Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 01:58 pm BST

PDB ID	:	5L85
BMRB ID	:	34007
Title	:	Solution structure of the complex between human ZNHIT3 and NUFIP1 proteins
Authors	:	Quinternet, M.; Chagot, M.-E.; Manival, X.
Deposited on	:	2016-06-07

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

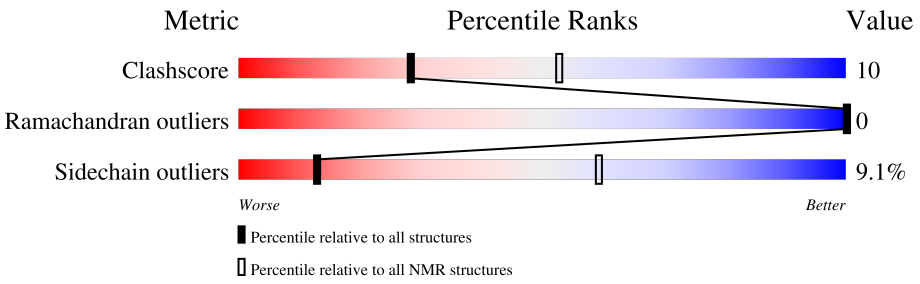
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 92%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	75	61% 21% • 16%
2	B	34	35% 18% 47%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:86-A:148, B:463-B:480 (81)	0.44	11

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

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

The models can be grouped into 5 clusters and 5 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1757 atoms, of which 883 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc finger HIT domain-containing protein 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	75	1181	366	590	104	115	6	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	GLY	-	expression tag	UNP Q15649
A	82	PRO	-	expression tag	UNP Q15649
A	83	HIS	-	expression tag	UNP Q15649
A	84	MET	-	expression tag	UNP Q15649

- Molecule 2 is a protein called Nuclear fragile X mental retardation-interacting protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	34	576	178	293	52	52	1	0

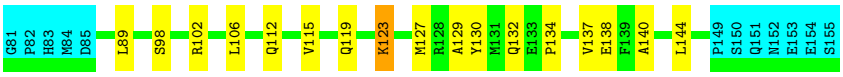
4 Residue-property plots (i)

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.

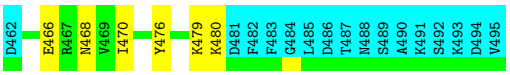
• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 61% 21% • 16%



• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B: 35% 18% 47%



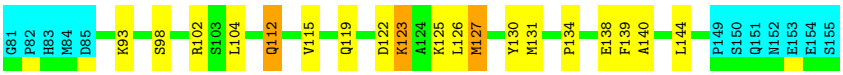
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

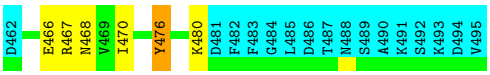
• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 59% 21% • 16%



• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

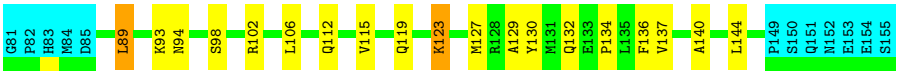
Chain B: 35% 15% • 47%



4.2.2 Score per residue for model 2

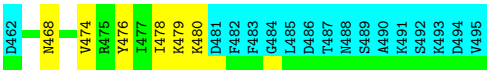
• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 59% 23% • 16%



• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

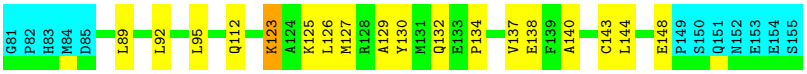
Chain B: 35% 18% 47%



4.2.3 Score per residue for model 3

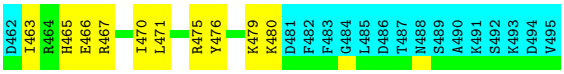
• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 60% 23% • 16%



• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

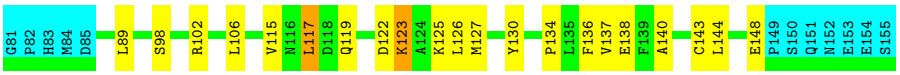
Chain B: 24% 29% 47%



4.2.4 Score per residue for model 4

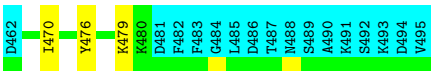
• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 56% 25% • 16%



• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

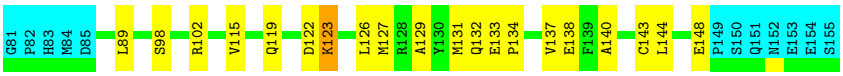
Chain B: 44% 9% 47%



4.2.5 Score per residue for model 5

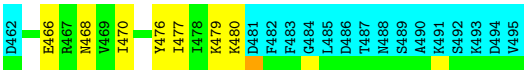
- Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 57% 25% • 16%



- Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

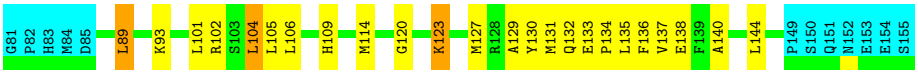
Chain B: 32% 21% 47%



4.2.6 Score per residue for model 6

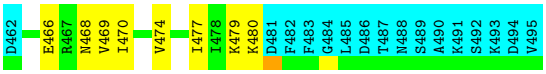
- Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 52% 28% • 16%



- Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

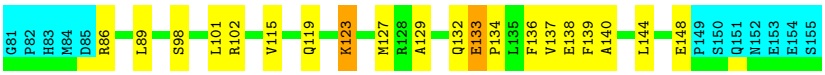
Chain B: 29% 24% 47%



4.2.7 Score per residue for model 7

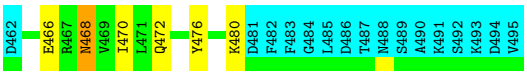
- Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 57% 24% • 16%



- Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B: 35% 15% • 47%



4.2.8 Score per residue for model 8

- Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 63% 20% • 16%

G81 P82 H83 M84 D85 L89 R111 V115 N116 L117 K123 M127 R128 A129 Y130 M131 Q132 E133 P134 L135 F136 V137 E138 F139 A140 L144 E148 P149 S150 Q151 N152 E153 E154 S155

- Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B: 24% 29% 47%

D462 E466 R467 N468 V469 I470 L471 V474 R475 Y476 I477 I478 K479 K480 D481 F482 F483 G484 L485 D486 T487 N488 S489 A490 K491 S492 K493 D494 V495

4.2.9 Score per residue for model 9

- Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 57% 25% • 16%

G81 P82 H83 M84 D85 L89 K93 S98 R102 L106 H109 L113 M114 V115 Q119 D122 K123 L126 A129 Q132 E133 P134 E138 F139 A140 C143 L144 P149 S150 Q151 N152 E153 E154 S155

- Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B: 35% 15% • 47%

D462 T463 R464 L471 R475 Y476 K479 K480 D481 F482 F483 G484 L485 D486 T487 N488 S489 A490 K491 S492 K493 D494 V495

4.2.10 Score per residue for model 10

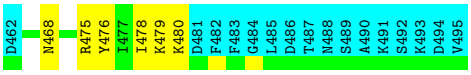
- Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 49% 32% • 16%

G81 P82 H83 M84 D85 L89 L92 K93 N94 L95 S98 R102 S103 L104 L105 L106 L110 V115 Q119 G120 E121 D122 K123 A124 K125 L126 M127 R128 A129 Y130 M131 Q132 E133 P134 L135 F136 V137 E138 F139 A140 D141 C142 C143 L144 G145 I146 P149 S150 Q151 N152 E153 E154 S155

- Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

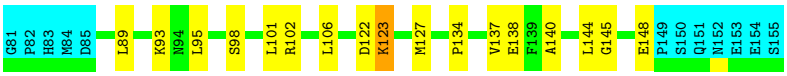
Chain B: 35% 18% 47%



4.2.11 Score per residue for model 11 (medoid)

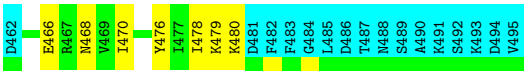
• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A:



• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B:



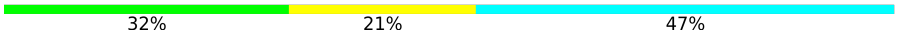
4.2.12 Score per residue for model 12

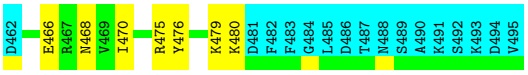
• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A:

• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B:





4.2.13 Score per residue for model 13

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A:

• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B: 26% 24% • 47%

D462 I463 R464 H465 E466 R467 N468 V469 I470 R475 Y476 K479 K480 D481 F482 F483 G484 L485 D486 T487 N488 S489 A490 K491 S492 K493 D494 V495

4.2.14 Score per residue for model 14

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 60% 24% 16%

G81 P82 H83 M84 D85 L89 S98 R102 L106 V115 Q119 D122 K123 L126 M127 R128 A129 Q132 E133 P134 V137 E138 F139 A140 C143 L144 P149 S150 Q151 N152 E153 E154 S155

• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B: 35% 15% • 47%

D462 H465 N468 L471 Y476 K479 K480 D481 F482 F483 G484 L485 D486 T487 N488 S489 A490 K491 S492 K493 D494 V495

4.2.15 Score per residue for model 15

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 61% 21% • 16%

G81 P82 H83 M84 D85 L89 R102 L106 H109 Q112 L113 M114 V115 Q119 K123 M127 R128 A129 Q132 E133 V137 A140 L144 E148 P149 S150 Q151 N152 E153 E154 S155

• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B: 41% 9% • 47%

D462 L471 Y476 K479 K480 D481 F482 F483 G484 L485 D486 T487 N488 S489 A490 K491 S492 K493 D494 V495

4.2.16 Score per residue for model 16

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 59% 24% • 16%

G81 P82 H83 M84 D85 L89 S98 L101 R102 Q112 L117 K123 M127 R128 A129 Y130 M131 Q132 E133 P134 L135 F136 V137 E138 F139 A140 L144 P149 S150 Q151 N152 E153 E154 S155

• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B: 32% 18% • 47%

D462 I463 R464 H465 N468 R475 Y476 K479 K480 D481 F482 F483 G484 L485 D486 T487 N488 S489 A490 K491 S492 K493 D494 V495

4.2.17 Score per residue for model 17

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 55% 28% • 16%

G81 P82 H83 M84 D85 L89 K93 S98 R102 L105 R111 Q112 L113 M114 V115 G120 K123 A124 K125 L126 M127 R128 A129 Y130 M131 Q132 E133 V137 A140 L144 P149 S150 Q151 N152 E153 E154 S155

• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B: 24% 29% 47%

D462 I463 R464 H465 E466 R467 N468 V469 I470 V474 R475 I478 K479 K480 D481 F482 F483 G484 L485 D486 T487 N488 S489 A490 K491 S492 K493 D494 V495

4.2.18 Score per residue for model 18

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 61% 20% • 16%

G81 P82 H83 M84 D85 S88 L89 Q90 S98 R102 Q112 V115 Q119 G120 K123 A124 M127 P134 V137 E138 F139 A140 L144 P149 S150 Q151 N152 E153 E154 S155

• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B: 26% 26% 47%

D462 E466 R467 N468 V469 I470 C473 Y476 I477 I478 K479 K480 D481 F482 F483 G484 L485 D486 T487 N488 S489 A490 K491 S492 K493 D494 V495

4.2.19 Score per residue for model 19

• Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 53% 28% • 16%

G81 P82 H83 M84 D85 S98 L101 R102 S103 L104 L105 L106 N107 R111 V115 N116 L117 D118 Q119 K123 A124 K125 L126 M127 R128 A129 Q132 E133 P134 V137 E138 F139 A140 L144 P149 S150 Q151 N152 E153 E154 S155

• Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B: 26% 26% 47%

D462 I463 E466 R467 N468 V469 I470 R475 Y476 I477 I478 K479 K480 D481 F482 F483 G484 L485 D486 T487 N488 S489 A490 K491 S492 K493 D494 V495

4.2.20 Score per residue for model 20

- Molecule 1: Zinc finger HIT domain-containing protein 3

Chain A: 59% 25% 16%

G81 P82 H83 M84 D85 R86 L89 R102 L106 M114 D122 K123 L126 M127 R128 A129 Y130 M131 Q132 E133 P134 L135 F136 V137 A140 C143 L144 E148 P149 S150 Q151 N152 E153 E154 S155

- Molecule 2: Nuclear fragile X mental retardation-interacting protein 1

Chain B: 32% 21% 47%

D462 E466 R467 N468 V469 I470 V474 R475 Y476 K479 K480 D481 F482 F483 G484 L485 D486 T487 N488 S489 A490 K491 S492 K493 D494 V495

5 Refinement protocol and experimental data overview (i)

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

Of the 160 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure calculation	3.0
CNS	refinement	1.21

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	1418
Number of shifts mapped to atoms	1418
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	499	515	515	12±2
2	B	159	180	179	3±2
All	All	13160	13900	13880	283

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:ALA:O	1:A:144:LEU:HG	0.70	1.87	6	20
1:A:134:PRO:HA	1:A:137:VAL:CG2	0.65	2.20	5	12
1:A:129:ALA:O	1:A:132:GLN:HG2	0.64	1.92	16	16
1:A:134:PRO:HA	1:A:137:VAL:HG22	0.64	1.69	6	12
1:A:115:VAL:O	1:A:119:GLN:HG3	0.60	1.96	1	13
1:A:140:ALA:HA	1:A:143:CYS:SG	0.60	2.37	14	7
1:A:134:PRO:O	1:A:138:GLU:HG2	0.59	1.96	1	5
1:A:102:ARG:O	1:A:106:LEU:HG	0.58	1.97	6	11
2:B:474:VAL:O	2:B:478:ILE:HG12	0.57	1.99	2	2
1:A:123:LYS:HD2	1:A:124:ALA:N	0.57	2.15	18	2
1:A:98:SER:O	1:A:102:ARG:HG2	0.57	2.00	9	15
1:A:104:LEU:HD21	1:A:142:CYS:SG	0.56	2.40	12	1
2:B:466:GLU:O	2:B:470:ILE:HG12	0.55	2.01	19	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:471:LEU:H	2:B:471:LEU:CD2	0.54	2.16	14	3
1:A:126:LEU:HD22	1:A:130:TYR:CE1	0.54	2.38	4	3
1:A:144:LEU:O	1:A:148:GLU:HG2	0.53	2.03	5	4
1:A:122:ASP:O	1:A:126:LEU:HG	0.53	2.03	14	4
1:A:144:LEU:O	1:A:148:GLU:HG3	0.53	2.04	8	2
1:A:123:LYS:HD3	1:A:123:LYS:H	0.53	1.64	7	13
2:B:475:ARG:O	2:B:479:LYS:HB2	0.52	2.04	17	8
1:A:123:LYS:N	1:A:123:LYS:HD3	0.52	2.19	2	4
1:A:123:LYS:O	1:A:127:MET:HG2	0.52	2.04	2	2
1:A:123:LYS:HD3	1:A:123:LYS:N	0.51	2.20	9	7
1:A:89:LEU:O	1:A:93:LYS:HG3	0.50	2.05	2	6
1:A:134:PRO:O	1:A:138:GLU:HG3	0.50	2.06	7	2
2:B:471:LEU:CD2	2:B:471:LEU:N	0.50	2.75	15	3
1:A:105:LEU:HD21	2:B:477:ILE:HD13	0.49	1.82	19	1
1:A:137:VAL:HG23	1:A:138:GLU:N	0.49	2.22	6	9
1:A:88:SER:OG	1:A:90:GLN:HG2	0.49	2.08	18	1
1:A:117:LEU:HD11	1:A:127:MET:SD	0.48	2.48	19	1
1:A:130:TYR:HB3	1:A:136:PHE:CD2	0.48	2.44	10	4
2:B:465:HIS:HA	2:B:468:ASN:OD1	0.48	2.09	14	4
1:A:130:TYR:HB3	1:A:136:PHE:CD1	0.47	2.43	16	3
1:A:133:GLU:O	1:A:137:VAL:HG23	0.47	2.09	19	5
1:A:123:LYS:HD2	1:A:124:ALA:H	0.47	1.69	17	2
2:B:463:ILE:O	2:B:467:ARG:HB2	0.47	2.09	3	1
2:B:473:CYS:O	2:B:477:ILE:HG12	0.47	2.08	18	1
1:A:122:ASP:OD2	1:A:125:LYS:HG2	0.47	2.10	4	1
1:A:115:VAL:HA	2:B:478:ILE:HD13	0.47	1.86	17	1
1:A:122:ASP:O	1:A:126:LEU:HD13	0.47	2.09	5	1
2:B:463:ILE:HA	2:B:466:GLU:HG2	0.47	1.86	13	1
1:A:107:ASN:O	1:A:111:ARG:HG3	0.47	2.10	19	1
1:A:126:LEU:HD22	1:A:130:TYR:CE2	0.46	2.46	1	1
1:A:113:LEU:HD21	1:A:133:GLU:OE2	0.46	2.11	15	1
1:A:101:LEU:O	1:A:105:LEU:HD13	0.46	2.11	19	2
1:A:117:LEU:HB2	1:A:130:TYR:CE2	0.46	2.46	8	1
1:A:127:MET:SD	2:B:467:ARG:HB3	0.46	2.51	1	1
1:A:95:LEU:HB3	1:A:101:LEU:CD2	0.45	2.41	12	2
1:A:101:LEU:O	1:A:104:LEU:HD12	0.45	2.10	12	3
2:B:475:ARG:O	2:B:479:LYS:HE2	0.45	2.11	17	1
1:A:136:PHE:CZ	2:B:470:ILE:HG21	0.45	2.47	4	3
1:A:120:GLY:HA2	1:A:123:LYS:HG3	0.45	1.88	17	3
1:A:86:ARG:HA	2:B:472:GLN:NE2	0.45	2.27	7	1
1:A:117:LEU:HB2	1:A:130:TYR:CE1	0.44	2.47	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:HD12	1:A:130:TYR:CD2	0.44	2.48	4	1
1:A:109:HIS:CD2	1:A:135:LEU:HD22	0.44	2.48	6	1
1:A:109:HIS:NE2	1:A:113:LEU:HD11	0.44	2.28	9	1
1:A:105:LEU:O	1:A:111:ARG:HD2	0.44	2.13	17	1
2:B:471:LEU:O	2:B:475:ARG:HG2	0.44	2.13	8	1
1:A:104:LEU:O	1:A:110:LEU:HD13	0.43	2.12	10	1
1:A:142:CYS:O	1:A:146:ILE:HG13	0.43	2.13	10	1
1:A:114:MET:HG3	2:B:474:VAL:HG13	0.43	1.90	20	2
1:A:104:LEU:O	1:A:110:LEU:HD23	0.43	2.11	12	1
1:A:92:LEU:HA	1:A:95:LEU:HD13	0.43	1.90	10	2
2:B:471:LEU:O	2:B:475:ARG:HG3	0.43	2.13	3	1
2:B:466:GLU:O	2:B:469:VAL:HB	0.43	2.13	6	1
1:A:113:LEU:HD21	1:A:133:GLU:OE1	0.43	2.13	9	1
2:B:471:LEU:N	2:B:471:LEU:HD22	0.43	2.28	15	2
1:A:145:GLY:HA2	1:A:148:GLU:OE2	0.43	2.14	11	1
2:B:464:ARG:HD2	2:B:464:ARG:C	0.43	2.34	17	1
1:A:109:HIS:O	1:A:112:GLN:HB2	0.43	2.14	15	1
1:A:125:LYS:HD2	1:A:125:LYS:C	0.42	2.34	17	1
1:A:134:PRO:CA	1:A:137:VAL:HG22	0.42	2.44	4	3
1:A:118:ASP:OD1	2:B:475:ARG:HG2	0.42	2.15	19	1
1:A:101:LEU:HD11	1:A:139:PHE:CD1	0.42	2.50	16	1
1:A:122:ASP:OD2	1:A:125:LYS:HE2	0.42	2.14	13	1
1:A:111:ARG:O	1:A:115:VAL:HG23	0.41	2.15	8	1
1:A:93:LYS:HA	2:B:476:TYR:CZ	0.41	2.50	1	1
1:A:112:GLN:HA	1:A:112:GLN:HE21	0.41	1.76	18	2
2:B:463:ILE:HD12	2:B:463:ILE:H	0.41	1.75	19	1
1:A:104:LEU:CD1	1:A:139:PHE:HA	0.40	2.46	1	1
1:A:101:LEU:HD11	1:A:139:PHE:CD2	0.40	2.52	7	1
2:B:464:ARG:H	2:B:464:ARG:HD2	0.40	1.76	16	1
1:A:114:MET:HG3	2:B:474:VAL:HG22	0.40	1.94	6	1
1:A:112:GLN:HE21	1:A:112:GLN:HA	0.40	1.77	12	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	63/75 (84%)	62±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100
2	B	18/34 (53%)	18±0 (99±2%)	0±0 (1±2%)	0±0 (0±0%)	100	100
All	All	1620/2180 (74%)	1605 (99%)	15 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	56/67 (84%)	52±1 (93±2%)	4±1 (7±2%)	18	67
2	B	18/32 (56%)	15±1 (84±4%)	3±1 (16±4%)	5	43
All	All	1480/1980 (75%)	1345 (91%)	135 (9%)	13	59

All 21 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	123	LYS	20
2	B	480	LYS	19
2	B	476	TYR	18
1	A	127	MET	16
1	A	89	LEU	14
2	B	468	ASN	12
1	A	112	GLN	7
1	A	125	LYS	4
1	A	104	LEU	4
1	A	131	MET	3
1	A	133	GLU	3
2	B	471	LEU	3
1	A	94	ASN	2
1	A	117	LEU	2
2	B	464	ARG	2
1	A	148	GLU	1
1	A	121	GLU	1
1	A	122	ASP	1
2	B	475	ARG	1

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Mol	Chain	Res	Type	Models (Total)
2	B	467	ARG	1
1	A	86	ARG	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *ZNHIT3NUFIP_ref_dss_298K.str*

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	1418
Number of shifts mapped to atoms	1418
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	109	-0.42 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	104	0.31 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	103	-0.36 ± 0.13	None needed (< 0.5 ppm)
^{15}N	103	0.31 ± 0.27	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 92%, i.e. 1109 atoms were assigned a chemical shift out of a possible 1201. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	401/404 (99%)	163/163 (100%)	159/162 (98%)	79/79 (100%)
Sidechain	672/743 (90%)	451/483 (93%)	208/224 (93%)	13/36 (36%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	36/54 (67%)	20/26 (77%)	12/24 (50%)	4/4 (100%)
Overall	1109/1201 (92%)	634/672 (94%)	379/410 (92%)	96/119 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1415 atoms were assigned a chemical shift out of a possible 1533. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	532/542 (98%)	217/219 (99%)	212/218 (97%)	103/105 (98%)
Sidechain	829/909 (91%)	555/587 (95%)	258/281 (92%)	16/41 (39%)
Aromatic	54/82 (66%)	30/40 (75%)	18/36 (50%)	6/6 (100%)
Overall	1415/1533 (92%)	802/846 (95%)	488/535 (91%)	125/152 (82%)

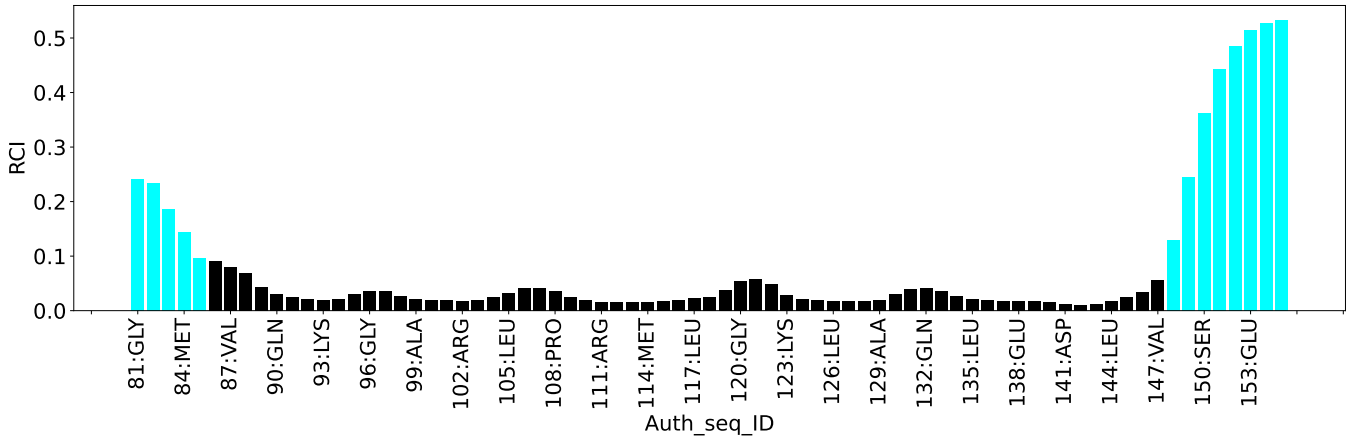
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

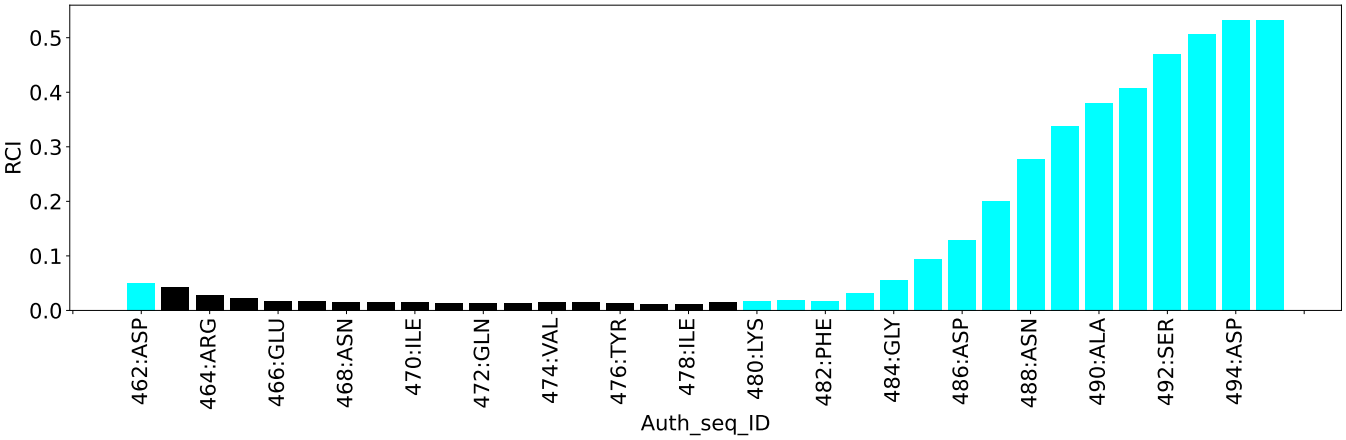
7.1.5 Random Coil Index (RCI) plots (i)

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:



Random coil index (RCI) for chain B:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
462:ASP
464:ARG
466:GLU
468:ASN
470:ILE
472:GLN
474:VAL
476:TYR
478:ILE
480:LYS
482:PHE
484:GLY
486:ASP
488:ASN
490:ALA
492:SER
494:ASP
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	2163
Intra-residue (|i-j|=0)	548
Sequential (|i-j|=1)	569
Medium range (|i-j|>1 and |i-j|<5)	599
Long range (|i-j|≥5)	261
Inter-chain	186
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	19.8
Number of long range restraints per residue[1]	2.4

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

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	15.8	0.2
0.2-0.5 (Medium)	5.9	0.5
>0.5 (Large)	6.9	2.42

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

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

9 Distance violation analysis (i)

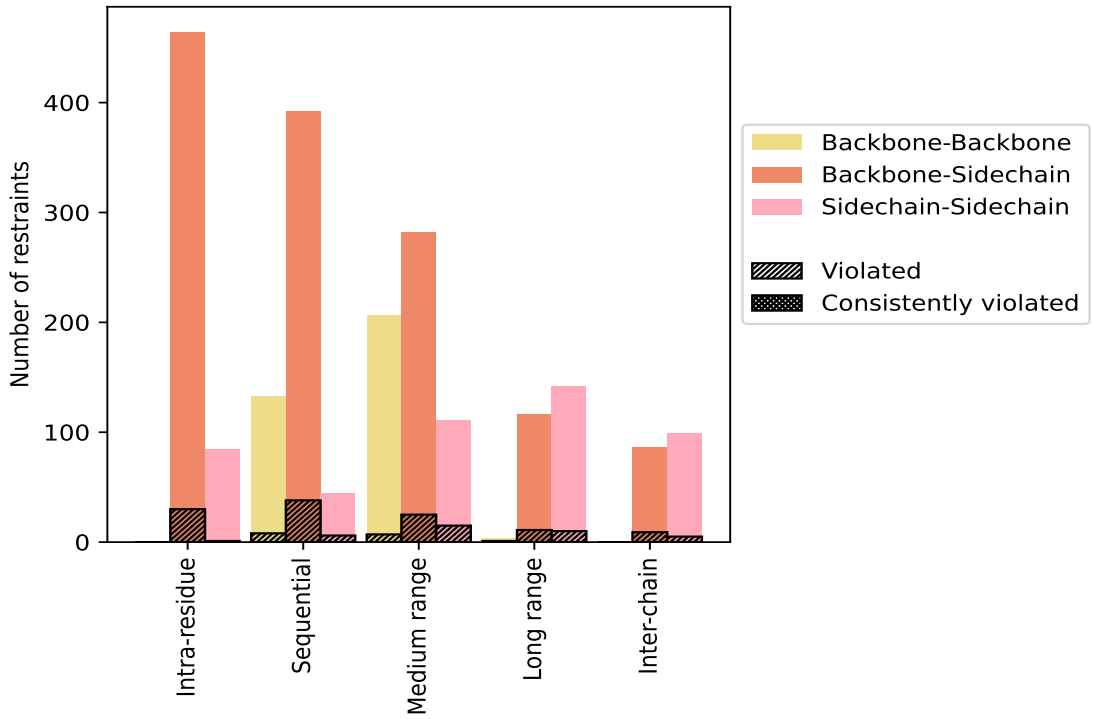
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	548	25.3	31	5.7	1.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	464	21.5	30	6.5	1.4	0	0.0	0.0
Sidechain-Sidechain	84	3.9	1	1.2	0.0	0	0.0	0.0
Sequential (|i-j|=1)	569	26.3	52	9.1	2.4	0	0.0	0.0
Backbone-Backbone	133	6.1	8	6.0	0.4	0	0.0	0.0
Backbone-Sidechain	392	18.1	38	9.7	1.8	0	0.0	0.0
Sidechain-Sidechain	44	2.0	6	13.6	0.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	599	27.7	47	7.8	2.2	0	0.0	0.0
Backbone-Backbone	206	9.5	7	3.4	0.3	0	0.0	0.0
Backbone-Sidechain	282	13.0	25	8.9	1.2	0	0.0	0.0
Sidechain-Sidechain	111	5.1	15	13.5	0.7	0	0.0	0.0
Long range (|i-j|≥5)	261	12.1	22	8.4	1.0	0	0.0	0.0
Backbone-Backbone	3	0.1	1	33.3	0.0	0	0.0	0.0
Backbone-Sidechain	116	5.4	11	9.5	0.5	0	0.0	0.0
Sidechain-Sidechain	142	6.6	10	7.0	0.5	0	0.0	0.0
Inter-chain	186	8.6	14	7.5	0.6	0	0.0	0.0
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	86	4.0	9	10.5	0.4	0	0.0	0.0
Sidechain-Sidechain	99	4.6	5	5.1	0.2	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2163	100.0	166	7.7	7.7	0	0.0	0.0
Backbone-Backbone	343	15.9	16	4.7	0.7	0	0.0	0.0
Backbone-Sidechain	1340	62.0	113	8.4	5.2	0	0.0	0.0
Sidechain-Sidechain	480	22.2	37	7.7	1.7	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 disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	3	4	7	0	1	15	0.16	0.33	0.06	0.14
2	1	10	13	6	4	34	0.49	1.55	0.43	0.26
3	6	8	8	4	1	27	0.45	1.72	0.49	0.18
4	5	8	8	13	1	35	0.55	2.36	0.55	0.32
5	8	7	7	3	1	26	0.4	1.56	0.43	0.19
6	12	9	9	6	3	39	0.49	1.75	0.48	0.25
7	5	6	4	1	0	16	0.17	0.27	0.05	0.16
8	5	12	11	4	4	36	0.41	1.74	0.42	0.18
9	7	7	7	1	1	23	0.27	1.14	0.27	0.16
10	7	10	7	4	2	30	0.45	1.74	0.47	0.2
11	6	10	9	5	1	31	0.44	1.6	0.47	0.18

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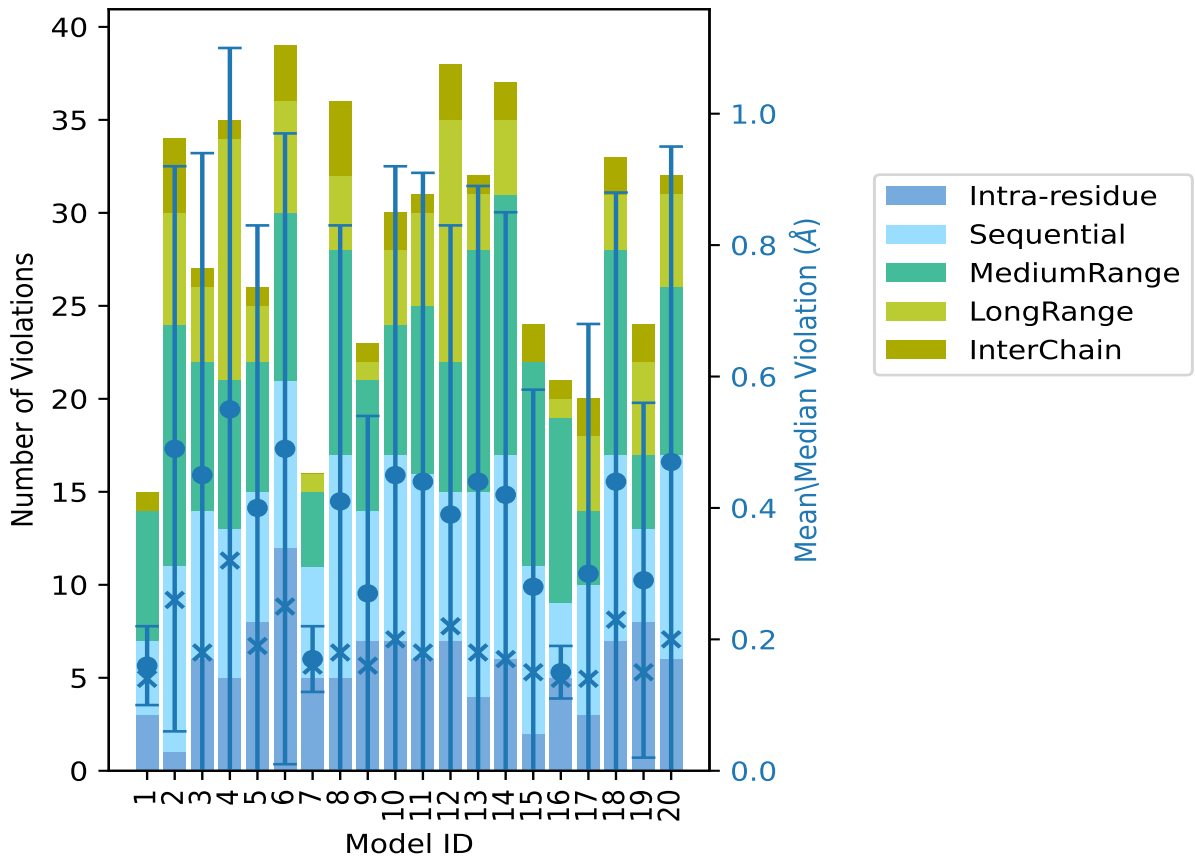
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	7	8	7	13	3	38	0.39	2.42	0.44	0.22
13	4	11	13	3	1	32	0.44	1.58	0.45	0.18
14	6	11	14	4	2	37	0.42	1.61	0.43	0.17
15	2	9	11	0	2	24	0.28	1.33	0.3	0.15
16	5	4	10	1	1	21	0.15	0.26	0.04	0.14
17	3	7	4	4	2	20	0.3	1.47	0.38	0.14
18	7	10	11	3	2	33	0.44	1.75	0.44	0.23
19	8	5	4	5	2	24	0.29	1.03	0.27	0.15
20	6	11	9	5	1	32	0.47	1.6	0.48	0.2

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

9.2.1 Bar graph : Distance Violation statistics for each model (i)



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

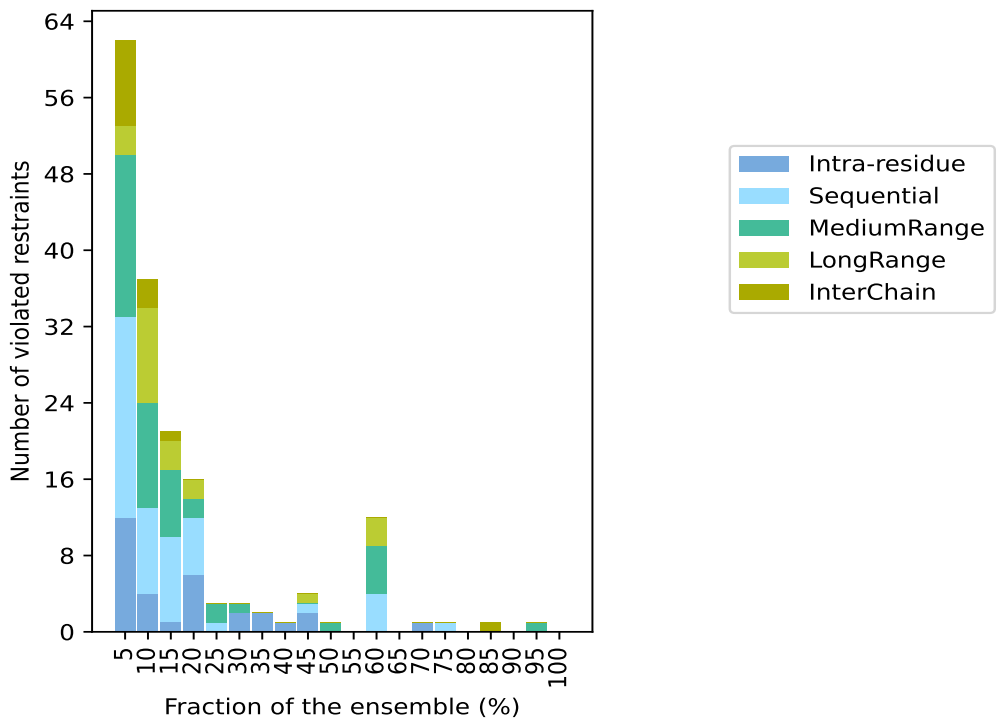
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1997(IR:517, SQ:517, MR:552, LR:239, IC:172) 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]	%
12	21	17	3	9	62	1	5.0
4	9	11	10	3	37	2	10.0
1	9	7	3	1	21	3	15.0
6	6	2	2	0	16	4	20.0
0	1	2	0	0	3	5	25.0
2	0	1	0	0	3	6	30.0
2	0	0	0	0	2	7	35.0
1	0	0	0	0	1	8	40.0
2	1	0	1	0	4	9	45.0
0	0	1	0	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	4	5	3	0	12	12	60.0
0	0	0	0	0	0	13	65.0
1	0	0	0	0	1	14	70.0
0	1	0	0	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	1	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	1	0	0	1	19	95.0
0	0	0	0	0	0	20	100.0

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

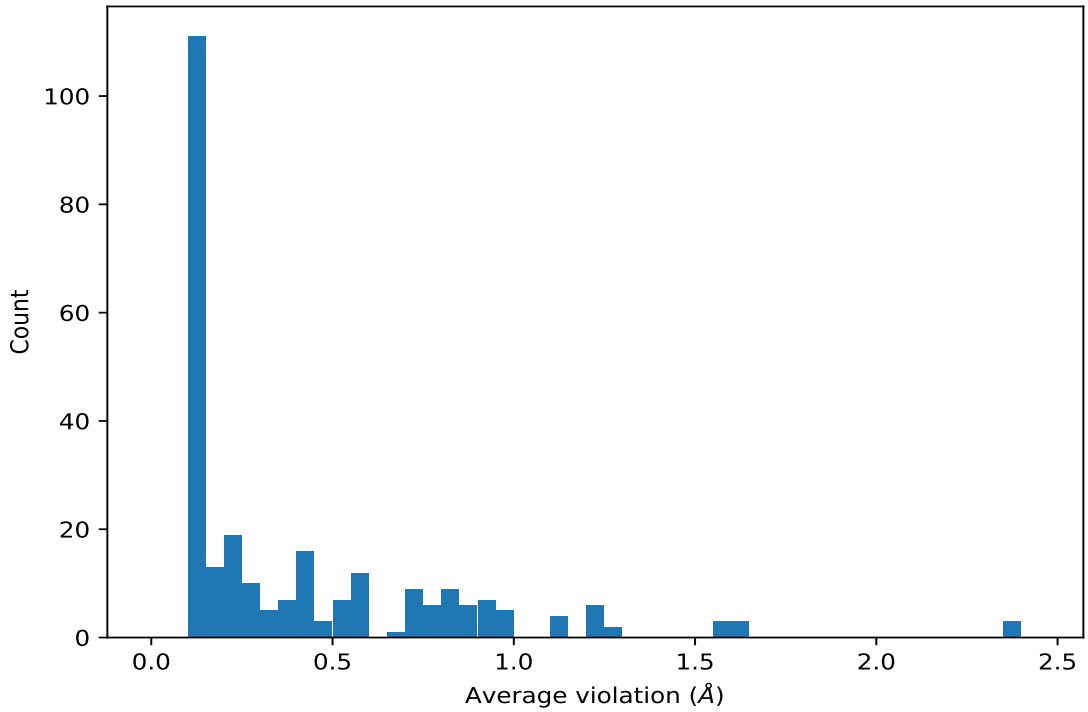
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	19	0.2	0.04	0.2
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	19	0.2	0.04	0.2
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	17	0.37	0.48	0.15
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	15	0.14	0.01	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	15	0.14	0.01	0.13
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	14	0.13	0.01	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	14	0.13	0.01	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	14	0.13	0.01	0.12
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG21	12	1.63	0.14	1.66
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG22	12	1.63	0.14	1.66
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG23	12	1.63	0.14	1.66
(1,1153)	1:A:137:VAL:HG11	1:A:138:GLU:HA	12	1.59	0.03	1.59
(1,1153)	1:A:137:VAL:HG12	1:A:138:GLU:HA	12	1.59	0.03	1.59
(1,1153)	1:A:137:VAL:HG13	1:A:138:GLU:HA	12	1.59	0.03	1.59
(1,480)	1:A:136:PHE:H	1:A:137:VAL:HB	12	1.11	0.02	1.11
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG21	12	1.1	0.1	1.1

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG22	12	1.1	0.1	1.1
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG23	12	1.1	0.1	1.1
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG21	12	0.95	0.19	0.93
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG22	12	0.95	0.19	0.93
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG23	12	0.95	0.19	0.93
(1,520)	1:A:137:VAL:HG11	1:A:141:ASP:H	12	0.73	0.12	0.75
(1,520)	1:A:137:VAL:HG12	1:A:141:ASP:H	12	0.73	0.12	0.75
(1,520)	1:A:137:VAL:HG13	1:A:141:ASP:H	12	0.73	0.12	0.75
(1,495)	1:A:137:VAL:HG11	1:A:138:GLU:H	12	0.38	0.04	0.38
(1,495)	1:A:137:VAL:HG12	1:A:138:GLU:H	12	0.38	0.04	0.38
(1,495)	1:A:137:VAL:HG13	1:A:138:GLU:H	12	0.38	0.04	0.38
(1,1483)	1:A:134:PRO:HA	1:A:137:VAL:HB	12	0.33	0.02	0.34
(1,496)	1:A:137:VAL:HB	1:A:138:GLU:H	12	0.25	0.03	0.24
(1,813)	2:B:479:LYS:HA	2:B:481:ASP:H	12	0.14	0.02	0.15
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD1	12	0.14	0.02	0.14
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD2	12	0.14	0.02	0.14
(2,55)	2:B:477:ILE:HD11	2:B:479:LYS:H	12	0.12	0.01	0.12
(2,55)	2:B:477:ILE:HD12	2:B:479:LYS:H	12	0.12	0.01	0.12
(2,55)	2:B:477:ILE:HD13	2:B:479:LYS:H	12	0.12	0.01	0.12
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG21	10	0.9	0.19	0.92
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG22	10	0.9	0.19	0.92
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG23	10	0.9	0.19	0.92
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG11	9	0.27	0.01	0.27
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG12	9	0.27	0.01	0.27
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG13	9	0.27	0.01	0.27
(1,1977)	2:B:462:ASP:HB2	2:B:463:ILE:H	9	0.14	0.03	0.14
(1,1977)	2:B:462:ASP:HB3	2:B:463:ILE:H	9	0.14	0.03	0.14
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD11	9	0.12	0.01	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD12	9	0.12	0.01	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD13	9	0.12	0.01	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD21	9	0.12	0.01	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD22	9	0.12	0.01	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD23	9	0.12	0.01	0.12
(1,1430)	1:A:110:LEU:H	1:A:110:LEU:HG	9	0.12	0.01	0.12
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG21	8	0.22	0.01	0.22
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG22	8	0.22	0.01	0.22
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG23	8	0.22	0.01	0.22
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD21	7	0.14	0.01	0.14
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD22	7	0.14	0.01	0.14
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE2	7	0.14	0.02	0.14
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE3	7	0.14	0.02	0.14
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD11	6	0.23	0.08	0.25

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD12	6	0.23	0.08	0.25
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD13	6	0.23	0.08	0.25
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD1	6	0.12	0.01	0.12
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD2	6	0.12	0.01	0.12
(1,481)	1:A:133:GLU:HG3	1:A:136:PHE:H	6	0.12	0.01	0.11
(1,1602)	1:A:90:GLN:HG2	1:A:94:ASN:HD21	5	0.78	0.57	0.84
(1,1602)	1:A:90:GLN:HG3	1:A:94:ASN:HD21	5	0.78	0.57	0.84
(1,864)	2:B:488:ASN:H	2:B:489:SER:H	5	0.15	0.06	0.12
(1,1465)	1:A:122:ASP:HA	1:A:124:ALA:HA	5	0.15	0.03	0.13
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD21	4	0.99	0.03	1.0
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD22	4	0.99	0.03	1.0
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD23	4	0.99	0.03	1.0
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD21	4	0.88	0.02	0.88
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD22	4	0.88	0.02	0.88
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD23	4	0.88	0.02	0.88
(1,537)	1:A:104:LEU:HD11	1:A:142:CYS:H	4	0.56	0.19	0.58
(1,537)	1:A:104:LEU:HD12	1:A:142:CYS:H	4	0.56	0.19	0.58
(1,537)	1:A:104:LEU:HD13	1:A:142:CYS:H	4	0.56	0.19	0.58
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD21	4	0.36	0.03	0.34
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD22	4	0.36	0.03	0.34
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD23	4	0.36	0.03	0.34
(1,1429)	1:A:125:LYS:H	1:A:125:LYS:HD2	4	0.2	0.05	0.22
(1,1429)	1:A:125:LYS:H	1:A:125:LYS:HD3	4	0.2	0.05	0.22
(1,878)	2:B:490:ALA:HA	2:B:491:LYS:H	4	0.2	0.06	0.17
(1,1427)	1:A:105:LEU:H	1:A:105:LEU:HG	4	0.18	0.03	0.18
(1,626)	1:A:153:GLU:HA	1:A:154:GLU:H	4	0.16	0.04	0.15
(1,1255)	2:B:486:ASP:HA	2:B:487:THR:H	4	0.14	0.01	0.14
(2,5)	1:A:94:ASN:HD21	1:A:95:LEU:HG	4	0.14	0.01	0.14
(1,2001)	2:B:467:ARG:H	2:B:467:ARG:HG2	4	0.13	0.02	0.13
(1,2001)	2:B:467:ARG:H	2:B:467:ARG:HG3	4	0.13	0.02	0.13
(1,871)	2:B:490:ALA:HB1	2:B:491:LYS:H	4	0.13	0.01	0.12
(1,871)	2:B:490:ALA:HB2	2:B:491:LYS:H	4	0.13	0.01	0.12
(1,871)	2:B:490:ALA:HB3	2:B:491:LYS:H	4	0.13	0.01	0.12
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG11	4	0.13	0.01	0.12
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG12	4	0.13	0.01	0.12
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG13	4	0.13	0.01	0.12
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG21	4	0.13	0.01	0.12
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG22	4	0.13	0.01	0.12
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG23	4	0.13	0.01	0.12
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG11	4	0.13	0.01	0.12
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG12	4	0.13	0.01	0.12
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG13	4	0.13	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG21	4	0.13	0.01	0.12
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG22	4	0.13	0.01	0.12
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG23	4	0.13	0.01	0.12
(1,236)	1:A:109:HIS:HD2	1:A:111:ARG:H	4	0.12	0.01	0.12
(1,919)	1:A:109:HIS:HD2	1:A:135:LEU:HG	4	0.12	0.01	0.12
(1,1484)	2:B:480:LYS:HA	2:B:480:LYS:HD2	4	0.12	0.01	0.12
(1,1484)	2:B:480:LYS:HA	2:B:480:LYS:HD3	4	0.12	0.01	0.12
(1,1445)	1:A:114:MET:HG2	1:A:139:PHE:HE1	3	1.26	0.04	1.24
(1,1445)	1:A:114:MET:HG2	1:A:139:PHE:HE2	3	1.26	0.04	1.24
(1,668)	2:B:468:ASN:H	2:B:471:LEU:HD11	3	1.23	0.08	1.21
(1,668)	2:B:468:ASN:H	2:B:471:LEU:HD12	3	1.23	0.08	1.21
(1,668)	2:B:468:ASN:H	2:B:471:LEU:HD13	3	1.23	0.08	1.21
(1,1128)	1:A:117:LEU:HD11	2:B:471:LEU:HD21	3	0.83	0.16	0.89
(1,1128)	1:A:117:LEU:HD11	2:B:471:LEU:HD22	3	0.83	0.16	0.89
(1,1128)	1:A:117:LEU:HD11	2:B:471:LEU:HD23	3	0.83	0.16	0.89
(1,1128)	1:A:117:LEU:HD12	2:B:471:LEU:HD21	3	0.83	0.16	0.89
(1,1128)	1:A:117:LEU:HD12	2:B:471:LEU:HD22	3	0.83	0.16	0.89
(1,1128)	1:A:117:LEU:HD12	2:B:471:LEU:HD23	3	0.83	0.16	0.89
(1,1128)	1:A:117:LEU:HD13	2:B:471:LEU:HD21	3	0.83	0.16	0.89
(1,1128)	1:A:117:LEU:HD13	2:B:471:LEU:HD22	3	0.83	0.16	0.89
(1,1128)	1:A:117:LEU:HD13	2:B:471:LEU:HD23	3	0.83	0.16	0.89
(2,17)	1:A:113:LEU:H	1:A:114:MET:HG3	3	0.75	0.03	0.73
(1,2015)	2:B:468:ASN:HD21	2:B:471:LEU:HD11	3	0.71	0.03	0.71
(1,2015)	2:B:468:ASN:HD21	2:B:471:LEU:HD12	3	0.71	0.03	0.71
(1,2015)	2:B:468:ASN:HD21	2:B:471:LEU:HD13	3	0.71	0.03	0.71
(1,2015)	2:B:468:ASN:HD22	2:B:471:LEU:HD11	3	0.71	0.03	0.71
(1,2015)	2:B:468:ASN:HD22	2:B:471:LEU:HD12	3	0.71	0.03	0.71
(1,2015)	2:B:468:ASN:HD22	2:B:471:LEU:HD13	3	0.71	0.03	0.71
(1,752)	2:B:471:LEU:HD21	2:B:475:ARG:H	3	0.46	0.06	0.45
(1,752)	2:B:471:LEU:HD22	2:B:475:ARG:H	3	0.46	0.06	0.45
(1,752)	2:B:471:LEU:HD23	2:B:475:ARG:H	3	0.46	0.06	0.45
(1,511)	1:A:104:LEU:HD11	1:A:139:PHE:H	3	0.33	0.12	0.41
(1,511)	1:A:104:LEU:HD12	1:A:139:PHE:H	3	0.33	0.12	0.41
(1,511)	1:A:104:LEU:HD13	1:A:139:PHE:H	3	0.33	0.12	0.41
(1,1424)	1:A:114:MET:H	1:A:114:MET:HG3	3	0.31	0.0	0.31
(1,695)	2:B:470:ILE:H	2:B:471:LEU:HG	3	0.27	0.01	0.27
(1,1473)	2:B:468:ASN:HA	2:B:471:LEU:HD11	3	0.2	0.06	0.16
(1,1473)	2:B:468:ASN:HA	2:B:471:LEU:HD12	3	0.2	0.06	0.16
(1,1473)	2:B:468:ASN:HA	2:B:471:LEU:HD13	3	0.2	0.06	0.16
(1,714)	2:B:471:LEU:HG	2:B:472:GLN:H	3	0.17	0.02	0.17
(1,627)	1:A:154:GLU:H	1:A:155:SER:H	3	0.14	0.02	0.14
(1,1970)	1:A:152:ASN:HB2	1:A:153:GLU:H	3	0.13	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1970)	1:A:152:ASN:HB3	1:A:153:GLU:H	3	0.13	0.02	0.14
(1,1678)	1:A:101:LEU:HD11	1:A:104:LEU:H	3	0.13	0.02	0.13
(1,1678)	1:A:101:LEU:HD12	1:A:104:LEU:H	3	0.13	0.02	0.13
(1,1678)	1:A:101:LEU:HD13	1:A:104:LEU:H	3	0.13	0.02	0.13
(1,1678)	1:A:101:LEU:HD21	1:A:104:LEU:H	3	0.13	0.02	0.13
(1,1678)	1:A:101:LEU:HD22	1:A:104:LEU:H	3	0.13	0.02	0.13
(1,1678)	1:A:101:LEU:HD23	1:A:104:LEU:H	3	0.13	0.02	0.13
(1,1879)	1:A:123:LYS:HE2	1:A:124:ALA:HA	3	0.13	0.02	0.11
(1,1879)	1:A:123:LYS:HE3	1:A:124:ALA:HA	3	0.13	0.02	0.11
(2,24)	1:A:116:ASN:HD22	1:A:117:LEU:H	3	0.13	0.0	0.13
(2,27)	1:A:117:LEU:HA	1:A:126:LEU:H	3	0.13	0.02	0.12
(1,167)	1:A:101:LEU:H	1:A:102:ARG:HG3	3	0.12	0.01	0.12
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD11	3	0.12	0.01	0.12
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD12	3	0.12	0.01	0.12
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD13	3	0.12	0.01	0.12
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD21	3	0.12	0.01	0.12
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD22	3	0.12	0.01	0.12
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD23	3	0.12	0.01	0.12
(1,545)	1:A:143:CYS:H	1:A:144:LEU:HD21	3	0.11	0.0	0.11
(1,545)	1:A:143:CYS:H	1:A:144:LEU:HD22	3	0.11	0.0	0.11
(1,545)	1:A:143:CYS:H	1:A:144:LEU:HD23	3	0.11	0.0	0.11
(1,833)	2:B:483:PHE:H	2:B:485:LEU:H	3	0.11	0.0	0.11
(1,370)	1:A:117:LEU:HD11	1:A:123:LYS:H	2	2.39	0.03	2.39
(1,370)	1:A:117:LEU:HD12	1:A:123:LYS:H	2	2.39	0.03	2.39
(1,370)	1:A:117:LEU:HD13	1:A:123:LYS:H	2	2.39	0.03	2.39
(1,1131)	1:A:117:LEU:HD11	1:A:123:LYS:HA	2	1.24	0.0	1.24
(1,1131)	1:A:117:LEU:HD12	1:A:123:LYS:HA	2	1.24	0.0	1.24
(1,1131)	1:A:117:LEU:HD13	1:A:123:LYS:HA	2	1.24	0.0	1.24
(1,1600)	1:A:90:GLN:HB2	1:A:94:ASN:HD21	2	0.96	0.51	0.96
(1,1600)	1:A:90:GLN:HB3	1:A:94:ASN:HD21	2	0.96	0.51	0.96
(1,1354)	1:A:91:ASN:H	1:A:94:ASN:HD21	2	0.9	0.23	0.9
(1,384)	1:A:117:LEU:HD11	1:A:126:LEU:H	2	0.86	0.04	0.86
(1,384)	1:A:117:LEU:HD12	1:A:126:LEU:H	2	0.86	0.04	0.86
(1,384)	1:A:117:LEU:HD13	1:A:126:LEU:H	2	0.86	0.04	0.86
(1,1035)	1:A:114:MET:HE1	2:B:478:ILE:HG13	2	0.76	0.14	0.76
(1,1035)	1:A:114:MET:HE2	2:B:478:ILE:HG13	2	0.76	0.14	0.76
(1,1035)	1:A:114:MET:HE3	2:B:478:ILE:HG13	2	0.76	0.14	0.76
(1,327)	1:A:117:LEU:HG	1:A:118:ASP:H	2	0.68	0.08	0.68
(1,1074)	2:B:477:ILE:HG21	2:B:478:ILE:HG13	2	0.6	0.03	0.6
(1,1074)	2:B:477:ILE:HG22	2:B:478:ILE:HG13	2	0.6	0.03	0.6
(1,1074)	2:B:477:ILE:HG23	2:B:478:ILE:HG13	2	0.6	0.03	0.6
(1,894)	1:A:117:LEU:HD21	1:A:130:TYR:HE1	2	0.58	0.08	0.58

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,894)	1:A:117:LEU:HD21	1:A:130:TYR:HE2	2	0.58	0.08	0.58
(1,894)	1:A:117:LEU:HD22	1:A:130:TYR:HE1	2	0.58	0.08	0.58
(1,894)	1:A:117:LEU:HD22	1:A:130:TYR:HE2	2	0.58	0.08	0.58
(1,894)	1:A:117:LEU:HD23	1:A:130:TYR:HE1	2	0.58	0.08	0.58
(1,894)	1:A:117:LEU:HD23	1:A:130:TYR:HE2	2	0.58	0.08	0.58
(1,1842)	1:A:117:LEU:HD11	1:A:123:LYS:HB2	2	0.54	0.14	0.54
(1,1842)	1:A:117:LEU:HD11	1:A:123:LYS:HB3	2	0.54	0.14	0.54
(1,1842)	1:A:117:LEU:HD12	1:A:123:LYS:HB2	2	0.54	0.14	0.54
(1,1842)	1:A:117:LEU:HD12	1:A:123:LYS:HB3	2	0.54	0.14	0.54
(1,1842)	1:A:117:LEU:HD13	1:A:123:LYS:HB2	2	0.54	0.14	0.54
(1,1842)	1:A:117:LEU:HD13	1:A:123:LYS:HB3	2	0.54	0.14	0.54
(1,837)	2:B:478:ILE:HG12	2:B:483:PHE:H	2	0.53	0.08	0.53
(1,1440)	1:A:117:LEU:HD21	2:B:471:LEU:H	2	0.44	0.18	0.44
(1,1440)	1:A:117:LEU:HD22	2:B:471:LEU:H	2	0.44	0.18	0.44
(1,1440)	1:A:117:LEU:HD23	2:B:471:LEU:H	2	0.44	0.18	0.44
(1,1015)	1:A:117:LEU:HD21	1:A:127:MET:HE1	2	0.44	0.07	0.44
(1,1015)	1:A:117:LEU:HD21	1:A:127:MET:HE2	2	0.44	0.07	0.44
(1,1015)	1:A:117:LEU:HD21	1:A:127:MET:HE3	2	0.44	0.07	0.44
(1,1015)	1:A:117:LEU:HD22	1:A:127:MET:HE1	2	0.44	0.07	0.44
(1,1015)	1:A:117:LEU:HD22	1:A:127:MET:HE2	2	0.44	0.07	0.44
(1,1015)	1:A:117:LEU:HD22	1:A:127:MET:HE3	2	0.44	0.07	0.44
(1,1015)	1:A:117:LEU:HD23	1:A:127:MET:HE1	2	0.44	0.07	0.44
(1,1015)	1:A:117:LEU:HD23	1:A:127:MET:HE2	2	0.44	0.07	0.44
(1,1015)	1:A:117:LEU:HD23	1:A:127:MET:HE3	2	0.44	0.07	0.44
(1,1132)	1:A:117:LEU:HA	1:A:117:LEU:HD11	2	0.42	0.01	0.42
(1,1132)	1:A:117:LEU:HA	1:A:117:LEU:HD12	2	0.42	0.01	0.42
(1,1132)	1:A:117:LEU:HA	1:A:117:LEU:HD13	2	0.42	0.01	0.42
(2,51)	2:B:474:VAL:H	2:B:478:ILE:HG13	2	0.41	0.06	0.41
(1,1129)	1:A:117:LEU:HD11	1:A:126:LEU:HB2	2	0.3	0.08	0.3
(1,1129)	1:A:117:LEU:HD12	1:A:126:LEU:HB2	2	0.3	0.08	0.3
(1,1129)	1:A:117:LEU:HD13	1:A:126:LEU:HB2	2	0.3	0.08	0.3
(1,797)	2:B:478:ILE:HG13	2:B:479:LYS:H	2	0.28	0.01	0.28
(1,1275)	2:B:466:GLU:HA	2:B:469:VAL:HB	2	0.28	0.04	0.28
(1,332)	1:A:117:LEU:HG	1:A:119:GLN:H	2	0.24	0.01	0.24
(1,1133)	1:A:117:LEU:HD11	1:A:127:MET:H	2	0.24	0.05	0.24
(1,1133)	1:A:117:LEU:HD12	1:A:127:MET:H	2	0.24	0.05	0.24
(1,1133)	1:A:117:LEU:HD13	1:A:127:MET:H	2	0.24	0.05	0.24
(1,724)	2:B:472:GLN:HA	2:B:472:GLN:HE21	2	0.2	0.01	0.2
(1,869)	2:B:489:SER:HA	2:B:490:ALA:H	2	0.17	0.06	0.17
(1,1972)	1:A:153:GLU:H	1:A:153:GLU:HB2	2	0.17	0.01	0.17
(1,1972)	1:A:153:GLU:H	1:A:153:GLU:HB3	2	0.17	0.01	0.17
(1,349)	1:A:117:LEU:HG	1:A:120:GLY:H	2	0.16	0.01	0.16

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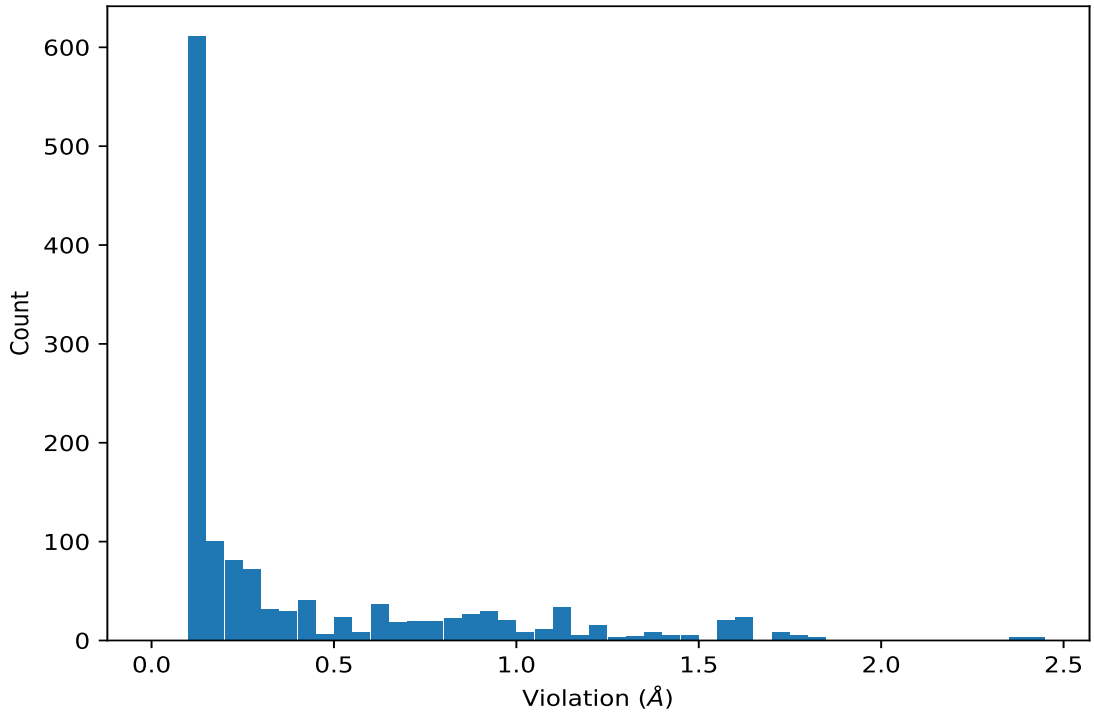
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1860)	1:A:121:GLU:H	1:A:122:ASP:HB2	2	0.16	0.03	0.16
(1,1860)	1:A:121:GLU:H	1:A:122:ASP:HB3	2	0.16	0.03	0.16
(1,942)	1:A:109:HIS:HE1	1:A:113:LEU:HG	2	0.16	0.02	0.16
(1,1536)	1:A:117:LEU:HD11	1:A:126:LEU:HB3	2	0.16	0.04	0.16
(1,1536)	1:A:117:LEU:HD12	1:A:126:LEU:HB3	2	0.16	0.04	0.16
(1,1536)	1:A:117:LEU:HD13	1:A:126:LEU:HB3	2	0.16	0.04	0.16
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG11	2	0.15	0.01	0.15
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG12	2	0.15	0.01	0.15
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG13	2	0.15	0.01	0.15
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG21	2	0.15	0.01	0.15
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG22	2	0.15	0.01	0.15
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG23	2	0.15	0.01	0.15
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG11	2	0.15	0.01	0.15
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG12	2	0.15	0.01	0.15
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG13	2	0.15	0.01	0.15
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG21	2	0.15	0.01	0.15
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG22	2	0.15	0.01	0.15
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG23	2	0.15	0.01	0.15
(1,42)	1:A:89:LEU:HB2	1:A:90:GLN:H	2	0.15	0.0	0.15
(1,252)	1:A:111:ARG:H	1:A:111:ARG:HE	2	0.14	0.01	0.14
(1,1683)	1:A:101:LEU:HD11	1:A:105:LEU:HG	2	0.14	0.02	0.14
(1,1683)	1:A:101:LEU:HD12	1:A:105:LEU:HG	2	0.14	0.02	0.14
(1,1683)	1:A:101:LEU:HD13	1:A:105:LEU:HG	2	0.14	0.02	0.14
(1,1683)	1:A:101:LEU:HD21	1:A:105:LEU:HG	2	0.14	0.02	0.14
(1,1683)	1:A:101:LEU:HD22	1:A:105:LEU:HG	2	0.14	0.02	0.14
(1,1683)	1:A:101:LEU:HD23	1:A:105:LEU:HG	2	0.14	0.02	0.14
(1,2090)	2:B:487:THR:HB	2:B:488:ASN:HD21	2	0.14	0.01	0.14
(1,2090)	2:B:487:THR:HB	2:B:488:ASN:HD22	2	0.14	0.01	0.14
(1,1315)	2:B:469:VAL:H	2:B:471:LEU:HG	2	0.13	0.0	0.13
(1,425)	1:A:127:MET:HB2	1:A:130:TYR:H	2	0.12	0.01	0.12
(1,425)	1:A:127:MET:HB3	1:A:130:TYR:H	2	0.12	0.01	0.12
(1,746)	2:B:474:VAL:H	2:B:476:TYR:HD1	2	0.12	0.01	0.12
(1,746)	2:B:474:VAL:H	2:B:476:TYR:HD2	2	0.12	0.01	0.12
(1,1677)	1:A:101:LEU:HD11	1:A:102:ARG:HA	2	0.12	0.02	0.12
(1,1677)	1:A:101:LEU:HD12	1:A:102:ARG:HA	2	0.12	0.02	0.12
(1,1677)	1:A:101:LEU:HD13	1:A:102:ARG:HA	2	0.12	0.02	0.12
(1,1677)	1:A:101:LEU:HD21	1:A:102:ARG:HA	2	0.12	0.02	0.12
(1,1677)	1:A:101:LEU:HD22	1:A:102:ARG:HA	2	0.12	0.02	0.12
(1,1677)	1:A:101:LEU:HD23	1:A:102:ARG:HA	2	0.12	0.02	0.12
(1,1667)	1:A:97:GLU:HB2	1:A:98:SER:H	2	0.12	0.0	0.12
(1,1667)	1:A:97:GLU:HB3	1:A:98:SER:H	2	0.12	0.0	0.12

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:A:117:LEU:HD11	1:A:123:LYS:H	12	2.42
(1,370)	1:A:117:LEU:HD12	1:A:123:LYS:H	12	2.42
(1,370)	1:A:117:LEU:HD13	1:A:123:LYS:H	12	2.42
(1,370)	1:A:117:LEU:HD11	1:A:123:LYS:H	4	2.36
(1,370)	1:A:117:LEU:HD12	1:A:123:LYS:H	4	2.36
(1,370)	1:A:117:LEU:HD13	1:A:123:LYS:H	4	2.36
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG21	4	1.82
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG22	4	1.82
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG23	4	1.82
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG21	6	1.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG22	6	1.75
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG23	6	1.75
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG21	18	1.75
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG22	18	1.75
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG23	18	1.75
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG21	8	1.74
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG22	8	1.74
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG23	8	1.74
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG21	10	1.74
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG22	10	1.74
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG23	10	1.74
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG21	3	1.72
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG22	3	1.72
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG23	3	1.72
(1,1153)	1:A:137:VAL:HG11	1:A:138:GLU:HA	3	1.63
(1,1153)	1:A:137:VAL:HG12	1:A:138:GLU:HA	3	1.63
(1,1153)	1:A:137:VAL:HG13	1:A:138:GLU:HA	3	1.63
(1,1153)	1:A:137:VAL:HG11	1:A:138:GLU:HA	4	1.62
(1,1153)	1:A:137:VAL:HG12	1:A:138:GLU:HA	4	1.62
(1,1153)	1:A:137:VAL:HG13	1:A:138:GLU:HA	4	1.62
(1,1153)	1:A:137:VAL:HG11	1:A:138:GLU:HA	10	1.62
(1,1153)	1:A:137:VAL:HG12	1:A:138:GLU:HA	10	1.62
(1,1153)	1:A:137:VAL:HG13	1:A:138:GLU:HA	10	1.62
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG21	14	1.61
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG22	14	1.61
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG23	14	1.61
(1,1153)	1:A:137:VAL:HG11	1:A:138:GLU:HA	8	1.61
(1,1153)	1:A:137:VAL:HG12	1:A:138:GLU:HA	8	1.61
(1,1153)	1:A:137:VAL:HG13	1:A:138:GLU:HA	8	1.61
(1,1153)	1:A:137:VAL:HG11	1:A:138:GLU:HA	14	1.61
(1,1153)	1:A:137:VAL:HG12	1:A:138:GLU:HA	14	1.61
(1,1153)	1:A:137:VAL:HG13	1:A:138:GLU:HA	14	1.61
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG21	11	1.6
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG22	11	1.6
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG23	11	1.6
(1,1153)	1:A:137:VAL:HG11	1:A:138:GLU:HA	20	1.6
(1,1153)	1:A:137:VAL:HG12	1:A:138:GLU:HA	20	1.6
(1,1153)	1:A:137:VAL:HG13	1:A:138:GLU:HA	20	1.6
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG21	20	1.59
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG22	20	1.59
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG23	20	1.59
(1,1153)	1:A:137:VAL:HG11	1:A:138:GLU:HA	13	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1153)	1:A:137:VAL:HG12	1:A:138:GLU:HA	13	1.58
(1,1153)	1:A:137:VAL:HG13	1:A:138:GLU:HA	13	1.58
(1,1153)	1:A:137:VAL:HG11	1:A:138:GLU:HA	18	1.58
(1,1153)	1:A:137:VAL:HG12	1:A:138:GLU:HA	18	1.58
(1,1153)	1:A:137:VAL:HG13	1:A:138:GLU:HA	18	1.58
(1,1153)	1:A:137:VAL:HG11	1:A:138:GLU:HA	5	1.56
(1,1153)	1:A:137:VAL:HG12	1:A:138:GLU:HA	5	1.56
(1,1153)	1:A:137:VAL:HG13	1:A:138:GLU:HA	5	1.56
(1,1153)	1:A:137:VAL:HG11	1:A:138:GLU:HA	6	1.56
(1,1153)	1:A:137:VAL:HG12	1:A:138:GLU:HA	6	1.56
(1,1153)	1:A:137:VAL:HG13	1:A:138:GLU:HA	6	1.56
(1,1153)	1:A:137:VAL:HG11	1:A:138:GLU:HA	11	1.56
(1,1153)	1:A:137:VAL:HG12	1:A:138:GLU:HA	11	1.56
(1,1153)	1:A:137:VAL:HG13	1:A:138:GLU:HA	11	1.56
(1,1153)	1:A:137:VAL:HG11	1:A:138:GLU:HA	2	1.55
(1,1153)	1:A:137:VAL:HG12	1:A:138:GLU:HA	2	1.55
(1,1153)	1:A:137:VAL:HG13	1:A:138:GLU:HA	2	1.55
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG21	13	1.49
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG22	13	1.49
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG23	13	1.49
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	17	1.47
(1,1600)	1:A:90:GLN:HB2	1:A:94:ASN:HD21	2	1.47
(1,1600)	1:A:90:GLN:HB3	1:A:94:ASN:HD21	2	1.47
(1,1602)	1:A:90:GLN:HG2	1:A:94:ASN:HD21	13	1.45
(1,1602)	1:A:90:GLN:HG3	1:A:94:ASN:HD21	13	1.45
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	20	1.42
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG21	6	1.42
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG22	6	1.42
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG23	6	1.42
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG21	5	1.4
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG22	5	1.4
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG23	5	1.4
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG21	2	1.39
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG22	2	1.39
(1,448)	1:A:132:GLN:H	1:A:137:VAL:HG23	2	1.39
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	6	1.35
(1,1602)	1:A:90:GLN:HG2	1:A:94:ASN:HD21	11	1.35
(1,1602)	1:A:90:GLN:HG3	1:A:94:ASN:HD21	11	1.35
(1,668)	2:B:468:ASN:H	2:B:471:LEU:HD11	15	1.33
(1,668)	2:B:468:ASN:H	2:B:471:LEU:HD12	15	1.33
(1,668)	2:B:468:ASN:H	2:B:471:LEU:HD13	15	1.33
(1,1445)	1:A:114:MET:HG2	1:A:139:PHE:HE1	20	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1445)	1:A:114:MET:HG2	1:A:139:PHE:HE2	20	1.31
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG21	10	1.25
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG22	10	1.25
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG23	10	1.25
(1,1445)	1:A:114:MET:HG2	1:A:139:PHE:HE1	17	1.24
(1,1445)	1:A:114:MET:HG2	1:A:139:PHE:HE2	17	1.24
(1,1131)	1:A:117:LEU:HD11	1:A:123:LYS:HA	4	1.24
(1,1131)	1:A:117:LEU:HD12	1:A:123:LYS:HA	4	1.24
(1,1131)	1:A:117:LEU:HD13	1:A:123:LYS:HA	4	1.24
(1,1131)	1:A:117:LEU:HD11	1:A:123:LYS:HA	12	1.24
(1,1131)	1:A:117:LEU:HD12	1:A:123:LYS:HA	12	1.24
(1,1131)	1:A:117:LEU:HD13	1:A:123:LYS:HA	12	1.24
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG21	3	1.24
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG22	3	1.24
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG23	3	1.24
(1,1445)	1:A:114:MET:HG2	1:A:139:PHE:HE1	6	1.23
(1,1445)	1:A:114:MET:HG2	1:A:139:PHE:HE2	6	1.23
(1,668)	2:B:468:ASN:H	2:B:471:LEU:HD11	14	1.21
(1,668)	2:B:468:ASN:H	2:B:471:LEU:HD12	14	1.21
(1,668)	2:B:468:ASN:H	2:B:471:LEU:HD13	14	1.21
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG21	8	1.16
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG22	8	1.16
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG23	8	1.16
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG21	14	1.16
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG22	14	1.16
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG23	14	1.16
(1,668)	2:B:468:ASN:H	2:B:471:LEU:HD11	9	1.14
(1,668)	2:B:468:ASN:H	2:B:471:LEU:HD12	9	1.14
(1,668)	2:B:468:ASN:H	2:B:471:LEU:HD13	9	1.14
(1,480)	1:A:136:PHE:H	1:A:137:VAL:HB	13	1.14
(1,480)	1:A:136:PHE:H	1:A:137:VAL:HB	8	1.13
(1,1354)	1:A:91:ASN:H	1:A:94:ASN:HD21	2	1.13
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG21	3	1.13
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG22	3	1.13
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG23	3	1.13
(1,480)	1:A:136:PHE:H	1:A:137:VAL:HB	4	1.12
(1,480)	1:A:136:PHE:H	1:A:137:VAL:HB	14	1.12
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG21	4	1.12
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG22	4	1.12
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG23	4	1.12
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG21	18	1.12
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG22	18	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG23	18	1.12
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG21	4	1.12
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG22	4	1.12
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG23	4	1.12
(1,480)	1:A:136:PHE:H	1:A:137:VAL:HB	3	1.11
(1,480)	1:A:136:PHE:H	1:A:137:VAL:HB	10	1.11
(1,480)	1:A:136:PHE:H	1:A:137:VAL:HB	11	1.11
(1,480)	1:A:136:PHE:H	1:A:137:VAL:HB	18	1.11
(1,480)	1:A:136:PHE:H	1:A:137:VAL:HB	20	1.11
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG21	10	1.11
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG22	10	1.11
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG23	10	1.11
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG21	11	1.11
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG22	11	1.11
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG23	11	1.11
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG21	5	1.1
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG22	5	1.1
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG23	5	1.1
(1,480)	1:A:136:PHE:H	1:A:137:VAL:HB	5	1.09
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG21	6	1.09
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG22	6	1.09
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG23	6	1.09
(1,480)	1:A:136:PHE:H	1:A:137:VAL:HB	2	1.08
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG21	20	1.08
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG22	20	1.08
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG23	20	1.08
(1,480)	1:A:136:PHE:H	1:A:137:VAL:HB	6	1.07
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG21	4	1.07
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG22	4	1.07
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG23	4	1.07
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD21	19	1.03
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD22	19	1.03
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD23	19	1.03
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD21	12	1.01
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD22	12	1.01
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD23	12	1.01
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG21	11	1.01
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG22	11	1.01
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG23	11	1.01
(1,1128)	1:A:117:LEU:HD11	2:B:471:LEU:HD21	15	0.99
(1,1128)	1:A:117:LEU:HD11	2:B:471:LEU:HD22	15	0.99
(1,1128)	1:A:117:LEU:HD11	2:B:471:LEU:HD23	15	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1128)	1:A:117:LEU:HD12	2:B:471:LEU:HD21	15	0.99
(1,1128)	1:A:117:LEU:HD12	2:B:471:LEU:HD22	15	0.99
(1,1128)	1:A:117:LEU:HD12	2:B:471:LEU:HD23	15	0.99
(1,1128)	1:A:117:LEU:HD13	2:B:471:LEU:HD21	15	0.99
(1,1128)	1:A:117:LEU:HD13	2:B:471:LEU:HD22	15	0.99
(1,1128)	1:A:117:LEU:HD13	2:B:471:LEU:HD23	15	0.99
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG21	13	0.99
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG22	13	0.99
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG23	13	0.99
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD21	6	0.98
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD22	6	0.98
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD23	6	0.98
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG21	14	0.98
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG22	14	0.98
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG23	14	0.98
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG21	8	0.97
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG22	8	0.97
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG23	8	0.97
(1,520)	1:A:137:VAL:HG11	1:A:141:ASP:H	6	0.95
(1,520)	1:A:137:VAL:HG12	1:A:141:ASP:H	6	0.95
(1,520)	1:A:137:VAL:HG13	1:A:141:ASP:H	6	0.95
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD21	10	0.95
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD22	10	0.95
(1,184)	1:A:103:SER:H	1:A:104:LEU:HD23	10	0.95
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG21	18	0.95
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG22	18	0.95
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG23	18	0.95
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG21	20	0.94
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG22	20	0.94
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG23	20	0.94
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG21	11	0.93
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG22	11	0.93
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG23	11	0.93
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG21	3	0.92
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG22	3	0.92
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG23	3	0.92
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG21	18	0.92
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG22	18	0.92
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG23	18	0.92
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD21	19	0.91
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD22	19	0.91
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD23	19	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:A:117:LEU:HD11	1:A:126:LEU:H	12	0.9
(1,384)	1:A:117:LEU:HD12	1:A:126:LEU:H	12	0.9
(1,384)	1:A:117:LEU:HD13	1:A:126:LEU:H	12	0.9
(1,1035)	1:A:114:MET:HE1	2:B:478:ILE:HG13	2	0.9
(1,1035)	1:A:114:MET:HE2	2:B:478:ILE:HG13	2	0.9
(1,1035)	1:A:114:MET:HE3	2:B:478:ILE:HG13	2	0.9
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD21	6	0.89
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD22	6	0.89
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD23	6	0.89
(1,1128)	1:A:117:LEU:HD11	2:B:471:LEU:HD21	9	0.89
(1,1128)	1:A:117:LEU:HD11	2:B:471:LEU:HD22	9	0.89
(1,1128)	1:A:117:LEU:HD11	2:B:471:LEU:HD23	9	0.89
(1,1128)	1:A:117:LEU:HD12	2:B:471:LEU:HD21	9	0.89
(1,1128)	1:A:117:LEU:HD12	2:B:471:LEU:HD22	9	0.89
(1,1128)	1:A:117:LEU:HD12	2:B:471:LEU:HD23	9	0.89
(1,1128)	1:A:117:LEU:HD13	2:B:471:LEU:HD21	9	0.89
(1,1128)	1:A:117:LEU:HD13	2:B:471:LEU:HD22	9	0.89
(1,1128)	1:A:117:LEU:HD13	2:B:471:LEU:HD23	9	0.89
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD21	12	0.87
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD22	12	0.87
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD23	12	0.87
(1,520)	1:A:137:VAL:HG11	1:A:141:ASP:H	11	0.86
(1,520)	1:A:137:VAL:HG12	1:A:141:ASP:H	11	0.86
(1,520)	1:A:137:VAL:HG13	1:A:141:ASP:H	11	0.86
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD21	10	0.86
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD22	10	0.86
(1,1250)	1:A:104:LEU:HA	1:A:104:LEU:HD23	10	0.86
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG21	5	0.86
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG22	5	0.86
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG23	5	0.86
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG21	2	0.86
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG22	2	0.86
(1,1103)	1:A:131:MET:HA	1:A:137:VAL:HG23	2	0.86
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG21	20	0.85
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG22	20	0.85
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG23	20	0.85
(1,1602)	1:A:90:GLN:HG2	1:A:94:ASN:HD21	2	0.84
(1,1602)	1:A:90:GLN:HG3	1:A:94:ASN:HD21	2	0.84
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG21	2	0.84
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG22	2	0.84
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG23	2	0.84
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG21	13	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG22	13	0.83
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG23	13	0.83
(1,912)	2:B:476:TYR:HE1	2:B:477:ILE:HG13	18	0.82
(1,912)	2:B:476:TYR:HE2	2:B:477:ILE:HG13	18	0.82
(1,769)	2:B:476:TYR:H	2:B:477:ILE:HG13	18	0.82
(1,384)	1:A:117:LEU:HD11	1:A:126:LEU:H	4	0.82
(1,384)	1:A:117:LEU:HD12	1:A:126:LEU:H	4	0.82
(1,384)	1:A:117:LEU:HD13	1:A:126:LEU:H	4	0.82
(1,537)	1:A:104:LEU:HD11	1:A:142:CYS:H	19	0.81
(1,537)	1:A:104:LEU:HD12	1:A:142:CYS:H	19	0.81
(1,537)	1:A:104:LEU:HD13	1:A:142:CYS:H	19	0.81
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG21	8	0.8
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG22	8	0.8
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG23	8	0.8
(2,17)	1:A:113:LEU:H	1:A:114:MET:HG3	6	0.79
(1,520)	1:A:137:VAL:HG11	1:A:141:ASP:H	14	0.79
(1,520)	1:A:137:VAL:HG12	1:A:141:ASP:H	14	0.79
(1,520)	1:A:137:VAL:HG13	1:A:141:ASP:H	14	0.79
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG21	13	0.79
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG22	13	0.79
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG23	13	0.79
(1,520)	1:A:137:VAL:HG11	1:A:141:ASP:H	3	0.78
(1,520)	1:A:137:VAL:HG12	1:A:141:ASP:H	3	0.78
(1,520)	1:A:137:VAL:HG13	1:A:141:ASP:H	3	0.78
(1,520)	1:A:137:VAL:HG11	1:A:141:ASP:H	13	0.78
(1,520)	1:A:137:VAL:HG12	1:A:141:ASP:H	13	0.78
(1,520)	1:A:137:VAL:HG13	1:A:141:ASP:H	13	0.78
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG21	14	0.78
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG22	14	0.78
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG23	14	0.78
(1,520)	1:A:137:VAL:HG11	1:A:141:ASP:H	4	0.76
(1,520)	1:A:137:VAL:HG12	1:A:141:ASP:H	4	0.76
(1,520)	1:A:137:VAL:HG13	1:A:141:ASP:H	4	0.76
(1,327)	1:A:117:LEU:HG	1:A:118:ASP:H	12	0.75
(1,520)	1:A:137:VAL:HG11	1:A:141:ASP:H	2	0.74
(1,520)	1:A:137:VAL:HG12	1:A:141:ASP:H	2	0.74
(1,520)	1:A:137:VAL:HG13	1:A:141:ASP:H	2	0.74
(1,520)	1:A:137:VAL:HG11	1:A:141:ASP:H	5	0.74
(1,520)	1:A:137:VAL:HG12	1:A:141:ASP:H	5	0.74
(1,520)	1:A:137:VAL:HG13	1:A:141:ASP:H	5	0.74
(1,2015)	2:B:468:ASN:HD21	2:B:471:LEU:HD11	9	0.74
(1,2015)	2:B:468:ASN:HD21	2:B:471:LEU:HD12	9	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2015)	2:B:468:ASN:HD21	2:B:471:LEU:HD13	9	0.74
(1,2015)	2:B:468:ASN:HD22	2:B:471:LEU:HD11	9	0.74
(1,2015)	2:B:468:ASN:HD22	2:B:471:LEU:HD12	9	0.74
(1,2015)	2:B:468:ASN:HD22	2:B:471:LEU:HD13	9	0.74
(2,17)	1:A:113:LEU:H	1:A:114:MET:HG3	17	0.73
(2,17)	1:A:113:LEU:H	1:A:114:MET:HG3	20	0.73
(1,2015)	2:B:468:ASN:HD21	2:B:471:LEU:HD11	15	0.71
(1,2015)	2:B:468:ASN:HD21	2:B:471:LEU:HD12	15	0.71
(1,2015)	2:B:468:ASN:HD21	2:B:471:LEU:HD13	15	0.71
(1,2015)	2:B:468:ASN:HD22	2:B:471:LEU:HD11	15	0.71
(1,2015)	2:B:468:ASN:HD22	2:B:471:LEU:HD12	15	0.71
(1,2015)	2:B:468:ASN:HD22	2:B:471:LEU:HD13	15	0.71
(1,1842)	1:A:117:LEU:HD11	1:A:123:LYS:HB2	12	0.68
(1,1842)	1:A:117:LEU:HD11	1:A:123:LYS:HB3	12	0.68
(1,1842)	1:A:117:LEU:HD12	1:A:123:LYS:HB2	12	0.68
(1,1842)	1:A:117:LEU:HD12	1:A:123:LYS:HB3	12	0.68
(1,1842)	1:A:117:LEU:HD13	1:A:123:LYS:HB2	12	0.68
(1,1842)	1:A:117:LEU:HD13	1:A:123:LYS:HB3	12	0.68
(1,2015)	2:B:468:ASN:HD21	2:B:471:LEU:HD11	14	0.67
(1,2015)	2:B:468:ASN:HD21	2:B:471:LEU:HD12	14	0.67
(1,2015)	2:B:468:ASN:HD21	2:B:471:LEU:HD13	14	0.67
(1,2015)	2:B:468:ASN:HD22	2:B:471:LEU:HD11	14	0.67
(1,2015)	2:B:468:ASN:HD22	2:B:471:LEU:HD12	14	0.67
(1,2015)	2:B:468:ASN:HD22	2:B:471:LEU:HD13	14	0.67
(1,1354)	1:A:91:ASN:H	1:A:94:ASN:HD21	13	0.67
(1,894)	1:A:117:LEU:HD21	1:A:130:TYR:HE1	4	0.66
(1,894)	1:A:117:LEU:HD21	1:A:130:TYR:HE2	4	0.66
(1,894)	1:A:117:LEU:HD22	1:A:130:TYR:HE1	4	0.66
(1,894)	1:A:117:LEU:HD22	1:A:130:TYR:HE2	4	0.66
(1,894)	1:A:117:LEU:HD23	1:A:130:TYR:HE1	4	0.66
(1,894)	1:A:117:LEU:HD23	1:A:130:TYR:HE2	4	0.66
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG21	2	0.64
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG22	2	0.64
(1,1104)	1:A:133:GLU:H	1:A:137:VAL:HG23	2	0.64
(1,520)	1:A:137:VAL:HG11	1:A:141:ASP:H	18	0.63
(1,520)	1:A:137:VAL:HG12	1:A:141:ASP:H	18	0.63
(1,520)	1:A:137:VAL:HG13	1:A:141:ASP:H	18	0.63
(1,520)	1:A:137:VAL:HG11	1:A:141:ASP:H	20	0.63
(1,520)	1:A:137:VAL:HG12	1:A:141:ASP:H	20	0.63
(1,520)	1:A:137:VAL:HG13	1:A:141:ASP:H	20	0.63
(1,1440)	1:A:117:LEU:HD21	2:B:471:LEU:H	12	0.63
(1,1440)	1:A:117:LEU:HD22	2:B:471:LEU:H	12	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1440)	1:A:117:LEU:HD23	2:B:471:LEU:H	12	0.63
(1,1074)	2:B:477:ILE:HG21	2:B:478:ILE:HG13	8	0.63
(1,1074)	2:B:477:ILE:HG22	2:B:478:ILE:HG13	8	0.63
(1,1074)	2:B:477:ILE:HG23	2:B:478:ILE:HG13	8	0.63
(1,537)	1:A:104:LEU:HD11	1:A:142:CYS:H	6	0.62
(1,537)	1:A:104:LEU:HD12	1:A:142:CYS:H	6	0.62
(1,537)	1:A:104:LEU:HD13	1:A:142:CYS:H	6	0.62
(1,1709)	1:A:104:LEU:HD11	1:A:138:GLU:HG2	19	0.62
(1,1709)	1:A:104:LEU:HD11	1:A:138:GLU:HG3	19	0.62
(1,1709)	1:A:104:LEU:HD12	1:A:138:GLU:HG2	19	0.62
(1,1709)	1:A:104:LEU:HD12	1:A:138:GLU:HG3	19	0.62
(1,1709)	1:A:104:LEU:HD13	1:A:138:GLU:HG2	19	0.62
(1,1709)	1:A:104:LEU:HD13	1:A:138:GLU:HG3	19	0.62
(1,1035)	1:A:114:MET:HE1	2:B:478:ILE:HG13	8	0.62
(1,1035)	1:A:114:MET:HE2	2:B:478:ILE:HG13	8	0.62
(1,1035)	1:A:114:MET:HE3	2:B:478:ILE:HG13	8	0.62
(1,837)	2:B:478:ILE:HG12	2:B:483:PHE:H	8	0.61
(1,1128)	1:A:117:LEU:HD11	2:B:471:LEU:HD21	14	0.61
(1,1128)	1:A:117:LEU:HD11	2:B:471:LEU:HD22	14	0.61
(1,1128)	1:A:117:LEU:HD11	2:B:471:LEU:HD23	14	0.61
(1,1128)	1:A:117:LEU:HD12	2:B:471:LEU:HD21	14	0.61
(1,1128)	1:A:117:LEU:HD12	2:B:471:LEU:HD22	14	0.61
(1,1128)	1:A:117:LEU:HD12	2:B:471:LEU:HD23	14	0.61
(1,1128)	1:A:117:LEU:HD13	2:B:471:LEU:HD21	14	0.61
(1,1128)	1:A:117:LEU:HD13	2:B:471:LEU:HD22	14	0.61
(1,1128)	1:A:117:LEU:HD13	2:B:471:LEU:HD23	14	0.61
(1,327)	1:A:117:LEU:HG	1:A:118:ASP:H	4	0.6
(1,1074)	2:B:477:ILE:HG21	2:B:478:ILE:HG13	2	0.58
(1,1074)	2:B:477:ILE:HG22	2:B:478:ILE:HG13	2	0.58
(1,1074)	2:B:477:ILE:HG23	2:B:478:ILE:HG13	2	0.58
(1,959)	2:B:476:TYR:HD1	2:B:477:ILE:HG13	18	0.57
(1,959)	2:B:476:TYR:HD2	2:B:477:ILE:HG13	18	0.57
(1,520)	1:A:137:VAL:HG11	1:A:141:ASP:H	10	0.55
(1,520)	1:A:137:VAL:HG12	1:A:141:ASP:H	10	0.55
(1,520)	1:A:137:VAL:HG13	1:A:141:ASP:H	10	0.55
(1,537)	1:A:104:LEU:HD11	1:A:142:CYS:H	10	0.54
(1,537)	1:A:104:LEU:HD12	1:A:142:CYS:H	10	0.54
(1,537)	1:A:104:LEU:HD13	1:A:142:CYS:H	10	0.54
(1,752)	2:B:471:LEU:HD21	2:B:475:ARG:H	15	0.53
(1,752)	2:B:471:LEU:HD22	2:B:475:ARG:H	15	0.53
(1,752)	2:B:471:LEU:HD23	2:B:475:ARG:H	15	0.53
(1,520)	1:A:137:VAL:HG11	1:A:141:ASP:H	8	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,520)	1:A:137:VAL:HG12	1:A:141:ASP:H	8	0.52
(1,520)	1:A:137:VAL:HG13	1:A:141:ASP:H	8	0.52
(1,1015)	1:A:117:LEU:HD21	1:A:127:MET:HE1	12	0.51
(1,1015)	1:A:117:LEU:HD21	1:A:127:MET:HE2	12	0.51
(1,1015)	1:A:117:LEU:HD21	1:A:127:MET:HE3	12	0.51
(1,1015)	1:A:117:LEU:HD22	1:A:127:MET:HE1	12	0.51
(1,1015)	1:A:117:LEU:HD22	1:A:127:MET:HE2	12	0.51
(1,1015)	1:A:117:LEU:HD22	1:A:127:MET:HE3	12	0.51
(1,1015)	1:A:117:LEU:HD23	1:A:127:MET:HE1	12	0.51
(1,1015)	1:A:117:LEU:HD23	1:A:127:MET:HE2	12	0.51
(1,1015)	1:A:117:LEU:HD23	1:A:127:MET:HE3	12	0.51
(1,894)	1:A:117:LEU:HD21	1:A:130:TYR:HE1	12	0.5
(1,894)	1:A:117:LEU:HD21	1:A:130:TYR:HE2	12	0.5
(1,894)	1:A:117:LEU:HD22	1:A:130:TYR:HE1	12	0.5
(1,894)	1:A:117:LEU:HD22	1:A:130:TYR:HE2	12	0.5
(1,894)	1:A:117:LEU:HD23	1:A:130:TYR:HE1	12	0.5
(1,894)	1:A:117:LEU:HD23	1:A:130:TYR:HE2	12	0.5
(2,51)	2:B:474:VAL:H	2:B:478:ILE:HG13	2	0.47
(1,837)	2:B:478:ILE:HG12	2:B:483:PHE:H	2	0.45
(1,752)	2:B:471:LEU:HD21	2:B:475:ARG:H	14	0.45
(1,752)	2:B:471:LEU:HD22	2:B:475:ARG:H	14	0.45
(1,752)	2:B:471:LEU:HD23	2:B:475:ARG:H	14	0.45
(1,1600)	1:A:90:GLN:HB2	1:A:94:ASN:HD21	13	0.45
(1,1600)	1:A:90:GLN:HB3	1:A:94:ASN:HD21	13	0.45
(1,1132)	1:A:117:LEU:HA	1:A:117:LEU:HD11	12	0.43
(1,1132)	1:A:117:LEU:HA	1:A:117:LEU:HD12	12	0.43
(1,1132)	1:A:117:LEU:HA	1:A:117:LEU:HD13	12	0.43
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG21	6	0.43
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG22	6	0.43
(1,1101)	1:A:133:GLU:HG3	1:A:137:VAL:HG23	6	0.43
(1,511)	1:A:104:LEU:HD11	1:A:139:PHE:H	6	0.42
(1,511)	1:A:104:LEU:HD12	1:A:139:PHE:H	6	0.42
(1,511)	1:A:104:LEU:HD13	1:A:139:PHE:H	6	0.42
(1,495)	1:A:137:VAL:HG11	1:A:138:GLU:H	2	0.42
(1,495)	1:A:137:VAL:HG12	1:A:138:GLU:H	2	0.42
(1,495)	1:A:137:VAL:HG13	1:A:138:GLU:H	2	0.42
(1,495)	1:A:137:VAL:HG11	1:A:138:GLU:H	20	0.42
(1,495)	1:A:137:VAL:HG12	1:A:138:GLU:H	20	0.42
(1,495)	1:A:137:VAL:HG13	1:A:138:GLU:H	20	0.42
(1,511)	1:A:104:LEU:HD11	1:A:139:PHE:H	19	0.41
(1,511)	1:A:104:LEU:HD12	1:A:139:PHE:H	19	0.41
(1,511)	1:A:104:LEU:HD13	1:A:139:PHE:H	19	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:A:137:VAL:HG11	1:A:138:GLU:H	10	0.41
(1,495)	1:A:137:VAL:HG12	1:A:138:GLU:H	10	0.41
(1,495)	1:A:137:VAL:HG13	1:A:138:GLU:H	10	0.41
(1,1132)	1:A:117:LEU:HA	1:A:117:LEU:HD11	4	0.41
(1,1132)	1:A:117:LEU:HA	1:A:117:LEU:HD12	4	0.41
(1,1132)	1:A:117:LEU:HA	1:A:117:LEU:HD13	4	0.41
(1,495)	1:A:137:VAL:HG11	1:A:138:GLU:H	8	0.4
(1,495)	1:A:137:VAL:HG12	1:A:138:GLU:H	8	0.4
(1,495)	1:A:137:VAL:HG13	1:A:138:GLU:H	8	0.4
(1,495)	1:A:137:VAL:HG11	1:A:138:GLU:H	18	0.4
(1,495)	1:A:137:VAL:HG12	1:A:138:GLU:H	18	0.4
(1,495)	1:A:137:VAL:HG13	1:A:138:GLU:H	18	0.4
(1,255)	1:A:112:GLN:H	1:A:112:GLN:HG2	5	0.4
(1,255)	1:A:112:GLN:H	1:A:112:GLN:HG3	5	0.4
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD21	19	0.4
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD22	19	0.4
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD23	19	0.4
(1,1842)	1:A:117:LEU:HD11	1:A:123:LYS:HB2	4	0.4
(1,1842)	1:A:117:LEU:HD11	1:A:123:LYS:HB3	4	0.4
(1,1842)	1:A:117:LEU:HD12	1:A:123:LYS:HB2	4	0.4
(1,1842)	1:A:117:LEU:HD12	1:A:123:LYS:HB3	4	0.4
(1,1842)	1:A:117:LEU:HD13	1:A:123:LYS:HB2	4	0.4
(1,1842)	1:A:117:LEU:HD13	1:A:123:LYS:HB3	4	0.4
(1,752)	2:B:471:LEU:HD21	2:B:475:ARG:H	9	0.39
(1,752)	2:B:471:LEU:HD22	2:B:475:ARG:H	9	0.39
(1,752)	2:B:471:LEU:HD23	2:B:475:ARG:H	9	0.39
(1,495)	1:A:137:VAL:HG11	1:A:138:GLU:H	13	0.39
(1,495)	1:A:137:VAL:HG12	1:A:138:GLU:H	13	0.39
(1,495)	1:A:137:VAL:HG13	1:A:138:GLU:H	13	0.39
(1,495)	1:A:137:VAL:HG11	1:A:138:GLU:H	14	0.38
(1,495)	1:A:137:VAL:HG12	1:A:138:GLU:H	14	0.38
(1,495)	1:A:137:VAL:HG13	1:A:138:GLU:H	14	0.38
(1,495)	1:A:137:VAL:HG11	1:A:138:GLU:H	5	0.37
(1,495)	1:A:137:VAL:HG12	1:A:138:GLU:H	5	0.37
(1,495)	1:A:137:VAL:HG13	1:A:138:GLU:H	5	0.37
(1,1129)	1:A:117:LEU:HD11	1:A:126:LEU:HB2	4	0.37
(1,1129)	1:A:117:LEU:HD12	1:A:126:LEU:HB2	4	0.37
(1,1129)	1:A:117:LEU:HD13	1:A:126:LEU:HB2	4	0.37
(1,1015)	1:A:117:LEU:HD21	1:A:127:MET:HE1	4	0.37
(1,1015)	1:A:117:LEU:HD21	1:A:127:MET:HE2	4	0.37
(1,1015)	1:A:117:LEU:HD21	1:A:127:MET:HE3	4	0.37
(1,1015)	1:A:117:LEU:HD22	1:A:127:MET:HE1	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:A:117:LEU:HD22	1:A:127:MET:HE2	4	0.37
(1,1015)	1:A:117:LEU:HD22	1:A:127:MET:HE3	4	0.37
(1,1015)	1:A:117:LEU:HD23	1:A:127:MET:HE1	4	0.37
(1,1015)	1:A:117:LEU:HD23	1:A:127:MET:HE2	4	0.37
(1,1015)	1:A:117:LEU:HD23	1:A:127:MET:HE3	4	0.37
(1,495)	1:A:137:VAL:HG11	1:A:138:GLU:H	11	0.36
(1,495)	1:A:137:VAL:HG12	1:A:138:GLU:H	11	0.36
(1,495)	1:A:137:VAL:HG13	1:A:138:GLU:H	11	0.36
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD21	12	0.36
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD22	12	0.36
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD23	12	0.36
(2,51)	2:B:474:VAL:H	2:B:478:ILE:HG13	8	0.35
(1,495)	1:A:137:VAL:HG11	1:A:138:GLU:H	3	0.35
(1,495)	1:A:137:VAL:HG12	1:A:138:GLU:H	3	0.35
(1,495)	1:A:137:VAL:HG13	1:A:138:GLU:H	3	0.35
(1,1483)	1:A:134:PRO:HA	1:A:137:VAL:HB	10	0.35
(1,1483)	1:A:134:PRO:HA	1:A:137:VAL:HB	13	0.35
(1,1483)	1:A:134:PRO:HA	1:A:137:VAL:HB	2	0.34
(1,1483)	1:A:134:PRO:HA	1:A:137:VAL:HB	11	0.34
(1,1483)	1:A:134:PRO:HA	1:A:137:VAL:HB	14	0.34
(1,1483)	1:A:134:PRO:HA	1:A:137:VAL:HB	18	0.34
(1,1483)	1:A:134:PRO:HA	1:A:137:VAL:HB	20	0.34
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD21	6	0.33
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD22	6	0.33
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD23	6	0.33
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD21	10	0.33
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD22	10	0.33
(1,195)	1:A:104:LEU:H	1:A:104:LEU:HD23	10	0.33
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD11	1	0.33
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD12	1	0.33
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD13	1	0.33
(1,496)	1:A:137:VAL:HB	1:A:138:GLU:H	6	0.32
(1,495)	1:A:137:VAL:HG11	1:A:138:GLU:H	4	0.32
(1,495)	1:A:137:VAL:HG12	1:A:138:GLU:H	4	0.32
(1,495)	1:A:137:VAL:HG13	1:A:138:GLU:H	4	0.32
(1,1483)	1:A:134:PRO:HA	1:A:137:VAL:HB	3	0.32
(1,1483)	1:A:134:PRO:HA	1:A:137:VAL:HB	4	0.32
(1,1483)	1:A:134:PRO:HA	1:A:137:VAL:HB	5	0.32
(1,1483)	1:A:134:PRO:HA	1:A:137:VAL:HB	8	0.32
(1,1275)	2:B:466:GLU:HA	2:B:469:VAL:HB	18	0.32
(1,1424)	1:A:114:MET:H	1:A:114:MET:HG3	6	0.31
(1,1424)	1:A:114:MET:H	1:A:114:MET:HG3	17	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1424)	1:A:114:MET:H	1:A:114:MET:HG3	20	0.31
(1,878)	2:B:490:ALA:HA	2:B:491:LYS:H	17	0.3
(1,1334)	1:A:89:LEU:HA	1:A:89:LEU:HD21	9	0.3
(1,1334)	1:A:89:LEU:HA	1:A:89:LEU:HD22	9	0.3
(1,1334)	1:A:89:LEU:HA	1:A:89:LEU:HD23	9	0.3
(1,797)	2:B:478:ILE:HG13	2:B:479:LYS:H	8	0.29
(1,695)	2:B:470:ILE:H	2:B:471:LEU:HG	14	0.29
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG11	8	0.29
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG12	8	0.29
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG13	8	0.29
(1,1473)	2:B:468:ASN:HA	2:B:471:LEU:HD11	15	0.29
(1,1473)	2:B:468:ASN:HA	2:B:471:LEU:HD12	15	0.29
(1,1473)	2:B:468:ASN:HA	2:B:471:LEU:HD13	15	0.29
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD11	8	0.29
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD12	8	0.29
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD13	8	0.29
(1,1133)	1:A:117:LEU:HD11	1:A:127:MET:H	12	0.29
(1,1133)	1:A:117:LEU:HD12	1:A:127:MET:H	12	0.29
(1,1133)	1:A:117:LEU:HD13	1:A:127:MET:H	12	0.29
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	4	0.28
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	4	0.28
(1,537)	1:A:104:LEU:HD11	1:A:142:CYS:H	12	0.28
(1,537)	1:A:104:LEU:HD12	1:A:142:CYS:H	12	0.28
(1,537)	1:A:104:LEU:HD13	1:A:142:CYS:H	12	0.28
(1,495)	1:A:137:VAL:HG11	1:A:138:GLU:H	6	0.28
(1,495)	1:A:137:VAL:HG12	1:A:138:GLU:H	6	0.28
(1,495)	1:A:137:VAL:HG13	1:A:138:GLU:H	6	0.28
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG11	11	0.28
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG12	11	0.28
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG13	11	0.28
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG11	13	0.28
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG12	13	0.28
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG13	13	0.28
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD11	18	0.28
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD12	18	0.28
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD13	18	0.28
(1,864)	2:B:488:ASN:H	2:B:489:SER:H	7	0.27
(1,797)	2:B:478:ILE:HG13	2:B:479:LYS:H	2	0.27
(1,695)	2:B:470:ILE:H	2:B:471:LEU:HG	9	0.27
(1,496)	1:A:137:VAL:HB	1:A:138:GLU:H	3	0.27
(1,496)	1:A:137:VAL:HB	1:A:138:GLU:H	8	0.27
(1,496)	1:A:137:VAL:HB	1:A:138:GLU:H	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG11	3	0.27
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG12	3	0.27
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG13	3	0.27
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG11	5	0.27
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG12	5	0.27
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG13	5	0.27
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG11	7	0.27
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG12	7	0.27
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG13	7	0.27
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG11	18	0.27
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG12	18	0.27
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG13	18	0.27
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	12	0.26
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	12	0.26
(1,695)	2:B:470:ILE:H	2:B:471:LEU:HG	15	0.26
(1,496)	1:A:137:VAL:HB	1:A:138:GLU:H	11	0.26
(1,386)	1:A:126:LEU:H	1:A:126:LEU:HG	5	0.26
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG11	16	0.26
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG12	16	0.26
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG13	16	0.26
(1,1483)	1:A:134:PRO:HA	1:A:137:VAL:HB	6	0.26
(1,1440)	1:A:117:LEU:HD21	2:B:471:LEU:H	4	0.26
(1,1440)	1:A:117:LEU:HD22	2:B:471:LEU:H	4	0.26
(1,1440)	1:A:117:LEU:HD23	2:B:471:LEU:H	4	0.26
(1,1429)	1:A:125:LYS:H	1:A:125:LYS:HD2	11	0.26
(1,1429)	1:A:125:LYS:H	1:A:125:LYS:HD3	11	0.26
(1,496)	1:A:137:VAL:HB	1:A:138:GLU:H	4	0.25
(1,332)	1:A:117:LEU:HG	1:A:119:GLN:H	4	0.25
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG11	6	0.25
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG12	6	0.25
(1,286)	1:A:115:VAL:H	1:A:115:VAL:HG13	6	0.25
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	15	0.24
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	15	0.24
(1,496)	1:A:137:VAL:HB	1:A:138:GLU:H	2	0.24
(1,496)	1:A:137:VAL:HB	1:A:138:GLU:H	20	0.24
(1,1275)	2:B:466:GLU:HA	2:B:469:VAL:HB	16	0.24
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	18	0.23
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	18	0.23
(1,869)	2:B:489:SER:HA	2:B:490:ALA:H	7	0.23
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	12	0.23
(1,496)	1:A:137:VAL:HB	1:A:138:GLU:H	13	0.23
(1,496)	1:A:137:VAL:HB	1:A:138:GLU:H	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:A:137:VAL:HB	1:A:138:GLU:H	18	0.23
(1,332)	1:A:117:LEU:HG	1:A:119:GLN:H	12	0.23
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG21	3	0.23
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG22	3	0.23
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG23	3	0.23
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG21	5	0.23
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG22	5	0.23
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG23	5	0.23
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG21	10	0.23
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG22	10	0.23
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG23	10	0.23
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG21	19	0.23
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG22	19	0.23
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG23	19	0.23
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	2	0.22
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	2	0.22
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	14	0.22
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	14	0.22
(1,1973)	1:A:153:GLU:HB2	1:A:154:GLU:H	14	0.22
(1,1973)	1:A:153:GLU:HB3	1:A:154:GLU:H	14	0.22
(1,1429)	1:A:125:LYS:H	1:A:125:LYS:HD2	13	0.22
(1,1429)	1:A:125:LYS:H	1:A:125:LYS:HD3	13	0.22
(1,1427)	1:A:105:LEU:H	1:A:105:LEU:HG	19	0.22
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD11	19	0.22
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD12	19	0.22
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD13	19	0.22
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG21	7	0.22
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG22	7	0.22
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG23	7	0.22
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG21	12	0.22
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG22	12	0.22
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG23	12	0.22
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG21	20	0.22
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG22	20	0.22
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG23	20	0.22
(1,1129)	1:A:117:LEU:HD11	1:A:126:LEU:HB2	12	0.22
(1,1129)	1:A:117:LEU:HD12	1:A:126:LEU:HB2	12	0.22
(1,1129)	1:A:117:LEU:HD13	1:A:126:LEU:HB2	12	0.22
(1,910)	2:B:476:TYR:HE1	2:B:480:LYS:HD2	12	0.21
(1,910)	2:B:476:TYR:HE1	2:B:480:LYS:HD3	12	0.21
(1,910)	2:B:476:TYR:HE2	2:B:480:LYS:HD2	12	0.21
(1,910)	2:B:476:TYR:HE2	2:B:480:LYS:HD3	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	11	0.21
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	11	0.21
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	19	0.21
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	19	0.21
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	10	0.21
(1,626)	1:A:153:GLU:HA	1:A:154:GLU:H	1	0.21
(1,496)	1:A:137:VAL:HB	1:A:138:GLU:H	5	0.21
(1,1977)	2:B:462:ASP:HB2	2:B:463:ILE:H	3	0.21
(1,1977)	2:B:462:ASP:HB3	2:B:463:ILE:H	3	0.21
(1,15)	1:A:84:MET:HA	1:A:85:ASP:H	12	0.21
(1,1429)	1:A:125:LYS:H	1:A:125:LYS:HD2	14	0.21
(1,1429)	1:A:125:LYS:H	1:A:125:LYS:HD3	14	0.21
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG21	4	0.21
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG22	4	0.21
(1,1220)	2:B:487:THR:HA	2:B:487:THR:HG23	4	0.21
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	6	0.2
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	6	0.2
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	7	0.2
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	7	0.2
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	17	0.2
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	17	0.2
(1,850)	2:B:486:ASP:H	2:B:487:THR:HG21	6	0.2
(1,850)	2:B:486:ASP:H	2:B:487:THR:HG22	6	0.2
(1,850)	2:B:486:ASP:H	2:B:487:THR:HG23	6	0.2
(1,724)	2:B:472:GLN:HA	2:B:472:GLN:HE21	7	0.2
(1,714)	2:B:471:LEU:HG	2:B:472:GLN:H	9	0.2
(1,1465)	1:A:122:ASP:HA	1:A:124:ALA:HA	20	0.2
(1,1427)	1:A:105:LEU:H	1:A:105:LEU:HG	6	0.2
(2,64)	1:A:152:ASN:HD22	1:A:153:GLU:H	1	0.19
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	1	0.19
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	1	0.19
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	10	0.19
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	10	0.19
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	20	0.19
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	20	0.19
(1,878)	2:B:490:ALA:HA	2:B:491:LYS:H	7	0.19
(1,724)	2:B:472:GLN:HA	2:B:472:GLN:HE21	9	0.19
(1,615)	1:A:152:ASN:H	1:A:152:ASN:HB3	9	0.19
(1,390)	1:A:125:LYS:HE2	1:A:126:LEU:H	19	0.19
(1,390)	1:A:125:LYS:HE3	1:A:126:LEU:H	19	0.19
(1,1860)	1:A:121:GLU:H	1:A:122:ASP:HB2	11	0.19
(1,1860)	1:A:121:GLU:H	1:A:122:ASP:HB3	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1536)	1:A:117:LEU:HD11	1:A:126:LEU:HB3	12	0.19
(1,1536)	1:A:117:LEU:HD12	1:A:126:LEU:HB3	12	0.19
(1,1536)	1:A:117:LEU:HD13	1:A:126:LEU:HB3	12	0.19
(1,1133)	1:A:117:LEU:HD11	1:A:127:MET:H	4	0.19
(1,1133)	1:A:117:LEU:HD12	1:A:127:MET:H	4	0.19
(1,1133)	1:A:117:LEU:HD13	1:A:127:MET:H	4	0.19
(1,989)	1:A:118:ASP:HA	2:B:478:ILE:HD11	2	0.18
(1,989)	1:A:118:ASP:HA	2:B:478:ILE:HD12	2	0.18
(1,989)	1:A:118:ASP:HA	2:B:478:ILE:HD13	2	0.18
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	3	0.18
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	3	0.18
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	9	0.18
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	9	0.18
(1,813)	2:B:479:LYS:HA	2:B:481:ASP:H	13	0.18
(1,626)	1:A:153:GLU:HA	1:A:154:GLU:H	11	0.18
(1,387)	1:A:125:LYS:HD2	1:A:126:LEU:H	2	0.18
(1,387)	1:A:125:LYS:HD3	1:A:126:LEU:H	2	0.18
(1,1977)	2:B:462:ASP:HB2	2:B:463:ILE:H	16	0.18
(1,1977)	2:B:462:ASP:HB3	2:B:463:ILE:H	16	0.18
(1,1972)	1:A:153:GLU:H	1:A:153:GLU:HB2	1	0.18
(1,1972)	1:A:153:GLU:H	1:A:153:GLU:HB3	1	0.18
(1,1497)	1:A:115:VAL:HA	2:B:478:ILE:HG12	8	0.18
(1,1309)	2:B:475:ARG:HA	2:B:475:ARG:HD2	8	0.18
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD1	13	0.17
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD2	13	0.17
(1,942)	1:A:109:HIS:HE1	1:A:113:LEU:HG	15	0.17
(1,868)	2:B:489:SER:HB2	2:B:490:ALA:H	14	0.17
(1,868)	2:B:489:SER:HB3	2:B:490:ALA:H	14	0.17
(1,813)	2:B:479:LYS:HA	2:B:481:ASP:H	5	0.17
(1,813)	2:B:479:LYS:HA	2:B:481:ASP:H	9	0.17
(1,780)	2:B:477:ILE:HD11	2:B:478:ILE:H	18	0.17
(1,780)	2:B:477:ILE:HD12	2:B:478:ILE:H	18	0.17
(1,780)	2:B:477:ILE:HD13	2:B:478:ILE:H	18	0.17
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	2	0.17
(1,714)	2:B:471:LEU:HG	2:B:472:GLN:H	15	0.17
(1,349)	1:A:117:LEU:HG	1:A:120:GLY:H	4	0.17
(1,1977)	2:B:462:ASP:HB2	2:B:463:ILE:H	15	0.17
(1,1977)	2:B:462:ASP:HB3	2:B:463:ILE:H	15	0.17
(1,1465)	1:A:122:ASP:HA	1:A:124:ALA:HA	11	0.17
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD1	3	0.16
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD2	3	0.16
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD1	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD2	8	0.16
(2,53)	1:A:136:PHE:HE1	2:B:474:VAL:H	6	0.16
(2,53)	1:A:136:PHE:HE2	2:B:474:VAL:H	6	0.16
(1,813)	2:B:479:LYS:HA	2:B:481:ASP:H	1	0.16
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE2	7	0.16
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE3	7	0.16
(1,763)	2:B:475:ARG:H	2:B:475:ARG:HE	16	0.16
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	18	0.16
(1,729)	2:B:472:GLN:HA	2:B:472:GLN:HE22	6	0.16
(1,627)	1:A:154:GLU:H	1:A:155:SER:H	9	0.16
(1,616)	1:A:151:GLN:HB2	1:A:152:ASN:H	15	0.16
(1,511)	1:A:104:LEU:HD11	1:A:139:PHE:H	12	0.16
(1,511)	1:A:104:LEU:HD12	1:A:139:PHE:H	12	0.16
(1,511)	1:A:104:LEU:HD13	1:A:139:PHE:H	12	0.16
(1,270)	1:A:113:LEU:H	1:A:113:LEU:HG	9	0.16
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD21	8	0.16
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD22	8	0.16
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD21	10	0.16
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD22	10	0.16
(1,2001)	2:B:467:ARG:H	2:B:467:ARG:HG2	4	0.16
(1,2001)	2:B:467:ARG:H	2:B:467:ARG:HG3	4	0.16
(1,1972)	1:A:153:GLU:H	1:A:153:GLU:HB2	3	0.16
(1,1972)	1:A:153:GLU:H	1:A:153:GLU:HB3	3	0.16
(1,1954)	1:A:147:VAL:H	1:A:149:PRO:HD2	16	0.16
(1,1954)	1:A:147:VAL:H	1:A:149:PRO:HD3	16	0.16
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	2	0.16
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	2	0.16
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG11	10	0.16
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG12	10	0.16
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG13	10	0.16
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG21	10	0.16
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG22	10	0.16
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG23	10	0.16
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG11	10	0.16
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG12	10	0.16
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG13	10	0.16
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG21	10	0.16
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG22	10	0.16
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG23	10	0.16
(1,1879)	1:A:123:LYS:HE2	1:A:124:ALA:HA	17	0.16
(1,1879)	1:A:123:LYS:HE3	1:A:124:ALA:HA	17	0.16
(1,1473)	2:B:468:ASN:HA	2:B:471:LEU:HD11	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1473)	2:B:468:ASN:HA	2:B:471:LEU:HD12	14	0.16
(1,1473)	2:B:468:ASN:HA	2:B:471:LEU:HD13	14	0.16
(1,1427)	1:A:105:LEU:H	1:A:105:LEU:HG	10	0.16
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD1	16	0.15
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD2	16	0.15
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD1	20	0.15
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD2	20	0.15
(2,55)	2:B:477:ILE:HD11	2:B:479:LYS:H	17	0.15
(2,55)	2:B:477:ILE:HD12	2:B:479:LYS:H	17	0.15
(2,55)	2:B:477:ILE:HD13	2:B:479:LYS:H	17	0.15
(2,27)	1:A:117:LEU:HA	1:A:126:LEU:H	2	0.15
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	8	0.15
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	8	0.15
(1,878)	2:B:490:ALA:HA	2:B:491:LYS:H	2	0.15
(1,813)	2:B:479:LYS:HA	2:B:481:ASP:H	7	0.15
(1,813)	2:B:479:LYS:HA	2:B:481:ASP:H	15	0.15
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE2	3	0.15
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE3	3	0.15
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE2	11	0.15
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE3	11	0.15
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	8	0.15
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	11	0.15
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	14	0.15
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	16	0.15
(1,714)	2:B:471:LEU:HG	2:B:472:GLN:H	14	0.15
(1,617)	1:A:151:GLN:HA	1:A:152:ASN:H	3	0.15
(1,42)	1:A:89:LEU:HB2	1:A:90:GLN:H	9	0.15
(1,42)	1:A:89:LEU:HB2	1:A:90:GLN:H	17	0.15
(1,349)	1:A:117:LEU:HG	1:A:120:GLY:H	12	0.15
(1,325)	1:A:118:ASP:H	2:B:478:ILE:HD11	8	0.15
(1,325)	1:A:118:ASP:H	2:B:478:ILE:HD12	8	0.15
(1,325)	1:A:118:ASP:H	2:B:478:ILE:HD13	8	0.15
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD21	6	0.15
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD22	6	0.15
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG11	6	0.15
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG12	6	0.15
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG13	6	0.15
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG21	6	0.15
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG22	6	0.15
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG23	6	0.15
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG11	6	0.15
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG12	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG13	6	0.15
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG21	6	0.15
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG22	6	0.15
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG23	6	0.15
(1,1977)	2:B:462:ASP:HB2	2:B:463:ILE:H	8	0.15
(1,1977)	2:B:462:ASP:HB3	2:B:463:ILE:H	8	0.15
(1,1970)	1:A:152:ASN:HB2	1:A:153:GLU:H	15	0.15
(1,1970)	1:A:152:ASN:HB3	1:A:153:GLU:H	15	0.15
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	5	0.15
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	5	0.15
(1,1683)	1:A:101:LEU:HD11	1:A:105:LEU:HG	16	0.15
(1,1683)	1:A:101:LEU:HD12	1:A:105:LEU:HG	16	0.15
(1,1683)	1:A:101:LEU:HD13	1:A:105:LEU:HG	16	0.15
(1,1683)	1:A:101:LEU:HD21	1:A:105:LEU:HG	16	0.15
(1,1683)	1:A:101:LEU:HD22	1:A:105:LEU:HG	16	0.15
(1,1683)	1:A:101:LEU:HD23	1:A:105:LEU:HG	16	0.15
(1,1678)	1:A:101:LEU:HD11	1:A:104:LEU:H	19	0.15
(1,1678)	1:A:101:LEU:HD12	1:A:104:LEU:H	19	0.15
(1,1678)	1:A:101:LEU:HD13	1:A:104:LEU:H	19	0.15
(1,1678)	1:A:101:LEU:HD21	1:A:104:LEU:H	19	0.15
(1,1678)	1:A:101:LEU:HD22	1:A:104:LEU:H	19	0.15
(1,1678)	1:A:101:LEU:HD23	1:A:104:LEU:H	19	0.15
(1,1602)	1:A:90:GLN:HG2	1:A:94:ASN:HD21	1	0.15
(1,1602)	1:A:90:GLN:HG3	1:A:94:ASN:HD21	1	0.15
(1,1546)	1:A:85:ASP:HB2	1:A:86:ARG:H	2	0.15
(1,1546)	1:A:85:ASP:HB3	1:A:86:ARG:H	2	0.15
(1,1473)	2:B:468:ASN:HA	2:B:471:LEU:HD11	9	0.15
(1,1473)	2:B:468:ASN:HA	2:B:471:LEU:HD12	9	0.15
(1,1473)	2:B:468:ASN:HA	2:B:471:LEU:HD13	9	0.15
(1,1427)	1:A:105:LEU:H	1:A:105:LEU:HG	12	0.15
(1,1255)	2:B:486:ASP:HA	2:B:487:THR:H	7	0.15
(1,1255)	2:B:486:ASP:HA	2:B:487:THR:H	12	0.15
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	6	0.15
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	6	0.15
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	6	0.15
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	12	0.15
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	12	0.15
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	12	0.15
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	19	0.15
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	19	0.15
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	19	0.15
(1,1063)	2:B:463:ILE:HG21	2:B:466:GLU:HB2	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1063)	2:B:463:ILE:HG21	2:B:466:GLU:HB3	13	0.15
(1,1063)	2:B:463:ILE:HG22	2:B:466:GLU:HB2	13	0.15
(1,1063)	2:B:463:ILE:HG22	2:B:466:GLU:HB3	13	0.15
(1,1063)	2:B:463:ILE:HG23	2:B:466:GLU:HB2	13	0.15
(1,1063)	2:B:463:ILE:HG23	2:B:466:GLU:HB3	13	0.15
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD1	2	0.14
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD2	2	0.14
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD1	10	0.14
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD2	10	0.14
(2,55)	2:B:477:ILE:HD11	2:B:479:LYS:H	8	0.14
(2,55)	2:B:477:ILE:HD12	2:B:479:LYS:H	8	0.14
(2,55)	2:B:477:ILE:HD13	2:B:479:LYS:H	8	0.14
(2,5)	1:A:94:ASN:HD21	1:A:95:LEU:HG	10	0.14
(2,5)	1:A:94:ASN:HD21	1:A:95:LEU:HG	16	0.14
(1,942)	1:A:109:HIS:HE1	1:A:113:LEU:HG	9	0.14
(1,919)	1:A:109:HIS:HD2	1:A:135:LEU:HG	2	0.14
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	13	0.14
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	13	0.14
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE1	16	0.14
(1,895)	1:A:126:LEU:HG	1:A:130:TYR:HE2	16	0.14
(1,878)	2:B:490:ALA:HA	2:B:491:LYS:H	16	0.14
(1,871)	2:B:490:ALA:HB1	2:B:491:LYS:H	11	0.14
(1,871)	2:B:490:ALA:HB2	2:B:491:LYS:H	11	0.14
(1,871)	2:B:490:ALA:HB3	2:B:491:LYS:H	11	0.14
(1,813)	2:B:479:LYS:HA	2:B:481:ASP:H	3	0.14
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE2	18	0.14
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE3	18	0.14
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	5	0.14
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	13	0.14
(1,627)	1:A:154:GLU:H	1:A:155:SER:H	17	0.14
(1,350)	1:A:120:GLY:H	1:A:123:LYS:HD2	18	0.14
(1,350)	1:A:120:GLY:H	1:A:123:LYS:HD3	18	0.14
(1,252)	1:A:111:ARG:H	1:A:111:ARG:HE	19	0.14
(1,236)	1:A:109:HIS:HD2	1:A:111:ARG:H	2	0.14
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD21	5	0.14
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD22	5	0.14
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD21	14	0.14
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD22	14	0.14
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD21	20	0.14
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD22	20	0.14
(1,2090)	2:B:487:THR:HB	2:B:488:ASN:HD21	4	0.14
(1,2090)	2:B:487:THR:HB	2:B:488:ASN:HD22	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2038)	2:B:472:GLN:HA	2:B:475:ARG:HB2	8	0.14
(1,2038)	2:B:472:GLN:HA	2:B:475:ARG:HB3	8	0.14
(1,1992)	2:B:465:HIS:HD2	2:B:466:GLU:HG2	13	0.14
(1,1992)	2:B:465:HIS:HD2	2:B:466:GLU:HG3	13	0.14
(1,1977)	2:B:462:ASP:HB2	2:B:463:ILE:H	20	0.14
(1,1977)	2:B:462:ASP:HB3	2:B:463:ILE:H	20	0.14
(1,1970)	1:A:152:ASN:HB2	1:A:153:GLU:H	11	0.14
(1,1970)	1:A:152:ASN:HB3	1:A:153:GLU:H	11	0.14
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	3	0.14
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	3	0.14
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	4	0.14
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	4	0.14
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	8	0.14
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	8	0.14
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	14	0.14
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	14	0.14
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	15	0.14
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	15	0.14
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG11	12	0.14
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG12	12	0.14
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG13	12	0.14
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG21	12	0.14
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG22	12	0.14
(1,1941)	1:A:139:PHE:HD1	2:B:474:VAL:HG23	12	0.14
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG11	12	0.14
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG12	12	0.14
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG13	12	0.14
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG21	12	0.14
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG22	12	0.14
(1,1941)	1:A:139:PHE:HD2	2:B:474:VAL:HG23	12	0.14
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD11	1	0.14
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD12	1	0.14
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD13	1	0.14
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD21	1	0.14
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD22	1	0.14
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD23	1	0.14
(1,1680)	1:A:101:LEU:HD11	1:A:104:LEU:HG	1	0.14
(1,1680)	1:A:101:LEU:HD12	1:A:104:LEU:HG	1	0.14
(1,1680)	1:A:101:LEU:HD13	1:A:104:LEU:HG	1	0.14
(1,1680)	1:A:101:LEU:HD21	1:A:104:LEU:HG	1	0.14
(1,1680)	1:A:101:LEU:HD22	1:A:104:LEU:HG	1	0.14
(1,1680)	1:A:101:LEU:HD23	1:A:104:LEU:HG	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1677)	1:A:101:LEU:HD11	1:A:102:ARG:HA	10	0.14
(1,1677)	1:A:101:LEU:HD12	1:A:102:ARG:HA	10	0.14
(1,1677)	1:A:101:LEU:HD13	1:A:102:ARG:HA	10	0.14
(1,1677)	1:A:101:LEU:HD21	1:A:102:ARG:HA	10	0.14
(1,1677)	1:A:101:LEU:HD22	1:A:102:ARG:HA	10	0.14
(1,1677)	1:A:101:LEU:HD23	1:A:102:ARG:HA	10	0.14
(1,167)	1:A:101:LEU:H	1:A:102:ARG:HG3	13	0.14
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD11	11	0.14
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD12	11	0.14
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD13	11	0.14
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD21	11	0.14
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD22	11	0.14
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD23	11	0.14
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD11	18	0.14
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD12	18	0.14
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD13	18	0.14
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD21	18	0.14
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD22	18	0.14
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD23	18	0.14
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	4	0.14
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	4	0.14
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	4	0.14
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	10	0.14
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	10	0.14
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	10	0.14
(2,63)	1:A:92:LEU:HB3	2:B:472:GLN:HA	6	0.13
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD1	6	0.13
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD2	6	0.13
(2,55)	2:B:477:ILE:HD11	2:B:479:LYS:H	3	0.13
(2,55)	2:B:477:ILE:HD12	2:B:479:LYS:H	3	0.13
(2,55)	2:B:477:ILE:HD13	2:B:479:LYS:H	3	0.13
(2,55)	2:B:477:ILE:HD11	2:B:479:LYS:H	20	0.13
(2,55)	2:B:477:ILE:HD12	2:B:479:LYS:H	20	0.13
(2,55)	2:B:477:ILE:HD13	2:B:479:LYS:H	20	0.13
(2,5)	1:A:94:ASN:HD21	1:A:95:LEU:HG	3	0.13
(2,5)	1:A:94:ASN:HD21	1:A:95:LEU:HG	9	0.13
(2,24)	1:A:116:ASN:HD22	1:A:117:LEU:H	12	0.13
(2,24)	1:A:116:ASN:HD22	1:A:117:LEU:H	20	0.13
(1,871)	2:B:490:ALA:HB1	2:B:491:LYS:H	20	0.13
(1,871)	2:B:490:ALA:HB2	2:B:491:LYS:H	20	0.13
(1,871)	2:B:490:ALA:HB3	2:B:491:LYS:H	20	0.13
(1,864)	2:B:488:ASN:H	2:B:489:SER:H	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,813)	2:B:479:LYS:HA	2:B:481:ASP:H	19	0.13
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE2	13	0.13
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE3	13	0.13
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD1	17	0.13
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD2	17	0.13
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD1	18	0.13
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD2	18	0.13
(1,746)	2:B:474:VAL:H	2:B:476:TYR:HD1	16	0.13
(1,746)	2:B:474:VAL:H	2:B:476:TYR:HD2	16	0.13
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	1	0.13
(1,655)	2:B:465:HIS:H	2:B:466:GLU:HB2	13	0.13
(1,655)	2:B:465:HIS:H	2:B:466:GLU:HB3	13	0.13
(1,481)	1:A:133:GLU:HG3	1:A:136:PHE:H	11	0.13
(1,425)	1:A:127:MET:HB2	1:A:130:TYR:H	16	0.13
(1,425)	1:A:127:MET:HB3	1:A:130:TYR:H	16	0.13
(1,252)	1:A:111:ARG:H	1:A:111:ARG:HE	16	0.13
(1,236)	1:A:109:HIS:HD2	1:A:111:ARG:H	17	0.13
(1,2090)	2:B:487:THR:HB	2:B:488:ASN:HD21	15	0.13
(1,2090)	2:B:487:THR:HB	2:B:488:ASN:HD22	15	0.13
(1,2001)	2:B:467:ARG:H	2:B:467:ARG:HG2	3	0.13
(1,2001)	2:B:467:ARG:H	2:B:467:ARG:HG3	3	0.13
(1,2001)	2:B:467:ARG:H	2:B:467:ARG:HG2	14	0.13
(1,2001)	2:B:467:ARG:H	2:B:467:ARG:HG3	14	0.13
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG11	2	0.13
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG12	2	0.13
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG13	2	0.13
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG21	2	0.13
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG22	2	0.13
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG23	2	0.13
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG11	2	0.13
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG12	2	0.13
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG13	2	0.13
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG21	2	0.13
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG22	2	0.13
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG23	2	0.13
(1,1966)	1:A:152:ASN:H	1:A:152:ASN:HB2	9	0.13
(1,1966)	1:A:152:ASN:H	1:A:152:ASN:HB3	9	0.13
(1,1964)	1:A:151:GLN:HB2	1:A:152:ASN:H	15	0.13
(1,1964)	1:A:151:GLN:HB3	1:A:152:ASN:H	15	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	6	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	6	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	9	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	11	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	11	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	12	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	12	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	13	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	13	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	18	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	18	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	20	0.13
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	20	0.13
(1,1860)	1:A:121:GLU:H	1:A:122:ASP:HB2	13	0.13
(1,1860)	1:A:121:GLU:H	1:A:122:ASP:HB3	13	0.13
(1,1678)	1:A:101:LEU:HD11	1:A:104:LEU:H	10	0.13
(1,1678)	1:A:101:LEU:HD12	1:A:104:LEU:H	10	0.13
(1,1678)	1:A:101:LEU:HD13	1:A:104:LEU:H	10	0.13
(1,1678)	1:A:101:LEU:HD21	1:A:104:LEU:H	10	0.13
(1,1678)	1:A:101:LEU:HD22	1:A:104:LEU:H	10	0.13
(1,1678)	1:A:101:LEU:HD23	1:A:104:LEU:H	10	0.13
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD11	12	0.13
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD12	12	0.13
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD13	12	0.13
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD21	12	0.13
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD22	12	0.13
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD23	12	0.13
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD11	14	0.13
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD12	14	0.13
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD13	14	0.13
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD21	14	0.13
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD22	14	0.13
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD23	14	0.13
(1,1484)	2:B:480:LYS:HA	2:B:480:LYS:HD2	17	0.13
(1,1484)	2:B:480:LYS:HA	2:B:480:LYS:HD3	17	0.13
(1,1465)	1:A:122:ASP:HA	1:A:124:ALA:HA	14	0.13
(1,1430)	1:A:110:LEU:H	1:A:110:LEU:HG	7	0.13
(1,1430)	1:A:110:LEU:H	1:A:110:LEU:HG	14	0.13
(1,1430)	1:A:110:LEU:H	1:A:110:LEU:HG	18	0.13
(1,1430)	1:A:110:LEU:H	1:A:110:LEU:HG	19	0.13
(1,1315)	2:B:469:VAL:H	2:B:471:LEU:HG	14	0.13
(1,1315)	2:B:469:VAL:H	2:B:471:LEU:HG	15	0.13
(1,1255)	2:B:486:ASP:HA	2:B:487:THR:H	5	0.13
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD11	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD12	12	0.13
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD13	12	0.13
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	2	0.13
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	2	0.13
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	2	0.13
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	15	0.13
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	15	0.13
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	15	0.13
(1,100)	1:A:91:ASN:HA	1:A:94:ASN:H	13	0.13
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD1	14	0.12
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD2	14	0.12
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD1	17	0.12
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD2	17	0.12
(2,55)	2:B:477:ILE:HD11	2:B:479:LYS:H	7	0.12
(2,55)	2:B:477:ILE:HD12	2:B:479:LYS:H	7	0.12
(2,55)	2:B:477:ILE:HD13	2:B:479:LYS:H	7	0.12
(2,55)	2:B:477:ILE:HD11	2:B:479:LYS:H	10	0.12
(2,55)	2:B:477:ILE:HD12	2:B:479:LYS:H	10	0.12
(2,55)	2:B:477:ILE:HD13	2:B:479:LYS:H	10	0.12
(2,55)	2:B:477:ILE:HD11	2:B:479:LYS:H	16	0.12
(2,55)	2:B:477:ILE:HD12	2:B:479:LYS:H	16	0.12
(2,55)	2:B:477:ILE:HD13	2:B:479:LYS:H	16	0.12
(2,27)	1:A:117:LEU:HA	1:A:126:LEU:H	19	0.12
(2,24)	1:A:116:ASN:HD22	1:A:117:LEU:H	17	0.12
(1,943)	2:B:465:HIS:HE1	2:B:469:VAL:HB	18	0.12
(1,919)	1:A:109:HIS:HD2	1:A:135:LEU:HG	3	0.12
(1,919)	1:A:109:HIS:HD2	1:A:135:LEU:HG	11	0.12
(1,871)	2:B:490:ALA:HB1	2:B:491:LYS:H	8	0.12
(1,871)	2:B:490:ALA:HB2	2:B:491:LYS:H	8	0.12
(1,871)	2:B:490:ALA:HB3	2:B:491:LYS:H	8	0.12
(1,871)	2:B:490:ALA:HB1	2:B:491:LYS:H	14	0.12
(1,871)	2:B:490:ALA:HB2	2:B:491:LYS:H	14	0.12
(1,871)	2:B:490:ALA:HB3	2:B:491:LYS:H	14	0.12
(1,864)	2:B:488:ASN:H	2:B:489:SER:H	6	0.12
(1,864)	2:B:488:ASN:H	2:B:489:SER:H	13	0.12
(1,864)	2:B:488:ASN:H	2:B:489:SER:H	19	0.12
(1,813)	2:B:479:LYS:HA	2:B:481:ASP:H	12	0.12
(1,813)	2:B:479:LYS:HA	2:B:481:ASP:H	16	0.12
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE2	14	0.12
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE3	14	0.12
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD1	11	0.12
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,746)	2:B:474:VAL:H	2:B:476:TYR:HD1	5	0.12
(1,746)	2:B:474:VAL:H	2:B:476:TYR:HD2	5	0.12
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	3	0.12
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	15	0.12
(1,64)	1:A:91:ASN:HD22	1:A:147:VAL:HA	12	0.12
(1,627)	1:A:154:GLU:H	1:A:155:SER:H	20	0.12
(1,626)	1:A:153:GLU:HA	1:A:154:GLU:H	13	0.12
(1,481)	1:A:133:GLU:HG3	1:A:136:PHE:H	14	0.12
(1,425)	1:A:127:MET:HB2	1:A:130:TYR:H	20	0.12
(1,425)	1:A:127:MET:HB3	1:A:130:TYR:H	20	0.12
(1,355)	1:A:118:ASP:H	1:A:120:GLY:H	4	0.12
(1,236)	1:A:109:HIS:HD2	1:A:111:ARG:H	3	0.12
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD21	13	0.12
(1,2093)	2:B:488:ASN:HB2	2:B:488:ASN:HD22	13	0.12
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG11	8	0.12
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG12	8	0.12
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG13	8	0.12
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG21	8	0.12
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG22	8	0.12
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG23	8	0.12
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG11	8	0.12
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG12	8	0.12
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG13	8	0.12
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG21	8	0.12
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG22	8	0.12
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG23	8	0.12
(1,1977)	2:B:462:ASP:HB2	2:B:463:ILE:H	17	0.12
(1,1977)	2:B:462:ASP:HB3	2:B:463:ILE:H	17	0.12
(1,1909)	1:A:131:MET:HE1	2:B:467:ARG:HD2	2	0.12
(1,1909)	1:A:131:MET:HE1	2:B:467:ARG:HD3	2	0.12
(1,1909)	1:A:131:MET:HE2	2:B:467:ARG:HD2	2	0.12
(1,1909)	1:A:131:MET:HE2	2:B:467:ARG:HD3	2	0.12
(1,1909)	1:A:131:MET:HE3	2:B:467:ARG:HD2	2	0.12
(1,1909)	1:A:131:MET:HE3	2:B:467:ARG:HD3	2	0.12
(1,1744)	1:A:108:PRO:HA	1:A:111:ARG:HB2	2	0.12
(1,1744)	1:A:108:PRO:HA	1:A:111:ARG:HB3	2	0.12
(1,1699)	1:A:103:SER:H	1:A:106:LEU:HD11	19	0.12
(1,1699)	1:A:103:SER:H	1:A:106:LEU:HD12	19	0.12
(1,1699)	1:A:103:SER:H	1:A:106:LEU:HD13	19	0.12
(1,1699)	1:A:103:SER:H	1:A:106:LEU:HD21	19	0.12
(1,1699)	1:A:103:SER:H	1:A:106:LEU:HD22	19	0.12
(1,1699)	1:A:103:SER:H	1:A:106:LEU:HD23	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD11	15	0.12
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD12	15	0.12
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD13	15	0.12
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD21	15	0.12
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD22	15	0.12
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD23	15	0.12
(1,1683)	1:A:101:LEU:HD11	1:A:105:LEU:HG	7	0.12
(1,1683)	1:A:101:LEU:HD12	1:A:105:LEU:HG	7	0.12
(1,1683)	1:A:101:LEU:HD13	1:A:105:LEU:HG	7	0.12
(1,1683)	1:A:101:LEU:HD21	1:A:105:LEU:HG	7	0.12
(1,1683)	1:A:101:LEU:HD22	1:A:105:LEU:HG	7	0.12
(1,1683)	1:A:101:LEU:HD23	1:A:105:LEU:HG	7	0.12
(1,167)	1:A:101:LEU:H	1:A:102:ARG:HG3	5	0.12
(1,1667)	1:A:97:GLU:HB2	1:A:98:SER:H	10	0.12
(1,1667)	1:A:97:GLU:HB3	1:A:98:SER:H	10	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD11	4	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD12	4	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD13	4	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD21	4	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD22	4	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD23	4	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD11	7	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD12	7	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD13	7	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD21	7	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD22	7	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD23	7	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD11	20	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD12	20	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD13	20	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD21	20	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD22	20	0.12
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD23	20	0.12
(1,1605)	1:A:91:ASN:HD21	2:B:469:VAL:HG11	18	0.12
(1,1605)	1:A:91:ASN:HD21	2:B:469:VAL:HG12	18	0.12
(1,1605)	1:A:91:ASN:HD21	2:B:469:VAL:HG13	18	0.12
(1,1605)	1:A:91:ASN:HD21	2:B:469:VAL:HG21	18	0.12
(1,1605)	1:A:91:ASN:HD21	2:B:469:VAL:HG22	18	0.12
(1,1605)	1:A:91:ASN:HD21	2:B:469:VAL:HG23	18	0.12
(1,1536)	1:A:117:LEU:HD11	1:A:126:LEU:HB3	4	0.12
(1,1536)	1:A:117:LEU:HD12	1:A:126:LEU:HB3	4	0.12
(1,1536)	1:A:117:LEU:HD13	1:A:126:LEU:HB3	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1484)	2:B:480:LYS:HA	2:B:480:LYS:HD2	5	0.12
(1,1484)	2:B:480:LYS:HA	2:B:480:LYS:HD3	5	0.12
(1,1484)	2:B:480:LYS:HA	2:B:480:LYS:HD2	20	0.12
(1,1484)	2:B:480:LYS:HA	2:B:480:LYS:HD3	20	0.12
(1,1465)	1:A:122:ASP:HA	1:A:124:ALA:HA	16	0.12
(1,1430)	1:A:110:LEU:H	1:A:110:LEU:HG	20	0.12
(1,1429)	1:A:125:LYS:H	1:A:125:LYS:HD2	5	0.12
(1,1429)	1:A:125:LYS:H	1:A:125:LYS:HD3	5	0.12
(1,1378)	2:B:476:TYR:HE1	2:B:480:LYS:HG2	8	0.12
(1,1378)	2:B:476:TYR:HE1	2:B:480:LYS:HG3	8	0.12
(1,1378)	2:B:476:TYR:HE2	2:B:480:LYS:HG2	8	0.12
(1,1378)	2:B:476:TYR:HE2	2:B:480:LYS:HG3	8	0.12
(1,1283)	2:B:479:LYS:HA	2:B:479:LYS:HD2	6	0.12
(1,1283)	2:B:479:LYS:HA	2:B:479:LYS:HD3	6	0.12
(1,1255)	2:B:486:ASP:HA	2:B:487:THR:H	20	0.12
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD11	11	0.12
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD12	11	0.12
(1,1240)	1:A:89:LEU:HA	1:A:89:LEU:HD13	11	0.12
(1,1209)	1:A:110:LEU:HA	1:A:113:LEU:HG	15	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	8	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	8	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	8	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	9	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	9	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	9	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	18	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	18	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	18	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	20	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	20	0.12
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	20	0.12
(1,1039)	1:A:114:MET:HE1	2:B:474:VAL:HA	17	0.12
(1,1039)	1:A:114:MET:HE2	2:B:474:VAL:HA	17	0.12
(1,1039)	1:A:114:MET:HE3	2:B:474:VAL:HA	17	0.12
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD1	9	0.11
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD2	9	0.11
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD1	11	0.11
(2,58)	1:A:116:ASN:HB3	1:A:130:TYR:HD2	11	0.11
(2,55)	2:B:477:ILE:HD11	2:B:479:LYS:H	2	0.11
(2,55)	2:B:477:ILE:HD12	2:B:479:LYS:H	2	0.11
(2,55)	2:B:477:ILE:HD13	2:B:479:LYS:H	2	0.11
(2,55)	2:B:477:ILE:HD11	2:B:479:LYS:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,55)	2:B:477:ILE:HD12	2:B:479:LYS:H	5	0.11
(2,55)	2:B:477:ILE:HD13	2:B:479:LYS:H	5	0.11
(2,55)	2:B:477:ILE:HD11	2:B:479:LYS:H	6	0.11
(2,55)	2:B:477:ILE:HD12	2:B:479:LYS:H	6	0.11
(2,55)	2:B:477:ILE:HD13	2:B:479:LYS:H	6	0.11
(2,55)	2:B:477:ILE:HD11	2:B:479:LYS:H	13	0.11
(2,55)	2:B:477:ILE:HD12	2:B:479:LYS:H	13	0.11
(2,55)	2:B:477:ILE:HD13	2:B:479:LYS:H	13	0.11
(2,55)	2:B:477:ILE:HD11	2:B:479:LYS:H	14	0.11
(2,55)	2:B:477:ILE:HD12	2:B:479:LYS:H	14	0.11
(2,55)	2:B:477:ILE:HD13	2:B:479:LYS:H	14	0.11
(2,27)	1:A:117:LEU:HA	1:A:126:LEU:H	4	0.11
(1,996)	1:A:96:GLY:H	2:B:477:ILE:HD11	19	0.11
(1,996)	1:A:96:GLY:H	2:B:477:ILE:HD12	19	0.11
(1,996)	1:A:96:GLY:H	2:B:477:ILE:HD13	19	0.11
(1,933)	2:B:463:ILE:HA	2:B:465:HIS:HD2	15	0.11
(1,919)	1:A:109:HIS:HD2	1:A:135:LEU:HG	17	0.11
(1,877)	2:B:491:LYS:H	2:B:492:SER:HB2	19	0.11
(1,877)	2:B:491:LYS:H	2:B:492:SER:HB3	19	0.11
(1,869)	2:B:489:SER:HA	2:B:490:ALA:H	15	0.11
(1,833)	2:B:483:PHE:H	2:B:485:LEU:H	5	0.11
(1,833)	2:B:483:PHE:H	2:B:485:LEU:H	11	0.11
(1,833)	2:B:483:PHE:H	2:B:485:LEU:H	14	0.11
(1,813)	2:B:479:LYS:HA	2:B:481:ASP:H	10	0.11
(1,813)	2:B:479:LYS:HA	2:B:481:ASP:H	18	0.11
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE2	16	0.11
(1,801)	2:B:479:LYS:H	2:B:479:LYS:HE3	16	0.11
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD1	1	0.11
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD2	1	0.11
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD1	10	0.11
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD2	10	0.11
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD1	16	0.11
(1,774)	2:B:476:TYR:H	2:B:476:TYR:HD2	16	0.11
(1,756)	2:B:474:VAL:HB	2:B:475:ARG:H	12	0.11
(1,739)	1:A:114:MET:HG2	2:B:474:VAL:H	19	0.11
(1,626)	1:A:153:GLU:HA	1:A:154:GLU:H	16	0.11
(1,545)	1:A:143:CYS:H	1:A:144:LEU:HD21	8	0.11
(1,545)	1:A:143:CYS:H	1:A:144:LEU:HD22	8	0.11
(1,545)	1:A:143:CYS:H	1:A:144:LEU:HD23	8	0.11
(1,545)	1:A:143:CYS:H	1:A:144:LEU:HD21	10	0.11
(1,545)	1:A:143:CYS:H	1:A:144:LEU:HD22	10	0.11
(1,545)	1:A:143:CYS:H	1:A:144:LEU:HD23	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,545)	1:A:143:CYS:H	1:A:144:LEU:HD21	11	0.11
(1,545)	1:A:143:CYS:H	1:A:144:LEU:HD22	11	0.11
(1,545)	1:A:143:CYS:H	1:A:144:LEU:HD23	11	0.11
(1,488)	1:A:136:PHE:H	1:A:138:GLU:H	6	0.11
(1,481)	1:A:133:GLU:HG3	1:A:136:PHE:H	13	0.11
(1,481)	1:A:133:GLU:HG3	1:A:136:PHE:H	16	0.11
(1,481)	1:A:133:GLU:HG3	1:A:136:PHE:H	17	0.11
(1,481)	1:A:133:GLU:HG3	1:A:136:PHE:H	18	0.11
(1,462)	1:A:133:GLU:H	1:A:135:LEU:H	1	0.11
(1,348)	1:A:119:GLN:H	1:A:119:GLN:HE21	6	0.11
(1,236)	1:A:109:HIS:HD2	1:A:111:ARG:H	8	0.11
(1,2084)	2:B:485:LEU:HD11	2:B:486:ASP:H	8	0.11
(1,2084)	2:B:485:LEU:HD12	2:B:486:ASP:H	8	0.11
(1,2084)	2:B:485:LEU:HD13	2:B:486:ASP:H	8	0.11
(1,2084)	2:B:485:LEU:HD21	2:B:486:ASP:H	8	0.11
(1,2084)	2:B:485:LEU:HD22	2:B:486:ASP:H	8	0.11
(1,2084)	2:B:485:LEU:HD23	2:B:486:ASP:H	8	0.11
(1,2079)	2:B:485:LEU:H	2:B:485:LEU:HD11	18	0.11
(1,2079)	2:B:485:LEU:H	2:B:485:LEU:HD12	18	0.11
(1,2079)	2:B:485:LEU:H	2:B:485:LEU:HD13	18	0.11
(1,2079)	2:B:485:LEU:H	2:B:485:LEU:HD21	18	0.11
(1,2079)	2:B:485:LEU:H	2:B:485:LEU:HD22	18	0.11
(1,2079)	2:B:485:LEU:H	2:B:485:LEU:HD23	18	0.11
(1,2061)	2:B:478:ILE:HB	2:B:484:GLY:HA2	17	0.11
(1,2061)	2:B:478:ILE:HB	2:B:484:GLY:HA3	17	0.11
(1,2001)	2:B:467:ARG:H	2:B:467:ARG:HG2	15	0.11
(1,2001)	2:B:467:ARG:H	2:B:467:ARG:HG3	15	0.11
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG11	20	0.11
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG12	20	0.11
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG13	20	0.11
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG21	20	0.11
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG22	20	0.11
(1,1998)	2:B:466:GLU:HB2	2:B:469:VAL:HG23	20	0.11
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG11	20	0.11
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG12	20	0.11
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG13	20	0.11
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG21	20	0.11
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG22	20	0.11
(1,1998)	2:B:466:GLU:HB3	2:B:469:VAL:HG23	20	0.11
(1,1977)	2:B:462:ASP:HB2	2:B:463:ILE:H	4	0.11
(1,1977)	2:B:462:ASP:HB3	2:B:463:ILE:H	4	0.11
(1,1977)	2:B:462:ASP:HB2	2:B:463:ILE:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1977)	2:B:462:ASP:HB3	2:B:463:ILE:H	9	0.11
(1,1977)	2:B:462:ASP:HB2	2:B:463:ILE:H	12	0.11
(1,1977)	2:B:462:ASP:HB3	2:B:463:ILE:H	12	0.11
(1,1970)	1:A:152:ASN:HB2	1:A:153:GLU:H	1	0.11
(1,1970)	1:A:152:ASN:HB3	1:A:153:GLU:H	1	0.11
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB2	7	0.11
(1,1946)	1:A:141:ASP:H	1:A:142:CYS:HB3	7	0.11
(1,1879)	1:A:123:LYS:HE2	1:A:124:ALA:HA	14	0.11
(1,1879)	1:A:123:LYS:HE3	1:A:124:ALA:HA	14	0.11
(1,1879)	1:A:123:LYS:HE2	1:A:124:ALA:HA	18	0.11
(1,1879)	1:A:123:LYS:HE3	1:A:124:ALA:HA	18	0.11
(1,1867)	1:A:122:ASP:HA	1:A:123:LYS:HE2	7	0.11
(1,1867)	1:A:122:ASP:HA	1:A:123:LYS:HE3	7	0.11
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD11	18	0.11
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD12	18	0.11
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD13	18	0.11
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD21	18	0.11
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD22	18	0.11
(1,1697)	1:A:102:ARG:HE	1:A:106:LEU:HD23	18	0.11
(1,1678)	1:A:101:LEU:HD11	1:A:104:LEU:H	6	0.11
(1,1678)	1:A:101:LEU:HD12	1:A:104:LEU:H	6	0.11
(1,1678)	1:A:101:LEU:HD13	1:A:104:LEU:H	6	0.11
(1,1678)	1:A:101:LEU:HD21	1:A:104:LEU:H	6	0.11
(1,1678)	1:A:101:LEU:HD22	1:A:104:LEU:H	6	0.11
(1,1678)	1:A:101:LEU:HD23	1:A:104:LEU:H	6	0.11
(1,1677)	1:A:101:LEU:HD11	1:A:102:ARG:HA	19	0.11
(1,1677)	1:A:101:LEU:HD12	1:A:102:ARG:HA	19	0.11
(1,1677)	1:A:101:LEU:HD13	1:A:102:ARG:HA	19	0.11
(1,1677)	1:A:101:LEU:HD21	1:A:102:ARG:HA	19	0.11
(1,1677)	1:A:101:LEU:HD22	1:A:102:ARG:HA	19	0.11
(1,1677)	1:A:101:LEU:HD23	1:A:102:ARG:HA	19	0.11
(1,167)	1:A:101:LEU:H	1:A:102:ARG:HG3	1	0.11
(1,1667)	1:A:97:GLU:HB2	1:A:98:SER:H	8	0.11
(1,1667)	1:A:97:GLU:HB3	1:A:98:SER:H	8	0.11
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD11	5	0.11
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD12	5	0.11
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD13	5	0.11
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD21	5	0.11
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD22	5	0.11
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD23	5	0.11
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD11	19	0.11
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD12	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD13	19	0.11
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD21	19	0.11
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD22	19	0.11
(1,1641)	1:A:95:LEU:HG	1:A:101:LEU:HD23	19	0.11
(1,1602)	1:A:90:GLN:HG2	1:A:94:ASN:HD21	12	0.11
(1,1602)	1:A:90:GLN:HG3	1:A:94:ASN:HD21	12	0.11
(1,1484)	2:B:480:LYS:HA	2:B:480:LYS:HD2	6	0.11
(1,1484)	2:B:480:LYS:HA	2:B:480:LYS:HD3	6	0.11
(1,1465)	1:A:122:ASP:HA	1:A:124:ALA:HA	12	0.11
(1,1449)	2:B:476:TYR:HD1	2:B:480:LYS:HE2	1	0.11
(1,1449)	2:B:476:TYR:HD1	2:B:480:LYS:HE3	1	0.11
(1,1449)	2:B:476:TYR:HD2	2:B:480:LYS:HE2	1	0.11
(1,1449)	2:B:476:TYR:HD2	2:B:480:LYS:HE3	1	0.11
(1,1430)	1:A:110:LEU:H	1:A:110:LEU:HG	4	0.11
(1,1430)	1:A:110:LEU:H	1:A:110:LEU:HG	5	0.11
(1,1430)	1:A:110:LEU:H	1:A:110:LEU:HG	6	0.11
(1,1430)	1:A:110:LEU:H	1:A:110:LEU:HG	9	0.11
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	3	0.11
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	3	0.11
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	3	0.11
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	11	0.11
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	11	0.11
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	11	0.11
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD11	14	0.11
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD12	14	0.11
(1,1159)	1:A:106:LEU:HA	1:A:106:LEU:HD13	14	0.11

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value