1:B:235:MET:HB2	1:B:269:GLN:CG	0.43	2.43	6	1
1:B:241:LEU:O	1:B:242:PRO:C	0.43	2.56	11	3
1:A:40:GLN:CD	1:A:66:TRP:CD1	0.43	2.92	10	2
1:A:92:ALA:CB	1:A:118:LEU:CD2	0.43	2.81	7	1
1:A:94:PRO:HG2	1:A:121:GLU:OE2	0.43	2.13	7	1
1:B:281:GLN:HG3	1:B:312:PHE:HZ	0.43	1.72	11	2
1:B:284:ILE:HB	1:B:312:PHE:CZ	0.43	2.49	9	1
1:A:104:VAL:CA	1:B:304:VAL:HA	0.43	2.29	10	1
1:B:264:GLU:N	1:B:264:GLU:OE2	0.43	2.51	10	1
1:A:24:PHE:HE1	1:A:61:HIS:CE1	0.43	2.30	11	1
1:A:71:LEU:HD13	1:A:75:GLU:OE2	0.43	2.13	11	1
1:A:77:THR:HB	1:B:334:GLY:HA3	0.43	1.91	11	2
1:B:319:LEU:HD23	1:B:344:VAL:HG12	0.43	1.88	11	1
1:A:28:VAL:CB	1:A:33:ASN:HB2	0.43	2.42	13	1
1:A:47:ILE:CG1	1:A:57:VAL:HG21	0.43	2.44	13	1
1:A:155:GLN:HA	1:A:155:GLN:HE21	0.43	1.71	13	1
1:B:219:PHE:CB	1:B:287:ALA:HB1	0.43	2.44	13	1
1:A:20:LEU:HA	1:A:20:LEU:HD23	0.43	1.57	14	1
1:B:324:ARG:O	1:B:326:GLU:N	0.43	2.52	1	2
1:A:98:PRO:HB2	1:B:300:PRO:CB	0.43	2.44	2	1
1:A:21:ALA:CB	1:A:59:ASN:ND2	0.43	2.75	3	1
1:A:113:ASP:OD1	1:A:113:ASP:O	0.43	2.37	3	1
1:A:35:MET:HB2	1:A:69:GLN:HG3	0.43	1.88	5	1
1:B:325:GLU:CG	1:B:345:HIS:HE2	0.43	2.26	5	1
1:A:133:ARG:NH1	1:A:133:ARG:HG2	0.43	2.28	6	1
1:B:356:ILE:CG2	1:B:357:ASP:N	0.43	2.82	7	2
1:A:153:LYS:HD2	1:A:154:PRO:HD3	0.43	1.90	9	1
1:B:263:ARG:HD3	1:B:263:ARG:H	0.43	1.73	10	1
1:A:22:GLY:C	1:A:102:THR:HG1	0.43	2.18	15	2
1:A:155:GLN:NE2	1:A:155:GLN:N	0.43	2.66	11	1
1:B:244:LEU:CD2	1:B:244:LEU:H	0.43	2.18	12	1
1:A:122:GLU:C	1:A:125:GLU:OE1	0.43	2.57	13	1
1:A:157:ASP:OD1	1:A:161:ARG:NH1	0.43	2.52	14	1
1:B:240:GLN:HE21	1:B:266:TRP:HE1	0.43	1.56	14	1
1:A:37:SER:HA	1:A:40:GLN:CD	0.43	2.34	15	1
1:B:295:GLY:C	1:B:328:TYR:HH	0.43	2.15	15	1
1:B:298:PRO:CA	1:B:328:TYR:CE2	0.43	2.96	15	1
1:A:82:LEU:HD22	1:A:82:LEU:N	0.43	2.29	1	1
1:B:218:VAL:HG13	1:B:291:VAL:CB	0.43	2.40	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:308:TRP:CD1	1:B:312:PHE:HE1	0.43	2.32	1	1
1:B:218:VAL:CG1	1:B:250:PHE:CZ	0.43	2.81	2	1
1:B:285:ARG:CB	1:B:312:PHE:CG	0.43	3.02	3	1
1:A:75:GLU:O	1:A:79:LEU:HB3	0.43	2.13	4	1
1:B:296:ILE:HG22	1:B:324:ARG:NE	0.43	2.29	6	1
1:A:31:GLU:OE2	1:A:31:GLU:HA	0.43	2.14	8	1
1:A:49:HIS:NE2	1:A:50:PHE:CZ	0.43	2.86	8	1
1:B:245:THR:CG2	1:B:353:LYS:NZ	0.43	2.82	8	1
1:B:347:LYS:O	1:B:347:LYS:HD2	0.43	2.13	8	1
1:A:61:HIS:CD2	1:A:69:GLN:NE2	0.43	2.87	9	1
1:B:246:LEU:C	1:B:248:GLU:H	0.43	2.17	10	1
1:B:324:ARG:HG3	1:B:324:ARG:HH11	0.43	1.74	10	1
1:A:41:LEU:HD12	1:A:44:LEU:HD11	0.43	1.89	11	1
1:A:39:GLU:CG	1:A:66:TRP:CZ3	0.43	3.02	12	1
1:B:331:LEU:CD1	1:B:335:LEU:HD12	0.43	2.44	3	2
1:A:78:PRO:C	1:A:82:LEU:HD22	0.43	2.34	4	1
1:A:80:ASP:C	1:A:84:ILE:HG13	0.43	2.30	4	1
1:A:84:ILE:CG2	1:A:112:PHE:CE1	0.43	3.02	5	1
1:A:149:ILE:HD13	1:A:149:ILE:HA	0.43	1.65	14	4
1:B:321:GLU:C	1:B:323:GLY:H	0.43	2.15	5	1
1:A:17:SER:OG	1:A:88:ASP:HB2	0.43	2.14	6	1
1:A:104:VAL:CG2	1:B:331:LEU:HG	0.43	2.44	6	1
1:A:28:VAL:CG2	1:A:33:ASN:N	0.43	2.80	8	1
1:A:37:SER:C	1:A:39:GLU:H	0.43	2.17	8	1
1:B:262:ARG:HB3	1:B:262:ARG:CZ	0.43	2.44	9	1
1:A:114:LYS:HZ3	1:A:114:LYS:CA	0.43	2.26	11	1
1:B:228:VAL:CG2	1:B:232:THR:HB	0.43	2.44	14	1
1:B:229:ASN:HB3	1:B:232:THR:HG1	0.43	1.74	14	1
1:B:302:THR:HG22	1:B:306:ILE:CD1	0.43	2.44	14	1
1:A:81:GLN:C	1:A:81:GLN:NE2	0.43	2.72	15	1
1:B:261:HIS:CD2	1:B:271:LEU:HD11	0.42	2.48	1	1
1:A:19:PHE:HD2	1:A:83:GLU:HB3	0.42	1.73	2	2
1:A:107:GLY:HA2	1:B:308:TRP:NE1	0.42	2.27	12	2
1:B:335:LEU:C	1:B:337:THR:N	0.42	2.72	4	2
1:A:71:LEU:O	1:B:330:PHE:CZ	0.42	2.71	5	1
1:A:71:LEU:N	1:A:71:LEU:CD2	0.42	2.74	5	1
1:B:217:SER:OG	1:B:288:ASP:HB2	0.42	2.14	6	1
1:A:24:PHE:O	1:A:28:VAL:HG12	0.42	2.14	10	1
1:A:146:TYR:CD2	1:A:146:TYR:C	0.42	2.91	13	1
1:B:348:ASP:O	1:B:351:LEU:HB2	0.42	2.14	13	1
1:B:256:GLU:HB3	1:B:258:PHE:CE1	0.42	2.49	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:PRO:CB	1:A:99:SER:HB2	0.42	2.43	15	1
1:B:296:ILE:N	1:B:328:TYR:HH	0.42	2.08	15	1
1:B:319:LEU:CD2	1:B:344:VAL:HG11	0.42	2.44	15	1
1:A:25:MET:HE3	1:B:330:PHE:CD1	0.42	2.49	1	1
1:A:40:GLN:CD	1:A:41:LEU:HD13	0.42	2.34	2	1
1:B:249:HIS:CE1	1:B:250:PHE:CD2	0.42	3.06	2	1
1:A:128:TYR:CB	1:A:132:VAL:HB	0.42	2.43	3	2
1:B:342:GLU:OE2	1:B:362:LYS:HD2	0.42	2.14	3	1
1:A:44:LEU:CD1	1:A:66:TRP:CH2	0.42	3.00	6	1
1:A:46:LEU:HD11	1:A:153:LYS:N	0.42	2.28	6	1
1:A:104:VAL:HB	1:B:331:LEU:HG	0.42	1.91	6	1
1:A:31:GLU:O	1:A:31:GLU:HG3	0.42	2.14	7	1
1:A:35:MET:HB2	1:A:69:GLN:OE1	0.42	2.11	8	1
1:A:73:PRO:C	1:A:75:GLU:N	0.42	2.72	8	3
1:A:35:MET:HG3	1:A:36:PRO:HD2	0.42	1.90	9	1
1:B:274:GLU:O	1:B:275:GLU:CD	0.42	2.57	9	1
1:A:108:TRP:C	1:A:110:SER:N	0.42	2.73	10	1
1:A:148:ASP:O	1:A:151:LEU:HB2	0.42	2.14	13	1
1:B:229:ASN:CG	1:B:232:THR:O	0.42	2.57	13	1
1:B:246:LEU:HD13	1:B:349:ILE:HD12	0.42	1.90	14	1
1:A:111:ALA:C	1:B:312:PHE:CD2	0.42	2.93	2	1
1:B:223:PRO:O	1:B:225:MET:HE2	0.42	2.14	2	1
1:B:346:TYR:C	1:B:347:LYS:CG	0.42	2.87	3	1
1:B:233:ASN:OD1	1:B:233:ASN:C	0.42	2.57	4	1
1:B:288:ASP:OD2	1:B:288:ASP:N	0.42	2.52	5	1
1:B:355:GLN:OE1	1:B:355:GLN:O	0.42	2.38	6	1
1:A:120:LEU:CD1	1:A:145:HIS:CD2	0.42	2.97	7	1
1:B:317:VAL:HG13	1:B:342:GLU:HB3	0.42	1.91	8	1
1:A:35:MET:SD	1:A:65:ALA:CA	0.42	3.07	11	1
1:B:224:PHE:HE1	1:B:261:HIS:CE1	0.42	2.32	11	1
1:A:162:LYS:CG	1:A:163:VAL:N	0.42	2.79	12	1
1:A:39:GLU:OE2	1:A:43:PHE:HZ	0.42	1.96	13	1
1:B:228:VAL:CB	1:B:233:ASN:HB2	0.42	2.44	13	1
1:A:61:HIS:HD2	1:A:65:ALA:CB	0.42	2.24	2	1
1:A:84:ILE:HG23	1:A:90:PHE:CE2	0.42	2.50	2	1
1:B:309:ALA:CA	1:B:312:PHE:HB2	0.42	2.45	4	2
1:B:341:VAL:HG11	1:B:343:PHE:CE2	0.42	2.49	4	3
1:A:84:ILE:HG22	1:A:109:ALA:HA	0.42	1.89	7	1
1:A:96:ILE:HG13	1:A:97:PRO:CA	0.42	2.44	7	1
1:A:35:MET:HE3	1:A:40:GLN:OE1	0.42	2.15	8	1
1:B:273:PRO:C	1:B:275:GLU:N	0.42	2.72	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:284:ILE:HG21	1:B:309:ALA:N	0.42	2.28	15	2
1:B:344:VAL:HG21	1:B:356:ILE:HG13	0.42	1.91	8	1
1:B:236:PRO:HB2	1:B:240:GLN:CB	0.42	2.45	10	1
1:B:227:LEU:HB2	1:B:236:PRO:HD2	0.42	1.91	11	1
1:B:243:PHE:HZ	1:B:293:ILE:HB	0.42	1.72	12	1
1:A:98:PRO:O	1:A:100:PRO:HD3	0.42	2.15	13	1
1:A:107:GLY:C	1:A:110:SER:OG	0.42	2.57	15	2
1:B:348:ASP:OD1	1:B:348:ASP:C	0.42	2.57	14	1
1:A:19:PHE:HZ	1:A:105:GLU:OE1	0.42	1.94	4	2
1:A:103:HIS:N	1:A:106:ILE:CD1	0.42	2.82	2	1
1:B:249:HIS:ND1	1:B:249:HIS:C	0.42	2.70	8	3
1:B:249:HIS:HE1	1:B:250:PHE:CG	0.42	2.29	2	1
1:A:96:ILE:HB	1:A:124:ARG:HD2	0.42	1.91	4	1
1:A:103:HIS:O	1:A:104:VAL:C	0.42	2.55	5	3
1:A:20:LEU:HD11	1:A:43:PHE:CE2	0.42	2.50	6	1
1:A:85:ARG:CB	1:A:114:LYS:HE2	0.42	2.44	6	1
1:A:152:ALA:O	1:A:155:GLN:N	0.42	2.53	6	1
1:A:20:LEU:HD11	1:A:50:PHE:CE1	0.42	2.50	7	1
1:A:33:ASN:ND2	1:A:34:SER:H	0.42	2.12	7	2
1:A:165:ASP:HA	1:A:168:ASN:ND2	0.42	2.30	7	1
1:B:294:PRO:HG2	1:B:321:GLU:OE2	0.42	2.14	7	1
1:A:120:LEU:HB3	1:A:125:GLU:HB3	0.42	1.91	8	1
1:B:295:GLY:N	1:B:328:TYR:CZ	0.42	2.81	8	2
1:B:340:ALA:HB1	1:B:363:VAL:HG22	0.42	1.90	8	1
1:B:308:TRP:O	1:B:312:PHE:HD2	0.42	1.95	9	1
1:A:41:LEU:O	1:A:42:PRO:C	0.42	2.56	11	2
1:A:40:GLN:NE2	1:A:66:TRP:HB2	0.42	2.30	12	1
1:A:93:ILE:CD1	1:A:119:LEU:HB2	0.42	2.44	13	1
1:A:25:MET:HB3	1:B:330:PHE:HD2	0.42	1.68	15	1
1:A:90:PHE:CG	1:A:109:ALA:HB2	0.42	2.49	15	1
1:B:349:ILE:HD13	1:B:349:ILE:HA	0.42	1.62	4	3
1:B:229:ASN:HB2	1:B:233:ASN:HB2	0.42	1.90	3	1
1:A:19:PHE:CE1	1:A:105:GLU:OE1	0.42	2.73	4	1
1:A:161:ARG:O	1:A:165:ASP:HB3	0.42	2.13	4	1
1:B:221:ALA:HB2	1:B:305:GLU:OE1	0.42	2.14	4	1
1:A:130:PHE:HE2	1:B:224:PHE:CD2	0.42	2.33	5	1
1:A:119:LEU:HD23	1:A:144:VAL:HG12	0.42	1.91	11	2
1:A:131:LEU:HG	1:B:304:VAL:HG21	0.42	1.89	6	1
1:B:333:ARG:CG	1:B:333:ARG:HH11	0.42	2.26	6	1
1:B:320:LEU:HA	1:B:325:GLU:HB3	0.42	1.92	7	1
1:B:342:GLU:HG2	1:B:359:ALA:O	0.42	2.15	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:VAL:CB	1:A:33:ASN:HB3	0.42	2.44	8	1
1:B:297:PRO:CB	1:B:298:PRO:HD2	0.42	2.44	8	1
1:A:46:LEU:C	1:A:48:GLU:H	0.42	2.18	10	1
1:A:134:GLY:HA3	1:B:277:THR:HB	0.42	1.91	11	1
1:A:40:GLN:HB3	1:A:66:TRP:CD2	0.42	2.37	12	1
1:B:289:VAL:HG21	1:B:360:ILE:HG23	0.42	1.91	13	1
1:A:72:THR:O	1:A:73:PRO:C	0.42	2.56	14	1
1:B:217:SER:HB3	1:B:258:PHE:HE2	0.42	1.74	15	1
1:B:289:VAL:CG1	1:B:291:VAL:HG23	0.42	2.44	15	1
1:A:17:SER:CB	1:A:58:PHE:CE2	0.42	3.03	2	1
1:A:20:LEU:CD1	1:A:50:PHE:HE2	0.42	2.24	2	1
1:A:85:ARG:CB	1:A:112:PHE:CG	0.42	3.02	3	1
1:A:105:GLU:HA	1:A:108:TRP:HB2	0.42	1.92	3	1
1:B:223:PRO:C	1:B:224:PHE:O	0.42	2.57	3	1
1:B:235:MET:SD	1:B:239:GLU:OE2	0.42	2.78	3	1
1:A:85:ARG:CB	1:A:114:LYS:NZ	0.42	2.83	4	1
1:A:124:ARG:O	1:A:127:GLU:HB2	0.42	2.14	14	3
1:A:124:ARG:CB	1:A:128:TYR:HE2	0.42	2.28	6	2
1:B:295:GLY:CA	1:B:324:ARG:HD3	0.42	2.45	5	1
1:B:296:ILE:HD13	1:B:327:GLU:CB	0.42	2.44	6	1
1:A:61:HIS:O	1:A:63:ARG:N	0.42	2.51	8	1
1:B:265:ALA:HA	1:B:269:GLN:HB2	0.42	1.91	9	2
1:A:36:PRO:HB2	1:A:40:GLN:CB	0.42	2.44	10	1
1:A:134:GLY:HA2	1:A:137:THR:HG22	0.42	1.92	10	1
1:A:43:PHE:HD1	1:A:66:TRP:HH2	0.42	1.58	12	1
1:A:15:VAL:CG2	1:A:160:ILE:HG21	0.42	2.44	13	1
1:B:329:GLY:CA	1:B:333:ARG:HD3	0.42	2.45	13	1
1:B:272:THR:OG1	1:B:275:GLU:HG3	0.42	2.15	14	1
1:A:79:LEU:CG	1:A:80:ASP:N	0.42	2.82	15	1
1:B:238:ALA:O	1:B:242:PRO:HD3	0.42	2.13	15	1
1:B:279:LEU:CG	1:B:280:ASP:N	0.42	2.82	15	1
1:A:21:ALA:CB	1:A:59:ASN:OD1	0.42	2.66	1	1
1:A:46:LEU:CD1	1:A:47:ILE:HD12	0.42	2.38	1	1
1:B:320:LEU:O	1:B:346:TYR:CB	0.42	2.67	3	2
1:B:281:GLN:HB3	1:B:308:TRP:CE2	0.42	2.48	4	1
1:B:337:THR:HG23	1:B:338:VAL:N	0.42	2.30	4	1
1:B:225:MET:O	1:B:228:VAL:CA	0.42	2.68	5	1
1:A:69:GLN:OE1	1:A:70:VAL:N	0.42	2.53	7	1
1:B:320:LEU:CD1	1:B:345:HIS:CD2	0.42	3.00	7	1
1:A:29:ASN:O	1:A:32:THR:N	0.42	2.53	10	3
1:A:106:ILE:HG21	1:A:135:LEU:CG	0.42	2.45	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:291:VAL:CG2	1:B:360:ILE:HD11	0.42	2.45	10	1
1:B:292:ALA:O	1:B:318:LEU:CA	0.42	2.68	11	1
1:A:108:TRP:HE1	1:B:307:GLY:HA2	0.42	1.75	12	1
1:B:217:SER:CB	1:B:256:GLU:HB3	0.42	2.45	12	1
1:B:218:VAL:HG21	1:B:250:PHE:HE1	0.42	1.67	12	1
1:A:122:GLU:OE1	1:A:147:LYS:HE3	0.42	2.15	14	1
1:A:31:GLU:OE2	1:B:330:PHE:CD1	0.42	2.73	3	1
1:A:96:ILE:CD1	1:A:127:GLU:CB	0.42	2.98	6	2
1:B:227:LEU:CD1	1:B:239:GLU:OE2	0.42	2.68	3	1
1:B:361:ARG:O	1:B:365:ASP:HB3	0.42	2.14	4	1
1:A:35:MET:H	1:A:69:GLN:CG	0.42	2.27	5	1
1:B:217:SER:HB3	1:B:256:GLU:CB	0.42	2.44	5	1
1:B:361:ARG:O	1:B:361:ARG:HG3	0.42	2.13	5	1
1:A:65:ALA:HB1	1:A:69:GLN:HE22	0.42	1.75	6	1
1:B:282:LEU:O	1:B:285:ARG:CG	0.42	2.67	6	1
1:A:135:LEU:N	1:B:277:THR:HG21	0.42	2.22	8	1
1:B:228:VAL:O	1:B:230:PRO:CD	0.42	2.68	9	1
1:B:321:GLU:OE1	1:B:321:GLU:CA	0.42	2.66	9	1
1:A:34:SER:OG	1:A:36:PRO:HD2	0.42	2.12	10	1
1:A:123:GLY:C	1:A:125:GLU:OE1	0.42	2.58	11	1
1:A:21:ALA:O	1:A:93:ILE:HB	0.42	2.15	13	1
1:A:81:GLN:CA	1:A:84:ILE:CG1	0.42	2.90	13	1
1:A:83:GLU:O	1:A:87:ALA:CB	0.42	2.68	13	1
1:A:155:GLN:NE2	1:A:155:GLN:O	0.42	2.50	13	1
1:A:43:PHE:CE2	1:A:93:ILE:HD12	0.42	2.50	1	1
1:A:18:VAL:HG13	1:A:91:VAL:CG2	0.42	2.45	2	2
1:A:81:GLN:NE2	1:A:85:ARG:HH11	0.42	2.12	2	1
1:B:219:PHE:HE2	1:B:259:ASN:ND2	0.42	2.12	2	1
1:B:225:MET:CE	1:B:225:MET:N	0.42	2.83	2	1
1:A:144:VAL:HG13	1:A:155:GLN:HG3	0.42	1.92	3	1
1:B:302:THR:HA	1:B:305:GLU:OE1	0.42	2.15	3	1
1:A:46:LEU:HD11	1:A:149:ILE:HG23	0.42	1.91	4	1
1:A:81:GLN:CG	1:A:108:TRP:CH2	0.42	3.02	4	1
1:A:81:GLN:HG2	1:A:108:TRP:CH2	0.42	2.50	14	2
1:A:121:GLU:HG2	1:A:124:ARG:HB2	0.42	1.90	7	1
1:A:34:SER:O	1:A:35:MET:O	0.42	2.38	9	1
1:A:135:LEU:CD2	1:A:141:VAL:HG21	0.42	2.45	9	1
1:B:246:LEU:HG	1:B:353:LYS:HG2	0.42	1.92	10	1
1:A:73:PRO:HG3	1:B:333:ARG:HE	0.42	1.75	11	1
1:A:122:GLU:OE2	1:A:147:LYS:HE2	0.42	2.15	12	1
1:A:129:GLY:CA	1:A:133:ARG:HB2	0.42	2.39	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:GLU:OE2	1:A:162:LYS:HE2	0.42	2.14	14	1
1:A:24:PHE:CD2	1:B:330:PHE:HZ	0.41	2.31	6	2
1:A:76:CYS:O	1:A:80:ASP:HB3	0.41	2.14	2	1
1:A:142:GLU:OE1	1:A:163:VAL:HG23	0.41	2.15	3	1
1:A:162:LYS:HD3	1:A:166:ARG:NH2	0.41	2.30	3	1
1:A:29:ASN:HB3	1:A:32:THR:HB	0.41	1.91	4	1
1:A:93:ILE:HD11	1:A:119:LEU:HD13	0.41	1.91	4	1
1:B:331:LEU:O	1:B:332:VAL:C	0.41	2.57	5	1
1:B:239:GLU:CG	1:B:240:GLN:N	0.41	2.82	8	1
1:B:316:ILE:CB	1:B:341:VAL:HG22	0.41	2.45	8	1
1:A:27:LEU:HB2	1:A:35:MET:HB3	0.41	1.90	10	1
1:A:35:MET:H	1:A:68:ALA:HA	0.41	1.71	11	1
1:A:71:LEU:N	1:A:71:LEU:HD23	0.41	2.30	11	1
1:A:96:ILE:CG1	1:A:127:GLU:HB3	0.41	2.45	11	1
1:A:19:PHE:CD1	1:A:58:PHE:O	0.41	2.73	12	1
1:A:43:PHE:HZ	1:A:93:ILE:HB	0.41	1.74	12	1
1:A:84:ILE:CD1	1:A:90:PHE:HE1	0.41	2.22	12	1
1:B:247:ILE:O	1:B:250:PHE:HB2	0.41	2.15	12	1
1:A:125:GLU:HG3	1:A:145:HIS:NE2	0.41	2.30	13	1
1:A:25:MET:HG2	1:A:26:GLY:N	0.41	2.30	2	1
1:A:120:LEU:CD1	1:A:125:GLU:CB	0.41	2.84	3	1
1:A:20:LEU:HD12	1:A:21:ALA:N	0.41	2.30	5	1
1:A:104:VAL:HG13	1:B:307:GLY:CA	0.41	2.39	6	2
1:A:131:LEU:O	1:A:132:VAL:C	0.41	2.58	5	1
1:B:298:PRO:CB	1:B:303:HIS:CE1	0.41	3.03	5	1
1:B:228:VAL:CB	1:B:233:ASN:HB3	0.41	2.45	8	1
1:B:235:MET:HE3	1:B:261:HIS:CD2	0.41	2.50	9	1
1:A:25:MET:HB3	1:A:30:PRO:HA	0.41	1.91	14	2
1:A:89:VAL:HG11	1:A:160:ILE:HG12	0.41	1.91	11	1
1:A:17:SER:CB	1:A:56:GLU:HB3	0.41	2.45	12	1
1:A:141:VAL:CG1	1:A:143:PHE:CE1	0.41	3.04	13	1
1:B:220:LEU:CD1	1:B:247:ILE:HD12	0.41	2.44	13	1
1:B:259:ASN:CA	1:B:283:GLU:OE1	0.41	2.66	13	1
1:A:16:ARG:HB2	1:A:88:ASP:OD1	0.41	2.15	14	1
1:A:45:THR:CG2	1:A:46:LEU:N	0.41	2.78	14	1
1:B:307:GLY:O	1:B:310:SER:CB	0.41	2.68	14	1
1:A:19:PHE:CD2	1:A:59:ASN:OD1	0.41	2.73	15	1
1:B:350:ALA:O	1:B:354:PRO:HG3	0.41	2.14	15	1
1:B:221:ALA:CB	1:B:259:ASN:OD1	0.41	2.67	1	1
1:A:119:LEU:HD22	1:A:146:TYR:CG	0.41	2.49	2	1
1:A:130:PHE:HD2	1:A:130:PHE:HA	0.41	1.59	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:219:PHE:CZ	1:B:259:ASN:ND2	0.41	2.88	3	1
1:B:304:VAL:O	1:B:308:TRP:CG	0.41	2.73	3	1
1:B:324:ARG:HA	1:B:327:GLU:OE1	0.41	2.15	3	1
1:B:241:LEU:O	1:B:244:LEU:CB	0.41	2.69	6	2
1:A:131:LEU:HG	1:B:304:VAL:HB	0.41	1.93	5	2
1:A:25:MET:CE	1:B:330:PHE:CG	0.41	3.04	6	1
1:A:130:PHE:HD2	1:B:225:MET:CG	0.41	2.28	8	1
1:A:61:HIS:O	1:A:66:TRP:CD1	0.41	2.73	9	1
1:B:261:HIS:CD2	1:B:269:GLN:NE2	0.41	2.89	9	1
1:B:263:ARG:O	1:B:263:ARG:NH1	0.41	2.53	9	1
1:A:82:LEU:C	1:A:86:LYS:HE2	0.41	2.34	10	1
1:B:227:LEU:HG	1:B:228:VAL:HG23	0.41	1.92	11	1
1:B:353:LYS:CG	1:B:354:PRO:HD3	0.41	2.45	11	1
1:A:43:PHE:HB3	1:A:44:LEU:HD23	0.41	1.92	12	1
1:B:346:TYR:CD2	1:B:346:TYR:C	0.41	2.94	13	1
1:A:74:GLU:N	1:A:74:GLU:OE2	0.41	2.53	15	1
1:B:225:MET:HG2	1:B:226:GLY:N	0.41	2.29	2	1
1:A:109:ALA:HB3	1:A:116:ILE:CG1	0.41	2.44	3	1
1:A:33:ASN:CG	1:A:33:ASN:O	0.41	2.58	4	1
1:A:38:ALA:C	1:A:42:PRO:CD	0.41	2.89	4	1
1:B:296:ILE:HB	1:B:324:ARG:HD2	0.41	1.91	6	2
1:B:225:MET:SD	1:B:228:VAL:CG1	0.41	3.09	5	1
1:B:225:MET:SD	1:B:228:VAL:HG12	0.41	2.55	5	1
1:B:294:PRO:CB	1:B:321:GLU:OE2	0.41	2.69	7	1
1:A:25:MET:CG	1:B:330:PHE:HD2	0.41	2.28	8	1
1:A:63:ARG:CD	1:A:63:ARG:H	0.41	2.28	10	1
1:A:93:ILE:HG12	1:A:119:LEU:HB3	0.41	1.91	11	1
1:B:275:GLU:HG3	1:B:279:LEU:CD1	0.41	2.46	12	1
1:A:134:GLY:O	1:A:137:THR:HG23	0.41	2.15	13	1
1:A:117:VAL:CG1	1:A:142:GLU:HB2	0.41	2.44	15	1
1:B:329:GLY:CA	1:B:333:ARG:HB2	0.41	2.43	15	1
1:B:249:HIS:HD1	1:B:250:PHE:N	0.41	2.13	2	1
1:B:264:GLU:C	1:B:266:TRP:N	0.41	2.73	2	1
1:A:157:ASP:O	1:A:160:ILE:HG22	0.41	2.16	3	1
1:B:320:LEU:CD1	1:B:325:GLU:CB	0.41	2.84	3	1
1:B:216:ARG:N	1:B:216:ARG:HD3	0.41	2.30	4	1
1:B:265:ALA:HA	1:B:269:GLN:HA	0.41	1.92	4	1
1:B:231:GLU:O	1:B:231:GLU:OE1	0.41	2.39	5	1
1:A:61:HIS:O	1:A:64:GLU:HB2	0.41	2.15	6	1
1:A:119:LEU:HA	1:A:144:VAL:O	0.41	2.16	6	1
1:A:147:LYS:O	1:A:147:LYS:HD2	0.41	2.15	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:298:PRO:HA	1:B:328:TYR:HE1	0.41	1.64	8	1
1:A:153:LYS:CG	1:A:154:PRO:HD3	0.41	2.45	9	1
1:A:63:ARG:HD3	1:A:63:ARG:N	0.41	2.30	10	1
1:A:157:ASP:OD1	1:A:157:ASP:C	0.41	2.57	12	1
1:B:336:GLY:N	1:B:341:VAL:HB	0.41	2.30	12	1
1:B:322:GLU:N	1:B:325:GLU:OE1	0.41	2.54	13	1
1:A:77:THR:HG22	1:A:78:PRO:HD3	0.41	1.90	14	1
1:B:242:PRO:HB3	1:B:349:ILE:CG1	0.41	2.44	15	1
1:B:255:LEU:CD2	1:B:255:LEU:N	0.41	2.79	15	1
1:A:96:ILE:N	1:A:124:ARG:HD2	0.41	2.30	1	1
1:A:113:ASP:O	1:A:114:LYS:C	0.41	2.57	2	1
1:A:117:VAL:CG2	1:A:163:VAL:HG11	0.41	2.46	10	4
1:A:45:THR:O	1:A:48:GLU:N	0.41	2.53	5	1
1:A:124:ARG:C	1:A:128:TYR:CE2	0.41	2.94	5	1
1:B:246:LEU:CA	1:B:249:HIS:HD2	0.41	2.26	5	1
1:B:322:GLU:HA	1:B:345:HIS:CD2	0.41	2.51	5	1
1:A:82:LEU:HD13	1:A:85:ARG:NE	0.41	2.27	7	1
1:B:231:GLU:OE1	1:B:273:PRO:HD3	0.41	2.16	8	1
1:A:19:PHE:CE2	1:A:59:ASN:HB3	0.41	2.50	10	1
1:A:24:PHE:O	1:A:28:VAL:CG1	0.41	2.69	10	1
1:A:74:GLU:O	1:A:74:GLU:HG2	0.41	2.16	10	1
1:A:44:LEU:CD2	1:A:44:LEU:N	0.41	2.79	11	1
1:B:233:ASN:CA	1:B:269:GLN:OE1	0.41	2.69	12	1
1:B:247:ILE:HG23	1:B:257:VAL:CG2	0.41	2.42	12	1
1:B:291:VAL:CA	1:B:317:VAL:O	0.41	2.68	12	1
1:A:29:ASN:ND2	1:A:32:THR:O	0.41	2.53	13	1
1:B:220:LEU:HD12	1:B:247:ILE:HD12	0.41	1.92	13	1
1:B:280:ASP:OD2	1:B:305:GLU:OE2	0.41	2.39	13	1
1:B:319:LEU:HD23	1:B:319:LEU:HA	0.41	1.72	13	2
1:A:69:GLN:NE2	1:A:70:VAL:CG2	0.41	2.76	14	1
1:A:71:LEU:HD13	1:A:71:LEU:HA	0.41	1.54	15	1
1:B:333:ARG:O	1:B:334:GLY:C	0.41	2.59	15	1
1:A:35:MET:HG2	1:A:36:PRO:CD	0.41	2.44	1	1
1:B:268:ALA:C	1:B:269:GLN:O	0.41	2.58	1	2
1:B:284:ILE:CD1	1:B:305:GLU:HB3	0.41	2.45	2	1
1:B:324:ARG:CB	1:B:328:TYR:HE2	0.41	2.28	5	1
1:A:84:ILE:HD11	1:A:105:GLU:OE2	0.41	2.16	7	1
1:A:133:ARG:C	1:A:135:LEU:N	0.41	2.72	7	1
1:A:108:TRP:CZ2	1:B:331:LEU:CD2	0.41	3.03	12	2
1:B:320:LEU:HB3	1:B:325:GLU:HB3	0.41	1.93	8	1
1:A:28:VAL:O	1:A:30:PRO:N	0.41	2.54	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:ARG:NH1	1:A:63:ARG:HG3	0.41	2.31	9	1
1:B:290:PHE:CD2	1:B:309:ALA:CB	0.41	3.03	9	1
1:B:227:LEU:HB2	1:B:235:MET:HB3	0.41	1.90	10	1
1:B:316:ILE:CD1	1:B:335:LEU:CD2	0.41	2.99	11	1
1:B:329:GLY:HA2	1:B:333:ARG:CG	0.41	2.46	11	1
1:A:117:VAL:HG21	1:A:160:ILE:HG13	0.41	1.91	12	1
1:A:114:LYS:HA	1:A:114:LYS:HD2	0.41	1.72	14	1
1:B:277:THR:HG22	1:B:278:PRO:CD	0.41	2.45	14	1
1:B:277:THR:HG22	1:B:278:PRO:HD3	0.41	1.93	14	1
1:B:321:GLU:CA	1:B:321:GLU:OE1	0.41	2.66	15	1
1:A:16:ARG:O	1:A:56:GLU:CD	0.41	2.59	1	1
1:A:59:ASN:H	1:A:83:GLU:HG2	0.41	1.70	2	1
1:B:225:MET:SD	1:B:225:MET:N	0.41	2.94	2	1
1:B:250:PHE:CD1	1:B:255:LEU:CB	0.41	3.00	2	2
1:B:284:ILE:HD11	1:B:305:GLU:CB	0.41	2.46	3	1
1:B:309:ALA:HB3	1:B:316:ILE:CG1	0.41	2.44	3	1
1:B:236:PRO:HB2	1:B:239:GLU:HB2	0.41	1.93	4	1
1:B:229:ASN:ND2	1:B:232:THR:CB	0.41	2.81	5	1
1:A:28:VAL:CB	1:A:70:VAL:HG21	0.41	2.37	11	2
1:B:220:LEU:H	1:B:259:ASN:CB	0.41	2.28	7	1
1:A:35:MET:CE	1:A:40:GLN:OE1	0.41	2.68	8	1
1:A:15:VAL:HG13	1:A:88:ASP:OD2	0.41	2.15	9	1
1:A:75:GLU:HG3	1:A:79:LEU:CD1	0.41	2.45	12	1
1:A:29:ASN:HB3	1:A:32:THR:CG2	0.41	2.44	14	1
1:A:73:PRO:CB	1:B:333:ARG:HB3	0.41	2.46	14	1
1:B:240:GLN:HE22	1:B:266:TRP:HA	0.41	1.75	15	1
1:B:291:VAL:HG13	1:B:356:ILE:HD11	0.41	1.93	1	1
1:B:325:GLU:OE2	1:B:326:GLU:HB2	0.41	2.15	1	2
1:A:102:THR:HB	1:A:106:ILE:HD11	0.41	1.92	2	1
1:A:108:TRP:CG	1:B:311:ALA:HB2	0.41	2.50	2	1
1:B:249:HIS:HE1	1:B:250:PHE:CE1	0.41	2.32	2	1
1:B:283:GLU:O	1:B:287:ALA:CB	0.41	2.69	2	1
1:A:23:PRO:C	1:A:24:PHE:O	0.41	2.58	3	1
1:A:84:ILE:HD13	1:A:90:PHE:CZ	0.41	2.47	3	2
1:B:240:GLN:OE1	1:B:240:GLN:HA	0.41	2.13	3	1
1:B:243:PHE:CD1	1:B:243:PHE:N	0.41	2.89	3	1
1:B:305:GLU:HA	1:B:308:TRP:HB2	0.41	1.93	3	1
1:A:24:PHE:HB3	1:B:330:PHE:HE1	0.41	1.76	4	1
1:A:28:VAL:HG13	1:A:32:THR:CG2	0.41	2.33	4	1
1:A:29:ASN:N	1:A:32:THR:CG2	0.41	2.84	4	1
1:A:24:PHE:CG	1:B:330:PHE:HE2	0.41	2.34	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ARG:CG	1:A:85:ARG:NH1	0.41	2.82	5	1
1:A:153:LYS:HD3	1:A:154:PRO:HD3	0.41	1.92	5	1
1:B:223:PRO:CA	1:B:299:SER:OG	0.41	2.69	5	1
1:B:303:HIS:C	1:B:305:GLU:N	0.41	2.74	5	1
1:B:325:GLU:HG2	1:B:345:HIS:HE2	0.41	1.74	5	1
1:A:29:ASN:HB2	1:A:33:ASN:CG	0.41	2.36	6	1
1:A:38:ALA:O	1:A:42:PRO:HD2	0.41	2.14	6	1
1:A:50:PHE:HD1	1:A:50:PHE:HA	0.41	1.61	6	1
1:A:80:ASP:O	1:A:84:ILE:N	0.41	2.53	6	1
1:B:281:GLN:CG	1:B:312:PHE:CZ	0.41	3.04	6	1
1:B:285:ARG:CB	1:B:314:LYS:HE2	0.41	2.45	6	1
1:B:290:PHE:CE2	1:B:292:ALA:HB2	0.41	2.51	6	1
1:A:120:LEU:HA	1:A:125:GLU:HB3	0.41	1.92	7	1
1:A:127:GLU:OE1	1:B:230:PRO:O	0.41	2.39	7	1
1:B:320:LEU:CD1	1:B:345:HIS:HE2	0.41	2.26	7	1
1:B:272:THR:O	1:B:273:PRO:C	0.41	2.59	14	2
1:B:295:GLY:C	1:B:296:ILE:O	0.41	2.59	14	2
1:B:341:VAL:HG12	1:B:341:VAL:O	0.41	2.14	9	1
1:A:28:VAL:CG2	1:A:34:SER:N	0.41	2.84	10	1
1:A:36:PRO:O	1:A:39:GLU:CG	0.41	2.52	10	1
1:A:65:ALA:HA	1:A:69:GLN:HB2	0.41	1.93	10	1
1:B:308:TRP:C	1:B:310:SER:N	0.41	2.73	10	1
1:A:28:VAL:CG2	1:A:70:VAL:HG23	0.41	2.46	11	1
1:A:35:MET:CB	1:A:68:ALA:HA	0.41	2.45	11	1
1:B:234:SER:HB2	1:B:268:ALA:HB1	0.41	1.92	11	1
1:B:264:GLU:OE1	1:B:264:GLU:N	0.41	2.54	11	1
1:B:296:ILE:CG1	1:B:297:PRO:HA	0.41	2.40	12	1
1:B:321:GLU:H	1:B:325:GLU:HB3	0.41	1.73	13	1
1:B:215:VAL:HG22	1:B:289:VAL:CG2	0.41	2.46	14	1
1:B:220:LEU:HD23	1:B:220:LEU:HA	0.41	1.55	14	1
1:B:229:ASN:HB3	1:B:232:THR:CG2	0.41	2.45	14	1
1:B:306:ILE:HG22	1:B:335:LEU:CD1	0.41	2.45	14	1
1:A:81:GLN:CG	1:A:108:TRP:CZ2	0.41	3.03	15	1
1:A:161:ARG:CZ	1:A:161:ARG:CB	0.41	2.99	15	1
1:B:248:GLU:O	1:B:252:LYS:CB	0.41	2.69	15	1
1:B:356:ILE:O	1:B:360:ILE:CD1	0.41	2.68	15	1
1:A:68:ALA:C	1:A:69:GLN:O	0.41	2.59	1	1
1:A:156:ILE:HG23	1:A:157:ASP:N	0.41	2.31	1	2
1:A:108:TRP:HA	1:B:311:ALA:CB	0.41	2.45	2	1
1:B:269:GLN:O	1:B:271:LEU:HD23	0.41	2.15	2	1
1:A:124:ARG:HA	1:A:127:GLU:OE1	0.41	2.15	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ASN:H	1:A:83:GLU:CG	0.41	2.29	4	1
1:A:120:LEU:HD12	1:A:125:GLU:OE2	0.41	2.12	4	1
1:B:264:GLU:O	1:B:268:ALA:N	0.41	2.54	4	1
1:B:294:PRO:HB2	1:B:295:GLY:H	0.41	1.45	4	1
1:A:103:HIS:CE1	1:B:300:PRO:HB3	0.41	2.51	5	1
1:A:63:ARG:HG2	1:A:64:GLU:N	0.41	2.31	6	1
1:A:119:LEU:HD21	1:A:156:ILE:HD12	0.41	1.93	7	1
1:B:334:GLY:O	1:B:338:VAL:CG1	0.41	2.62	7	1
1:A:22:GLY:H	1:A:61:HIS:CE1	0.41	2.33	9	1
1:A:20:LEU:CD1	1:A:47:ILE:HD12	0.41	2.46	13	1
1:A:25:MET:C	1:A:25:MET:SD	0.41	2.98	13	1
1:A:35:MET:SD	1:A:36:PRO:N	0.41	2.94	15	1
1:A:61:HIS:HB3	1:A:71:LEU:HD23	0.41	1.93	15	1
1:A:46:LEU:HD13	1:A:47:ILE:N	0.40	2.26	1	1
1:A:82:LEU:CD2	1:A:82:LEU:N	0.40	2.83	1	1
1:B:235:MET:HG2	1:B:236:PRO:CD	0.40	2.46	1	1
1:B:342:GLU:CD	1:B:343:PHE:N	0.40	2.75	1	1
1:A:49:HIS:CE1	1:A:50:PHE:CZ	0.40	3.08	2	1
1:B:225:MET:HB2	1:B:230:PRO:HA	0.40	1.91	2	1
1:A:105:GLU:CA	1:A:108:TRP:HB2	0.40	2.46	3	1
1:B:235:MET:HB3	1:B:269:GLN:CD	0.40	2.37	3	1
1:A:85:ARG:HH11	1:A:85:ARG:CG	0.40	2.29	5	1
1:B:225:MET:CE	1:B:225:MET:CA	0.40	2.94	5	1
1:B:235:MET:HB2	1:B:269:GLN:HG3	0.40	1.93	5	1
1:B:240:GLN:HE21	1:B:244:LEU:HD21	0.40	1.75	6	1
1:B:259:ASN:HB2	1:B:283:GLU:CG	0.40	2.46	8	1
1:B:264:GLU:CD	1:B:264:GLU:N	0.40	2.71	9	1
1:A:64:GLU:C	1:A:69:GLN:CG	0.40	2.89	11	1
1:B:228:VAL:HG21	1:B:270:VAL:CB	0.40	2.46	11	1
1:A:24:PHE:HE1	1:A:70:VAL:HA	0.40	1.75	12	1
1:A:137:THR:HG23	1:A:138:VAL:HG13	0.40	1.93	12	1
1:B:291:VAL:CG2	1:B:317:VAL:O	0.40	2.66	12	1
1:A:49:HIS:O	1:A:49:HIS:CG	0.40	2.72	13	1
1:B:325:GLU:HG3	1:B:345:HIS:CE1	0.40	2.52	15	1
1:A:20:LEU:CG	1:A:47:ILE:HD11	0.40	2.46	1	1
1:B:224:PHE:C	1:B:228:VAL:HG12	0.40	2.36	1	1
1:A:27:LEU:CD1	1:A:39:GLU:OE2	0.40	2.68	3	1
1:A:49:HIS:HE1	1:A:53:GLN:HG3	0.40	1.75	3	1
1:A:121:GLU:OE2	1:A:121:GLU:CA	0.40	2.67	3	1
1:A:93:ILE:HD13	1:A:146:TYR:CE1	0.40	2.51	4	1
1:B:220:LEU:HD11	1:B:250:PHE:CE1	0.40	2.51	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LEU:HB3	1:A:86:LYS:HD2	0.40	1.92	8	1
1:A:110:SER:CB	1:B:308:TRP:CE2	0.40	3.04	9	1
1:A:25:MET:O	1:A:30:PRO:CD	0.40	2.69	10	1
1:A:46:LEU:HG	1:A:153:LYS:HG2	0.40	1.92	10	1
1:B:219:PHE:HD2	1:B:283:GLU:HB3	0.40	1.75	10	1
1:B:225:MET:HB3	1:B:230:PRO:HA	0.40	1.93	10	1
1:B:367:VAL:O	1:B:367:VAL:HG12	0.40	2.15	10	1
1:A:35:MET:HG2	1:A:65:ALA:O	0.40	2.17	11	1
1:A:70:VAL:C	1:B:330:PHE:CZ	0.40	2.95	11	1
1:A:122:GLU:H	1:A:146:TYR:HB2	0.40	1.76	11	1
1:B:264:GLU:HB3	1:B:269:GLN:HG3	0.40	1.93	11	1
1:A:130:PHE:HD1	1:A:130:PHE:HA	0.40	1.57	12	1
1:B:303:HIS:HE2	1:B:332:VAL:HG23	0.40	1.75	12	1
1:A:24:PHE:HE1	1:A:71:LEU:N	0.40	2.14	13	1
1:A:29:ASN:N	1:A:33:ASN:OD1	0.40	2.54	13	1
1:A:40:GLN:N	1:A:42:PRO:HD2	0.40	2.30	13	1
1:A:102:THR:HG22	1:A:106:ILE:CD1	0.40	2.46	14	1
1:B:224:PHE:HB3	1:B:225:MET:H	0.40	1.51	14	1
1:B:250:PHE:CD1	1:B:257:VAL:HG21	0.40	2.51	15	1
1:B:342:GLU:CG	1:B:363:VAL:CB	0.40	2.98	15	1
1:A:89:VAL:HG21	1:A:164:VAL:HG21	0.40	1.91	1	1
1:A:108:TRP:O	1:A:112:PHE:HD1	0.40	2.00	1	1
1:A:110:SER:HB3	1:B:308:TRP:CE2	0.40	2.52	1	1
1:A:130:PHE:CE1	1:B:225:MET:HB2	0.40	2.50	1	1
1:B:283:GLU:HA	1:B:286:LYS:HB3	0.40	1.94	1	1
1:A:18:VAL:CG1	1:A:50:PHE:CZ	0.40	2.90	2	1
1:B:284:ILE:HG23	1:B:290:PHE:CE2	0.40	2.52	2	1
1:B:318:LEU:CD1	1:B:341:VAL:HG13	0.40	2.46	2	1
1:A:104:VAL:O	1:A:108:TRP:CG	0.40	2.73	3	1
1:B:296:ILE:CG2	1:B:324:ARG:HD3	0.40	2.47	3	1
1:A:79:LEU:HA	1:A:83:GLU:OE2	0.40	2.17	5	1
1:B:220:LEU:HD22	1:B:291:VAL:CG1	0.40	2.47	5	1
1:B:285:ARG:HD3	1:B:312:PHE:CE1	0.40	2.50	5	1
1:B:306:ILE:HG23	1:B:335:LEU:CD2	0.40	2.45	9	1
1:A:25:MET:HE1	1:A:101:GLY:N	0.40	2.25	10	1
1:A:63:ARG:H	1:A:63:ARG:HD3	0.40	1.76	10	1
1:B:248:GLU:C	1:B:250:PHE:N	0.40	2.74	10	2
1:A:129:GLY:HA2	1:A:133:ARG:CG	0.40	2.46	11	1
1:B:219:PHE:CD1	1:B:258:PHE:O	0.40	2.74	12	1
1:B:221:ALA:HA	1:B:259:ASN:OD1	0.40	2.17	12	1
1:B:228:VAL:CB	1:B:233:ASN:CB	0.40	2.99	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:GLY:C	1:A:96:ILE:O	0.40	2.58	14	1
1:A:61:HIS:CG	1:A:71:LEU:HD11	0.40	2.51	1	1
1:B:249:HIS:CE1	1:B:250:PHE:CZ	0.40	3.09	2	1
1:B:302:THR:HB	1:B:306:ILE:HD11	0.40	1.93	2	1
1:B:294:PRO:HD3	1:B:318:LEU:HB3	0.40	1.92	4	1
1:A:119:LEU:HD23	1:A:119:LEU:HA	0.40	1.80	7	1
1:A:35:MET:HG2	1:A:69:GLN:OE1	0.40	2.13	8	1
1:B:223:PRO:C	1:B:225:MET:HE3	0.40	2.36	10	1
1:A:120:LEU:O	1:A:146:TYR:N	0.40	2.55	11	1
1:B:267:GLY:C	1:B:269:GLN:OE1	0.40	2.59	11	1
1:A:106:ILE:HG12	1:A:118:LEU:HD22	0.40	1.94	13	1
1:A:150:ALA:O	1:A:154:PRO:HD3	0.40	2.15	14	1
1:B:329:GLY:O	1:B:333:ARG:HB3	0.40	2.17	1	1
1:A:85:ARG:O	1:A:114:LYS:NZ	0.40	2.53	2	1
1:A:105:GLU:O	1:A:108:TRP:CB	0.40	2.68	6	1
1:B:329:GLY:O	1:B:333:ARG:N	0.40	2.54	6	1
1:B:359:ALA:O	1:B:363:VAL:HG12	0.40	2.16	7	1
1:A:25:MET:CG	1:B:330:PHE:CD1	0.40	3.04	10	1
1:A:53:GLN:OE1	1:A:53:GLN:O	0.40	2.38	10	1
1:A:24:PHE:HD2	1:A:70:VAL:CG2	0.40	2.21	11	1
1:A:120:LEU:O	1:A:146:TYR:CB	0.40	2.69	11	1
1:B:293:ILE:HG12	1:B:319:LEU:HB3	0.40	1.91	11	1
1:B:348:ASP:O	1:B:350:ALA:N	0.40	2.54	11	1
1:A:36:PRO:HB2	1:A:39:GLU:HB3	0.40	1.92	12	1
1:A:29:ASN:CG	1:A:32:THR:O	0.40	2.60	13	1
1:B:244:LEU:HA	1:B:247:ILE:CG2	0.40	2.47	13	1
1:A:94:PRO:HB2	1:A:95:GLY:H	0.40	1.49	14	1
1:B:342:GLU:CD	1:B:362:LYS:HE2	0.40	2.37	14	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	154/163 (94%)	106±3 (69±2%)	24±3 (15±2%)	24±2 (16±1%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	154/163 (94%)	107±3 (69±2%)	24±4 (15±2%)	24±2 (15±1%)	0	4
All	All	4620/4890 (94%)	3192 (69%)	716 (15%)	712 (15%)	0	4

All 95 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	24	PHE	15
1	A	30	PRO	15
1	A	62	ARG	15
1	A	63	ARG	15
1	A	94	PRO	15
1	A	98	PRO	15
1	A	122	GLU	15
1	A	130	PHE	15
1	A	140	ALA	15
1	B	224	PHE	15
1	B	230	PRO	15
1	B	262	ARG	15
1	B	294	PRO	15
1	B	298	PRO	15
1	B	322	GLU	15
1	B	330	PHE	15
1	B	340	ALA	15
1	A	59	ASN	14
1	A	60	ALA	14
1	A	96	ILE	14
1	A	129	GLY	14
1	B	225	MET	14
1	B	259	ASN	14
1	B	260	ALA	14
1	B	263	ARG	14
1	B	329	GLY	14
1	A	25	MET	13
1	A	31	GLU	13
1	A	71	LEU	13
1	B	231	GLU	13
1	B	271	LEU	13
1	B	296	ILE	13
1	A	69	GLN	10
1	B	269	GLN	10
1	A	117	VAL	9

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Mol	Chain	Res	Type	Models (Total)
1	B	303	HIS	9
1	A	103	HIS	8
1	B	317	VAL	8
1	A	33	ASN	8
1	B	233	ASN	8
1	A	99	SER	7
1	B	299	SER	7
1	A	68	ALA	7
1	B	268	ALA	7
1	A	32	THR	7
1	B	232	THR	7
1	A	70	VAL	6
1	B	270	VAL	6
1	A	27	LEU	5
1	A	87	ALA	5
1	B	287	ALA	5
1	A	15	VAL	4
1	A	115	PRO	4
1	B	215	VAL	4
1	A	47	ILE	4
1	A	150	ALA	4
1	B	247	ILE	4
1	A	147	LYS	4
1	B	347	LYS	4
1	A	61	HIS	4
1	B	261	HIS	4
1	A	26	GLY	4
1	B	226	GLY	4
1	B	227	LEU	4
1	A	34	SER	3
1	A	102	THR	3
1	A	128	TYR	3
1	B	234	SER	3
1	B	302	THR	3
1	B	315	PRO	3
1	B	328	TYR	3
1	B	350	ALA	3
1	A	23	PRO	3
1	A	113	ASP	3
1	B	223	PRO	3
1	A	148	ASP	2
1	B	348	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	B	313	ASP	2
1	A	35	MET	2
1	B	235	MET	2
1	A	36	PRO	2
1	A	67	GLY	2
1	B	236	PRO	2
1	B	267	GLY	2
1	A	125	GLU	1
1	A	28	VAL	1
1	A	123	GLY	1
1	B	323	GLY	1
1	A	38	ALA	1
1	B	238	ALA	1
1	B	274	GLU	1
1	A	77	THR	1
1	A	100	PRO	1
1	B	277	THR	1
1	B	300	PRO	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	128/133 (96%)	81±5 (63±4%)	47±5 (37±4%)	1 8
1	B	128/133 (96%)	81±5 (63±4%)	47±5 (37±4%)	1 8
All	All	3840/3990 (96%)	2432 (63%)	1408 (37%)	1 8

All 209 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	24	PHE	15
1	A	96	ILE	15
1	A	102	THR	15
1	A	130	PHE	15
1	A	131	LEU	15
1	B	224	PHE	15

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Mol	Chain	Res	Type	Models (Total)
1	B	296	ILE	15
1	B	302	THR	15
1	B	330	PHE	15
1	B	331	LEU	15
1	A	108	TRP	14
1	A	135	LEU	14
1	B	335	LEU	14
1	A	85	ARG	13
1	B	285	ARG	13
1	B	308	TRP	13
1	A	46	LEU	13
1	A	49	HIS	13
1	B	246	LEU	13
1	B	249	HIS	13
1	A	19	PHE	12
1	A	69	GLN	12
1	A	110	SER	12
1	A	153	LYS	12
1	B	219	PHE	12
1	B	310	SER	12
1	B	353	LYS	12
1	A	55	LEU	11
1	A	93	ILE	11
1	A	166	ARG	11
1	B	269	GLN	11
1	B	289	VAL	11
1	B	293	ILE	11
1	B	321	GLU	11
1	A	20	LEU	11
1	A	133	ARG	11
1	B	220	LEU	11
1	A	41	LEU	10
1	A	76	CYS	10
1	A	89	VAL	10
1	A	121	GLU	10
1	A	163	VAL	10
1	B	241	LEU	10
1	B	276	CYS	10
1	B	363	VAL	10
1	B	366	ARG	10
1	A	83	GLU	10
1	B	283	GLU	10

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Mol	Chain	Res	Type	Models (Total)
1	B	333	ARG	10
1	A	61	HIS	9
1	A	63	ARG	9
1	B	227	LEU	9
1	B	255	LEU	9
1	B	263	ARG	9
1	A	34	SER	9
1	B	234	SER	9
1	A	33	ASN	8
1	A	81	GLN	8
1	A	151	LEU	8
1	A	165	ASP	8
1	B	261	HIS	8
1	B	365	ASP	8
1	A	112	PHE	8
1	A	147	LYS	8
1	B	312	PHE	8
1	B	347	LYS	8
1	A	16	ARG	8
1	B	216	ARG	8
1	B	229	ASN	8
1	A	161	ARG	8
1	B	361	ARG	8
1	A	27	LEU	7
1	A	32	THR	7
1	A	106	ILE	7
1	A	113	ASP	7
1	A	120	LEU	7
1	B	232	THR	7
1	B	233	ASN	7
1	B	281	GLN	7
1	B	306	ILE	7
1	B	313	ASP	7
1	B	320	LEU	7
1	B	351	LEU	7
1	A	40	GLN	7
1	A	48	GLU	7
1	A	62	ARG	7
1	A	99	SER	7
1	A	149	ILE	7
1	B	240	GLN	7
1	B	248	GLU	7

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Mol	Chain	Res	Type	Models (Total)
1	B	252	LYS	7
1	B	262	ARG	7
1	B	299	SER	7
1	B	349	ILE	7
1	A	35	MET	7
1	A	45	THR	7
1	A	103	HIS	7
1	A	160	ILE	7
1	B	235	MET	7
1	B	245	THR	7
1	B	303	HIS	7
1	B	360	ILE	7
1	A	29	ASN	7
1	A	125	GLU	7
1	B	325	GLU	7
1	B	357	ASP	7
1	A	75	GLU	6
1	A	84	ILE	6
1	B	217	SER	6
1	B	275	GLU	6
1	B	284	ILE	6
1	B	362	LYS	6
1	A	52	LYS	6
1	A	122	GLU	6
1	A	148	ASP	6
1	B	322	GLU	6
1	B	348	ASP	6
1	A	37	SER	6
1	A	124	ARG	6
1	B	237	SER	6
1	B	324	ARG	6
1	A	155	GLN	6
1	B	355	GLN	6
1	A	64	GLU	6
1	A	157	ASP	6
1	B	264	GLU	6
1	A	17	SER	5
1	A	25	MET	5
1	A	162	LYS	5
1	A	168	ASN	5
1	B	225	MET	5
1	B	239	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	B	256	GLU	5
1	B	368	ASN	5
1	A	56	GLU	5
1	B	326	GLU	5
1	A	47	ILE	5
1	A	88	ASP	5
1	B	247	ILE	5
1	A	82	LEU	5
1	B	282	LEU	5
1	A	43	PHE	5
1	A	114	LYS	5
1	B	243	PHE	5
1	B	244	LEU	5
1	A	39	GLU	4
1	A	51	GLU	4
1	B	251	GLU	4
1	A	79	LEU	4
1	B	279	LEU	4
1	A	146	TYR	4
1	B	288	ASP	4
1	B	346	TYR	4
1	A	28	VAL	4
1	A	50	PHE	4
1	A	142	GLU	4
1	B	228	VAL	4
1	B	250	PHE	4
1	A	105	GLU	4
1	B	305	GLU	4
1	B	314	LYS	4
1	A	53	GLN	4
1	B	253	GLN	4
1	A	44	LEU	4
1	A	66	TRP	3
1	B	231	GLU	3
1	B	266	TRP	3
1	A	164	VAL	3
1	B	364	VAL	3
1	B	342	GLU	3
1	A	80	ASP	3
1	A	132	VAL	3
1	B	332	VAL	3
1	A	18	VAL	3

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Mol	Chain	Res	Type	Models (Total)
1	A	70	VAL	3
1	A	127	GLU	3
1	B	270	VAL	3
1	B	327	GLU	3
1	A	74	GLU	3
1	B	274	GLU	3
1	A	156	ILE	2
1	B	356	ILE	2
1	A	31	GLU	2
1	A	86	LYS	2
1	A	126	GLU	2
1	B	286	LYS	2
1	A	71	LEU	2
1	A	91	VAL	2
1	A	117	VAL	2
1	B	271	LEU	2
1	B	280	ASP	2
1	B	291	VAL	2
1	B	218	VAL	2
1	A	119	LEU	2
1	B	319	LEU	2
1	A	104	VAL	1
1	A	59	ASN	1
1	B	259	ASN	1
1	B	317	VAL	1
1	A	77	THR	1
1	A	167	VAL	1
1	B	277	THR	1
1	B	367	VAL	1
1	A	118	LEU	1
1	B	318	LEU	1
1	A	137	THR	1
1	A	58	PHE	1
1	B	258	PHE	1
1	B	345	HIS	1

6.3.3 RNA

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 39% for the well-defined parts and 38% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *ChemicalShift_v3.txt*

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	1686
Number of shifts mapped to atoms	1686
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	12

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	159	0.23 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	146	0.78 ± 0.10	Should be checked
$^{13}\text{C}'$	138	-0.05 ± 0.11	None needed (< 0.5 ppm)
^{15}N	138	0.16 ± 0.19	None needed (< 0.5 ppm)

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 39%, i.e. 1640 atoms were assigned a chemical shift out of a possible 4244. 0 out of 62 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	703/1514 (46%)	286/614 (47%)	286/616 (46%)	131/284 (46%)
Sidechain	902/2402 (38%)	586/1574 (37%)	316/750 (42%)	0/78 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	35/328 (11%)	33/162 (20%)	0/146 (0%)	2/20 (10%)
Overall	1640/4244 (39%)	905/2350 (39%)	602/1512 (40%)	133/382 (35%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 38%, i.e. 1684 atoms were assigned a chemical shift out of a possible 4440. 0 out of 62 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	732/1598 (46%)	297/648 (46%)	297/652 (46%)	138/298 (46%)
Sidechain	917/2514 (36%)	593/1648 (36%)	324/784 (41%)	0/82 (0%)
Aromatic	35/328 (11%)	33/162 (20%)	0/146 (0%)	2/20 (10%)
Overall	1684/4440 (38%)	923/2458 (38%)	621/1582 (39%)	140/400 (35%)

7.1.4 Statistically unusual chemical shifts [i](#)

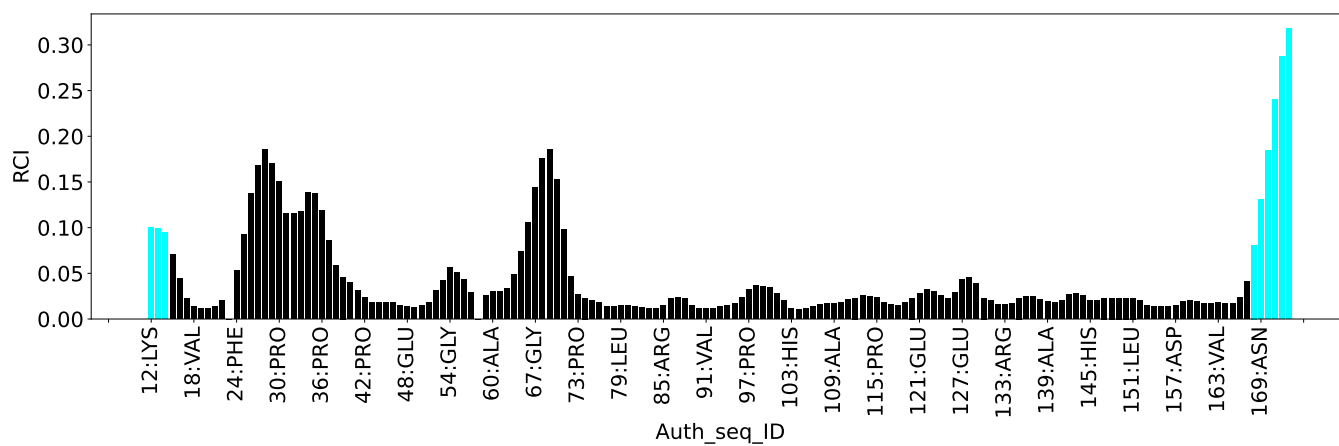
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	162	LYS	HE2	42.02	1.95 – 3.88	202.6
1	A	143	PHE	HE2	0.00	5.54 – 8.63	-22.9
1	A	58	PHE	HZ	0.00	4.94 – 9.06	-17.0
1	A	81	GLN	HG2	0.58	1.01 – 3.62	-6.7
1	A	134	GLY	N	130.68	91.59 – 127.52	5.9
1	A	104	VAL	HG11	-0.64	-0.48 – 2.12	-5.7
1	A	104	VAL	HG12	-0.64	-0.48 – 2.12	-5.7
1	A	104	VAL	HG13	-0.64	-0.48 – 2.12	-5.7
1	A	136	GLY	N	129.29	91.59 – 127.52	5.5
1	A	109	ALA	HB1	0.03	0.14 – 2.58	-5.5
1	A	109	ALA	HB2	0.03	0.14 – 2.58	-5.5
1	A	109	ALA	HB3	0.03	0.14 – 2.58	-5.5

7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	3018
Intra-residue ($ i-j =0$)	8
Sequential ($ i-j =1$)	412
Medium range ($ i-j >1$ and $ i-j <5$)	744
Long range ($ i-j \geq 5$)	1296
Inter-chain	210
Hydrogen bond restraints	348
Disulfide bond restraints	0
Total dihedral-angle restraints	174
Number of unmapped restraints	0
Number of restraints per residue	9.8
Number of long range restraints per residue ¹	4.2

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	62.6	0.2
0.2-0.5 (Medium)	10.5	0.49
>0.5 (Large)	4.0	0.63

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)	4.6	9.6
10.0-20.0 (Medium)	1.0	19.4
>20.0 (Large)	0.3	36.9

9 Distance violation analysis

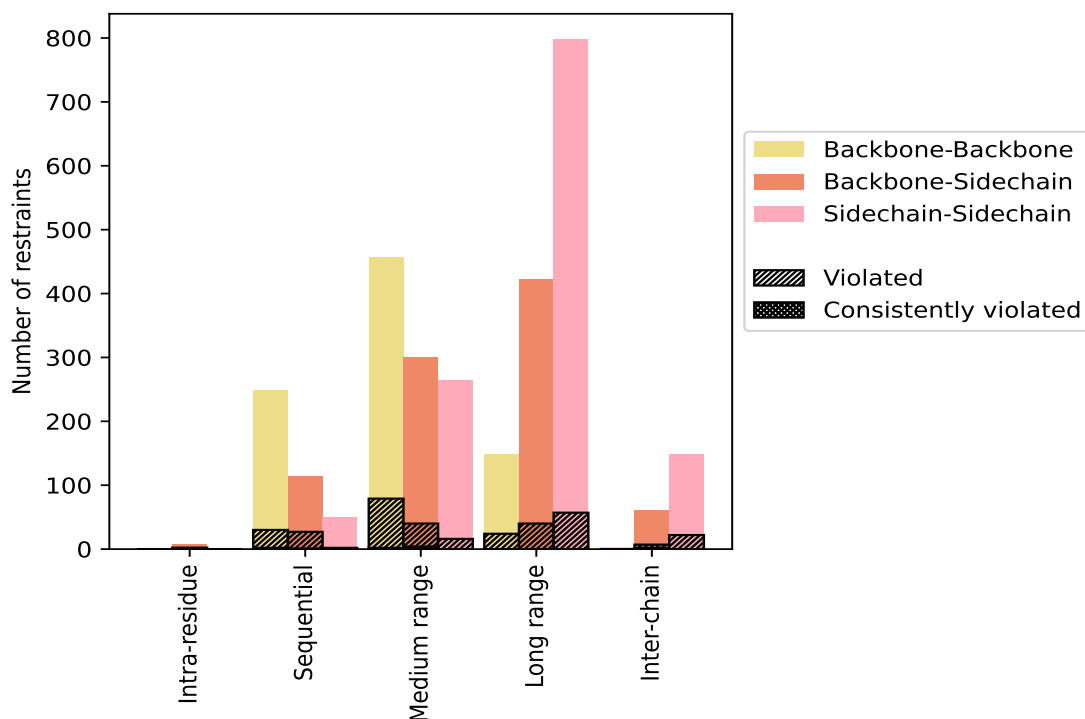
9.1 Summary of distance violations

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	8	0.3	2	25.0	0.1	2	25.0	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	8	0.3	2	25.0	0.1	2	25.0	0.1
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	412	13.7	59	14.3	2.0	3	0.7	0.1
Backbone-Backbone	248	8.2	30	12.1	1.0	2	0.8	0.1
Backbone-Sidechain	114	3.8	27	23.7	0.9	1	0.9	0.0
Sidechain-Sidechain	50	1.7	2	4.0	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	744	24.7	81	10.9	2.7	4	0.5	0.1
Backbone-Backbone	180	6.0	25	13.9	0.8	0	0.0	0.0
Backbone-Sidechain	300	9.9	40	13.3	1.3	4	1.3	0.1
Sidechain-Sidechain	264	8.7	16	6.1	0.5	0	0.0	0.0
Long range ($i-j \geq 5$)	1296	42.9	103	7.9	3.4	0	0.0	0.0
Backbone-Backbone	76	2.5	6	7.9	0.2	0	0.0	0.0
Backbone-Sidechain	422	14.0	40	9.5	1.3	0	0.0	0.0
Sidechain-Sidechain	798	26.4	57	7.1	1.9	0	0.0	0.0
Inter-chain	210	7.0	29	13.8	1.0	2	1.0	0.1
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	60	2.0	7	11.7	0.2	2	3.3	0.1
Sidechain-Sidechain	148	4.9	22	14.9	0.7	0	0.0	0.0
Hydrogen bond	348	11.5	72	20.7	2.4	2	0.6	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3018	100.0	346	11.5	11.5	13	0.4	0.4
Backbone-Backbone	854	28.3	133	15.6	4.4	4	0.5	0.1
Backbone-Sidechain	904	30.0	116	12.8	3.8	9	1.0	0.3
Sidechain-Sidechain	1260	41.7	97	7.7	3.2	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfid 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	14	28	10	6	60	0.18	0.58	0.12	0.14
2	2	16	32	21	3	74	0.18	0.59	0.11	0.14
3	2	11	34	28	5	80	0.18	0.6	0.1	0.14
4	2	13	42	16	4	77	0.18	0.57	0.1	0.15
5	2	15	23	19	2	61	0.19	0.6	0.12	0.14
6	2	13	28	17	11	71	0.17	0.59	0.11	0.13
7	2	16	30	21	6	75	0.17	0.6	0.11	0.14
8	2	13	32	27	2	76	0.18	0.6	0.11	0.14
9	2	7	33	18	4	64	0.19	0.58	0.11	0.14
10	2	17	32	25	5	81	0.19	0.6	0.12	0.14
11	2	21	38	25	7	93	0.17	0.59	0.09	0.14

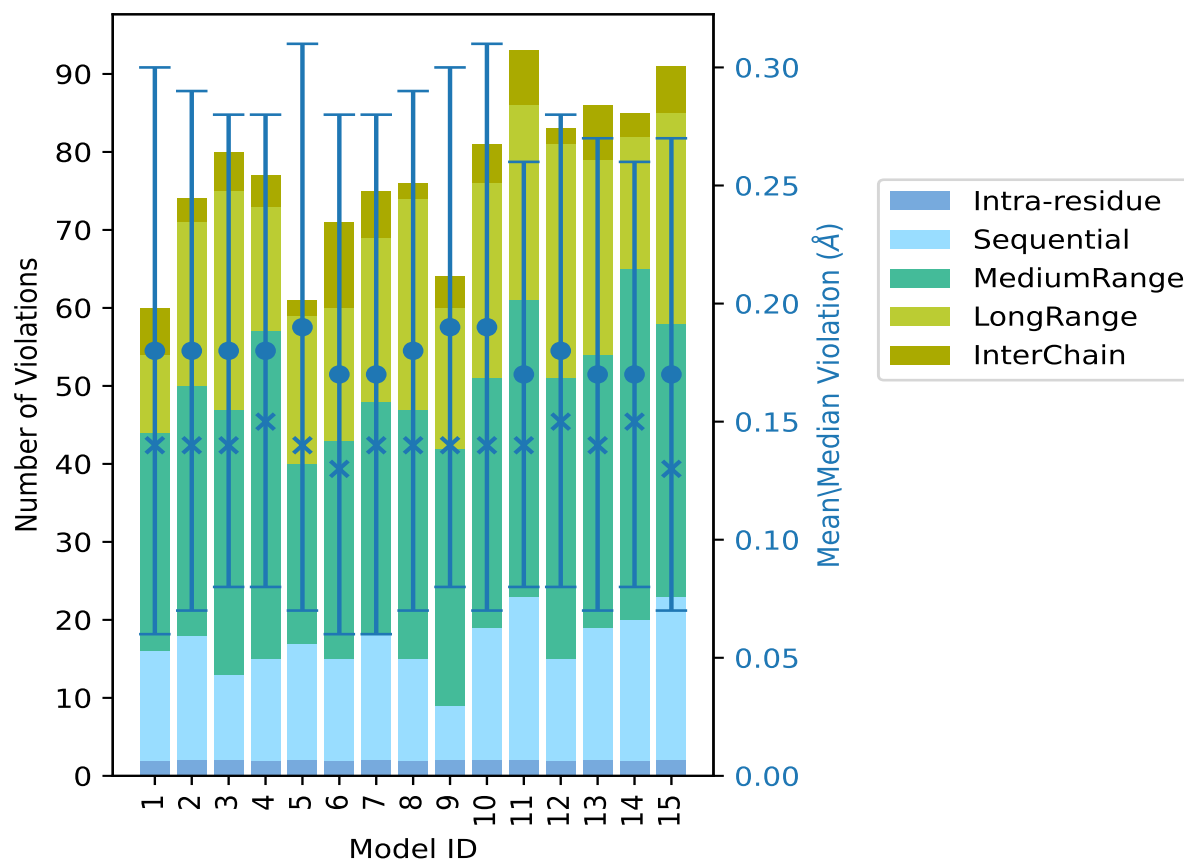
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
12	2	13	36	30	2	83	0.18	0.59	0.1	0.15
13	2	17	35	25	7	86	0.17	0.57	0.1	0.14
14	2	18	45	17	3	85	0.17	0.55	0.09	0.15
15	2	21	35	27	6	91	0.17	0.63	0.1	0.13

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard 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](#)

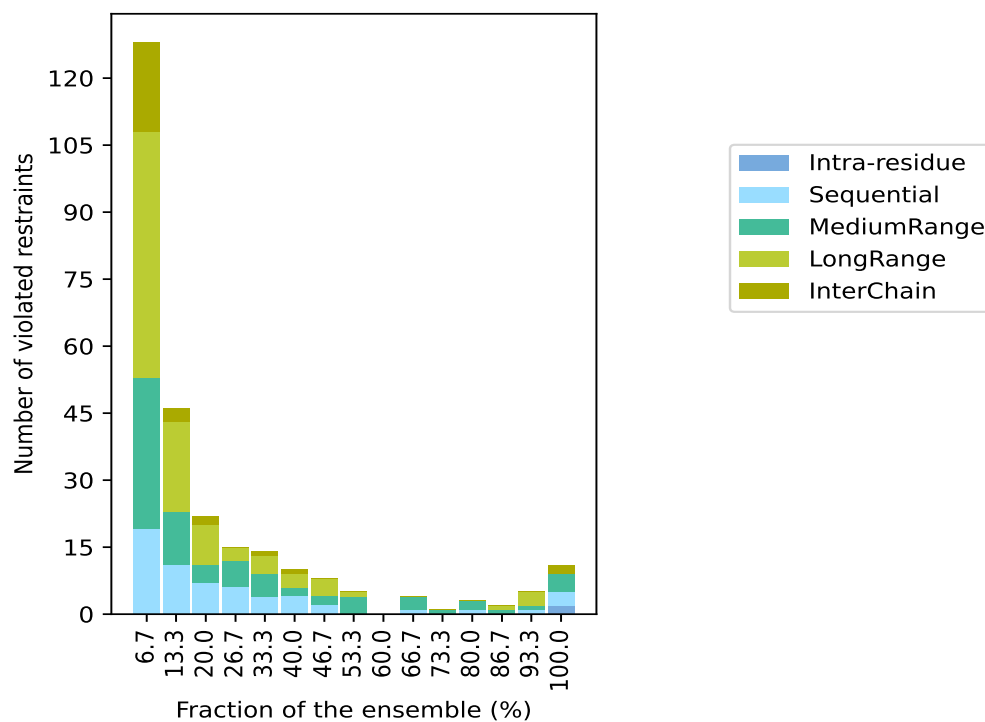
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for

a given fraction of the ensemble. In total, 2396(IR:6, SQ:353, MR:663, LR:1193, IC:181) 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	%
0	19	34	55	20	128	1	6.7
0	11	12	20	3	46	2	13.3
0	7	4	9	2	22	3	20.0
0	6	6	3	0	15	4	26.7
0	4	5	4	1	14	5	33.3
0	4	2	3	1	10	6	40.0
0	2	2	4	0	8	7	46.7
0	0	4	1	0	5	8	53.3
0	0	0	0	0	0	9	60.0
0	1	3	0	0	4	10	66.7
0	0	1	0	0	1	11	73.3
0	1	2	0	0	3	12	80.0
0	0	1	1	0	2	13	86.7
0	1	1	3	0	5	14	93.3
2	3	4	0	2	11	15	100.0

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

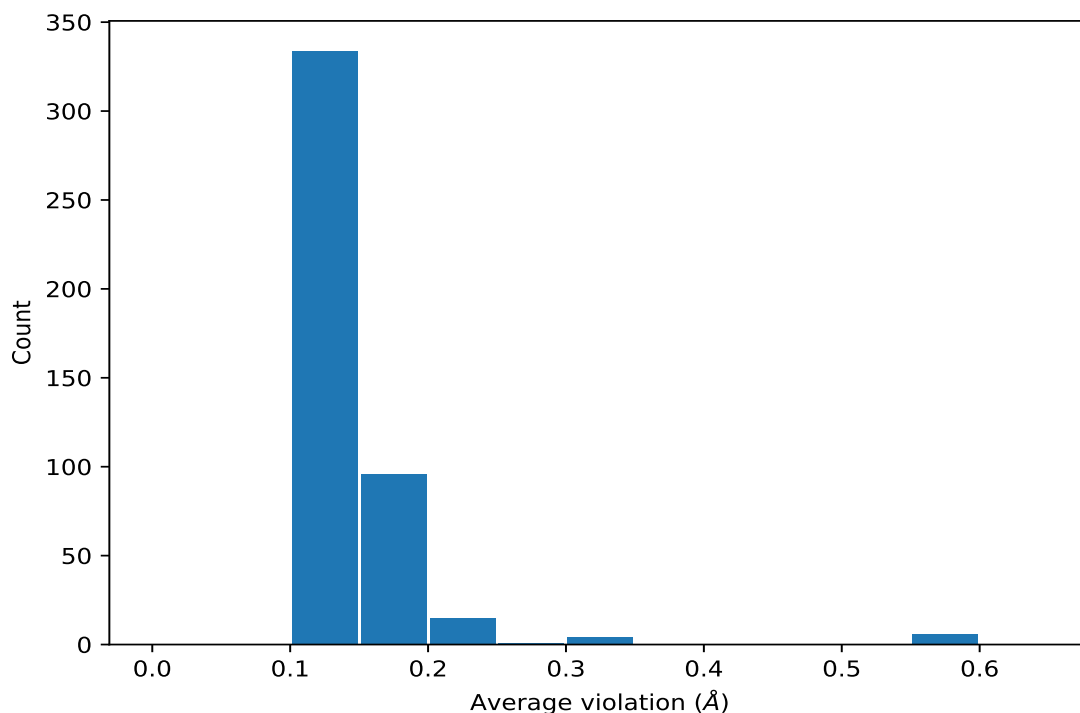
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	15	0.58	0.02	0.58
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	15	0.58	0.02	0.57
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	15	0.55	0.03	0.55
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	15	0.55	0.03	0.55
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	15	0.55	0.03	0.55
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	15	0.55	0.03	0.55
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	15	0.32	0.04	0.32
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	15	0.32	0.04	0.32
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	15	0.32	0.04	0.31
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	15	0.32	0.04	0.31
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	15	0.22	0.02	0.22
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	15	0.22	0.02	0.22
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	15	0.22	0.05	0.22
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	15	0.22	0.05	0.22
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	15	0.2	0.03	0.2
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	15	0.2	0.03	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	15	0.19	0.05	0.19
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	15	0.19	0.05	0.19
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	15	0.18	0.05	0.19
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	15	0.18	0.05	0.19
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	15	0.18	0.07	0.15
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	15	0.18	0.07	0.15
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	15	0.18	0.07	0.15
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	14	0.22	0.04	0.2
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	14	0.22	0.04	0.2
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	14	0.21	0.04	0.21
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	14	0.21	0.04	0.21
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	14	0.18	0.07	0.18
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	14	0.18	0.07	0.18
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	14	0.18	0.07	0.18
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	14	0.17	0.03	0.18
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	14	0.17	0.03	0.18
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	14	0.16	0.04	0.15
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	14	0.16	0.04	0.15
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	14	0.16	0.04	0.15
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	14	0.16	0.04	0.15
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	14	0.16	0.04	0.15
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	14	0.16	0.04	0.15
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	14	0.16	0.04	0.15
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	14	0.16	0.04	0.15
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	14	0.16	0.04	0.15
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	13	0.18	0.03	0.19
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	13	0.18	0.03	0.19
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	13	0.15	0.02	0.15
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	13	0.15	0.02	0.15
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	13	0.15	0.02	0.15
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	13	0.15	0.02	0.15
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	13	0.15	0.02	0.15
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	13	0.15	0.02	0.15
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	13	0.15	0.02	0.15
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	13	0.15	0.02	0.15
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	13	0.15	0.02	0.15
(2,783)	1:B:303:HIS:HD2	1:B:304:VAL:H	12	0.17	0.06	0.14
(4,120)	1:B:344:VAL:O	1:B:320:LEU:N	12	0.16	0.04	0.16
(3,120)	1:A:144:VAL:O	1:A:120:LEU:N	12	0.16	0.04	0.15
(3,119)	1:A:144:VAL:O	1:A:120:LEU:H	12	0.15	0.03	0.14
(4,119)	1:B:344:VAL:O	1:B:320:LEU:H	12	0.14	0.03	0.14
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD1	12	0.14	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD2	12	0.14	0.02	0.15
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD1	12	0.14	0.01	0.14
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD2	12	0.14	0.01	0.14
(1,699)	1:A:93:ILE:HA	1:A:95:GLY:H	11	0.14	0.03	0.13
(1,783)	1:A:103:HIS:HD2	1:A:104:VAL:H	10	0.18	0.05	0.18
(4,22)	1:B:229:ASN:O	1:B:232:THR:N	10	0.14	0.02	0.15
(2,884)	1:B:312:PHE:HD1	1:B:314:LYS:H	10	0.14	0.02	0.14
(2,884)	1:B:312:PHE:HD2	1:B:314:LYS:H	10	0.14	0.02	0.14
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG21	10	0.14	0.03	0.14
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG22	10	0.14	0.03	0.14
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG23	10	0.14	0.03	0.14
(2,699)	1:B:293:ILE:HA	1:B:295:GLY:H	10	0.13	0.02	0.12
(1,1102)	1:A:132:VAL:HA	1:A:135:LEU:H	8	0.16	0.03	0.16
(1,734)	1:A:96:ILE:H	1:A:125:GLU:HA	8	0.16	0.03	0.15
(2,1102)	1:B:332:VAL:HA	1:B:335:LEU:H	8	0.16	0.03	0.15
(3,22)	1:A:29:ASN:O	1:A:32:THR:N	8	0.15	0.02	0.15
(1,884)	1:A:112:PHE:HD1	1:A:114:LYS:H	8	0.14	0.03	0.14
(1,884)	1:A:112:PHE:HD2	1:A:114:LYS:H	8	0.14	0.03	0.14
(1,780)	1:A:103:HIS:HA	1:A:107:GLY:H	8	0.14	0.02	0.14
(3,135)	1:A:133:ARG:O	1:A:137:THR:H	8	0.14	0.02	0.15
(2,734)	1:B:296:ILE:H	1:B:325:GLU:HA	7	0.17	0.03	0.17
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG21	7	0.15	0.03	0.14
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG22	7	0.15	0.03	0.14
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG23	7	0.15	0.03	0.14
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG21	7	0.15	0.03	0.14
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG22	7	0.15	0.03	0.14
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG23	7	0.15	0.03	0.14
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG21	7	0.15	0.03	0.14
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG22	7	0.15	0.03	0.14
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG23	7	0.15	0.03	0.14
(2,780)	1:B:303:HIS:HA	1:B:307:GLY:H	7	0.15	0.02	0.15
(4,61)	1:B:273:PRO:O	1:B:277:THR:H	7	0.15	0.03	0.15
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG21	7	0.14	0.02	0.13
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG22	7	0.14	0.02	0.13
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG23	7	0.14	0.02	0.13
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD1	7	0.14	0.03	0.13
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD2	7	0.14	0.03	0.13
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD11	7	0.13	0.02	0.12
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD12	7	0.13	0.02	0.12
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD13	7	0.13	0.02	0.12
(2,767)	1:B:301:GLY:H	1:B:302:THR:H	7	0.13	0.01	0.13
(1,48)	1:A:18:VAL:H	1:A:55:LEU:HA	7	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,152)	1:A:24:PHE:HD1	1:A:25:MET:HA	6	0.17	0.06	0.16
(1,152)	1:A:24:PHE:HD2	1:A:25:MET:HA	6	0.17	0.06	0.16
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD1	6	0.17	0.02	0.18
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD2	6	0.17	0.02	0.18
(2,152)	1:B:224:PHE:HD1	1:B:225:MET:HA	6	0.17	0.05	0.16
(2,152)	1:B:224:PHE:HD2	1:B:225:MET:HA	6	0.17	0.05	0.16
(1,459)	1:A:65:ALA:HA	1:A:66:TRP:HE1	6	0.16	0.04	0.15
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG21	6	0.16	0.03	0.16
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG22	6	0.16	0.03	0.16
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG23	6	0.16	0.03	0.16
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG21	6	0.16	0.03	0.16
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG22	6	0.16	0.03	0.16
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG23	6	0.16	0.03	0.16
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG21	6	0.16	0.03	0.16
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG22	6	0.16	0.03	0.16
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG23	6	0.16	0.03	0.16
(2,446)	1:B:260:ALA:HB1	1:B:262:ARG:HA	6	0.16	0.03	0.16
(2,446)	1:B:260:ALA:HB2	1:B:262:ARG:HA	6	0.16	0.03	0.16
(2,446)	1:B:260:ALA:HB3	1:B:262:ARG:HA	6	0.16	0.03	0.16
(4,135)	1:B:333:ARG:O	1:B:337:THR:H	6	0.15	0.03	0.15
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE1	6	0.14	0.02	0.15
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE2	6	0.14	0.02	0.15
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE1	6	0.14	0.02	0.15
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE2	6	0.14	0.02	0.15
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE1	6	0.14	0.02	0.15
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE2	6	0.14	0.02	0.15
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD11	6	0.13	0.02	0.13
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD12	6	0.13	0.02	0.13
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD13	6	0.13	0.02	0.13
(4,132)	1:B:331:LEU:O	1:B:335:LEU:N	6	0.13	0.01	0.12
(3,103)	1:A:106:ILE:O	1:A:110:SER:H	6	0.12	0.01	0.12
(2,48)	1:B:218:VAL:H	1:B:255:LEU:HA	6	0.12	0.01	0.12
(2,569)	1:B:279:LEU:HA	1:B:282:LEU:H	6	0.12	0.01	0.12
(2,459)	1:B:265:ALA:HA	1:B:266:TRP:HE1	5	0.19	0.04	0.19
(1,446)	1:A:60:ALA:HB1	1:A:62:ARG:HA	5	0.17	0.04	0.16
(1,446)	1:A:60:ALA:HB2	1:A:62:ARG:HA	5	0.17	0.04	0.16
(1,446)	1:A:60:ALA:HB3	1:A:62:ARG:HA	5	0.17	0.04	0.16
(1,201)	1:A:27:LEU:HD21	1:B:330:PHE:HE1	5	0.16	0.03	0.15
(1,201)	1:A:27:LEU:HD21	1:B:330:PHE:HE2	5	0.16	0.03	0.15
(1,201)	1:A:27:LEU:HD22	1:B:330:PHE:HE1	5	0.16	0.03	0.15
(1,201)	1:A:27:LEU:HD22	1:B:330:PHE:HE2	5	0.16	0.03	0.15
(1,201)	1:A:27:LEU:HD23	1:B:330:PHE:HE1	5	0.16	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,201)	1:A:27:LEU:HD23	1:B:330:PHE:HE2	5	0.16	0.03	0.15
(2,373)	1:B:249:HIS:HA	1:B:253:GLN:H	5	0.14	0.01	0.14
(1,582)	1:A:82:LEU:HA	1:A:85:ARG:H	5	0.14	0.02	0.14
(1,767)	1:A:101:GLY:H	1:A:102:THR:H	5	0.14	0.02	0.14
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD21	5	0.14	0.04	0.12
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD22	5	0.14	0.04	0.12
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD23	5	0.14	0.04	0.12
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD21	5	0.14	0.04	0.12
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD22	5	0.14	0.04	0.12
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD23	5	0.14	0.04	0.12
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD21	5	0.14	0.04	0.12
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD22	5	0.14	0.04	0.12
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD23	5	0.14	0.04	0.12
(1,373)	1:A:49:HIS:HA	1:A:53:GLN:H	5	0.14	0.01	0.14
(1,791)	1:A:104:VAL:H	1:A:105:GLU:H	5	0.13	0.02	0.13
(2,271)	1:B:241:LEU:HD11	1:B:266:TRP:HZ2	5	0.13	0.02	0.13
(2,271)	1:B:241:LEU:HD12	1:B:266:TRP:HZ2	5	0.13	0.02	0.13
(2,271)	1:B:241:LEU:HD13	1:B:266:TRP:HZ2	5	0.13	0.02	0.13
(2,791)	1:B:304:VAL:H	1:B:305:GLU:H	5	0.13	0.02	0.12
(4,103)	1:B:306:ILE:O	1:B:310:SER:H	5	0.13	0.01	0.14
(2,582)	1:B:282:LEU:HA	1:B:285:ARG:H	5	0.13	0.01	0.13
(3,132)	1:A:131:LEU:O	1:A:135:LEU:N	5	0.13	0.02	0.12
(2,623)	1:B:285:ARG:HD2	1:B:312:PHE:HD1	5	0.12	0.0	0.12
(2,623)	1:B:285:ARG:HD2	1:B:312:PHE:HD2	5	0.12	0.0	0.12
(2,623)	1:B:285:ARG:HD3	1:B:312:PHE:HD1	5	0.12	0.0	0.12
(2,623)	1:B:285:ARG:HD3	1:B:312:PHE:HD2	5	0.12	0.0	0.12
(1,1188)	1:A:144:VAL:HG21	1:A:155:GLN:H	5	0.12	0.01	0.12
(1,1188)	1:A:144:VAL:HG22	1:A:155:GLN:H	5	0.12	0.01	0.12
(1,1188)	1:A:144:VAL:HG23	1:A:155:GLN:H	5	0.12	0.01	0.12
(4,27)	1:B:239:GLU:O	1:B:243:PHE:H	5	0.12	0.01	0.12
(3,98)	1:A:103:HIS:O	1:A:107:GLY:N	5	0.11	0.0	0.11
(1,1205)	1:A:146:TYR:HE1	1:A:147:LYS:HA	4	0.22	0.01	0.22
(1,1205)	1:A:146:TYR:HE2	1:A:147:LYS:HA	4	0.22	0.01	0.22
(2,460)	1:B:265:ALA:HA	1:B:266:TRP:HD1	4	0.22	0.1	0.21
(2,1205)	1:B:346:TYR:HE1	1:B:347:LYS:HA	4	0.21	0.01	0.22
(2,1205)	1:B:346:TYR:HE2	1:B:347:LYS:HA	4	0.21	0.01	0.22
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG21	4	0.17	0.04	0.18
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG22	4	0.17	0.04	0.18
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG23	4	0.17	0.04	0.18
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG21	4	0.17	0.03	0.18
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG22	4	0.17	0.03	0.18
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG23	4	0.17	0.03	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,487)	1:A:71:LEU:HA	1:A:72:THR:H	4	0.16	0.04	0.15
(3,61)	1:A:73:PRO:O	1:A:77:THR:H	4	0.16	0.01	0.16
(1,271)	1:A:41:LEU:HD11	1:A:66:TRP:HZ2	4	0.15	0.03	0.16
(1,271)	1:A:41:LEU:HD12	1:A:66:TRP:HZ2	4	0.15	0.03	0.16
(1,271)	1:A:41:LEU:HD13	1:A:66:TRP:HZ2	4	0.15	0.03	0.16
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD21	4	0.14	0.04	0.12
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD22	4	0.14	0.04	0.12
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD23	4	0.14	0.04	0.12
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD21	4	0.14	0.04	0.12
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD22	4	0.14	0.04	0.12
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD23	4	0.14	0.04	0.12
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD21	4	0.14	0.04	0.12
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD22	4	0.14	0.04	0.12
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD23	4	0.14	0.04	0.12
(1,1184)	1:A:144:VAL:HG11	1:A:146:TYR:HD1	4	0.14	0.02	0.14
(1,1184)	1:A:144:VAL:HG11	1:A:146:TYR:HD2	4	0.14	0.02	0.14
(1,1184)	1:A:144:VAL:HG12	1:A:146:TYR:HD1	4	0.14	0.02	0.14
(1,1184)	1:A:144:VAL:HG12	1:A:146:TYR:HD2	4	0.14	0.02	0.14
(1,1184)	1:A:144:VAL:HG13	1:A:146:TYR:HD1	4	0.14	0.02	0.14
(1,1184)	1:A:144:VAL:HG13	1:A:146:TYR:HD2	4	0.14	0.02	0.14
(1,502)	1:A:72:THR:H	1:A:74:GLU:H	4	0.13	0.03	0.12
(1,906)	1:A:116:ILE:HG12	1:A:117:VAL:H	4	0.13	0.02	0.13
(4,36)	1:B:243:PHE:O	1:B:247:ILE:N	4	0.13	0.02	0.12
(1,239)	1:A:34:SER:HB2	1:A:35:MET:H	4	0.13	0.02	0.12
(1,239)	1:A:34:SER:HB3	1:A:35:MET:H	4	0.13	0.02	0.12
(3,75)	1:A:81:GLN:O	1:A:85:ARG:H	4	0.13	0.01	0.13
(1,569)	1:A:79:LEU:HA	1:A:82:LEU:H	4	0.12	0.01	0.12
(2,1188)	1:B:344:VAL:HG21	1:B:355:GLN:H	4	0.12	0.01	0.12
(2,1188)	1:B:344:VAL:HG22	1:B:355:GLN:H	4	0.12	0.01	0.12
(2,1188)	1:B:344:VAL:HG23	1:B:355:GLN:H	4	0.12	0.01	0.12
(3,27)	1:A:39:GLU:O	1:A:43:PHE:H	4	0.12	0.01	0.12
(1,1075)	1:A:125:GLU:HA	1:A:128:TYR:HB2	4	0.12	0.01	0.11
(4,98)	1:B:303:HIS:O	1:B:307:GLY:N	4	0.11	0.0	0.11
(1,460)	1:A:65:ALA:HA	1:A:66:TRP:HD1	3	0.26	0.09	0.31
(1,225)	1:A:30:PRO:HD2	1:A:70:VAL:HG11	3	0.18	0.02	0.18
(1,225)	1:A:30:PRO:HD2	1:A:70:VAL:HG12	3	0.18	0.02	0.18
(1,225)	1:A:30:PRO:HD2	1:A:70:VAL:HG13	3	0.18	0.02	0.18
(1,225)	1:A:30:PRO:HD3	1:A:70:VAL:HG11	3	0.18	0.02	0.18
(1,225)	1:A:30:PRO:HD3	1:A:70:VAL:HG12	3	0.18	0.02	0.18
(1,225)	1:A:30:PRO:HD3	1:A:70:VAL:HG13	3	0.18	0.02	0.18
(2,225)	1:B:230:PRO:HD2	1:B:270:VAL:HG11	3	0.17	0.02	0.18
(2,225)	1:B:230:PRO:HD2	1:B:270:VAL:HG12	3	0.17	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,225)	1:B:230:PRO:HD2	1:B:270:VAL:HG13	3	0.17	0.02	0.18
(2,225)	1:B:230:PRO:HD3	1:B:270:VAL:HG11	3	0.17	0.02	0.18
(2,225)	1:B:230:PRO:HD3	1:B:270:VAL:HG12	3	0.17	0.02	0.18
(2,225)	1:B:230:PRO:HD3	1:B:270:VAL:HG13	3	0.17	0.02	0.18
(2,487)	1:B:271:LEU:HA	1:B:272:THR:H	3	0.17	0.03	0.15
(1,270)	1:A:41:LEU:HD11	1:A:66:TRP:HD1	3	0.16	0.05	0.14
(1,270)	1:A:41:LEU:HD12	1:A:66:TRP:HD1	3	0.16	0.05	0.14
(1,270)	1:A:41:LEU:HD13	1:A:66:TRP:HD1	3	0.16	0.05	0.14
(2,224)	1:B:230:PRO:HD2	1:B:270:VAL:HG21	3	0.16	0.02	0.16
(2,224)	1:B:230:PRO:HD2	1:B:270:VAL:HG22	3	0.16	0.02	0.16
(2,224)	1:B:230:PRO:HD2	1:B:270:VAL:HG23	3	0.16	0.02	0.16
(2,224)	1:B:230:PRO:HD3	1:B:270:VAL:HG21	3	0.16	0.02	0.16
(2,224)	1:B:230:PRO:HD3	1:B:270:VAL:HG22	3	0.16	0.02	0.16
(2,224)	1:B:230:PRO:HD3	1:B:270:VAL:HG23	3	0.16	0.02	0.16
(1,233)	1:A:32:THR:HA	1:A:33:ASN:H	3	0.15	0.04	0.15
(2,233)	1:B:232:THR:HA	1:B:233:ASN:H	3	0.15	0.04	0.14
(4,21)	1:B:229:ASN:O	1:B:232:THR:H	3	0.15	0.02	0.14
(1,224)	1:A:30:PRO:HD2	1:A:70:VAL:HG21	3	0.14	0.02	0.13
(1,224)	1:A:30:PRO:HD2	1:A:70:VAL:HG22	3	0.14	0.02	0.13
(1,224)	1:A:30:PRO:HD2	1:A:70:VAL:HG23	3	0.14	0.02	0.13
(1,224)	1:A:30:PRO:HD3	1:A:70:VAL:HG21	3	0.14	0.02	0.13
(1,224)	1:A:30:PRO:HD3	1:A:70:VAL:HG22	3	0.14	0.02	0.13
(1,224)	1:A:30:PRO:HD3	1:A:70:VAL:HG23	3	0.14	0.02	0.13
(1,1115)	1:A:135:LEU:H	1:A:143:PHE:HZ	3	0.14	0.02	0.14
(2,590)	1:B:282:LEU:HD11	1:A:110:SER:HB2	3	0.14	0.01	0.14
(2,590)	1:B:282:LEU:HD11	1:A:110:SER:HB3	3	0.14	0.01	0.14
(2,590)	1:B:282:LEU:HD12	1:A:110:SER:HB2	3	0.14	0.01	0.14
(2,590)	1:B:282:LEU:HD12	1:A:110:SER:HB3	3	0.14	0.01	0.14
(2,590)	1:B:282:LEU:HD13	1:A:110:SER:HB2	3	0.14	0.01	0.14
(2,590)	1:B:282:LEU:HD13	1:A:110:SER:HB3	3	0.14	0.01	0.14
(2,590)	1:B:282:LEU:HD21	1:A:110:SER:HB2	3	0.14	0.01	0.14
(2,590)	1:B:282:LEU:HD21	1:A:110:SER:HB3	3	0.14	0.01	0.14
(2,590)	1:B:282:LEU:HD22	1:A:110:SER:HB2	3	0.14	0.01	0.14
(2,590)	1:B:282:LEU:HD22	1:A:110:SER:HB3	3	0.14	0.01	0.14
(2,590)	1:B:282:LEU:HD23	1:A:110:SER:HB2	3	0.14	0.01	0.14
(2,590)	1:B:282:LEU:HD23	1:A:110:SER:HB3	3	0.14	0.01	0.14
(1,720)	1:A:94:PRO:HA	1:A:103:HIS:HE1	3	0.14	0.02	0.14
(2,237)	1:B:233:ASN:HB2	1:B:270:VAL:HG11	3	0.13	0.02	0.12
(2,237)	1:B:233:ASN:HB2	1:B:270:VAL:HG12	3	0.13	0.02	0.12
(2,237)	1:B:233:ASN:HB2	1:B:270:VAL:HG13	3	0.13	0.02	0.12
(2,237)	1:B:233:ASN:HB3	1:B:270:VAL:HG11	3	0.13	0.02	0.12
(2,237)	1:B:233:ASN:HB3	1:B:270:VAL:HG12	3	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,237)	1:B:233:ASN:HB3	1:B:270:VAL:HG13	3	0.13	0.02	0.12
(1,418)	1:A:53:GLN:H	1:A:55:LEU:H	3	0.13	0.01	0.13
(3,128)	1:A:129:GLY:O	1:A:133:ARG:N	3	0.13	0.03	0.11
(1,389)	1:A:50:PHE:HD1	1:A:55:LEU:HD11	3	0.13	0.01	0.13
(1,389)	1:A:50:PHE:HD1	1:A:55:LEU:HD12	3	0.13	0.01	0.13
(1,389)	1:A:50:PHE:HD1	1:A:55:LEU:HD13	3	0.13	0.01	0.13
(1,389)	1:A:50:PHE:HD2	1:A:55:LEU:HD11	3	0.13	0.01	0.13
(1,389)	1:A:50:PHE:HD2	1:A:55:LEU:HD12	3	0.13	0.01	0.13
(1,389)	1:A:50:PHE:HD2	1:A:55:LEU:HD13	3	0.13	0.01	0.13
(2,906)	1:B:316:ILE:HG12	1:B:317:VAL:H	3	0.13	0.01	0.13
(1,631)	1:A:87:ALA:HB1	1:A:90:PHE:HE1	3	0.12	0.0	0.12
(1,631)	1:A:87:ALA:HB1	1:A:90:PHE:HE2	3	0.12	0.0	0.12
(1,631)	1:A:87:ALA:HB2	1:A:90:PHE:HE1	3	0.12	0.0	0.12
(1,631)	1:A:87:ALA:HB2	1:A:90:PHE:HE2	3	0.12	0.0	0.12
(1,631)	1:A:87:ALA:HB3	1:A:90:PHE:HE1	3	0.12	0.0	0.12
(1,631)	1:A:87:ALA:HB3	1:A:90:PHE:HE2	3	0.12	0.0	0.12
(2,1075)	1:B:325:GLU:HA	1:B:328:TYR:HB2	3	0.12	0.01	0.12
(3,100)	1:A:104:VAL:O	1:A:108:TRP:N	3	0.12	0.01	0.12
(1,477)	1:A:69:GLN:HB2	1:A:71:LEU:HD11	3	0.12	0.01	0.12
(1,477)	1:A:69:GLN:HB2	1:A:71:LEU:HD12	3	0.12	0.01	0.12
(1,477)	1:A:69:GLN:HB2	1:A:71:LEU:HD13	3	0.12	0.01	0.12
(1,477)	1:A:69:GLN:HB3	1:A:71:LEU:HD11	3	0.12	0.01	0.12
(1,477)	1:A:69:GLN:HB3	1:A:71:LEU:HD12	3	0.12	0.01	0.12
(1,477)	1:A:69:GLN:HB3	1:A:71:LEU:HD13	3	0.12	0.01	0.12
(1,1064)	1:A:125:GLU:H	1:A:126:GLU:H	3	0.12	0.0	0.12
(1,590)	1:A:82:LEU:HD11	1:B:310:SER:HB2	3	0.11	0.0	0.11
(1,590)	1:A:82:LEU:HD11	1:B:310:SER:HB3	3	0.11	0.0	0.11
(1,590)	1:A:82:LEU:HD12	1:B:310:SER:HB2	3	0.11	0.0	0.11
(1,590)	1:A:82:LEU:HD12	1:B:310:SER:HB3	3	0.11	0.0	0.11
(1,590)	1:A:82:LEU:HD13	1:B:310:SER:HB2	3	0.11	0.0	0.11
(1,590)	1:A:82:LEU:HD13	1:B:310:SER:HB3	3	0.11	0.0	0.11
(1,590)	1:A:82:LEU:HD21	1:B:310:SER:HB2	3	0.11	0.0	0.11
(1,590)	1:A:82:LEU:HD21	1:B:310:SER:HB3	3	0.11	0.0	0.11
(1,590)	1:A:82:LEU:HD22	1:B:310:SER:HB2	3	0.11	0.0	0.11
(1,590)	1:A:82:LEU:HD22	1:B:310:SER:HB3	3	0.11	0.0	0.11
(1,590)	1:A:82:LEU:HD23	1:B:310:SER:HB2	3	0.11	0.0	0.11
(1,590)	1:A:82:LEU:HD23	1:B:310:SER:HB3	3	0.11	0.0	0.11
(3,21)	1:A:29:ASN:O	1:A:32:THR:H	3	0.11	0.0	0.11
(1,1222)	1:A:149:ILE:H	1:A:150:ALA:H	3	0.11	0.0	0.11
(2,270)	1:B:241:LEU:HD11	1:B:266:TRP:HD1	2	0.16	0.05	0.16
(2,270)	1:B:241:LEU:HD12	1:B:266:TRP:HD1	2	0.16	0.05	0.16
(2,270)	1:B:241:LEU:HD13	1:B:266:TRP:HD1	2	0.16	0.05	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,844)	1:A:108:TRP:HE3	1:B:331:LEU:HD21	2	0.16	0.01	0.16
(1,844)	1:A:108:TRP:HE3	1:B:331:LEU:HD22	2	0.16	0.01	0.16
(1,844)	1:A:108:TRP:HE3	1:B:331:LEU:HD23	2	0.16	0.01	0.16
(2,210)	1:B:228:VAL:HG11	1:B:233:ASN:HA	2	0.15	0.02	0.15
(2,210)	1:B:228:VAL:HG12	1:B:233:ASN:HA	2	0.15	0.02	0.15
(2,210)	1:B:228:VAL:HG13	1:B:233:ASN:HA	2	0.15	0.02	0.15
(2,150)	1:B:224:PHE:HA	1:B:270:VAL:HG11	2	0.15	0.0	0.15
(2,150)	1:B:224:PHE:HA	1:B:270:VAL:HG12	2	0.15	0.0	0.15
(2,150)	1:B:224:PHE:HA	1:B:270:VAL:HG13	2	0.15	0.0	0.15
(2,239)	1:B:234:SER:HB2	1:B:235:MET:H	2	0.15	0.03	0.15
(2,239)	1:B:234:SER:HB3	1:B:235:MET:H	2	0.15	0.03	0.15
(2,720)	1:B:294:PRO:HA	1:B:303:HIS:HE1	2	0.15	0.0	0.15
(4,128)	1:B:329:GLY:O	1:B:333:ARG:N	2	0.15	0.02	0.15
(1,1120)	1:A:135:LEU:HA	1:A:138:VAL:HG21	2	0.14	0.02	0.14
(1,1120)	1:A:135:LEU:HA	1:A:138:VAL:HG22	2	0.14	0.02	0.14
(1,1120)	1:A:135:LEU:HA	1:A:138:VAL:HG23	2	0.14	0.02	0.14
(2,418)	1:B:253:GLN:H	1:B:255:LEU:H	2	0.14	0.0	0.14
(2,502)	1:B:272:THR:H	1:B:274:GLU:H	2	0.14	0.03	0.14
(2,1115)	1:B:335:LEU:H	1:B:343:PHE:HZ	2	0.14	0.03	0.14
(4,75)	1:B:281:GLN:O	1:B:285:ARG:H	2	0.14	0.01	0.14
(1,150)	1:A:24:PHE:HA	1:A:70:VAL:HG11	2	0.14	0.01	0.14
(1,150)	1:A:24:PHE:HA	1:A:70:VAL:HG12	2	0.14	0.01	0.14
(1,150)	1:A:24:PHE:HA	1:A:70:VAL:HG13	2	0.14	0.01	0.14
(1,228)	1:A:31:GLU:HA	1:A:32:THR:H	2	0.14	0.02	0.14
(1,491)	1:A:71:LEU:HD21	1:A:72:THR:H	2	0.14	0.01	0.14
(1,491)	1:A:71:LEU:HD22	1:A:72:THR:H	2	0.14	0.01	0.14
(1,491)	1:A:71:LEU:HD23	1:A:72:THR:H	2	0.14	0.01	0.14
(2,389)	1:B:250:PHE:HD1	1:B:255:LEU:HD11	2	0.14	0.01	0.14
(2,389)	1:B:250:PHE:HD1	1:B:255:LEU:HD12	2	0.14	0.01	0.14
(2,389)	1:B:250:PHE:HD1	1:B:255:LEU:HD13	2	0.14	0.01	0.14
(2,389)	1:B:250:PHE:HD2	1:B:255:LEU:HD11	2	0.14	0.01	0.14
(2,389)	1:B:250:PHE:HD2	1:B:255:LEU:HD12	2	0.14	0.01	0.14
(2,389)	1:B:250:PHE:HD2	1:B:255:LEU:HD13	2	0.14	0.01	0.14
(2,449)	1:B:262:ARG:HA	1:B:266:TRP:HD1	2	0.14	0.01	0.14
(2,491)	1:B:271:LEU:HD21	1:B:272:THR:H	2	0.14	0.01	0.14
(2,491)	1:B:271:LEU:HD22	1:B:272:THR:H	2	0.14	0.01	0.14
(2,491)	1:B:271:LEU:HD23	1:B:272:THR:H	2	0.14	0.01	0.14
(2,1184)	1:B:344:VAL:HG11	1:B:346:TYR:HD1	2	0.14	0.01	0.14
(2,1184)	1:B:344:VAL:HG11	1:B:346:TYR:HD2	2	0.14	0.01	0.14
(2,1184)	1:B:344:VAL:HG12	1:B:346:TYR:HD1	2	0.14	0.01	0.14
(2,1184)	1:B:344:VAL:HG12	1:B:346:TYR:HD2	2	0.14	0.01	0.14
(2,1184)	1:B:344:VAL:HG13	1:B:346:TYR:HD1	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)
(2,1184)	1:B:344:VAL:HG13	1:B:346:TYR:HD2	2	0.14	0.01	0.14
(3,108)	1:A:108:TRP:O	1:A:112:PHE:N	2	0.14	0.01	0.14
(4,96)	1:B:302:THR:O	1:B:306:ILE:N	2	0.14	0.02	0.14
(1,622)	1:A:85:ARG:HG2	1:A:112:PHE:HD1	2	0.13	0.0	0.13
(1,622)	1:A:85:ARG:HG2	1:A:112:PHE:HD2	2	0.13	0.0	0.13
(1,622)	1:A:85:ARG:HG3	1:A:112:PHE:HD1	2	0.13	0.0	0.13
(1,622)	1:A:85:ARG:HG3	1:A:112:PHE:HD2	2	0.13	0.0	0.13
(2,209)	1:B:228:VAL:HG11	1:B:231:GLU:HA	2	0.13	0.02	0.13
(2,209)	1:B:228:VAL:HG12	1:B:231:GLU:HA	2	0.13	0.02	0.13
(2,209)	1:B:228:VAL:HG13	1:B:231:GLU:HA	2	0.13	0.02	0.13
(2,477)	1:B:269:GLN:HB2	1:B:271:LEU:HD11	2	0.13	0.01	0.13
(2,477)	1:B:269:GLN:HB2	1:B:271:LEU:HD12	2	0.13	0.01	0.13
(2,477)	1:B:269:GLN:HB2	1:B:271:LEU:HD13	2	0.13	0.01	0.13
(2,477)	1:B:269:GLN:HB3	1:B:271:LEU:HD11	2	0.13	0.01	0.13
(2,477)	1:B:269:GLN:HB3	1:B:271:LEU:HD12	2	0.13	0.01	0.13
(2,477)	1:B:269:GLN:HB3	1:B:271:LEU:HD13	2	0.13	0.01	0.13
(2,622)	1:B:285:ARG:HG2	1:B:312:PHE:HD1	2	0.13	0.0	0.13
(2,622)	1:B:285:ARG:HG2	1:B:312:PHE:HD2	2	0.13	0.0	0.13
(2,622)	1:B:285:ARG:HG3	1:B:312:PHE:HD1	2	0.13	0.0	0.13
(2,622)	1:B:285:ARG:HG3	1:B:312:PHE:HD2	2	0.13	0.0	0.13
(3,58)	1:A:64:GLU:O	1:A:68:ALA:N	2	0.13	0.02	0.13
(1,1198)	1:A:144:VAL:HG21	1:A:159:ALA:HB1	2	0.12	0.01	0.12
(1,1198)	1:A:144:VAL:HG21	1:A:159:ALA:HB2	2	0.12	0.01	0.12
(1,1198)	1:A:144:VAL:HG21	1:A:159:ALA:HB3	2	0.12	0.01	0.12
(1,1198)	1:A:144:VAL:HG22	1:A:159:ALA:HB1	2	0.12	0.01	0.12
(1,1198)	1:A:144:VAL:HG22	1:A:159:ALA:HB2	2	0.12	0.01	0.12
(1,1198)	1:A:144:VAL:HG22	1:A:159:ALA:HB3	2	0.12	0.01	0.12
(1,1198)	1:A:144:VAL:HG23	1:A:159:ALA:HB1	2	0.12	0.01	0.12
(1,1198)	1:A:144:VAL:HG23	1:A:159:ALA:HB2	2	0.12	0.01	0.12
(1,1198)	1:A:144:VAL:HG23	1:A:159:ALA:HB3	2	0.12	0.01	0.12
(4,108)	1:B:308:TRP:O	1:B:312:PHE:N	2	0.12	0.02	0.12
(1,237)	1:A:33:ASN:HB2	1:A:70:VAL:HG11	2	0.12	0.01	0.12
(1,237)	1:A:33:ASN:HB2	1:A:70:VAL:HG12	2	0.12	0.01	0.12
(1,237)	1:A:33:ASN:HB2	1:A:70:VAL:HG13	2	0.12	0.01	0.12
(1,237)	1:A:33:ASN:HB3	1:A:70:VAL:HG11	2	0.12	0.01	0.12
(1,237)	1:A:33:ASN:HB3	1:A:70:VAL:HG12	2	0.12	0.01	0.12
(1,237)	1:A:33:ASN:HB3	1:A:70:VAL:HG13	2	0.12	0.01	0.12
(1,430)	1:A:55:LEU:HD21	1:A:56:GLU:H	2	0.12	0.01	0.12
(1,430)	1:A:55:LEU:HD22	1:A:56:GLU:H	2	0.12	0.01	0.12
(1,430)	1:A:55:LEU:HD23	1:A:56:GLU:H	2	0.12	0.01	0.12
(1,610)	1:A:84:ILE:HG21	1:A:108:TRP:HZ3	2	0.12	0.0	0.12
(1,610)	1:A:84:ILE:HG22	1:A:108:TRP:HZ3	2	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,610)	1:A:84:ILE:HG23	1:A:108:TRP:HZ3	2	0.12	0.0	0.12
(1,1179)	1:A:143:PHE:HA	1:A:144:VAL:HG21	2	0.12	0.0	0.12
(1,1179)	1:A:143:PHE:HA	1:A:144:VAL:HG22	2	0.12	0.0	0.12
(1,1179)	1:A:143:PHE:HA	1:A:144:VAL:HG23	2	0.12	0.0	0.12
(2,833)	1:B:308:TRP:H	1:B:309:ALA:H	2	0.12	0.0	0.12
(2,834)	1:B:308:TRP:HA	1:B:311:ALA:H	2	0.12	0.01	0.12
(2,1002)	1:B:320:LEU:HD11	1:B:325:GLU:HB2	2	0.12	0.01	0.12
(2,1002)	1:B:320:LEU:HD11	1:B:325:GLU:HB3	2	0.12	0.01	0.12
(2,1002)	1:B:320:LEU:HD12	1:B:325:GLU:HB2	2	0.12	0.01	0.12
(2,1002)	1:B:320:LEU:HD12	1:B:325:GLU:HB3	2	0.12	0.01	0.12
(2,1002)	1:B:320:LEU:HD13	1:B:325:GLU:HB2	2	0.12	0.01	0.12
(2,1002)	1:B:320:LEU:HD13	1:B:325:GLU:HB3	2	0.12	0.01	0.12
(2,1050)	1:B:322:GLU:HB2	1:B:346:TYR:H	2	0.12	0.0	0.12
(2,1050)	1:B:322:GLU:HB3	1:B:346:TYR:H	2	0.12	0.0	0.12
(2,1101)	1:B:332:VAL:H	1:B:333:ARG:H	2	0.12	0.01	0.12
(2,1198)	1:B:344:VAL:HG21	1:B:359:ALA:HB1	2	0.12	0.0	0.12
(2,1198)	1:B:344:VAL:HG21	1:B:359:ALA:HB2	2	0.12	0.0	0.12
(2,1198)	1:B:344:VAL:HG21	1:B:359:ALA:HB3	2	0.12	0.0	0.12
(2,1198)	1:B:344:VAL:HG22	1:B:359:ALA:HB1	2	0.12	0.0	0.12
(2,1198)	1:B:344:VAL:HG22	1:B:359:ALA:HB2	2	0.12	0.0	0.12
(2,1198)	1:B:344:VAL:HG22	1:B:359:ALA:HB3	2	0.12	0.0	0.12
(2,1198)	1:B:344:VAL:HG23	1:B:359:ALA:HB1	2	0.12	0.0	0.12
(2,1198)	1:B:344:VAL:HG23	1:B:359:ALA:HB2	2	0.12	0.0	0.12
(2,1198)	1:B:344:VAL:HG23	1:B:359:ALA:HB3	2	0.12	0.0	0.12
(4,137)	1:B:334:GLY:O	1:B:338:VAL:H	2	0.12	0.0	0.12
(1,279)	1:A:43:PHE:HA	1:A:46:LEU:H	2	0.12	0.0	0.12
(1,449)	1:A:62:ARG:HA	1:A:66:TRP:HD1	2	0.12	0.0	0.12
(1,577)	1:A:81:GLN:HA	1:A:112:PHE:HD1	2	0.12	0.0	0.12
(1,577)	1:A:81:GLN:HA	1:A:112:PHE:HD2	2	0.12	0.0	0.12
(1,623)	1:A:85:ARG:HD2	1:A:112:PHE:HD1	2	0.12	0.0	0.12
(1,623)	1:A:85:ARG:HD2	1:A:112:PHE:HD2	2	0.12	0.0	0.12
(1,623)	1:A:85:ARG:HD3	1:A:112:PHE:HD1	2	0.12	0.0	0.12
(1,623)	1:A:85:ARG:HD3	1:A:112:PHE:HD2	2	0.12	0.0	0.12
(1,1101)	1:A:132:VAL:H	1:A:133:ARG:H	2	0.12	0.0	0.12
(1,1210)	1:A:146:TYR:HD1	1:A:152:ALA:HA	2	0.12	0.0	0.12
(1,1210)	1:A:146:TYR:HD2	1:A:152:ALA:HA	2	0.12	0.0	0.12
(2,176)	1:B:225:MET:HA	1:B:228:VAL:HG11	2	0.12	0.0	0.12
(2,176)	1:B:225:MET:HA	1:B:228:VAL:HG12	2	0.12	0.0	0.12
(2,176)	1:B:225:MET:HA	1:B:228:VAL:HG13	2	0.12	0.0	0.12
(2,577)	1:B:281:GLN:HA	1:B:312:PHE:HD1	2	0.12	0.0	0.12
(2,577)	1:B:281:GLN:HA	1:B:312:PHE:HD2	2	0.12	0.0	0.12
(2,716)	1:B:294:PRO:HA	1:B:298:PRO:HA	2	0.12	0.0	0.12

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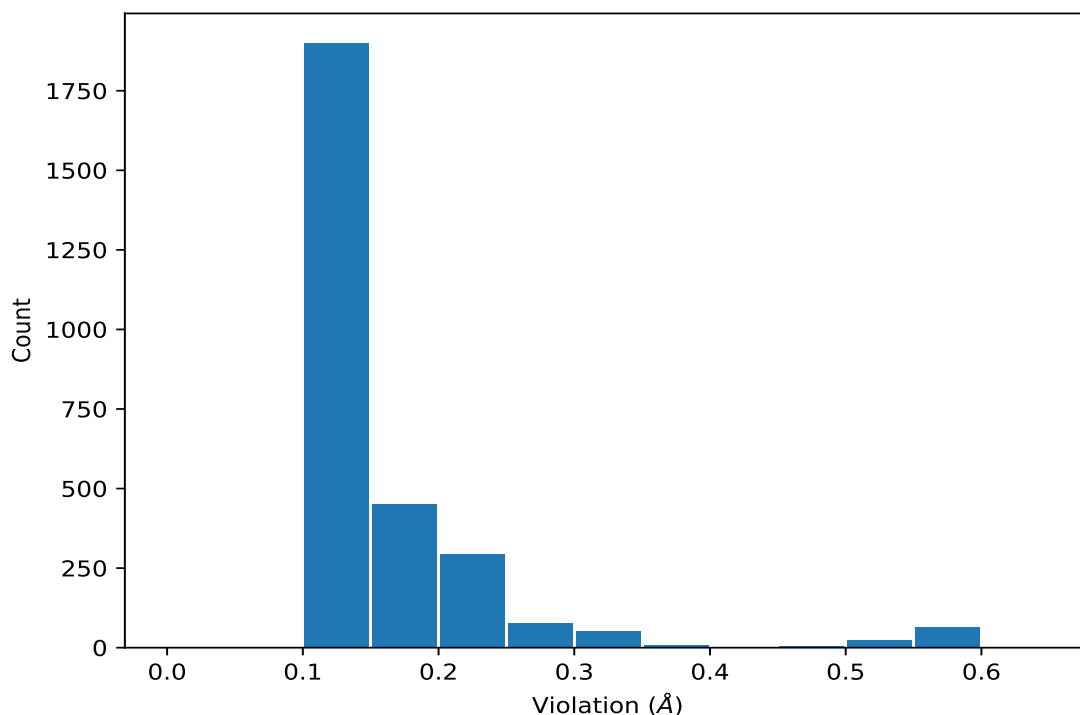
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1179)	1:B:343:PHE:HA	1:B:344:VAL:HG21	2	0.12	0.0	0.12
(2,1179)	1:B:343:PHE:HA	1:B:344:VAL:HG22	2	0.12	0.0	0.12
(2,1179)	1:B:343:PHE:HA	1:B:344:VAL:HG23	2	0.12	0.0	0.12
(4,105)	1:B:307:GLY:O	1:B:311:ALA:H	2	0.12	0.0	0.12
(4,121)	1:B:320:LEU:O	1:B:346:TYR:H	2	0.12	0.0	0.12
(1,879)	1:A:111:ALA:HB1	1:B:312:PHE:HD1	2	0.11	0.0	0.11
(1,879)	1:A:111:ALA:HB1	1:B:312:PHE:HD2	2	0.11	0.0	0.11
(1,879)	1:A:111:ALA:HB2	1:B:312:PHE:HD1	2	0.11	0.0	0.11
(1,879)	1:A:111:ALA:HB2	1:B:312:PHE:HD2	2	0.11	0.0	0.11
(1,879)	1:A:111:ALA:HB3	1:B:312:PHE:HD1	2	0.11	0.0	0.11
(1,879)	1:A:111:ALA:HB3	1:B:312:PHE:HD2	2	0.11	0.0	0.11
(2,430)	1:B:255:LEU:HD21	1:B:256:GLU:H	2	0.11	0.0	0.11
(2,430)	1:B:255:LEU:HD22	1:B:256:GLU:H	2	0.11	0.0	0.11
(2,430)	1:B:255:LEU:HD23	1:B:256:GLU:H	2	0.11	0.0	0.11
(2,537)	1:B:277:THR:HB	1:A:131:LEU:HD11	2	0.11	0.0	0.11
(2,537)	1:B:277:THR:HB	1:A:131:LEU:HD12	2	0.11	0.0	0.11
(2,537)	1:B:277:THR:HB	1:A:131:LEU:HD13	2	0.11	0.0	0.11
(2,998)	1:B:320:LEU:HA	1:B:346:TYR:HE1	2	0.11	0.0	0.11
(2,998)	1:B:320:LEU:HA	1:B:346:TYR:HE2	2	0.11	0.0	0.11
(3,39)	1:A:45:THR:O	1:A:49:HIS:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard 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)
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	15	0.63
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	15	0.62
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	3	0.6
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	8	0.6
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	10	0.6
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	5	0.6
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	5	0.6
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	5	0.6
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	5	0.6
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	7	0.6
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	7	0.6
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	6	0.59
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	12	0.59
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	6	0.59
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	6	0.59
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	3	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	6	0.59
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	11	0.59
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	2	0.59
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	2	0.59
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	5	0.58
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	9	0.58
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	11	0.58
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	7	0.58
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	7	0.58
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	1	0.58
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	10	0.58
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	12	0.58
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	6	0.58
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	6	0.58
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	1	0.57
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	2	0.57
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	7	0.57
(2,244)	1:B:236:PRO:HA	1:B:237:SER:H	10	0.57
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	2	0.57
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	2	0.57
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	4	0.57
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	4	0.57
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	2	0.57
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	5	0.57
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	7	0.57
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	8	0.57
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	9	0.57
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	13	0.57
(1,244)	1:A:36:PRO:HA	1:A:37:SER:H	10	0.57
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	1	0.57
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	1	0.57
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	13	0.56
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	1	0.56
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	1	0.56
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	8	0.56
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	8	0.56
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	8	0.56
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	8	0.56
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	4	0.55
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	13	0.55
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	13	0.55
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	14	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	14	0.55
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	14	0.55
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	4	0.55
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	4	0.55
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	9	0.55
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	9	0.55
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	14	0.55
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	14	0.55
(2,715)	1:B:294:PRO:HA	1:B:295:GLY:H	14	0.54
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	12	0.54
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	12	0.54
(1,715)	1:A:94:PRO:HA	1:A:95:GLY:H	4	0.54
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	13	0.54
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	13	0.54
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	15	0.54
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	15	0.54
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	9	0.53
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	9	0.53
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	15	0.53
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	15	0.53
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	3	0.53
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	3	0.53
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	12	0.53
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	12	0.53
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	3	0.52
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	3	0.52
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	10	0.52
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	10	0.52
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	10	0.51
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	10	0.51
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE1	11	0.49
(2,1083)	1:B:328:TYR:HA	1:B:328:TYR:HE2	11	0.49
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE1	11	0.49
(1,1083)	1:A:128:TYR:HA	1:A:128:TYR:HE2	11	0.49
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	13	0.39
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	13	0.39
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	13	0.38
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	13	0.38
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	10	0.37
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	10	0.37
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	1	0.36
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	8	0.35
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	8	0.35
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	8	0.35
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	1	0.35
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	1	0.35
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	5	0.35
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	5	0.35
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	10	0.35
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	10	0.35
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	5	0.34
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	5	0.34
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	15	0.34
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	15	0.34
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	4	0.34
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	4	0.34
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	9	0.34
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	9	0.34
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	8	0.33
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	8	0.33
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	8	0.33
(2,460)	1:B:265:ALA:HA	1:B:266:TRP:HD1	12	0.33
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	8	0.33
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	8	0.33
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	3	0.33
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	3	0.33
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	3	0.33
(1,460)	1:A:65:ALA:HA	1:A:66:TRP:HD1	12	0.33
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	15	0.33
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	15	0.33
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	3	0.32
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	3	0.32
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	3	0.32
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	11	0.32
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	11	0.32
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	3	0.32
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	3	0.32
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	8	0.32
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	8	0.32
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	11	0.32
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	11	0.32
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	9	0.32
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	4	0.31
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	4	0.31
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	9	0.31
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	9	0.31
(1,460)	1:A:65:ALA:HA	1:A:66:TRP:HD1	13	0.31
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	2	0.31
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	2	0.31
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	6	0.31
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	6	0.31
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	7	0.3
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	7	0.3
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	2	0.3
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	2	0.3
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	14	0.3
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	14	0.3
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	14	0.3
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	14	0.3
(2,783)	1:B:303:HIS:HD2	1:B:304:VAL:H	10	0.29
(2,460)	1:B:265:ALA:HA	1:B:266:TRP:HD1	13	0.29
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	3	0.29
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	3	0.29
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	9	0.29
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	9	0.29
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	2	0.28
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	2	0.28
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	1	0.28
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	1	0.28
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	6	0.28
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	6	0.28
(1,783)	1:A:103:HIS:HD2	1:A:104:VAL:H	10	0.28
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	2	0.28
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	2	0.28
(1,152)	1:A:24:PHE:HD1	1:A:25:MET:HA	10	0.28
(1,152)	1:A:24:PHE:HD2	1:A:25:MET:HA	10	0.28
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	12	0.28
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	12	0.28
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	15	0.27
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	15	0.27
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	14	0.27
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	14	0.27
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	2	0.27
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	7	0.27
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	7	0.27
(1,310)	1:A:45:THR:HG21	1:A:49:HIS:HB2	5	0.27
(1,310)	1:A:45:THR:HG21	1:A:49:HIS:HB3	5	0.27
(1,310)	1:A:45:THR:HG22	1:A:49:HIS:HB2	5	0.27
(1,310)	1:A:45:THR:HG22	1:A:49:HIS:HB3	5	0.27
(1,310)	1:A:45:THR:HG23	1:A:49:HIS:HB2	5	0.27
(1,310)	1:A:45:THR:HG23	1:A:49:HIS:HB3	5	0.27
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	11	0.26
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	13	0.26
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	3	0.26
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	3	0.26
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	4	0.26
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	4	0.26
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	12	0.26
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	12	0.26
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	9	0.25
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	10	0.25
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	10	0.25
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	8	0.25
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	8	0.25
(2,310)	1:B:245:THR:HG21	1:B:249:HIS:HB2	5	0.25
(2,310)	1:B:245:THR:HG21	1:B:249:HIS:HB3	5	0.25
(2,310)	1:B:245:THR:HG22	1:B:249:HIS:HB2	5	0.25
(2,310)	1:B:245:THR:HG22	1:B:249:HIS:HB3	5	0.25
(2,310)	1:B:245:THR:HG23	1:B:249:HIS:HB2	5	0.25
(2,310)	1:B:245:THR:HG23	1:B:249:HIS:HB3	5	0.25
(2,198)	1:B:227:LEU:HD11	1:B:269:GLN:HG2	11	0.25
(2,198)	1:B:227:LEU:HD11	1:B:269:GLN:HG3	11	0.25
(2,198)	1:B:227:LEU:HD12	1:B:269:GLN:HG2	11	0.25
(2,198)	1:B:227:LEU:HD12	1:B:269:GLN:HG3	11	0.25
(2,198)	1:B:227:LEU:HD13	1:B:269:GLN:HG2	11	0.25
(2,198)	1:B:227:LEU:HD13	1:B:269:GLN:HG3	11	0.25
(2,1084)	1:B:328:TYR:HB2	1:B:331:LEU:H	7	0.25
(2,1084)	1:B:328:TYR:HB3	1:B:331:LEU:H	7	0.25
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	8	0.25
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	8	0.25
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	9	0.25
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	9	0.25
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	1	0.25
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	1	0.25
(1,459)	1:A:65:ALA:HA	1:A:66:TRP:HE1	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	4	0.25
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	4	0.25
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	11	0.24
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	12	0.24
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	12	0.24
(2,783)	1:B:303:HIS:HD2	1:B:304:VAL:H	1	0.24
(2,783)	1:B:303:HIS:HD2	1:B:304:VAL:H	4	0.24
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	8	0.24
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	8	0.24
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	15	0.24
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	15	0.24
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	15	0.24
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	15	0.24
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	15	0.24
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	15	0.24
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	15	0.24
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	15	0.24
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	15	0.24
(2,459)	1:B:265:ALA:HA	1:B:266:TRP:HE1	9	0.24
(2,152)	1:B:224:PHE:HD1	1:B:225:MET:HA	10	0.24
(2,152)	1:B:224:PHE:HD2	1:B:225:MET:HA	10	0.24
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	4	0.24
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	4	0.24
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	11	0.24
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	11	0.24
(1,783)	1:A:103:HIS:HD2	1:A:104:VAL:H	4	0.24
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	10	0.24
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	10	0.24
(1,198)	1:A:27:LEU:HD11	1:A:69:GLN:HG2	11	0.24
(1,198)	1:A:27:LEU:HD11	1:A:69:GLN:HG3	11	0.24
(1,198)	1:A:27:LEU:HD12	1:A:69:GLN:HG2	11	0.24
(1,198)	1:A:27:LEU:HD12	1:A:69:GLN:HG3	11	0.24
(1,198)	1:A:27:LEU:HD13	1:A:69:GLN:HG2	11	0.24
(1,198)	1:A:27:LEU:HD13	1:A:69:GLN:HG3	11	0.24
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	1	0.23
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	3	0.23
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	13	0.23
(4,120)	1:B:344:VAL:O	1:B:320:LEU:N	15	0.23
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	1	0.23
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	9	0.23
(3,119)	1:A:144:VAL:O	1:A:120:LEU:H	2	0.23
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	9	0.23
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	14	0.23
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	14	0.23
(2,734)	1:B:296:ILE:H	1:B:325:GLU:HA	4	0.23
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG21	5	0.23
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG22	5	0.23
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG23	5	0.23
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	9	0.23
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	9	0.23
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	12	0.23
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	12	0.23
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	14	0.23
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	14	0.23
(1,270)	1:A:41:LEU:HD11	1:A:66:TRP:HD1	12	0.23
(1,270)	1:A:41:LEU:HD12	1:A:66:TRP:HD1	12	0.23
(1,270)	1:A:41:LEU:HD13	1:A:66:TRP:HD1	12	0.23
(1,1205)	1:A:146:TYR:HE1	1:A:147:LYS:HA	8	0.23
(1,1205)	1:A:146:TYR:HE2	1:A:147:LYS:HA	8	0.23
(1,1084)	1:A:128:TYR:HB2	1:A:131:LEU:H	7	0.23
(1,1084)	1:A:128:TYR:HB3	1:A:131:LEU:H	7	0.23
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	7	0.22
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	12	0.22
(4,120)	1:B:344:VAL:O	1:B:320:LEU:N	11	0.22
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	8	0.22
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	12	0.22
(3,120)	1:A:144:VAL:O	1:A:120:LEU:N	11	0.22
(3,120)	1:A:144:VAL:O	1:A:120:LEU:N	15	0.22
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	1	0.22
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	1	0.22
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	7	0.22
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	7	0.22
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	11	0.22
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	11	0.22
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	15	0.22
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	15	0.22
(2,459)	1:B:265:ALA:HA	1:B:266:TRP:HE1	11	0.22
(2,152)	1:B:224:PHE:HD1	1:B:225:MET:HA	14	0.22
(2,152)	1:B:224:PHE:HD2	1:B:225:MET:HA	14	0.22
(2,1205)	1:B:346:TYR:HE1	1:B:347:LYS:HA	11	0.22
(2,1205)	1:B:346:TYR:HE2	1:B:347:LYS:HA	11	0.22
(2,1205)	1:B:346:TYR:HE1	1:B:347:LYS:HA	15	0.22
(2,1205)	1:B:346:TYR:HE2	1:B:347:LYS:HA	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	14	0.22
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	14	0.22
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	15	0.22
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	15	0.22
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	15	0.22
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	1	0.22
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	1	0.22
(1,783)	1:A:103:HIS:HD2	1:A:104:VAL:H	1	0.22
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	8	0.22
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	8	0.22
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	9	0.22
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	9	0.22
(1,734)	1:A:96:ILE:H	1:A:125:GLU:HA	4	0.22
(1,487)	1:A:71:LEU:HA	1:A:72:THR:H	7	0.22
(1,446)	1:A:60:ALA:HB1	1:A:62:ARG:HA	14	0.22
(1,446)	1:A:60:ALA:HB2	1:A:62:ARG:HA	14	0.22
(1,446)	1:A:60:ALA:HB3	1:A:62:ARG:HA	14	0.22
(1,1205)	1:A:146:TYR:HE1	1:A:147:LYS:HA	3	0.22
(1,1205)	1:A:146:TYR:HE2	1:A:147:LYS:HA	3	0.22
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	5	0.22
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	5	0.22
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	9	0.22
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	9	0.22
(4,135)	1:B:333:ARG:O	1:B:337:THR:H	4	0.21
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	4	0.21
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	8	0.21
(4,120)	1:B:344:VAL:O	1:B:320:LEU:N	8	0.21
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	3	0.21
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	6	0.21
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	7	0.21
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	12	0.21
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	12	0.21
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	12	0.21
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	5	0.21
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	5	0.21
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD21	7	0.21
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD22	7	0.21
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD23	7	0.21
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD21	7	0.21
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD22	7	0.21
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD23	7	0.21
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD21	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD22	7	0.21
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD23	7	0.21
(2,783)	1:B:303:HIS:HD2	1:B:304:VAL:H	11	0.21
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	6	0.21
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	6	0.21
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	9	0.21
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	9	0.21
(2,487)	1:B:271:LEU:HA	1:B:272:THR:H	7	0.21
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	3	0.21
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	3	0.21
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	3	0.21
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	3	0.21
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	3	0.21
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	3	0.21
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	3	0.21
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	3	0.21
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	3	0.21
(2,270)	1:B:241:LEU:HD11	1:B:266:TRP:HD1	12	0.21
(2,270)	1:B:241:LEU:HD12	1:B:266:TRP:HD1	12	0.21
(2,270)	1:B:241:LEU:HD13	1:B:266:TRP:HD1	12	0.21
(2,1205)	1:B:346:TYR:HE1	1:B:347:LYS:HA	8	0.21
(2,1205)	1:B:346:TYR:HE2	1:B:347:LYS:HA	8	0.21
(2,1102)	1:B:332:VAL:HA	1:B:335:LEU:H	15	0.21
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	2	0.21
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	2	0.21
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	5	0.21
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	5	0.21
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	13	0.21
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	13	0.21
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	4	0.21
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	4	0.21
(1,783)	1:A:103:HIS:HD2	1:A:104:VAL:H	11	0.21
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	4	0.21
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	4	0.21
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	6	0.21
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	6	0.21
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	14	0.21
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	14	0.21
(1,201)	1:A:27:LEU:HD21	1:B:330:PHE:HE1	7	0.21
(1,201)	1:A:27:LEU:HD21	1:B:330:PHE:HE2	7	0.21
(1,201)	1:A:27:LEU:HD22	1:B:330:PHE:HE1	7	0.21
(1,201)	1:A:27:LEU:HD22	1:B:330:PHE:HE2	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:A:27:LEU:HD23	1:B:330:PHE:HE1	7	0.21
(1,201)	1:A:27:LEU:HD23	1:B:330:PHE:HE2	7	0.21
(1,152)	1:A:24:PHE:HD1	1:A:25:MET:HA	14	0.21
(1,152)	1:A:24:PHE:HD2	1:A:25:MET:HA	14	0.21
(1,1205)	1:A:146:TYR:HE1	1:A:147:LYS:HA	11	0.21
(1,1205)	1:A:146:TYR:HE2	1:A:147:LYS:HA	11	0.21
(1,1205)	1:A:146:TYR:HE1	1:A:147:LYS:HA	15	0.21
(1,1205)	1:A:146:TYR:HE2	1:A:147:LYS:HA	15	0.21
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	8	0.21
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	8	0.21
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	5	0.21
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	5	0.21
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	6	0.2
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	14	0.2
(4,119)	1:B:344:VAL:O	1:B:320:LEU:H	12	0.2
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	2	0.2
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	4	0.2
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	5	0.2
(3,129)	1:A:130:PHE:O	1:A:134:GLY:H	14	0.2
(3,120)	1:A:144:VAL:O	1:A:120:LEU:N	8	0.2
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	10	0.2
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	10	0.2
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	10	0.2
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	15	0.2
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	15	0.2
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	15	0.2
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	4	0.2
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	4	0.2
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	10	0.2
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	10	0.2
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	12	0.2
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	12	0.2
(2,233)	1:B:232:THR:HA	1:B:233:ASN:H	2	0.2
(2,225)	1:B:230:PRO:HD2	1:B:270:VAL:HG11	14	0.2
(2,225)	1:B:230:PRO:HD2	1:B:270:VAL:HG12	14	0.2
(2,225)	1:B:230:PRO:HD2	1:B:270:VAL:HG13	14	0.2
(2,225)	1:B:230:PRO:HD3	1:B:270:VAL:HG11	14	0.2
(2,225)	1:B:230:PRO:HD3	1:B:270:VAL:HG12	14	0.2
(2,225)	1:B:230:PRO:HD3	1:B:270:VAL:HG13	14	0.2
(2,1205)	1:B:346:TYR:HE1	1:B:347:LYS:HA	3	0.2
(2,1205)	1:B:346:TYR:HE2	1:B:347:LYS:HA	3	0.2
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG21	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG22	3	0.2
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG23	3	0.2
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG21	3	0.2
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG22	3	0.2
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG23	3	0.2
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG21	3	0.2
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG22	3	0.2
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG23	3	0.2
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG21	15	0.2
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG22	15	0.2
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG23	15	0.2
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG21	15	0.2
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG22	15	0.2
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG23	15	0.2
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG21	15	0.2
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG22	15	0.2
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG23	15	0.2
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	8	0.2
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	8	0.2
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	13	0.2
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	13	0.2
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	5	0.2
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	5	0.2
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	2	0.2
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	2	0.2
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	2	0.2
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	10	0.2
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	10	0.2
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	10	0.2
(1,884)	1:A:112:PHE:HD1	1:A:114:LYS:H	9	0.2
(1,884)	1:A:112:PHE:HD2	1:A:114:LYS:H	9	0.2
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	2	0.2
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	2	0.2
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	6	0.2
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	6	0.2
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD21	7	0.2
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD22	7	0.2
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD23	7	0.2
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD21	7	0.2
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD22	7	0.2
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD23	7	0.2
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD21	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD22	7	0.2
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD23	7	0.2
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD1	8	0.2
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD2	8	0.2
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	3	0.2
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	3	0.2
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	3	0.2
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	3	0.2
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	3	0.2
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	3	0.2
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	3	0.2
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	3	0.2
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	3	0.2
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	15	0.2
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	15	0.2
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	15	0.2
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	15	0.2
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	15	0.2
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	15	0.2
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	15	0.2
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	15	0.2
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	15	0.2
(1,446)	1:A:60:ALA:HB1	1:A:62:ARG:HA	4	0.2
(1,446)	1:A:60:ALA:HB2	1:A:62:ARG:HA	4	0.2
(1,446)	1:A:60:ALA:HB3	1:A:62:ARG:HA	4	0.2
(1,233)	1:A:32:THR:HA	1:A:33:ASN:H	2	0.2
(1,225)	1:A:30:PRO:HD2	1:A:70:VAL:HG11	14	0.2
(1,225)	1:A:30:PRO:HD2	1:A:70:VAL:HG12	14	0.2
(1,225)	1:A:30:PRO:HD2	1:A:70:VAL:HG13	14	0.2
(1,225)	1:A:30:PRO:HD3	1:A:70:VAL:HG11	14	0.2
(1,225)	1:A:30:PRO:HD3	1:A:70:VAL:HG12	14	0.2
(1,225)	1:A:30:PRO:HD3	1:A:70:VAL:HG13	14	0.2
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG21	5	0.2
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG22	5	0.2
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG23	5	0.2
(1,1102)	1:A:132:VAL:HA	1:A:135:LEU:H	4	0.2
(1,1102)	1:A:132:VAL:HA	1:A:135:LEU:H	15	0.2
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	2	0.2
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	2	0.2
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	13	0.2
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	13	0.2
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	6	0.2
(4,61)	1:B:273:PRO:O	1:B:277:THR:H	9	0.19
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	2	0.19
(4,129)	1:B:330:PHE:O	1:B:334:GLY:H	5	0.19
(4,119)	1:B:344:VAL:O	1:B:320:LEU:H	2	0.19
(3,119)	1:A:144:VAL:O	1:A:120:LEU:H	8	0.19
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	1	0.19
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	1	0.19
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	1	0.19
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	5	0.19
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	5	0.19
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	10	0.19
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	10	0.19
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	10	0.19
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	10	0.19
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	10	0.19
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	10	0.19
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	10	0.19
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	10	0.19
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	10	0.19
(2,459)	1:B:265:ALA:HA	1:B:266:TRP:HE1	10	0.19
(2,446)	1:B:260:ALA:HB1	1:B:262:ARG:HA	4	0.19
(2,446)	1:B:260:ALA:HB2	1:B:262:ARG:HA	4	0.19
(2,446)	1:B:260:ALA:HB3	1:B:262:ARG:HA	4	0.19
(2,446)	1:B:260:ALA:HB1	1:B:262:ARG:HA	14	0.19
(2,446)	1:B:260:ALA:HB2	1:B:262:ARG:HA	14	0.19
(2,446)	1:B:260:ALA:HB3	1:B:262:ARG:HA	14	0.19
(2,224)	1:B:230:PRO:HD2	1:B:270:VAL:HG21	8	0.19
(2,224)	1:B:230:PRO:HD2	1:B:270:VAL:HG22	8	0.19
(2,224)	1:B:230:PRO:HD2	1:B:270:VAL:HG23	8	0.19
(2,224)	1:B:230:PRO:HD3	1:B:270:VAL:HG21	8	0.19
(2,224)	1:B:230:PRO:HD3	1:B:270:VAL:HG22	8	0.19
(2,224)	1:B:230:PRO:HD3	1:B:270:VAL:HG23	8	0.19
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG21	11	0.19
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG22	11	0.19
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG23	11	0.19
(2,152)	1:B:224:PHE:HD1	1:B:225:MET:HA	11	0.19
(2,152)	1:B:224:PHE:HD2	1:B:225:MET:HA	11	0.19
(2,1102)	1:B:332:VAL:HA	1:B:335:LEU:H	4	0.19
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	12	0.19
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	12	0.19
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	6	0.19
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	7	0.19
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	7	0.19
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	8	0.19
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	8	0.19
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	10	0.19
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	10	0.19
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	5	0.19
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	5	0.19
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	7	0.19
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	7	0.19
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD1	3	0.19
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD2	3	0.19
(1,483)	1:A:70:VAL:HA	1:B:330:PHE:HD1	11	0.19
(1,483)	1:A:70:VAL:HA	1:B:330:PHE:HD2	11	0.19
(1,459)	1:A:65:ALA:HA	1:A:66:TRP:HE1	9	0.19
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG21	15	0.19
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG22	15	0.19
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG23	15	0.19
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG21	15	0.19
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG22	15	0.19
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG23	15	0.19
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG21	15	0.19
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG22	15	0.19
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG23	15	0.19
(1,1103)	1:A:132:VAL:HA	1:A:135:LEU:HD11	14	0.19
(1,1103)	1:A:132:VAL:HA	1:A:135:LEU:HD12	14	0.19
(1,1103)	1:A:132:VAL:HA	1:A:135:LEU:HD13	14	0.19
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	3	0.19
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	3	0.19
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	14	0.19
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	14	0.19
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	7	0.19
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	7	0.19
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	11	0.19
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	11	0.19
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	12	0.19
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	12	0.19
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	13	0.19
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	13	0.19
(4,61)	1:B:273:PRO:O	1:B:277:THR:H	12	0.18
(4,22)	1:B:229:ASN:O	1:B:232:THR:N	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,21)	1:B:229:ASN:O	1:B:232:THR:H	11	0.18
(4,120)	1:B:344:VAL:O	1:B:320:LEU:N	2	0.18
(4,119)	1:B:344:VAL:O	1:B:320:LEU:H	8	0.18
(3,120)	1:A:144:VAL:O	1:A:120:LEU:N	4	0.18
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	2	0.18
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	2	0.18
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	2	0.18
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	9	0.18
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	9	0.18
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	9	0.18
(2,884)	1:B:312:PHE:HD1	1:B:314:LYS:H	9	0.18
(2,884)	1:B:312:PHE:HD2	1:B:314:LYS:H	9	0.18
(2,791)	1:B:304:VAL:H	1:B:305:GLU:H	4	0.18
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	3	0.18
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	3	0.18
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	13	0.18
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	13	0.18
(2,734)	1:B:296:ILE:H	1:B:325:GLU:HA	5	0.18
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD1	8	0.18
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD2	8	0.18
(2,446)	1:B:260:ALA:HB1	1:B:262:ARG:HA	5	0.18
(2,446)	1:B:260:ALA:HB2	1:B:262:ARG:HA	5	0.18
(2,446)	1:B:260:ALA:HB3	1:B:262:ARG:HA	5	0.18
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG21	12	0.18
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG22	12	0.18
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG23	12	0.18
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG21	14	0.18
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG22	14	0.18
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG23	14	0.18
(2,225)	1:B:230:PRO:HD2	1:B:270:VAL:HG11	12	0.18
(2,225)	1:B:230:PRO:HD2	1:B:270:VAL:HG12	12	0.18
(2,225)	1:B:230:PRO:HD2	1:B:270:VAL:HG13	12	0.18
(2,225)	1:B:230:PRO:HD3	1:B:270:VAL:HG11	12	0.18
(2,225)	1:B:230:PRO:HD3	1:B:270:VAL:HG12	12	0.18
(2,225)	1:B:230:PRO:HD3	1:B:270:VAL:HG13	12	0.18
(2,1120)	1:B:335:LEU:HA	1:B:338:VAL:HG21	11	0.18
(2,1120)	1:B:335:LEU:HA	1:B:338:VAL:HG22	11	0.18
(2,1120)	1:B:335:LEU:HA	1:B:338:VAL:HG23	11	0.18
(2,1103)	1:B:332:VAL:HA	1:B:335:LEU:HD11	14	0.18
(2,1103)	1:B:332:VAL:HA	1:B:335:LEU:HD12	14	0.18
(2,1103)	1:B:332:VAL:HA	1:B:335:LEU:HD13	14	0.18
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	3	0.18
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	12	0.18
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	12	0.18
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	5	0.18
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	5	0.18
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	5	0.18
(1,783)	1:A:103:HIS:HD2	1:A:104:VAL:H	2	0.18
(1,780)	1:A:103:HIS:HA	1:A:107:GLY:H	11	0.18
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	5	0.18
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	5	0.18
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	12	0.18
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	12	0.18
(1,734)	1:A:96:ILE:H	1:A:125:GLU:HA	5	0.18
(1,699)	1:A:93:ILE:HA	1:A:95:GLY:H	2	0.18
(1,699)	1:A:93:ILE:HA	1:A:95:GLY:H	4	0.18
(1,699)	1:A:93:ILE:HA	1:A:95:GLY:H	14	0.18
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD1	7	0.18
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD2	7	0.18
(1,502)	1:A:72:THR:H	1:A:74:GLU:H	12	0.18
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG21	12	0.18
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG22	12	0.18
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG23	12	0.18
(1,271)	1:A:41:LEU:HD11	1:A:66:TRP:HZ2	12	0.18
(1,271)	1:A:41:LEU:HD12	1:A:66:TRP:HZ2	12	0.18
(1,271)	1:A:41:LEU:HD13	1:A:66:TRP:HZ2	12	0.18
(1,225)	1:A:30:PRO:HD2	1:A:70:VAL:HG11	12	0.18
(1,225)	1:A:30:PRO:HD2	1:A:70:VAL:HG12	12	0.18
(1,225)	1:A:30:PRO:HD2	1:A:70:VAL:HG13	12	0.18
(1,225)	1:A:30:PRO:HD3	1:A:70:VAL:HG11	12	0.18
(1,225)	1:A:30:PRO:HD3	1:A:70:VAL:HG12	12	0.18
(1,225)	1:A:30:PRO:HD3	1:A:70:VAL:HG13	12	0.18
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG21	11	0.18
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG22	11	0.18
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG23	11	0.18
(1,151)	1:A:24:PHE:HA	1:A:70:VAL:HG21	13	0.18
(1,151)	1:A:24:PHE:HA	1:A:70:VAL:HG22	13	0.18
(1,151)	1:A:24:PHE:HA	1:A:70:VAL:HG23	13	0.18
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG21	3	0.18
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG22	3	0.18
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG23	3	0.18
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG21	3	0.18
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG22	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG23	3	0.18
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG21	3	0.18
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG22	3	0.18
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG23	3	0.18
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG21	14	0.18
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG22	14	0.18
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG23	14	0.18
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG21	14	0.18
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG22	14	0.18
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG23	14	0.18
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG21	14	0.18
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG22	14	0.18
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG23	14	0.18
(1,1102)	1:A:132:VAL:HA	1:A:135:LEU:H	12	0.18
(4,36)	1:B:243:PHE:O	1:B:247:ILE:N	14	0.17
(4,22)	1:B:229:ASN:O	1:B:232:THR:N	14	0.17
(3,74)	1:A:80:ASP:O	1:A:84:ILE:N	6	0.17
(3,61)	1:A:73:PRO:O	1:A:77:THR:H	9	0.17
(3,22)	1:A:29:ASN:O	1:A:32:THR:N	10	0.17
(3,22)	1:A:29:ASN:O	1:A:32:THR:N	14	0.17
(3,135)	1:A:133:ARG:O	1:A:137:THR:H	4	0.17
(3,128)	1:A:129:GLY:O	1:A:133:ARG:N	6	0.17
(3,120)	1:A:144:VAL:O	1:A:120:LEU:N	2	0.17
(2,884)	1:B:312:PHE:HD1	1:B:314:LYS:H	3	0.17
(2,884)	1:B:312:PHE:HD2	1:B:314:LYS:H	3	0.17
(2,790)	1:B:303:HIS:HD2	1:A:104:VAL:HG21	9	0.17
(2,790)	1:B:303:HIS:HD2	1:A:104:VAL:HG22	9	0.17
(2,790)	1:B:303:HIS:HD2	1:A:104:VAL:HG23	9	0.17
(2,780)	1:B:303:HIS:HA	1:B:307:GLY:H	10	0.17
(2,780)	1:B:303:HIS:HA	1:B:307:GLY:H	11	0.17
(2,734)	1:B:296:ILE:H	1:B:325:GLU:HA	6	0.17
(2,734)	1:B:296:ILE:H	1:B:325:GLU:HA	9	0.17
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD1	7	0.17
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD2	7	0.17
(2,502)	1:B:272:THR:H	1:B:274:GLU:H	12	0.17
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	4	0.17
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	4	0.17
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	4	0.17
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	4	0.17
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	4	0.17
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	4	0.17
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	4	0.17
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	4	0.17
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	7	0.17
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	7	0.17
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	7	0.17
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	7	0.17
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	7	0.17
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	7	0.17
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	7	0.17
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	7	0.17
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	7	0.17
(2,459)	1:B:265:ALA:HA	1:B:266:TRP:HE1	14	0.17
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD11	12	0.17
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD12	12	0.17
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD13	12	0.17
(2,299)	1:B:244:LEU:HD11	1:B:266:TRP:HZ2	12	0.17
(2,299)	1:B:244:LEU:HD12	1:B:266:TRP:HZ2	12	0.17
(2,299)	1:B:244:LEU:HD13	1:B:266:TRP:HZ2	12	0.17
(2,271)	1:B:241:LEU:HD11	1:B:266:TRP:HZ2	12	0.17
(2,271)	1:B:241:LEU:HD12	1:B:266:TRP:HZ2	12	0.17
(2,271)	1:B:241:LEU:HD13	1:B:266:TRP:HZ2	12	0.17
(2,239)	1:B:234:SER:HB2	1:B:235:MET:H	8	0.17
(2,239)	1:B:234:SER:HB3	1:B:235:MET:H	8	0.17
(2,210)	1:B:228:VAL:HG11	1:B:233:ASN:HA	8	0.17
(2,210)	1:B:228:VAL:HG12	1:B:233:ASN:HA	8	0.17
(2,210)	1:B:228:VAL:HG13	1:B:233:ASN:HA	8	0.17
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG21	14	0.17
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG22	14	0.17
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG23	14	0.17
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG21	14	0.17
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG22	14	0.17
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG23	14	0.17
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG21	14	0.17
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG22	14	0.17
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG23	14	0.17
(2,1115)	1:B:335:LEU:H	1:B:343:PHE:HZ	6	0.17
(2,1035)	1:B:321:GLU:H	1:B:346:TYR:HE1	3	0.17
(2,1035)	1:B:321:GLU:H	1:B:346:TYR:HE2	3	0.17
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	11	0.17
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	11	0.17
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	12	0.17
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	12	0.17
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	3	0.17
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	3	0.17
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	15	0.17
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	15	0.17
(1,783)	1:A:103:HIS:HD2	1:A:104:VAL:H	13	0.17
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	3	0.17
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	3	0.17
(1,767)	1:A:101:GLY:H	1:A:102:THR:H	13	0.17
(1,734)	1:A:96:ILE:H	1:A:125:GLU:HA	9	0.17
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD1	15	0.17
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD2	15	0.17
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	6	0.17
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	6	0.17
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	6	0.17
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	6	0.17
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	6	0.17
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	6	0.17
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	6	0.17
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	6	0.17
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	6	0.17
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD11	12	0.17
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD12	12	0.17
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD13	12	0.17
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG21	14	0.17
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG22	14	0.17
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG23	14	0.17
(1,224)	1:A:30:PRO:HD2	1:A:70:VAL:HG21	8	0.17
(1,224)	1:A:30:PRO:HD2	1:A:70:VAL:HG22	8	0.17
(1,224)	1:A:30:PRO:HD2	1:A:70:VAL:HG23	8	0.17
(1,224)	1:A:30:PRO:HD3	1:A:70:VAL:HG21	8	0.17
(1,224)	1:A:30:PRO:HD3	1:A:70:VAL:HG22	8	0.17
(1,224)	1:A:30:PRO:HD3	1:A:70:VAL:HG23	8	0.17
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG21	3	0.17
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG22	3	0.17
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG23	3	0.17
(1,152)	1:A:24:PHE:HD1	1:A:25:MET:HA	11	0.17
(1,152)	1:A:24:PHE:HD2	1:A:25:MET:HA	11	0.17
(1,1102)	1:A:132:VAL:HA	1:A:135:LEU:H	13	0.17
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	1	0.17
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	1	0.17
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	12	0.17
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD1	1	0.17
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD2	1	0.17
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD1	10	0.17
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD2	10	0.17
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD1	12	0.17
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD2	12	0.17
(1,1035)	1:A:121:GLU:H	1:A:146:TYR:HE1	3	0.17
(1,1035)	1:A:121:GLU:H	1:A:146:TYR:HE2	3	0.17
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	10	0.17
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	10	0.17
(4,61)	1:B:273:PRO:O	1:B:277:THR:H	5	0.16
(4,58)	1:B:264:GLU:O	1:B:268:ALA:N	4	0.16
(4,22)	1:B:229:ASN:O	1:B:232:THR:N	15	0.16
(4,135)	1:B:333:ARG:O	1:B:337:THR:H	1	0.16
(4,128)	1:B:329:GLY:O	1:B:333:ARG:N	6	0.16
(4,120)	1:B:344:VAL:O	1:B:320:LEU:N	1	0.16
(4,120)	1:B:344:VAL:O	1:B:320:LEU:N	3	0.16
(4,120)	1:B:344:VAL:O	1:B:320:LEU:N	4	0.16
(3,96)	1:A:102:THR:O	1:A:106:ILE:N	13	0.16
(3,90)	1:A:99:SER:O	1:A:103:HIS:N	14	0.16
(3,61)	1:A:73:PRO:O	1:A:77:THR:H	12	0.16
(3,22)	1:A:29:ASN:O	1:A:32:THR:N	15	0.16
(3,135)	1:A:133:ARG:O	1:A:137:THR:H	1	0.16
(3,119)	1:A:144:VAL:O	1:A:120:LEU:H	1	0.16
(3,119)	1:A:144:VAL:O	1:A:120:LEU:H	4	0.16
(3,119)	1:A:144:VAL:O	1:A:120:LEU:H	11	0.16
(2,884)	1:B:312:PHE:HD1	1:B:314:LYS:H	2	0.16
(2,884)	1:B:312:PHE:HD2	1:B:314:LYS:H	2	0.16
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	6	0.16
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	6	0.16
(2,783)	1:B:303:HIS:HD2	1:B:304:VAL:H	7	0.16
(2,780)	1:B:303:HIS:HA	1:B:307:GLY:H	6	0.16
(2,699)	1:B:293:ILE:HA	1:B:295:GLY:H	2	0.16
(2,699)	1:B:293:ILE:HA	1:B:295:GLY:H	14	0.16
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	6	0.16
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	6	0.16
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	6	0.16
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	6	0.16
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	6	0.16
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	6	0.16
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	6	0.16
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	6	0.16
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG21	6	0.16
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG22	6	0.16
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG23	6	0.16
(2,237)	1:B:233:ASN:HB2	1:B:270:VAL:HG11	15	0.16
(2,237)	1:B:233:ASN:HB2	1:B:270:VAL:HG12	15	0.16
(2,237)	1:B:233:ASN:HB2	1:B:270:VAL:HG13	15	0.16
(2,237)	1:B:233:ASN:HB3	1:B:270:VAL:HG11	15	0.16
(2,237)	1:B:233:ASN:HB3	1:B:270:VAL:HG12	15	0.16
(2,237)	1:B:233:ASN:HB3	1:B:270:VAL:HG13	15	0.16
(2,224)	1:B:230:PRO:HD2	1:B:270:VAL:HG21	13	0.16
(2,224)	1:B:230:PRO:HD2	1:B:270:VAL:HG22	13	0.16
(2,224)	1:B:230:PRO:HD2	1:B:270:VAL:HG23	13	0.16
(2,224)	1:B:230:PRO:HD3	1:B:270:VAL:HG21	13	0.16
(2,224)	1:B:230:PRO:HD3	1:B:270:VAL:HG22	13	0.16
(2,224)	1:B:230:PRO:HD3	1:B:270:VAL:HG23	13	0.16
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE1	6	0.16
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE2	6	0.16
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE1	6	0.16
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE2	6	0.16
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE1	6	0.16
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE2	6	0.16
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG21	3	0.16
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG22	3	0.16
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG23	3	0.16
(2,166)	1:B:224:PHE:HE1	1:B:265:ALA:HB1	10	0.16
(2,166)	1:B:224:PHE:HE1	1:B:265:ALA:HB2	10	0.16
(2,166)	1:B:224:PHE:HE1	1:B:265:ALA:HB3	10	0.16
(2,166)	1:B:224:PHE:HE2	1:B:265:ALA:HB1	10	0.16
(2,166)	1:B:224:PHE:HE2	1:B:265:ALA:HB2	10	0.16
(2,166)	1:B:224:PHE:HE2	1:B:265:ALA:HB3	10	0.16
(2,151)	1:B:224:PHE:HA	1:B:270:VAL:HG21	13	0.16
(2,151)	1:B:224:PHE:HA	1:B:270:VAL:HG22	13	0.16
(2,151)	1:B:224:PHE:HA	1:B:270:VAL:HG23	13	0.16
(2,1102)	1:B:332:VAL:HA	1:B:335:LEU:H	12	0.16
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	1	0.16
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	1	0.16
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD1	4	0.16
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD2	4	0.16
(1,906)	1:A:116:ILE:HG12	1:A:117:VAL:H	5	0.16
(1,884)	1:A:112:PHE:HD1	1:A:114:LYS:H	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,884)	1:A:112:PHE:HD2	1:A:114:LYS:H	15	0.16
(1,844)	1:A:108:TRP:HE3	1:B:331:LEU:HD21	14	0.16
(1,844)	1:A:108:TRP:HE3	1:B:331:LEU:HD22	14	0.16
(1,844)	1:A:108:TRP:HE3	1:B:331:LEU:HD23	14	0.16
(1,791)	1:A:104:VAL:H	1:A:105:GLU:H	4	0.16
(1,790)	1:A:103:HIS:HD2	1:B:304:VAL:HG21	9	0.16
(1,790)	1:A:103:HIS:HD2	1:B:304:VAL:HG22	9	0.16
(1,790)	1:A:103:HIS:HD2	1:B:304:VAL:HG23	9	0.16
(1,780)	1:A:103:HIS:HA	1:A:107:GLY:H	15	0.16
(1,734)	1:A:96:ILE:H	1:A:125:GLU:HA	3	0.16
(1,720)	1:A:94:PRO:HA	1:A:103:HIS:HE1	14	0.16
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD1	2	0.16
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD2	2	0.16
(1,582)	1:A:82:LEU:HA	1:A:85:ARG:H	2	0.16
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	7	0.16
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	7	0.16
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	7	0.16
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	7	0.16
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	7	0.16
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	7	0.16
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	7	0.16
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	7	0.16
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	7	0.16
(1,459)	1:A:65:ALA:HA	1:A:66:TRP:HE1	10	0.16
(1,446)	1:A:60:ALA:HB1	1:A:62:ARG:HA	5	0.16
(1,446)	1:A:60:ALA:HB2	1:A:62:ARG:HA	5	0.16
(1,446)	1:A:60:ALA:HB3	1:A:62:ARG:HA	5	0.16
(1,433)	1:A:56:GLU:H	1:A:58:PHE:HD1	15	0.16
(1,433)	1:A:56:GLU:H	1:A:58:PHE:HD2	15	0.16
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG21	10	0.16
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG22	10	0.16
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG23	10	0.16
(1,271)	1:A:41:LEU:HD11	1:A:66:TRP:HZ2	13	0.16
(1,271)	1:A:41:LEU:HD12	1:A:66:TRP:HZ2	13	0.16
(1,271)	1:A:41:LEU:HD13	1:A:66:TRP:HZ2	13	0.16
(1,239)	1:A:34:SER:HB2	1:A:35:MET:H	8	0.16
(1,239)	1:A:34:SER:HB3	1:A:35:MET:H	8	0.16
(1,228)	1:A:31:GLU:HA	1:A:32:THR:H	11	0.16
(1,201)	1:A:27:LEU:HD21	1:B:330:PHE:HE1	3	0.16
(1,201)	1:A:27:LEU:HD21	1:B:330:PHE:HE2	3	0.16
(1,201)	1:A:27:LEU:HD22	1:B:330:PHE:HE1	3	0.16
(1,201)	1:A:27:LEU:HD22	1:B:330:PHE:HE2	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:A:27:LEU:HD23	1:B:330:PHE:HE1	3	0.16
(1,201)	1:A:27:LEU:HD23	1:B:330:PHE:HE2	3	0.16
(1,200)	1:A:27:LEU:HD21	1:B:330:PHE:HD1	7	0.16
(1,200)	1:A:27:LEU:HD21	1:B:330:PHE:HD2	7	0.16
(1,200)	1:A:27:LEU:HD22	1:B:330:PHE:HD1	7	0.16
(1,200)	1:A:27:LEU:HD22	1:B:330:PHE:HD2	7	0.16
(1,200)	1:A:27:LEU:HD23	1:B:330:PHE:HD1	7	0.16
(1,200)	1:A:27:LEU:HD23	1:B:330:PHE:HD2	7	0.16
(1,166)	1:A:24:PHE:HE1	1:A:65:ALA:HB1	10	0.16
(1,166)	1:A:24:PHE:HE1	1:A:65:ALA:HB2	10	0.16
(1,166)	1:A:24:PHE:HE1	1:A:65:ALA:HB3	10	0.16
(1,166)	1:A:24:PHE:HE2	1:A:65:ALA:HB1	10	0.16
(1,166)	1:A:24:PHE:HE2	1:A:65:ALA:HB2	10	0.16
(1,166)	1:A:24:PHE:HE2	1:A:65:ALA:HB3	10	0.16
(1,152)	1:A:24:PHE:HD1	1:A:25:MET:HA	2	0.16
(1,152)	1:A:24:PHE:HD2	1:A:25:MET:HA	2	0.16
(1,1184)	1:A:144:VAL:HG11	1:A:146:TYR:HD1	3	0.16
(1,1184)	1:A:144:VAL:HG11	1:A:146:TYR:HD2	3	0.16
(1,1184)	1:A:144:VAL:HG12	1:A:146:TYR:HD1	3	0.16
(1,1184)	1:A:144:VAL:HG12	1:A:146:TYR:HD2	3	0.16
(1,1184)	1:A:144:VAL:HG13	1:A:146:TYR:HD1	3	0.16
(1,1184)	1:A:144:VAL:HG13	1:A:146:TYR:HD2	3	0.16
(1,1120)	1:A:135:LEU:HA	1:A:138:VAL:HG21	11	0.16
(1,1120)	1:A:135:LEU:HA	1:A:138:VAL:HG22	11	0.16
(1,1120)	1:A:135:LEU:HA	1:A:138:VAL:HG23	11	0.16
(1,1115)	1:A:135:LEU:H	1:A:143:PHE:HZ	6	0.16
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	11	0.16
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	11	0.16
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD1	13	0.16
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD2	13	0.16
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	2	0.16
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	2	0.16
(4,96)	1:B:302:THR:O	1:B:306:ILE:N	13	0.15
(4,90)	1:B:299:SER:O	1:B:303:HIS:N	14	0.15
(4,75)	1:B:281:GLN:O	1:B:285:ARG:H	6	0.15
(4,61)	1:B:273:PRO:O	1:B:277:THR:H	14	0.15
(4,22)	1:B:229:ASN:O	1:B:232:THR:N	4	0.15
(4,22)	1:B:229:ASN:O	1:B:232:THR:N	12	0.15
(4,135)	1:B:333:ARG:O	1:B:337:THR:H	7	0.15
(4,132)	1:B:331:LEU:O	1:B:335:LEU:N	10	0.15
(4,119)	1:B:344:VAL:O	1:B:320:LEU:H	4	0.15
(4,119)	1:B:344:VAL:O	1:B:320:LEU:H	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,61)	1:A:73:PRO:O	1:A:77:THR:H	2	0.15
(3,61)	1:A:73:PRO:O	1:A:77:THR:H	14	0.15
(3,58)	1:A:64:GLU:O	1:A:68:ALA:N	4	0.15
(3,36)	1:A:43:PHE:O	1:A:47:ILE:N	14	0.15
(3,22)	1:A:29:ASN:O	1:A:32:THR:N	8	0.15
(3,135)	1:A:133:ARG:O	1:A:137:THR:H	2	0.15
(3,135)	1:A:133:ARG:O	1:A:137:THR:H	7	0.15
(3,132)	1:A:131:LEU:O	1:A:135:LEU:N	10	0.15
(3,132)	1:A:131:LEU:O	1:A:135:LEU:N	12	0.15
(3,122)	1:A:120:LEU:O	1:A:146:TYR:N	11	0.15
(3,120)	1:A:144:VAL:O	1:A:120:LEU:N	3	0.15
(2,884)	1:B:312:PHE:HD1	1:B:314:LYS:H	8	0.15
(2,884)	1:B:312:PHE:HD2	1:B:314:LYS:H	8	0.15
(2,783)	1:B:303:HIS:HD2	1:B:304:VAL:H	13	0.15
(2,780)	1:B:303:HIS:HA	1:B:307:GLY:H	13	0.15
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD1	11	0.15
(2,778)	1:B:303:HIS:H	1:B:328:TYR:HD2	11	0.15
(2,734)	1:B:296:ILE:H	1:B:325:GLU:HA	14	0.15
(2,720)	1:B:294:PRO:HA	1:B:303:HIS:HE1	14	0.15
(2,704)	1:B:293:ILE:HG21	1:B:296:ILE:H	4	0.15
(2,704)	1:B:293:ILE:HG22	1:B:296:ILE:H	4	0.15
(2,704)	1:B:293:ILE:HG23	1:B:296:ILE:H	4	0.15
(2,699)	1:B:293:ILE:HA	1:B:295:GLY:H	1	0.15
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD1	2	0.15
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD2	2	0.15
(2,590)	1:B:282:LEU:HD11	1:A:110:SER:HB2	13	0.15
(2,590)	1:B:282:LEU:HD11	1:A:110:SER:HB3	13	0.15
(2,590)	1:B:282:LEU:HD12	1:A:110:SER:HB2	13	0.15
(2,590)	1:B:282:LEU:HD12	1:A:110:SER:HB3	13	0.15
(2,590)	1:B:282:LEU:HD13	1:A:110:SER:HB2	13	0.15
(2,590)	1:B:282:LEU:HD13	1:A:110:SER:HB3	13	0.15
(2,590)	1:B:282:LEU:HD21	1:A:110:SER:HB2	13	0.15
(2,590)	1:B:282:LEU:HD21	1:A:110:SER:HB3	13	0.15
(2,590)	1:B:282:LEU:HD22	1:A:110:SER:HB2	13	0.15
(2,590)	1:B:282:LEU:HD22	1:A:110:SER:HB3	13	0.15
(2,590)	1:B:282:LEU:HD23	1:A:110:SER:HB2	13	0.15
(2,590)	1:B:282:LEU:HD23	1:A:110:SER:HB3	13	0.15
(2,490)	1:B:271:LEU:HD21	1:B:272:THR:HG21	14	0.15
(2,490)	1:B:271:LEU:HD21	1:B:272:THR:HG22	14	0.15
(2,490)	1:B:271:LEU:HD21	1:B:272:THR:HG23	14	0.15
(2,490)	1:B:271:LEU:HD22	1:B:272:THR:HG21	14	0.15
(2,490)	1:B:271:LEU:HD22	1:B:272:THR:HG22	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,490)	1:B:271:LEU:HD22	1:B:272:THR:HG23	14	0.15
(2,490)	1:B:271:LEU:HD23	1:B:272:THR:HG21	14	0.15
(2,490)	1:B:271:LEU:HD23	1:B:272:THR:HG22	14	0.15
(2,490)	1:B:271:LEU:HD23	1:B:272:THR:HG23	14	0.15
(2,487)	1:B:271:LEU:HA	1:B:272:THR:H	13	0.15
(2,483)	1:B:270:VAL:HA	1:A:130:PHE:HD1	11	0.15
(2,483)	1:B:270:VAL:HA	1:A:130:PHE:HD2	11	0.15
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	2	0.15
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	2	0.15
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	2	0.15
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	2	0.15
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	2	0.15
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	2	0.15
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	2	0.15
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	2	0.15
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	2	0.15
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	5	0.15
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	5	0.15
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	5	0.15
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	5	0.15
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	5	0.15
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	5	0.15
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	5	0.15
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	5	0.15
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	5	0.15
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	13	0.15
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	13	0.15
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	13	0.15
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	13	0.15
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	13	0.15
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	13	0.15
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	13	0.15
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	13	0.15
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	13	0.15
(2,433)	1:B:256:GLU:H	1:B:258:PHE:HD1	15	0.15
(2,433)	1:B:256:GLU:H	1:B:258:PHE:HD2	15	0.15
(2,42)	1:B:217:SER:HB2	1:B:257:VAL:HG11	3	0.15
(2,42)	1:B:217:SER:HB2	1:B:257:VAL:HG12	3	0.15
(2,42)	1:B:217:SER:HB2	1:B:257:VAL:HG13	3	0.15
(2,42)	1:B:217:SER:HB3	1:B:257:VAL:HG11	3	0.15
(2,42)	1:B:217:SER:HB3	1:B:257:VAL:HG12	3	0.15
(2,42)	1:B:217:SER:HB3	1:B:257:VAL:HG13	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,373)	1:B:249:HIS:HA	1:B:253:GLN:H	4	0.15
(2,373)	1:B:249:HIS:HA	1:B:253:GLN:H	13	0.15
(2,209)	1:B:228:VAL:HG11	1:B:231:GLU:HA	12	0.15
(2,209)	1:B:228:VAL:HG12	1:B:231:GLU:HA	12	0.15
(2,209)	1:B:228:VAL:HG13	1:B:231:GLU:HA	12	0.15
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE1	1	0.15
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE2	1	0.15
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE1	1	0.15
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE2	1	0.15
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE1	1	0.15
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE2	1	0.15
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE1	4	0.15
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE2	4	0.15
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE1	4	0.15
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE2	4	0.15
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE1	4	0.15
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE2	4	0.15
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE1	13	0.15
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE2	13	0.15
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE1	13	0.15
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE2	13	0.15
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE1	13	0.15
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE2	13	0.15
(2,155)	1:B:224:PHE:HD1	1:B:227:LEU:HD11	1	0.15
(2,155)	1:B:224:PHE:HD1	1:B:227:LEU:HD12	1	0.15
(2,155)	1:B:224:PHE:HD1	1:B:227:LEU:HD13	1	0.15
(2,155)	1:B:224:PHE:HD2	1:B:227:LEU:HD11	1	0.15
(2,155)	1:B:224:PHE:HD2	1:B:227:LEU:HD12	1	0.15
(2,155)	1:B:224:PHE:HD2	1:B:227:LEU:HD13	1	0.15
(2,150)	1:B:224:PHE:HA	1:B:270:VAL:HG11	11	0.15
(2,150)	1:B:224:PHE:HA	1:B:270:VAL:HG12	11	0.15
(2,150)	1:B:224:PHE:HA	1:B:270:VAL:HG13	11	0.15
(2,1102)	1:B:332:VAL:HA	1:B:335:LEU:H	13	0.15
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD1	1	0.15
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD2	1	0.15
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD1	12	0.15
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD2	12	0.15
(2,1049)	1:B:322:GLU:HA	1:B:345:HIS:HD2	15	0.15
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	3	0.15
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	3	0.15
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	15	0.15
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	1	0.15
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	1	0.15
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	1	0.15
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	13	0.15
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	13	0.15
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	13	0.15
(1,884)	1:A:112:PHE:HD1	1:A:114:LYS:H	3	0.15
(1,884)	1:A:112:PHE:HD2	1:A:114:LYS:H	3	0.15
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	10	0.15
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	10	0.15
(1,844)	1:A:108:TRP:HE3	1:B:331:LEU:HD21	3	0.15
(1,844)	1:A:108:TRP:HE3	1:B:331:LEU:HD22	3	0.15
(1,844)	1:A:108:TRP:HE3	1:B:331:LEU:HD23	3	0.15
(1,783)	1:A:103:HIS:HD2	1:A:104:VAL:H	8	0.15
(1,780)	1:A:103:HIS:HA	1:A:107:GLY:H	10	0.15
(1,780)	1:A:103:HIS:HA	1:A:107:GLY:H	13	0.15
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	11	0.15
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	11	0.15
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD1	13	0.15
(1,778)	1:A:103:HIS:H	1:A:128:TYR:HD2	13	0.15
(1,767)	1:A:101:GLY:H	1:A:102:THR:H	15	0.15
(1,699)	1:A:93:ILE:HA	1:A:95:GLY:H	10	0.15
(1,582)	1:A:82:LEU:HA	1:A:85:ARG:H	8	0.15
(1,487)	1:A:71:LEU:HA	1:A:72:THR:H	11	0.15
(1,487)	1:A:71:LEU:HA	1:A:72:THR:H	13	0.15
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	4	0.15
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	4	0.15
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	4	0.15
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	4	0.15
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	4	0.15
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	4	0.15
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	4	0.15
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	4	0.15
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	4	0.15
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	10	0.15
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	10	0.15
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	10	0.15
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	10	0.15
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	10	0.15
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	10	0.15
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	10	0.15
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	10	0.15
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	14	0.15
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	14	0.15
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	14	0.15
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	14	0.15
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	14	0.15
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	14	0.15
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	14	0.15
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	14	0.15
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	14	0.15
(1,373)	1:A:49:HIS:HA	1:A:53:GLN:H	3	0.15
(1,271)	1:A:41:LEU:HD11	1:A:66:TRP:HZ2	11	0.15
(1,271)	1:A:41:LEU:HD12	1:A:66:TRP:HZ2	11	0.15
(1,271)	1:A:41:LEU:HD13	1:A:66:TRP:HZ2	11	0.15
(1,233)	1:A:32:THR:HA	1:A:33:ASN:H	14	0.15
(1,225)	1:A:30:PRO:HD2	1:A:70:VAL:HG11	7	0.15
(1,225)	1:A:30:PRO:HD2	1:A:70:VAL:HG12	7	0.15
(1,225)	1:A:30:PRO:HD2	1:A:70:VAL:HG13	7	0.15
(1,225)	1:A:30:PRO:HD3	1:A:70:VAL:HG11	7	0.15
(1,225)	1:A:30:PRO:HD3	1:A:70:VAL:HG12	7	0.15
(1,225)	1:A:30:PRO:HD3	1:A:70:VAL:HG13	7	0.15
(1,201)	1:A:27:LEU:HD21	1:B:330:PHE:HE1	1	0.15
(1,201)	1:A:27:LEU:HD21	1:B:330:PHE:HE2	1	0.15
(1,201)	1:A:27:LEU:HD22	1:B:330:PHE:HE1	1	0.15
(1,201)	1:A:27:LEU:HD22	1:B:330:PHE:HE2	1	0.15
(1,201)	1:A:27:LEU:HD23	1:B:330:PHE:HE1	1	0.15
(1,201)	1:A:27:LEU:HD23	1:B:330:PHE:HE2	1	0.15
(1,17)	1:A:15:VAL:HG21	1:A:50:PHE:HZ	5	0.15
(1,17)	1:A:15:VAL:HG22	1:A:50:PHE:HZ	5	0.15
(1,17)	1:A:15:VAL:HG23	1:A:50:PHE:HZ	5	0.15
(1,167)	1:A:24:PHE:HZ	1:A:65:ALA:HB1	9	0.15
(1,167)	1:A:24:PHE:HZ	1:A:65:ALA:HB2	9	0.15
(1,167)	1:A:24:PHE:HZ	1:A:65:ALA:HB3	9	0.15
(1,1184)	1:A:144:VAL:HG11	1:A:146:TYR:HD1	8	0.15
(1,1184)	1:A:144:VAL:HG11	1:A:146:TYR:HD2	8	0.15
(1,1184)	1:A:144:VAL:HG12	1:A:146:TYR:HD1	8	0.15
(1,1184)	1:A:144:VAL:HG12	1:A:146:TYR:HD2	8	0.15
(1,1184)	1:A:144:VAL:HG13	1:A:146:TYR:HD1	8	0.15
(1,1184)	1:A:144:VAL:HG13	1:A:146:TYR:HD2	8	0.15
(1,1100)	1:A:131:LEU:HD11	1:A:138:VAL:HG21	12	0.15
(1,1100)	1:A:131:LEU:HD11	1:A:138:VAL:HG22	12	0.15
(1,1100)	1:A:131:LEU:HD11	1:A:138:VAL:HG23	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1100)	1:A:131:LEU:HD12	1:A:138:VAL:HG21	12	0.15
(1,1100)	1:A:131:LEU:HD12	1:A:138:VAL:HG22	12	0.15
(1,1100)	1:A:131:LEU:HD12	1:A:138:VAL:HG23	12	0.15
(1,1100)	1:A:131:LEU:HD13	1:A:138:VAL:HG21	12	0.15
(1,1100)	1:A:131:LEU:HD13	1:A:138:VAL:HG22	12	0.15
(1,1100)	1:A:131:LEU:HD13	1:A:138:VAL:HG23	12	0.15
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	6	0.15
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	6	0.15
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	10	0.15
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	10	0.15
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD1	8	0.15
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD2	8	0.15
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD1	11	0.15
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD2	11	0.15
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	3	0.15
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	3	0.15
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	8	0.15
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	8	0.15
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	15	0.15
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	15	0.15
(4,74)	1:B:280:ASP:O	1:B:284:ILE:N	6	0.14
(4,36)	1:B:243:PHE:O	1:B:247:ILE:N	11	0.14
(4,22)	1:B:229:ASN:O	1:B:232:THR:N	8	0.14
(4,21)	1:B:229:ASN:O	1:B:232:THR:H	7	0.14
(4,148)	1:B:352:ALA:O	1:B:356:ILE:N	1	0.14
(4,135)	1:B:333:ARG:O	1:B:337:THR:H	2	0.14
(4,132)	1:B:331:LEU:O	1:B:335:LEU:N	12	0.14
(4,119)	1:B:344:VAL:O	1:B:320:LEU:H	10	0.14
(4,108)	1:B:308:TRP:O	1:B:312:PHE:N	1	0.14
(4,103)	1:B:306:ILE:O	1:B:310:SER:H	3	0.14
(4,103)	1:B:306:ILE:O	1:B:310:SER:H	7	0.14
(4,103)	1:B:306:ILE:O	1:B:310:SER:H	14	0.14
(3,75)	1:A:81:GLN:O	1:A:85:ARG:H	6	0.14
(3,53)	1:A:62:ARG:O	1:A:66:TRP:H	12	0.14
(3,22)	1:A:29:ASN:O	1:A:32:THR:N	4	0.14
(3,22)	1:A:29:ASN:O	1:A:32:THR:N	9	0.14
(3,137)	1:A:134:GLY:O	1:A:138:VAL:H	6	0.14
(3,135)	1:A:133:ARG:O	1:A:137:THR:H	15	0.14
(3,120)	1:A:144:VAL:O	1:A:120:LEU:N	1	0.14
(3,120)	1:A:144:VAL:O	1:A:120:LEU:N	6	0.14
(3,120)	1:A:144:VAL:O	1:A:120:LEU:N	12	0.14
(3,119)	1:A:144:VAL:O	1:A:120:LEU:H	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,108)	1:A:108:TRP:O	1:A:112:PHE:N	1	0.14
(3,103)	1:A:106:ILE:O	1:A:110:SER:H	7	0.14
(3,100)	1:A:104:VAL:O	1:A:108:TRP:N	13	0.14
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	4	0.14
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	4	0.14
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	4	0.14
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	13	0.14
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	13	0.14
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	13	0.14
(2,906)	1:B:316:ILE:HG12	1:B:317:VAL:H	5	0.14
(2,884)	1:B:312:PHE:HD1	1:B:314:LYS:H	12	0.14
(2,884)	1:B:312:PHE:HD2	1:B:314:LYS:H	12	0.14
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD21	2	0.14
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD22	2	0.14
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD23	2	0.14
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD21	2	0.14
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD22	2	0.14
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD23	2	0.14
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD21	2	0.14
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD22	2	0.14
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD23	2	0.14
(2,780)	1:B:303:HIS:HA	1:B:307:GLY:H	15	0.14
(2,767)	1:B:301:GLY:H	1:B:302:THR:H	7	0.14
(2,734)	1:B:296:ILE:H	1:B:325:GLU:HA	3	0.14
(2,720)	1:B:294:PRO:HA	1:B:303:HIS:HE1	3	0.14
(2,590)	1:B:282:LEU:HD11	1:A:110:SER:HB2	6	0.14
(2,590)	1:B:282:LEU:HD11	1:A:110:SER:HB3	6	0.14
(2,590)	1:B:282:LEU:HD12	1:A:110:SER:HB2	6	0.14
(2,590)	1:B:282:LEU:HD12	1:A:110:SER:HB3	6	0.14
(2,590)	1:B:282:LEU:HD13	1:A:110:SER:HB2	6	0.14
(2,590)	1:B:282:LEU:HD13	1:A:110:SER:HB3	6	0.14
(2,590)	1:B:282:LEU:HD21	1:A:110:SER:HB2	6	0.14
(2,590)	1:B:282:LEU:HD21	1:A:110:SER:HB3	6	0.14
(2,590)	1:B:282:LEU:HD22	1:A:110:SER:HB2	6	0.14
(2,590)	1:B:282:LEU:HD22	1:A:110:SER:HB3	6	0.14
(2,590)	1:B:282:LEU:HD23	1:A:110:SER:HB2	6	0.14
(2,590)	1:B:282:LEU:HD23	1:A:110:SER:HB3	6	0.14
(2,582)	1:B:282:LEU:HA	1:B:285:ARG:H	2	0.14
(2,582)	1:B:282:LEU:HA	1:B:285:ARG:H	8	0.14
(2,569)	1:B:279:LEU:HA	1:B:282:LEU:H	14	0.14
(2,491)	1:B:271:LEU:HD21	1:B:272:THR:H	14	0.14
(2,491)	1:B:271:LEU:HD22	1:B:272:THR:H	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,491)	1:B:271:LEU:HD23	1:B:272:THR:H	14	0.14
(2,487)	1:B:271:LEU:HA	1:B:272:THR:H	11	0.14
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	9	0.14
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	9	0.14
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	9	0.14
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	9	0.14
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	9	0.14
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	9	0.14
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	9	0.14
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	9	0.14
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	9	0.14
(2,477)	1:B:269:GLN:HB2	1:B:271:LEU:HD11	15	0.14
(2,477)	1:B:269:GLN:HB2	1:B:271:LEU:HD12	15	0.14
(2,477)	1:B:269:GLN:HB2	1:B:271:LEU:HD13	15	0.14
(2,477)	1:B:269:GLN:HB3	1:B:271:LEU:HD11	15	0.14
(2,477)	1:B:269:GLN:HB3	1:B:271:LEU:HD12	15	0.14
(2,477)	1:B:269:GLN:HB3	1:B:271:LEU:HD13	15	0.14
(2,469)	1:B:265:ALA:HB1	1:B:270:VAL:HG11	12	0.14
(2,469)	1:B:265:ALA:HB1	1:B:270:VAL:HG12	12	0.14
(2,469)	1:B:265:ALA:HB1	1:B:270:VAL:HG13	12	0.14
(2,469)	1:B:265:ALA:HB1	1:B:270:VAL:HG21	12	0.14
(2,469)	1:B:265:ALA:HB1	1:B:270:VAL:HG22	12	0.14
(2,469)	1:B:265:ALA:HB1	1:B:270:VAL:HG23	12	0.14
(2,469)	1:B:265:ALA:HB2	1:B:270:VAL:HG11	12	0.14
(2,469)	1:B:265:ALA:HB2	1:B:270:VAL:HG12	12	0.14
(2,469)	1:B:265:ALA:HB2	1:B:270:VAL:HG13	12	0.14
(2,469)	1:B:265:ALA:HB2	1:B:270:VAL:HG21	12	0.14
(2,469)	1:B:265:ALA:HB2	1:B:270:VAL:HG22	12	0.14
(2,469)	1:B:265:ALA:HB2	1:B:270:VAL:HG23	12	0.14
(2,469)	1:B:265:ALA:HB3	1:B:270:VAL:HG11	12	0.14
(2,469)	1:B:265:ALA:HB3	1:B:270:VAL:HG12	12	0.14
(2,469)	1:B:265:ALA:HB3	1:B:270:VAL:HG13	12	0.14
(2,469)	1:B:265:ALA:HB3	1:B:270:VAL:HG21	12	0.14
(2,469)	1:B:265:ALA:HB3	1:B:270:VAL:HG22	12	0.14
(2,469)	1:B:265:ALA:HB3	1:B:270:VAL:HG23	12	0.14
(2,449)	1:B:262:ARG:HA	1:B:266:TRP:HD1	14	0.14
(2,446)	1:B:260:ALA:HB1	1:B:262:ARG:HA	2	0.14
(2,446)	1:B:260:ALA:HB2	1:B:262:ARG:HA	2	0.14
(2,446)	1:B:260:ALA:HB3	1:B:262:ARG:HA	2	0.14
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD11	13	0.14
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD12	13	0.14
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD13	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,418)	1:B:253:GLN:H	1:B:255:LEU:H	3	0.14
(2,418)	1:B:253:GLN:H	1:B:255:LEU:H	9	0.14
(2,391)	1:B:250:PHE:HZ	1:B:255:LEU:HD11	8	0.14
(2,391)	1:B:250:PHE:HZ	1:B:255:LEU:HD12	8	0.14
(2,391)	1:B:250:PHE:HZ	1:B:255:LEU:HD13	8	0.14
(2,389)	1:B:250:PHE:HD1	1:B:255:LEU:HD11	15	0.14
(2,389)	1:B:250:PHE:HD1	1:B:255:LEU:HD12	15	0.14
(2,389)	1:B:250:PHE:HD1	1:B:255:LEU:HD13	15	0.14
(2,389)	1:B:250:PHE:HD2	1:B:255:LEU:HD11	15	0.14
(2,389)	1:B:250:PHE:HD2	1:B:255:LEU:HD12	15	0.14
(2,389)	1:B:250:PHE:HD2	1:B:255:LEU:HD13	15	0.14
(2,373)	1:B:249:HIS:HA	1:B:253:GLN:H	1	0.14
(2,373)	1:B:249:HIS:HA	1:B:253:GLN:H	3	0.14
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG21	3	0.14
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG22	3	0.14
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG23	3	0.14
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG21	10	0.14
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG22	10	0.14
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG23	10	0.14
(2,245)	1:B:236:PRO:HB2	1:B:237:SER:H	10	0.14
(2,245)	1:B:236:PRO:HB3	1:B:237:SER:H	10	0.14
(2,233)	1:B:232:THR:HA	1:B:233:ASN:H	14	0.14
(2,225)	1:B:230:PRO:HD2	1:B:270:VAL:HG11	7	0.14
(2,225)	1:B:230:PRO:HD2	1:B:270:VAL:HG12	7	0.14
(2,225)	1:B:230:PRO:HD2	1:B:270:VAL:HG13	7	0.14
(2,225)	1:B:230:PRO:HD3	1:B:270:VAL:HG11	7	0.14
(2,225)	1:B:230:PRO:HD3	1:B:270:VAL:HG12	7	0.14
(2,225)	1:B:230:PRO:HD3	1:B:270:VAL:HG13	7	0.14
(2,212)	1:B:228:VAL:HG11	1:A:130:PHE:HZ	11	0.14
(2,212)	1:B:228:VAL:HG12	1:A:130:PHE:HZ	11	0.14
(2,212)	1:B:228:VAL:HG13	1:A:130:PHE:HZ	11	0.14
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE1	15	0.14
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE2	15	0.14
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE1	15	0.14
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE2	15	0.14
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE1	15	0.14
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE2	15	0.14
(2,199)	1:B:227:LEU:HD21	1:B:295:GLY:HA2	9	0.14
(2,199)	1:B:227:LEU:HD21	1:B:295:GLY:HA3	9	0.14
(2,199)	1:B:227:LEU:HD22	1:B:295:GLY:HA2	9	0.14
(2,199)	1:B:227:LEU:HD22	1:B:295:GLY:HA3	9	0.14
(2,199)	1:B:227:LEU:HD23	1:B:295:GLY:HA2	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,199)	1:B:227:LEU:HD23	1:B:295:GLY:HA3	9	0.14
(2,150)	1:B:224:PHE:HA	1:B:270:VAL:HG11	7	0.14
(2,150)	1:B:224:PHE:HA	1:B:270:VAL:HG12	7	0.14
(2,150)	1:B:224:PHE:HA	1:B:270:VAL:HG13	7	0.14
(2,1188)	1:B:344:VAL:HG21	1:B:355:GLN:H	5	0.14
(2,1188)	1:B:344:VAL:HG22	1:B:355:GLN:H	5	0.14
(2,1188)	1:B:344:VAL:HG23	1:B:355:GLN:H	5	0.14
(2,1184)	1:B:344:VAL:HG11	1:B:346:TYR:HD1	3	0.14
(2,1184)	1:B:344:VAL:HG11	1:B:346:TYR:HD2	3	0.14
(2,1184)	1:B:344:VAL:HG12	1:B:346:TYR:HD1	3	0.14
(2,1184)	1:B:344:VAL:HG12	1:B:346:TYR:HD2	3	0.14
(2,1184)	1:B:344:VAL:HG13	1:B:346:TYR:HD1	3	0.14
(2,1184)	1:B:344:VAL:HG13	1:B:346:TYR:HD2	3	0.14
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG21	2	0.14
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG22	2	0.14
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG23	2	0.14
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG21	2	0.14
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG22	2	0.14
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG23	2	0.14
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG21	2	0.14
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG22	2	0.14
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG23	2	0.14
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG21	4	0.14
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG22	4	0.14
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG23	4	0.14
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG21	4	0.14
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG22	4	0.14
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG23	4	0.14
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG21	4	0.14
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG22	4	0.14
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG23	4	0.14
(2,1102)	1:B:332:VAL:HA	1:B:335:LEU:H	11	0.14
(2,1100)	1:B:331:LEU:HD11	1:B:338:VAL:HG21	12	0.14
(2,1100)	1:B:331:LEU:HD11	1:B:338:VAL:HG22	12	0.14
(2,1100)	1:B:331:LEU:HD11	1:B:338:VAL:HG23	12	0.14
(2,1100)	1:B:331:LEU:HD12	1:B:338:VAL:HG21	12	0.14
(2,1100)	1:B:331:LEU:HD12	1:B:338:VAL:HG22	12	0.14
(2,1100)	1:B:331:LEU:HD12	1:B:338:VAL:HG23	12	0.14
(2,1100)	1:B:331:LEU:HD13	1:B:338:VAL:HG21	12	0.14
(2,1100)	1:B:331:LEU:HD13	1:B:338:VAL:HG22	12	0.14
(2,1100)	1:B:331:LEU:HD13	1:B:338:VAL:HG23	12	0.14
(2,1075)	1:B:325:GLU:HA	1:B:328:TYR:HB2	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD1	2	0.14
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD2	2	0.14
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD1	5	0.14
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD2	5	0.14
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD1	10	0.14
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD2	10	0.14
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD1	13	0.14
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD2	13	0.14
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	9	0.14
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	9	0.14
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	9	0.14
(1,998)	1:A:120:LEU:HA	1:A:146:TYR:HE1	8	0.14
(1,998)	1:A:120:LEU:HA	1:A:146:TYR:HE2	8	0.14
(1,906)	1:A:116:ILE:HG12	1:A:117:VAL:H	2	0.14
(1,884)	1:A:112:PHE:HD1	1:A:114:LYS:H	8	0.14
(1,884)	1:A:112:PHE:HD2	1:A:114:LYS:H	8	0.14
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD1	13	0.14
(1,873)	1:A:111:ALA:H	1:B:312:PHE:HD2	13	0.14
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD21	2	0.14
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD22	2	0.14
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD23	2	0.14
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD21	2	0.14
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD22	2	0.14
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD23	2	0.14
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD21	2	0.14
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD22	2	0.14
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD23	2	0.14
(1,811)	1:A:104:VAL:HG11	1:B:338:VAL:HG21	1	0.14
(1,811)	1:A:104:VAL:HG11	1:B:338:VAL:HG22	1	0.14
(1,811)	1:A:104:VAL:HG11	1:B:338:VAL:HG23	1	0.14
(1,811)	1:A:104:VAL:HG12	1:B:338:VAL:HG21	1	0.14
(1,811)	1:A:104:VAL:HG12	1:B:338:VAL:HG22	1	0.14
(1,811)	1:A:104:VAL:HG12	1:B:338:VAL:HG23	1	0.14
(1,811)	1:A:104:VAL:HG13	1:B:338:VAL:HG21	1	0.14
(1,811)	1:A:104:VAL:HG13	1:B:338:VAL:HG22	1	0.14
(1,811)	1:A:104:VAL:HG13	1:B:338:VAL:HG23	1	0.14
(1,805)	1:A:104:VAL:HG11	1:B:331:LEU:HD11	6	0.14
(1,805)	1:A:104:VAL:HG11	1:B:331:LEU:HD12	6	0.14
(1,805)	1:A:104:VAL:HG11	1:B:331:LEU:HD13	6	0.14
(1,805)	1:A:104:VAL:HG12	1:B:331:LEU:HD11	6	0.14
(1,805)	1:A:104:VAL:HG12	1:B:331:LEU:HD12	6	0.14
(1,805)	1:A:104:VAL:HG12	1:B:331:LEU:HD13	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,805)	1:A:104:VAL:HG13	1:B:331:LEU:HD11	6	0.14
(1,805)	1:A:104:VAL:HG13	1:B:331:LEU:HD12	6	0.14
(1,805)	1:A:104:VAL:HG13	1:B:331:LEU:HD13	6	0.14
(1,791)	1:A:104:VAL:H	1:A:105:GLU:H	1	0.14
(1,783)	1:A:103:HIS:HD2	1:A:104:VAL:H	7	0.14
(1,767)	1:A:101:GLY:H	1:A:102:THR:H	7	0.14
(1,734)	1:A:96:ILE:H	1:A:125:GLU:HA	6	0.14
(1,734)	1:A:96:ILE:H	1:A:125:GLU:HA	14	0.14
(1,720)	1:A:94:PRO:HA	1:A:103:HIS:HE1	3	0.14
(1,598)	1:A:84:ILE:H	1:A:85:ARG:H	7	0.14
(1,582)	1:A:82:LEU:HA	1:A:85:ARG:H	11	0.14
(1,569)	1:A:79:LEU:HA	1:A:82:LEU:H	14	0.14
(1,491)	1:A:71:LEU:HD21	1:A:72:THR:H	14	0.14
(1,491)	1:A:71:LEU:HD22	1:A:72:THR:H	14	0.14
(1,491)	1:A:71:LEU:HD23	1:A:72:THR:H	14	0.14
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	1	0.14
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	1	0.14
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	1	0.14
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	1	0.14
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	1	0.14
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	1	0.14
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	1	0.14
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	1	0.14
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	1	0.14
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	13	0.14
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	13	0.14
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	13	0.14
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	13	0.14
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	13	0.14
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	13	0.14
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	13	0.14
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	13	0.14
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	13	0.14
(1,460)	1:A:65:ALA:HA	1:A:66:TRP:HD1	15	0.14
(1,459)	1:A:65:ALA:HA	1:A:66:TRP:HE1	14	0.14
(1,446)	1:A:60:ALA:HB1	1:A:62:ARG:HA	2	0.14
(1,446)	1:A:60:ALA:HB2	1:A:62:ARG:HA	2	0.14
(1,446)	1:A:60:ALA:HB3	1:A:62:ARG:HA	2	0.14
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD11	10	0.14
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD12	10	0.14
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD13	10	0.14
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD11	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD12	13	0.14
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD13	13	0.14
(1,418)	1:A:53:GLN:H	1:A:55:LEU:H	9	0.14
(1,389)	1:A:50:PHE:HD1	1:A:55:LEU:HD11	7	0.14
(1,389)	1:A:50:PHE:HD1	1:A:55:LEU:HD12	7	0.14
(1,389)	1:A:50:PHE:HD1	1:A:55:LEU:HD13	7	0.14
(1,389)	1:A:50:PHE:HD2	1:A:55:LEU:HD11	7	0.14
(1,389)	1:A:50:PHE:HD2	1:A:55:LEU:HD12	7	0.14
(1,389)	1:A:50:PHE:HD2	1:A:55:LEU:HD13	7	0.14
(1,387)	1:A:50:PHE:HB2	1:A:57:VAL:HG21	11	0.14
(1,387)	1:A:50:PHE:HB2	1:A:57:VAL:HG22	11	0.14
(1,387)	1:A:50:PHE:HB2	1:A:57:VAL:HG23	11	0.14
(1,387)	1:A:50:PHE:HB3	1:A:57:VAL:HG21	11	0.14
(1,387)	1:A:50:PHE:HB3	1:A:57:VAL:HG22	11	0.14
(1,387)	1:A:50:PHE:HB3	1:A:57:VAL:HG23	11	0.14
(1,373)	1:A:49:HIS:HA	1:A:53:GLN:H	1	0.14
(1,373)	1:A:49:HIS:HA	1:A:53:GLN:H	9	0.14
(1,270)	1:A:41:LEU:HD11	1:A:66:TRP:HD1	13	0.14
(1,270)	1:A:41:LEU:HD12	1:A:66:TRP:HD1	13	0.14
(1,270)	1:A:41:LEU:HD13	1:A:66:TRP:HD1	13	0.14
(1,210)	1:A:28:VAL:HG11	1:A:33:ASN:HA	8	0.14
(1,210)	1:A:28:VAL:HG12	1:A:33:ASN:HA	8	0.14
(1,210)	1:A:28:VAL:HG13	1:A:33:ASN:HA	8	0.14
(1,201)	1:A:27:LEU:HD21	1:B:330:PHE:HE1	4	0.14
(1,201)	1:A:27:LEU:HD21	1:B:330:PHE:HE2	4	0.14
(1,201)	1:A:27:LEU:HD22	1:B:330:PHE:HE1	4	0.14
(1,201)	1:A:27:LEU:HD22	1:B:330:PHE:HE2	4	0.14
(1,201)	1:A:27:LEU:HD23	1:B:330:PHE:HE1	4	0.14
(1,201)	1:A:27:LEU:HD23	1:B:330:PHE:HE2	4	0.14
(1,177)	1:A:25:MET:HE1	1:A:28:VAL:HG21	8	0.14
(1,177)	1:A:25:MET:HE1	1:A:28:VAL:HG22	8	0.14
(1,177)	1:A:25:MET:HE1	1:A:28:VAL:HG23	8	0.14
(1,177)	1:A:25:MET:HE2	1:A:28:VAL:HG21	8	0.14
(1,177)	1:A:25:MET:HE2	1:A:28:VAL:HG22	8	0.14
(1,177)	1:A:25:MET:HE2	1:A:28:VAL:HG23	8	0.14
(1,177)	1:A:25:MET:HE3	1:A:28:VAL:HG21	8	0.14
(1,177)	1:A:25:MET:HE3	1:A:28:VAL:HG22	8	0.14
(1,177)	1:A:25:MET:HE3	1:A:28:VAL:HG23	8	0.14
(1,150)	1:A:24:PHE:HA	1:A:70:VAL:HG11	7	0.14
(1,150)	1:A:24:PHE:HA	1:A:70:VAL:HG12	7	0.14
(1,150)	1:A:24:PHE:HA	1:A:70:VAL:HG13	7	0.14
(1,1188)	1:A:144:VAL:HG21	1:A:155:GLN:H	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1188)	1:A:144:VAL:HG22	1:A:155:GLN:H	5	0.14
(1,1188)	1:A:144:VAL:HG23	1:A:155:GLN:H	5	0.14
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG21	2	0.14
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG22	2	0.14
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG23	2	0.14
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG21	2	0.14
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG22	2	0.14
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG23	2	0.14
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG21	2	0.14
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG22	2	0.14
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG23	2	0.14
(1,1115)	1:A:135:LEU:H	1:A:143:PHE:HZ	5	0.14
(1,1102)	1:A:132:VAL:HA	1:A:135:LEU:H	11	0.14
(1,1075)	1:A:125:GLU:HA	1:A:128:TYR:HB2	13	0.14
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD1	15	0.14
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD2	15	0.14
(1,1050)	1:A:122:GLU:HB2	1:A:146:TYR:H	6	0.14
(1,1050)	1:A:122:GLU:HB3	1:A:146:TYR:H	6	0.14
(1,1049)	1:A:122:GLU:HA	1:A:145:HIS:HD2	15	0.14
(4,75)	1:B:281:GLN:O	1:B:285:ARG:H	9	0.13
(4,27)	1:B:239:GLU:O	1:B:243:PHE:H	11	0.13
(4,22)	1:B:229:ASN:O	1:B:232:THR:N	2	0.13
(4,21)	1:B:229:ASN:O	1:B:232:THR:H	9	0.13
(4,132)	1:B:331:LEU:O	1:B:335:LEU:N	11	0.13
(4,128)	1:B:329:GLY:O	1:B:333:ARG:N	13	0.13
(4,122)	1:B:320:LEU:O	1:B:346:TYR:N	11	0.13
(4,120)	1:B:344:VAL:O	1:B:320:LEU:N	6	0.13
(4,120)	1:B:344:VAL:O	1:B:320:LEU:N	10	0.13
(4,119)	1:B:344:VAL:O	1:B:320:LEU:H	3	0.13
(4,119)	1:B:344:VAL:O	1:B:320:LEU:H	13	0.13
(4,103)	1:B:306:ILE:O	1:B:310:SER:H	12	0.13
(3,85)	1:A:117:VAL:O	1:A:92:ALA:H	10	0.13
(3,75)	1:A:81:GLN:O	1:A:85:ARG:H	9	0.13
(3,75)	1:A:81:GLN:O	1:A:85:ARG:H	15	0.13
(3,3)	1:A:17:SER:O	1:A:89:VAL:H	8	0.13
(3,27)	1:A:39:GLU:O	1:A:43:PHE:H	14	0.13
(3,22)	1:A:29:ASN:O	1:A:32:THR:N	12	0.13
(3,120)	1:A:144:VAL:O	1:A:120:LEU:N	10	0.13
(3,119)	1:A:144:VAL:O	1:A:120:LEU:H	5	0.13
(3,119)	1:A:144:VAL:O	1:A:120:LEU:H	10	0.13
(3,108)	1:A:108:TRP:O	1:A:112:PHE:N	9	0.13
(3,103)	1:A:106:ILE:O	1:A:110:SER:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,103)	1:A:106:ILE:O	1:A:110:SER:H	14	0.13
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	5	0.13
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	5	0.13
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	5	0.13
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	6	0.13
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	6	0.13
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	6	0.13
(2,906)	1:B:316:ILE:HG12	1:B:317:VAL:H	2	0.13
(2,886)	1:B:312:PHE:HD1	1:A:112:PHE:HD1	15	0.13
(2,886)	1:B:312:PHE:HD1	1:A:112:PHE:HD2	15	0.13
(2,886)	1:B:312:PHE:HD2	1:A:112:PHE:HD1	15	0.13
(2,886)	1:B:312:PHE:HD2	1:A:112:PHE:HD2	15	0.13
(2,884)	1:B:312:PHE:HD1	1:B:314:LYS:H	15	0.13
(2,884)	1:B:312:PHE:HD2	1:B:314:LYS:H	15	0.13
(2,879)	1:B:311:ALA:HB1	1:A:112:PHE:HD1	6	0.13
(2,879)	1:B:311:ALA:HB1	1:A:112:PHE:HD2	6	0.13
(2,879)	1:B:311:ALA:HB2	1:A:112:PHE:HD1	6	0.13
(2,879)	1:B:311:ALA:HB2	1:A:112:PHE:HD2	6	0.13
(2,879)	1:B:311:ALA:HB3	1:A:112:PHE:HD1	6	0.13
(2,879)	1:B:311:ALA:HB3	1:A:112:PHE:HD2	6	0.13
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	10	0.13
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	10	0.13
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD1	13	0.13
(2,873)	1:B:311:ALA:H	1:A:112:PHE:HD2	13	0.13
(2,834)	1:B:308:TRP:HA	1:B:311:ALA:H	10	0.13
(2,805)	1:B:304:VAL:HG11	1:A:131:LEU:HD11	6	0.13
(2,805)	1:B:304:VAL:HG11	1:A:131:LEU:HD12	6	0.13
(2,805)	1:B:304:VAL:HG11	1:A:131:LEU:HD13	6	0.13
(2,805)	1:B:304:VAL:HG12	1:A:131:LEU:HD11	6	0.13
(2,805)	1:B:304:VAL:HG12	1:A:131:LEU:HD12	6	0.13
(2,805)	1:B:304:VAL:HG12	1:A:131:LEU:HD13	6	0.13
(2,805)	1:B:304:VAL:HG13	1:A:131:LEU:HD11	6	0.13
(2,805)	1:B:304:VAL:HG13	1:A:131:LEU:HD12	6	0.13
(2,805)	1:B:304:VAL:HG13	1:A:131:LEU:HD13	6	0.13
(2,791)	1:B:304:VAL:H	1:B:305:GLU:H	7	0.13
(2,783)	1:B:303:HIS:HD2	1:B:304:VAL:H	2	0.13
(2,783)	1:B:303:HIS:HD2	1:B:304:VAL:H	8	0.13
(2,780)	1:B:303:HIS:HA	1:B:307:GLY:H	12	0.13
(2,769)	1:B:301:GLY:HA2	1:A:131:LEU:HD11	6	0.13
(2,769)	1:B:301:GLY:HA2	1:A:131:LEU:HD12	6	0.13
(2,769)	1:B:301:GLY:HA2	1:A:131:LEU:HD13	6	0.13
(2,769)	1:B:301:GLY:HA3	1:A:131:LEU:HD11	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,769)	1:B:301:GLY:HA3	1:A:131:LEU:HD12	6	0.13
(2,769)	1:B:301:GLY:HA3	1:A:131:LEU:HD13	6	0.13
(2,767)	1:B:301:GLY:H	1:B:302:THR:H	13	0.13
(2,767)	1:B:301:GLY:H	1:B:302:THR:H	14	0.13
(2,767)	1:B:301:GLY:H	1:B:302:THR:H	15	0.13
(2,699)	1:B:293:ILE:HA	1:B:295:GLY:H	4	0.13
(2,623)	1:B:285:ARG:HD2	1:B:312:PHE:HD1	6	0.13
(2,623)	1:B:285:ARG:HD2	1:B:312:PHE:HD2	6	0.13
(2,623)	1:B:285:ARG:HD3	1:B:312:PHE:HD1	6	0.13
(2,623)	1:B:285:ARG:HD3	1:B:312:PHE:HD2	6	0.13
(2,623)	1:B:285:ARG:HD2	1:B:312:PHE:HD1	15	0.13
(2,623)	1:B:285:ARG:HD2	1:B:312:PHE:HD2	15	0.13
(2,623)	1:B:285:ARG:HD3	1:B:312:PHE:HD1	15	0.13
(2,623)	1:B:285:ARG:HD3	1:B:312:PHE:HD2	15	0.13
(2,622)	1:B:285:ARG:HG2	1:B:312:PHE:HD1	2	0.13
(2,622)	1:B:285:ARG:HG2	1:B:312:PHE:HD2	2	0.13
(2,622)	1:B:285:ARG:HG3	1:B:312:PHE:HD1	2	0.13
(2,622)	1:B:285:ARG:HG3	1:B:312:PHE:HD2	2	0.13
(2,622)	1:B:285:ARG:HG2	1:B:312:PHE:HD1	12	0.13
(2,622)	1:B:285:ARG:HG2	1:B:312:PHE:HD2	12	0.13
(2,622)	1:B:285:ARG:HG3	1:B:312:PHE:HD1	12	0.13
(2,622)	1:B:285:ARG:HG3	1:B:312:PHE:HD2	12	0.13
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD1	3	0.13
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD2	3	0.13
(2,590)	1:B:282:LEU:HD11	1:A:110:SER:HB2	10	0.13
(2,590)	1:B:282:LEU:HD11	1:A:110:SER:HB3	10	0.13
(2,590)	1:B:282:LEU:HD12	1:A:110:SER:HB2	10	0.13
(2,590)	1:B:282:LEU:HD12	1:A:110:SER:HB3	10	0.13
(2,590)	1:B:282:LEU:HD13	1:A:110:SER:HB2	10	0.13
(2,590)	1:B:282:LEU:HD13	1:A:110:SER:HB3	10	0.13
(2,590)	1:B:282:LEU:HD21	1:A:110:SER:HB2	10	0.13
(2,590)	1:B:282:LEU:HD21	1:A:110:SER:HB3	10	0.13
(2,590)	1:B:282:LEU:HD22	1:A:110:SER:HB2	10	0.13
(2,590)	1:B:282:LEU:HD22	1:A:110:SER:HB3	10	0.13
(2,590)	1:B:282:LEU:HD23	1:A:110:SER:HB2	10	0.13
(2,590)	1:B:282:LEU:HD23	1:A:110:SER:HB3	10	0.13
(2,582)	1:B:282:LEU:HA	1:B:285:ARG:H	4	0.13
(2,582)	1:B:282:LEU:HA	1:B:285:ARG:H	11	0.13
(2,569)	1:B:279:LEU:HA	1:B:282:LEU:H	10	0.13
(2,515)	1:B:274:GLU:H	1:B:275:GLU:H	8	0.13
(2,491)	1:B:271:LEU:HD21	1:B:272:THR:H	15	0.13
(2,491)	1:B:271:LEU:HD22	1:B:272:THR:H	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,491)	1:B:271:LEU:HD23	1:B:272:THR:H	15	0.13
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	14	0.13
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	14	0.13
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	14	0.13
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	14	0.13
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	14	0.13
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	14	0.13
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	14	0.13
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	14	0.13
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	14	0.13
(2,48)	1:B:218:VAL:H	1:B:255:LEU:HA	8	0.13
(2,48)	1:B:218:VAL:H	1:B:255:LEU:HA	12	0.13
(2,48)	1:B:218:VAL:H	1:B:255:LEU:HA	15	0.13
(2,460)	1:B:265:ALA:HA	1:B:266:TRP:HD1	15	0.13
(2,459)	1:B:265:ALA:HA	1:B:266:TRP:HE1	6	0.13
(2,449)	1:B:262:ARG:HA	1:B:266:TRP:HD1	10	0.13
(2,446)	1:B:260:ALA:HB1	1:B:262:ARG:HA	8	0.13
(2,446)	1:B:260:ALA:HB2	1:B:262:ARG:HA	8	0.13
(2,446)	1:B:260:ALA:HB3	1:B:262:ARG:HA	8	0.13
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD11	10	0.13
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD12	10	0.13
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD13	10	0.13
(2,389)	1:B:250:PHE:HD1	1:B:255:LEU:HD11	7	0.13
(2,389)	1:B:250:PHE:HD1	1:B:255:LEU:HD12	7	0.13
(2,389)	1:B:250:PHE:HD1	1:B:255:LEU:HD13	7	0.13
(2,389)	1:B:250:PHE:HD2	1:B:255:LEU:HD11	7	0.13
(2,389)	1:B:250:PHE:HD2	1:B:255:LEU:HD12	7	0.13
(2,389)	1:B:250:PHE:HD2	1:B:255:LEU:HD13	7	0.13
(2,387)	1:B:250:PHE:HB2	1:B:257:VAL:HG21	11	0.13
(2,387)	1:B:250:PHE:HB2	1:B:257:VAL:HG22	11	0.13
(2,387)	1:B:250:PHE:HB2	1:B:257:VAL:HG23	11	0.13
(2,387)	1:B:250:PHE:HB3	1:B:257:VAL:HG21	11	0.13
(2,387)	1:B:250:PHE:HB3	1:B:257:VAL:HG22	11	0.13
(2,387)	1:B:250:PHE:HB3	1:B:257:VAL:HG23	11	0.13
(2,373)	1:B:249:HIS:HA	1:B:253:GLN:H	9	0.13
(2,322)	1:B:246:LEU:HD21	1:B:249:HIS:H	4	0.13
(2,322)	1:B:246:LEU:HD22	1:B:249:HIS:H	4	0.13
(2,322)	1:B:246:LEU:HD23	1:B:249:HIS:H	4	0.13
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG21	4	0.13
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG22	4	0.13
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG23	4	0.13
(2,271)	1:B:241:LEU:HD11	1:B:266:TRP:HZ2	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,271)	1:B:241:LEU:HD12	1:B:266:TRP:HZ2	11	0.13
(2,271)	1:B:241:LEU:HD13	1:B:266:TRP:HZ2	11	0.13
(2,271)	1:B:241:LEU:HD11	1:B:266:TRP:HZ2	13	0.13
(2,271)	1:B:241:LEU:HD12	1:B:266:TRP:HZ2	13	0.13
(2,271)	1:B:241:LEU:HD13	1:B:266:TRP:HZ2	13	0.13
(2,224)	1:B:230:PRO:HD2	1:B:270:VAL:HG21	5	0.13
(2,224)	1:B:230:PRO:HD2	1:B:270:VAL:HG22	5	0.13
(2,224)	1:B:230:PRO:HD2	1:B:270:VAL:HG23	5	0.13
(2,224)	1:B:230:PRO:HD3	1:B:270:VAL:HG21	5	0.13
(2,224)	1:B:230:PRO:HD3	1:B:270:VAL:HG22	5	0.13
(2,224)	1:B:230:PRO:HD3	1:B:270:VAL:HG23	5	0.13
(2,210)	1:B:228:VAL:HG11	1:B:233:ASN:HA	13	0.13
(2,210)	1:B:228:VAL:HG12	1:B:233:ASN:HA	13	0.13
(2,210)	1:B:228:VAL:HG13	1:B:233:ASN:HA	13	0.13
(2,152)	1:B:224:PHE:HD1	1:B:225:MET:HA	2	0.13
(2,152)	1:B:224:PHE:HD2	1:B:225:MET:HA	2	0.13
(2,152)	1:B:224:PHE:HD1	1:B:225:MET:HA	7	0.13
(2,152)	1:B:224:PHE:HD2	1:B:225:MET:HA	7	0.13
(2,1210)	1:B:346:TYR:HD1	1:B:352:ALA:HA	15	0.13
(2,1210)	1:B:346:TYR:HD2	1:B:352:ALA:HA	15	0.13
(2,1184)	1:B:344:VAL:HG11	1:B:346:TYR:HD1	15	0.13
(2,1184)	1:B:344:VAL:HG11	1:B:346:TYR:HD2	15	0.13
(2,1184)	1:B:344:VAL:HG12	1:B:346:TYR:HD1	15	0.13
(2,1184)	1:B:344:VAL:HG12	1:B:346:TYR:HD2	15	0.13
(2,1184)	1:B:344:VAL:HG13	1:B:346:TYR:HD1	15	0.13
(2,1184)	1:B:344:VAL:HG13	1:B:346:TYR:HD2	15	0.13
(2,1102)	1:B:332:VAL:HA	1:B:335:LEU:H	7	0.13
(2,1102)	1:B:332:VAL:HA	1:B:335:LEU:H	8	0.13
(2,1102)	1:B:332:VAL:HA	1:B:335:LEU:H	9	0.13
(2,1101)	1:B:332:VAL:H	1:B:333:ARG:H	5	0.13
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	6	0.13
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	6	0.13
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	7	0.13
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	7	0.13
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	10	0.13
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	10	0.13
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	15	0.13
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	15	0.13
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD1	8	0.13
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD2	8	0.13
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD1	11	0.13
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD2	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD1	15	0.13
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD2	15	0.13
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	2	0.13
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	2	0.13
(2,1027)	1:B:320:LEU:HD21	1:B:345:HIS:HE1	15	0.13
(2,1027)	1:B:320:LEU:HD22	1:B:345:HIS:HE1	15	0.13
(2,1027)	1:B:320:LEU:HD23	1:B:345:HIS:HE1	15	0.13
(2,1002)	1:B:320:LEU:HD11	1:B:325:GLU:HB2	3	0.13
(2,1002)	1:B:320:LEU:HD11	1:B:325:GLU:HB3	3	0.13
(2,1002)	1:B:320:LEU:HD12	1:B:325:GLU:HB2	3	0.13
(2,1002)	1:B:320:LEU:HD12	1:B:325:GLU:HB3	3	0.13
(2,1002)	1:B:320:LEU:HD13	1:B:325:GLU:HB2	3	0.13
(2,1002)	1:B:320:LEU:HD13	1:B:325:GLU:HB3	3	0.13
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	6	0.13
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	6	0.13
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	6	0.13
(1,98)	1:A:19:PHE:H	1:A:89:VAL:H	15	0.13
(1,886)	1:A:112:PHE:HD1	1:B:312:PHE:HD1	15	0.13
(1,886)	1:A:112:PHE:HD1	1:B:312:PHE:HD2	15	0.13
(1,886)	1:A:112:PHE:HD2	1:B:312:PHE:HD1	15	0.13
(1,886)	1:A:112:PHE:HD2	1:B:312:PHE:HD2	15	0.13
(1,884)	1:A:112:PHE:HD1	1:A:114:LYS:H	12	0.13
(1,884)	1:A:112:PHE:HD2	1:A:114:LYS:H	12	0.13
(1,803)	1:A:104:VAL:HG11	1:B:307:GLY:HA2	3	0.13
(1,803)	1:A:104:VAL:HG11	1:B:307:GLY:HA3	3	0.13
(1,803)	1:A:104:VAL:HG12	1:B:307:GLY:HA2	3	0.13
(1,803)	1:A:104:VAL:HG12	1:B:307:GLY:HA3	3	0.13
(1,803)	1:A:104:VAL:HG13	1:B:307:GLY:HA2	3	0.13
(1,803)	1:A:104:VAL:HG13	1:B:307:GLY:HA3	3	0.13
(1,791)	1:A:104:VAL:H	1:A:105:GLU:H	7	0.13
(1,780)	1:A:103:HIS:HA	1:A:107:GLY:H	3	0.13
(1,734)	1:A:96:ILE:H	1:A:125:GLU:HA	10	0.13
(1,699)	1:A:93:ILE:HA	1:A:95:GLY:H	12	0.13
(1,699)	1:A:93:ILE:HA	1:A:95:GLY:H	13	0.13
(1,631)	1:A:87:ALA:HB1	1:A:90:PHE:HE1	4	0.13
(1,631)	1:A:87:ALA:HB1	1:A:90:PHE:HE2	4	0.13
(1,631)	1:A:87:ALA:HB2	1:A:90:PHE:HE1	4	0.13
(1,631)	1:A:87:ALA:HB2	1:A:90:PHE:HE2	4	0.13
(1,631)	1:A:87:ALA:HB3	1:A:90:PHE:HE1	4	0.13
(1,631)	1:A:87:ALA:HB3	1:A:90:PHE:HE2	4	0.13
(1,622)	1:A:85:ARG:HG2	1:A:112:PHE:HD1	2	0.13
(1,622)	1:A:85:ARG:HG2	1:A:112:PHE:HD2	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,622)	1:A:85:ARG:HG3	1:A:112:PHE:HD1	2	0.13
(1,622)	1:A:85:ARG:HG3	1:A:112:PHE:HD2	2	0.13
(1,622)	1:A:85:ARG:HG2	1:A:112:PHE:HD1	12	0.13
(1,622)	1:A:85:ARG:HG2	1:A:112:PHE:HD2	12	0.13
(1,622)	1:A:85:ARG:HG3	1:A:112:PHE:HD1	12	0.13
(1,622)	1:A:85:ARG:HG3	1:A:112:PHE:HD2	12	0.13
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD1	12	0.13
(1,620)	1:A:85:ARG:H	1:A:112:PHE:HD2	12	0.13
(1,582)	1:A:82:LEU:HA	1:A:85:ARG:H	4	0.13
(1,569)	1:A:79:LEU:HA	1:A:82:LEU:H	10	0.13
(1,502)	1:A:72:THR:H	1:A:74:GLU:H	5	0.13
(1,491)	1:A:71:LEU:HD21	1:A:72:THR:H	15	0.13
(1,491)	1:A:71:LEU:HD22	1:A:72:THR:H	15	0.13
(1,491)	1:A:71:LEU:HD23	1:A:72:THR:H	15	0.13
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	2	0.13
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	2	0.13
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	2	0.13
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	2	0.13
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	2	0.13
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	2	0.13
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	2	0.13
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	2	0.13
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	2	0.13
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	5	0.13
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	5	0.13
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	5	0.13
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	5	0.13
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	5	0.13
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	5	0.13
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	5	0.13
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	5	0.13
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	5	0.13
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	9	0.13
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	9	0.13
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	9	0.13
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	9	0.13
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	9	0.13
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	9	0.13
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	9	0.13
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	9	0.13
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	9	0.13
(1,48)	1:A:18:VAL:H	1:A:55:LEU:HA	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:A:18:VAL:H	1:A:55:LEU:HA	15	0.13
(1,477)	1:A:69:GLN:HB2	1:A:71:LEU:HD11	14	0.13
(1,477)	1:A:69:GLN:HB2	1:A:71:LEU:HD12	14	0.13
(1,477)	1:A:69:GLN:HB2	1:A:71:LEU:HD13	14	0.13
(1,477)	1:A:69:GLN:HB3	1:A:71:LEU:HD11	14	0.13
(1,477)	1:A:69:GLN:HB3	1:A:71:LEU:HD12	14	0.13
(1,477)	1:A:69:GLN:HB3	1:A:71:LEU:HD13	14	0.13
(1,469)	1:A:65:ALA:HB1	1:A:70:VAL:HG11	12	0.13
(1,469)	1:A:65:ALA:HB1	1:A:70:VAL:HG12	12	0.13
(1,469)	1:A:65:ALA:HB1	1:A:70:VAL:HG13	12	0.13
(1,469)	1:A:65:ALA:HB1	1:A:70:VAL:HG21	12	0.13
(1,469)	1:A:65:ALA:HB1	1:A:70:VAL:HG22	12	0.13
(1,469)	1:A:65:ALA:HB1	1:A:70:VAL:HG23	12	0.13
(1,469)	1:A:65:ALA:HB2	1:A:70:VAL:HG11	12	0.13
(1,469)	1:A:65:ALA:HB2	1:A:70:VAL:HG12	12	0.13
(1,469)	1:A:65:ALA:HB2	1:A:70:VAL:HG13	12	0.13
(1,469)	1:A:65:ALA:HB2	1:A:70:VAL:HG21	12	0.13
(1,469)	1:A:65:ALA:HB2	1:A:70:VAL:HG22	12	0.13
(1,469)	1:A:65:ALA:HB2	1:A:70:VAL:HG23	12	0.13
(1,469)	1:A:65:ALA:HB3	1:A:70:VAL:HG11	12	0.13
(1,469)	1:A:65:ALA:HB3	1:A:70:VAL:HG12	12	0.13
(1,469)	1:A:65:ALA:HB3	1:A:70:VAL:HG13	12	0.13
(1,469)	1:A:65:ALA:HB3	1:A:70:VAL:HG21	12	0.13
(1,469)	1:A:65:ALA:HB3	1:A:70:VAL:HG22	12	0.13
(1,469)	1:A:65:ALA:HB3	1:A:70:VAL:HG23	12	0.13
(1,459)	1:A:65:ALA:HA	1:A:66:TRP:HE1	6	0.13
(1,430)	1:A:55:LEU:HD21	1:A:56:GLU:H	10	0.13
(1,430)	1:A:55:LEU:HD22	1:A:56:GLU:H	10	0.13
(1,430)	1:A:55:LEU:HD23	1:A:56:GLU:H	10	0.13
(1,418)	1:A:53:GLN:H	1:A:55:LEU:H	3	0.13
(1,391)	1:A:50:PHE:HZ	1:A:55:LEU:HD11	8	0.13
(1,391)	1:A:50:PHE:HZ	1:A:55:LEU:HD12	8	0.13
(1,391)	1:A:50:PHE:HZ	1:A:55:LEU:HD13	8	0.13
(1,389)	1:A:50:PHE:HD1	1:A:55:LEU:HD11	1	0.13
(1,389)	1:A:50:PHE:HD1	1:A:55:LEU:HD12	1	0.13
(1,389)	1:A:50:PHE:HD1	1:A:55:LEU:HD13	1	0.13
(1,389)	1:A:50:PHE:HD2	1:A:55:LEU:HD11	1	0.13
(1,389)	1:A:50:PHE:HD2	1:A:55:LEU:HD12	1	0.13
(1,389)	1:A:50:PHE:HD2	1:A:55:LEU:HD13	1	0.13
(1,373)	1:A:49:HIS:HA	1:A:53:GLN:H	4	0.13
(1,350)	1:A:47:ILE:HG21	1:A:50:PHE:HE1	7	0.13
(1,350)	1:A:47:ILE:HG21	1:A:50:PHE:HE2	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,350)	1:A:47:ILE:HG22	1:A:50:PHE:HE1	7	0.13
(1,350)	1:A:47:ILE:HG22	1:A:50:PHE:HE2	7	0.13
(1,350)	1:A:47:ILE:HG23	1:A:50:PHE:HE1	7	0.13
(1,350)	1:A:47:ILE:HG23	1:A:50:PHE:HE2	7	0.13
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG21	3	0.13
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG22	3	0.13
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG23	3	0.13
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG21	6	0.13
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG22	6	0.13
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG23	6	0.13
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG21	7	0.13
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG22	7	0.13
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG23	7	0.13
(1,245)	1:A:36:PRO:HB2	1:A:37:SER:H	10	0.13
(1,245)	1:A:36:PRO:HB3	1:A:37:SER:H	10	0.13
(1,237)	1:A:33:ASN:HB2	1:A:70:VAL:HG11	15	0.13
(1,237)	1:A:33:ASN:HB2	1:A:70:VAL:HG12	15	0.13
(1,237)	1:A:33:ASN:HB2	1:A:70:VAL:HG13	15	0.13
(1,237)	1:A:33:ASN:HB3	1:A:70:VAL:HG11	15	0.13
(1,237)	1:A:33:ASN:HB3	1:A:70:VAL:HG12	15	0.13
(1,237)	1:A:33:ASN:HB3	1:A:70:VAL:HG13	15	0.13
(1,224)	1:A:30:PRO:HD2	1:A:70:VAL:HG21	5	0.13
(1,224)	1:A:30:PRO:HD2	1:A:70:VAL:HG22	5	0.13
(1,224)	1:A:30:PRO:HD2	1:A:70:VAL:HG23	5	0.13
(1,224)	1:A:30:PRO:HD3	1:A:70:VAL:HG21	5	0.13
(1,224)	1:A:30:PRO:HD3	1:A:70:VAL:HG22	5	0.13
(1,224)	1:A:30:PRO:HD3	1:A:70:VAL:HG23	5	0.13
(1,224)	1:A:30:PRO:HD2	1:A:70:VAL:HG21	13	0.13
(1,224)	1:A:30:PRO:HD2	1:A:70:VAL:HG22	13	0.13
(1,224)	1:A:30:PRO:HD2	1:A:70:VAL:HG23	13	0.13
(1,224)	1:A:30:PRO:HD3	1:A:70:VAL:HG21	13	0.13
(1,224)	1:A:30:PRO:HD3	1:A:70:VAL:HG22	13	0.13
(1,224)	1:A:30:PRO:HD3	1:A:70:VAL:HG23	13	0.13
(1,212)	1:A:28:VAL:HG11	1:B:330:PHE:HZ	11	0.13
(1,212)	1:A:28:VAL:HG12	1:B:330:PHE:HZ	11	0.13
(1,212)	1:A:28:VAL:HG13	1:B:330:PHE:HZ	11	0.13
(1,209)	1:A:28:VAL:HG11	1:A:31:GLU:HA	12	0.13
(1,209)	1:A:28:VAL:HG12	1:A:31:GLU:HA	12	0.13
(1,209)	1:A:28:VAL:HG13	1:A:31:GLU:HA	12	0.13
(1,181)	1:A:25:MET:HE1	1:A:100:PRO:HD2	1	0.13
(1,181)	1:A:25:MET:HE1	1:A:100:PRO:HD3	1	0.13
(1,181)	1:A:25:MET:HE2	1:A:100:PRO:HD2	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:A:25:MET:HE2	1:A:100:PRO:HD3	1	0.13
(1,181)	1:A:25:MET:HE3	1:A:100:PRO:HD2	1	0.13
(1,181)	1:A:25:MET:HE3	1:A:100:PRO:HD3	1	0.13
(1,150)	1:A:24:PHE:HA	1:A:70:VAL:HG11	11	0.13
(1,150)	1:A:24:PHE:HA	1:A:70:VAL:HG12	11	0.13
(1,150)	1:A:24:PHE:HA	1:A:70:VAL:HG13	11	0.13
(1,1198)	1:A:144:VAL:HG21	1:A:159:ALA:HB1	6	0.13
(1,1198)	1:A:144:VAL:HG21	1:A:159:ALA:HB2	6	0.13
(1,1198)	1:A:144:VAL:HG21	1:A:159:ALA:HB3	6	0.13
(1,1198)	1:A:144:VAL:HG22	1:A:159:ALA:HB1	6	0.13
(1,1198)	1:A:144:VAL:HG22	1:A:159:ALA:HB2	6	0.13
(1,1198)	1:A:144:VAL:HG22	1:A:159:ALA:HB3	6	0.13
(1,1198)	1:A:144:VAL:HG23	1:A:159:ALA:HB1	6	0.13
(1,1198)	1:A:144:VAL:HG23	1:A:159:ALA:HB2	6	0.13
(1,1198)	1:A:144:VAL:HG23	1:A:159:ALA:HB3	6	0.13
(1,1184)	1:A:144:VAL:HG11	1:A:146:TYR:HD1	15	0.13
(1,1184)	1:A:144:VAL:HG11	1:A:146:TYR:HD2	15	0.13
(1,1184)	1:A:144:VAL:HG12	1:A:146:TYR:HD1	15	0.13
(1,1184)	1:A:144:VAL:HG12	1:A:146:TYR:HD2	15	0.13
(1,1184)	1:A:144:VAL:HG13	1:A:146:TYR:HD1	15	0.13
(1,1184)	1:A:144:VAL:HG13	1:A:146:TYR:HD2	15	0.13
(1,1102)	1:A:132:VAL:HA	1:A:135:LEU:H	7	0.13
(1,1102)	1:A:132:VAL:HA	1:A:135:LEU:H	8	0.13
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	7	0.13
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	7	0.13
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD1	5	0.13
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD2	5	0.13
(4,98)	1:B:303:HIS:O	1:B:307:GLY:N	7	0.12
(4,96)	1:B:302:THR:O	1:B:306:ILE:N	1	0.12
(4,85)	1:B:317:VAL:O	1:B:292:ALA:H	10	0.12
(4,61)	1:B:273:PRO:O	1:B:277:THR:H	2	0.12
(4,53)	1:B:262:ARG:O	1:B:266:TRP:H	11	0.12
(4,3)	1:B:217:SER:O	1:B:289:VAL:H	8	0.12
(4,27)	1:B:239:GLU:O	1:B:243:PHE:H	14	0.12
(4,27)	1:B:239:GLU:O	1:B:243:PHE:H	15	0.12
(4,22)	1:B:229:ASN:O	1:B:232:THR:N	6	0.12
(4,22)	1:B:229:ASN:O	1:B:232:THR:N	9	0.12
(4,137)	1:B:334:GLY:O	1:B:338:VAL:H	5	0.12
(4,137)	1:B:334:GLY:O	1:B:338:VAL:H	6	0.12
(4,135)	1:B:333:ARG:O	1:B:337:THR:H	15	0.12
(4,132)	1:B:331:LEU:O	1:B:335:LEU:N	8	0.12
(4,132)	1:B:331:LEU:O	1:B:335:LEU:N	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,121)	1:B:320:LEU:O	1:B:346:TYR:H	3	0.12
(4,120)	1:B:344:VAL:O	1:B:320:LEU:N	12	0.12
(4,119)	1:B:344:VAL:O	1:B:320:LEU:H	1	0.12
(4,119)	1:B:344:VAL:O	1:B:320:LEU:H	15	0.12
(4,105)	1:B:307:GLY:O	1:B:311:ALA:H	14	0.12
(3,98)	1:A:103:HIS:O	1:A:107:GLY:N	7	0.12
(3,7)	1:A:18:VAL:O	1:A:58:PHE:H	15	0.12
(3,27)	1:A:39:GLU:O	1:A:43:PHE:H	11	0.12
(3,27)	1:A:39:GLU:O	1:A:43:PHE:H	15	0.12
(3,21)	1:A:29:ASN:O	1:A:32:THR:H	12	0.12
(3,148)	1:A:152:ALA:O	1:A:156:ILE:N	1	0.12
(3,135)	1:A:133:ARG:O	1:A:137:THR:H	3	0.12
(3,132)	1:A:131:LEU:O	1:A:135:LEU:N	14	0.12
(3,119)	1:A:144:VAL:O	1:A:120:LEU:H	7	0.12
(3,119)	1:A:144:VAL:O	1:A:120:LEU:H	13	0.12
(3,119)	1:A:144:VAL:O	1:A:120:LEU:H	15	0.12
(3,103)	1:A:106:ILE:O	1:A:110:SER:H	4	0.12
(3,103)	1:A:106:ILE:O	1:A:110:SER:H	13	0.12
(3,100)	1:A:104:VAL:O	1:A:108:TRP:N	7	0.12
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	7	0.12
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	7	0.12
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	7	0.12
(2,887)	1:B:313:ASP:H	1:B:314:LYS:H	15	0.12
(2,884)	1:B:312:PHE:HD1	1:B:314:LYS:H	11	0.12
(2,884)	1:B:312:PHE:HD2	1:B:314:LYS:H	11	0.12
(2,884)	1:B:312:PHE:HD1	1:B:314:LYS:H	14	0.12
(2,884)	1:B:312:PHE:HD2	1:B:314:LYS:H	14	0.12
(2,833)	1:B:308:TRP:H	1:B:309:ALA:H	12	0.12
(2,833)	1:B:308:TRP:H	1:B:309:ALA:H	15	0.12
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD21	8	0.12
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD22	8	0.12
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD23	8	0.12
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD21	8	0.12
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD22	8	0.12
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD23	8	0.12
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD21	8	0.12
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD22	8	0.12
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD23	8	0.12
(2,791)	1:B:304:VAL:H	1:B:305:GLU:H	1	0.12
(2,791)	1:B:304:VAL:H	1:B:305:GLU:H	5	0.12
(2,785)	1:B:303:HIS:HE1	1:B:306:ILE:HD11	9	0.12
(2,785)	1:B:303:HIS:HE1	1:B:306:ILE:HD12	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,785)	1:B:303:HIS:HE1	1:B:306:ILE:HD13	9	0.12
(2,783)	1:B:303:HIS:HD2	1:B:304:VAL:H	5	0.12
(2,780)	1:B:303:HIS:HA	1:B:307:GLY:H	3	0.12
(2,767)	1:B:301:GLY:H	1:B:302:THR:H	2	0.12
(2,767)	1:B:301:GLY:H	1:B:302:THR:H	6	0.12
(2,734)	1:B:296:ILE:H	1:B:325:GLU:HA	10	0.12
(2,716)	1:B:294:PRO:HA	1:B:298:PRO:HA	1	0.12
(2,699)	1:B:293:ILE:HA	1:B:295:GLY:H	7	0.12
(2,699)	1:B:293:ILE:HA	1:B:295:GLY:H	9	0.12
(2,699)	1:B:293:ILE:HA	1:B:295:GLY:H	12	0.12
(2,623)	1:B:285:ARG:HD2	1:B:312:PHE:HD1	2	0.12
(2,623)	1:B:285:ARG:HD2	1:B:312:PHE:HD2	2	0.12
(2,623)	1:B:285:ARG:HD3	1:B:312:PHE:HD1	2	0.12
(2,623)	1:B:285:ARG:HD3	1:B:312:PHE:HD2	2	0.12
(2,623)	1:B:285:ARG:HD2	1:B:312:PHE:HD1	9	0.12
(2,623)	1:B:285:ARG:HD2	1:B:312:PHE:HD2	9	0.12
(2,623)	1:B:285:ARG:HD3	1:B:312:PHE:HD1	9	0.12
(2,623)	1:B:285:ARG:HD3	1:B:312:PHE:HD2	9	0.12
(2,623)	1:B:285:ARG:HD2	1:B:312:PHE:HD1	10	0.12
(2,623)	1:B:285:ARG:HD2	1:B:312:PHE:HD2	10	0.12
(2,623)	1:B:285:ARG:HD3	1:B:312:PHE:HD1	10	0.12
(2,623)	1:B:285:ARG:HD3	1:B:312:PHE:HD2	10	0.12
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD1	12	0.12
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD2	12	0.12
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD1	15	0.12
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD2	15	0.12
(2,596)	1:B:283:GLU:HA	1:B:286:LYS:HG2	8	0.12
(2,596)	1:B:283:GLU:HA	1:B:286:LYS:HG3	8	0.12
(2,577)	1:B:281:GLN:HA	1:B:312:PHE:HD1	13	0.12
(2,577)	1:B:281:GLN:HA	1:B:312:PHE:HD2	13	0.12
(2,569)	1:B:279:LEU:HA	1:B:282:LEU:H	2	0.12
(2,569)	1:B:279:LEU:HA	1:B:282:LEU:H	5	0.12
(2,48)	1:B:218:VAL:H	1:B:255:LEU:HA	13	0.12
(2,477)	1:B:269:GLN:HB2	1:B:271:LEU:HD11	14	0.12
(2,477)	1:B:269:GLN:HB2	1:B:271:LEU:HD12	14	0.12
(2,477)	1:B:269:GLN:HB2	1:B:271:LEU:HD13	14	0.12
(2,477)	1:B:269:GLN:HB3	1:B:271:LEU:HD11	14	0.12
(2,477)	1:B:269:GLN:HB3	1:B:271:LEU:HD12	14	0.12
(2,477)	1:B:269:GLN:HB3	1:B:271:LEU:HD13	14	0.12
(2,446)	1:B:260:ALA:HB1	1:B:262:ARG:HA	3	0.12
(2,446)	1:B:260:ALA:HB2	1:B:262:ARG:HA	3	0.12
(2,446)	1:B:260:ALA:HB3	1:B:262:ARG:HA	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD11	14	0.12
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD12	14	0.12
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD13	14	0.12
(2,350)	1:B:247:ILE:HG21	1:B:250:PHE:HE1	7	0.12
(2,350)	1:B:247:ILE:HG21	1:B:250:PHE:HE2	7	0.12
(2,350)	1:B:247:ILE:HG22	1:B:250:PHE:HE1	7	0.12
(2,350)	1:B:247:ILE:HG22	1:B:250:PHE:HE2	7	0.12
(2,350)	1:B:247:ILE:HG23	1:B:250:PHE:HE1	7	0.12
(2,350)	1:B:247:ILE:HG23	1:B:250:PHE:HE2	7	0.12
(2,321)	1:B:246:LEU:HD11	1:B:249:HIS:H	12	0.12
(2,321)	1:B:246:LEU:HD12	1:B:249:HIS:H	12	0.12
(2,321)	1:B:246:LEU:HD13	1:B:249:HIS:H	12	0.12
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG21	2	0.12
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG22	2	0.12
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG23	2	0.12
(2,271)	1:B:241:LEU:HD11	1:B:266:TRP:HZ2	3	0.12
(2,271)	1:B:241:LEU:HD12	1:B:266:TRP:HZ2	3	0.12
(2,271)	1:B:241:LEU:HD13	1:B:266:TRP:HZ2	3	0.12
(2,25)	1:B:215:VAL:HG21	1:B:361:ARG:HD2	5	0.12
(2,25)	1:B:215:VAL:HG21	1:B:361:ARG:HD3	5	0.12
(2,25)	1:B:215:VAL:HG22	1:B:361:ARG:HD2	5	0.12
(2,25)	1:B:215:VAL:HG22	1:B:361:ARG:HD3	5	0.12
(2,25)	1:B:215:VAL:HG23	1:B:361:ARG:HD2	5	0.12
(2,25)	1:B:215:VAL:HG23	1:B:361:ARG:HD3	5	0.12
(2,239)	1:B:234:SER:HB2	1:B:235:MET:H	6	0.12
(2,239)	1:B:234:SER:HB3	1:B:235:MET:H	6	0.12
(2,237)	1:B:233:ASN:HB2	1:B:270:VAL:HG11	10	0.12
(2,237)	1:B:233:ASN:HB2	1:B:270:VAL:HG12	10	0.12
(2,237)	1:B:233:ASN:HB2	1:B:270:VAL:HG13	10	0.12
(2,237)	1:B:233:ASN:HB3	1:B:270:VAL:HG11	10	0.12
(2,237)	1:B:233:ASN:HB3	1:B:270:VAL:HG12	10	0.12
(2,237)	1:B:233:ASN:HB3	1:B:270:VAL:HG13	10	0.12
(2,237)	1:B:233:ASN:HB2	1:B:270:VAL:HG11	14	0.12
(2,237)	1:B:233:ASN:HB2	1:B:270:VAL:HG12	14	0.12
(2,237)	1:B:233:ASN:HB2	1:B:270:VAL:HG13	14	0.12
(2,237)	1:B:233:ASN:HB3	1:B:270:VAL:HG11	14	0.12
(2,237)	1:B:233:ASN:HB3	1:B:270:VAL:HG12	14	0.12
(2,237)	1:B:233:ASN:HB3	1:B:270:VAL:HG13	14	0.12
(2,228)	1:B:231:GLU:HA	1:B:232:THR:H	11	0.12
(2,200)	1:B:227:LEU:HD21	1:A:130:PHE:HD1	13	0.12
(2,200)	1:B:227:LEU:HD21	1:A:130:PHE:HD2	13	0.12
(2,200)	1:B:227:LEU:HD22	1:A:130:PHE:HD1	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,200)	1:B:227:LEU:HD22	1:A:130:PHE:HD2	13	0.12
(2,200)	1:B:227:LEU:HD23	1:A:130:PHE:HD1	13	0.12
(2,200)	1:B:227:LEU:HD23	1:A:130:PHE:HD2	13	0.12
(2,191)	1:B:227:LEU:HD11	1:B:235:MET:HA	11	0.12
(2,191)	1:B:227:LEU:HD12	1:B:235:MET:HA	11	0.12
(2,191)	1:B:227:LEU:HD13	1:B:235:MET:HA	11	0.12
(2,181)	1:B:225:MET:HE1	1:B:300:PRO:HD2	1	0.12
(2,181)	1:B:225:MET:HE1	1:B:300:PRO:HD3	1	0.12
(2,181)	1:B:225:MET:HE2	1:B:300:PRO:HD2	1	0.12
(2,181)	1:B:225:MET:HE2	1:B:300:PRO:HD3	1	0.12
(2,181)	1:B:225:MET:HE3	1:B:300:PRO:HD2	1	0.12
(2,181)	1:B:225:MET:HE3	1:B:300:PRO:HD3	1	0.12
(2,176)	1:B:225:MET:HA	1:B:228:VAL:HG11	3	0.12
(2,176)	1:B:225:MET:HA	1:B:228:VAL:HG12	3	0.12
(2,176)	1:B:225:MET:HA	1:B:228:VAL:HG13	3	0.12
(2,152)	1:B:224:PHE:HD1	1:B:225:MET:HA	15	0.12
(2,152)	1:B:224:PHE:HD2	1:B:225:MET:HA	15	0.12
(2,1252)	1:B:352:ALA:HA	1:B:355:GLN:HG2	10	0.12
(2,1252)	1:B:352:ALA:HA	1:B:355:GLN:HG3	10	0.12
(2,1198)	1:B:344:VAL:HG21	1:B:359:ALA:HB1	6	0.12
(2,1198)	1:B:344:VAL:HG21	1:B:359:ALA:HB2	6	0.12
(2,1198)	1:B:344:VAL:HG21	1:B:359:ALA:HB3	6	0.12
(2,1198)	1:B:344:VAL:HG22	1:B:359:ALA:HB1	6	0.12
(2,1198)	1:B:344:VAL:HG22	1:B:359:ALA:HB2	6	0.12
(2,1198)	1:B:344:VAL:HG22	1:B:359:ALA:HB3	6	0.12
(2,1198)	1:B:344:VAL:HG23	1:B:359:ALA:HB1	6	0.12
(2,1198)	1:B:344:VAL:HG23	1:B:359:ALA:HB2	6	0.12
(2,1198)	1:B:344:VAL:HG23	1:B:359:ALA:HB3	6	0.12
(2,1198)	1:B:344:VAL:HG21	1:B:359:ALA:HB1	10	0.12
(2,1198)	1:B:344:VAL:HG21	1:B:359:ALA:HB2	10	0.12
(2,1198)	1:B:344:VAL:HG21	1:B:359:ALA:HB3	10	0.12
(2,1198)	1:B:344:VAL:HG22	1:B:359:ALA:HB1	10	0.12
(2,1198)	1:B:344:VAL:HG22	1:B:359:ALA:HB2	10	0.12
(2,1198)	1:B:344:VAL:HG22	1:B:359:ALA:HB3	10	0.12
(2,1198)	1:B:344:VAL:HG23	1:B:359:ALA:HB1	10	0.12
(2,1198)	1:B:344:VAL:HG23	1:B:359:ALA:HB2	10	0.12
(2,1198)	1:B:344:VAL:HG23	1:B:359:ALA:HB3	10	0.12
(2,1188)	1:B:344:VAL:HG21	1:B:355:GLN:H	7	0.12
(2,1188)	1:B:344:VAL:HG22	1:B:355:GLN:H	7	0.12
(2,1188)	1:B:344:VAL:HG23	1:B:355:GLN:H	7	0.12
(2,1188)	1:B:344:VAL:HG21	1:B:355:GLN:H	12	0.12
(2,1188)	1:B:344:VAL:HG22	1:B:355:GLN:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1188)	1:B:344:VAL:HG23	1:B:355:GLN:H	12	0.12
(2,1179)	1:B:343:PHE:HA	1:B:344:VAL:HG21	1	0.12
(2,1179)	1:B:343:PHE:HA	1:B:344:VAL:HG22	1	0.12
(2,1179)	1:B:343:PHE:HA	1:B:344:VAL:HG23	1	0.12
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG21	9	0.12
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG22	9	0.12
(2,1165)	1:B:340:ALA:HB1	1:B:367:VAL:HG23	9	0.12
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG21	9	0.12
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG22	9	0.12
(2,1165)	1:B:340:ALA:HB2	1:B:367:VAL:HG23	9	0.12
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG21	9	0.12
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG22	9	0.12
(2,1165)	1:B:340:ALA:HB3	1:B:367:VAL:HG23	9	0.12
(2,1154)	1:B:339:ALA:HA	1:B:367:VAL:HG21	8	0.12
(2,1154)	1:B:339:ALA:HA	1:B:367:VAL:HG22	8	0.12
(2,1154)	1:B:339:ALA:HA	1:B:367:VAL:HG23	8	0.12
(2,1153)	1:B:339:ALA:HA	1:B:367:VAL:HG11	3	0.12
(2,1153)	1:B:339:ALA:HA	1:B:367:VAL:HG12	3	0.12
(2,1153)	1:B:339:ALA:HA	1:B:367:VAL:HG13	3	0.12
(2,1075)	1:B:325:GLU:HA	1:B:328:TYR:HB2	2	0.12
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD1	11	0.12
(2,1067)	1:B:325:GLU:HA	1:B:328:TYR:HD2	11	0.12
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD1	3	0.12
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD2	3	0.12
(2,1050)	1:B:322:GLU:HB2	1:B:346:TYR:H	2	0.12
(2,1050)	1:B:322:GLU:HB3	1:B:346:TYR:H	2	0.12
(2,1050)	1:B:322:GLU:HB2	1:B:346:TYR:H	6	0.12
(2,1050)	1:B:322:GLU:HB3	1:B:346:TYR:H	6	0.12
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	4	0.12
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	4	0.12
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	7	0.12
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	7	0.12
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	7	0.12
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	11	0.12
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	11	0.12
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	11	0.12
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	14	0.12
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	14	0.12
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	14	0.12
(1,968)	1:A:119:LEU:HD21	1:A:144:VAL:HG11	15	0.12
(1,968)	1:A:119:LEU:HD21	1:A:144:VAL:HG12	15	0.12
(1,968)	1:A:119:LEU:HD21	1:A:144:VAL:HG13	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,968)	1:A:119:LEU:HD22	1:A:144:VAL:HG11	15	0.12
(1,968)	1:A:119:LEU:HD22	1:A:144:VAL:HG12	15	0.12
(1,968)	1:A:119:LEU:HD22	1:A:144:VAL:HG13	15	0.12
(1,968)	1:A:119:LEU:HD23	1:A:144:VAL:HG11	15	0.12
(1,968)	1:A:119:LEU:HD23	1:A:144:VAL:HG12	15	0.12
(1,968)	1:A:119:LEU:HD23	1:A:144:VAL:HG13	15	0.12
(1,921)	1:A:116:ILE:HG21	1:A:141:VAL:HG11	4	0.12
(1,921)	1:A:116:ILE:HG21	1:A:141:VAL:HG12	4	0.12
(1,921)	1:A:116:ILE:HG21	1:A:141:VAL:HG13	4	0.12
(1,921)	1:A:116:ILE:HG22	1:A:141:VAL:HG11	4	0.12
(1,921)	1:A:116:ILE:HG22	1:A:141:VAL:HG12	4	0.12
(1,921)	1:A:116:ILE:HG22	1:A:141:VAL:HG13	4	0.12
(1,921)	1:A:116:ILE:HG23	1:A:141:VAL:HG11	4	0.12
(1,921)	1:A:116:ILE:HG23	1:A:141:VAL:HG12	4	0.12
(1,921)	1:A:116:ILE:HG23	1:A:141:VAL:HG13	4	0.12
(1,906)	1:A:116:ILE:HG12	1:A:117:VAL:H	1	0.12
(1,887)	1:A:113:ASP:H	1:A:114:LYS:H	2	0.12
(1,884)	1:A:112:PHE:HD1	1:A:114:LYS:H	2	0.12
(1,884)	1:A:112:PHE:HD2	1:A:114:LYS:H	2	0.12
(1,884)	1:A:112:PHE:HD1	1:A:114:LYS:H	14	0.12
(1,884)	1:A:112:PHE:HD2	1:A:114:LYS:H	14	0.12
(1,833)	1:A:108:TRP:H	1:A:109:ALA:H	12	0.12
(1,791)	1:A:104:VAL:H	1:A:105:GLU:H	12	0.12
(1,783)	1:A:103:HIS:HD2	1:A:104:VAL:H	5	0.12
(1,783)	1:A:103:HIS:HD2	1:A:104:VAL:H	15	0.12
(1,780)	1:A:103:HIS:HA	1:A:107:GLY:H	6	0.12
(1,780)	1:A:103:HIS:HA	1:A:107:GLY:H	8	0.12
(1,780)	1:A:103:HIS:HA	1:A:107:GLY:H	12	0.12
(1,767)	1:A:101:GLY:H	1:A:102:THR:H	14	0.12
(1,734)	1:A:96:ILE:H	1:A:125:GLU:HA	8	0.12
(1,704)	1:A:93:ILE:HG21	1:A:96:ILE:H	4	0.12
(1,704)	1:A:93:ILE:HG22	1:A:96:ILE:H	4	0.12
(1,704)	1:A:93:ILE:HG23	1:A:96:ILE:H	4	0.12
(1,699)	1:A:93:ILE:HA	1:A:95:GLY:H	1	0.12
(1,699)	1:A:93:ILE:HA	1:A:95:GLY:H	5	0.12
(1,699)	1:A:93:ILE:HA	1:A:95:GLY:H	9	0.12
(1,631)	1:A:87:ALA:HB1	1:A:90:PHE:HE1	3	0.12
(1,631)	1:A:87:ALA:HB1	1:A:90:PHE:HE2	3	0.12
(1,631)	1:A:87:ALA:HB2	1:A:90:PHE:HE1	3	0.12
(1,631)	1:A:87:ALA:HB2	1:A:90:PHE:HE2	3	0.12
(1,631)	1:A:87:ALA:HB3	1:A:90:PHE:HE1	3	0.12
(1,631)	1:A:87:ALA:HB3	1:A:90:PHE:HE2	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,631)	1:A:87:ALA:HB1	1:A:90:PHE:HE1	9	0.12
(1,631)	1:A:87:ALA:HB1	1:A:90:PHE:HE2	9	0.12
(1,631)	1:A:87:ALA:HB2	1:A:90:PHE:HE1	9	0.12
(1,631)	1:A:87:ALA:HB2	1:A:90:PHE:HE2	9	0.12
(1,631)	1:A:87:ALA:HB3	1:A:90:PHE:HE1	9	0.12
(1,631)	1:A:87:ALA:HB3	1:A:90:PHE:HE2	9	0.12
(1,623)	1:A:85:ARG:HD2	1:A:112:PHE:HD1	10	0.12
(1,623)	1:A:85:ARG:HD2	1:A:112:PHE:HD2	10	0.12
(1,623)	1:A:85:ARG:HD3	1:A:112:PHE:HD1	10	0.12
(1,623)	1:A:85:ARG:HD3	1:A:112:PHE:HD2	10	0.12
(1,610)	1:A:84:ILE:HG21	1:A:108:TRP:HZ3	13	0.12
(1,610)	1:A:84:ILE:HG22	1:A:108:TRP:HZ3	13	0.12
(1,610)	1:A:84:ILE:HG23	1:A:108:TRP:HZ3	13	0.12
(1,610)	1:A:84:ILE:HG21	1:A:108:TRP:HZ3	14	0.12
(1,610)	1:A:84:ILE:HG22	1:A:108:TRP:HZ3	14	0.12
(1,610)	1:A:84:ILE:HG23	1:A:108:TRP:HZ3	14	0.12
(1,590)	1:A:82:LEU:HD11	1:B:310:SER:HB2	6	0.12
(1,590)	1:A:82:LEU:HD11	1:B:310:SER:HB3	6	0.12
(1,590)	1:A:82:LEU:HD12	1:B:310:SER:HB2	6	0.12
(1,590)	1:A:82:LEU:HD12	1:B:310:SER:HB3	6	0.12
(1,590)	1:A:82:LEU:HD13	1:B:310:SER:HB2	6	0.12
(1,590)	1:A:82:LEU:HD13	1:B:310:SER:HB3	6	0.12
(1,590)	1:A:82:LEU:HD21	1:B:310:SER:HB2	6	0.12
(1,590)	1:A:82:LEU:HD21	1:B:310:SER:HB3	6	0.12
(1,590)	1:A:82:LEU:HD22	1:B:310:SER:HB2	6	0.12
(1,590)	1:A:82:LEU:HD22	1:B:310:SER:HB3	6	0.12
(1,590)	1:A:82:LEU:HD23	1:B:310:SER:HB2	6	0.12
(1,590)	1:A:82:LEU:HD23	1:B:310:SER:HB3	6	0.12
(1,577)	1:A:81:GLN:HA	1:A:112:PHE:HD1	10	0.12
(1,577)	1:A:81:GLN:HA	1:A:112:PHE:HD2	10	0.12
(1,569)	1:A:79:LEU:HA	1:A:82:LEU:H	8	0.12
(1,515)	1:A:74:GLU:H	1:A:75:GLU:H	8	0.12
(1,490)	1:A:71:LEU:HD21	1:A:72:THR:HG21	14	0.12
(1,490)	1:A:71:LEU:HD21	1:A:72:THR:HG22	14	0.12
(1,490)	1:A:71:LEU:HD21	1:A:72:THR:HG23	14	0.12
(1,490)	1:A:71:LEU:HD22	1:A:72:THR:HG21	14	0.12
(1,490)	1:A:71:LEU:HD22	1:A:72:THR:HG22	14	0.12
(1,490)	1:A:71:LEU:HD22	1:A:72:THR:HG23	14	0.12
(1,490)	1:A:71:LEU:HD23	1:A:72:THR:HG21	14	0.12
(1,490)	1:A:71:LEU:HD23	1:A:72:THR:HG22	14	0.12
(1,490)	1:A:71:LEU:HD23	1:A:72:THR:HG23	14	0.12
(1,487)	1:A:71:LEU:HA	1:A:72:THR:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG21	12	0.12
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG22	12	0.12
(1,481)	1:A:70:VAL:HG21	1:A:72:THR:HG23	12	0.12
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG21	12	0.12
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG22	12	0.12
(1,481)	1:A:70:VAL:HG22	1:A:72:THR:HG23	12	0.12
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG21	12	0.12
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG22	12	0.12
(1,481)	1:A:70:VAL:HG23	1:A:72:THR:HG23	12	0.12
(1,48)	1:A:18:VAL:H	1:A:55:LEU:HA	7	0.12
(1,48)	1:A:18:VAL:H	1:A:55:LEU:HA	8	0.12
(1,48)	1:A:18:VAL:H	1:A:55:LEU:HA	12	0.12
(1,48)	1:A:18:VAL:H	1:A:55:LEU:HA	13	0.12
(1,477)	1:A:69:GLN:HB2	1:A:71:LEU:HD11	9	0.12
(1,477)	1:A:69:GLN:HB2	1:A:71:LEU:HD12	9	0.12
(1,477)	1:A:69:GLN:HB2	1:A:71:LEU:HD13	9	0.12
(1,477)	1:A:69:GLN:HB3	1:A:71:LEU:HD11	9	0.12
(1,477)	1:A:69:GLN:HB3	1:A:71:LEU:HD12	9	0.12
(1,477)	1:A:69:GLN:HB3	1:A:71:LEU:HD13	9	0.12
(1,459)	1:A:65:ALA:HA	1:A:66:TRP:HE1	4	0.12
(1,449)	1:A:62:ARG:HA	1:A:66:TRP:HD1	14	0.12
(1,446)	1:A:60:ALA:HB1	1:A:62:ARG:HA	8	0.12
(1,446)	1:A:60:ALA:HB2	1:A:62:ARG:HA	8	0.12
(1,446)	1:A:60:ALA:HB3	1:A:62:ARG:HA	8	0.12
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD11	1	0.12
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD12	1	0.12
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD13	1	0.12
(1,419)	1:A:53:GLN:H	1:A:55:LEU:HD11	15	0.12
(1,419)	1:A:53:GLN:H	1:A:55:LEU:HD12	15	0.12
(1,419)	1:A:53:GLN:H	1:A:55:LEU:HD13	15	0.12
(1,418)	1:A:53:GLN:H	1:A:55:LEU:H	13	0.12
(1,373)	1:A:49:HIS:HA	1:A:53:GLN:H	13	0.12
(1,322)	1:A:46:LEU:HD21	1:A:49:HIS:H	4	0.12
(1,322)	1:A:46:LEU:HD22	1:A:49:HIS:H	4	0.12
(1,322)	1:A:46:LEU:HD23	1:A:49:HIS:H	4	0.12
(1,314)	1:A:45:THR:HG21	1:A:150:ALA:HB1	4	0.12
(1,314)	1:A:45:THR:HG21	1:A:150:ALA:HB2	4	0.12
(1,314)	1:A:45:THR:HG21	1:A:150:ALA:HB3	4	0.12
(1,314)	1:A:45:THR:HG22	1:A:150:ALA:HB1	4	0.12
(1,314)	1:A:45:THR:HG22	1:A:150:ALA:HB2	4	0.12
(1,314)	1:A:45:THR:HG22	1:A:150:ALA:HB3	4	0.12
(1,314)	1:A:45:THR:HG23	1:A:150:ALA:HB1	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:A:45:THR:HG23	1:A:150:ALA:HB2	4	0.12
(1,314)	1:A:45:THR:HG23	1:A:150:ALA:HB3	4	0.12
(1,299)	1:A:44:LEU:HD11	1:A:66:TRP:HZ2	12	0.12
(1,299)	1:A:44:LEU:HD12	1:A:66:TRP:HZ2	12	0.12
(1,299)	1:A:44:LEU:HD13	1:A:66:TRP:HZ2	12	0.12
(1,279)	1:A:43:PHE:HA	1:A:46:LEU:H	11	0.12
(1,270)	1:A:41:LEU:HD11	1:A:66:TRP:HD1	2	0.12
(1,270)	1:A:41:LEU:HD12	1:A:66:TRP:HD1	2	0.12
(1,270)	1:A:41:LEU:HD13	1:A:66:TRP:HD1	2	0.12
(1,239)	1:A:34:SER:HB2	1:A:35:MET:H	2	0.12
(1,239)	1:A:34:SER:HB3	1:A:35:MET:H	2	0.12
(1,239)	1:A:34:SER:HB2	1:A:35:MET:H	13	0.12
(1,239)	1:A:34:SER:HB3	1:A:35:MET:H	13	0.12
(1,201)	1:A:27:LEU:HD21	1:B:330:PHE:HE1	15	0.12
(1,201)	1:A:27:LEU:HD21	1:B:330:PHE:HE2	15	0.12
(1,201)	1:A:27:LEU:HD22	1:B:330:PHE:HE1	15	0.12
(1,201)	1:A:27:LEU:HD22	1:B:330:PHE:HE2	15	0.12
(1,201)	1:A:27:LEU:HD23	1:B:330:PHE:HE1	15	0.12
(1,201)	1:A:27:LEU:HD23	1:B:330:PHE:HE2	15	0.12
(1,191)	1:A:27:LEU:HD11	1:A:35:MET:HA	11	0.12
(1,191)	1:A:27:LEU:HD12	1:A:35:MET:HA	11	0.12
(1,191)	1:A:27:LEU:HD13	1:A:35:MET:HA	11	0.12
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG21	2	0.12
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG22	2	0.12
(1,175)	1:A:25:MET:HA	1:A:28:VAL:HG23	2	0.12
(1,1210)	1:A:146:TYR:HD1	1:A:152:ALA:HA	15	0.12
(1,1210)	1:A:146:TYR:HD2	1:A:152:ALA:HA	15	0.12
(1,1198)	1:A:144:VAL:HG21	1:A:159:ALA:HB1	10	0.12
(1,1198)	1:A:144:VAL:HG21	1:A:159:ALA:HB2	10	0.12
(1,1198)	1:A:144:VAL:HG21	1:A:159:ALA:HB3	10	0.12
(1,1198)	1:A:144:VAL:HG22	1:A:159:ALA:HB1	10	0.12
(1,1198)	1:A:144:VAL:HG22	1:A:159:ALA:HB2	10	0.12
(1,1198)	1:A:144:VAL:HG22	1:A:159:ALA:HB3	10	0.12
(1,1198)	1:A:144:VAL:HG23	1:A:159:ALA:HB1	10	0.12
(1,1198)	1:A:144:VAL:HG23	1:A:159:ALA:HB2	10	0.12
(1,1198)	1:A:144:VAL:HG23	1:A:159:ALA:HB3	10	0.12
(1,1188)	1:A:144:VAL:HG21	1:A:155:GLN:H	10	0.12
(1,1188)	1:A:144:VAL:HG22	1:A:155:GLN:H	10	0.12
(1,1188)	1:A:144:VAL:HG23	1:A:155:GLN:H	10	0.12
(1,1188)	1:A:144:VAL:HG21	1:A:155:GLN:H	12	0.12
(1,1188)	1:A:144:VAL:HG22	1:A:155:GLN:H	12	0.12
(1,1188)	1:A:144:VAL:HG23	1:A:155:GLN:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1184)	1:A:144:VAL:HG11	1:A:146:TYR:HD1	11	0.12
(1,1184)	1:A:144:VAL:HG11	1:A:146:TYR:HD2	11	0.12
(1,1184)	1:A:144:VAL:HG12	1:A:146:TYR:HD1	11	0.12
(1,1184)	1:A:144:VAL:HG12	1:A:146:TYR:HD2	11	0.12
(1,1184)	1:A:144:VAL:HG13	1:A:146:TYR:HD1	11	0.12
(1,1184)	1:A:144:VAL:HG13	1:A:146:TYR:HD2	11	0.12
(1,1182)	1:A:144:VAL:HG11	1:A:145:HIS:H	11	0.12
(1,1182)	1:A:144:VAL:HG12	1:A:145:HIS:H	11	0.12
(1,1182)	1:A:144:VAL:HG13	1:A:145:HIS:H	11	0.12
(1,1179)	1:A:143:PHE:HA	1:A:144:VAL:HG21	1	0.12
(1,1179)	1:A:143:PHE:HA	1:A:144:VAL:HG22	1	0.12
(1,1179)	1:A:143:PHE:HA	1:A:144:VAL:HG23	1	0.12
(1,1179)	1:A:143:PHE:HA	1:A:144:VAL:HG21	12	0.12
(1,1179)	1:A:143:PHE:HA	1:A:144:VAL:HG22	12	0.12
(1,1179)	1:A:143:PHE:HA	1:A:144:VAL:HG23	12	0.12
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG21	4	0.12
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG22	4	0.12
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG23	4	0.12
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG21	4	0.12
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG22	4	0.12
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG23	4	0.12
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG21	4	0.12
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG22	4	0.12
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG23	4	0.12
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG21	9	0.12
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG22	9	0.12
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG23	9	0.12
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG21	9	0.12
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG22	9	0.12
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG23	9	0.12
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG21	9	0.12
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG22	9	0.12
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG23	9	0.12
(1,1120)	1:A:135:LEU:HA	1:A:138:VAL:HG21	7	0.12
(1,1120)	1:A:135:LEU:HA	1:A:138:VAL:HG22	7	0.12
(1,1120)	1:A:135:LEU:HA	1:A:138:VAL:HG23	7	0.12
(1,1115)	1:A:135:LEU:H	1:A:143:PHE:HZ	4	0.12
(1,1102)	1:A:132:VAL:HA	1:A:135:LEU:H	9	0.12
(1,1101)	1:A:132:VAL:H	1:A:133:ARG:H	6	0.12
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD1	2	0.12
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD2	2	0.12
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD1	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD2	4	0.12
(1,1064)	1:A:125:GLU:H	1:A:126:GLU:H	3	0.12
(1,1064)	1:A:125:GLU:H	1:A:126:GLU:H	14	0.12
(1,1052)	1:A:122:GLU:HG2	1:A:145:HIS:HA	1	0.12
(1,1052)	1:A:122:GLU:HG3	1:A:145:HIS:HA	1	0.12
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE1	4	0.12
(1,1034)	1:A:121:GLU:H	1:A:128:TYR:HE2	4	0.12
(1,1002)	1:A:120:LEU:HD11	1:A:125:GLU:HB2	3	0.12
(1,1002)	1:A:120:LEU:HD11	1:A:125:GLU:HB3	3	0.12
(1,1002)	1:A:120:LEU:HD12	1:A:125:GLU:HB2	3	0.12
(1,1002)	1:A:120:LEU:HD12	1:A:125:GLU:HB3	3	0.12
(1,1002)	1:A:120:LEU:HD13	1:A:125:GLU:HB2	3	0.12
(1,1002)	1:A:120:LEU:HD13	1:A:125:GLU:HB3	3	0.12
(4,98)	1:B:303:HIS:O	1:B:307:GLY:N	1	0.11
(4,98)	1:B:303:HIS:O	1:B:307:GLY:N	8	0.11
(4,98)	1:B:303:HIS:O	1:B:307:GLY:N	14	0.11
(4,93)	1:B:301:GLY:O	1:B:305:GLU:H	13	0.11
(4,91)	1:B:300:PRO:O	1:B:304:VAL:H	7	0.11
(4,78)	1:B:282:LEU:O	1:B:286:LYS:N	9	0.11
(4,73)	1:B:280:ASP:O	1:B:284:ILE:H	7	0.11
(4,7)	1:B:218:VAL:O	1:B:258:PHE:H	15	0.11
(4,61)	1:B:273:PRO:O	1:B:277:THR:H	10	0.11
(4,61)	1:B:273:PRO:O	1:B:277:THR:H	15	0.11
(4,5)	1:B:256:GLU:O	1:B:218:VAL:H	9	0.11
(4,46)	1:B:248:GLU:O	1:B:252:LYS:N	1	0.11
(4,36)	1:B:243:PHE:O	1:B:247:ILE:N	2	0.11
(4,36)	1:B:243:PHE:O	1:B:247:ILE:N	4	0.11
(4,32)	1:B:241:LEU:O	1:B:245:THR:N	12	0.11
(4,27)	1:B:239:GLU:O	1:B:243:PHE:H	3	0.11
(4,27)	1:B:239:GLU:O	1:B:243:PHE:H	6	0.11
(4,22)	1:B:229:ASN:O	1:B:232:THR:N	5	0.11
(4,135)	1:B:333:ARG:O	1:B:337:THR:H	3	0.11
(4,133)	1:B:332:VAL:O	1:B:336:GLY:H	10	0.11
(4,132)	1:B:331:LEU:O	1:B:335:LEU:N	4	0.11
(4,121)	1:B:320:LEU:O	1:B:346:TYR:H	10	0.11
(4,120)	1:B:344:VAL:O	1:B:320:LEU:N	5	0.11
(4,120)	1:B:344:VAL:O	1:B:320:LEU:N	13	0.11
(4,119)	1:B:344:VAL:O	1:B:320:LEU:H	5	0.11
(4,119)	1:B:344:VAL:O	1:B:320:LEU:H	6	0.11
(4,108)	1:B:308:TRP:O	1:B:312:PHE:N	9	0.11
(4,105)	1:B:307:GLY:O	1:B:311:ALA:H	11	0.11
(4,103)	1:B:306:ILE:O	1:B:310:SER:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,100)	1:B:304:VAL:O	1:B:308:TRP:N	6	0.11
(3,98)	1:A:103:HIS:O	1:A:107:GLY:N	1	0.11
(3,98)	1:A:103:HIS:O	1:A:107:GLY:N	4	0.11
(3,98)	1:A:103:HIS:O	1:A:107:GLY:N	8	0.11
(3,98)	1:A:103:HIS:O	1:A:107:GLY:N	10	0.11
(3,89)	1:A:99:SER:O	1:A:103:HIS:H	13	0.11
(3,81)	1:A:115:PRO:O	1:A:90:PHE:H	14	0.11
(3,75)	1:A:81:GLN:O	1:A:85:ARG:H	13	0.11
(3,58)	1:A:64:GLU:O	1:A:68:ALA:N	10	0.11
(3,5)	1:A:56:GLU:O	1:A:18:VAL:H	9	0.11
(3,39)	1:A:45:THR:O	1:A:49:HIS:H	11	0.11
(3,39)	1:A:45:THR:O	1:A:49:HIS:H	13	0.11
(3,31)	1:A:41:LEU:O	1:A:45:THR:H	10	0.11
(3,27)	1:A:39:GLU:O	1:A:43:PHE:H	6	0.11
(3,22)	1:A:29:ASN:O	1:A:32:THR:N	2	0.11
(3,21)	1:A:29:ASN:O	1:A:32:THR:H	4	0.11
(3,21)	1:A:29:ASN:O	1:A:32:THR:H	9	0.11
(3,135)	1:A:133:ARG:O	1:A:137:THR:H	13	0.11
(3,135)	1:A:133:ARG:O	1:A:137:THR:H	14	0.11
(3,133)	1:A:132:VAL:O	1:A:136:GLY:H	10	0.11
(3,132)	1:A:131:LEU:O	1:A:135:LEU:N	4	0.11
(3,132)	1:A:131:LEU:O	1:A:135:LEU:N	11	0.11
(3,13)	1:A:58:PHE:O	1:A:20:LEU:H	7	0.11
(3,128)	1:A:129:GLY:O	1:A:133:ARG:N	11	0.11
(3,128)	1:A:129:GLY:O	1:A:133:ARG:N	13	0.11
(3,121)	1:A:120:LEU:O	1:A:146:TYR:H	3	0.11
(3,120)	1:A:144:VAL:O	1:A:120:LEU:N	5	0.11
(3,120)	1:A:144:VAL:O	1:A:120:LEU:N	13	0.11
(3,119)	1:A:144:VAL:O	1:A:120:LEU:H	6	0.11
(3,103)	1:A:106:ILE:O	1:A:110:SER:H	3	0.11
(3,100)	1:A:104:VAL:O	1:A:108:TRP:N	6	0.11
(2,999)	1:B:320:LEU:HD11	1:B:321:GLU:H	11	0.11
(2,999)	1:B:320:LEU:HD12	1:B:321:GLU:H	11	0.11
(2,999)	1:B:320:LEU:HD13	1:B:321:GLU:H	11	0.11
(2,998)	1:B:320:LEU:HA	1:B:346:TYR:HE1	8	0.11
(2,998)	1:B:320:LEU:HA	1:B:346:TYR:HE2	8	0.11
(2,998)	1:B:320:LEU:HA	1:B:346:TYR:HE1	11	0.11
(2,998)	1:B:320:LEU:HA	1:B:346:TYR:HE2	11	0.11
(2,968)	1:B:319:LEU:HD21	1:B:344:VAL:HG11	3	0.11
(2,968)	1:B:319:LEU:HD21	1:B:344:VAL:HG12	3	0.11
(2,968)	1:B:319:LEU:HD21	1:B:344:VAL:HG13	3	0.11
(2,968)	1:B:319:LEU:HD22	1:B:344:VAL:HG11	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,968)	1:B:319:LEU:HD22	1:B:344:VAL:HG12	3	0.11
(2,968)	1:B:319:LEU:HD22	1:B:344:VAL:HG13	3	0.11
(2,968)	1:B:319:LEU:HD23	1:B:344:VAL:HG11	3	0.11
(2,968)	1:B:319:LEU:HD23	1:B:344:VAL:HG12	3	0.11
(2,968)	1:B:319:LEU:HD23	1:B:344:VAL:HG13	3	0.11
(2,945)	1:B:318:LEU:H	1:B:343:PHE:HA	14	0.11
(2,906)	1:B:316:ILE:HG12	1:B:317:VAL:H	11	0.11
(2,884)	1:B:312:PHE:HD1	1:B:314:LYS:H	4	0.11
(2,884)	1:B:312:PHE:HD2	1:B:314:LYS:H	4	0.11
(2,884)	1:B:312:PHE:HD1	1:B:314:LYS:H	10	0.11
(2,884)	1:B:312:PHE:HD2	1:B:314:LYS:H	10	0.11
(2,834)	1:B:308:TRP:HA	1:B:311:ALA:H	11	0.11
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD21	10	0.11
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD22	10	0.11
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD23	10	0.11
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD21	10	0.11
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD22	10	0.11
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD23	10	0.11
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD21	10	0.11
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD22	10	0.11
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD23	10	0.11
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD21	13	0.11
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD22	13	0.11
(2,828)	1:B:306:ILE:HG21	1:B:335:LEU:HD23	13	0.11
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD21	13	0.11
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD22	13	0.11
(2,828)	1:B:306:ILE:HG22	1:B:335:LEU:HD23	13	0.11
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD21	13	0.11
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD22	13	0.11
(2,828)	1:B:306:ILE:HG23	1:B:335:LEU:HD23	13	0.11
(2,806)	1:B:304:VAL:HG11	1:A:131:LEU:HD21	13	0.11
(2,806)	1:B:304:VAL:HG11	1:A:131:LEU:HD22	13	0.11
(2,806)	1:B:304:VAL:HG11	1:A:131:LEU:HD23	13	0.11
(2,806)	1:B:304:VAL:HG12	1:A:131:LEU:HD21	13	0.11
(2,806)	1:B:304:VAL:HG12	1:A:131:LEU:HD22	13	0.11
(2,806)	1:B:304:VAL:HG12	1:A:131:LEU:HD23	13	0.11
(2,806)	1:B:304:VAL:HG13	1:A:131:LEU:HD21	13	0.11
(2,806)	1:B:304:VAL:HG13	1:A:131:LEU:HD22	13	0.11
(2,806)	1:B:304:VAL:HG13	1:A:131:LEU:HD23	13	0.11
(2,800)	1:B:304:VAL:HG21	1:A:106:ILE:HG21	2	0.11
(2,800)	1:B:304:VAL:HG21	1:A:106:ILE:HG22	2	0.11
(2,800)	1:B:304:VAL:HG21	1:A:106:ILE:HG23	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,800)	1:B:304:VAL:HG22	1:A:106:ILE:HG21	2	0.11
(2,800)	1:B:304:VAL:HG22	1:A:106:ILE:HG22	2	0.11
(2,800)	1:B:304:VAL:HG22	1:A:106:ILE:HG23	2	0.11
(2,800)	1:B:304:VAL:HG23	1:A:106:ILE:HG21	2	0.11
(2,800)	1:B:304:VAL:HG23	1:A:106:ILE:HG22	2	0.11
(2,800)	1:B:304:VAL:HG23	1:A:106:ILE:HG23	2	0.11
(2,791)	1:B:304:VAL:H	1:B:305:GLU:H	12	0.11
(2,786)	1:B:303:HIS:HD2	1:B:332:VAL:HG11	13	0.11
(2,786)	1:B:303:HIS:HD2	1:B:332:VAL:HG12	13	0.11
(2,786)	1:B:303:HIS:HD2	1:B:332:VAL:HG13	13	0.11
(2,783)	1:B:303:HIS:HD2	1:B:304:VAL:H	6	0.11
(2,783)	1:B:303:HIS:HD2	1:B:304:VAL:H	14	0.11
(2,783)	1:B:303:HIS:HD2	1:B:304:VAL:H	15	0.11
(2,767)	1:B:301:GLY:H	1:B:302:THR:H	3	0.11
(2,716)	1:B:294:PRO:HA	1:B:298:PRO:HA	6	0.11
(2,699)	1:B:293:ILE:HA	1:B:295:GLY:H	5	0.11
(2,699)	1:B:293:ILE:HA	1:B:295:GLY:H	6	0.11
(2,699)	1:B:293:ILE:HA	1:B:295:GLY:H	13	0.11
(2,631)	1:B:287:ALA:HB1	1:B:290:PHE:HE1	3	0.11
(2,631)	1:B:287:ALA:HB1	1:B:290:PHE:HE2	3	0.11
(2,631)	1:B:287:ALA:HB2	1:B:290:PHE:HE1	3	0.11
(2,631)	1:B:287:ALA:HB2	1:B:290:PHE:HE2	3	0.11
(2,631)	1:B:287:ALA:HB3	1:B:290:PHE:HE1	3	0.11
(2,631)	1:B:287:ALA:HB3	1:B:290:PHE:HE2	3	0.11
(2,624)	1:B:285:ARG:HD2	1:B:312:PHE:HE1	12	0.11
(2,624)	1:B:285:ARG:HD2	1:B:312:PHE:HE2	12	0.11
(2,624)	1:B:285:ARG:HD3	1:B:312:PHE:HE1	12	0.11
(2,624)	1:B:285:ARG:HD3	1:B:312:PHE:HE2	12	0.11
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD1	13	0.11
(2,620)	1:B:285:ARG:H	1:B:312:PHE:HD2	13	0.11
(2,610)	1:B:284:ILE:HG21	1:B:308:TRP:HZ3	14	0.11
(2,610)	1:B:284:ILE:HG22	1:B:308:TRP:HZ3	14	0.11
(2,610)	1:B:284:ILE:HG23	1:B:308:TRP:HZ3	14	0.11
(2,598)	1:B:284:ILE:H	1:B:285:ARG:H	7	0.11
(2,582)	1:B:282:LEU:HA	1:B:285:ARG:H	1	0.11
(2,577)	1:B:281:GLN:HA	1:B:312:PHE:HD1	9	0.11
(2,577)	1:B:281:GLN:HA	1:B:312:PHE:HD2	9	0.11
(2,569)	1:B:279:LEU:HA	1:B:282:LEU:H	7	0.11
(2,569)	1:B:279:LEU:HA	1:B:282:LEU:H	8	0.11
(2,537)	1:B:277:THR:HB	1:A:131:LEU:HD11	7	0.11
(2,537)	1:B:277:THR:HB	1:A:131:LEU:HD12	7	0.11
(2,537)	1:B:277:THR:HB	1:A:131:LEU:HD13	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,537)	1:B:277:THR:HB	1:A:131:LEU:HD11	10	0.11
(2,537)	1:B:277:THR:HB	1:A:131:LEU:HD12	10	0.11
(2,537)	1:B:277:THR:HB	1:A:131:LEU:HD13	10	0.11
(2,502)	1:B:272:THR:H	1:B:274:GLU:H	4	0.11
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	1	0.11
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	1	0.11
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	1	0.11
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	1	0.11
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	1	0.11
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	1	0.11
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	1	0.11
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	1	0.11
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	1	0.11
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	8	0.11
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	8	0.11
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	8	0.11
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	8	0.11
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	8	0.11
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	8	0.11
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	8	0.11
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	8	0.11
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	8	0.11
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG21	12	0.11
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG22	12	0.11
(2,481)	1:B:270:VAL:HG21	1:B:272:THR:HG23	12	0.11
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG21	12	0.11
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG22	12	0.11
(2,481)	1:B:270:VAL:HG22	1:B:272:THR:HG23	12	0.11
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG21	12	0.11
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG22	12	0.11
(2,481)	1:B:270:VAL:HG23	1:B:272:THR:HG23	12	0.11
(2,48)	1:B:218:VAL:H	1:B:255:LEU:HA	7	0.11
(2,48)	1:B:218:VAL:H	1:B:255:LEU:HA	11	0.11
(2,460)	1:B:265:ALA:HA	1:B:266:TRP:HD1	2	0.11
(2,430)	1:B:255:LEU:HD21	1:B:256:GLU:H	6	0.11
(2,430)	1:B:255:LEU:HD22	1:B:256:GLU:H	6	0.11
(2,430)	1:B:255:LEU:HD23	1:B:256:GLU:H	6	0.11
(2,430)	1:B:255:LEU:HD21	1:B:256:GLU:H	11	0.11
(2,430)	1:B:255:LEU:HD22	1:B:256:GLU:H	11	0.11
(2,430)	1:B:255:LEU:HD23	1:B:256:GLU:H	11	0.11
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD11	1	0.11
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD12	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD13	1	0.11
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD11	3	0.11
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD12	3	0.11
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD13	3	0.11
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD11	4	0.11
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD12	4	0.11
(2,428)	1:B:254:GLY:H	1:B:255:LEU:HD13	4	0.11
(2,426)	1:B:254:GLY:H	1:B:255:LEU:H	5	0.11
(2,314)	1:B:245:THR:HG21	1:B:350:ALA:HB1	3	0.11
(2,314)	1:B:245:THR:HG21	1:B:350:ALA:HB2	3	0.11
(2,314)	1:B:245:THR:HG21	1:B:350:ALA:HB3	3	0.11
(2,314)	1:B:245:THR:HG22	1:B:350:ALA:HB1	3	0.11
(2,314)	1:B:245:THR:HG22	1:B:350:ALA:HB2	3	0.11
(2,314)	1:B:245:THR:HG22	1:B:350:ALA:HB3	3	0.11
(2,314)	1:B:245:THR:HG23	1:B:350:ALA:HB1	3	0.11
(2,314)	1:B:245:THR:HG23	1:B:350:ALA:HB2	3	0.11
(2,314)	1:B:245:THR:HG23	1:B:350:ALA:HB3	3	0.11
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG21	7	0.11
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG22	7	0.11
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG23	7	0.11
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG21	13	0.11
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG22	13	0.11
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG23	13	0.11
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG21	15	0.11
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG22	15	0.11
(2,281)	1:B:243:PHE:HA	1:B:247:ILE:HG23	15	0.11
(2,280)	1:B:243:PHE:HA	1:B:246:LEU:HD11	6	0.11
(2,280)	1:B:243:PHE:HA	1:B:246:LEU:HD12	6	0.11
(2,280)	1:B:243:PHE:HA	1:B:246:LEU:HD13	6	0.11
(2,271)	1:B:241:LEU:HD11	1:B:266:TRP:HZ2	14	0.11
(2,271)	1:B:241:LEU:HD12	1:B:266:TRP:HZ2	14	0.11
(2,271)	1:B:241:LEU:HD13	1:B:266:TRP:HZ2	14	0.11
(2,270)	1:B:241:LEU:HD11	1:B:266:TRP:HD1	13	0.11
(2,270)	1:B:241:LEU:HD12	1:B:266:TRP:HD1	13	0.11
(2,270)	1:B:241:LEU:HD13	1:B:266:TRP:HD1	13	0.11
(2,233)	1:B:232:THR:HA	1:B:233:ASN:H	15	0.11
(2,209)	1:B:228:VAL:HG11	1:B:231:GLU:HA	4	0.11
(2,209)	1:B:228:VAL:HG12	1:B:231:GLU:HA	4	0.11
(2,209)	1:B:228:VAL:HG13	1:B:231:GLU:HA	4	0.11
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE1	7	0.11
(2,201)	1:B:227:LEU:HD21	1:A:130:PHE:HE2	7	0.11
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE1	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,201)	1:B:227:LEU:HD22	1:A:130:PHE:HE2	7	0.11
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE1	7	0.11
(2,201)	1:B:227:LEU:HD23	1:A:130:PHE:HE2	7	0.11
(2,177)	1:B:225:MET:HE1	1:B:228:VAL:HG21	8	0.11
(2,177)	1:B:225:MET:HE1	1:B:228:VAL:HG22	8	0.11
(2,177)	1:B:225:MET:HE1	1:B:228:VAL:HG23	8	0.11
(2,177)	1:B:225:MET:HE2	1:B:228:VAL:HG21	8	0.11
(2,177)	1:B:225:MET:HE2	1:B:228:VAL:HG22	8	0.11
(2,177)	1:B:225:MET:HE2	1:B:228:VAL:HG23	8	0.11
(2,177)	1:B:225:MET:HE3	1:B:228:VAL:HG21	8	0.11
(2,177)	1:B:225:MET:HE3	1:B:228:VAL:HG22	8	0.11
(2,177)	1:B:225:MET:HE3	1:B:228:VAL:HG23	8	0.11
(2,176)	1:B:225:MET:HA	1:B:228:VAL:HG11	2	0.11
(2,176)	1:B:225:MET:HA	1:B:228:VAL:HG12	2	0.11
(2,176)	1:B:225:MET:HA	1:B:228:VAL:HG13	2	0.11
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG21	2	0.11
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG22	2	0.11
(2,175)	1:B:225:MET:HA	1:B:228:VAL:HG23	2	0.11
(2,17)	1:B:215:VAL:HG21	1:B:250:PHE:HZ	11	0.11
(2,17)	1:B:215:VAL:HG22	1:B:250:PHE:HZ	11	0.11
(2,17)	1:B:215:VAL:HG23	1:B:250:PHE:HZ	11	0.11
(2,167)	1:B:224:PHE:HZ	1:B:265:ALA:HB1	9	0.11
(2,167)	1:B:224:PHE:HZ	1:B:265:ALA:HB2	9	0.11
(2,167)	1:B:224:PHE:HZ	1:B:265:ALA:HB3	9	0.11
(2,1268)	1:B:355:GLN:HA	1:B:358:ALA:H	14	0.11
(2,1188)	1:B:344:VAL:HG21	1:B:355:GLN:H	2	0.11
(2,1188)	1:B:344:VAL:HG22	1:B:355:GLN:H	2	0.11
(2,1188)	1:B:344:VAL:HG23	1:B:355:GLN:H	2	0.11
(2,1179)	1:B:343:PHE:HA	1:B:344:VAL:HG21	13	0.11
(2,1179)	1:B:343:PHE:HA	1:B:344:VAL:HG22	13	0.11
(2,1179)	1:B:343:PHE:HA	1:B:344:VAL:HG23	13	0.11
(2,1115)	1:B:335:LEU:H	1:B:343:PHE:HZ	5	0.11
(2,1101)	1:B:332:VAL:H	1:B:333:ARG:H	6	0.11
(2,1075)	1:B:325:GLU:HA	1:B:328:TYR:HB2	11	0.11
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD1	7	0.11
(2,1065)	1:B:325:GLU:H	1:B:328:TYR:HD2	7	0.11
(2,1064)	1:B:325:GLU:H	1:B:326:GLU:H	4	0.11
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE1	14	0.11
(2,1034)	1:B:321:GLU:H	1:B:328:TYR:HE2	14	0.11
(2,1002)	1:B:320:LEU:HD11	1:B:325:GLU:HB2	4	0.11
(2,1002)	1:B:320:LEU:HD11	1:B:325:GLU:HB3	4	0.11
(2,1002)	1:B:320:LEU:HD12	1:B:325:GLU:HB2	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1002)	1:B:320:LEU:HD12	1:B:325:GLU:HB3	4	0.11
(2,1002)	1:B:320:LEU:HD13	1:B:325:GLU:HB2	4	0.11
(2,1002)	1:B:320:LEU:HD13	1:B:325:GLU:HB3	4	0.11
(1,999)	1:A:120:LEU:HD11	1:A:121:GLU:H	4	0.11
(1,999)	1:A:120:LEU:HD12	1:A:121:GLU:H	4	0.11
(1,999)	1:A:120:LEU:HD13	1:A:121:GLU:H	4	0.11
(1,906)	1:A:116:ILE:HG12	1:A:117:VAL:H	3	0.11
(1,888)	1:A:113:ASP:HA	1:A:139:ALA:HB1	9	0.11
(1,888)	1:A:113:ASP:HA	1:A:139:ALA:HB2	9	0.11
(1,888)	1:A:113:ASP:HA	1:A:139:ALA:HB3	9	0.11
(1,884)	1:A:112:PHE:HD1	1:A:114:LYS:H	11	0.11
(1,884)	1:A:112:PHE:HD2	1:A:114:LYS:H	11	0.11
(1,879)	1:A:111:ALA:HB1	1:B:312:PHE:HD1	6	0.11
(1,879)	1:A:111:ALA:HB1	1:B:312:PHE:HD2	6	0.11
(1,879)	1:A:111:ALA:HB2	1:B:312:PHE:HD1	6	0.11
(1,879)	1:A:111:ALA:HB2	1:B:312:PHE:HD2	6	0.11
(1,879)	1:A:111:ALA:HB3	1:B:312:PHE:HD1	6	0.11
(1,879)	1:A:111:ALA:HB3	1:B:312:PHE:HD2	6	0.11
(1,879)	1:A:111:ALA:HB1	1:B:312:PHE:HD1	11	0.11
(1,879)	1:A:111:ALA:HB1	1:B:312:PHE:HD2	11	0.11
(1,879)	1:A:111:ALA:HB2	1:B:312:PHE:HD1	11	0.11
(1,879)	1:A:111:ALA:HB2	1:B:312:PHE:HD2	11	0.11
(1,879)	1:A:111:ALA:HB3	1:B:312:PHE:HD1	11	0.11
(1,879)	1:A:111:ALA:HB3	1:B:312:PHE:HD2	11	0.11
(1,864)	1:A:110:SER:H	1:A:111:ALA:H	4	0.11
(1,852)	1:A:109:ALA:HA	1:A:112:PHE:H	15	0.11
(1,834)	1:A:108:TRP:HA	1:A:111:ALA:H	10	0.11
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD21	8	0.11
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD22	8	0.11
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD23	8	0.11
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD21	8	0.11
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD22	8	0.11
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD23	8	0.11
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD21	8	0.11
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD22	8	0.11
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD23	8	0.11
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD21	10	0.11
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD22	10	0.11
(1,828)	1:A:106:ILE:HG21	1:A:135:LEU:HD23	10	0.11
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD21	10	0.11
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD22	10	0.11
(1,828)	1:A:106:ILE:HG22	1:A:135:LEU:HD23	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD21	10	0.11
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD22	10	0.11
(1,828)	1:A:106:ILE:HG23	1:A:135:LEU:HD23	10	0.11
(1,806)	1:A:104:VAL:HG11	1:B:331:LEU:HD21	1	0.11
(1,806)	1:A:104:VAL:HG11	1:B:331:LEU:HD22	1	0.11
(1,806)	1:A:104:VAL:HG11	1:B:331:LEU:HD23	1	0.11
(1,806)	1:A:104:VAL:HG12	1:B:331:LEU:HD21	1	0.11
(1,806)	1:A:104:VAL:HG12	1:B:331:LEU:HD22	1	0.11
(1,806)	1:A:104:VAL:HG12	1:B:331:LEU:HD23	1	0.11
(1,806)	1:A:104:VAL:HG13	1:B:331:LEU:HD21	1	0.11
(1,806)	1:A:104:VAL:HG13	1:B:331:LEU:HD22	1	0.11
(1,806)	1:A:104:VAL:HG13	1:B:331:LEU:HD23	1	0.11
(1,792)	1:A:104:VAL:HA	1:A:107:GLY:H	11	0.11
(1,791)	1:A:104:VAL:H	1:A:105:GLU:H	5	0.11
(1,769)	1:A:101:GLY:HA2	1:B:331:LEU:HD11	6	0.11
(1,769)	1:A:101:GLY:HA2	1:B:331:LEU:HD12	6	0.11
(1,769)	1:A:101:GLY:HA2	1:B:331:LEU:HD13	6	0.11
(1,769)	1:A:101:GLY:HA3	1:B:331:LEU:HD11	6	0.11
(1,769)	1:A:101:GLY:HA3	1:B:331:LEU:HD12	6	0.11
(1,769)	1:A:101:GLY:HA3	1:B:331:LEU:HD13	6	0.11
(1,767)	1:A:101:GLY:H	1:A:102:THR:H	6	0.11
(1,750)	1:A:96:ILE:HD11	1:A:125:GLU:H	7	0.11
(1,750)	1:A:96:ILE:HD12	1:A:125:GLU:H	7	0.11
(1,750)	1:A:96:ILE:HD13	1:A:125:GLU:H	7	0.11
(1,720)	1:A:94:PRO:HA	1:A:103:HIS:HE1	12	0.11
(1,699)	1:A:93:ILE:HA	1:A:95:GLY:H	7	0.11
(1,699)	1:A:93:ILE:HA	1:A:95:GLY:H	8	0.11
(1,623)	1:A:85:ARG:HD2	1:A:112:PHE:HD1	15	0.11
(1,623)	1:A:85:ARG:HD2	1:A:112:PHE:HD2	15	0.11
(1,623)	1:A:85:ARG:HD3	1:A:112:PHE:HD1	15	0.11
(1,623)	1:A:85:ARG:HD3	1:A:112:PHE:HD2	15	0.11
(1,590)	1:A:82:LEU:HD11	1:B:310:SER:HB2	10	0.11
(1,590)	1:A:82:LEU:HD11	1:B:310:SER:HB3	10	0.11
(1,590)	1:A:82:LEU:HD12	1:B:310:SER:HB2	10	0.11
(1,590)	1:A:82:LEU:HD12	1:B:310:SER:HB3	10	0.11
(1,590)	1:A:82:LEU:HD13	1:B:310:SER:HB2	10	0.11
(1,590)	1:A:82:LEU:HD13	1:B:310:SER:HB3	10	0.11
(1,590)	1:A:82:LEU:HD21	1:B:310:SER:HB2	10	0.11
(1,590)	1:A:82:LEU:HD21	1:B:310:SER:HB3	10	0.11
(1,590)	1:A:82:LEU:HD22	1:B:310:SER:HB2	10	0.11
(1,590)	1:A:82:LEU:HD22	1:B:310:SER:HB3	10	0.11
(1,590)	1:A:82:LEU:HD23	1:B:310:SER:HB2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:A:82:LEU:HD23	1:B:310:SER:HB3	10	0.11
(1,590)	1:A:82:LEU:HD11	1:B:310:SER:HB2	13	0.11
(1,590)	1:A:82:LEU:HD11	1:B:310:SER:HB3	13	0.11
(1,590)	1:A:82:LEU:HD12	1:B:310:SER:HB2	13	0.11
(1,590)	1:A:82:LEU:HD12	1:B:310:SER:HB3	13	0.11
(1,590)	1:A:82:LEU:HD13	1:B:310:SER:HB2	13	0.11
(1,590)	1:A:82:LEU:HD13	1:B:310:SER:HB3	13	0.11
(1,590)	1:A:82:LEU:HD21	1:B:310:SER:HB2	13	0.11
(1,590)	1:A:82:LEU:HD21	1:B:310:SER:HB3	13	0.11
(1,590)	1:A:82:LEU:HD22	1:B:310:SER:HB2	13	0.11
(1,590)	1:A:82:LEU:HD22	1:B:310:SER:HB3	13	0.11
(1,590)	1:A:82:LEU:HD23	1:B:310:SER:HB2	13	0.11
(1,590)	1:A:82:LEU:HD23	1:B:310:SER:HB3	13	0.11
(1,582)	1:A:82:LEU:HA	1:A:85:ARG:H	3	0.11
(1,577)	1:A:81:GLN:HA	1:A:112:PHE:HD1	13	0.11
(1,577)	1:A:81:GLN:HA	1:A:112:PHE:HD2	13	0.11
(1,569)	1:A:79:LEU:HA	1:A:82:LEU:H	2	0.11
(1,502)	1:A:72:THR:H	1:A:74:GLU:H	11	0.11
(1,502)	1:A:72:THR:H	1:A:74:GLU:H	15	0.11
(1,48)	1:A:18:VAL:H	1:A:55:LEU:HA	5	0.11
(1,477)	1:A:69:GLN:HB2	1:A:71:LEU:HD11	15	0.11
(1,477)	1:A:69:GLN:HB2	1:A:71:LEU:HD12	15	0.11
(1,477)	1:A:69:GLN:HB2	1:A:71:LEU:HD13	15	0.11
(1,477)	1:A:69:GLN:HB3	1:A:71:LEU:HD11	15	0.11
(1,477)	1:A:69:GLN:HB3	1:A:71:LEU:HD12	15	0.11
(1,477)	1:A:69:GLN:HB3	1:A:71:LEU:HD13	15	0.11
(1,449)	1:A:62:ARG:HA	1:A:66:TRP:HD1	4	0.11
(1,430)	1:A:55:LEU:HD21	1:A:56:GLU:H	11	0.11
(1,430)	1:A:55:LEU:HD22	1:A:56:GLU:H	11	0.11
(1,430)	1:A:55:LEU:HD23	1:A:56:GLU:H	11	0.11
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD11	5	0.11
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD12	5	0.11
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD13	5	0.11
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD11	8	0.11
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD12	8	0.11
(1,428)	1:A:54:GLY:H	1:A:55:LEU:HD13	8	0.11
(1,426)	1:A:54:GLY:H	1:A:55:LEU:H	5	0.11
(1,42)	1:A:17:SER:HB2	1:A:57:VAL:HG11	8	0.11
(1,42)	1:A:17:SER:HB2	1:A:57:VAL:HG12	8	0.11
(1,42)	1:A:17:SER:HB2	1:A:57:VAL:HG13	8	0.11
(1,42)	1:A:17:SER:HB3	1:A:57:VAL:HG11	8	0.11
(1,42)	1:A:17:SER:HB3	1:A:57:VAL:HG12	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:A:17:SER:HB3	1:A:57:VAL:HG13	8	0.11
(1,389)	1:A:50:PHE:HD1	1:A:55:LEU:HD11	15	0.11
(1,389)	1:A:50:PHE:HD1	1:A:55:LEU:HD12	15	0.11
(1,389)	1:A:50:PHE:HD1	1:A:55:LEU:HD13	15	0.11
(1,389)	1:A:50:PHE:HD2	1:A:55:LEU:HD11	15	0.11
(1,389)	1:A:50:PHE:HD2	1:A:55:LEU:HD12	15	0.11
(1,389)	1:A:50:PHE:HD2	1:A:55:LEU:HD13	15	0.11
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG21	13	0.11
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG22	13	0.11
(1,281)	1:A:43:PHE:HA	1:A:47:ILE:HG23	13	0.11
(1,280)	1:A:43:PHE:HA	1:A:46:LEU:HD11	14	0.11
(1,280)	1:A:43:PHE:HA	1:A:46:LEU:HD12	14	0.11
(1,280)	1:A:43:PHE:HA	1:A:46:LEU:HD13	14	0.11
(1,279)	1:A:43:PHE:HA	1:A:46:LEU:H	8	0.11
(1,271)	1:A:41:LEU:HD11	1:A:66:TRP:HZ2	9	0.11
(1,271)	1:A:41:LEU:HD12	1:A:66:TRP:HZ2	9	0.11
(1,271)	1:A:41:LEU:HD13	1:A:66:TRP:HZ2	9	0.11
(1,239)	1:A:34:SER:HB2	1:A:35:MET:H	15	0.11
(1,239)	1:A:34:SER:HB3	1:A:35:MET:H	15	0.11
(1,237)	1:A:33:ASN:HB2	1:A:70:VAL:HG11	10	0.11
(1,237)	1:A:33:ASN:HB2	1:A:70:VAL:HG12	10	0.11
(1,237)	1:A:33:ASN:HB2	1:A:70:VAL:HG13	10	0.11
(1,237)	1:A:33:ASN:HB3	1:A:70:VAL:HG11	10	0.11
(1,237)	1:A:33:ASN:HB3	1:A:70:VAL:HG12	10	0.11
(1,237)	1:A:33:ASN:HB3	1:A:70:VAL:HG13	10	0.11
(1,233)	1:A:32:THR:HA	1:A:33:ASN:H	15	0.11
(1,228)	1:A:31:GLU:HA	1:A:32:THR:H	9	0.11
(1,199)	1:A:27:LEU:HD21	1:A:95:GLY:HA2	9	0.11
(1,199)	1:A:27:LEU:HD21	1:A:95:GLY:HA3	9	0.11
(1,199)	1:A:27:LEU:HD22	1:A:95:GLY:HA2	9	0.11
(1,199)	1:A:27:LEU:HD22	1:A:95:GLY:HA3	9	0.11
(1,199)	1:A:27:LEU:HD23	1:A:95:GLY:HA2	9	0.11
(1,199)	1:A:27:LEU:HD23	1:A:95:GLY:HA3	9	0.11
(1,176)	1:A:25:MET:HA	1:A:28:VAL:HG11	3	0.11
(1,176)	1:A:25:MET:HA	1:A:28:VAL:HG12	3	0.11
(1,176)	1:A:25:MET:HA	1:A:28:VAL:HG13	3	0.11
(1,152)	1:A:24:PHE:HD1	1:A:25:MET:HA	7	0.11
(1,152)	1:A:24:PHE:HD2	1:A:25:MET:HA	7	0.11
(1,152)	1:A:24:PHE:HD1	1:A:25:MET:HA	15	0.11
(1,152)	1:A:24:PHE:HD2	1:A:25:MET:HA	15	0.11
(1,1312)	1:A:162:LYS:HA	1:A:165:ASP:H	8	0.11
(1,1268)	1:A:155:GLN:HA	1:A:158:ALA:H	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1253)	1:A:152:ALA:HA	1:A:156:ILE:HD11	9	0.11
(1,1253)	1:A:152:ALA:HA	1:A:156:ILE:HD12	9	0.11
(1,1253)	1:A:152:ALA:HA	1:A:156:ILE:HD13	9	0.11
(1,1222)	1:A:149:ILE:H	1:A:150:ALA:H	1	0.11
(1,1222)	1:A:149:ILE:H	1:A:150:ALA:H	11	0.11
(1,1222)	1:A:149:ILE:H	1:A:150:ALA:H	13	0.11
(1,1210)	1:A:146:TYR:HD1	1:A:152:ALA:HA	3	0.11
(1,1210)	1:A:146:TYR:HD2	1:A:152:ALA:HA	3	0.11
(1,1188)	1:A:144:VAL:HG21	1:A:155:GLN:H	2	0.11
(1,1188)	1:A:144:VAL:HG22	1:A:155:GLN:H	2	0.11
(1,1188)	1:A:144:VAL:HG23	1:A:155:GLN:H	2	0.11
(1,1188)	1:A:144:VAL:HG21	1:A:155:GLN:H	7	0.11
(1,1188)	1:A:144:VAL:HG22	1:A:155:GLN:H	7	0.11
(1,1188)	1:A:144:VAL:HG23	1:A:155:GLN:H	7	0.11
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG21	11	0.11
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG22	11	0.11
(1,1165)	1:A:140:ALA:HB1	1:A:167:VAL:HG23	11	0.11
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG21	11	0.11
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG22	11	0.11
(1,1165)	1:A:140:ALA:HB2	1:A:167:VAL:HG23	11	0.11
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG21	11	0.11
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG22	11	0.11
(1,1165)	1:A:140:ALA:HB3	1:A:167:VAL:HG23	11	0.11
(1,1153)	1:A:139:ALA:HA	1:A:167:VAL:HG11	3	0.11
(1,1153)	1:A:139:ALA:HA	1:A:167:VAL:HG12	3	0.11
(1,1153)	1:A:139:ALA:HA	1:A:167:VAL:HG13	3	0.11
(1,1151)	1:A:139:ALA:H	1:A:141:VAL:HG11	11	0.11
(1,1151)	1:A:139:ALA:H	1:A:141:VAL:HG12	11	0.11
(1,1151)	1:A:139:ALA:H	1:A:141:VAL:HG13	11	0.11
(1,1101)	1:A:132:VAL:H	1:A:133:ARG:H	5	0.11
(1,1075)	1:A:125:GLU:HA	1:A:128:TYR:HB2	1	0.11
(1,1075)	1:A:125:GLU:HA	1:A:128:TYR:HB2	11	0.11
(1,1075)	1:A:125:GLU:HA	1:A:128:TYR:HB2	15	0.11
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD1	15	0.11
(1,1067)	1:A:125:GLU:HA	1:A:128:TYR:HD2	15	0.11
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD1	7	0.11
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD2	7	0.11
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD1	14	0.11
(1,1065)	1:A:125:GLU:H	1:A:128:TYR:HD2	14	0.11
(1,1064)	1:A:125:GLU:H	1:A:126:GLU:H	4	0.11

10 Dihedral-angle violation analysis [i](#)

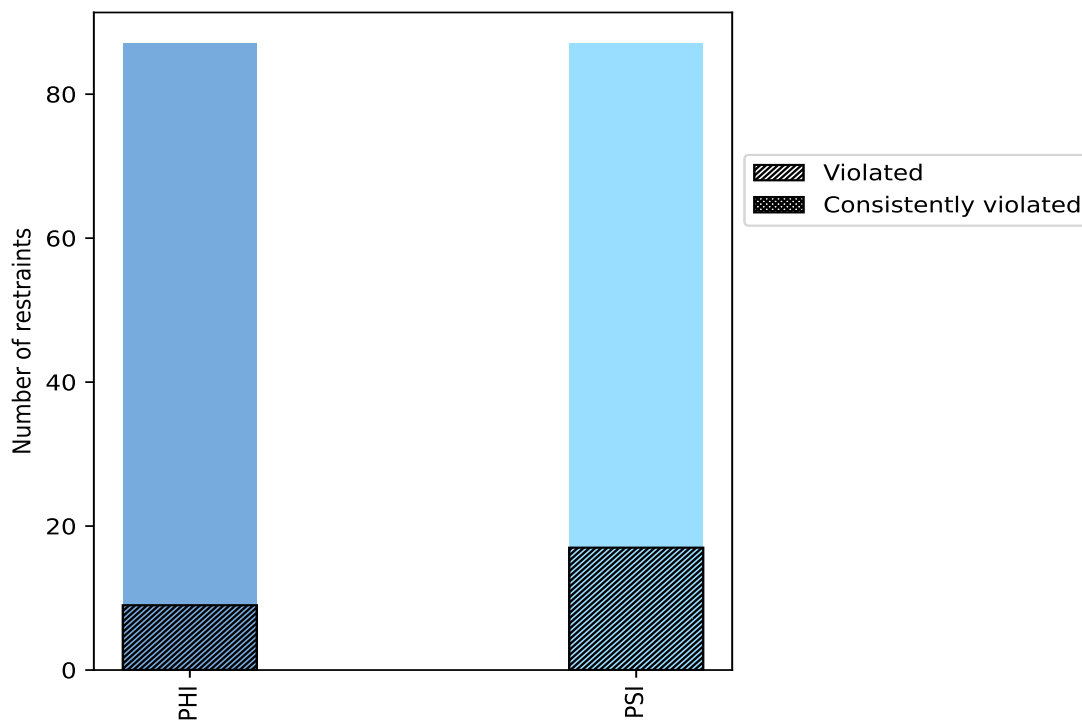
10.1 Summary of dihedral-angle violations [i](#)

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
PHI	87	50.0	9	10.3	5.2	0	0.0	0.0
PSI	87	50.0	17	19.5	9.8	0	0.0	0.0
Total	174	100.0	26	14.9	14.9	0	0.0	0.0

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

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



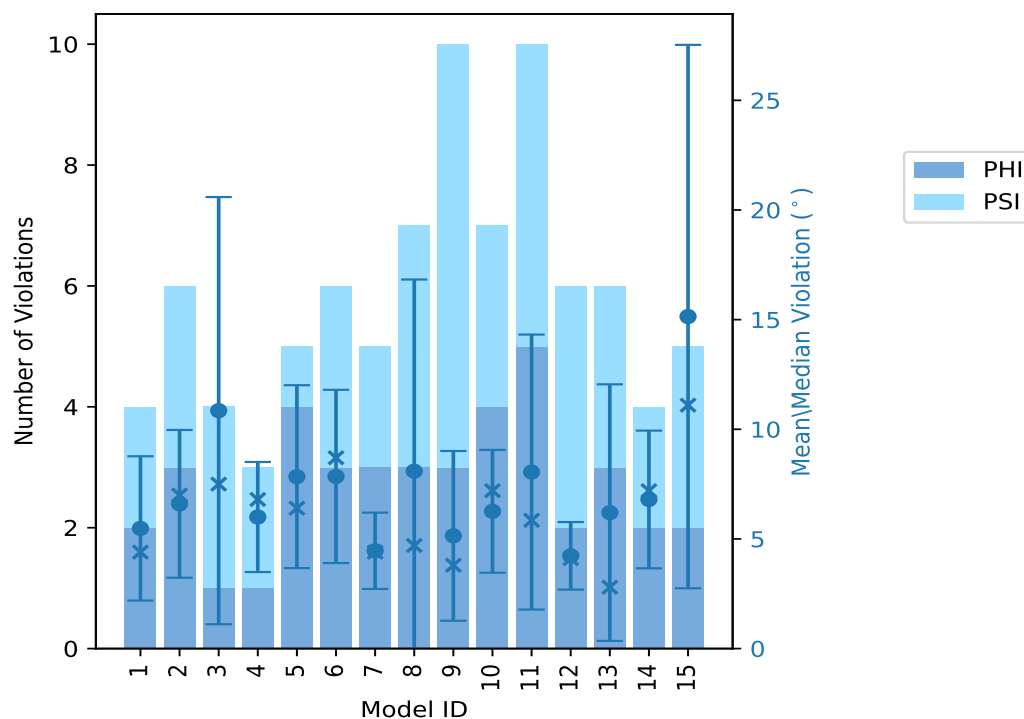
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PHI	PSI	Total				
1	2	2	4	5.48	10.9	3.29	4.4
2	3	3	6	6.6	12.3	3.37	7.0
3	1	3	4	10.85	27.0	9.74	7.5
4	1	2	3	6.0	8.6	2.51	6.8
5	4	1	5	7.84	13.1	4.17	6.4
6	3	3	6	7.85	12.5	3.95	8.7
7	3	2	5	4.46	7.4	1.74	4.4
8	3	4	7	8.09	28.4	8.74	4.7
9	3	7	10	5.14	14.8	3.87	3.8
10	4	3	7	6.26	10.2	2.8	7.2
11	5	5	10	8.05	24.9	6.27	5.85
12	2	4	6	4.23	6.4	1.54	4.1
13	3	3	6	6.2	18.1	5.85	2.8
14	2	2	4	6.8	10.1	3.14	7.2
15	2	3	5	15.14	36.9	12.39	11.1

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

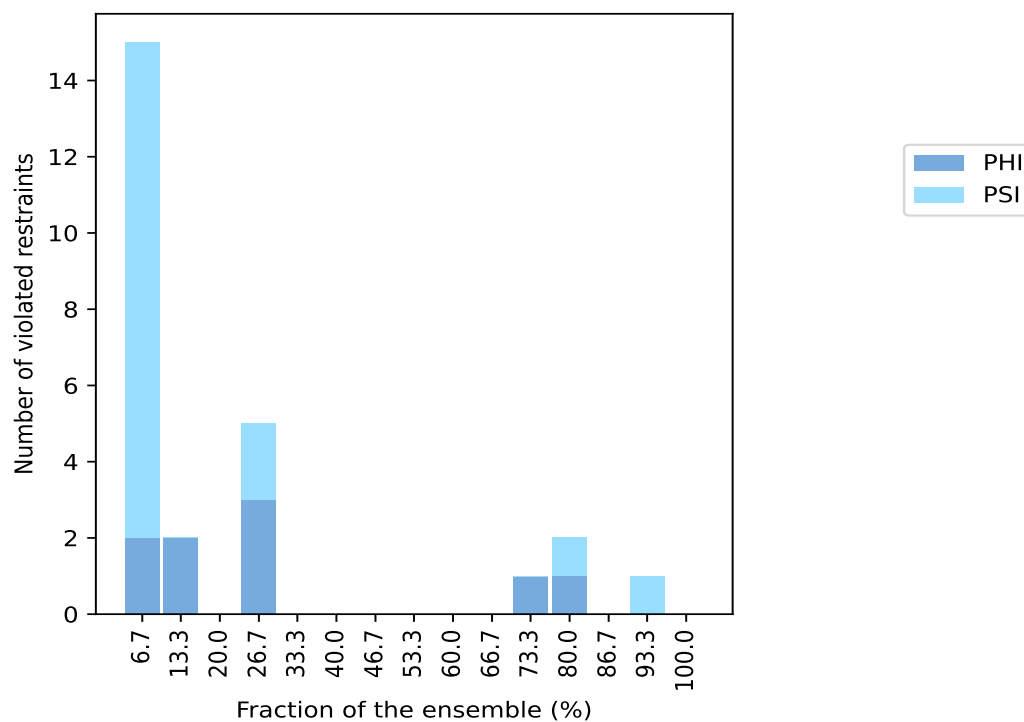
10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
2	13	15	1	6.7
2	0	2	2	13.3
0	0	0	3	20.0
3	2	5	4	26.7
0	0	0	5	33.3
0	0	0	6	40.0
0	0	0	7	46.7
0	0	0	8	53.3
0	0	0	9	60.0
0	0	0	10	66.7
1	0	1	11	73.3
1	1	2	12	80.0
0	0	0	13	86.7
0	1	1	14	93.3
0	0	0	15	100.0

¹ Number of models with violations

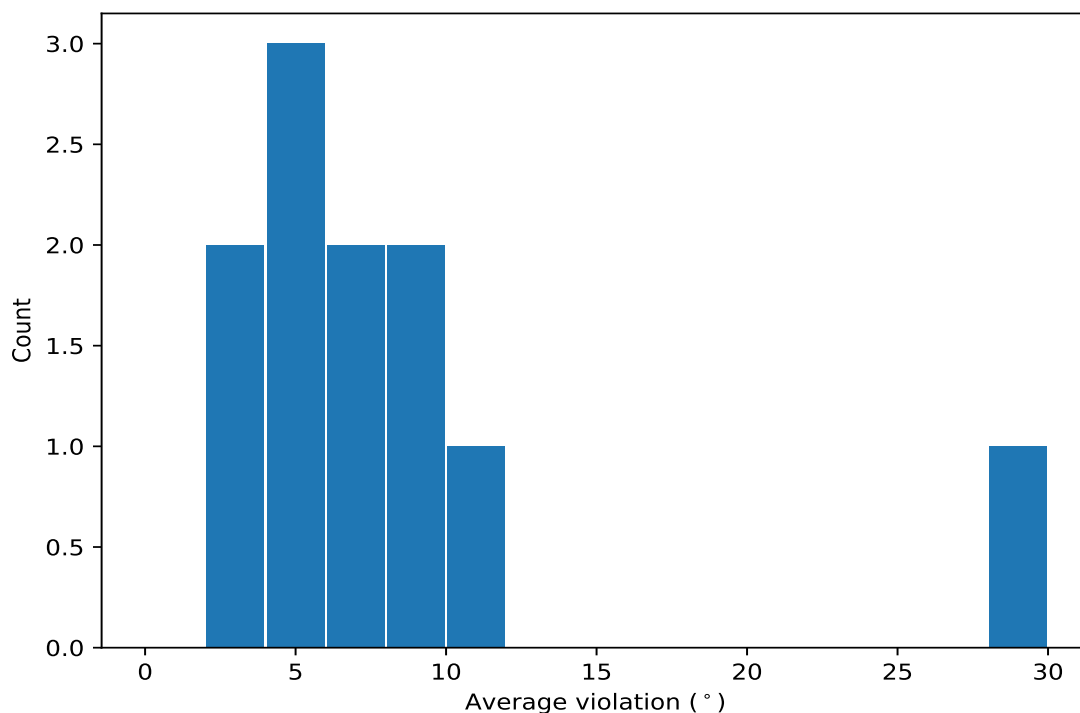
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

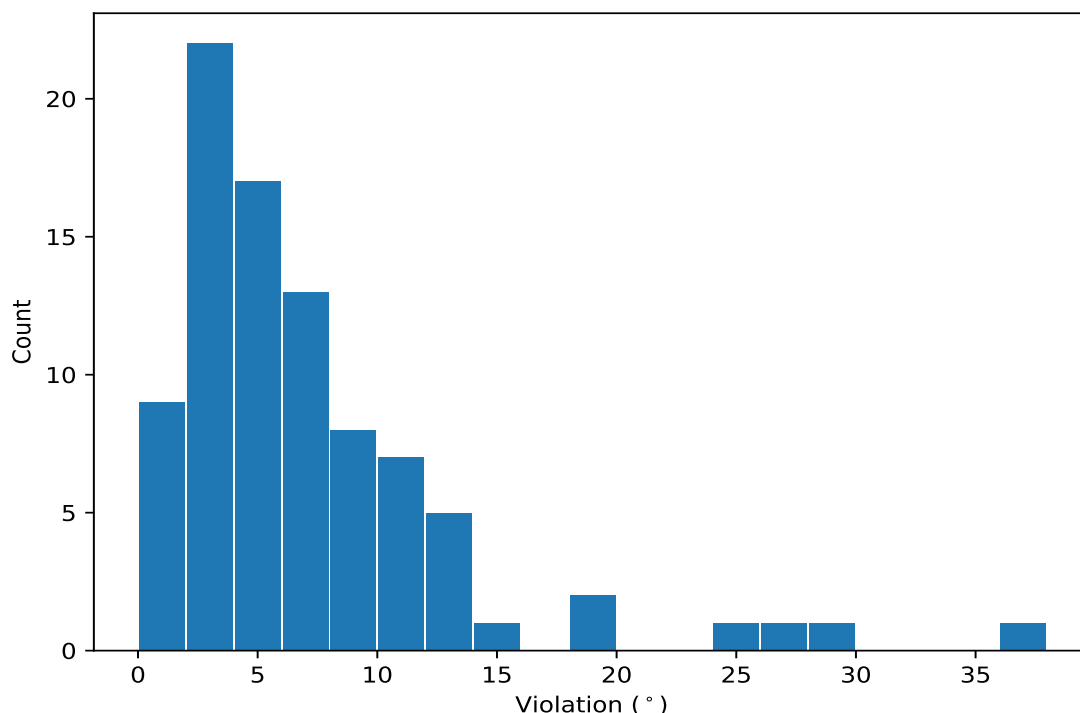
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	14	8.39	3.7	8.85
(2,73)	1:B:290:PHE:C	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	12	7.11	4.33	5.75
(2,6)	1:B:219:PHE:N	1:B:219:PHE:CA	1:B:219:PHE:C	1:B:220:LEU:N	12	5.26	2.65	5.2
(2,81)	1:B:302:THR:C	1:B:303:HIS:N	1:B:303:HIS:CA	1:B:303:HIS:C	11	4.55	1.89	4.9
(2,135)	1:B:345:HIS:C	1:B:346:TYR:N	1:B:346:TYR:CA	1:B:346:TYR:C	4	29.3	4.56	27.7
(2,136)	1:B:346:TYR:N	1:B:346:TYR:CA	1:B:346:TYR:C	1:B:347:LYS:N	4	11.8	4.46	9.85
(2,75)	1:B:291:VAL:C	1:B:292:ALA:N	1:B:292:ALA:CA	1:B:292:ALA:C	4	8.98	4.26	10.15
(2,122)	1:B:339:ALA:N	1:B:339:ALA:CA	1:B:339:ALA:C	1:B:340:ALA:N	4	6.15	4.15	5.1
(2,123)	1:B:339:ALA:C	1:B:340:ALA:N	1:B:340:ALA:CA	1:B:340:ALA:C	4	4.18	1.84	3.65
(2,113)	1:B:329:GLY:C	1:B:330:PHE:N	1:B:330:PHE:CA	1:B:330:PHE:C	2	3.85	1.75	3.85
(2,101)	1:B:317:VAL:C	1:B:318:LEU:N	1:B:318:LEU:CA	1:B:318:LEU:C	2	3.5	0.6	3.5

¹ Number of violated models, ²Standard 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 (°)
(2,135)	1:B:345:HIS:C	1:B:346:TYR:N	1:B:346:TYR:CA	1:B:346:TYR:C	15	36.9
(2,135)	1:B:345:HIS:C	1:B:346:TYR:N	1:B:346:TYR:CA	1:B:346:TYR:C	8	28.4
(2,135)	1:B:345:HIS:C	1:B:346:TYR:N	1:B:346:TYR:CA	1:B:346:TYR:C	3	27.0
(2,135)	1:B:345:HIS:C	1:B:346:TYR:N	1:B:346:TYR:CA	1:B:346:TYR:C	11	24.9
(2,136)	1:B:346:TYR:N	1:B:346:TYR:CA	1:B:346:TYR:C	1:B:347:LYS:N	15	19.4
(2,73)	1:B:290:PHE:C	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	13	18.1
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	9	14.8
(2,75)	1:B:291:VAL:C	1:B:292:ALA:N	1:B:292:ALA:CA	1:B:292:ALA:C	5	13.1
(2,122)	1:B:339:ALA:N	1:B:339:ALA:CA	1:B:339:ALA:C	1:B:340:ALA:N	11	12.7
(2,75)	1:B:291:VAL:C	1:B:292:ALA:N	1:B:292:ALA:CA	1:B:292:ALA:C	6	12.5
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	2	12.3
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	5	12.1
(2,73)	1:B:290:PHE:C	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	6	11.2
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	6	11.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,73)	1:B:290:PHE:C	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	15	11.1
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	1	10.9
(2,136)	1:B:346:TYR:N	1:B:346:TYR:CA	1:B:346:TYR:C	1:B:347:LYS:N	8	10.3
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	10	10.2
(2,6)	1:B:219:PHE:N	1:B:219:PHE:CA	1:B:219:PHE:C	1:B:220:LEU:N	14	10.1
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	14	9.6
(2,136)	1:B:346:TYR:N	1:B:346:TYR:CA	1:B:346:TYR:C	1:B:347:LYS:N	3	9.4
(2,70)	1:B:289:VAL:N	1:B:289:VAL:CA	1:B:289:VAL:C	1:B:290:PHE:N	10	9.1
(2,6)	1:B:219:PHE:N	1:B:219:PHE:CA	1:B:219:PHE:C	1:B:220:LEU:N	13	9.1
(2,73)	1:B:290:PHE:C	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	4	8.6
(2,82)	1:B:303:HIS:N	1:B:303:HIS:CA	1:B:303:HIS:C	1:B:304:VAL:N	9	8.1
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	11	8.1
(2,136)	1:B:346:TYR:N	1:B:346:TYR:CA	1:B:346:TYR:C	1:B:347:LYS:N	11	8.1
(2,81)	1:B:302:THR:C	1:B:303:HIS:N	1:B:303:HIS:CA	1:B:303:HIS:C	2	7.9
(2,75)	1:B:291:VAL:C	1:B:292:ALA:N	1:B:292:ALA:CA	1:B:292:ALA:C	2	7.8
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	7	7.4
(2,81)	1:B:302:THR:C	1:B:303:HIS:N	1:B:303:HIS:CA	1:B:303:HIS:C	10	7.2
(2,6)	1:B:219:PHE:N	1:B:219:PHE:CA	1:B:219:PHE:C	1:B:220:LEU:N	15	7.2
(2,123)	1:B:339:ALA:C	1:B:340:ALA:N	1:B:340:ALA:CA	1:B:340:ALA:C	10	7.2
(2,6)	1:B:219:PHE:N	1:B:219:PHE:CA	1:B:219:PHE:C	1:B:220:LEU:N	4	6.8
(2,122)	1:B:339:ALA:N	1:B:339:ALA:CA	1:B:339:ALA:C	1:B:340:ALA:N	9	6.5
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	12	6.4
(2,73)	1:B:290:PHE:C	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	5	6.4
(2,81)	1:B:302:THR:C	1:B:303:HIS:N	1:B:303:HIS:CA	1:B:303:HIS:C	6	6.3
(2,10)	1:B:221:ALA:N	1:B:221:ALA:CA	1:B:221:ALA:C	1:B:222:GLY:N	2	6.2
(2,84)	1:B:304:VAL:N	1:B:304:VAL:CA	1:B:304:VAL:C	1:B:305:GLU:N	9	6.1
(2,6)	1:B:219:PHE:N	1:B:219:PHE:CA	1:B:219:PHE:C	1:B:220:LEU:N	11	5.9
(2,73)	1:B:290:PHE:C	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	11	5.8
(2,73)	1:B:290:PHE:C	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	8	5.7
(2,6)	1:B:219:PHE:N	1:B:219:PHE:CA	1:B:219:PHE:C	1:B:220:LEU:N	12	5.7
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	3	5.6
(2,113)	1:B:329:GLY:C	1:B:330:PHE:N	1:B:330:PHE:CA	1:B:330:PHE:C	5	5.6
(2,81)	1:B:302:THR:C	1:B:303:HIS:N	1:B:303:HIS:CA	1:B:303:HIS:C	11	5.1
(2,81)	1:B:302:THR:C	1:B:303:HIS:N	1:B:303:HIS:CA	1:B:303:HIS:C	1	5.0
(2,73)	1:B:290:PHE:C	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	10	5.0
(2,81)	1:B:302:THR:C	1:B:303:HIS:N	1:B:303:HIS:CA	1:B:303:HIS:C	7	4.9
(2,73)	1:B:290:PHE:C	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	14	4.8
(2,6)	1:B:219:PHE:N	1:B:219:PHE:CA	1:B:219:PHE:C	1:B:220:LEU:N	9	4.7
(2,44)	1:B:274:GLU:N	1:B:274:GLU:CA	1:B:274:GLU:C	1:B:275:GLU:N	8	4.7
(2,68)	1:B:286:LYS:N	1:B:286:LYS:CA	1:B:286:LYS:C	1:B:287:ALA:N	12	4.6
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	8	4.5
(2,6)	1:B:219:PHE:N	1:B:219:PHE:CA	1:B:219:PHE:C	1:B:220:LEU:N	7	4.4
(2,101)	1:B:317:VAL:C	1:B:318:LEU:N	1:B:318:LEU:CA	1:B:318:LEU:C	11	4.1
(2,6)	1:B:219:PHE:N	1:B:219:PHE:CA	1:B:219:PHE:C	1:B:220:LEU:N	1	3.8
(2,123)	1:B:339:ALA:C	1:B:340:ALA:N	1:B:340:ALA:CA	1:B:340:ALA:C	2	3.7
(2,122)	1:B:339:ALA:N	1:B:339:ALA:CA	1:B:339:ALA:C	1:B:340:ALA:N	6	3.7
(2,73)	1:B:290:PHE:C	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	12	3.6
(2,123)	1:B:339:ALA:C	1:B:340:ALA:N	1:B:340:ALA:CA	1:B:340:ALA:C	11	3.6
(2,67)	1:B:285:ARG:C	1:B:286:LYS:N	1:B:286:LYS:CA	1:B:286:LYS:C	7	3.4
(2,81)	1:B:302:THR:C	1:B:303:HIS:N	1:B:303:HIS:CA	1:B:303:HIS:C	12	3.3
(2,81)	1:B:302:THR:C	1:B:303:HIS:N	1:B:303:HIS:CA	1:B:303:HIS:C	13	3.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,66)	1:B:285:ARG:N	1:B:285:ARG:CA	1:B:285:ARG:C	1:B:286:LYS:N	10	3.0
(2,101)	1:B:317:VAL:C	1:B:318:LEU:N	1:B:318:LEU:CA	1:B:318:LEU:C	9	2.9
(2,73)	1:B:290:PHE:C	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	9	2.8
(2,81)	1:B:302:THR:C	1:B:303:HIS:N	1:B:303:HIS:CA	1:B:303:HIS:C	9	2.7
(2,81)	1:B:302:THR:C	1:B:303:HIS:N	1:B:303:HIS:CA	1:B:303:HIS:C	14	2.7
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	4	2.6
(2,72)	1:B:290:PHE:N	1:B:290:PHE:CA	1:B:290:PHE:C	1:B:291:VAL:N	13	2.6
(2,75)	1:B:291:VAL:C	1:B:292:ALA:N	1:B:292:ALA:CA	1:B:292:ALA:C	13	2.5
(2,6)	1:B:219:PHE:N	1:B:219:PHE:CA	1:B:219:PHE:C	1:B:220:LEU:N	6	2.3
(2,73)	1:B:290:PHE:C	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	7	2.2
(2,124)	1:B:340:ALA:N	1:B:340:ALA:CA	1:B:340:ALA:C	1:B:341:VAL:N	11	2.2
(2,123)	1:B:339:ALA:C	1:B:340:ALA:N	1:B:340:ALA:CA	1:B:340:ALA:C	1	2.2
(2,113)	1:B:329:GLY:C	1:B:330:PHE:N	1:B:330:PHE:CA	1:B:330:PHE:C	10	2.1
(2,81)	1:B:302:THR:C	1:B:303:HIS:N	1:B:303:HIS:CA	1:B:303:HIS:C	5	2.0
(2,80)	1:B:302:THR:N	1:B:302:THR:CA	1:B:302:THR:C	1:B:303:HIS:N	13	1.9
(2,22)	1:B:243:PHE:N	1:B:243:PHE:CA	1:B:243:PHE:C	1:B:244:LEU:N	12	1.8
(2,6)	1:B:219:PHE:N	1:B:219:PHE:CA	1:B:219:PHE:C	1:B:220:LEU:N	2	1.7
(2,122)	1:B:339:ALA:N	1:B:339:ALA:CA	1:B:339:ALA:C	1:B:340:ALA:N	8	1.7
(2,74)	1:B:291:VAL:N	1:B:291:VAL:CA	1:B:291:VAL:C	1:B:292:ALA:N	9	1.5
(2,6)	1:B:219:PHE:N	1:B:219:PHE:CA	1:B:219:PHE:C	1:B:220:LEU:N	3	1.4
(2,156)	1:B:358:ALA:N	1:B:358:ALA:CA	1:B:358:ALA:C	1:B:359:ALA:N	9	1.3
(2,111)	1:B:326:GLU:C	1:B:327:GLU:N	1:B:327:GLU:CA	1:B:327:GLU:C	8	1.3
(2,56)	1:B:280:ASP:N	1:B:280:ASP:CA	1:B:280:ASP:C	1:B:281:GLN:N	15	1.1