



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 06:02 PM UTC

PDB ID : 2LOW / pdb_00002low
BMRB ID : 18227
Title : Solution structure of AR55 in 50% HFIP
Authors : Langelaan, D.N.; Rainey, J.K.
Deposited on : 2012-01-27

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

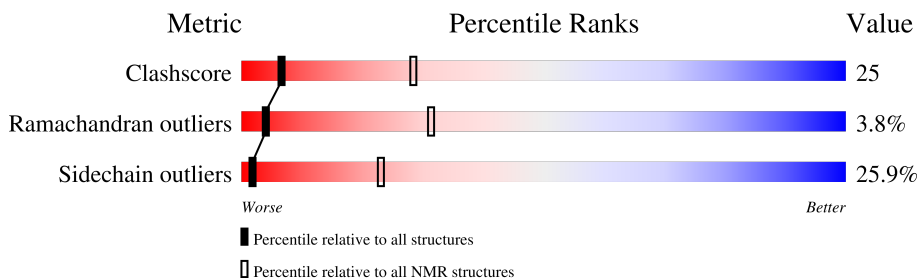
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	64	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 30%; height: 10px; background-color: #00FF00;"></div> <div style="width: 44%; height: 10px; background-color: #FFFF00;"></div> <div style="width: 27%; height: 10px; background-color: #00FFFF;"></div> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 30% 44% 27% </div>

2 Ensemble composition and analysis i

This entry contains 40 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *extended conformation*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:12-A:30 (19)	1.08	23
2	A:32-A:59 (28)	0.94	10

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

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

The models can be grouped into 6 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 6, 10, 11, 14, 19, 24, 27, 34, 36
2	9, 16, 18, 21, 22, 23, 25, 30, 39
3	3, 4, 5, 8, 13, 17, 31
4	2, 12, 20, 26, 28, 29
5	15, 40
6	37, 38
Single-model clusters	7; 32; 33; 35

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 988 atoms, of which 472 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apelin receptor.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	64	988	329	472	88	96	3	0

There are 9 discrepancies between the modelled and reference sequences:

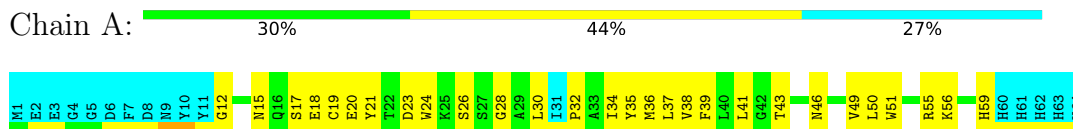
Chain	Residue	Modelled	Actual	Comment	Reference
A	56	LYS	-	expression tag	UNP P35414
A	57	LYS	-	expression tag	UNP P35414
A	58	GLY	-	expression tag	UNP P35414
A	59	HIS	-	expression tag	UNP P35414
A	60	HIS	-	expression tag	UNP P35414
A	61	HIS	-	expression tag	UNP P35414
A	62	HIS	-	expression tag	UNP P35414
A	63	HIS	-	expression tag	UNP P35414
A	64	HIS	-	expression tag	UNP P35414

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Apelin receptor

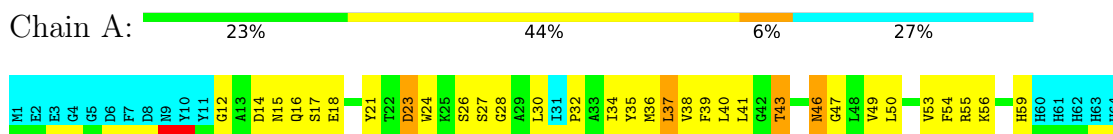


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

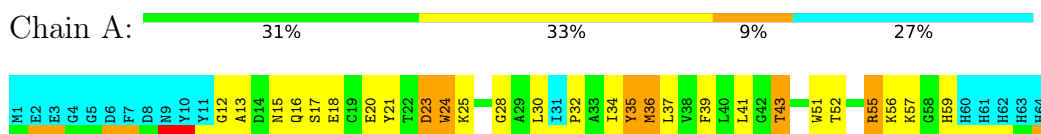
4.2.1 Score per residue for model 1

- Molecule 1: Apelin receptor



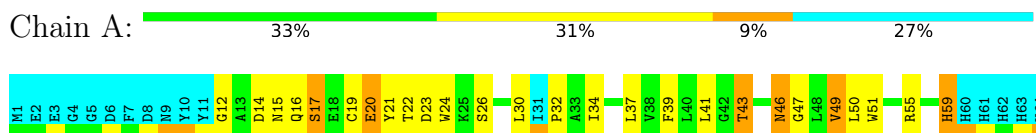
4.2.2 Score per residue for model 2

- Molecule 1: Apelin receptor



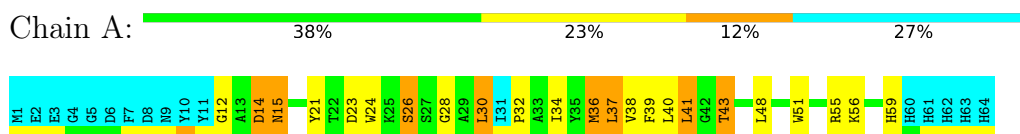
4.2.3 Score per residue for model 3

- Molecule 1: Apelin receptor



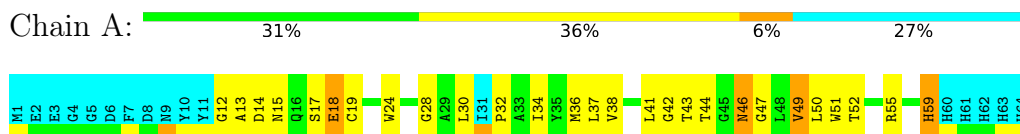
4.2.4 Score per residue for model 4

- Molecule 1: Apelin receptor



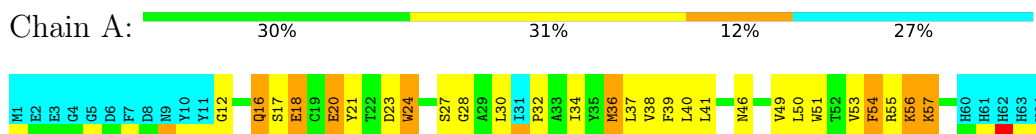
4.2.5 Score per residue for model 5

- Molecule 1: Apelin receptor



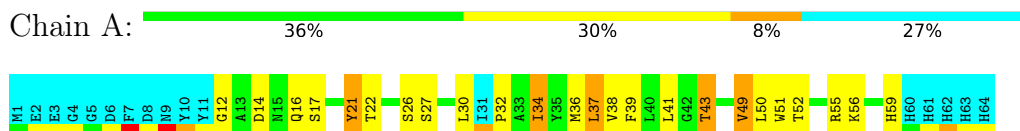
4.2.6 Score per residue for model 6

- Molecule 1: Apelin receptor



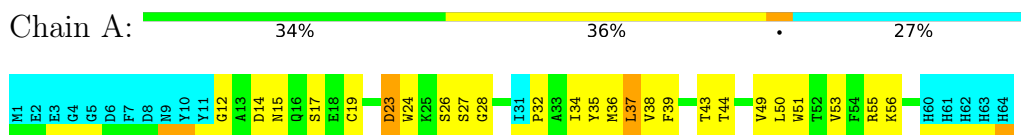
4.2.7 Score per residue for model 7

- Molecule 1: Apelin receptor



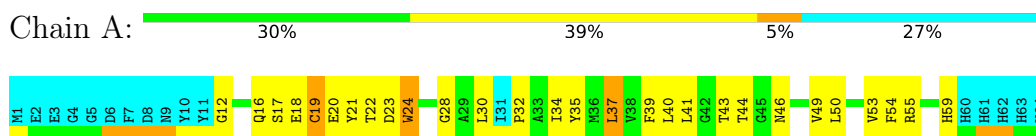
4.2.8 Score per residue for model 8

- Molecule 1: Apelin receptor



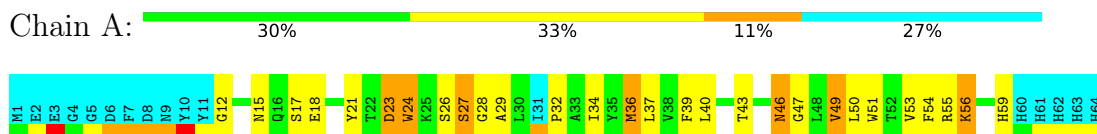
4.2.9 Score per residue for model 9

- Molecule 1: Apelin receptor



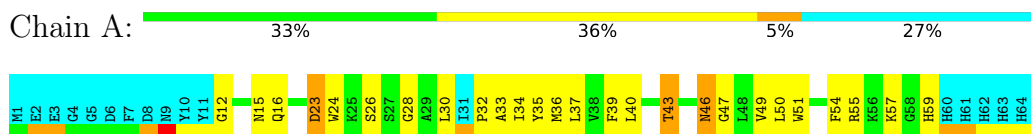
4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Apelin receptor



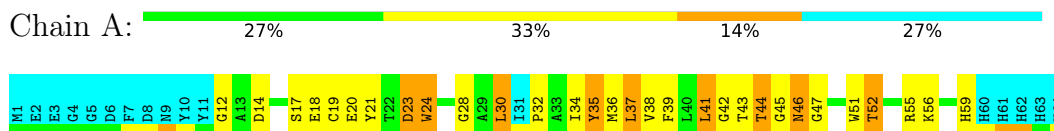
4.2.11 Score per residue for model 11

- Molecule 1: Apelin receptor



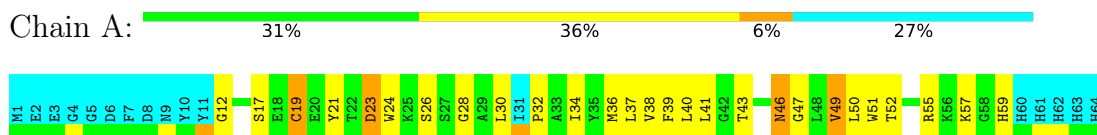
4.2.12 Score per residue for model 12

- Molecule 1: Apelin receptor



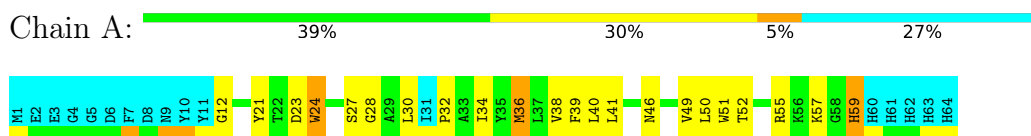
4.2.13 Score per residue for model 13

- Molecule 1: Apelin receptor



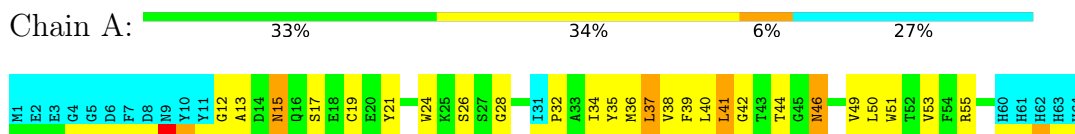
4.2.14 Score per residue for model 14

- Molecule 1: Apelin receptor



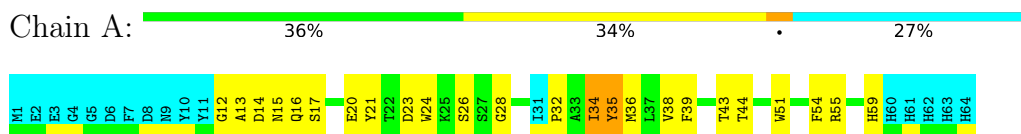
4.2.15 Score per residue for model 15

- Molecule 1: Apelin receptor



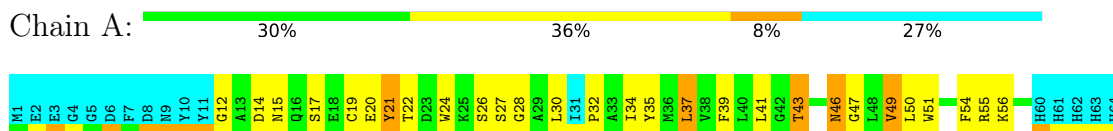
4.2.16 Score per residue for model 16

- Molecule 1: Apelin receptor



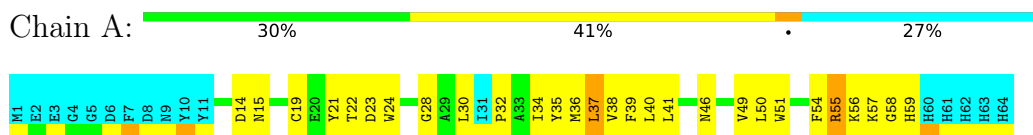
4.2.17 Score per residue for model 17

- Molecule 1: Apelin receptor



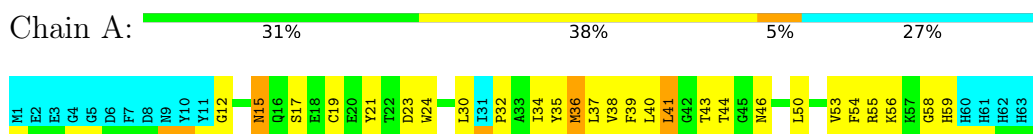
4.2.18 Score per residue for model 18

- Molecule 1: Apelin receptor



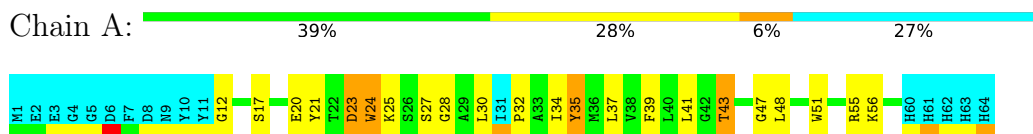
4.2.19 Score per residue for model 19

- Molecule 1: Apelin receptor



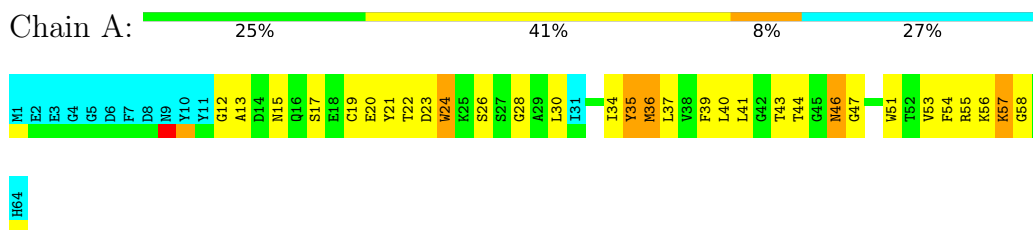
4.2.20 Score per residue for model 20

- Molecule 1: Apelin receptor



4.2.21 Score per residue for model 21

- Molecule 1: Apelin receptor



4.2.22 Score per residue for model 22

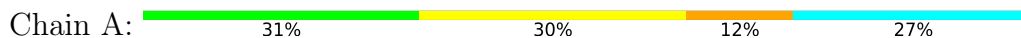
- Molecule 1: Apelin receptor





4.2.23 Score per residue for model 23

- Molecule 1: Apelin receptor



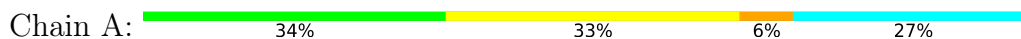
4.2.24 Score per residue for model 24

- Molecule 1: Apelin receptor



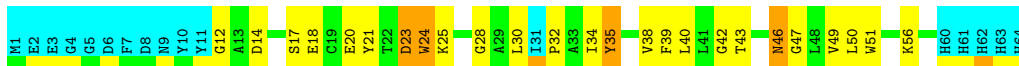
4.2.25 Score per residue for model 25

- Molecule 1: Apelin receptor



4.2.26 Score per residue for model 26

- Molecule 1: Apelin receptor



4.2.27 Score per residue for model 27

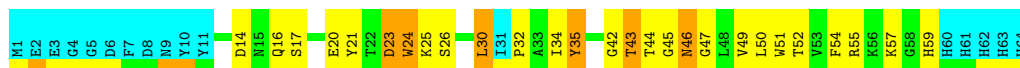
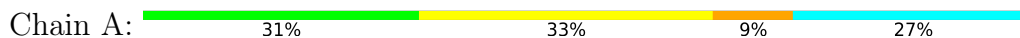
- Molecule 1: Apelin receptor





4.2.28 Score per residue for model 28

- Molecule 1: Apelin receptor



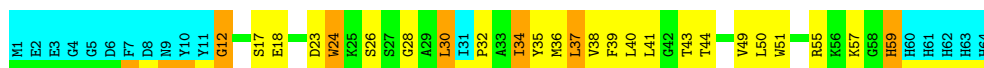
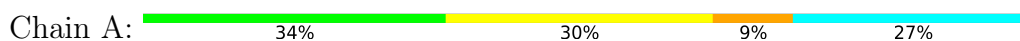
4.2.29 Score per residue for model 29

- Molecule 1: Apelin receptor



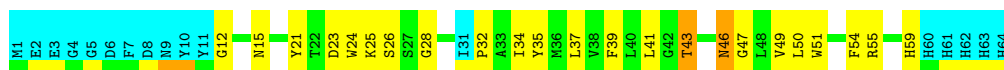
4.2.30 Score per residue for model 30

- Molecule 1: Apelin receptor



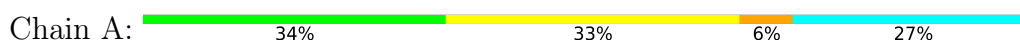
4.2.31 Score per residue for model 31

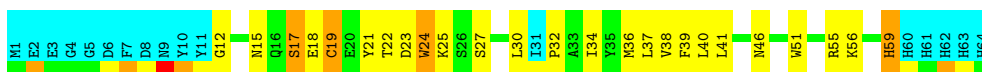
- Molecule 1: Apelin receptor



4.2.32 Score per residue for model 32

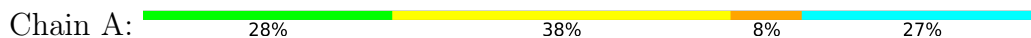
- Molecule 1: Apelin receptor





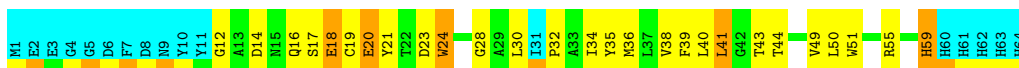
4.2.33 Score per residue for model 33

- Molecule 1: Apelin receptor



4.2.34 Score per residue for model 34

- Molecule 1: Apelin receptor



4.2.35 Score per residue for model 35

- Molecule 1: Apelin receptor



4.2.36 Score per residue for model 36

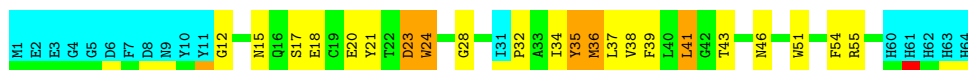
- Molecule 1: Apelin receptor



4.2.37 Score per residue for model 37

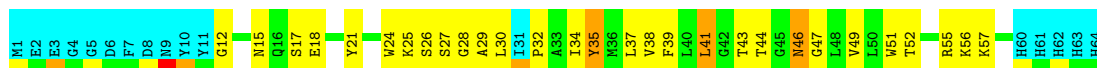
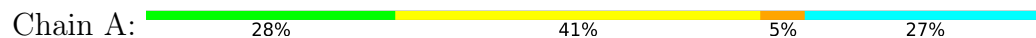
- Molecule 1: Apelin receptor





4.2.38 Score per residue for model 38

- Molecule 1: Apelin receptor



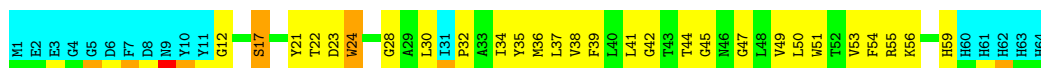
4.2.39 Score per residue for model 39

- Molecule 1: Apelin receptor



4.2.40 Score per residue for model 40

- Molecule 1: Apelin receptor



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 40 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	741
Number of shifts mapped to atoms	741
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

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	364	356	356	18±4
All	All	14560	14240	14240	717

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:HD12	1:A:41:LEU:O	0.79	1.77	38	6
1:A:37:LEU:O	1:A:41:LEU:HD12	0.71	1.85	1	16
1:A:41:LEU:HD12	1:A:41:LEU:C	0.67	2.15	37	7
1:A:40:LEU:C	1:A:40:LEU:HD12	0.66	2.16	30	1
1:A:43:THR:HG22	1:A:43:THR:O	0.65	1.90	34	2
1:A:38:VAL:HG12	1:A:38:VAL:O	0.64	1.92	38	16
1:A:51:TRP:CD1	1:A:55:ARG:NH2	0.64	2.66	34	19
1:A:59:HIS:O	1:A:59:HIS:CG	0.63	2.50	39	1
1:A:51:TRP:CZ2	1:A:55:ARG:NE	0.62	2.68	12	5
1:A:51:TRP:CH2	1:A:55:ARG:NE	0.62	2.68	20	9
1:A:24:TRP:CE3	1:A:25:LYS:N	0.62	2.68	33	8
1:A:38:VAL:O	1:A:38:VAL:HG12	0.62	1.93	16	7
1:A:46:ASN:ND2	1:A:47:GLY:N	0.61	2.48	31	14
1:A:46:ASN:HD22	1:A:46:ASN:N	0.58	1.95	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:TRP:CZ2	1:A:55:ARG:NH1	0.57	2.73	36	1
1:A:51:TRP:CH2	1:A:55:ARG:CZ	0.57	2.88	8	7
1:A:35:TYR:O	1:A:39:PHE:N	0.55	2.40	38	19
1:A:51:TRP:CE2	1:A:55:ARG:NE	0.54	2.75	5	16
1:A:50:LEU:O	1:A:54:PHE:CD1	0.54	2.60	36	5
1:A:36:MET:SD	1:A:36:MET:N	0.54	2.80	2	3
1:A:42:GLY:O	1:A:46:ASN:N	0.54	2.40	28	4
1:A:42:GLY:C	1:A:44:THR:N	0.54	2.66	12	5
1:A:17:SER:O	1:A:21:TYR:N	0.54	2.41	37	16
1:A:51:TRP:O	1:A:55:ARG:NE	0.54	2.41	31	11
1:A:21:TYR:CD1	1:A:22:THR:N	0.53	2.77	17	2
1:A:23:ASP:O	1:A:27:SER:N	0.53	2.41	32	3
1:A:18:GLU:O	1:A:21:TYR:N	0.53	2.42	23	6
1:A:24:TRP:O	1:A:28:GLY:N	0.53	2.42	11	32
1:A:42:GLY:O	1:A:46:ASN:ND2	0.53	2.42	26	1
1:A:46:ASN:CG	1:A:47:GLY:N	0.53	2.68	38	15
1:A:56:LYS:O	1:A:59:HIS:ND1	0.53	2.42	18	1
1:A:14:ASP:OD1	1:A:15:ASN:N	0.52	2.42	23	3
1:A:41:LEU:O	1:A:46:ASN:ND2	0.52	2.43	6	8
1:A:41:LEU:HD12	1:A:42:GLY:N	0.52	2.19	40	1
1:A:17:SER:O	1:A:20:GLU:N	0.52	2.43	34	10
1:A:51:TRP:CZ2	1:A:55:ARG:CZ	0.52	2.93	36	1
1:A:45:GLY:C	1:A:46:ASN:ND2	0.52	2.67	35	1
1:A:51:TRP:O	1:A:55:ARG:NH2	0.52	2.42	18	2
1:A:36:MET:C	1:A:38:VAL:N	0.52	2.68	30	8
1:A:53:VAL:C	1:A:55:ARG:N	0.52	2.68	6	9
1:A:17:SER:C	1:A:19:CYS:N	0.52	2.68	8	16
1:A:14:ASP:O	1:A:17:SER:N	0.51	2.42	33	6
1:A:14:ASP:OD1	1:A:14:ASP:N	0.51	2.44	28	3
1:A:41:LEU:C	1:A:41:LEU:CD1	0.51	2.82	37	6
1:A:51:TRP:CD1	1:A:55:ARG:HH21	0.51	2.23	31	18
1:A:39:PHE:O	1:A:43:THR:N	0.51	2.43	11	2
1:A:55:ARG:HE	1:A:55:ARG:N	0.51	2.03	23	2
1:A:42:GLY:O	1:A:44:THR:N	0.51	2.43	12	4
1:A:59:HIS:CD2	1:A:59:HIS:C	0.51	2.89	18	2
1:A:15:ASN:C	1:A:15:ASN:ND2	0.51	2.68	19	1
1:A:21:TYR:C	1:A:21:TYR:CD1	0.51	2.89	32	19
1:A:34:ILE:HD12	1:A:34:ILE:N	0.50	2.21	33	7
1:A:34:ILE:N	1:A:34:ILE:CD1	0.50	2.74	33	7
1:A:14:ASP:C	1:A:16:GLN:N	0.50	2.69	7	7
1:A:55:ARG:O	1:A:59:HIS:ND1	0.50	2.42	32	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:GLY:O	1:A:51:TRP:N	0.50	2.44	20	3
1:A:23:ASP:O	1:A:26:SER:N	0.50	2.45	10	7
1:A:21:TYR:CD1	1:A:21:TYR:C	0.50	2.88	17	7
1:A:20:GLU:CD	1:A:20:GLU:N	0.50	2.69	22	1
1:A:59:HIS:O	1:A:59:HIS:CD2	0.50	2.64	39	1
1:A:56:LYS:O	1:A:59:HIS:CE1	0.50	2.65	18	1
1:A:53:VAL:O	1:A:57:LYS:N	0.50	2.45	23	2
1:A:36:MET:O	1:A:39:PHE:N	0.49	2.44	30	12
1:A:24:TRP:CD2	1:A:24:TRP:C	0.49	2.89	33	2
1:A:55:ARG:HE	1:A:55:ARG:CA	0.49	2.19	23	2
1:A:38:VAL:O	1:A:38:VAL:CG1	0.48	2.62	16	16
1:A:42:GLY:C	1:A:44:THR:H	0.48	2.15	35	5
1:A:43:THR:O	1:A:43:THR:CG2	0.48	2.62	34	3
1:A:37:LEU:O	1:A:41:LEU:CB	0.48	2.62	36	1
1:A:28:GLY:O	1:A:32:PRO:CD	0.48	2.62	33	1
1:A:36:MET:O	1:A:38:VAL:N	0.47	2.47	30	3
1:A:37:LEU:O	1:A:41:LEU:CD2	0.47	2.62	40	1
1:A:51:TRP:CH2	1:A:55:ARG:NH2	0.47	2.83	2	4
1:A:20:GLU:CG	1:A:20:GLU:O	0.47	2.61	26	1
1:A:20:GLU:O	1:A:24:TRP:N	0.47	2.48	33	4
1:A:53:VAL:C	1:A:55:ARG:H	0.47	2.18	27	7
1:A:53:VAL:O	1:A:56:LYS:N	0.47	2.48	19	6
1:A:27:SER:C	1:A:29:ALA:N	0.47	2.72	38	2
1:A:32:PRO:O	1:A:36:MET:SD	0.47	2.73	35	3
1:A:36:MET:C	1:A:38:VAL:H	0.47	2.18	8	3
1:A:51:TRP:CG	1:A:55:ARG:HH21	0.47	2.28	18	1
1:A:34:ILE:CD1	1:A:34:ILE:N	0.46	2.77	25	1
1:A:34:ILE:N	1:A:34:ILE:HD12	0.46	2.23	25	1
1:A:52:THR:O	1:A:56:LYS:N	0.46	2.48	12	3
1:A:39:PHE:CZ	1:A:43:THR:HG21	0.46	2.45	26	1
1:A:45:GLY:O	1:A:46:ASN:ND2	0.46	2.49	35	1
1:A:36:MET:N	1:A:36:MET:SD	0.46	2.88	24	4
1:A:28:GLY:O	1:A:32:PRO:CG	0.46	2.64	37	1
1:A:17:SER:O	1:A:19:CYS:N	0.45	2.50	34	7
1:A:42:GLY:O	1:A:45:GLY:N	0.45	2.49	12	2
1:A:16:GLN:HE21	1:A:16:GLN:C	0.45	2.18	25	1
1:A:17:SER:C	1:A:19:CYS:H	0.45	2.19	3	7
1:A:53:VAL:O	1:A:55:ARG:N	0.45	2.49	6	6
1:A:27:SER:C	1:A:29:ALA:H	0.45	2.19	38	2
1:A:39:PHE:O	1:A:43:THR:CB	0.45	2.65	31	9
1:A:49:VAL:C	1:A:51:TRP:N	0.45	2.74	10	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:GLU:C	1:A:20:GLU:N	0.45	2.74	23	2
1:A:24:TRP:C	1:A:26:SER:N	0.45	2.74	38	3
1:A:16:GLN:HE21	1:A:16:GLN:H	0.45	1.54	6	1
1:A:39:PHE:C	1:A:41:LEU:H	0.44	2.20	20	8
1:A:20:GLU:O	1:A:23:ASP:N	0.44	2.48	20	3
1:A:46:ASN:N	1:A:46:ASN:ND2	0.44	2.62	15	1
1:A:39:PHE:CD1	1:A:39:PHE:C	0.44	2.94	24	2
1:A:39:PHE:O	1:A:43:THR:OG1	0.44	2.36	35	2
1:A:14:ASP:O	1:A:16:GLN:N	0.44	2.51	7	2
1:A:17:SER:OG	1:A:18:GLU:N	0.43	2.51	30	2
1:A:16:GLN:HE21	1:A:16:GLN:N	0.43	2.12	6	1
1:A:34:ILE:O	1:A:35:TYR:C	0.43	2.62	34	13
1:A:35:TYR:O	1:A:38:VAL:N	0.43	2.51	35	1
1:A:44:THR:CG2	1:A:45:GLY:N	0.43	2.82	40	1
1:A:49:VAL:HG12	1:A:50:LEU:N	0.43	2.28	3	23
1:A:23:ASP:O	1:A:24:TRP:C	0.43	2.60	2	16
1:A:55:ARG:CA	1:A:55:ARG:NE	0.43	2.82	23	1
1:A:16:GLN:O	1:A:20:GLU:OE1	0.43	2.37	22	1
1:A:17:SER:O	1:A:18:GLU:C	0.42	2.62	12	6
1:A:17:SER:O	1:A:21:TYR:CB	0.42	2.68	38	1
1:A:49:VAL:O	1:A:50:LEU:C	0.42	2.62	25	11
1:A:24:TRP:CD2	1:A:25:LYS:N	0.42	2.87	26	5
1:A:42:GLY:O	1:A:46:ASN:CG	0.42	2.62	36	1
1:A:39:PHE:C	1:A:41:LEU:N	0.42	2.78	24	7
1:A:24:TRP:O	1:A:25:LYS:C	0.42	2.63	38	1
1:A:20:GLU:O	1:A:20:GLU:OE1	0.42	2.37	3	1
1:A:18:GLU:O	1:A:18:GLU:OE1	0.42	2.37	5	1
1:A:43:THR:O	1:A:43:THR:HG22	0.42	2.14	28	1
1:A:40:LEU:O	1:A:44:THR:OG1	0.42	2.37	19	6
1:A:58:GLY:O	1:A:59:HIS:C	0.42	2.63	18	1
1:A:18:GLU:O	1:A:19:CYS:C	0.42	2.62	23	2
1:A:35:TYR:O	1:A:36:MET:C	0.42	2.62	35	2
1:A:16:GLN:CG	1:A:17:SER:N	0.42	2.82	23	1
1:A:18:GLU:O	1:A:20:GLU:N	0.42	2.52	23	1
1:A:14:ASP:C	1:A:16:GLN:H	0.42	2.23	3	1
1:A:47:GLY:O	1:A:51:TRP:CB	0.42	2.68	28	2
1:A:13:ALA:O	1:A:16:GLN:OE1	0.42	2.38	36	1
1:A:24:TRP:C	1:A:24:TRP:CD2	0.41	2.94	35	1
1:A:20:GLU:OE1	1:A:20:GLU:C	0.41	2.63	3	1
1:A:24:TRP:O	1:A:28:GLY:CA	0.41	2.68	10	1
1:A:37:LEU:O	1:A:41:LEU:N	0.41	2.50	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:GLU:CD	1:A:20:GLU:C	0.41	2.88	21	1
1:A:24:TRP:CE3	1:A:25:LYS:CA	0.41	3.03	33	3
1:A:49:VAL:O	1:A:51:TRP:N	0.41	2.54	34	2
1:A:36:MET:O	1:A:40:LEU:CD2	0.41	2.69	33	1
1:A:34:ILE:O	1:A:38:VAL:HG23	0.41	2.15	7	1
1:A:40:LEU:C	1:A:40:LEU:CD1	0.41	2.87	30	1
1:A:15:ASN:OD1	1:A:18:GLU:OE2	0.41	2.39	1	1
1:A:21:TYR:C	1:A:23:ASP:H	0.41	2.24	21	1
1:A:16:GLN:CD	1:A:16:GLN:C	0.41	2.88	27	1
1:A:24:TRP:O	1:A:26:SER:N	0.41	2.54	38	1
1:A:59:HIS:O	1:A:59:HIS:ND1	0.40	2.54	5	1
1:A:19:CYS:O	1:A:23:ASP:OD2	0.40	2.40	32	1
1:A:57:LYS:CB	1:A:57:LYS:NZ	0.40	2.84	6	1
1:A:14:ASP:N	1:A:14:ASP:OD1	0.40	2.53	8	1
1:A:50:LEU:O	1:A:54:PHE:CG	0.40	2.74	36	1
1:A:46:ASN:OD1	1:A:50:LEU:HD12	0.40	2.17	1	1
1:A:23:ASP:OD1	1:A:24:TRP:N	0.40	2.55	27	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	47/64 (73%)	37±2 (78±4%)	8±2 (18±4%)	2±1 (4±2%)	4	31
All	All	1880/2560 (73%)	1474 (78%)	335 (18%)	71 (4%)	4	31

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	12	GLY	34
1	A	30	LEU	14
1	A	49	VAL	7
1	A	18	GLU	6
1	A	43	THR	4

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Mol	Chain	Res	Type	Models (Total)
1	A	37	LEU	2
1	A	54	PHE	1
1	A	33	ALA	1
1	A	42	GLY	1
1	A	59	HIS	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	38/53 (72%)	28±2 (74±5%)	10±2 (26±5%)	2 23
All	All	1520/2120 (72%)	1126 (74%)	394 (26%)	2 23

All 31 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	59	HIS	28
1	A	23	ASP	27
1	A	30	LEU	26
1	A	43	THR	26
1	A	34	ILE	24
1	A	24	TRP	22
1	A	37	LEU	21
1	A	35	TYR	21
1	A	36	MET	21
1	A	15	ASN	20
1	A	46	ASN	18
1	A	56	LYS	15
1	A	41	LEU	13
1	A	40	LEU	12
1	A	57	LYS	12
1	A	26	SER	12
1	A	27	SER	11
1	A	54	PHE	10
1	A	22	THR	7
1	A	52	THR	7

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Mol	Chain	Res	Type	Models (Total)
1	A	16	GLN	6
1	A	44	THR	6
1	A	55	ARG	5
1	A	20	GLU	5
1	A	19	CYS	5
1	A	17	SER	4
1	A	21	TYR	3
1	A	14	ASP	3
1	A	48	LEU	2
1	A	18	GLU	1
1	A	25	LYS	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 oligosaccharides 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 91% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	741
Number of shifts mapped to atoms	741
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 \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	64	-1.19 ± 0.23	Should be checked
$^{13}\text{C}_\beta$	56	0.98 ± 0.16	Should be checked
$^{13}\text{C}'$	64	-0.80 ± 0.09	Should be applied
^{15}N	62	0.89 ± 0.31	Should be applied

7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 567 atoms were assigned a chemical shift out of a possible 620. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	236/239 (99%)	96/99 (97%)	94/94 (100%)	46/46 (100%)
Sidechain	281/312 (90%)	186/205 (91%)	90/98 (92%)	5/9 (56%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	50/69 (72%)	27/34 (79%)	21/32 (66%)	2/3 (67%)
Overall	567/620 (91%)	309/338 (91%)	205/224 (92%)	53/58 (91%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 741 atoms were assigned a chemical shift out of a possible 846. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	320/326 (98%)	130/135 (96%)	128/128 (100%)	62/63 (98%)
Sidechain	347/388 (89%)	229/253 (91%)	112/125 (90%)	6/10 (60%)
Aromatic	74/132 (56%)	41/67 (61%)	31/57 (54%)	2/8 (25%)
Overall	741/846 (88%)	400/455 (88%)	271/310 (87%)	70/81 (86%)

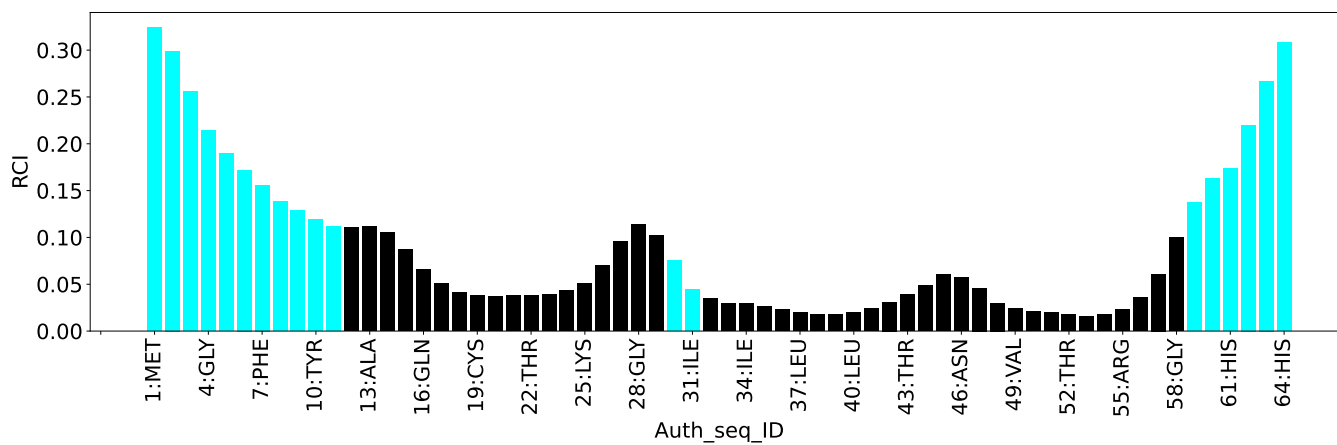
7.1.4 Statistically unusual chemical shifts [i](#)

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:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2439
Intra-residue ($ i-j =0$)	1131
Sequential ($ i-j =1$)	601
Medium range ($ i-j >1$ and $ i-j <5$)	700
Long range ($ i-j \geq 5$)	7
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	38.1
Number of long range restraints per residue ¹	0.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	10.9	0.2
0.2-0.5 (Medium)	20.3	0.5
>0.5 (Large)	16.6	1.99

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis [i](#)

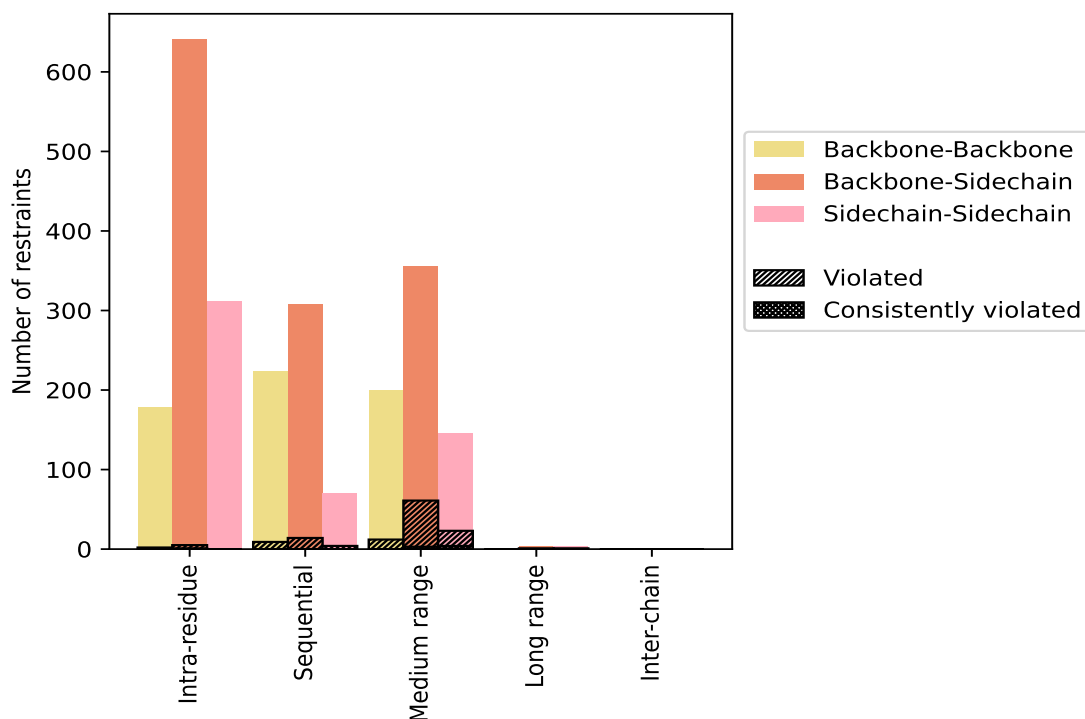
9.1 Summary of distance violations [i](#)

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1131	46.4	7	0.6	0.3	1	0.1	0.0
Backbone-Backbone	178	7.3	2	1.1	0.1	0	0.0	0.0
Backbone-Sidechain	641	26.3	5	0.8	0.2	1	0.2	0.0
Sidechain-Sidechain	312	12.8	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	601	24.6	27	4.5	1.1	0	0.0	0.0
Backbone-Backbone	223	9.1	9	4.0	0.4	0	0.0	0.0
Backbone-Sidechain	308	12.6	14	4.5	0.6	0	0.0	0.0
Sidechain-Sidechain	70	2.9	4	5.7	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	700	28.7	96	13.7	3.9	7	1.0	0.3
Backbone-Backbone	200	8.2	12	6.0	0.5	0	0.0	0.0
Backbone-Sidechain	355	14.6	61	17.2	2.5	3	0.8	0.1
Sidechain-Sidechain	145	5.9	23	15.9	0.9	4	2.8	0.2
Long range ($i-j \geq 5$)	7	0.3	2	28.6	0.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	3	0.1	1	33.3	0.0	0	0.0	0.0
Sidechain-Sidechain	4	0.2	1	25.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2439	100.0	132	5.4	5.4	8	0.3	0.3
Backbone-Backbone	601	24.6	23	3.8	0.9	0	0.0	0.0
Backbone-Sidechain	1307	53.6	81	6.2	3.3	4	0.3	0.2
Sidechain-Sidechain	531	21.8	28	5.3	1.1	4	0.8	0.2

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

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



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

9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	7	15	31	0	0	53	0.45	1.62	0.31	0.39
2	3	13	27	0	0	43	0.45	1.09	0.28	0.39
3	6	12	32	0	0	50	0.47	1.66	0.32	0.42
4	4	9	32	0	0	45	0.4	1.07	0.27	0.32
5	4	16	36	0	0	56	0.51	1.68	0.33	0.4
6	5	15	34	0	0	54	0.49	1.87	0.36	0.4
7	4	12	26	0	0	42	0.44	1.2	0.3	0.34
8	4	11	23	0	0	38	0.49	1.97	0.43	0.35
9	6	10	31	0	0	47	0.42	1.68	0.34	0.32
10	4	13	26	0	0	43	0.5	1.78	0.33	0.45

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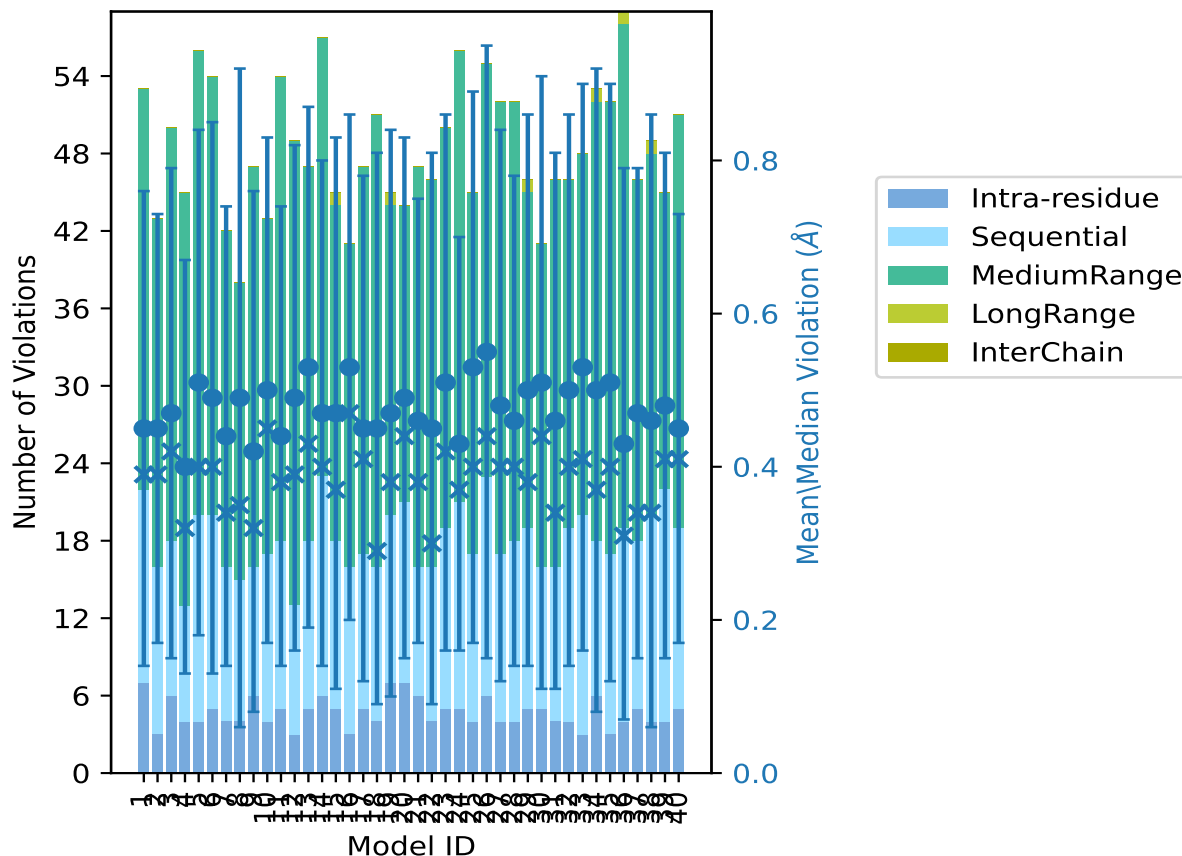
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	5	13	36	0	0	54	0.44	1.33	0.3	0.38
12	3	10	36	0	0	49	0.49	1.56	0.33	0.39
13	5	13	29	0	0	47	0.53	1.62	0.34	0.43
14	6	17	34	0	0	57	0.47	1.76	0.33	0.4
15	5	13	26	1	0	45	0.47	1.63	0.36	0.37
16	3	13	25	0	0	41	0.53	1.57	0.33	0.47
17	5	12	30	0	0	47	0.45	1.7	0.33	0.41
18	4	12	35	0	0	51	0.45	1.68	0.36	0.29
19	7	13	24	1	0	45	0.47	1.99	0.37	0.38
20	7	14	23	0	0	44	0.49	1.61	0.34	0.44
21	6	10	31	0	0	47	0.46	1.22	0.29	0.38
22	4	12	30	0	0	46	0.45	1.73	0.36	0.3
23	5	14	31	0	0	50	0.51	1.5	0.35	0.42
24	5	16	35	0	0	56	0.43	1.42	0.27	0.37
25	4	13	28	0	0	45	0.53	1.5	0.36	0.4
26	6	17	32	0	0	55	0.55	1.63	0.4	0.44
27	4	13	35	0	0	52	0.48	1.77	0.36	0.4
28	4	14	34	0	0	52	0.46	1.71	0.32	0.4
29	5	14	26	1	0	46	0.5	1.83	0.36	0.38
30	5	11	25	0	0	41	0.51	1.9	0.4	0.44
31	4	12	30	0	0	46	0.46	1.66	0.35	0.34
32	4	15	27	0	0	46	0.5	1.7	0.36	0.4
33	3	17	28	0	0	48	0.53	1.66	0.37	0.41
34	6	12	34	1	0	53	0.5	1.99	0.42	0.37
35	3	14	35	0	0	52	0.51	1.64	0.39	0.4
36	4	15	39	1	0	59	0.43	1.81	0.36	0.31
37	5	13	28	0	0	46	0.47	1.41	0.32	0.34
38	4	16	28	1	0	49	0.46	1.82	0.4	0.34
39	4	18	23	0	0	45	0.48	1.68	0.33	0.41
40	5	14	32	0	0	51	0.45	1.33	0.28	0.41

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

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



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2307(IR:1124, SQ:574, MR:604, LR:5, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
3	7	21	0	0	31	1	2.5
0	2	7	0	0	9	2	5.0
1	3	5	0	0	9	3	7.5
0	1	5	0	0	6	4	10.0
0	0	2	0	0	2	5	12.5
0	1	5	0	0	6	6	15.0

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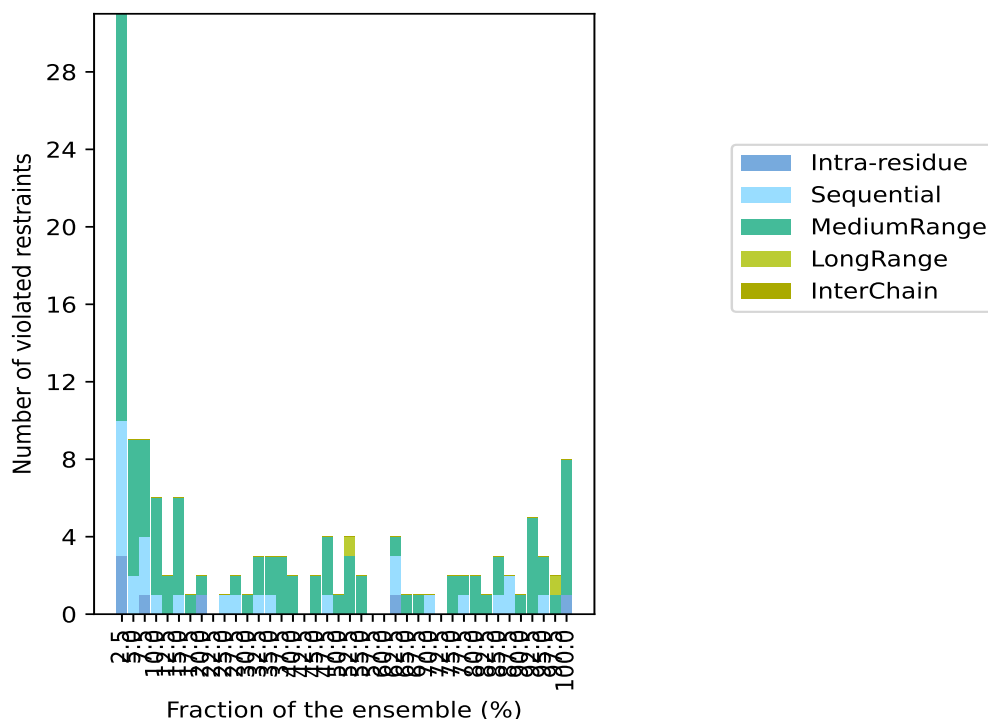
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	1	0	0	1	7	17.5
1	0	1	0	0	2	8	20.0
0	0	0	0	0	0	9	22.5
0	1	0	0	0	1	10	25.0
0	1	1	0	0	2	11	27.5
0	0	1	0	0	1	12	30.0
0	1	2	0	0	3	13	32.5
0	1	2	0	0	3	14	35.0
0	0	3	0	0	3	15	37.5
0	0	2	0	0	2	16	40.0
0	0	0	0	0	0	17	42.5
0	0	2	0	0	2	18	45.0
0	1	3	0	0	4	19	47.5
0	0	1	0	0	1	20	50.0
0	0	3	1	0	4	21	52.5
0	0	2	0	0	2	22	55.0
0	0	0	0	0	0	23	57.5
0	0	0	0	0	0	24	60.0
1	2	1	0	0	4	25	62.5
0	0	1	0	0	1	26	65.0
0	0	1	0	0	1	27	67.5
0	1	0	0	0	1	28	70.0
0	0	0	0	0	0	29	72.5
0	0	2	0	0	2	30	75.0
0	1	1	0	0	2	31	77.5
0	0	2	0	0	2	32	80.0
0	0	1	0	0	1	33	82.5
0	1	2	0	0	3	34	85.0
0	2	0	0	0	2	35	87.5
0	0	1	0	0	1	36	90.0
0	0	5	0	0	5	37	92.5
0	1	2	0	0	3	38	95.0
0	0	1	1	0	2	39	97.5
1	0	7	0	0	8	40	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

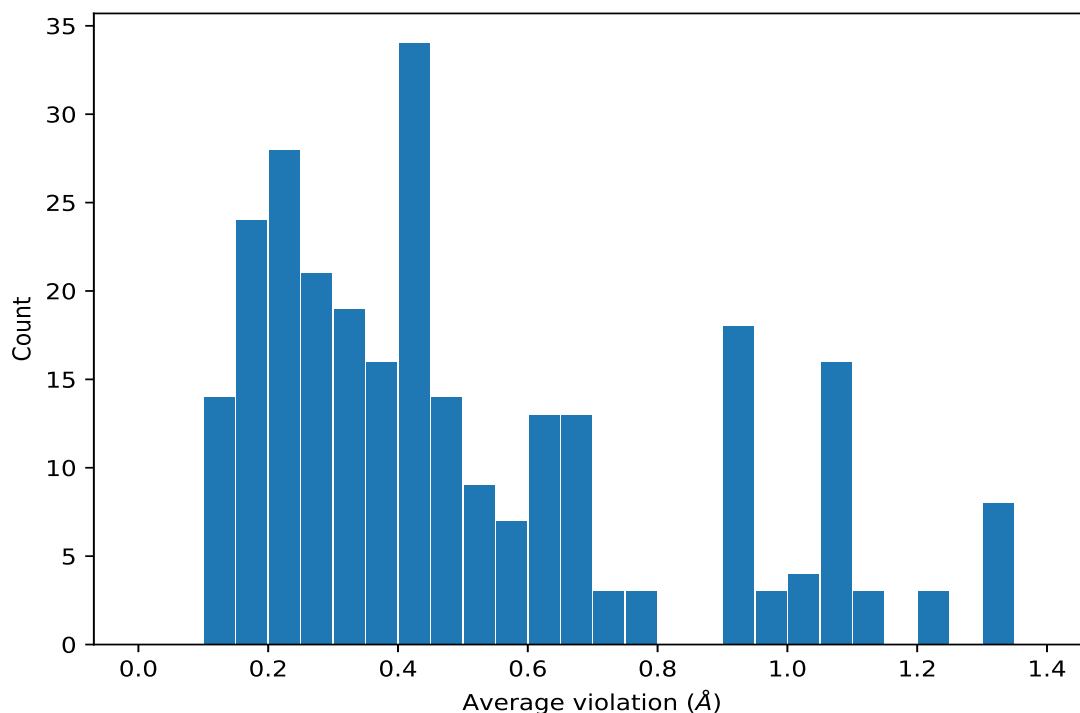
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



9.4.2 Table: Most violated distance restraints [i](#)

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	40	1.22	0.45	1.4
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	40	1.22	0.45	1.4
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG2	40	1.22	0.45	1.4
(1,803)	1:40:A:LEU:HD11	1:44:A:THR:HG22	40	1.09	0.28	1.08
(1,803)	1:40:A:LEU:HD11	1:44:A:THR:HG21	40	1.09	0.28	1.08
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG23	40	1.09	0.28	1.08
(1,803)	1:40:A:LEU:HD13	1:44:A:THR:HG23	40	1.09	0.28	1.08
(1,803)	1:40:A:LEU:HD12	1:44:A:THR:HG21	40	1.09	0.28	1.08
(1,803)	1:49:A:VAL:HG12	1:52:A:THR:HG21	40	1.09	0.28	1.08
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG21	40	1.09	0.28	1.08
(1,803)	1:40:A:LEU:HD12	1:44:A:THR:HG23	40	1.09	0.28	1.08
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG22	40	1.09	0.28	1.08
(1,803)	1:49:A:VAL:HG11	1:52:A:THR:HG22	40	1.09	0.28	1.08
(1,803)	1:49:A:VAL:HG12	1:52:A:THR:HG23	40	1.09	0.28	1.08
(1,803)	1:49:A:VAL:HG11	1:52:A:THR:HG23	40	1.09	0.28	1.08
(1,803)	1:49:A:VAL:HG11	1:52:A:THR:HG21	40	1.09	0.28	1.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,803)	1:40:A:LEU:HD13	1:44:A:THR:HG22	40	1.09	0.28	1.08
(1,803)	1:40:A:LEU:HD13	1:44:A:THR:HG21	40	1.09	0.28	1.08
(1,803)	1:40:A:LEU:HD12	1:44:A:THR:HG22	40	1.09	0.28	1.08
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	40	1.0	0.25	0.96
(1,1782)	1:36:A:MET:HE1	1:35:A:TYR:HA	40	1.0	0.25	0.96
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	40	1.0	0.25	0.96
(1,1782)	1:36:A:MET:HE3	1:37:A:LEU:HA	40	1.0	0.25	0.96
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	40	0.96	0.1	0.92
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD13	40	0.96	0.1	0.92
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD12	40	0.96	0.1	0.92
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB2	40	0.66	0.2	0.66
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB1	40	0.66	0.2	0.66
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB2	40	0.66	0.2	0.66
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB3	40	0.66	0.2	0.66
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB1	40	0.66	0.2	0.66
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB3	40	0.66	0.2	0.66
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	40	0.63	0.12	0.67
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	40	0.63	0.12	0.67
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	40	0.41	0.08	0.4
(1,171)	1:25:A:LYS:HG2	1:24:A:TRP:HE1	40	0.41	0.08	0.4
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	40	0.38	0.03	0.38
(1,1986)	1:48:A:LEU:H	1:48:A:LEU:HG	40	0.38	0.03	0.38
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD11	39	1.32	0.42	1.33
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD12	39	1.32	0.42	1.33
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD13	39	1.32	0.42	1.33
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD23	39	1.32	0.42	1.33
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD21	39	1.32	0.42	1.33
(1,1961)	1:39:A:PHE:HA	1:34:A:ILE:HG22	39	1.32	0.42	1.33
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD22	39	1.32	0.42	1.33
(1,1961)	1:39:A:PHE:HA	1:34:A:ILE:HG23	39	1.32	0.42	1.33
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	39	0.64	0.16	0.6
(1,412)	1:33:A:ALA:H	1:31:A:ILE:HG12	39	0.64	0.16	0.6
(1,412)	1:33:A:ALA:H	1:31:A:ILE:HG13	39	0.64	0.16	0.6
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG13	39	0.64	0.16	0.6
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	38	0.46	0.16	0.49
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG23	38	0.46	0.16	0.49
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG21	38	0.46	0.16	0.49
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	38	0.2	0.05	0.18
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	38	0.18	0.04	0.18
(1,1990)	1:36:A:MET:HE3	1:35:A:TYR:HE2	37	0.62	0.21	0.6
(1,1990)	1:36:A:MET:HE3	1:35:A:TYR:HE1	37	0.62	0.21	0.6
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	37	0.62	0.21	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1990)	1:36:A:MET:HE1	1:35:A:TYR:HE2	37	0.62	0.21	0.6
(1,1990)	1:36:A:MET:HE1	1:35:A:TYR:HE1	37	0.62	0.21	0.6
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE1	37	0.62	0.21	0.6
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	37	0.48	0.12	0.48
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HG	37	0.48	0.12	0.48
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG22	37	0.42	0.15	0.41
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG21	37	0.42	0.15	0.41
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	37	0.42	0.15	0.41
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	37	0.41	0.09	0.44
(1,553)	1:48:A:LEU:HB2	1:45:A:GLY:H	37	0.41	0.09	0.44
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	37	0.31	0.12	0.29
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD21	36	0.55	0.17	0.53
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD23	36	0.55	0.17	0.53
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD22	36	0.55	0.17	0.53
(1,1378)	1:47:A:GLY:H	1:48:A:LEU:HD13	36	0.55	0.17	0.53
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	35	0.46	0.23	0.44
(1,691)	1:15:A:ASN:HB2	1:16:A:GLN:HB3	35	0.46	0.23	0.44
(1,691)	1:46:A:ASN:HB2	1:49:A:VAL:HB	35	0.46	0.23	0.44
(1,691)	1:46:A:ASN:HB3	1:49:A:VAL:HB	35	0.46	0.23	0.44
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB2	35	0.46	0.23	0.44
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	35	0.15	0.01	0.15
(1,444)	1:13:A:ALA:H	1:10:A:TYR:HB3	34	0.73	0.13	0.76
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	34	0.73	0.13	0.76
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB2	34	0.73	0.13	0.76
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	34	0.33	0.17	0.3
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	34	0.33	0.17	0.3
(1,1313)	1:38:A:VAL:HG23	1:34:A:ILE:HB	34	0.33	0.17	0.3
(1,2401)	1:44:A:THR:HG21	1:44:A:THR:H	34	0.29	0.14	0.29
(1,2401)	1:44:A:THR:HG23	1:44:A:THR:H	34	0.29	0.14	0.29
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	34	0.29	0.14	0.29
(1,2401)	1:43:A:THR:HG22	1:44:A:THR:H	34	0.29	0.14	0.29
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	33	0.35	0.16	0.33
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	33	0.35	0.16	0.33
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	32	0.39	0.2	0.34
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG22	32	0.39	0.2	0.34
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG21	32	0.39	0.2	0.34
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	32	0.39	0.2	0.34
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG22	32	0.39	0.2	0.34
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG21	32	0.39	0.2	0.34
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	31	0.42	0.09	0.44
(1,1458)	1:22:A:THR:HG23	1:23:A:ASP:HA	31	0.42	0.09	0.44
(1,1458)	1:22:A:THR:HG21	1:23:A:ASP:HA	31	0.42	0.09	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	31	0.41	0.12	0.43
(1,14)	1:55:A:ARG:HH11	1:52:A:THR:HB	31	0.41	0.12	0.43
(1,1498)	1:31:A:ILE:HD11	1:33:A:ALA:HB3	30	0.91	0.49	0.81
(1,1498)	1:30:A:LEU:HD13	1:33:A:ALA:HB1	30	0.91	0.49	0.81
(1,1498)	1:30:A:LEU:HD13	1:33:A:ALA:HB2	30	0.91	0.49	0.81
(1,1498)	1:30:A:LEU:HD12	1:33:A:ALA:HB2	30	0.91	0.49	0.81
(1,1498)	1:30:A:LEU:HD12	1:33:A:ALA:HB3	30	0.91	0.49	0.81
(1,1498)	1:31:A:ILE:HD12	1:34:A:ILE:HG21	30	0.91	0.49	0.81
(1,1498)	1:31:A:ILE:HD13	1:33:A:ALA:HB2	30	0.91	0.49	0.81
(1,1498)	1:30:A:LEU:HD11	1:33:A:ALA:HB2	30	0.91	0.49	0.81
(1,1498)	1:30:A:LEU:HD11	1:33:A:ALA:HB1	30	0.91	0.49	0.81
(1,1498)	1:30:A:LEU:HD12	1:33:A:ALA:HB1	30	0.91	0.49	0.81
(1,1498)	1:30:A:LEU:HD22	1:33:A:ALA:HB3	30	0.91	0.49	0.81
(1,1498)	1:30:A:LEU:HD11	1:33:A:ALA:HB3	30	0.91	0.49	0.81
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB3	30	0.44	0.3	0.31
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	30	0.44	0.3	0.31
(1,2148)	1:22:A:THR:H	1:18:A:GLU:HB2	30	0.44	0.3	0.31
(1,2148)	1:22:A:THR:H	1:18:A:GLU:HB3	30	0.44	0.3	0.31
(1,1896)	1:36:A:MET:HE1	1:40:A:LEU:HB3	28	0.46	0.24	0.38
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	28	0.46	0.24	0.38
(1,1896)	1:36:A:MET:HE2	1:40:A:LEU:HB3	28	0.46	0.24	0.38
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB2	27	0.5	0.27	0.42
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB3	27	0.5	0.27	0.42
(1,983)	1:26:A:SER:HB2	1:29:A:ALA:HB3	27	0.5	0.27	0.42
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB1	27	0.5	0.27	0.42
(1,983)	1:27:A:SER:HB3	1:29:A:ALA:HB3	27	0.5	0.27	0.42
(1,983)	1:26:A:SER:HB2	1:29:A:ALA:HB2	27	0.5	0.27	0.42
(1,983)	1:27:A:SER:HB3	1:29:A:ALA:HB2	27	0.5	0.27	0.42
(1,983)	1:27:A:SER:HB3	1:29:A:ALA:HB1	27	0.5	0.27	0.42
(1,915)	1:49:A:VAL:HG23	1:46:A:ASN:HA	26	0.24	0.1	0.24
(1,915)	1:49:A:VAL:HG12	1:52:A:THR:HB	26	0.24	0.1	0.24
(1,915)	1:49:A:VAL:HG21	1:46:A:ASN:HA	26	0.24	0.1	0.24
(1,915)	1:49:A:VAL:HG13	1:52:A:THR:HB	26	0.24	0.1	0.24
(1,915)	1:49:A:VAL:HG22	1:46:A:ASN:HA	26	0.24	0.1	0.24
(1,915)	1:49:A:VAL:HG11	1:52:A:THR:HB	26	0.24	0.1	0.24
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD23	25	0.4	0.09	0.43
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD22	25	0.4	0.09	0.43
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD21	25	0.4	0.09	0.43
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD13	25	0.4	0.09	0.43
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD11	25	0.4	0.09	0.43
(1,1046)	1:50:A:LEU:HD23	1:51:A:TRP:HA	25	0.4	0.09	0.43
(1,1046)	1:50:A:LEU:HD22	1:51:A:TRP:HA	25	0.4	0.09	0.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1046)	1:50:A:LEU:HD21	1:51:A:TRP:HA	25	0.4	0.09	0.43
(1,1046)	1:50:A:LEU:HD13	1:51:A:TRP:HA	25	0.4	0.09	0.43
(1,1046)	1:53:A:VAL:HG12	1:51:A:TRP:HA	25	0.4	0.09	0.43
(1,1046)	1:50:A:LEU:HD11	1:51:A:TRP:HA	25	0.4	0.09	0.43
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	25	0.3	0.07	0.29
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	25	0.12	0.02	0.12
(1,1858)	1:28:A:GLY:H	1:27:A:SER:HA	25	0.12	0.02	0.12
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD12	22	0.9	0.03	0.91
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD13	22	0.9	0.03	0.91
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD11	22	0.9	0.03	0.91
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD12	22	0.68	0.43	0.66
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD13	22	0.68	0.43	0.66
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD11	22	0.68	0.43	0.66
(1,970)	1:33:A:ALA:HA	1:31:A:ILE:HG23	22	0.68	0.43	0.66
(1,970)	1:33:A:ALA:HA	1:31:A:ILE:HG22	22	0.68	0.43	0.66
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD22	22	0.68	0.43	0.66
(1,970)	1:33:A:ALA:HA	1:31:A:ILE:HG21	22	0.68	0.43	0.66
(1,1156)	1:52:A:THR:HG22	1:55:A:ARG:HH21	21	1.1	0.22	1.17
(1,1156)	1:52:A:THR:HG21	1:55:A:ARG:HH21	21	1.1	0.22	1.17
(1,1156)	1:52:A:THR:HG23	1:55:A:ARG:HH21	21	1.1	0.22	1.17
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	21	0.39	0.17	0.39
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB2	21	0.39	0.17	0.39
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	21	0.39	0.17	0.39
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB2	21	0.39	0.17	0.39
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	21	0.34	0.22	0.27
(1,21)	1:55:A:ARG:HB3	1:51:A:TRP:HE1	21	0.34	0.22	0.27
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	20	0.43	0.12	0.46
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB1	19	0.43	0.25	0.34
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB2	19	0.43	0.25	0.34
(1,491)	1:37:A:LEU:H	1:41:A:LEU:HB2	19	0.43	0.25	0.34
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB3	19	0.43	0.25	0.34
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	19	0.39	0.1	0.39
(1,480)	1:51:A:TRP:HA	1:55:A:ARG:HE	19	0.39	0.1	0.39
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	19	0.34	0.08	0.33
(1,699)	1:16:A:GLN:HA	1:18:A:GLU:H	19	0.22	0.09	0.19
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	19	0.22	0.09	0.19
(1,685)	1:27:A:SER:HB2	1:29:A:ALA:H	18	0.34	0.12	0.36
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	18	0.34	0.12	0.36
(1,2329)	1:27:A:SER:HB2	1:29:A:ALA:H	18	0.34	0.12	0.36
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	18	0.34	0.12	0.36
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	16	0.25	0.08	0.24
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB2	16	0.25	0.08	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG11	16	0.24	0.12	0.21
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG13	16	0.24	0.12	0.21
(1,2079)	1:40:A:LEU:H	1:43:A:THR:HG21	16	0.24	0.12	0.21
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG12	16	0.24	0.12	0.21
(1,475)	1:41:A:LEU:HB2	1:44:A:THR:H	15	0.31	0.2	0.3
(1,475)	1:41:A:LEU:HB3	1:44:A:THR:H	15	0.31	0.2	0.3
(1,427)	1:40:A:LEU:HG	1:43:A:THR:H	15	0.28	0.1	0.26
(1,427)	1:41:A:LEU:HB3	1:43:A:THR:H	15	0.28	0.1	0.26
(1,427)	1:41:A:LEU:HB2	1:43:A:THR:H	15	0.28	0.1	0.26
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	15	0.25	0.06	0.28
(1,2203)	1:23:A:ASP:HB2	1:25:A:LYS:H	14	0.24	0.09	0.22
(1,2203)	1:23:A:ASP:HB2	1:20:A:GLU:H	14	0.24	0.09	0.22
(1,2203)	1:23:A:ASP:HB3	1:25:A:LYS:H	14	0.24	0.09	0.22
(1,2121)	1:22:A:THR:H	1:18:A:GLU:HA	14	0.2	0.07	0.18
(1,2121)	1:22:A:THR:H	1:20:A:GLU:HA	14	0.2	0.07	0.18
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	14	0.13	0.01	0.13
(1,920)	1:34:A:ILE:HB	1:35:A:TYR:HE1	13	0.76	0.38	0.69
(1,920)	1:32:A:PRO:HG3	1:35:A:TYR:HE2	13	0.76	0.38	0.69
(1,920)	1:34:A:ILE:HB	1:35:A:TYR:HE2	13	0.76	0.38	0.69
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD11	13	0.57	0.39	0.29
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD13	13	0.57	0.39	0.29
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD12	13	0.57	0.39	0.29
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	13	0.13	0.02	0.12
(1,1964)	1:47:A:GLY:HA2	1:50:A:LEU:HG	12	0.14	0.03	0.14
(1,430)	1:15:A:ASN:H	1:16:A:GLN:HB3	11	0.26	0.09	0.24
(1,430)	1:15:A:ASN:H	1:18:A:GLU:HB2	11	0.26	0.09	0.24
(1,1181)	1:32:A:PRO:HA	1:34:A:ILE:H	11	0.15	0.04	0.14
(1,592)	1:62:A:HIS:H	1:61:A:HIS:HA	10	0.13	0.02	0.14
(1,592)	1:62:A:HIS:H	1:62:A:HIS:HA	10	0.13	0.02	0.14
(1,89)	1:20:A:GLU:HG2	1:20:A:GLU:H	8	0.3	0.13	0.32
(1,89)	1:20:A:GLU:HG3	1:20:A:GLU:H	8	0.3	0.13	0.32
(1,1189)	1:30:A:LEU:HA	1:30:A:LEU:HD13	8	0.16	0.02	0.16
(1,1189)	1:30:A:LEU:HA	1:30:A:LEU:HD12	8	0.16	0.02	0.16
(1,1189)	1:30:A:LEU:HA	1:30:A:LEU:HD22	8	0.16	0.02	0.16
(1,466)	1:46:A:ASN:HD21	1:44:A:THR:HB	7	0.13	0.03	0.11
(1,1311)	1:44:A:THR:HG23	1:40:A:LEU:HA	6	0.94	0.33	1.04
(1,1311)	1:44:A:THR:HG21	1:40:A:LEU:HA	6	0.94	0.33	1.04
(1,1311)	1:44:A:THR:HG22	1:40:A:LEU:HA	6	0.94	0.33	1.04
(1,63)	1:53:A:VAL:H	1:56:A:LYS:HD3	6	0.48	0.08	0.48
(1,494)	1:46:A:ASN:H	1:50:A:LEU:HD12	6	0.42	0.12	0.37
(1,494)	1:46:A:ASN:H	1:50:A:LEU:HD13	6	0.42	0.12	0.37
(1,247)	1:53:A:VAL:H	1:55:A:ARG:H	6	0.34	0.12	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,247)	1:57:A:LYS:H	1:55:A:ARG:H	6	0.34	0.12	0.3
(1,1774)	1:21:A:TYR:HB3	1:22:A:THR:HG23	6	0.26	0.06	0.27
(1,1774)	1:21:A:TYR:HB3	1:22:A:THR:HG22	6	0.26	0.06	0.27
(1,1774)	1:21:A:TYR:HB3	1:22:A:THR:HG21	6	0.26	0.06	0.27
(1,1530)	1:39:A:PHE:HB2	1:38:A:VAL:HG11	6	0.18	0.06	0.15
(1,1530)	1:39:A:PHE:HB2	1:38:A:VAL:HG13	6	0.18	0.06	0.15
(1,1530)	1:39:A:PHE:HB2	1:38:A:VAL:HG12	6	0.18	0.06	0.15
(1,1409)	1:13:A:ALA:HB2	1:10:A:TYR:HA	5	0.25	0.07	0.28
(1,1409)	1:13:A:ALA:HB3	1:11:A:TYR:HA	5	0.25	0.07	0.28
(1,1409)	1:13:A:ALA:HB3	1:10:A:TYR:HA	5	0.25	0.07	0.28
(1,302)	1:39:A:PHE:H	1:37:A:LEU:HB3	5	0.15	0.03	0.16
(1,176)	1:36:A:MET:H	1:37:A:LEU:HB3	4	0.21	0.05	0.21
(1,176)	1:36:A:MET:H	1:32:A:PRO:HB3	4	0.21	0.05	0.21
(1,176)	1:36:A:MET:H	1:37:A:LEU:HB2	4	0.21	0.05	0.21
(1,2357)	1:30:A:LEU:H	1:27:A:SER:HA	4	0.2	0.15	0.12
(1,198)	1:51:A:TRP:H	1:47:A:GLY:HA2	4	0.2	0.04	0.2
(1,1158)	1:23:A:ASP:HB2	1:20:A:GLU:HA	4	0.18	0.09	0.14
(1,2392)	1:21:A:TYR:H	1:20:A:GLU:HB2	4	0.18	0.07	0.16
(1,2392)	1:21:A:TYR:H	1:20:A:GLU:HB3	4	0.18	0.07	0.16
(1,1759)	1:36:A:MET:HG3	1:33:A:ALA:HA	4	0.17	0.06	0.14
(1,1455)	1:51:A:TRP:HD1	1:55:A:ARG:HG2	3	0.61	0.23	0.76
(1,2341)	1:54:A:PHE:H	1:50:A:LEU:HG	3	0.54	0.18	0.42
(1,1358)	1:30:A:LEU:HA	1:33:A:ALA:HB1	3	0.26	0.06	0.23
(1,1358)	1:30:A:LEU:HA	1:33:A:ALA:HB3	3	0.26	0.06	0.23
(1,1358)	1:30:A:LEU:HA	1:33:A:ALA:HB2	3	0.26	0.06	0.23
(1,1494)	1:15:A:ASN:HA	1:18:A:GLU:HB3	3	0.21	0.03	0.22
(1,1494)	1:15:A:ASN:HA	1:18:A:GLU:HB2	3	0.21	0.03	0.22
(1,1095)	1:41:A:LEU:HG	1:37:A:LEU:HG	3	0.16	0.08	0.1
(1,434)	1:61:A:HIS:H	1:61:A:HIS:HB2	3	0.16	0.06	0.13
(1,434)	1:61:A:HIS:H	1:61:A:HIS:HB3	3	0.16	0.06	0.13
(1,908)	1:32:A:PRO:HG2	1:33:A:ALA:HA	3	0.15	0.04	0.12
(1,2255)	1:42:A:GLY:HA2	1:44:A:THR:H	3	0.14	0.02	0.15
(1,500)	1:64:A:HIS:HA	1:63:A:HIS:H	3	0.12	0.01	0.11
(1,2409)	1:18:A:GLU:HG3	1:17:A:SER:H	2	0.34	0.1	0.34
(1,664)	1:26:A:SER:HA	1:25:A:LYS:HB3	2	0.2	0.09	0.2
(1,664)	1:27:A:SER:HA	1:30:A:LEU:HG	2	0.2	0.09	0.2
(1,2377)	1:46:A:ASN:H	1:43:A:THR:HA	2	0.2	0.01	0.2
(1,550)	1:41:A:LEU:H	1:44:A:THR:H	2	0.18	0.02	0.18
(1,550)	1:41:A:LEU:H	1:37:A:LEU:H	2	0.18	0.02	0.18
(1,612)	1:35:A:TYR:H	1:34:A:ILE:HG13	2	0.18	0.01	0.18
(1,2053)	1:35:A:TYR:H	1:34:A:ILE:HG13	2	0.18	0.01	0.18
(1,1011)	1:28:A:GLY:HA3	1:29:A:ALA:HB1	2	0.16	0.02	0.16

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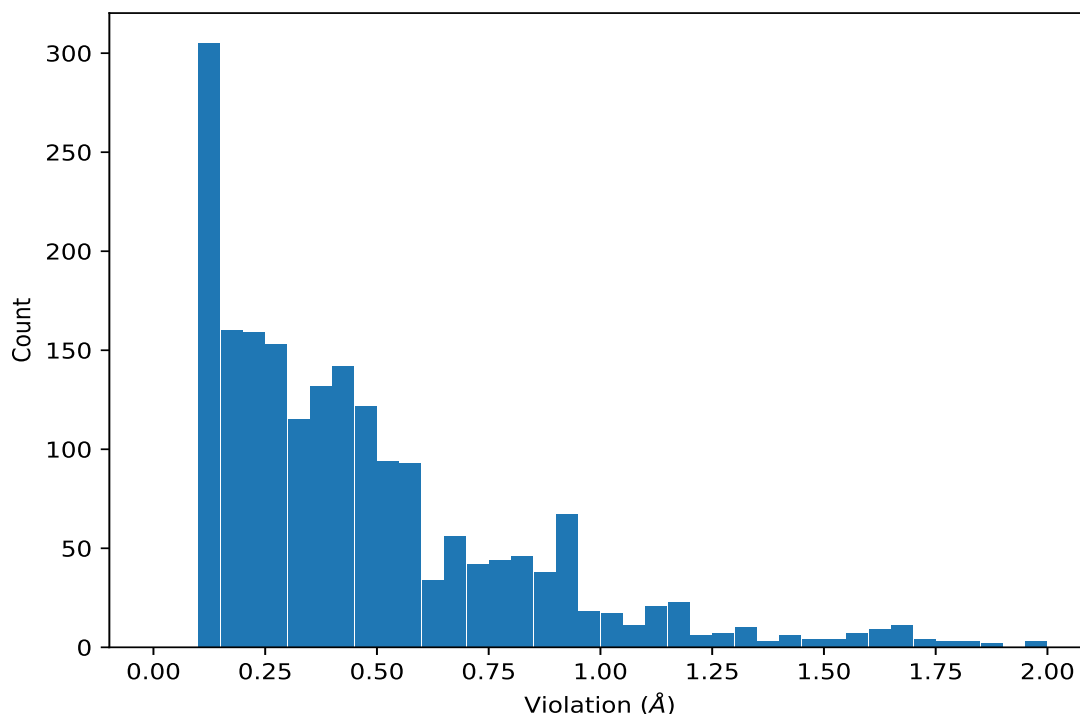
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1011)	1:28:A:GLY:HA3	1:29:A:ALA:HB3	2	0.16	0.02	0.16
(1,1664)	1:34:A:ILE:HB	1:35:A:TYR:HA	2	0.12	0.0	0.12
(1,1431)	1:38:A:VAL:H	1:34:A:ILE:HD11	2	0.11	0.0	0.11
(1,1431)	1:38:A:VAL:H	1:34:A:ILE:HD12	2	0.11	0.0	0.11
(1,1431)	1:38:A:VAL:H	1:34:A:ILE:HD13	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

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



9.5.2 Table : All distance violations [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1961)	1:39:A:PHE:HA	1:34:A:ILE:HG22	19	1.99
(1,1961)	1:39:A:PHE:HA	1:34:A:ILE:HG22	34	1.99
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD12	8	1.97
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD13	30	1.9
(1,1498)	1:30:A:LEU:HD13	1:33:A:ALA:HB2	6	1.87
(1,1961)	1:39:A:PHE:HA	1:34:A:ILE:HG23	29	1.83
(1,1961)	1:39:A:PHE:HA	1:34:A:ILE:HG23	38	1.82
(1,1961)	1:39:A:PHE:HA	1:34:A:ILE:HG23	36	1.81
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD23	10	1.78
(1,1498)	1:30:A:LEU:HD13	1:33:A:ALA:HB1	27	1.77
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD21	14	1.76
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD21	22	1.73
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG2	30	1.73
(1,803)	1:40:A:LEU:HD13	1:44:A:THR:HG21	36	1.72
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	28	1.71
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	17	1.7
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	32	1.7
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG2	5	1.68
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG2	9	1.68
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	18	1.68
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG2	39	1.68
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD22	18	1.67
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	8	1.67
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD21	33	1.66
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	3	1.66
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	31	1.66
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	34	1.65
(1,1498)	1:30:A:LEU:HD11	1:33:A:ALA:HB3	35	1.64
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG2	38	1.64
(1,1961)	1:39:A:PHE:HA	1:34:A:ILE:HG22	15	1.63
(1,803)	1:49:A:VAL:HG12	1:52:A:THR:HG23	26	1.63
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	1	1.62
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	13	1.62
(1,1498)	1:30:A:LEU:HD12	1:33:A:ALA:HB1	20	1.61
(1,1498)	1:30:A:LEU:HD12	1:33:A:ALA:HB1	34	1.6
(1,1156)	1:52:A:THR:HG23	1:55:A:ARG:HH21	31	1.59
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	20	1.59
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD13	13	1.57
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD12	16	1.57
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	12	1.56
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG2	15	1.56
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD12	26	1.55
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD12	6	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD13	32	1.54
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD11	23	1.5
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	25	1.5
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	25	1.49
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	33	1.48
(1,1498)	1:30:A:LEU:HD13	1:33:A:ALA:HB2	26	1.48
(1,1038)	1:32:A:PRO:HG3	1:36:A:MET:HG2	26	1.47
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG22	22	1.45
(1,803)	1:49:A:VAL:HG12	1:52:A:THR:HG21	23	1.45
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG22	35	1.44
(1,1498)	1:30:A:LEU:HD22	1:33:A:ALA:HB3	24	1.42
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	23	1.41
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	37	1.41
(1,970)	1:33:A:ALA:HA	1:31:A:ILE:HG22	26	1.4
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG21	8	1.38
(1,803)	1:49:A:VAL:HG12	1:52:A:THR:HG21	27	1.38
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	35	1.34
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD11	11	1.33
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	40	1.33
(1,1498)	1:30:A:LEU:HD12	1:33:A:ALA:HB2	5	1.32
(1,803)	1:49:A:VAL:HG12	1:52:A:THR:HG21	6	1.32
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG22	10	1.32
(1,970)	1:33:A:ALA:HA	1:31:A:ILE:HG23	25	1.31
(1,920)	1:34:A:ILE:HB	1:35:A:TYR:HE1	15	1.31
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	36	1.3
(1,803)	1:40:A:LEU:HD11	1:44:A:THR:HG21	29	1.3
(1,970)	1:33:A:ALA:HA	1:31:A:ILE:HG23	38	1.29
(1,920)	1:32:A:PRO:HG3	1:35:A:TYR:HE2	35	1.29
(1,803)	1:40:A:LEU:HD11	1:44:A:THR:HG22	1	1.29
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD13	12	1.28
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	27	1.28
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	16	1.26
(1,920)	1:34:A:ILE:HB	1:35:A:TYR:HE1	9	1.26
(1,1311)	1:44:A:THR:HG23	1:40:A:LEU:HA	28	1.23
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	21	1.22
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	11	1.21
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	27	1.21
(1,1156)	1:52:A:THR:HG23	1:55:A:ARG:HH21	38	1.21
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD13	35	1.21
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	40	1.2
(1,1498)	1:30:A:LEU:HD13	1:33:A:ALA:HB2	11	1.2
(1,1311)	1:44:A:THR:HG21	1:40:A:LEU:HA	12	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:52:A:THR:HG22	1:55:A:ARG:HH21	7	1.2
(1,1156)	1:52:A:THR:HG22	1:55:A:ARG:HH21	14	1.2
(1,1782)	1:36:A:MET:HE1	1:35:A:TYR:HA	6	1.19
(1,1782)	1:36:A:MET:HE1	1:35:A:TYR:HA	14	1.19
(1,1156)	1:52:A:THR:HG22	1:55:A:ARG:HH21	3	1.19
(1,1156)	1:52:A:THR:HG21	1:55:A:ARG:HH21	11	1.19
(1,1156)	1:52:A:THR:HG22	1:55:A:ARG:HH21	32	1.19
(1,803)	1:40:A:LEU:HD12	1:44:A:THR:HG23	24	1.19
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD12	5	1.18
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	21	1.18
(1,1156)	1:52:A:THR:HG22	1:55:A:ARG:HH21	34	1.18
(1,1156)	1:52:A:THR:HG21	1:55:A:ARG:HH21	5	1.17
(1,1156)	1:52:A:THR:HG22	1:55:A:ARG:HH21	13	1.17
(1,1156)	1:52:A:THR:HG22	1:55:A:ARG:HH21	30	1.17
(1,1156)	1:52:A:THR:HG22	1:55:A:ARG:HH21	33	1.17
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD11	35	1.17
(1,920)	1:32:A:PRO:HG3	1:35:A:TYR:HE2	26	1.17
(1,1156)	1:52:A:THR:HG22	1:55:A:ARG:HH21	17	1.16
(1,1156)	1:52:A:THR:HG23	1:55:A:ARG:HH21	39	1.16
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD12	29	1.16
(1,1156)	1:52:A:THR:HG22	1:55:A:ARG:HH21	25	1.15
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG22	37	1.15
(1,1498)	1:30:A:LEU:HD12	1:33:A:ALA:HB3	29	1.14
(1,1156)	1:52:A:THR:HG21	1:55:A:ARG:HH21	16	1.14
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD12	32	1.14
(1,1498)	1:30:A:LEU:HD11	1:33:A:ALA:HB2	36	1.13
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG23	3	1.13
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD12	23	1.13
(1,983)	1:27:A:SER:HB3	1:29:A:ALA:HB2	33	1.12
(1,803)	1:40:A:LEU:HD12	1:44:A:THR:HG23	20	1.12
(1,803)	1:49:A:VAL:HG12	1:52:A:THR:HG23	32	1.12
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	12	1.12
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	16	1.12
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	26	1.11
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD12	34	1.11
(1,803)	1:49:A:VAL:HG12	1:52:A:THR:HG23	14	1.11
(1,803)	1:40:A:LEU:HD12	1:44:A:THR:HG21	19	1.11
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	33	1.11
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD13	34	1.11
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD11	28	1.1
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG23	28	1.1
(1,803)	1:40:A:LEU:HD11	1:44:A:THR:HG21	2	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1782)	1:36:A:MET:HE1	1:35:A:TYR:HA	20	1.07
(1,1311)	1:44:A:THR:HG21	1:40:A:LEU:HA	5	1.07
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	2	1.07
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD12	30	1.07
(1,803)	1:40:A:LEU:HD13	1:44:A:THR:HG23	4	1.07
(1,803)	1:49:A:VAL:HG11	1:52:A:THR:HG21	15	1.07
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG22	16	1.07
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	22	1.06
(1,1498)	1:31:A:ILE:HD13	1:33:A:ALA:HB2	14	1.06
(1,803)	1:49:A:VAL:HG11	1:52:A:THR:HG23	18	1.05
(1,1782)	1:36:A:MET:HE1	1:35:A:TYR:HA	10	1.04
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD13	12	1.04
(1,691)	1:46:A:ASN:HB2	1:49:A:VAL:HB	13	1.04
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	29	1.03
(1,1990)	1:36:A:MET:HE1	1:35:A:TYR:HE1	35	1.03
(1,1782)	1:36:A:MET:HE1	1:35:A:TYR:HA	7	1.03
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD11	27	1.02
(1,1156)	1:52:A:THR:HG21	1:55:A:ARG:HH21	37	1.02
(1,970)	1:33:A:ALA:HA	1:31:A:ILE:HG21	37	1.02
(1,803)	1:49:A:VAL:HG11	1:52:A:THR:HG23	33	1.02
(1,803)	1:49:A:VAL:HG12	1:52:A:THR:HG21	39	1.02
(1,803)	1:40:A:LEU:HD13	1:44:A:THR:HG22	17	1.01
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG21	38	1.01
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD11	2	1.0
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD12	4	1.0
(1,1782)	1:36:A:MET:HE1	1:35:A:TYR:HA	2	1.0
(1,1311)	1:44:A:THR:HG21	1:40:A:LEU:HA	15	1.0
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD11	4	0.99
(1,803)	1:49:A:VAL:HG12	1:52:A:THR:HG23	25	0.99
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG23	34	0.99
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB2	26	0.99
(1,2148)	1:22:A:THR:H	1:18:A:GLU:HB3	37	0.98
(1,803)	1:49:A:VAL:HG11	1:52:A:THR:HG23	13	0.98
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	5	0.97
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD12	35	0.97
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	4	0.97
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD13	16	0.97
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB3	23	0.97
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG23	7	0.97
(1,803)	1:49:A:VAL:HG11	1:52:A:THR:HG22	11	0.97
(1,412)	1:33:A:ALA:H	1:31:A:ILE:HG13	25	0.97
(1,412)	1:33:A:ALA:H	1:31:A:ILE:HG13	34	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD13	29	0.96
(1,803)	1:49:A:VAL:HG12	1:52:A:THR:HG23	12	0.96
(1,412)	1:33:A:ALA:H	1:31:A:ILE:HG13	19	0.96
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	29	0.95
(1,970)	1:33:A:ALA:HA	1:31:A:ILE:HG21	33	0.95
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB1	22	0.95
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	26	0.95
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD13	28	0.95
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD13	36	0.95
(1,412)	1:33:A:ALA:H	1:31:A:ILE:HG13	33	0.95
(1,1498)	1:30:A:LEU:HD13	1:33:A:ALA:HB2	19	0.94
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	7	0.94
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB2	9	0.94
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB2	18	0.94
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB1	28	0.94
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB2	33	0.94
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD12	10	0.94
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	40	0.94
(1,412)	1:33:A:ALA:H	1:31:A:ILE:HG13	8	0.94
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	19	0.93
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD11	1	0.93
(1,1782)	1:36:A:MET:HE1	1:35:A:TYR:HA	39	0.93
(1,1311)	1:44:A:THR:HG23	1:40:A:LEU:HA	35	0.93
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD12	2	0.93
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD12	3	0.93
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD13	13	0.93
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD12	21	0.93
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD11	31	0.93
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD11	38	0.93
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD12	39	0.93
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	19	0.93
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD12	3	0.93
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	17	0.93
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	35	0.92
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD12	1	0.92
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD11	17	0.92
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD12	22	0.92
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB1	37	0.92
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD13	2	0.92
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD12	5	0.92
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	15	0.92
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD13	24	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	21	0.91
(1,1990)	1:36:A:MET:HE3	1:35:A:TYR:HE2	30	0.91
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD12	7	0.91
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD13	39	0.91
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD13	6	0.91
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD13	18	0.91
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD13	32	0.91
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB1	9	0.91
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	1	0.91
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD13	14	0.91
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD12	18	0.91
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	19	0.91
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	22	0.91
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	27	0.91
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	38	0.91
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	39	0.91
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD13	31	0.9
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD11	1	0.9
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD12	5	0.9
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD13	7	0.9
(1,983)	1:27:A:SER:HB3	1:29:A:ALA:HB2	39	0.9
(1,920)	1:34:A:ILE:HB	1:35:A:TYR:HE2	24	0.9
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	8	0.9
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD12	20	0.9
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	25	0.9
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD13	30	0.9
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	31	0.9
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	37	0.9
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	38	0.89
(1,1990)	1:36:A:MET:HE1	1:35:A:TYR:HE2	38	0.89
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD13	21	0.89
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	8	0.89
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	31	0.89
(1,1782)	1:36:A:MET:HE1	1:35:A:TYR:HA	38	0.89
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD12	14	0.89
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB1	24	0.89
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB2	22	0.89
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	9	0.89
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	11	0.89
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	34	0.88
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD11	17	0.88
(1,1498)	1:31:A:ILE:HD11	1:33:A:ALA:HB3	1	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	24	0.88
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD11	27	0.88
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	14	0.88
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD13	7	0.88
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB3	26	0.87
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD12	3	0.87
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	18	0.87
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	28	0.87
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD21	40	0.87
(1,1156)	1:52:A:THR:HG23	1:55:A:ARG:HH21	23	0.87
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD12	40	0.87
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD13	20	0.87
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	8	0.87
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	23	0.87
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	40	0.87
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD13	4	0.87
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD13	6	0.87
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD13	28	0.86
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD12	16	0.86
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD13	23	0.86
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB3	12	0.86
(1,803)	1:49:A:VAL:HG13	1:52:A:THR:HG21	31	0.86
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	26	0.86
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	37	0.86
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	9	0.85
(1,1782)	1:36:A:MET:HE1	1:35:A:TYR:HA	17	0.85
(1,1782)	1:36:A:MET:HE1	1:35:A:TYR:HA	19	0.85
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	14	0.85
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	22	0.85
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	33	0.85
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD11	30	0.85
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	12	0.85
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB2	31	0.85
(1,422)	1:51:A:TRP:HE1	1:48:A:LEU:HD11	13	0.85
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	13	0.84
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE1	27	0.84
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	10	0.84
(1,994)	1:35:A:TYR:HA	1:34:A:ILE:HD11	29	0.84
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB3	25	0.84
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB3	33	0.84
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG21	33	0.84
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	36	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1896)	1:36:A:MET:HE1	1:40:A:LEU:HB3	10	0.83
(1,1498)	1:30:A:LEU:HD12	1:33:A:ALA:HB2	40	0.83
(1,1378)	1:47:A:GLY:H	1:48:A:LEU:HD13	13	0.83
(1,691)	1:46:A:ASN:HB3	1:49:A:VAL:HB	15	0.83
(1,1990)	1:36:A:MET:HE3	1:35:A:TYR:HE1	3	0.82
(1,1990)	1:36:A:MET:HE3	1:35:A:TYR:HE2	32	0.82
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	32	0.82
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	6	0.82
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB2	4	0.82
(1,412)	1:33:A:ALA:H	1:31:A:ILE:HG12	35	0.82
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	3	0.81
(1,1990)	1:36:A:MET:HE3	1:35:A:TYR:HE1	26	0.81
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD21	25	0.81
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	24	0.81
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD23	18	0.81
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	11	0.81
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	17	0.81
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	34	0.81
(1,412)	1:33:A:ALA:H	1:31:A:ILE:HG12	26	0.81
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	5	0.8
(1,2341)	1:54:A:PHE:H	1:50:A:LEU:HG	23	0.8
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	5	0.8
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	12	0.8
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB2	17	0.8
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB2	25	0.8
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	5	0.8
(1,475)	1:41:A:LEU:HB3	1:44:A:THR:H	36	0.8
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	9	0.8
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD13	9	0.79
(1,1896)	1:36:A:MET:HE1	1:40:A:LEU:HB3	6	0.79
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	40	0.79
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	3	0.79
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	13	0.79
(1,1498)	1:30:A:LEU:HD12	1:33:A:ALA:HB1	32	0.79
(1,1378)	1:47:A:GLY:H	1:48:A:LEU:HD13	37	0.79
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	2	0.79
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB2	3	0.79
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	24	0.79
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD22	37	0.78
(1,1896)	1:36:A:MET:HE2	1:40:A:LEU:HB3	11	0.78
(1,1455)	1:51:A:TRP:HD1	1:55:A:ARG:HG2	18	0.78
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD23	19	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,983)	1:27:A:SER:HB3	1:29:A:ALA:HB2	21	0.78
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB3	21	0.78
(1,920)	1:34:A:ILE:HB	1:35:A:TYR:HE1	25	0.78
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	6	0.78
(1,1896)	1:36:A:MET:HE1	1:40:A:LEU:HB3	14	0.77
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	22	0.77
(1,1156)	1:52:A:THR:HG22	1:55:A:ARG:HH21	21	0.77
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	11	0.77
(1,983)	1:27:A:SER:HB3	1:29:A:ALA:HB3	29	0.77
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB3	6	0.77
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB2	39	0.77
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB1	26	0.77
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	12	0.77
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD12	24	0.76
(1,1455)	1:51:A:TRP:HD1	1:55:A:ARG:HG2	23	0.76
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD21	10	0.76
(1,803)	1:40:A:LEU:HD12	1:44:A:THR:HG21	5	0.76
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	25	0.76
(1,412)	1:33:A:ALA:H	1:31:A:ILE:HG12	4	0.76
(1,1990)	1:36:A:MET:HE3	1:35:A:TYR:HE2	1	0.75
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	31	0.75
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	5	0.75
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD13	14	0.75
(1,803)	1:40:A:LEU:HD12	1:44:A:THR:HG23	9	0.75
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	10	0.75
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	36	0.75
(1,412)	1:33:A:ALA:H	1:31:A:ILE:HG12	10	0.75
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	4	0.75
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	8	0.75
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	27	0.75
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	8	0.74
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	18	0.74
(1,1961)	1:39:A:PHE:HA	1:41:A:LEU:HD11	20	0.74
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	27	0.74
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB1	27	0.74
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB3	30	0.74
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	23	0.74
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	6	0.74
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	9	0.74
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	25	0.74
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	37	0.74
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	10	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	7	0.73
(1,1156)	1:52:A:THR:HG21	1:55:A:ARG:HH21	35	0.73
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	21	0.73
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	19	0.73
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	33	0.73
(1,412)	1:33:A:ALA:H	1:31:A:ILE:HG12	12	0.73
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	16	0.73
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	30	0.73
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	11	0.73
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	18	0.73
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	21	0.73
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	22	0.73
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	8	0.73
(1,1498)	1:30:A:LEU:HD13	1:33:A:ALA:HB1	3	0.72
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD23	16	0.72
(1,1313)	1:38:A:VAL:HG23	1:34:A:ILE:HB	26	0.72
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	35	0.72
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB1	20	0.72
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB3	29	0.72
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	7	0.72
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	13	0.72
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	30	0.72
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	31	0.72
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	31	0.72
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	33	0.71
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	35	0.71
(1,803)	1:40:A:LEU:HD11	1:44:A:THR:HG22	21	0.71
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	39	0.71
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB2	35	0.71
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	13	0.71
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG22	6	0.7
(1,1498)	1:30:A:LEU:HD13	1:33:A:ALA:HB1	30	0.7
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD13	23	0.7
(1,83)	1:49:A:VAL:H	1:51:A:TRP:HB3	34	0.7
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	25	0.69
(1,1498)	1:30:A:LEU:HD11	1:33:A:ALA:HB2	21	0.69
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD22	9	0.69
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	37	0.69
(1,920)	1:34:A:ILE:HB	1:35:A:TYR:HE1	2	0.69
(1,494)	1:46:A:ASN:H	1:50:A:LEU:HD13	36	0.69
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG23	2	0.69
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	19	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	15	0.68
(1,1782)	1:36:A:MET:HE2	1:35:A:TYR:HA	34	0.68
(1,1378)	1:47:A:GLY:H	1:48:A:LEU:HD13	22	0.68
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	21	0.68
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	21	0.68
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG23	10	0.68
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	39	0.68
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	6	0.68
(1,1990)	1:36:A:MET:HE1	1:35:A:TYR:HE1	20	0.67
(1,1896)	1:36:A:MET:HE1	1:40:A:LEU:HB3	2	0.67
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD21	6	0.67
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	4	0.67
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB2	19	0.67
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	21	0.67
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	29	0.67
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	23	0.67
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	40	0.67
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG21	25	0.67
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	15	0.67
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	16	0.67
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	40	0.66
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG22	9	0.66
(1,1896)	1:36:A:MET:HE1	1:40:A:LEU:HB3	7	0.66
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB2	7	0.66
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB2	35	0.66
(1,691)	1:15:A:ASN:HB2	1:16:A:GLN:HB3	5	0.66
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	40	0.66
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	38	0.66
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	2	0.66
(1,14)	1:55:A:ARG:HH11	1:52:A:THR:HB	36	0.66
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	34	0.65
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG22	27	0.65
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	1	0.65
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD21	1	0.65
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD21	17	0.65
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB1	12	0.65
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB2	10	0.65
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB1	26	0.65
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	32	0.65
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	34	0.65
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB1	25	0.65
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB3	38	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	5	0.65
(1,21)	1:55:A:ARG:HB3	1:51:A:TRP:HE1	31	0.65
(1,444)	1:13:A:ALA:H	1:10:A:TYR:HB3	1	0.64
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG23	3	0.64
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	14	0.64
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	33	0.64
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD21	7	0.63
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD21	32	0.63
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB2	16	0.63
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	16	0.63
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	29	0.63
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	15	0.63
(1,444)	1:13:A:ALA:H	1:10:A:TYR:HB3	25	0.63
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	6	0.63
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG23	13	0.63
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	21	0.62
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	15	0.62
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	23	0.62
(1,983)	1:26:A:SER:HB2	1:29:A:ALA:HB2	20	0.62
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD12	12	0.62
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB3	5	0.62
(1,920)	1:34:A:ILE:HB	1:35:A:TYR:HE2	36	0.62
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	30	0.62
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	34	0.62
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	35	0.62
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	21	0.62
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	27	0.62
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG23	17	0.62
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	1	0.62
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	13	0.61
(1,1498)	1:30:A:LEU:HD12	1:33:A:ALA:HB3	13	0.61
(1,1313)	1:38:A:VAL:HG23	1:34:A:ILE:HB	10	0.61
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	37	0.61
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	13	0.61
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG13	11	0.61
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	35	0.61
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE1	36	0.6
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB2	28	0.6
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	4	0.6
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	18	0.6
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	19	0.6
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	32	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	14	0.6
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	32	0.6
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG23	18	0.6
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	22	0.6
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	5	0.6
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	24	0.59
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG21	28	0.59
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD23	28	0.59
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	27	0.59
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB2	37	0.59
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	12	0.59
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	32	0.59
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	28	0.59
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	28	0.59
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	1	0.59
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	2	0.59
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	32	0.59
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG21	5	0.58
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	23	0.58
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG21	30	0.58
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	13	0.58
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	39	0.58
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	16	0.58
(1,1990)	1:36:A:MET:HE1	1:35:A:TYR:HE2	39	0.58
(1,1498)	1:30:A:LEU:HD11	1:33:A:ALA:HB1	23	0.58
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB1	16	0.58
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	1	0.58
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG21	5	0.58
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	23	0.58
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG21	30	0.58
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	40	0.58
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	26	0.58
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG21	7	0.58
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	24	0.58
(1,63)	1:53:A:VAL:H	1:56:A:LYS:HD3	2	0.58
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	3	0.57
(1,2329)	1:27:A:SER:HB2	1:29:A:ALA:H	14	0.57
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE1	40	0.57
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG21	35	0.57
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	15	0.57
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB3	40	0.57
(1,685)	1:27:A:SER:HB2	1:29:A:ALA:H	14	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	3	0.57
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB2	16	0.57
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG21	27	0.57
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	38	0.57
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	1	0.56
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	23	0.56
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	4	0.56
(1,1990)	1:36:A:MET:HE1	1:35:A:TYR:HE2	17	0.56
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	27	0.56
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG21	25	0.56
(1,1782)	1:36:A:MET:HE3	1:35:A:TYR:HA	30	0.56
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD22	21	0.56
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	19	0.56
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB3	13	0.56
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	26	0.56
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB2	3	0.56
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB2	34	0.56
(1,920)	1:34:A:ILE:HB	1:35:A:TYR:HE2	20	0.56
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	5	0.56
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	1	0.56
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	36	0.56
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	23	0.56
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG13	9	0.56
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	17	0.56
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	29	0.56
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	39	0.56
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	14	0.56
(1,63)	1:53:A:VAL:H	1:56:A:LYS:HD3	24	0.56
(1,2401)	1:44:A:THR:HG23	1:44:A:THR:H	19	0.55
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	28	0.55
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	15	0.55
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG22	32	0.55
(1,1498)	1:31:A:ILE:HD12	1:34:A:ILE:HG21	12	0.55
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB2	11	0.55
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB2	31	0.55
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB2	36	0.55
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	11	0.55
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	26	0.55
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	28	0.55
(1,480)	1:51:A:TRP:HA	1:55:A:ARG:HE	20	0.55
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	6	0.55
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	18	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,171)	1:25:A:LYS:HG2	1:24:A:TRP:HE1	5	0.55
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	23	0.55
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	35	0.55
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	16	0.54
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	13	0.54
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	28	0.54
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	6	0.54
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	17	0.54
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD23	31	0.54
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD21	33	0.54
(1,1313)	1:38:A:VAL:HG23	1:34:A:ILE:HB	22	0.54
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	16	0.54
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	23	0.54
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	29	0.54
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB3	14	0.54
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	16	0.54
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	13	0.54
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	5	0.54
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG21	32	0.54
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	6	0.53
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	24	0.53
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	1	0.53
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	19	0.53
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	30	0.53
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	19	0.53
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB1	37	0.53
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	6	0.53
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	24	0.53
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	22	0.53
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG23	37	0.53
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	40	0.53
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	23	0.53
(1,1990)	1:36:A:MET:HE3	1:35:A:TYR:HE1	6	0.52
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	26	0.52
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	2	0.52
(1,1458)	1:22:A:THR:HG21	1:23:A:ASP:HA	20	0.52
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD22	3	0.52
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD23	12	0.52
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD21	34	0.52
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	6	0.52
(1,1156)	1:52:A:THR:HG22	1:55:A:ARG:HH21	18	0.52
(1,691)	1:15:A:ASN:HB2	1:16:A:GLN:HB3	33	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	20	0.52
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	5	0.52
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	31	0.52
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	12	0.52
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	28	0.52
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	33	0.52
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	17	0.52
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG22	11	0.51
(1,2401)	1:44:A:THR:HG23	1:44:A:THR:H	30	0.51
(1,2148)	1:22:A:THR:H	1:18:A:GLU:HB3	34	0.51
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	40	0.51
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG21	40	0.51
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD13	32	0.51
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	16	0.51
(1,1046)	1:50:A:LEU:HD13	1:51:A:TRP:HA	32	0.51
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD22	27	0.51
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	2	0.51
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	34	0.51
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	28	0.51
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	6	0.51
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	39	0.51
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG22	11	0.51
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	2	0.51
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	21	0.51
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	38	0.51
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	21	0.51
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG21	31	0.51
(1,171)	1:25:A:LYS:HG2	1:24:A:TRP:HE1	11	0.51
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	20	0.51
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	3	0.51
(1,63)	1:53:A:VAL:H	1:56:A:LYS:HD3	29	0.51
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	25	0.5
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	3	0.5
(1,1986)	1:48:A:LEU:H	1:48:A:LEU:HG	40	0.5
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	15	0.5
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	24	0.5
(1,1782)	1:36:A:MET:HE3	1:37:A:LEU:HA	15	0.5
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD23	16	0.5
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	1	0.5
(1,1458)	1:22:A:THR:HG23	1:23:A:ASP:HA	4	0.5
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD22	29	0.5
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB1	23	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB2	1	0.5
(1,691)	1:15:A:ASN:HB2	1:16:A:GLN:HB3	6	0.5
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	40	0.5
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	21	0.5
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	22	0.5
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	3	0.5
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	35	0.5
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	7	0.5
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	13	0.5
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG13	28	0.5
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	40	0.5
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	2	0.5
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	37	0.5
(1,2401)	1:44:A:THR:HG21	1:44:A:THR:H	27	0.49
(1,2329)	1:27:A:SER:HB2	1:29:A:ALA:H	1	0.49
(1,1990)	1:36:A:MET:HE3	1:35:A:TYR:HE2	10	0.49
(1,1990)	1:36:A:MET:HE3	1:35:A:TYR:HE2	14	0.49
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	8	0.49
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	34	0.49
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD13	40	0.49
(1,1458)	1:22:A:THR:HG21	1:23:A:ASP:HA	13	0.49
(1,1458)	1:22:A:THR:HG23	1:23:A:ASP:HA	28	0.49
(1,1046)	1:50:A:LEU:HD13	1:51:A:TRP:HA	40	0.49
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	3	0.49
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	4	0.49
(1,685)	1:27:A:SER:HB2	1:29:A:ALA:H	1	0.49
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG12	3	0.49
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG13	20	0.49
(1,247)	1:57:A:LYS:H	1:55:A:ARG:H	5	0.49
(1,247)	1:53:A:VAL:H	1:55:A:ARG:H	24	0.49
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	39	0.49
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	29	0.49
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG22	29	0.48
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	26	0.48
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	34	0.48
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	36	0.48
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG13	26	0.48
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG13	33	0.48
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	27	0.48
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG22	3	0.48
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD23	20	0.48
(1,1458)	1:22:A:THR:HG21	1:23:A:ASP:HA	8	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1458)	1:22:A:THR:HG23	1:23:A:ASP:HA	27	0.48
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	30	0.48
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD23	14	0.48
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD21	30	0.48
(1,1046)	1:50:A:LEU:HD23	1:51:A:TRP:HA	20	0.48
(1,920)	1:34:A:ILE:HB	1:35:A:TYR:HE1	33	0.48
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	4	0.48
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	17	0.48
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	27	0.48
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	36	0.48
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	37	0.48
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG22	29	0.48
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	5	0.48
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	19	0.48
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	26	0.48
(1,475)	1:41:A:LEU:HB2	1:44:A:THR:H	26	0.48
(1,427)	1:40:A:LEU:HG	1:43:A:THR:H	36	0.48
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG21	39	0.48
(1,89)	1:20:A:GLU:HG2	1:20:A:GLU:H	20	0.48
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	14	0.47
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	12	0.47
(1,2357)	1:30:A:LEU:H	1:27:A:SER:HA	32	0.47
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	20	0.47
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	18	0.47
(1,1498)	1:30:A:LEU:HD13	1:33:A:ALA:HB2	4	0.47
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	37	0.47
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	18	0.47
(1,1046)	1:53:A:VAL:HG12	1:51:A:TRP:HA	16	0.47
(1,699)	1:16:A:GLN:HA	1:18:A:GLU:H	29	0.47
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	10	0.47
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	14	0.47
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	24	0.47
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB3	20	0.47
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	12	0.47
(1,480)	1:51:A:TRP:HA	1:55:A:ARG:HE	12	0.47
(1,475)	1:41:A:LEU:HB2	1:44:A:THR:H	6	0.47
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	8	0.47
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	18	0.47
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	26	0.47
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	29	0.47
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	35	0.47
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2401)	1:44:A:THR:HG23	1:44:A:THR:H	34	0.46
(1,2401)	1:43:A:THR:HG22	1:44:A:THR:H	36	0.46
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	10	0.46
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE1	24	0.46
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	22	0.46
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	14	0.46
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD23	1	0.46
(1,1458)	1:22:A:THR:HG23	1:23:A:ASP:HA	15	0.46
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	23	0.46
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD23	2	0.46
(1,1313)	1:38:A:VAL:HG23	1:34:A:ILE:HB	13	0.46
(1,1046)	1:50:A:LEU:HD23	1:51:A:TRP:HA	1	0.46
(1,915)	1:49:A:VAL:HG12	1:52:A:THR:HB	14	0.46
(1,915)	1:49:A:VAL:HG23	1:46:A:ASN:HA	20	0.46
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	18	0.46
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	1	0.46
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	25	0.46
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	10	0.46
(1,480)	1:51:A:TRP:HA	1:55:A:ARG:HE	24	0.46
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG13	15	0.46
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	10	0.46
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	40	0.46
(1,63)	1:53:A:VAL:H	1:56:A:LYS:HD3	31	0.46
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	7	0.45
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	38	0.45
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	39	0.45
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	6	0.45
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD21	10	0.45
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD21	17	0.45
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD23	24	0.45
(1,1498)	1:30:A:LEU:HD13	1:33:A:ALA:HB2	28	0.45
(1,1046)	1:50:A:LEU:HD21	1:51:A:TRP:HA	10	0.45
(1,1046)	1:50:A:LEU:HD21	1:51:A:TRP:HA	17	0.45
(1,1046)	1:50:A:LEU:HD23	1:51:A:TRP:HA	24	0.45
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	22	0.45
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	8	0.45
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	10	0.45
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	11	0.45
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	27	0.45
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	31	0.45
(1,475)	1:41:A:LEU:HB3	1:44:A:THR:H	10	0.45
(1,475)	1:41:A:LEU:HB2	1:44:A:THR:H	18	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:20:A:GLU:HG3	1:20:A:GLU:H	26	0.45
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	3	0.45
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	7	0.45
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	11	0.45
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	14	0.45
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	32	0.45
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	33	0.45
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	34	0.45
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	38	0.45
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	17	0.44
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	22	0.44
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG21	2	0.44
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	32	0.44
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	35	0.44
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	36	0.44
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD13	15	0.44
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD22	26	0.44
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD22	28	0.44
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD13	39	0.44
(1,1458)	1:22:A:THR:HG21	1:23:A:ASP:HA	22	0.44
(1,1458)	1:22:A:THR:HG21	1:23:A:ASP:HA	24	0.44
(1,1458)	1:22:A:THR:HG21	1:23:A:ASP:HA	25	0.44
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	26	0.44
(1,1458)	1:22:A:THR:HG23	1:23:A:ASP:HA	31	0.44
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD21	11	0.44
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD22	27	0.44
(1,1046)	1:50:A:LEU:HD13	1:51:A:TRP:HA	15	0.44
(1,1046)	1:50:A:LEU:HD22	1:51:A:TRP:HA	26	0.44
(1,1046)	1:50:A:LEU:HD22	1:51:A:TRP:HA	28	0.44
(1,1046)	1:50:A:LEU:HD13	1:51:A:TRP:HA	39	0.44
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB1	2	0.44
(1,803)	1:40:A:LEU:HD11	1:44:A:THR:HG21	30	0.44
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	9	0.44
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	38	0.44
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	14	0.44
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	17	0.44
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	18	0.44
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	39	0.44
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	17	0.44
(1,427)	1:41:A:LEU:HB3	1:43:A:THR:H	12	0.44
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	38	0.44
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	17	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	30	0.44
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	39	0.44
(1,2409)	1:18:A:GLU:HG3	1:17:A:SER:H	26	0.43
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	9	0.43
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	2	0.43
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	18	0.43
(1,2329)	1:27:A:SER:HB2	1:29:A:ALA:H	26	0.43
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG21	14	0.43
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	17	0.43
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	23	0.43
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	33	0.43
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD11	19	0.43
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	10	0.43
(1,1458)	1:22:A:THR:HG23	1:23:A:ASP:HA	19	0.43
(1,1046)	1:50:A:LEU:HD11	1:51:A:TRP:HA	19	0.43
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	6	0.43
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	30	0.43
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB2	8	0.43
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	37	0.43
(1,685)	1:27:A:SER:HB2	1:29:A:ALA:H	26	0.43
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	3	0.43
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	13	0.43
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	3	0.43
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	13	0.43
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB2	29	0.43
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	15	0.43
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	27	0.43
(1,475)	1:41:A:LEU:HB2	1:44:A:THR:H	33	0.43
(1,444)	1:13:A:ALA:H	1:11:A:TYR:HB3	20	0.43
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG13	36	0.43
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	40	0.43
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	28	0.43
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	13	0.43
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	16	0.43
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	25	0.43
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	13	0.42
(1,2341)	1:54:A:PHE:H	1:50:A:LEU:HG	35	0.42
(1,2203)	1:23:A:ASP:HB2	1:25:A:LYS:H	32	0.42
(1,1990)	1:36:A:MET:HE1	1:35:A:TYR:HE2	11	0.42
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	11	0.42
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	1	0.42
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD21	36	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1046)	1:50:A:LEU:HD21	1:51:A:TRP:HA	36	0.42
(1,983)	1:27:A:SER:HB3	1:29:A:ALA:HB3	15	0.42
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD11	9	0.42
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD13	24	0.42
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	28	0.42
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	33	0.42
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	7	0.42
(1,427)	1:41:A:LEU:HB2	1:43:A:THR:H	40	0.42
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	9	0.42
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	21	0.42
(1,2203)	1:23:A:ASP:HB3	1:25:A:LYS:H	5	0.41
(1,1990)	1:36:A:MET:HE3	1:35:A:TYR:HE2	19	0.41
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	13	0.41
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	13	0.41
(1,1896)	1:36:A:MET:HE2	1:40:A:LEU:HB3	35	0.41
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	9	0.41
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD23	3	0.41
(1,1498)	1:30:A:LEU:HD11	1:33:A:ALA:HB2	17	0.41
(1,1498)	1:30:A:LEU:HD11	1:33:A:ALA:HB3	39	0.41
(1,1458)	1:22:A:THR:HG23	1:23:A:ASP:HA	12	0.41
(1,1046)	1:50:A:LEU:HD23	1:51:A:TRP:HA	3	0.41
(1,1038)	1:40:A:LEU:HG	1:36:A:MET:HG3	36	0.41
(1,983)	1:26:A:SER:HB2	1:29:A:ALA:HB3	11	0.41
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	39	0.41
(1,915)	1:49:A:VAL:HG22	1:46:A:ASN:HA	26	0.41
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	6	0.41
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	9	0.41
(1,430)	1:15:A:ASN:H	1:16:A:GLN:HB3	40	0.41
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG21	12	0.41
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	22	0.41
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	24	0.41
(1,89)	1:20:A:GLU:HG3	1:20:A:GLU:H	23	0.41
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	28	0.41
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	5	0.41
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	27	0.4
(1,2341)	1:54:A:PHE:H	1:50:A:LEU:HG	18	0.4
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	27	0.4
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	33	0.4
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	12	0.4
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	13	0.4
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	14	0.4
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	22	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	28	0.4
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	33	0.4
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	5	0.4
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	11	0.4
(1,1458)	1:22:A:THR:HG21	1:23:A:ASP:HA	5	0.4
(1,1458)	1:22:A:THR:HG21	1:23:A:ASP:HA	14	0.4
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	34	0.4
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	38	0.4
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD23	36	0.4
(1,1313)	1:38:A:VAL:HG23	1:34:A:ILE:HB	14	0.4
(1,1313)	1:38:A:VAL:HG23	1:34:A:ILE:HB	25	0.4
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB1	24	0.4
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	23	0.4
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	35	0.4
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	27	0.4
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	33	0.4
(1,494)	1:46:A:ASN:H	1:50:A:LEU:HD12	24	0.4
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	1	0.4
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	6	0.4
(1,480)	1:51:A:TRP:HA	1:55:A:ARG:HE	29	0.4
(1,430)	1:15:A:ASN:H	1:16:A:GLN:HB3	39	0.4
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	4	0.4
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	6	0.4
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	23	0.4
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	27	0.4
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	27	0.39
(1,2401)	1:44:A:THR:HG21	1:44:A:THR:H	21	0.39
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	11	0.39
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	35	0.39
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	6	0.39
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG13	11	0.39
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	3	0.39
(1,1986)	1:48:A:LEU:H	1:48:A:LEU:HG	20	0.39
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	32	0.39
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	11	0.39
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG22	7	0.39
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	39	0.39
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD22	23	0.39
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD22	33	0.39
(1,1046)	1:50:A:LEU:HD22	1:51:A:TRP:HA	23	0.39
(1,1046)	1:50:A:LEU:HD22	1:51:A:TRP:HA	33	0.39
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB3	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,944)	1:30:A:LEU:HA	1:29:A:ALA:HB2	32	0.39
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	6	0.39
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	14	0.39
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	16	0.39
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	27	0.39
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	11	0.39
(1,480)	1:51:A:TRP:HA	1:55:A:ARG:HE	2	0.39
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	40	0.39
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	1	0.39
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	3	0.39
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	30	0.39
(1,89)	1:20:A:GLU:HG3	1:20:A:GLU:H	6	0.39
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	36	0.39
(1,63)	1:53:A:VAL:H	1:56:A:LYS:HD3	12	0.39
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	5	0.38
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	6	0.38
(1,2148)	1:22:A:THR:H	1:18:A:GLU:HB2	8	0.38
(1,2121)	1:22:A:THR:H	1:20:A:GLU:HA	37	0.38
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	4	0.38
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	7	0.38
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	10	0.38
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	11	0.38
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	12	0.38
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	18	0.38
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	19	0.38
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	21	0.38
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	24	0.38
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	25	0.38
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	36	0.38
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	37	0.38
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	5	0.38
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	20	0.38
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	4	0.38
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	21	0.38
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD22	38	0.38
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD22	5	0.38
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD22	23	0.38
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	40	0.38
(1,1046)	1:50:A:LEU:HD22	1:51:A:TRP:HA	38	0.38
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	36	0.38
(1,915)	1:49:A:VAL:HG11	1:52:A:THR:HB	33	0.38
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	16	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:46:A:ASN:H	1:50:A:LEU:HD12	1	0.38
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	19	0.38
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	4	0.38
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	15	0.38
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	19	0.38
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	25	0.38
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	36	0.38
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	27	0.38
(1,2401)	1:44:A:THR:HG23	1:44:A:THR:H	15	0.37
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	24	0.37
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	28	0.37
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	35	0.37
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	1	0.37
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	5	0.37
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	6	0.37
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	8	0.37
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	16	0.37
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	23	0.37
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	29	0.37
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	30	0.37
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	34	0.37
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	35	0.37
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	26	0.37
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	31	0.37
(1,1896)	1:36:A:MET:HE1	1:40:A:LEU:HB3	21	0.37
(1,1754)	1:53:A:VAL:HG22	1:56:A:LYS:HD3	5	0.37
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD22	29	0.37
(1,1046)	1:50:A:LEU:HD22	1:51:A:TRP:HA	29	0.37
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	14	0.37
(1,920)	1:34:A:ILE:HB	1:35:A:TYR:HE1	12	0.37
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	24	0.37
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	28	0.37
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	35	0.37
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	12	0.37
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	34	0.37
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	13	0.37
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	16	0.37
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	34	0.37
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	20	0.37
(1,63)	1:53:A:VAL:H	1:56:A:LYS:HD3	5	0.37
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	38	0.36
(1,2329)	1:27:A:SER:HB2	1:29:A:ALA:H	20	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	40	0.36
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	2	0.36
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	9	0.36
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	17	0.36
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	26	0.36
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	31	0.36
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	38	0.36
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	39	0.36
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	14	0.36
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG22	12	0.36
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD23	31	0.36
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD22	24	0.36
(1,1046)	1:50:A:LEU:HD23	1:51:A:TRP:HA	31	0.36
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB3	40	0.36
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	10	0.36
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	37	0.36
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	30	0.36
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	34	0.36
(1,685)	1:27:A:SER:HB2	1:29:A:ALA:H	20	0.36
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	9	0.36
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	12	0.36
(1,494)	1:46:A:ASN:H	1:50:A:LEU:HD12	16	0.36
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB1	12	0.36
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	38	0.36
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	8	0.36
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	28	0.36
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	20	0.36
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	23	0.36
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	8	0.36
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	14	0.36
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	40	0.36
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG21	32	0.35
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	34	0.35
(1,1990)	1:36:A:MET:HE3	1:35:A:TYR:HE2	7	0.35
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	13	0.35
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	18	0.35
(1,1458)	1:22:A:THR:HG23	1:23:A:ASP:HA	29	0.35
(1,1458)	1:22:A:THR:HG23	1:23:A:ASP:HA	39	0.35
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	17	0.35
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	34	0.35
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HG	24	0.35
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG21	32	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	29	0.35
(1,494)	1:46:A:ASN:H	1:50:A:LEU:HD12	17	0.35
(1,430)	1:15:A:ASN:H	1:16:A:GLN:HB3	12	0.35
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG21	16	0.35
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	19	0.35
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	10	0.35
(1,2401)	1:44:A:THR:HG21	1:44:A:THR:H	17	0.34
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	24	0.34
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	12	0.34
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	11	0.34
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	32	0.34
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	5	0.34
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	11	0.34
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	24	0.34
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD21	14	0.34
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD23	8	0.34
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD23	25	0.34
(1,1358)	1:30:A:LEU:HA	1:33:A:ALA:HB1	33	0.34
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	3	0.34
(1,1158)	1:23:A:ASP:HB2	1:20:A:GLU:HA	38	0.34
(1,1046)	1:50:A:LEU:HD21	1:51:A:TRP:HA	14	0.34
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB3	19	0.34
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	29	0.34
(1,691)	1:15:A:ASN:HB2	1:16:A:GLN:HB3	12	0.34
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	11	0.34
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	7	0.34
(1,491)	1:37:A:LEU:H	1:41:A:LEU:HB2	15	0.34
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	24	0.34
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	10	0.34
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	1	0.34
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG21	28	0.34
(1,83)	1:48:A:LEU:H	1:51:A:TRP:HB3	26	0.34
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	9	0.34
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	15	0.33
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	3	0.33
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	38	0.33
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	4	0.33
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	37	0.33
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	5	0.33
(1,2187)	1:41:A:LEU:H	1:42:A:GLY:HA3	5	0.33
(1,2148)	1:22:A:THR:H	1:18:A:GLU:HB2	17	0.33
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG22	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1896)	1:36:A:MET:HE1	1:40:A:LEU:HB3	26	0.33
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	1	0.33
(1,1774)	1:21:A:TYR:HB3	1:22:A:THR:HG22	7	0.33
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	32	0.33
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	25	0.33
(1,920)	1:34:A:ILE:HB	1:35:A:TYR:HE1	28	0.33
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	1	0.33
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	5	0.33
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	1	0.33
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	15	0.33
(1,553)	1:48:A:LEU:HB2	1:45:A:GLY:H	4	0.33
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	16	0.33
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	30	0.33
(1,494)	1:46:A:ASN:H	1:50:A:LEU:HD13	31	0.33
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	22	0.33
(1,475)	1:41:A:LEU:HB2	1:44:A:THR:H	11	0.33
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	34	0.33
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	10	0.33
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	24	0.33
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	37	0.33
(1,2401)	1:44:A:THR:HG23	1:44:A:THR:H	37	0.32
(1,1990)	1:36:A:MET:HE1	1:35:A:TYR:HE2	29	0.32
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	6	0.32
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	27	0.32
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	36	0.32
(1,1896)	1:36:A:MET:HE1	1:40:A:LEU:HB3	1	0.32
(1,1409)	1:13:A:ALA:HB3	1:10:A:TYR:HA	27	0.32
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD22	26	0.32
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	37	0.32
(1,915)	1:49:A:VAL:HG12	1:52:A:THR:HB	2	0.32
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	4	0.32
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	32	0.32
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	9	0.32
(1,430)	1:15:A:ASN:H	1:16:A:GLN:HB3	37	0.32
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG21	9	0.32
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	15	0.32
(1,247)	1:53:A:VAL:H	1:55:A:ARG:H	12	0.32
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	20	0.32
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	4	0.32
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	4	0.32
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	1	0.31
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB3	31	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	13	0.31
(1,2080)	1:46:A:ASN:H	1:44:A:THR:HB	40	0.31
(1,2079)	1:40:A:LEU:H	1:43:A:THR:HG21	35	0.31
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG21	21	0.31
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	8	0.31
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	31	0.31
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	34	0.31
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	2	0.31
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	24	0.31
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	27	0.31
(1,1774)	1:21:A:TYR:HB3	1:22:A:THR:HG23	36	0.31
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	21	0.31
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	36	0.31
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB3	5	0.31
(1,915)	1:49:A:VAL:HG12	1:52:A:THR:HB	29	0.31
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	14	0.31
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	25	0.31
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	23	0.31
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	1	0.31
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB3	31	0.31
(1,2401)	1:44:A:THR:HG23	1:44:A:THR:H	2	0.3
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	24	0.3
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	7	0.3
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	29	0.3
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG11	13	0.3
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG22	36	0.3
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	13	0.3
(1,1498)	1:30:A:LEU:HD12	1:33:A:ALA:HB3	22	0.3
(1,1409)	1:13:A:ALA:HB2	1:10:A:TYR:HA	4	0.3
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	5	0.3
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	39	0.3
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	11	0.3
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	16	0.3
(1,983)	1:26:A:SER:HB2	1:29:A:ALA:HB3	34	0.3
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	8	0.3
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	21	0.3
(1,699)	1:16:A:GLN:HA	1:18:A:GLU:H	36	0.3
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	26	0.3
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB2	9	0.3
(1,475)	1:41:A:LEU:HB3	1:44:A:THR:H	14	0.3
(1,427)	1:41:A:LEU:HB3	1:43:A:THR:H	15	0.3
(1,427)	1:41:A:LEU:HB2	1:43:A:THR:H	26	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG21	11	0.3
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	28	0.3
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	22	0.3
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG21	14	0.29
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	36	0.29
(1,2203)	1:23:A:ASP:HB3	1:25:A:LYS:H	16	0.29
(1,2203)	1:23:A:ASP:HB2	1:20:A:GLU:H	18	0.29
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	18	0.29
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	35	0.29
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG21	33	0.29
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	13	0.29
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	28	0.29
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	12	0.29
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	16	0.29
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	32	0.29
(1,1530)	1:39:A:PHE:HB2	1:38:A:VAL:HG11	33	0.29
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	33	0.29
(1,1455)	1:51:A:TRP:HD1	1:55:A:ARG:HG2	35	0.29
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD23	39	0.29
(1,1313)	1:38:A:VAL:HG23	1:34:A:ILE:HB	8	0.29
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	31	0.29
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	14	0.29
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	22	0.29
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	23	0.29
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD13	11	0.29
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	10	0.29
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	36	0.29
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG21	14	0.29
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB3	27	0.29
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB3	34	0.29
(1,430)	1:15:A:ASN:H	1:16:A:GLN:HB3	18	0.29
(1,427)	1:41:A:LEU:HB2	1:43:A:THR:H	14	0.29
(1,427)	1:41:A:LEU:HB3	1:43:A:THR:H	25	0.29
(1,247)	1:53:A:VAL:H	1:55:A:ARG:H	2	0.29
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	10	0.29
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	19	0.29
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG22	39	0.28
(1,2392)	1:21:A:TYR:H	1:20:A:GLU:HB3	5	0.28
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	8	0.28
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	25	0.28
(1,2121)	1:22:A:THR:H	1:20:A:GLU:HA	38	0.28
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	33	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	8	0.28
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	2	0.28
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	3	0.28
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	7	0.28
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	16	0.28
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	22	0.28
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	25	0.28
(1,1774)	1:21:A:TYR:HB3	1:22:A:THR:HG21	11	0.28
(1,1498)	1:30:A:LEU:HD11	1:33:A:ALA:HB1	18	0.28
(1,1409)	1:13:A:ALA:HB3	1:11:A:TYR:HA	7	0.28
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	6	0.28
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	24	0.28
(1,1095)	1:41:A:LEU:HG	1:37:A:LEU:HG	40	0.28
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	22	0.28
(1,915)	1:49:A:VAL:HG12	1:52:A:THR:HB	12	0.28
(1,915)	1:49:A:VAL:HG13	1:52:A:THR:HB	28	0.28
(1,664)	1:26:A:SER:HA	1:25:A:LYS:HB3	32	0.28
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	36	0.28
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	2	0.28
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG22	39	0.28
(1,480)	1:52:A:THR:HB	1:55:A:ARG:HE	4	0.28
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG23	38	0.28
(1,247)	1:53:A:VAL:H	1:55:A:ARG:H	29	0.28
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	40	0.28
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	1	0.28
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG21	36	0.27
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	4	0.27
(1,2203)	1:23:A:ASP:HB3	1:25:A:LYS:H	25	0.27
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	15	0.27
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	19	0.27
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	37	0.27
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	20	0.27
(1,1759)	1:36:A:MET:HG3	1:33:A:ALA:HA	5	0.27
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	20	0.27
(1,915)	1:49:A:VAL:HG23	1:46:A:ASN:HA	40	0.27
(1,699)	1:16:A:GLN:HA	1:18:A:GLU:H	6	0.27
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	11	0.27
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	8	0.27
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	22	0.27
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	31	0.27
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG21	36	0.27
(1,532)	1:8:A:ASP:H	1:9:A:ASN:H	31	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:36:A:MET:H	1:37:A:LEU:HB3	38	0.27
(1,171)	1:25:A:LYS:HG2	1:24:A:TRP:HE1	31	0.27
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	5	0.27
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	26	0.27
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	29	0.27
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	21	0.27
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	9	0.26
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB3	1	0.26
(1,2121)	1:22:A:THR:H	1:20:A:GLU:HA	22	0.26
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	37	0.26
(1,1986)	1:37:A:LEU:H	1:37:A:LEU:HG	15	0.26
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG23	37	0.26
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	4	0.26
(1,1774)	1:21:A:TYR:HB3	1:22:A:THR:HG22	6	0.26
(1,1774)	1:21:A:TYR:HB3	1:22:A:THR:HG23	17	0.26
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD22	25	0.26
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD21	30	0.26
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	18	0.26
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	7	0.26
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	10	0.26
(1,1046)	1:50:A:LEU:HD22	1:51:A:TRP:HA	25	0.26
(1,1046)	1:50:A:LEU:HD21	1:51:A:TRP:HA	30	0.26
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD12	5	0.26
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB3	36	0.26
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB3	15	0.26
(1,691)	1:15:A:ASN:HB2	1:16:A:GLN:HB3	24	0.26
(1,427)	1:41:A:LEU:HB3	1:43:A:THR:H	37	0.26
(1,171)	1:25:A:LYS:HG2	1:24:A:TRP:HE1	17	0.26
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	17	0.26
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB2	14	0.25
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	12	0.25
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	16	0.25
(1,1896)	1:36:A:MET:HE1	1:40:A:LEU:HB3	3	0.25
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	29	0.25
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	34	0.25
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	40	0.25
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD13	36	0.25
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	18	0.25
(1,915)	1:49:A:VAL:HG21	1:46:A:ASN:HA	24	0.25
(1,915)	1:49:A:VAL:HG21	1:46:A:ASN:HA	34	0.25
(1,915)	1:49:A:VAL:HG23	1:46:A:ASN:HA	38	0.25
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	40	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB2	14	0.25
(1,427)	1:41:A:LEU:HB3	1:43:A:THR:H	27	0.25
(1,412)	1:33:A:ALA:H	1:34:A:ILE:HG13	24	0.25
(1,198)	1:51:A:TRP:H	1:47:A:GLY:HA2	36	0.25
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	24	0.25
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG22	4	0.24
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG21	17	0.24
(1,2409)	1:18:A:GLU:HG3	1:17:A:SER:H	23	0.24
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	7	0.24
(1,2203)	1:23:A:ASP:HB2	1:20:A:GLU:H	34	0.24
(1,2121)	1:22:A:THR:H	1:20:A:GLU:HA	21	0.24
(1,1896)	1:36:A:MET:HE1	1:40:A:LEU:HB3	32	0.24
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	10	0.24
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	37	0.24
(1,1311)	1:44:A:THR:HG22	1:40:A:LEU:HA	27	0.24
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	10	0.24
(1,1181)	1:32:A:PRO:HA	1:34:A:ILE:H	11	0.24
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	17	0.24
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	20	0.24
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	28	0.24
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	40	0.24
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB3	30	0.24
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD11	40	0.24
(1,915)	1:49:A:VAL:HG21	1:46:A:ASN:HA	10	0.24
(1,691)	1:15:A:ASN:HB2	1:16:A:GLN:HB3	17	0.24
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG22	4	0.24
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG21	17	0.24
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	38	0.24
(1,434)	1:61:A:HIS:H	1:61:A:HIS:HB2	22	0.24
(1,434)	1:61:A:HIS:H	1:61:A:HIS:HB3	22	0.24
(1,430)	1:15:A:ASN:H	1:18:A:GLU:HB2	6	0.24
(1,430)	1:15:A:ASN:H	1:16:A:GLN:HB3	9	0.24
(1,427)	1:41:A:LEU:HB2	1:43:A:THR:H	10	0.24
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	35	0.24
(1,89)	1:20:A:GLU:HG2	1:20:A:GLU:H	24	0.24
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	35	0.24
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	9	0.24
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	28	0.23
(1,2401)	1:44:A:THR:HG23	1:44:A:THR:H	11	0.23
(1,2401)	1:44:A:THR:HG21	1:44:A:THR:H	22	0.23
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB2	9	0.23
(1,2203)	1:23:A:ASP:HB3	1:25:A:LYS:H	22	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB3	24	0.23
(1,2121)	1:22:A:THR:H	1:20:A:GLU:HA	15	0.23
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG11	18	0.23
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	20	0.23
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	35	0.23
(1,1896)	1:36:A:MET:HE2	1:40:A:LEU:HB3	20	0.23
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	37	0.23
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	28	0.23
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	31	0.23
(1,1494)	1:15:A:ASN:HA	1:18:A:GLU:HB3	28	0.23
(1,1358)	1:30:A:LEU:HA	1:33:A:ALA:HB2	38	0.23
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	2	0.23
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	4	0.23
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	11	0.23
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	23	0.23
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	28	0.23
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	5	0.23
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	29	0.23
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	35	0.23
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB1	14	0.23
(1,959)	1:57:A:LYS:HD2	1:57:A:LYS:HA	24	0.23
(1,959)	1:57:A:LYS:HD3	1:57:A:LYS:HA	24	0.23
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	31	0.23
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	33	0.23
(1,915)	1:49:A:VAL:HG23	1:46:A:ASN:HA	1	0.23
(1,915)	1:49:A:VAL:HG21	1:46:A:ASN:HA	7	0.23
(1,803)	1:40:A:LEU:HD12	1:44:A:THR:HG22	40	0.23
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	31	0.23
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	8	0.23
(1,606)	1:33:A:ALA:H	1:30:A:LEU:HB2	15	0.23
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	28	0.23
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB2	9	0.23
(1,176)	1:36:A:MET:H	1:37:A:LEU:HB2	29	0.23
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	23	0.23
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	28	0.23
(1,6)	1:54:A:PHE:H	1:50:A:LEU:HB3	31	0.23
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG22	2	0.22
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG21	21	0.22
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG22	26	0.22
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	10	0.22
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB3	20	0.22
(1,2121)	1:22:A:THR:H	1:18:A:GLU:HA	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG11	32	0.22
(1,1990)	1:36:A:MET:HE2	1:35:A:TYR:HE2	33	0.22
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	26	0.22
(1,1530)	1:39:A:PHE:HB2	1:38:A:VAL:HG13	35	0.22
(1,1498)	1:30:A:LEU:HD11	1:33:A:ALA:HB2	25	0.22
(1,1494)	1:15:A:ASN:HA	1:18:A:GLU:HB3	18	0.22
(1,1458)	1:22:A:THR:HG23	1:23:A:ASP:HA	3	0.22
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	21	0.22
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	23	0.22
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	26	0.22
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD11	7	0.22
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD13	26	0.22
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD13	34	0.22
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	32	0.22
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	24	0.22
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG22	2	0.22
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG21	21	0.22
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG22	26	0.22
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	37	0.22
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB3	16	0.22
(1,427)	1:41:A:LEU:HB2	1:43:A:THR:H	22	0.22
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG23	19	0.22
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG23	29	0.22
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	2	0.22
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	27	0.22
(1,2401)	1:44:A:THR:HG21	1:44:A:THR:H	1	0.21
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG13	2	0.21
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG11	6	0.21
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG22	1	0.21
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	8	0.21
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	38	0.21
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	7	0.21
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD12	35	0.21
(1,1000)	1:54:A:PHE:HB2	1:51:A:TRP:HE3	36	0.21
(1,1000)	1:54:A:PHE:HB3	1:51:A:TRP:HE3	36	0.21
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB2	3	0.21
(1,915)	1:49:A:VAL:HG22	1:46:A:ASN:HA	11	0.21
(1,915)	1:49:A:VAL:HG12	1:52:A:THR:HB	27	0.21
(1,908)	1:32:A:PRO:HG2	1:33:A:ALA:HA	33	0.21
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	28	0.21
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	38	0.21
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB2	11	0.21
(1,550)	1:41:A:LEU:H	1:44:A:THR:H	9	0.21
(1,466)	1:46:A:ASN:HD21	1:44:A:THR:HB	40	0.21
(1,427)	1:41:A:LEU:HB2	1:43:A:THR:H	6	0.21
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	18	0.21
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	34	0.21
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG22	18	0.2
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	22	0.2
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	39	0.2
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	11	0.2
(1,2377)	1:46:A:ASN:H	1:43:A:THR:HA	21	0.2
(1,2203)	1:23:A:ASP:HB3	1:25:A:LYS:H	4	0.2
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	25	0.2
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG21	38	0.2
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	10	0.2
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	9	0.2
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	18	0.2
(1,1358)	1:30:A:LEU:HA	1:33:A:ALA:HB3	35	0.2
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	15	0.2
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	18	0.2
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD12	2	0.2
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD11	28	0.2
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	1	0.2
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	7	0.2
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	29	0.2
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB2	5	0.2
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG22	18	0.2
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	22	0.2
(1,427)	1:41:A:LEU:HB2	1:43:A:THR:H	18	0.2
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG23	36	0.2
(1,302)	1:39:A:PHE:H	1:37:A:LEU:HB3	19	0.2
(1,198)	1:51:A:TRP:H	1:47:A:GLY:HA2	4	0.2
(1,198)	1:51:A:TRP:H	1:47:A:GLY:HA2	21	0.2
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	32	0.2
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	12	0.2
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	15	0.2
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	22	0.2
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	32	0.2
(1,2401)	1:44:A:THR:HG21	1:44:A:THR:H	31	0.19
(1,2384)	1:47:A:GLY:H	1:50:A:LEU:HG	21	0.19
(1,2377)	1:46:A:ASN:H	1:43:A:THR:HA	36	0.19
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	37	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2121)	1:22:A:THR:H	1:20:A:GLU:HA	3	0.19
(1,2053)	1:35:A:TYR:H	1:34:A:ILE:HG13	33	0.19
(1,1964)	1:47:A:GLY:HA2	1:50:A:LEU:HG	5	0.19
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD22	5	0.19
(1,1554)	1:51:A:TRP:HA	1:50:A:LEU:HD22	6	0.19
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	9	0.19
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	16	0.19
(1,1181)	1:32:A:PRO:HA	1:34:A:ILE:H	5	0.19
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	2	0.19
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	12	0.19
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	24	0.19
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	34	0.19
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	39	0.19
(1,1046)	1:50:A:LEU:HD22	1:51:A:TRP:HA	5	0.19
(1,1046)	1:50:A:LEU:HD22	1:51:A:TRP:HA	6	0.19
(1,898)	1:50:A:LEU:HB2	1:51:A:TRP:HD1	36	0.19
(1,898)	1:50:A:LEU:HB3	1:51:A:TRP:HD1	36	0.19
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	21	0.19
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	23	0.19
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	40	0.19
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	37	0.19
(1,612)	1:35:A:TYR:H	1:34:A:ILE:HG13	33	0.19
(1,553)	1:48:A:LEU:HB3	1:45:A:GLY:H	15	0.19
(1,430)	1:15:A:ASN:H	1:16:A:GLN:HB3	11	0.19
(1,176)	1:36:A:MET:H	1:32:A:PRO:HB3	37	0.19
(1,171)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	7	0.19
(1,2392)	1:21:A:TYR:H	1:20:A:GLU:HB3	39	0.18
(1,2203)	1:23:A:ASP:HB3	1:25:A:LYS:H	3	0.18
(1,2203)	1:23:A:ASP:HB3	1:25:A:LYS:H	23	0.18
(1,2203)	1:23:A:ASP:HB3	1:25:A:LYS:H	38	0.18
(1,2121)	1:22:A:THR:H	1:20:A:GLU:HA	6	0.18
(1,1964)	1:47:A:GLY:HA2	1:50:A:LEU:HG	18	0.18
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG21	30	0.18
(1,1896)	1:36:A:MET:HE3	1:40:A:LEU:HB3	31	0.18
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	14	0.18
(1,1189)	1:30:A:LEU:HA	1:30:A:LEU:HD13	3	0.18
(1,1189)	1:30:A:LEU:HA	1:30:A:LEU:HD12	40	0.18
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	3	0.18
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	16	0.18
(1,1011)	1:28:A:GLY:HA3	1:29:A:ALA:HB3	15	0.18
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	3	0.18
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	24	0.18
(1,915)	1:49:A:VAL:HG23	1:46:A:ASN:HA	3	0.18
(1,772)	1:53:A:VAL:HG11	1:57:A:LYS:HB2	2	0.18
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	35	0.18
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	13	0.18
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	34	0.18
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB1	11	0.18
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB1	28	0.18
(1,430)	1:15:A:ASN:H	1:16:A:GLN:HB3	10	0.18
(1,409)	1:36:A:MET:H	1:34:A:ILE:HG22	24	0.18
(1,89)	1:20:A:GLU:HG2	1:20:A:GLU:H	1	0.18
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	3	0.18
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	13	0.18
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	16	0.18
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	34	0.18
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	38	0.18
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	39	0.18
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	39	0.18
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB2	7	0.17
(1,2329)	1:27:A:SER:HB2	1:29:A:ALA:H	18	0.17
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	11	0.17
(1,2121)	1:22:A:THR:H	1:20:A:GLU:HA	29	0.17
(1,2053)	1:35:A:TYR:H	1:34:A:ILE:HG13	25	0.17
(1,1990)	1:36:A:MET:HE3	1:35:A:TYR:HE2	21	0.17
(1,1896)	1:36:A:MET:HE2	1:40:A:LEU:HB3	39	0.17
(1,1890)	1:38:A:VAL:HA	1:41:A:LEU:HB2	40	0.17
(1,1890)	1:38:A:VAL:HA	1:41:A:LEU:HB3	40	0.17
(1,1696)	1:38:A:VAL:HA	1:41:A:LEU:HB2	40	0.17
(1,1696)	1:38:A:VAL:HA	1:41:A:LEU:HB3	40	0.17
(1,1494)	1:15:A:ASN:HA	1:18:A:GLU:HB2	12	0.17
(1,1409)	1:13:A:ALA:HB3	1:10:A:TYR:HA	30	0.17
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	38	0.17
(1,1189)	1:30:A:LEU:HA	1:30:A:LEU:HD13	30	0.17
(1,1181)	1:32:A:PRO:HA	1:34:A:ILE:H	32	0.17
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	13	0.17
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	14	0.17
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	22	0.17
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	25	0.17
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	30	0.17
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	32	0.17
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	33	0.17
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	38	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1098)	1:58:A:GLY:HA2	1:59:A:HIS:HD2	39	0.17
(1,1098)	1:58:A:GLY:HA3	1:59:A:HIS:HD2	39	0.17
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB3	10	0.17
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	5	0.17
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	27	0.17
(1,685)	1:27:A:SER:HB2	1:29:A:ALA:H	18	0.17
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	25	0.17
(1,612)	1:35:A:TYR:H	1:34:A:ILE:HG13	25	0.17
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB1	2	0.17
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB2	7	0.17
(1,430)	1:15:A:ASN:H	1:16:A:GLN:HB3	28	0.17
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	8	0.17
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	14	0.17
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	25	0.17
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	30	0.17
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	1	0.17
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	9	0.16
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB2	8	0.16
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB2	27	0.16
(1,2255)	1:42:A:GLY:HA2	1:44:A:THR:H	18	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	3	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	7	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	11	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	13	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	14	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	16	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	20	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	21	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	25	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	28	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	30	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	33	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	37	0.16
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	38	0.16
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB2	4	0.16
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG13	7	0.16
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG12	14	0.16
(1,1964)	1:47:A:GLY:HA2	1:50:A:LEU:HG	2	0.16
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	2	0.16
(1,1896)	1:36:A:MET:HE2	1:40:A:LEU:HB3	17	0.16
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	29	0.16
(1,1409)	1:13:A:ALA:HB3	1:11:A:TYR:HA	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1378)	1:45:A:GLY:H	1:48:A:LEU:HD21	38	0.16
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	12	0.16
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	4	0.16
(1,1189)	1:30:A:LEU:HA	1:30:A:LEU:HD12	13	0.16
(1,1181)	1:32:A:PRO:HA	1:34:A:ILE:H	34	0.16
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	7	0.16
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	11	0.16
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	27	0.16
(1,955)	1:45:A:GLY:HA2	1:48:A:LEU:HG	17	0.16
(1,915)	1:49:A:VAL:HG12	1:52:A:THR:HB	6	0.16
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	19	0.16
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	15	0.16
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	9	0.16
(1,550)	1:41:A:LEU:H	1:37:A:LEU:H	36	0.16
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB3	23	0.16
(1,491)	1:37:A:LEU:H	1:33:A:ALA:HB1	40	0.16
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB2	8	0.16
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB2	27	0.16
(1,475)	1:41:A:LEU:HB3	1:44:A:THR:H	16	0.16
(1,463)	1:58:A:GLY:H	1:59:A:HIS:HA	39	0.16
(1,302)	1:39:A:PHE:H	1:37:A:LEU:HB3	12	0.16
(1,302)	1:39:A:PHE:H	1:37:A:LEU:HB3	30	0.16
(1,247)	1:53:A:VAL:H	1:55:A:ARG:H	31	0.16
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	4	0.16
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	6	0.16
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	7	0.16
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	11	0.16
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	27	0.16
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	33	0.16
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	15	0.16
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG23	31	0.15
(1,2255)	1:42:A:GLY:HA2	1:44:A:THR:H	6	0.15
(1,2203)	1:23:A:ASP:HB3	1:25:A:LYS:H	11	0.15
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	1	0.15
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	4	0.15
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	9	0.15
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	22	0.15
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	23	0.15
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	26	0.15
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	32	0.15
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	34	0.15
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	39	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB3	14	0.15
(1,2148)	1:22:A:THR:H	1:18:A:GLU:HB2	31	0.15
(1,2121)	1:22:A:THR:H	1:18:A:GLU:HA	31	0.15
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG13	3	0.15
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG13	36	0.15
(1,2069)	1:3:A:GLU:H	1:3:A:GLU:HA	29	0.15
(1,1964)	1:47:A:GLY:HA2	1:50:A:LEU:HG	6	0.15
(1,1945)	1:55:A:ARG:HA	1:54:A:PHE:HD2	36	0.15
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	39	0.15
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	2	0.15
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	10	0.15
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	12	0.15
(1,1774)	1:21:A:TYR:HB3	1:22:A:THR:HG21	21	0.15
(1,1530)	1:39:A:PHE:HB2	1:38:A:VAL:HG13	14	0.15
(1,1530)	1:39:A:PHE:HB2	1:38:A:VAL:HG12	27	0.15
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	1	0.15
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	29	0.15
(1,1189)	1:30:A:LEU:HA	1:30:A:LEU:HD13	19	0.15
(1,1189)	1:30:A:LEU:HA	1:30:A:LEU:HD13	28	0.15
(1,1181)	1:32:A:PRO:HA	1:34:A:ILE:H	1	0.15
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	4	0.15
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	37	0.15
(1,920)	1:34:A:ILE:HB	1:35:A:TYR:HE1	39	0.15
(1,915)	1:49:A:VAL:HG13	1:52:A:THR:HB	9	0.15
(1,915)	1:49:A:VAL:HG12	1:52:A:THR:HB	23	0.15
(1,737)	1:28:A:GLY:HA2	1:32:A:PRO:HG2	32	0.15
(1,737)	1:28:A:GLY:HA2	1:32:A:PRO:HG3	32	0.15
(1,737)	1:28:A:GLY:HA3	1:32:A:PRO:HG2	32	0.15
(1,737)	1:28:A:GLY:HA3	1:32:A:PRO:HG3	32	0.15
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	30	0.15
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	32	0.15
(1,695)	1:28:A:GLY:HA2	1:32:A:PRO:HG2	32	0.15
(1,695)	1:28:A:GLY:HA2	1:32:A:PRO:HG3	32	0.15
(1,695)	1:28:A:GLY:HA3	1:32:A:PRO:HG2	32	0.15
(1,695)	1:28:A:GLY:HA3	1:32:A:PRO:HG3	32	0.15
(1,592)	1:62:A:HIS:H	1:62:A:HIS:HA	21	0.15
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG23	31	0.15
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	3	0.15
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	13	0.15
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	36	0.15
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	40	0.15
(1,427)	1:41:A:LEU:HB2	1:43:A:THR:H	28	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:59:A:HIS:H	1:56:A:LYS:HB3	35	0.15
(1,231)	1:30:A:LEU:HD11	1:27:A:SER:H	32	0.15
(1,231)	1:30:A:LEU:HD12	1:27:A:SER:H	32	0.15
(1,231)	1:30:A:LEU:HD13	1:27:A:SER:H	32	0.15
(1,231)	1:30:A:LEU:HD21	1:27:A:SER:H	32	0.15
(1,231)	1:30:A:LEU:HD22	1:27:A:SER:H	32	0.15
(1,231)	1:30:A:LEU:HD23	1:27:A:SER:H	32	0.15
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	7	0.15
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	34	0.15
(1,89)	1:20:A:GLU:HG2	1:20:A:GLU:H	14	0.15
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG21	38	0.14
(1,2392)	1:21:A:TYR:H	1:20:A:GLU:HB2	29	0.14
(1,2203)	1:23:A:ASP:HB2	1:20:A:GLU:H	14	0.14
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	6	0.14
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	15	0.14
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	17	0.14
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	18	0.14
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	27	0.14
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	35	0.14
(1,2148)	1:22:A:THR:H	1:18:A:GLU:HB3	22	0.14
(1,1964)	1:47:A:GLY:HA2	1:50:A:LEU:HG	12	0.14
(1,1964)	1:47:A:GLY:HA2	1:50:A:LEU:HG	34	0.14
(1,1964)	1:47:A:GLY:HA2	1:50:A:LEU:HG	37	0.14
(1,1759)	1:36:A:MET:HG3	1:33:A:ALA:HA	17	0.14
(1,1530)	1:39:A:PHE:HB2	1:38:A:VAL:HG11	40	0.14
(1,1498)	1:30:A:LEU:HD12	1:33:A:ALA:HB3	9	0.14
(1,1458)	1:22:A:THR:HG22	1:23:A:ASP:HA	9	0.14
(1,1313)	1:38:A:VAL:HG22	1:34:A:ILE:HB	19	0.14
(1,1313)	1:38:A:VAL:HG23	1:34:A:ILE:HB	24	0.14
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	30	0.14
(1,1227)	1:33:A:ALA:H	1:36:A:MET:HG2	33	0.14
(1,1181)	1:32:A:PRO:HA	1:34:A:ILE:H	20	0.14
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	19	0.14
(1,1158)	1:23:A:ASP:HB2	1:20:A:GLU:HA	26	0.14
(1,1011)	1:28:A:GLY:HA3	1:29:A:ALA:HB1	13	0.14
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD12	39	0.14
(1,915)	1:49:A:VAL:HG21	1:46:A:ASN:HA	25	0.14
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	22	0.14
(1,592)	1:62:A:HIS:H	1:62:A:HIS:HA	19	0.14
(1,592)	1:62:A:HIS:H	1:62:A:HIS:HA	20	0.14
(1,592)	1:62:A:HIS:H	1:62:A:HIS:HA	26	0.14
(1,592)	1:62:A:HIS:H	1:62:A:HIS:HA	34	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,592)	1:62:A:HIS:H	1:62:A:HIS:HA	37	0.14
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG21	38	0.14
(1,500)	1:64:A:HIS:HA	1:63:A:HIS:H	22	0.14
(1,475)	1:41:A:LEU:HB3	1:44:A:THR:H	8	0.14
(1,469)	1:51:A:TRP:HE1	1:55:A:ARG:HD2	36	0.14
(1,469)	1:51:A:TRP:HE1	1:55:A:ARG:HD3	36	0.14
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	21	0.14
(1,198)	1:51:A:TRP:H	1:47:A:GLY:HA2	13	0.14
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	5	0.14
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	11	0.14
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	18	0.14
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	30	0.14
(1,176)	1:36:A:MET:H	1:37:A:LEU:HB3	34	0.14
(1,89)	1:20:A:GLU:HG2	1:20:A:GLU:H	19	0.14
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	19	0.14
(1,27)	1:58:A:GLY:HA2	1:61:A:HIS:H	34	0.14
(1,27)	1:58:A:GLY:HA3	1:61:A:HIS:H	34	0.14
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	13	0.14
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	15	0.14
(1,2401)	1:44:A:THR:HG21	1:44:A:THR:H	6	0.13
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	32	0.13
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	8	0.13
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	10	0.13
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	19	0.13
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	36	0.13
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	40	0.13
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB3	6	0.13
(1,2121)	1:22:A:THR:H	1:20:A:GLU:HA	5	0.13
(1,1964)	1:47:A:GLY:HA2	1:50:A:LEU:HG	22	0.13
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG22	19	0.13
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	19	0.13
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	1	0.13
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	6	0.13
(1,1858)	1:28:A:GLY:H	1:27:A:SER:HA	24	0.13
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	27	0.13
(1,1858)	1:28:A:GLY:H	1:27:A:SER:HA	35	0.13
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	40	0.13
(1,1759)	1:36:A:MET:HG3	1:33:A:ALA:HA	3	0.13
(1,1759)	1:36:A:MET:HG3	1:33:A:ALA:HA	18	0.13
(1,1189)	1:30:A:LEU:HA	1:30:A:LEU:HD22	12	0.13
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	6	0.13
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1158)	1:23:A:ASP:HB2	1:20:A:GLU:HA	15	0.13
(1,983)	1:26:A:SER:HB3	1:29:A:ALA:HB2	27	0.13
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD13	4	0.13
(1,915)	1:49:A:VAL:HG13	1:52:A:THR:HB	22	0.13
(1,699)	1:16:A:GLN:HA	1:18:A:GLU:H	2	0.13
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	20	0.13
(1,691)	1:15:A:ASN:HB3	1:16:A:GLN:HB3	8	0.13
(1,628)	1:27:A:SER:H	1:25:A:LYS:HB3	18	0.13
(1,592)	1:62:A:HIS:H	1:62:A:HIS:HA	23	0.13
(1,475)	1:41:A:LEU:HB3	1:44:A:THR:H	3	0.13
(1,466)	1:46:A:ASN:HD21	1:44:A:THR:HB	12	0.13
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	20	0.13
(1,434)	1:61:A:HIS:H	1:61:A:HIS:HB2	17	0.13
(1,434)	1:61:A:HIS:H	1:61:A:HIS:HB3	17	0.13
(1,427)	1:41:A:LEU:HB2	1:43:A:THR:H	11	0.13
(1,302)	1:39:A:PHE:H	1:37:A:LEU:HB3	4	0.13
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	8	0.13
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	31	0.13
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	35	0.13
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	37	0.13
(1,2414)	1:33:A:ALA:H	1:31:A:ILE:HG21	35	0.12
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	8	0.12
(1,2401)	1:44:A:THR:HG23	1:44:A:THR:H	18	0.12
(1,2401)	1:44:A:THR:HG22	1:44:A:THR:H	20	0.12
(1,2401)	1:44:A:THR:HG23	1:44:A:THR:H	23	0.12
(1,2401)	1:44:A:THR:HG21	1:44:A:THR:H	26	0.12
(1,2401)	1:44:A:THR:HG23	1:44:A:THR:H	29	0.12
(1,2357)	1:30:A:LEU:H	1:27:A:SER:HA	18	0.12
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	23	0.12
(1,2296)	1:42:A:GLY:H	1:41:A:LEU:HG	36	0.12
(1,2148)	1:22:A:THR:H	1:20:A:GLU:HB3	19	0.12
(1,2121)	1:22:A:THR:H	1:18:A:GLU:HA	34	0.12
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG11	12	0.12
(1,2048)	1:43:A:THR:H	1:40:A:LEU:HA	38	0.12
(1,1964)	1:47:A:GLY:HA2	1:50:A:LEU:HG	13	0.12
(1,1920)	1:35:A:TYR:H	1:38:A:VAL:HG22	23	0.12
(1,1909)	1:29:A:ALA:HA	1:30:A:LEU:HB3	38	0.12
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	9	0.12
(1,1858)	1:28:A:GLY:H	1:27:A:SER:HA	14	0.12
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	19	0.12
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	20	0.12
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	37	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	39	0.12
(1,1664)	1:34:A:ILE:HB	1:35:A:TYR:HA	26	0.12
(1,1664)	1:34:A:ILE:HB	1:35:A:TYR:HA	35	0.12
(1,1236)	1:35:A:TYR:HB2	1:31:A:ILE:HD11	24	0.12
(1,1236)	1:35:A:TYR:HB2	1:31:A:ILE:HD12	24	0.12
(1,1236)	1:35:A:TYR:HB2	1:31:A:ILE:HD13	24	0.12
(1,1236)	1:35:A:TYR:HB3	1:31:A:ILE:HD11	24	0.12
(1,1236)	1:35:A:TYR:HB3	1:31:A:ILE:HD12	24	0.12
(1,1236)	1:35:A:TYR:HB3	1:31:A:ILE:HD13	24	0.12
(1,1189)	1:30:A:LEU:HA	1:30:A:LEU:HD13	4	0.12
(1,1181)	1:32:A:PRO:HA	1:34:A:ILE:H	14	0.12
(1,1181)	1:32:A:PRO:HA	1:34:A:ILE:H	27	0.12
(1,983)	1:27:A:SER:HB3	1:29:A:ALA:HB1	38	0.12
(1,944)	1:27:A:SER:HA	1:29:A:ALA:HB1	38	0.12
(1,915)	1:49:A:VAL:HG23	1:46:A:ASN:HA	15	0.12
(1,915)	1:49:A:VAL:HG22	1:46:A:ASN:HA	19	0.12
(1,908)	1:32:A:PRO:HG2	1:33:A:ALA:HA	37	0.12
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	23	0.12
(1,592)	1:62:A:HIS:H	1:62:A:HIS:HA	9	0.12
(1,589)	1:33:A:ALA:H	1:31:A:ILE:HG21	35	0.12
(1,480)	1:51:A:TRP:HA	1:55:A:ARG:HE	36	0.12
(1,475)	1:41:A:LEU:HB3	1:44:A:THR:H	9	0.12
(1,475)	1:41:A:LEU:HB3	1:44:A:THR:H	23	0.12
(1,466)	1:46:A:ASN:HD21	1:44:A:THR:HB	17	0.12
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	1	0.12
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	9	0.12
(1,430)	1:15:A:ASN:H	1:16:A:GLN:HB3	38	0.12
(1,302)	1:39:A:PHE:H	1:37:A:LEU:HB3	8	0.12
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	1	0.12
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	14	0.12
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	15	0.12
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	17	0.12
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	33	0.12
(1,21)	1:55:A:ARG:HB2	1:51:A:TRP:HE1	37	0.12
(1,2401)	1:44:A:THR:HG23	1:44:A:THR:H	33	0.11
(1,2357)	1:30:A:LEU:H	1:27:A:SER:HA	17	0.11
(1,2357)	1:30:A:LEU:H	1:27:A:SER:HA	22	0.11
(1,2329)	1:27:A:SER:HB3	1:29:A:ALA:H	9	0.11
(1,2255)	1:42:A:GLY:HA2	1:44:A:THR:H	36	0.11
(1,2203)	1:23:A:ASP:HB2	1:20:A:GLU:H	7	0.11
(1,2155)	1:56:A:LYS:HA	1:56:A:LYS:H	5	0.11
(1,2121)	1:22:A:THR:H	1:18:A:GLU:HA	30	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2121)	1:22:A:THR:H	1:20:A:GLU:HA	40	0.11
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG13	31	0.11
(1,2047)	1:39:A:PHE:H	1:40:A:LEU:HB3	4	0.11
(1,1965)	1:46:A:ASN:HB2	1:44:A:THR:HA	35	0.11
(1,1965)	1:46:A:ASN:HB3	1:44:A:THR:HA	35	0.11
(1,1964)	1:47:A:GLY:HA2	1:50:A:LEU:HG	25	0.11
(1,1964)	1:47:A:GLY:HA2	1:50:A:LEU:HG	27	0.11
(1,1869)	1:23:A:ASP:HB2	1:22:A:THR:HB	26	0.11
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	5	0.11
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	15	0.11
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	16	0.11
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	21	0.11
(1,1858)	1:28:A:GLY:H	1:27:A:SER:HA	26	0.11
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	34	0.11
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	36	0.11
(1,1530)	1:39:A:PHE:HB2	1:38:A:VAL:HG13	26	0.11
(1,1431)	1:38:A:VAL:H	1:34:A:ILE:HD11	20	0.11
(1,1431)	1:38:A:VAL:H	1:34:A:ILE:HD12	20	0.11
(1,1431)	1:38:A:VAL:H	1:34:A:ILE:HD13	20	0.11
(1,1181)	1:32:A:PRO:HA	1:34:A:ILE:H	35	0.11
(1,1181)	1:32:A:PRO:HA	1:34:A:ILE:H	36	0.11
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	1	0.11
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	21	0.11
(1,1158)	1:23:A:ASP:HB2	1:20:A:GLU:HA	30	0.11
(1,1075)	1:53:A:VAL:HB	1:50:A:LEU:HA	36	0.11
(1,955)	1:34:A:ILE:HA	1:37:A:LEU:HG	27	0.11
(1,925)	1:35:A:TYR:HB2	1:32:A:PRO:HG2	24	0.11
(1,925)	1:35:A:TYR:HB2	1:32:A:PRO:HG3	24	0.11
(1,925)	1:35:A:TYR:HB3	1:32:A:PRO:HG2	24	0.11
(1,925)	1:35:A:TYR:HB3	1:32:A:PRO:HG3	24	0.11
(1,908)	1:32:A:PRO:HG2	1:33:A:ALA:HA	35	0.11
(1,699)	1:16:A:GLN:HA	1:18:A:GLU:H	3	0.11
(1,699)	1:16:A:GLN:HA	1:19:A:CYS:H	12	0.11
(1,685)	1:27:A:SER:HB3	1:29:A:ALA:H	9	0.11
(1,664)	1:27:A:SER:HA	1:30:A:LEU:HG	33	0.11
(1,592)	1:62:A:HIS:H	1:62:A:HIS:HA	38	0.11
(1,500)	1:64:A:HIS:HA	1:63:A:HIS:H	18	0.11
(1,500)	1:64:A:HIS:HA	1:63:A:HIS:H	24	0.11
(1,475)	1:41:A:LEU:HB3	1:44:A:THR:H	17	0.11
(1,466)	1:46:A:ASN:HD21	1:44:A:THR:HB	1	0.11
(1,466)	1:46:A:ASN:HD21	1:44:A:THR:HB	24	0.11
(1,466)	1:46:A:ASN:HD21	1:44:A:THR:HB	28	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,466)	1:46:A:ASN:HD21	1:44:A:THR:HB	31	0.11
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	14	0.11
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	24	0.11
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	28	0.11
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	32	0.11
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	3	0.11
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	21	0.11
(1,14)	1:55:A:ARG:HH21	1:52:A:THR:HB	21	0.11
(1,2398)	1:48:A:LEU:H	1:46:A:ASN:HB2	4	0.1
(1,2392)	1:21:A:TYR:H	1:20:A:GLU:HB3	35	0.1
(1,2116)	1:10:A:TYR:HA	1:11:A:TYR:H	33	0.1
(1,2079)	1:40:A:LEU:H	1:38:A:VAL:HG12	22	0.1
(1,1964)	1:47:A:GLY:HA2	1:50:A:LEU:HG	7	0.1
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	11	0.1
(1,1858)	1:27:A:SER:H	1:27:A:SER:HA	25	0.1
(1,1431)	1:38:A:VAL:H	1:34:A:ILE:HD11	28	0.1
(1,1431)	1:38:A:VAL:H	1:34:A:ILE:HD12	28	0.1
(1,1431)	1:38:A:VAL:H	1:34:A:ILE:HD13	28	0.1
(1,1313)	1:38:A:VAL:HG21	1:34:A:ILE:HB	34	0.1
(1,1181)	1:32:A:PRO:HA	1:34:A:ILE:H	6	0.1
(1,1174)	1:51:A:TRP:HD1	1:52:A:THR:HA	9	0.1
(1,1095)	1:41:A:LEU:HG	1:37:A:LEU:HG	27	0.1
(1,1095)	1:41:A:LEU:HG	1:37:A:LEU:HG	36	0.1
(1,1005)	1:28:A:GLY:HA2	1:31:A:ILE:HD13	10	0.1
(1,970)	1:33:A:ALA:HA	1:37:A:LEU:HD13	19	0.1
(1,915)	1:49:A:VAL:HG22	1:46:A:ASN:HA	17	0.1
(1,802)	1:52:A:THR:HG21	1:55:A:ARG:HE	36	0.1
(1,802)	1:52:A:THR:HG22	1:55:A:ARG:HE	36	0.1
(1,802)	1:52:A:THR:HG23	1:55:A:ARG:HE	36	0.1
(1,592)	1:62:A:HIS:H	1:61:A:HIS:HA	2	0.1
(1,573)	1:55:A:ARG:HB2	1:55:A:ARG:H	31	0.1
(1,573)	1:55:A:ARG:HB3	1:55:A:ARG:H	31	0.1
(1,490)	1:48:A:LEU:H	1:46:A:ASN:HB2	4	0.1
(1,475)	1:41:A:LEU:HB3	1:44:A:THR:H	22	0.1
(1,460)	1:19:A:CYS:H	1:19:A:CYS:HA	17	0.1
(1,434)	1:61:A:HIS:H	1:61:A:HIS:HB2	26	0.1
(1,434)	1:61:A:HIS:H	1:61:A:HIS:HB3	26	0.1
(1,380)	1:59:A:HIS:H	1:56:A:LYS:HA	34	0.1
(1,180)	1:61:A:HIS:H	1:61:A:HIS:HA	29	0.1
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	1	0.1
(1,67)	1:51:A:TRP:HE1	1:52:A:THR:HA	9	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found