



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 05:05 PM EST

PDB ID : 7B2B
BMRB ID : 34575
Title : Solution structure of a non-covalent extended docking domain complex of the Pax NRPS: PaxA T1-CDD/PaxB NDD
Authors : Watzel, J.; Sarawi, S.; Duchardt-Ferner, E.; Bode, H.B.; Woehnert, J.
Deposited on : 2020-11-26

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

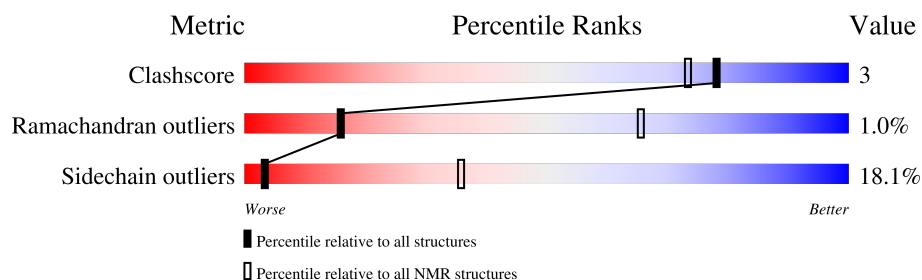
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	B	31	
2	A	104	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	B:2-B:27, A:991-A:1083 (119)	0.48	1

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

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

The models can be grouped into 3 clusters and 6 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2176 atoms, of which 1082 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Amino acid adenylation domain-containing protein.

Mol	Chain	Residues	Atoms						Trace
1	B	31	Total	C	H	N	O	S	0
			520	157	268	49	45	1	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	23	ALA	THR	variant	UNP A0A3D9UGN9
B	31	TYR	THR	engineered mutation	UNP A0A3D9UGN9

- Molecule 2 is a protein called Peptide synthetase PaxA.

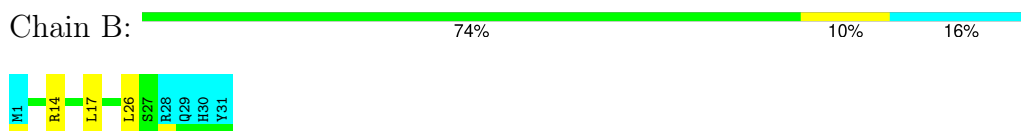
Mol	Chain	Residues	Atoms						Trace
2	A	104	Total	C	H	N	O	S	0
			1656	534	814	137	168	3	

4 Residue-property plots

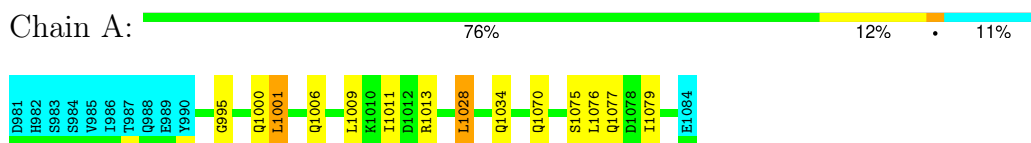
4.1 Average score per residue in the NMR ensemble

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: Amino acid adenylation domain-containing protein



- Molecule 2: Peptide synthetase PaxA



4.2 Scores per residue for each member of the ensemble

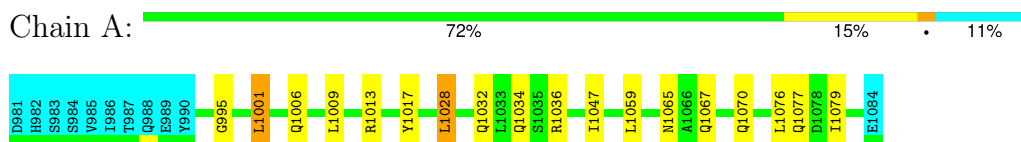
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Amino acid adenylation domain-containing protein

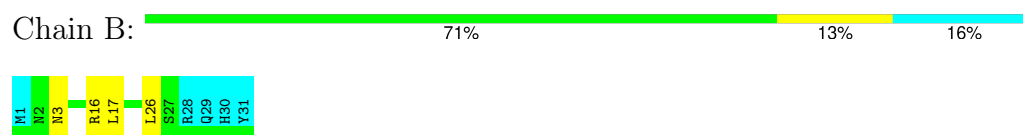


- Molecule 2: Peptide synthetase PaxA

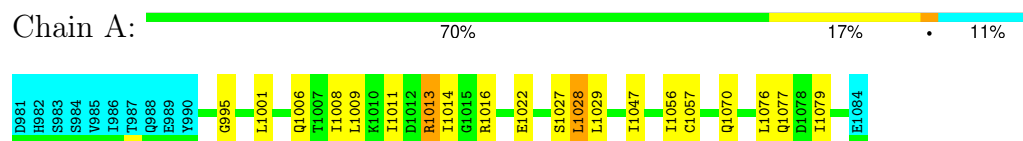


4.2.2 Score per residue for model 2

- Molecule 1: Amino acid adenylation domain-containing protein

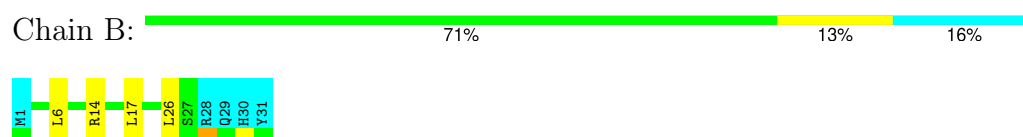


- Molecule 2: Peptide synthetase PaxA

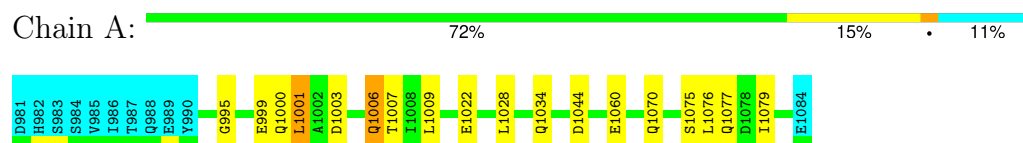


4.2.3 Score per residue for model 3

- Molecule 1: Amino acid adenylation domain-containing protein

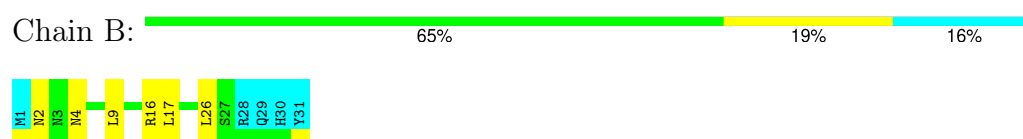


- Molecule 2: Peptide synthetase PaxA

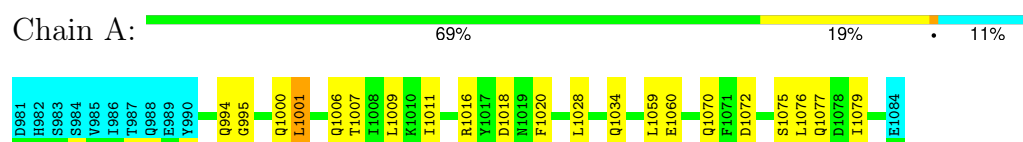


4.2.4 Score per residue for model 4

- Molecule 1: Amino acid adenylation domain-containing protein

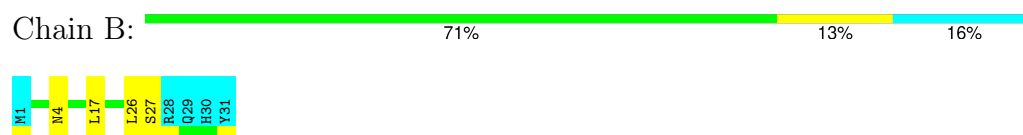


- Molecule 2: Peptide synthetase PaxA

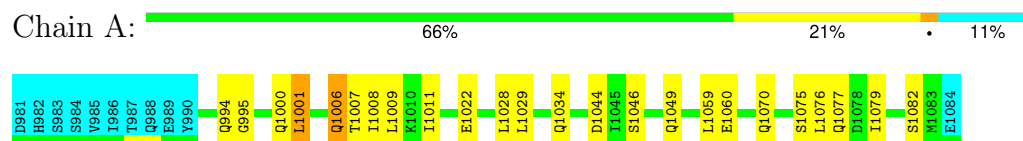


4.2.5 Score per residue for model 5

- Molecule 1: Amino acid adenylation domain-containing protein



- Molecule 2: Peptide synthetase PaxA

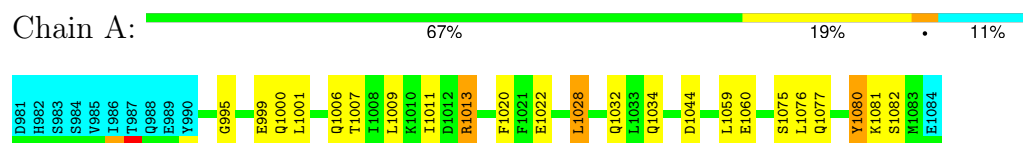


4.2.6 Score per residue for model 6

- Molecule 1: Amino acid adenylation domain-containing protein

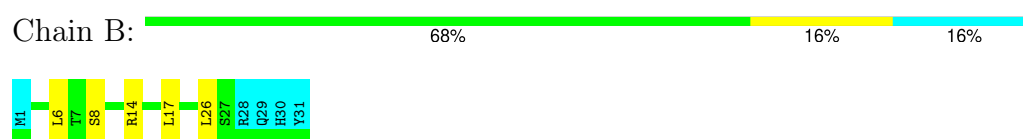


- Molecule 2: Peptide synthetase PaxA

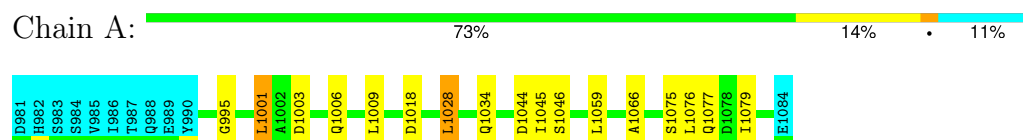


4.2.7 Score per residue for model 7

- Molecule 1: Amino acid adenylation domain-containing protein

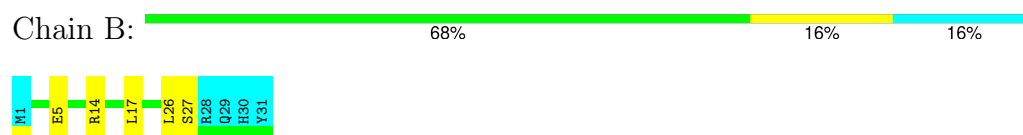


- Molecule 2: Peptide synthetase PaxA

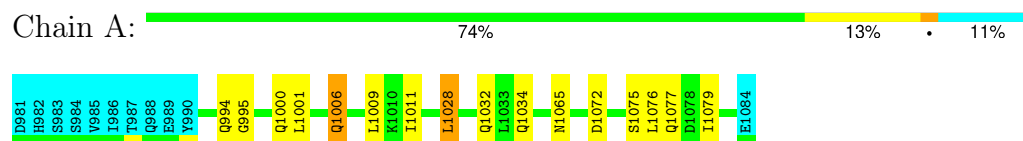


4.2.8 Score per residue for model 8

- Molecule 1: Amino acid adenylation domain-containing protein

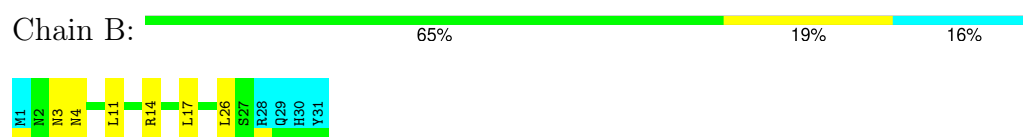


- Molecule 2: Peptide synthetase PaxA

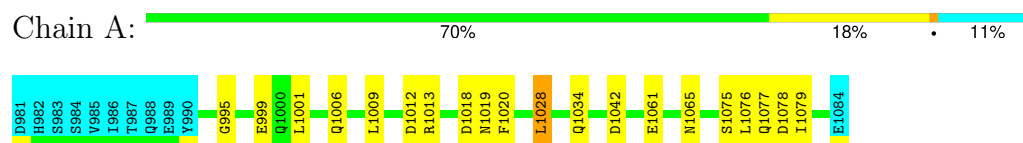


4.2.9 Score per residue for model 9

- Molecule 1: Amino acid adenylation domain-containing protein



- Molecule 2: Peptide synthetase PaxA

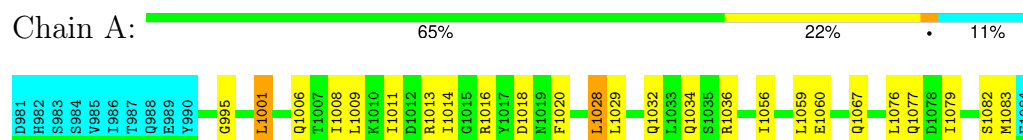


4.2.10 Score per residue for model 10

- Molecule 1: Amino acid adenylation domain-containing protein

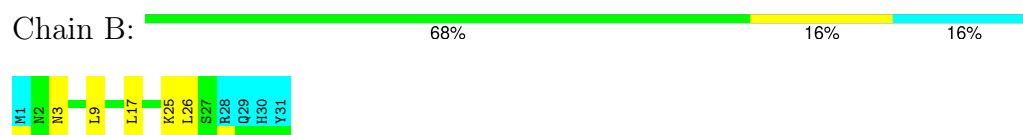


- Molecule 2: Peptide synthetase PaxA

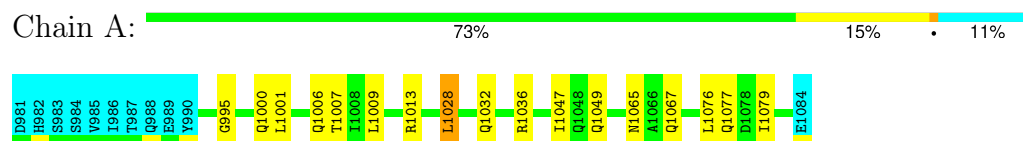


4.2.11 Score per residue for model 11

- Molecule 1: Amino acid adenylation domain-containing protein



- Molecule 2: Peptide synthetase PaxA

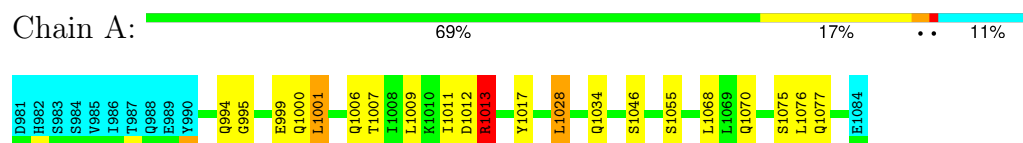


4.2.12 Score per residue for model 12

- Molecule 1: Amino acid adenylation domain-containing protein



- Molecule 2: Peptide synthetase PaxA

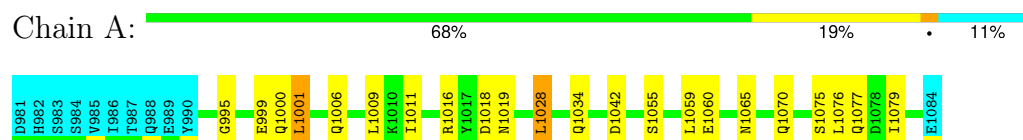


4.2.13 Score per residue for model 13

- Molecule 1: Amino acid adenylation domain-containing protein

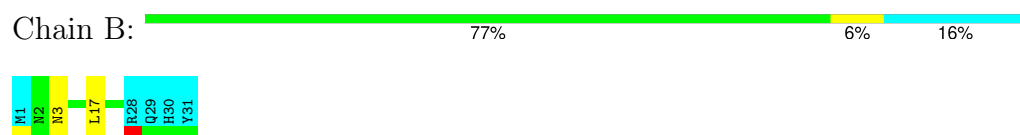


- Molecule 2: Peptide synthetase PaxA

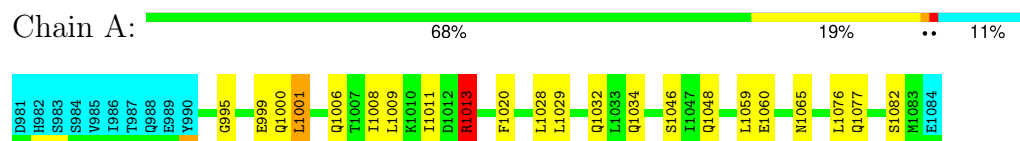


4.2.14 Score per residue for model 14

- Molecule 1: Amino acid adenylation domain-containing protein

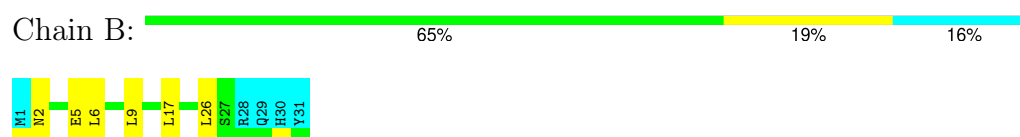


- Molecule 2: Peptide synthetase PaxA

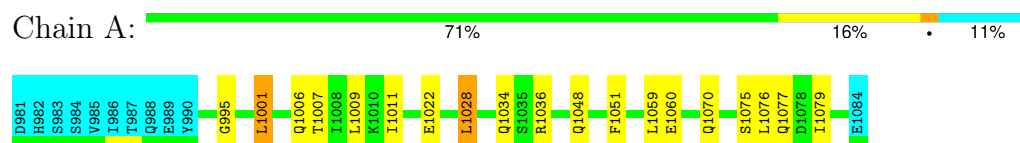


4.2.15 Score per residue for model 15

- Molecule 1: Amino acid adenylation domain-containing protein



- Molecule 2: Peptide synthetase PaxA

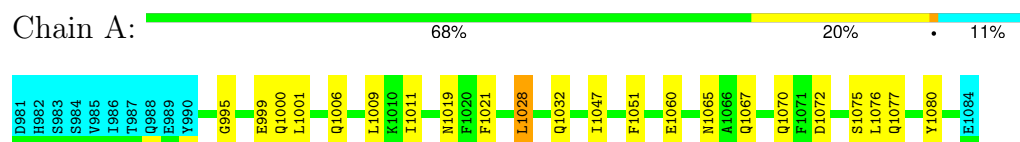


4.2.16 Score per residue for model 16

- Molecule 1: Amino acid adenylation domain-containing protein

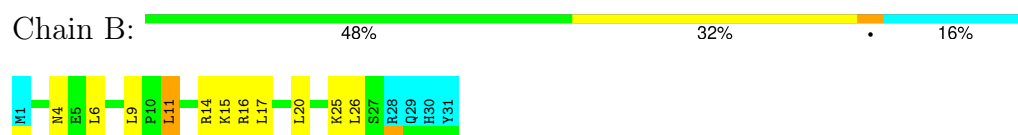


- Molecule 2: Peptide synthetase PaxA

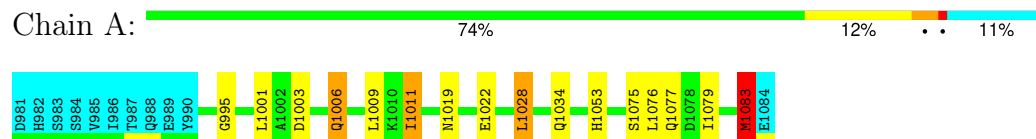


4.2.17 Score per residue for model 17

- Molecule 1: Amino acid adenylation domain-containing protein

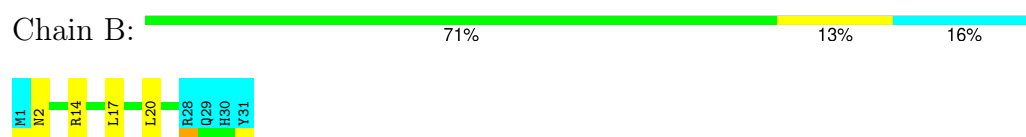


- Molecule 2: Peptide synthetase PaxA

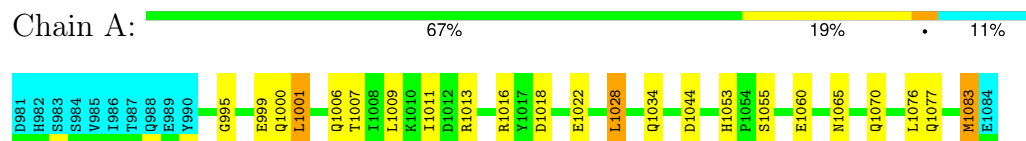


4.2.18 Score per residue for model 18

- Molecule 1: Amino acid adenylation domain-containing protein

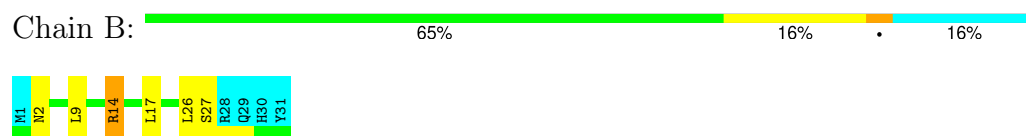


- Molecule 2: Peptide synthetase PaxA

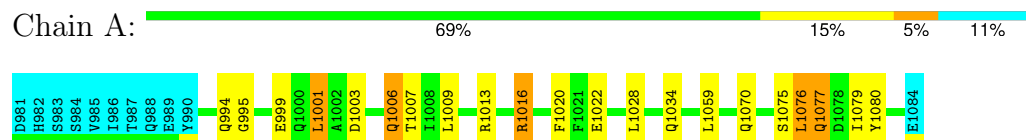


4.2.19 Score per residue for model 19

- Molecule 1: Amino acid adenylation domain-containing protein



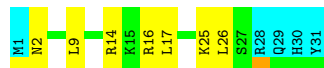
- Molecule 2: Peptide synthetase PaxA



4.2.20 Score per residue for model 20

- Molecule 1: Amino acid adenylation domain-containing protein

Chain B:  61% 23% 16%



- Molecule 2: Peptide synthetase PaxA

Chain A:  70% 18% 11%



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure calculation	3.98
OPALp	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	1718
Number of shifts mapped to atoms	1718
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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	B	0.45±0.02	0±0/203 (0.0± 0.0%)	0.98±0.04	0±0/273 (0.1± 0.2%)
2	A	0.57±0.01	0±0/764 (0.0± 0.0%)	1.01±0.03	1±1/1035 (0.1± 0.1%)
All	All	0.55	0/19340 (0.0%)	1.01	24/26160 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	B	0.0±0.0	0.6±0.6
2	A	0.0±0.0	0.7±0.8
All	All	0	24

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	1083	MET	CG-SD-CE	6.97	111.36	100.20	17	2
2	A	1013	ARG	CD-NE-CZ	6.88	133.23	123.60	12	2
2	A	1013	ARG	NE-CZ-NH1	6.79	123.69	120.30	19	1
2	A	1013	ARG	NE-CZ-NH2	-6.67	116.96	120.30	19	3
2	A	1018	ASP	CB-CG-OD1	-6.53	112.43	118.30	7	2
2	A	1016	ARG	NE-CZ-NH2	-6.07	117.27	120.30	19	1
1	B	14	ARG	NE-CZ-NH2	-5.88	117.36	120.30	20	2
1	B	16	ARG	NE-CZ-NH2	-5.74	117.43	120.30	1	3
2	A	1036	ARG	NE-CZ-NH2	-5.63	117.48	120.30	11	2
2	A	1016	ARG	NE-CZ-NH1	5.49	123.05	120.30	19	1
2	A	1006	GLN	CB-CA-C	-5.31	99.78	110.40	20	1
1	B	16	ARG	CD-NE-CZ	5.27	130.97	123.60	4	1
2	A	1036	ARG	CD-NE-CZ	5.05	130.68	123.60	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	1080	TYR	CB-CG-CD2	-5.05	117.97	121.00	19	2

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	B	14	ARG	Sidechain	9
2	A	1013	ARG	Sidechain	3
2	A	1016	ARG	Sidechain	3
2	A	1017	TYR	Sidechain	2
2	A	1080	TYR	Sidechain	2
2	A	1036	ARG	Sidechain	2
1	B	16	ARG	Sidechain	2
2	A	1020	PHE	Sidechain	1

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	B	202	222	222	2±1
2	A	751	737	737	5±2
All	All	19060	19180	19180	103

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:26:LEU:HD13	2:A:1079:ILE:HD12	0.61	1.73	3	9
1:B:26:LEU:HD12	2:A:1075:SER:HB3	0.59	1.75	5	6
2:A:1045:ILE:HD11	2:A:1066:ALA:HB2	0.58	1.75	7	1
2:A:1014:ILE:CG2	2:A:1056:ILE:HD11	0.58	2.29	10	3
2:A:1008:ILE:CG2	2:A:1029:LEU:HD22	0.57	2.30	2	4
1:B:20:LEU:HD11	2:A:1083:MET:CE	0.56	2.31	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:1001:LEU:HD13	2:A:1059:LEU:HD12	0.55	1.77	5	9
1:B:26:LEU:HD13	2:A:1079:ILE:CD1	0.53	2.34	11	12
1:B:20:LEU:HD11	2:A:1083:MET:SD	0.53	2.44	17	1
1:B:26:LEU:HD12	2:A:1075:SER:HB2	0.52	1.80	16	3
2:A:1014:ILE:HG21	2:A:1056:ILE:HD11	0.50	1.83	10	2
2:A:1006:GLN:HA	2:A:1011:ILE:HG22	0.50	1.82	17	1
2:A:1028:LEU:HD22	2:A:1028:LEU:C	0.50	2.27	13	12
2:A:1001:LEU:HD23	2:A:1001:LEU:H	0.48	1.67	3	5
2:A:994:GLN:NE2	2:A:1016:ARG:HH11	0.48	2.06	4	1
1:B:9:LEU:HD13	1:B:13:GLU:HB2	0.48	1.85	10	1
1:B:26:LEU:HD12	2:A:1075:SER:CB	0.48	2.38	8	9
1:B:20:LEU:HD12	2:A:1083:MET:SD	0.47	2.50	18	1
2:A:1059:LEU:C	2:A:1059:LEU:HD13	0.46	2.31	6	1
2:A:1001:LEU:HD13	2:A:1059:LEU:CD1	0.45	2.42	10	5
2:A:1006:GLN:H	2:A:1006:GLN:HE21	0.44	1.54	5	2
1:B:20:LEU:HD12	2:A:1083:MET:CE	0.44	2.41	18	1
2:A:1003:ASP:HA	2:A:1006:GLN:HE22	0.44	1.72	19	3
1:B:6:LEU:HD13	2:A:1068:LEU:HB2	0.43	1.88	12	1
1:B:2:ASN:ND2	1:B:4:ASN:HD22	0.43	2.11	13	1
1:B:11:LEU:HD12	1:B:15:LYS:CE	0.43	2.42	17	1
2:A:1045:ILE:HD11	2:A:1066:ALA:CB	0.43	2.44	7	1
2:A:1008:ILE:HG23	2:A:1029:LEU:HD22	0.41	1.93	2	1
2:A:1028:LEU:C	2:A:1028:LEU:HD22	0.41	2.36	15	2
2:A:1076:LEU:HD23	2:A:1077:GLN:N	0.41	2.31	19	1
1:B:19:GLU:OE2	1:B:22:LYS:HE2	0.41	2.16	13	1
1:B:16:ARG:HG2	2:A:1083:MET:SD	0.40	2.56	20	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	B	26/31 (84%)	25±1 (97±3%)	1±1 (2±3%)	0±0 (1±1%)	24	72
2	A	93/104 (89%)	88±1 (95±1%)	4±1 (4±1%)	1±0 (1±0%)	15	64
All	All	2380/2700 (88%)	2263 (95%)	94 (4%)	23 (1%)	16	65

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	995	GLY	20
1	B	27	SER	2
1	B	2	ASN	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	B	22/27 (81%)	18±1 (82±6%)	4±1 (18±6%)	3	37
2	A	83/94 (88%)	68±3 (82±3%)	15±3 (18±3%)	3	35
All	All	2100/2420 (87%)	1719 (82%)	381 (18%)	3	36

All 57 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	B	17	LEU	20
2	A	1001	LEU	20
2	A	1009	LEU	20
2	A	1028	LEU	20
2	A	1076	LEU	20
2	A	1077	GLN	20
2	A	1006	GLN	19
2	A	1034	GLN	17
2	A	1011	ILE	13
2	A	1070	GLN	12
2	A	1000	GLN	11
2	A	999	GLU	10
2	A	1060	GLU	10
2	A	1022	GLU	9
1	B	6	LEU	9
2	A	1007	THR	9
1	B	2	ASN	8
1	B	4	ASN	8
2	A	1032	GLN	8

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Mol	Chain	Res	Type	Models (Total)
2	A	1065	ASN	8
1	B	9	LEU	8
2	A	1013	ARG	6
1	B	25	LYS	5
1	B	3	ASN	5
2	A	1044	ASP	5
2	A	1018	ASP	5
2	A	1020	PHE	5
2	A	1047	ILE	4
2	A	1067	GLN	4
2	A	994	GLN	4
2	A	1046	SER	4
2	A	1082	SER	4
1	B	5	GLU	4
2	A	1019	ASN	4
2	A	1055	SER	4
1	B	16	ARG	3
2	A	1072	ASP	3
1	B	8	SER	3
2	A	1083	MET	3
1	B	27	SER	2
2	A	1049	GLN	2
1	B	11	LEU	2
2	A	1012	ASP	2
2	A	1042	ASP	2
2	A	1016	ARG	2
2	A	1048	GLN	2
2	A	1051	PHE	2
2	A	1053	HIS	2
2	A	1027	SER	1
2	A	1057	CYS	1
1	B	22	LYS	1
2	A	1081	LYS	1
2	A	1003	ASP	1
2	A	1061	GLU	1
2	A	1078	ASP	1
2	A	1021	PHE	1
2	A	1010	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no 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

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *JW140_JW146new2.star*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1718
Number of shifts mapped to atoms	1718
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	135	-0.38 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	130	0.04 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	127	-0.18 ± 0.15	None needed (< 0.5 ppm)
^{15}N	127	0.13 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1531 atoms were assigned a chemical shift out of a possible 1681. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	585/593 (99%)	237/239 (99%)	234/238 (98%)	114/116 (98%)
Sidechain	900/994 (91%)	613/646 (95%)	267/311 (86%)	20/37 (54%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	46/94 (49%)	23/47 (49%)	23/44 (52%)	0/3 (0%)
Overall	1531/1681 (91%)	873/932 (94%)	524/593 (88%)	134/156 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1718 atoms were assigned a chemical shift out of a possible 1906. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	655/673 (97%)	266/271 (98%)	262/270 (97%)	127/132 (96%)
Sidechain	997/1107 (90%)	678/718 (94%)	296/347 (85%)	23/42 (55%)
Aromatic	66/126 (52%)	33/63 (52%)	33/58 (57%)	0/5 (0%)
Overall	1718/1906 (90%)	977/1052 (93%)	591/675 (88%)	150/179 (84%)

7.1.4 Statistically unusual chemical shifts ⓘ

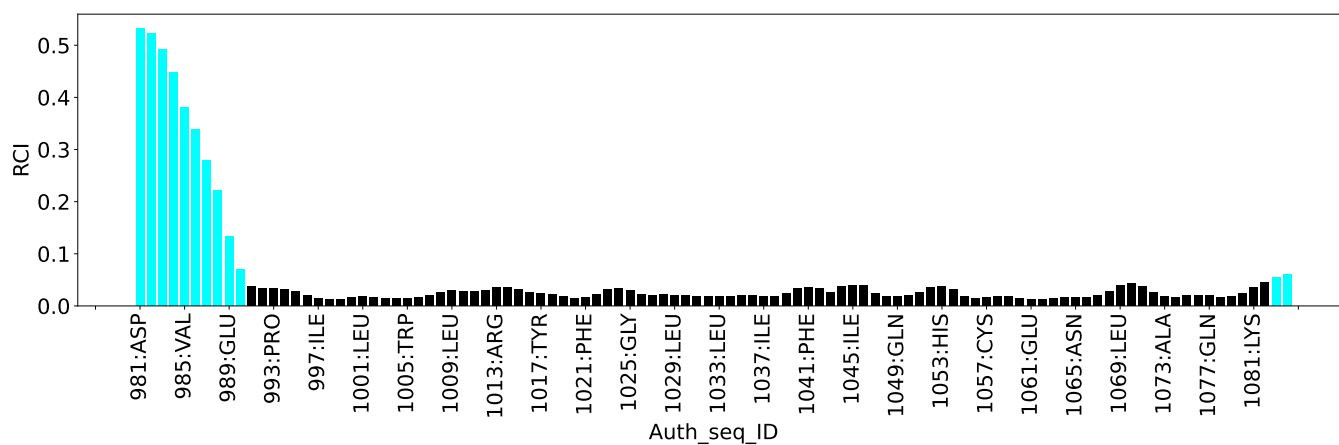
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	1013	ARG	NE	113.45	76.53 – 92.65	17.9
1	A	1036	ARG	NE	112.84	76.53 – 92.65	17.5
1	B	14	ARG	NE	112.77	76.53 – 92.65	17.5
1	A	1016	ARG	NE	112.10	76.53 – 92.65	17.1
1	B	16	ARG	NE	111.65	76.53 – 92.65	16.8
1	B	28	ARG	NE	110.78	76.53 – 92.65	16.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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	2826
Intra-residue ($ i-j =0$)	648
Sequential ($ i-j =1$)	703
Medium range ($ i-j >1$ and $ i-j <5$)	755
Long range ($ i-j \geq 5$)	451
Inter-chain	269
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	219
Number of unmapped restraints	0
Number of restraints per residue	22.6
Number of long range restraints per residue ¹	3.3

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)	9.2	0.14
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	14.9	9.16
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

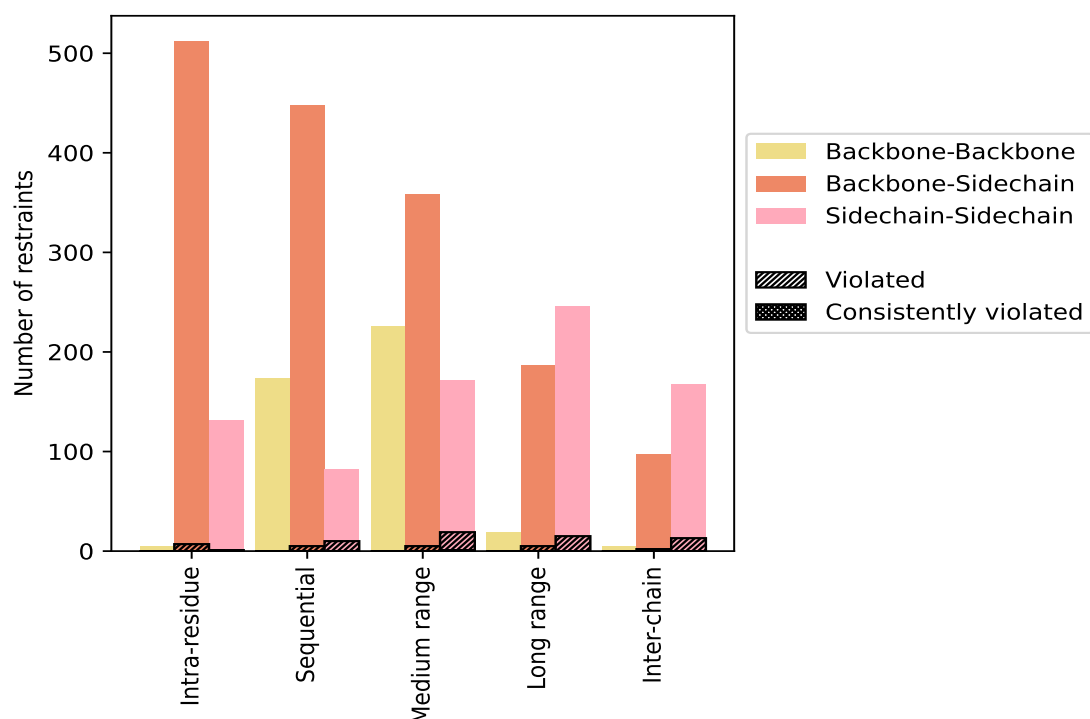
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	648	22.9	8	1.2	0.3	0	0.0	0.0
Backbone-Backbone	5	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	512	18.1	7	1.4	0.2	0	0.0	0.0
Sidechain-Sidechain	131	4.6	1	0.8	0.0	0	0.0	0.0
Sequential (i-j =1)	703	24.9	15	2.1	0.5	0	0.0	0.0
Backbone-Backbone	173	6.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	448	15.9	5	1.1	0.2	0	0.0	0.0
Sidechain-Sidechain	82	2.9	10	12.2	0.4	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	755	26.7	24	3.2	0.8	1	0.1	0.0
Backbone-Backbone	226	8.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	358	12.7	5	1.4	0.2	0	0.0	0.0
Sidechain-Sidechain	171	6.1	19	11.1	0.7	1	0.6	0.0
Long range (i-j ≥5)	451	16.0	20	4.4	0.7	0	0.0	0.0
Backbone-Backbone	19	0.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	186	6.6	5	2.7	0.2	0	0.0	0.0
Sidechain-Sidechain	246	8.7	15	6.1	0.5	0	0.0	0.0
Inter-chain	269	9.5	15	5.6	0.5	0	0.0	0.0
Backbone-Backbone	5	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	97	3.4	2	2.1	0.1	0	0.0	0.0
Sidechain-Sidechain	167	5.9	13	7.8	0.5	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	2826	100.0	82	2.9	2.9	1	0.0	0.0
Backbone-Backbone	428	15.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1601	56.7	24	1.5	0.8	0	0.0	0.0
Sidechain-Sidechain	797	28.2	58	7.3	2.1	1	0.1	0.0

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfide 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	0	1	2	5	1	9	0.11	0.13	0.01	0.11
2	0	0	1	3	1	5	0.12	0.13	0.01	0.11
3	1	1	7	2	0	11	0.11	0.14	0.01	0.11
4	0	1	6	3	1	11	0.11	0.13	0.01	0.11
5	0	1	4	5	4	14	0.11	0.12	0.01	0.11
6	0	3	4	5	0	12	0.11	0.13	0.01	0.11
7	0	0	5	3	4	12	0.11	0.12	0.0	0.11
8	0	4	3	5	1	13	0.11	0.13	0.01	0.11
9	1	2	4	4	1	12	0.11	0.13	0.01	0.12
10	0	2	5	3	3	13	0.11	0.14	0.01	0.11

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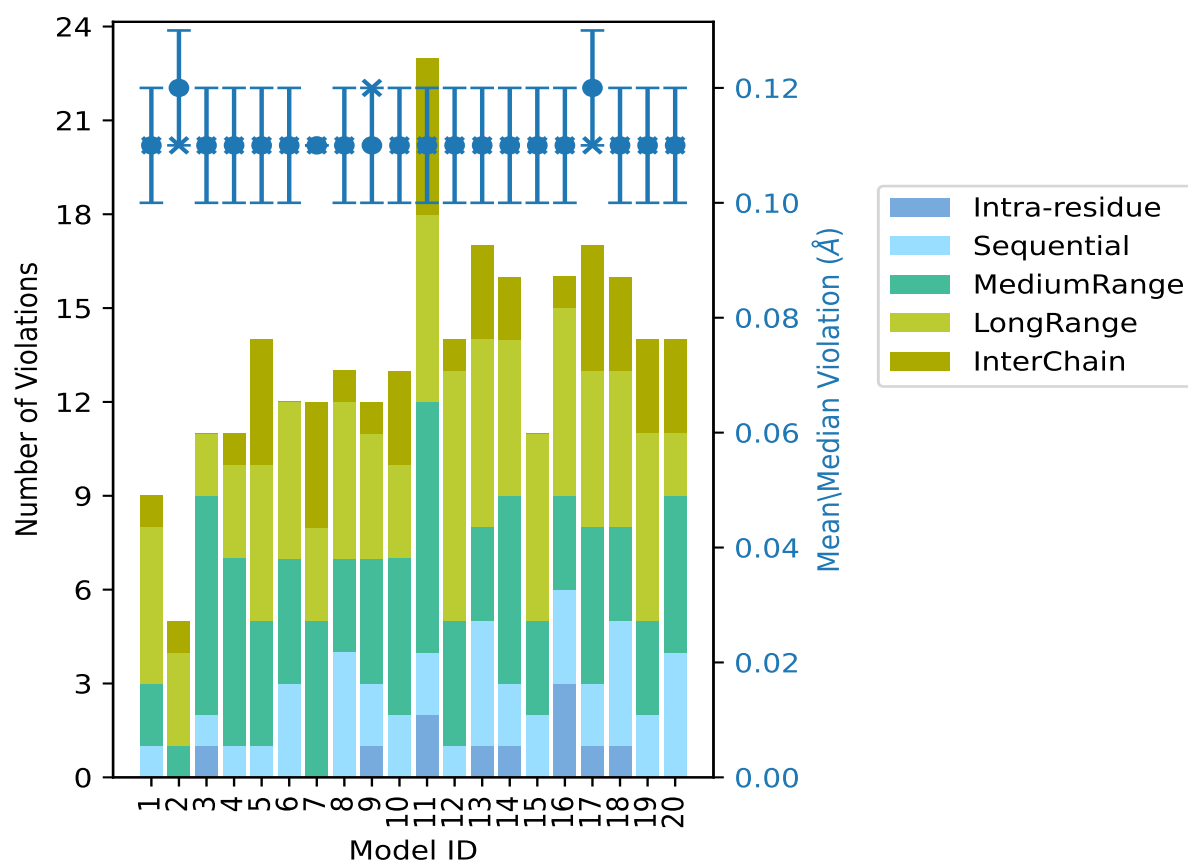
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	2	2	8	6	5	23	0.11	0.13	0.01	0.11
12	0	1	4	8	1	14	0.11	0.13	0.01	0.11
13	1	4	3	6	3	17	0.11	0.14	0.01	0.11
14	1	2	6	5	2	16	0.11	0.13	0.01	0.11
15	0	2	3	6	0	11	0.11	0.12	0.01	0.11
16	3	3	3	6	1	16	0.11	0.13	0.01	0.11
17	1	2	5	5	4	17	0.12	0.14	0.01	0.11
18	1	4	3	5	3	16	0.11	0.13	0.01	0.11
19	0	2	3	6	3	14	0.11	0.14	0.01	0.11
20	0	4	5	2	3	14	0.11	0.13	0.01	0.11

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 ⓘ



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

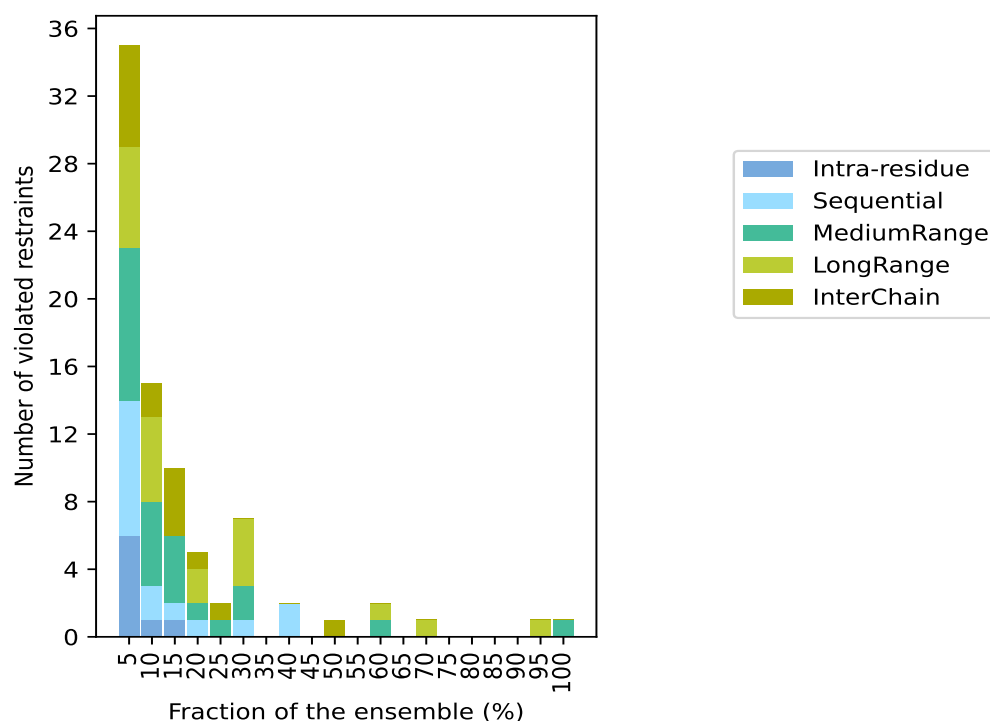
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2744(IR:640, SQ:688, MR:731, LR:431, IC:254) restraints are 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	%
6	8	9	6	6	35	1	5.0
1	2	5	5	2	15	2	10.0
1	1	4	0	4	10	3	15.0
0	1	1	2	1	5	4	20.0
0	0	1	0	1	2	5	25.0
0	1	2	4	0	7	6	30.0
0	0	0	0	0	0	7	35.0
0	2	0	0	0	2	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	1	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	1	1	0	2	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	1	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	1	0	1	19	95.0
0	0	1	0	0	1	20	100.0

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

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

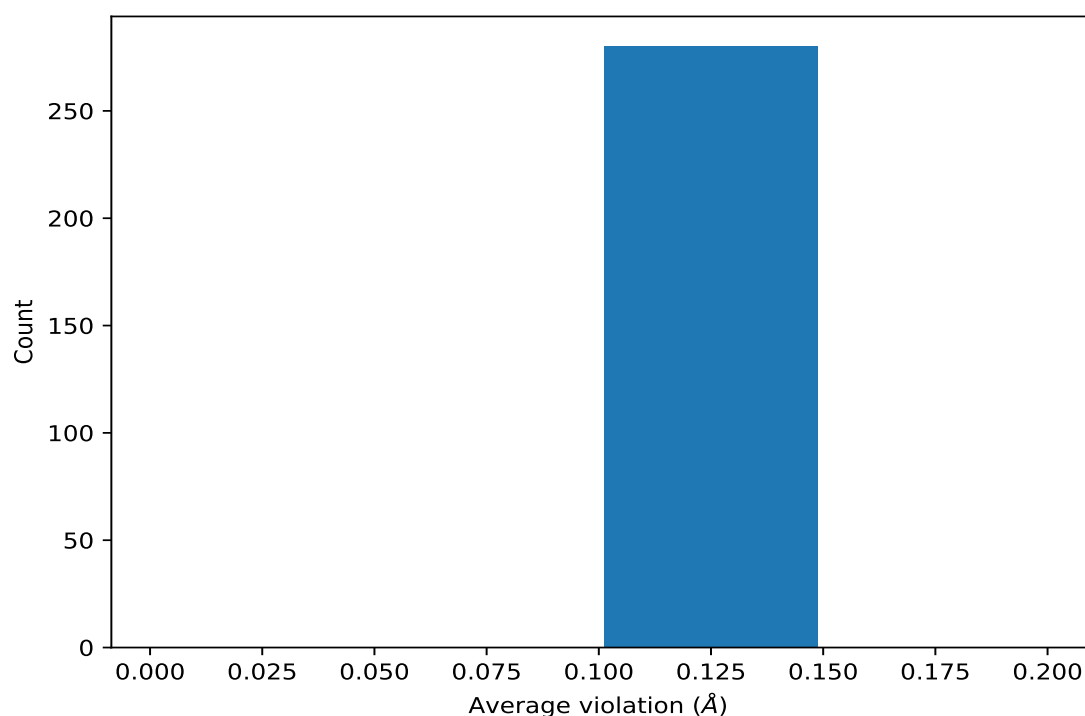
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	20	0.12	0.01	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	20	0.12	0.01	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	20	0.12	0.01	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	20	0.12	0.01	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	20	0.12	0.01	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	20	0.12	0.01	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	19	0.13	0.0	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	19	0.13	0.0	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	19	0.13	0.0	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	19	0.13	0.0	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	19	0.13	0.0	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	19	0.13	0.0	0.13
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	14	0.11	0.01	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	14	0.11	0.01	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	14	0.11	0.01	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	14	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	14	0.11	0.01	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	14	0.11	0.01	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	14	0.11	0.01	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	14	0.11	0.01	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	14	0.11	0.01	0.11
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD11	12	0.12	0.01	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD12	12	0.12	0.01	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD13	12	0.12	0.01	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD11	12	0.12	0.01	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD12	12	0.12	0.01	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD13	12	0.12	0.01	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD21	12	0.11	0.01	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD22	12	0.11	0.01	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD23	12	0.11	0.01	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD21	12	0.11	0.01	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD22	12	0.11	0.01	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD23	12	0.11	0.01	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD21	12	0.11	0.01	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD22	12	0.11	0.01	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD23	12	0.11	0.01	0.12
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD11	10	0.11	0.01	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD12	10	0.11	0.01	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD13	10	0.11	0.01	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD11	10	0.11	0.01	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD12	10	0.11	0.01	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD13	10	0.11	0.01	0.11
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD21	8	0.12	0.01	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD22	8	0.12	0.01	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD23	8	0.12	0.01	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD21	8	0.12	0.01	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD22	8	0.12	0.01	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD23	8	0.12	0.01	0.12
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE21	8	0.11	0.01	0.1
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE22	8	0.11	0.01	0.1
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE21	8	0.11	0.01	0.1
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE22	8	0.11	0.01	0.1
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE21	8	0.11	0.01	0.1
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE22	8	0.11	0.01	0.1
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD11	6	0.12	0.01	0.12
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD12	6	0.12	0.01	0.12
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD13	6	0.12	0.01	0.12
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD11	6	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD12	6	0.12	0.01	0.12
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD13	6	0.12	0.01	0.12
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD11	6	0.12	0.01	0.12
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD12	6	0.12	0.01	0.12
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD13	6	0.12	0.01	0.12
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD21	6	0.11	0.01	0.11
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD22	6	0.11	0.01	0.11
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD23	6	0.11	0.01	0.11
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD21	6	0.11	0.01	0.11
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD22	6	0.11	0.01	0.11
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD23	6	0.11	0.01	0.11
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD21	6	0.11	0.01	0.11
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD22	6	0.11	0.01	0.11
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD23	6	0.11	0.01	0.11
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE21	6	0.11	0.0	0.11
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE22	6	0.11	0.0	0.11
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE21	6	0.11	0.0	0.11
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE22	6	0.11	0.0	0.11
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE21	6	0.11	0.0	0.11
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE22	6	0.11	0.0	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD11	6	0.11	0.0	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD12	6	0.11	0.0	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD13	6	0.11	0.0	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD11	6	0.11	0.0	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD12	6	0.11	0.0	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD13	6	0.11	0.0	0.11
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD11	6	0.1	0.0	0.11
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD12	6	0.1	0.0	0.11
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD13	6	0.1	0.0	0.11
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD11	6	0.1	0.0	0.11
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD12	6	0.1	0.0	0.11
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD13	6	0.1	0.0	0.11
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD11	6	0.1	0.0	0.11
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD12	6	0.1	0.0	0.11
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD13	6	0.1	0.0	0.11
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG21	6	0.1	0.0	0.11
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG22	6	0.1	0.0	0.11
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG23	6	0.1	0.0	0.11
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG21	6	0.1	0.0	0.11
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG22	6	0.1	0.0	0.11
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG23	6	0.1	0.0	0.11
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG21	6	0.1	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG22	6	0.1	0.0	0.11
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG23	6	0.1	0.0	0.11
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB2	6	0.1	0.0	0.1
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB3	6	0.1	0.0	0.1
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB2	6	0.1	0.0	0.1
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB3	6	0.1	0.0	0.1
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB2	6	0.1	0.0	0.1
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB3	6	0.1	0.0	0.1
(1,2252)	1:20:B:LEU:HD11	2:1084:A:GLU:HG2	5	0.11	0.01	0.11
(1,2252)	1:20:B:LEU:HD11	2:1084:A:GLU:HG3	5	0.11	0.01	0.11
(1,2252)	1:20:B:LEU:HD12	2:1084:A:GLU:HG2	5	0.11	0.01	0.11
(1,2252)	1:20:B:LEU:HD12	2:1084:A:GLU:HG3	5	0.11	0.01	0.11
(1,2252)	1:20:B:LEU:HD13	2:1084:A:GLU:HG2	5	0.11	0.01	0.11
(1,2252)	1:20:B:LEU:HD13	2:1084:A:GLU:HG3	5	0.11	0.01	0.11
(1,2723)	2:1059:A:LEU:HD21	2:1063:A:ILE:HG12	5	0.11	0.0	0.11
(1,2723)	2:1059:A:LEU:HD21	2:1063:A:ILE:HG13	5	0.11	0.0	0.11
(1,2723)	2:1059:A:LEU:HD22	2:1063:A:ILE:HG12	5	0.11	0.0	0.11
(1,2723)	2:1059:A:LEU:HD22	2:1063:A:ILE:HG13	5	0.11	0.0	0.11
(1,2723)	2:1059:A:LEU:HD23	2:1063:A:ILE:HG12	5	0.11	0.0	0.11
(1,2723)	2:1059:A:LEU:HD23	2:1063:A:ILE:HG13	5	0.11	0.0	0.11
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD11	4	0.12	0.0	0.12
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD12	4	0.12	0.0	0.12
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD13	4	0.12	0.0	0.12
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD11	4	0.12	0.0	0.12
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD12	4	0.12	0.0	0.12
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD13	4	0.12	0.0	0.12
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD11	4	0.12	0.0	0.12
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD12	4	0.12	0.0	0.12
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD13	4	0.12	0.0	0.12
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD11	4	0.11	0.0	0.11
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD12	4	0.11	0.0	0.11
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD13	4	0.11	0.0	0.11
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD11	4	0.11	0.0	0.11
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD12	4	0.11	0.0	0.11
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD13	4	0.11	0.0	0.11
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD11	4	0.11	0.0	0.11
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD12	4	0.11	0.0	0.11
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD13	4	0.11	0.0	0.11
(1,1344)	2:986:A:ILE:HG21	2:988:A:GLN:HG2	4	0.11	0.01	0.11
(1,1344)	2:986:A:ILE:HG21	2:988:A:GLN:HG3	4	0.11	0.01	0.11
(1,1344)	2:986:A:ILE:HG22	2:988:A:GLN:HG2	4	0.11	0.01	0.11
(1,1344)	2:986:A:ILE:HG22	2:988:A:GLN:HG3	4	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1344)	2:986:A:ILE:HG23	2:988:A:GLN:HG2	4	0.11	0.01	0.11
(1,1344)	2:986:A:ILE:HG23	2:988:A:GLN:HG3	4	0.11	0.01	0.11
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD21	4	0.11	0.0	0.11
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD22	4	0.11	0.0	0.11
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD23	4	0.11	0.0	0.11
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD21	4	0.11	0.0	0.11
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD22	4	0.11	0.0	0.11
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD23	4	0.11	0.0	0.11
(1,838)	2:1004:A:ILE:HG21	2:1032:A:GLN:HE22	4	0.1	0.0	0.1
(1,838)	2:1004:A:ILE:HG22	2:1032:A:GLN:HE22	4	0.1	0.0	0.1
(1,838)	2:1004:A:ILE:HG23	2:1032:A:GLN:HE22	4	0.1	0.0	0.1
(1,2250)	1:20:B:LEU:HD11	2:1083:A:MET:HB2	3	0.13	0.0	0.13
(1,2250)	1:20:B:LEU:HD11	2:1083:A:MET:HB3	3	0.13	0.0	0.13
(1,2250)	1:20:B:LEU:HD12	2:1083:A:MET:HB2	3	0.13	0.0	0.13
(1,2250)	1:20:B:LEU:HD12	2:1083:A:MET:HB3	3	0.13	0.0	0.13
(1,2250)	1:20:B:LEU:HD13	2:1083:A:MET:HB2	3	0.13	0.0	0.13
(1,2250)	1:20:B:LEU:HD13	2:1083:A:MET:HB3	3	0.13	0.0	0.13
(1,2259)	1:22:B:LYS:HB2	1:23:B:ALA:HB1	3	0.13	0.01	0.12
(1,2259)	1:22:B:LYS:HB2	1:23:B:ALA:HB2	3	0.13	0.01	0.12
(1,2259)	1:22:B:LYS:HB2	1:23:B:ALA:HB3	3	0.13	0.01	0.12
(1,2259)	1:22:B:LYS:HB3	1:23:B:ALA:HB1	3	0.13	0.01	0.12
(1,2259)	1:22:B:LYS:HB3	1:23:B:ALA:HB2	3	0.13	0.01	0.12
(1,2259)	1:22:B:LYS:HB3	1:23:B:ALA:HB3	3	0.13	0.01	0.12
(1,2208)	1:16:B:ARG:HG2	1:20:B:LEU:HD11	3	0.11	0.0	0.11
(1,2208)	1:16:B:ARG:HG2	1:20:B:LEU:HD12	3	0.11	0.0	0.11
(1,2208)	1:16:B:ARG:HG2	1:20:B:LEU:HD13	3	0.11	0.0	0.11
(1,2208)	1:16:B:ARG:HG3	1:20:B:LEU:HD11	3	0.11	0.0	0.11
(1,2208)	1:16:B:ARG:HG3	1:20:B:LEU:HD12	3	0.11	0.0	0.11
(1,2208)	1:16:B:ARG:HG3	1:20:B:LEU:HD13	3	0.11	0.0	0.11
(1,2272)	1:26:B:LEU:HD21	2:1072:A:ASP:HB2	3	0.11	0.0	0.11
(1,2272)	1:26:B:LEU:HD21	2:1072:A:ASP:HB3	3	0.11	0.0	0.11
(1,2272)	1:26:B:LEU:HD22	2:1072:A:ASP:HB2	3	0.11	0.0	0.11
(1,2272)	1:26:B:LEU:HD22	2:1072:A:ASP:HB3	3	0.11	0.0	0.11
(1,2272)	1:26:B:LEU:HD23	2:1072:A:ASP:HB2	3	0.11	0.0	0.11
(1,2272)	1:26:B:LEU:HD23	2:1072:A:ASP:HB3	3	0.11	0.0	0.11
(1,2691)	2:1049:A:GLN:HG2	2:1052:A:ALA:HB1	3	0.11	0.0	0.11
(1,2691)	2:1049:A:GLN:HG2	2:1052:A:ALA:HB2	3	0.11	0.0	0.11
(1,2691)	2:1049:A:GLN:HG2	2:1052:A:ALA:HB3	3	0.11	0.0	0.11
(1,2691)	2:1049:A:GLN:HG3	2:1052:A:ALA:HB1	3	0.11	0.0	0.11
(1,2691)	2:1049:A:GLN:HG3	2:1052:A:ALA:HB2	3	0.11	0.0	0.11
(1,2691)	2:1049:A:GLN:HG3	2:1052:A:ALA:HB3	3	0.11	0.0	0.11
(1,1169)	1:3:B:ASN:HB2	1:7:B:THR:HG21	3	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1169)	1:3:B:ASN:HB2	1:7:B:THR:HG22	3	0.11	0.0	0.11
(1,1169)	1:3:B:ASN:HB2	1:7:B:THR:HG23	3	0.11	0.0	0.11
(1,1169)	1:3:B:ASN:HB3	1:7:B:THR:HG21	3	0.11	0.0	0.11
(1,1169)	1:3:B:ASN:HB3	1:7:B:THR:HG22	3	0.11	0.0	0.11
(1,1169)	1:3:B:ASN:HB3	1:7:B:THR:HG23	3	0.11	0.0	0.11
(1,2086)	1:20:B:LEU:HD11	2:1083:A:MET:HB2	3	0.11	0.01	0.1
(1,2086)	1:20:B:LEU:HD12	2:1083:A:MET:HB2	3	0.11	0.01	0.1
(1,2086)	1:20:B:LEU:HD13	2:1083:A:MET:HB2	3	0.11	0.01	0.1
(1,938)	1:7:B:THR:H	2:1068:A:LEU:HD11	3	0.1	0.0	0.1
(1,938)	1:7:B:THR:H	2:1068:A:LEU:HD12	3	0.1	0.0	0.1
(1,938)	1:7:B:THR:H	2:1068:A:LEU:HD13	3	0.1	0.0	0.1
(1,1500)	2:1007:A:THR:HG21	2:1010:A:LYS:H	3	0.1	0.0	0.1
(1,1500)	2:1007:A:THR:HG22	2:1010:A:LYS:H	3	0.1	0.0	0.1
(1,1500)	2:1007:A:THR:HG23	2:1010:A:LYS:H	3	0.1	0.0	0.1
(1,1819)	2:1047:A:ILE:HA	2:1047:A:ILE:HD11	3	0.1	0.0	0.1
(1,1819)	2:1047:A:ILE:HA	2:1047:A:ILE:HD12	3	0.1	0.0	0.1
(1,1819)	2:1047:A:ILE:HA	2:1047:A:ILE:HD13	3	0.1	0.0	0.1
(1,1349)	2:987:A:THR:HA	2:987:A:THR:HG21	2	0.13	0.0	0.13
(1,1349)	2:987:A:THR:HA	2:987:A:THR:HG22	2	0.13	0.0	0.13
(1,1349)	2:987:A:THR:HA	2:987:A:THR:HG23	2	0.13	0.0	0.13
(1,2172)	1:11:B:LEU:HD21	1:15:B:LYS:HE2	2	0.12	0.0	0.12
(1,2172)	1:11:B:LEU:HD21	1:15:B:LYS:HE3	2	0.12	0.0	0.12
(1,2172)	1:11:B:LEU:HD22	1:15:B:LYS:HE2	2	0.12	0.0	0.12
(1,2172)	1:11:B:LEU:HD22	1:15:B:LYS:HE3	2	0.12	0.0	0.12
(1,2172)	1:11:B:LEU:HD23	1:15:B:LYS:HE2	2	0.12	0.0	0.12
(1,2172)	1:11:B:LEU:HD23	1:15:B:LYS:HE3	2	0.12	0.0	0.12
(1,1296)	1:24:B:ALA:HB1	1:26:B:LEU:HD11	2	0.11	0.01	0.11
(1,1296)	1:24:B:ALA:HB1	1:26:B:LEU:HD12	2	0.11	0.01	0.11
(1,1296)	1:24:B:ALA:HB1	1:26:B:LEU:HD13	2	0.11	0.01	0.11
(1,1296)	1:24:B:ALA:HB2	1:26:B:LEU:HD11	2	0.11	0.01	0.11
(1,1296)	1:24:B:ALA:HB2	1:26:B:LEU:HD12	2	0.11	0.01	0.11
(1,1296)	1:24:B:ALA:HB2	1:26:B:LEU:HD13	2	0.11	0.01	0.11
(1,1296)	1:24:B:ALA:HB3	1:26:B:LEU:HD11	2	0.11	0.01	0.11
(1,1296)	1:24:B:ALA:HB3	1:26:B:LEU:HD12	2	0.11	0.01	0.11
(1,1296)	1:24:B:ALA:HB3	1:26:B:LEU:HD13	2	0.11	0.01	0.11
(1,1324)	1:20:B:LEU:HD11	2:1079:A:ILE:HD11	2	0.11	0.0	0.11
(1,1324)	1:20:B:LEU:HD11	2:1079:A:ILE:HD12	2	0.11	0.0	0.11
(1,1324)	1:20:B:LEU:HD11	2:1079:A:ILE:HD13	2	0.11	0.0	0.11
(1,1324)	1:20:B:LEU:HD12	2:1079:A:ILE:HD11	2	0.11	0.0	0.11
(1,1324)	1:20:B:LEU:HD12	2:1079:A:ILE:HD12	2	0.11	0.0	0.11
(1,1324)	1:20:B:LEU:HD12	2:1079:A:ILE:HD13	2	0.11	0.0	0.11
(1,1324)	1:20:B:LEU:HD13	2:1079:A:ILE:HD11	2	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1324)	1:20:B:LEU:HD13	2:1079:A:ILE:HD12	2	0.11	0.0	0.11
(1,1324)	1:20:B:LEU:HD13	2:1079:A:ILE:HD13	2	0.11	0.0	0.11
(1,2466)	2:1009:A:LEU:HD21	2:1024:A:GLY:HA2	2	0.11	0.0	0.11
(1,2466)	2:1009:A:LEU:HD21	2:1024:A:GLY:HA3	2	0.11	0.0	0.11
(1,2466)	2:1009:A:LEU:HD22	2:1024:A:GLY:HA2	2	0.11	0.0	0.11
(1,2466)	2:1009:A:LEU:HD22	2:1024:A:GLY:HA3	2	0.11	0.0	0.11
(1,2466)	2:1009:A:LEU:HD23	2:1024:A:GLY:HA2	2	0.11	0.0	0.11
(1,2466)	2:1009:A:LEU:HD23	2:1024:A:GLY:HA3	2	0.11	0.0	0.11
(1,242)	2:1014:A:ILE:H	2:1056:A:ILE:HD11	2	0.11	0.0	0.11
(1,242)	2:1014:A:ILE:H	2:1056:A:ILE:HD12	2	0.11	0.0	0.11
(1,242)	2:1014:A:ILE:H	2:1056:A:ILE:HD13	2	0.11	0.0	0.11
(1,1276)	1:18:B:LEU:HD11	1:22:B:LYS:HD2	2	0.11	0.0	0.11
(1,1276)	1:18:B:LEU:HD11	1:22:B:LYS:HD3	2	0.11	0.0	0.11
(1,1276)	1:18:B:LEU:HD12	1:22:B:LYS:HD2	2	0.11	0.0	0.11
(1,1276)	1:18:B:LEU:HD12	1:22:B:LYS:HD3	2	0.11	0.0	0.11
(1,1276)	1:18:B:LEU:HD13	1:22:B:LYS:HD2	2	0.11	0.0	0.11
(1,1276)	1:18:B:LEU:HD13	1:22:B:LYS:HD3	2	0.11	0.0	0.11
(1,1405)	2:997:A:ILE:HG21	2:1063:A:ILE:HD11	2	0.11	0.0	0.11
(1,1405)	2:997:A:ILE:HG21	2:1063:A:ILE:HD12	2	0.11	0.0	0.11
(1,1405)	2:997:A:ILE:HG21	2:1063:A:ILE:HD13	2	0.11	0.0	0.11
(1,1405)	2:997:A:ILE:HG22	2:1063:A:ILE:HD11	2	0.11	0.0	0.11
(1,1405)	2:997:A:ILE:HG22	2:1063:A:ILE:HD12	2	0.11	0.0	0.11
(1,1405)	2:997:A:ILE:HG22	2:1063:A:ILE:HD13	2	0.11	0.0	0.11
(1,1405)	2:997:A:ILE:HG23	2:1063:A:ILE:HD11	2	0.11	0.0	0.11
(1,1405)	2:997:A:ILE:HG23	2:1063:A:ILE:HD12	2	0.11	0.0	0.11
(1,1405)	2:997:A:ILE:HG23	2:1063:A:ILE:HD13	2	0.11	0.0	0.11
(1,1776)	2:1000:A:GLN:HB2	2:1040:A:ILE:HG21	2	0.11	0.0	0.11
(1,1776)	2:1000:A:GLN:HB2	2:1040:A:ILE:HG22	2	0.11	0.0	0.11
(1,1776)	2:1000:A:GLN:HB2	2:1040:A:ILE:HG23	2	0.11	0.0	0.11
(1,1975)	1:17:B:LEU:HD11	2:1079:A:ILE:HA	2	0.11	0.0	0.11
(1,1975)	1:17:B:LEU:HD12	2:1079:A:ILE:HA	2	0.11	0.0	0.11
(1,1975)	1:17:B:LEU:HD13	2:1079:A:ILE:HA	2	0.11	0.0	0.11
(1,2587)	2:1035:A:SER:H	2:1036:A:ARG:HD2	2	0.11	0.0	0.11
(1,2587)	2:1035:A:SER:H	2:1036:A:ARG:HD3	2	0.11	0.0	0.11
(1,1331)	2:984:A:SER:HB2	2:985:A:VAL:HG11	2	0.1	0.0	0.1
(1,1331)	2:984:A:SER:HB2	2:985:A:VAL:HG12	2	0.1	0.0	0.1
(1,1331)	2:984:A:SER:HB2	2:985:A:VAL:HG13	2	0.1	0.0	0.1
(1,1331)	2:984:A:SER:HB3	2:985:A:VAL:HG11	2	0.1	0.0	0.1
(1,1331)	2:984:A:SER:HB3	2:985:A:VAL:HG12	2	0.1	0.0	0.1
(1,1331)	2:984:A:SER:HB3	2:985:A:VAL:HG13	2	0.1	0.0	0.1
(1,1473)	2:1004:A:ILE:HD11	2:1041:A:PHE:HD1	2	0.1	0.0	0.1
(1,1473)	2:1004:A:ILE:HD11	2:1041:A:PHE:HD2	2	0.1	0.0	0.1

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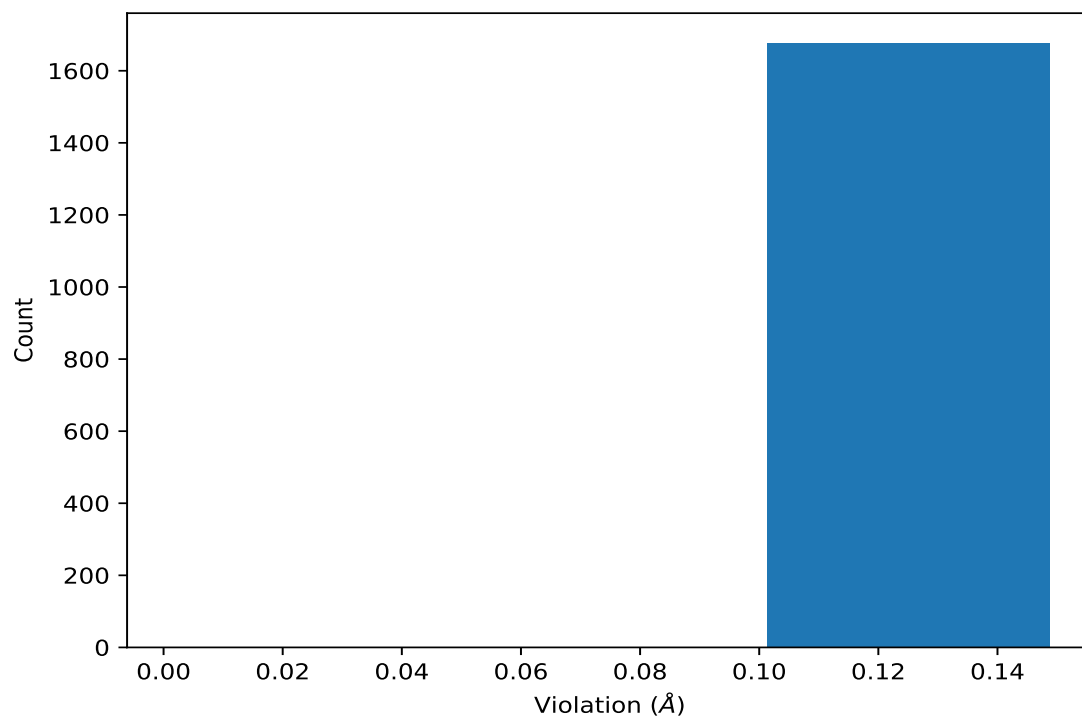
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1473)	2:1004:A:ILE:HD12	2:1041:A:PHE:HD1	2	0.1	0.0	0.1
(1,1473)	2:1004:A:ILE:HD12	2:1041:A:PHE:HD2	2	0.1	0.0	0.1
(1,1473)	2:1004:A:ILE:HD13	2:1041:A:PHE:HD1	2	0.1	0.0	0.1
(1,1473)	2:1004:A:ILE:HD13	2:1041:A:PHE:HD2	2	0.1	0.0	0.1
(1,2552)	2:1031:A:LEU:HD21	2:1034:A:GLN:HE21	2	0.1	0.0	0.1
(1,2552)	2:1031:A:LEU:HD21	2:1034:A:GLN:HE22	2	0.1	0.0	0.1
(1,2552)	2:1031:A:LEU:HD22	2:1034:A:GLN:HE21	2	0.1	0.0	0.1
(1,2552)	2:1031:A:LEU:HD22	2:1034:A:GLN:HE22	2	0.1	0.0	0.1
(1,2552)	2:1031:A:LEU:HD23	2:1034:A:GLN:HE21	2	0.1	0.0	0.1
(1,2552)	2:1031:A:LEU:HD23	2:1034:A:GLN:HE22	2	0.1	0.0	0.1
(1,2768)	2:1072:A:ASP:HB2	2:1076:A:LEU:H	2	0.1	0.0	0.1
(1,2768)	2:1072:A:ASP:HB3	2:1076:A:LEU:H	2	0.1	0.0	0.1

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)
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	3	0.14
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	3	0.14
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	3	0.14
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	3	0.14
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	3	0.14
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	3	0.14
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	17	0.14
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	17	0.14
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	17	0.14
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	17	0.14
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	17	0.14
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	17	0.14
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	19	0.14
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	19	0.14
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	19	0.14
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	19	0.14
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	19	0.14
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	19	0.14
(1,2259)	1:22:B:LYS:HB2	1:23:B:ALA:HB1	13	0.14
(1,2259)	1:22:B:LYS:HB2	1:23:B:ALA:HB2	13	0.14
(1,2259)	1:22:B:LYS:HB2	1:23:B:ALA:HB3	13	0.14
(1,2259)	1:22:B:LYS:HB3	1:23:B:ALA:HB1	13	0.14
(1,2259)	1:22:B:LYS:HB3	1:23:B:ALA:HB2	13	0.14
(1,2259)	1:22:B:LYS:HB3	1:23:B:ALA:HB3	13	0.14
(1,2252)	1:20:B:LEU:HD11	2:1084:A:GLU:HG2	17	0.14
(1,2252)	1:20:B:LEU:HD11	2:1084:A:GLU:HG3	17	0.14
(1,2252)	1:20:B:LEU:HD12	2:1084:A:GLU:HG2	17	0.14
(1,2252)	1:20:B:LEU:HD12	2:1084:A:GLU:HG3	17	0.14
(1,2252)	1:20:B:LEU:HD13	2:1084:A:GLU:HG2	17	0.14
(1,2252)	1:20:B:LEU:HD13	2:1084:A:GLU:HG3	17	0.14
(1,2250)	1:20:B:LEU:HD11	2:1083:A:MET:HB2	10	0.14
(1,2250)	1:20:B:LEU:HD11	2:1083:A:MET:HB3	10	0.14
(1,2250)	1:20:B:LEU:HD12	2:1083:A:MET:HB2	10	0.14
(1,2250)	1:20:B:LEU:HD12	2:1083:A:MET:HB3	10	0.14
(1,2250)	1:20:B:LEU:HD13	2:1083:A:MET:HB2	10	0.14
(1,2250)	1:20:B:LEU:HD13	2:1083:A:MET:HB3	10	0.14
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	1	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	1	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	1	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	1	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	1	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	2	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	2	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	2	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	2	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	2	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	2	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	3	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	3	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	3	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	3	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	3	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	3	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	4	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	4	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	4	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	4	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	4	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	4	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	9	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	9	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	9	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	9	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	9	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	9	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	10	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	10	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	10	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	10	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	10	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	10	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	11	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	11	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	11	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	11	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	11	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	11	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	12	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	12	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	12	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	12	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	12	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	13	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	13	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	13	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	13	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	13	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	13	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	16	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	16	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	16	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	16	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	16	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	16	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	17	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	17	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	17	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	17	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	17	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	17	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	18	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	18	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	18	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	18	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	18	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	18	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	19	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	19	0.13
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	19	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	19	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	19	0.13
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	19	0.13
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD11	6	0.13
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD12	6	0.13
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD13	6	0.13
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD11	6	0.13
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD12	6	0.13
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD13	6	0.13
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD11	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD12	8	0.13
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD13	8	0.13
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD11	8	0.13
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD12	8	0.13
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD13	8	0.13
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD11	12	0.13
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD12	12	0.13
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD13	12	0.13
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD11	12	0.13
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD12	12	0.13
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD13	12	0.13
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	4	0.13
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	4	0.13
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	4	0.13
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	4	0.13
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	4	0.13
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	4	0.13
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	10	0.13
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	10	0.13
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	10	0.13
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	10	0.13
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	10	0.13
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	10	0.13
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	20	0.13
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	20	0.13
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	20	0.13
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	20	0.13
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	20	0.13
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	20	0.13
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD21	4	0.13
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD22	4	0.13
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD23	4	0.13
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD21	4	0.13
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD22	4	0.13
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD23	4	0.13
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD21	14	0.13
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD22	14	0.13
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD23	14	0.13
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD21	14	0.13
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD22	14	0.13
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD23	14	0.13
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD21	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD22	18	0.13
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD23	18	0.13
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD21	18	0.13
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD22	18	0.13
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD23	18	0.13
(1,2250)	1:20:B:LEU:HD11	2:1083:A:MET:HB2	17	0.13
(1,2250)	1:20:B:LEU:HD11	2:1083:A:MET:HB3	17	0.13
(1,2250)	1:20:B:LEU:HD12	2:1083:A:MET:HB2	17	0.13
(1,2250)	1:20:B:LEU:HD12	2:1083:A:MET:HB3	17	0.13
(1,2250)	1:20:B:LEU:HD13	2:1083:A:MET:HB2	17	0.13
(1,2250)	1:20:B:LEU:HD13	2:1083:A:MET:HB3	17	0.13
(1,2250)	1:20:B:LEU:HD11	2:1083:A:MET:HB2	20	0.13
(1,2250)	1:20:B:LEU:HD11	2:1083:A:MET:HB3	20	0.13
(1,2250)	1:20:B:LEU:HD12	2:1083:A:MET:HB2	20	0.13
(1,2250)	1:20:B:LEU:HD12	2:1083:A:MET:HB3	20	0.13
(1,2250)	1:20:B:LEU:HD13	2:1083:A:MET:HB2	20	0.13
(1,2250)	1:20:B:LEU:HD13	2:1083:A:MET:HB3	20	0.13
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD11	20	0.13
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD12	20	0.13
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD13	20	0.13
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD11	20	0.13
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD12	20	0.13
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD13	20	0.13
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD11	20	0.13
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD12	20	0.13
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD13	20	0.13
(1,1349)	2:987:A:THR:HA	2:987:A:THR:HG21	9	0.13
(1,1349)	2:987:A:THR:HA	2:987:A:THR:HG22	9	0.13
(1,1349)	2:987:A:THR:HA	2:987:A:THR:HG23	9	0.13
(1,1349)	2:987:A:THR:HA	2:987:A:THR:HG21	16	0.13
(1,1349)	2:987:A:THR:HA	2:987:A:THR:HG22	16	0.13
(1,1349)	2:987:A:THR:HA	2:987:A:THR:HG23	16	0.13
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE21	17	0.12
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE22	17	0.12
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE21	17	0.12
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE22	17	0.12
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE21	17	0.12
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE22	17	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	6	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	6	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	6	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	6	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	6	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	7	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	7	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	7	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	7	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	7	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	7	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	8	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	8	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	8	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	8	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	8	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	8	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	14	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	14	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	14	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	14	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	14	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	14	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	15	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	15	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	15	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	15	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	15	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	15	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG21	20	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG22	20	0.12
(1,2441)	2:1006:A:GLN:HE21	2:1011:A:ILE:HG23	20	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG21	20	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG22	20	0.12
(1,2441)	2:1006:A:GLN:HE22	2:1011:A:ILE:HG23	20	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD11	5	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD12	5	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD13	5	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD11	5	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD12	5	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD13	5	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD11	7	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD12	7	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD13	7	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD11	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD12	7	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD13	7	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD11	9	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD12	9	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD13	9	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD11	9	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD12	9	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD13	9	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD11	11	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD12	11	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD13	11	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD11	11	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD12	11	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD13	11	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD11	13	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD12	13	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD13	13	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD11	13	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD12	13	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD13	13	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD11	15	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD12	15	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD13	15	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD11	15	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD12	15	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD13	15	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD11	16	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD12	16	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD13	16	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD11	16	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD12	16	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD13	16	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD11	18	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD12	18	0.12
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD13	18	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD11	18	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD12	18	0.12
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD13	18	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	1	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	1	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	1	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	1	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	1	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	6	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	6	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	6	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	6	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	6	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	6	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	8	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	8	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	8	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	8	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	8	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	8	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	9	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	9	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	9	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	9	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	9	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	9	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	11	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	11	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	11	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	11	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	11	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	11	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	12	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	12	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	12	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	12	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	12	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	12	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	13	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	13	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	13	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	13	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	13	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	13	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	14	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	14	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	14	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	14	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	14	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	18	0.12
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	18	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	18	0.12
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	18	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	18	0.12
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	18	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD21	3	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD22	3	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD23	3	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD21	3	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD22	3	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD23	3	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD21	12	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD22	12	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD23	12	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD21	12	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD22	12	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD23	12	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD21	13	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD22	13	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD23	13	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD21	13	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD22	13	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD23	13	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD21	16	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD22	16	0.12
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD23	16	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD21	16	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD22	16	0.12
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD23	16	0.12
(1,2259)	1:22:B:LYS:HB2	1:23:B:ALA:HB1	6	0.12
(1,2259)	1:22:B:LYS:HB2	1:23:B:ALA:HB2	6	0.12
(1,2259)	1:22:B:LYS:HB2	1:23:B:ALA:HB3	6	0.12
(1,2259)	1:22:B:LYS:HB3	1:23:B:ALA:HB1	6	0.12
(1,2259)	1:22:B:LYS:HB3	1:23:B:ALA:HB2	6	0.12
(1,2259)	1:22:B:LYS:HB3	1:23:B:ALA:HB3	6	0.12
(1,2259)	1:22:B:LYS:HB2	1:23:B:ALA:HB1	8	0.12
(1,2259)	1:22:B:LYS:HB2	1:23:B:ALA:HB2	8	0.12
(1,2259)	1:22:B:LYS:HB2	1:23:B:ALA:HB3	8	0.12
(1,2259)	1:22:B:LYS:HB3	1:23:B:ALA:HB1	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2259)	1:22:B:LYS:HB3	1:23:B:ALA:HB2	8	0.12
(1,2259)	1:22:B:LYS:HB3	1:23:B:ALA:HB3	8	0.12
(1,2172)	1:11:B:LEU:HD21	1:15:B:LYS:HE2	9	0.12
(1,2172)	1:11:B:LEU:HD21	1:15:B:LYS:HE3	9	0.12
(1,2172)	1:11:B:LEU:HD22	1:15:B:LYS:HE2	9	0.12
(1,2172)	1:11:B:LEU:HD22	1:15:B:LYS:HE3	9	0.12
(1,2172)	1:11:B:LEU:HD23	1:15:B:LYS:HE2	9	0.12
(1,2172)	1:11:B:LEU:HD23	1:15:B:LYS:HE3	9	0.12
(1,2172)	1:11:B:LEU:HD21	1:15:B:LYS:HE2	17	0.12
(1,2172)	1:11:B:LEU:HD21	1:15:B:LYS:HE3	17	0.12
(1,2172)	1:11:B:LEU:HD22	1:15:B:LYS:HE2	17	0.12
(1,2172)	1:11:B:LEU:HD22	1:15:B:LYS:HE3	17	0.12
(1,2172)	1:11:B:LEU:HD23	1:15:B:LYS:HE2	17	0.12
(1,2172)	1:11:B:LEU:HD23	1:15:B:LYS:HE3	17	0.12
(1,2086)	1:20:B:LEU:HD11	2:1083:A:MET:HB2	18	0.12
(1,2086)	1:20:B:LEU:HD12	2:1083:A:MET:HB2	18	0.12
(1,2086)	1:20:B:LEU:HD13	2:1083:A:MET:HB2	18	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD21	5	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD22	5	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD23	5	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD21	5	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD22	5	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD23	5	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD21	5	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD22	5	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD23	5	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD21	12	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD22	12	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD23	12	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD21	12	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD22	12	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD23	12	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD21	12	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD22	12	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD23	12	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD21	13	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD22	13	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD23	13	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD21	13	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD22	13	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD23	13	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD21	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD22	13	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD23	13	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD21	16	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD22	16	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD23	16	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD21	16	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD22	16	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD23	16	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD21	16	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD22	16	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD23	16	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD21	17	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD22	17	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD23	17	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD21	17	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD22	17	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD23	17	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD21	17	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD22	17	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD23	17	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD21	20	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD22	20	0.12
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD23	20	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD21	20	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD22	20	0.12
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD23	20	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD21	20	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD22	20	0.12
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD23	20	0.12
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD11	17	0.12
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD12	17	0.12
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD13	17	0.12
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD11	17	0.12
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD12	17	0.12
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD13	17	0.12
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD11	17	0.12
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD12	17	0.12
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD13	17	0.12
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD11	18	0.12
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD12	18	0.12
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD13	18	0.12
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD11	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD12	18	0.12
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD13	18	0.12
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD11	18	0.12
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD12	18	0.12
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD13	18	0.12
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD11	1	0.12
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD12	1	0.12
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD13	1	0.12
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD11	1	0.12
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD12	1	0.12
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD13	1	0.12
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD11	1	0.12
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD12	1	0.12
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD13	1	0.12
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD11	16	0.12
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD12	16	0.12
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD13	16	0.12
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD11	16	0.12
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD12	16	0.12
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD13	16	0.12
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD11	16	0.12
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD12	16	0.12
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD13	16	0.12
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD11	19	0.12
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD12	19	0.12
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD13	19	0.12
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD11	19	0.12
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD12	19	0.12
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD13	19	0.12
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD11	19	0.12
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD12	19	0.12
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD13	19	0.12
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD21	15	0.12
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD22	15	0.12
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD23	15	0.12
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD21	15	0.12
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD22	15	0.12
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD23	15	0.12
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD21	15	0.12
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD22	15	0.12
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD23	15	0.12
(1,1344)	2:986:A:ILE:HG21	2:988:A:GLN:HG2	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1344)	2:986:A:ILE:HG21	2:988:A:GLN:HG3	6	0.12
(1,1344)	2:986:A:ILE:HG22	2:988:A:GLN:HG2	6	0.12
(1,1344)	2:986:A:ILE:HG22	2:988:A:GLN:HG3	6	0.12
(1,1344)	2:986:A:ILE:HG23	2:988:A:GLN:HG2	6	0.12
(1,1344)	2:986:A:ILE:HG23	2:988:A:GLN:HG3	6	0.12
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	9	0.12
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	9	0.12
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	9	0.12
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	9	0.12
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	9	0.12
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	9	0.12
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	9	0.12
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	9	0.12
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	9	0.12
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	11	0.12
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	11	0.12
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	11	0.12
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	11	0.12
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	11	0.12
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	11	0.12
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	11	0.12
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	11	0.12
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	11	0.12
(1,1296)	1:24:B:ALA:HB1	1:26:B:LEU:HD11	1	0.12
(1,1296)	1:24:B:ALA:HB1	1:26:B:LEU:HD12	1	0.12
(1,1296)	1:24:B:ALA:HB1	1:26:B:LEU:HD13	1	0.12
(1,1296)	1:24:B:ALA:HB2	1:26:B:LEU:HD11	1	0.12
(1,1296)	1:24:B:ALA:HB2	1:26:B:LEU:HD12	1	0.12
(1,1296)	1:24:B:ALA:HB2	1:26:B:LEU:HD13	1	0.12
(1,1296)	1:24:B:ALA:HB3	1:26:B:LEU:HD11	1	0.12
(1,1296)	1:24:B:ALA:HB3	1:26:B:LEU:HD12	1	0.12
(1,1296)	1:24:B:ALA:HB3	1:26:B:LEU:HD13	1	0.12
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD11	8	0.12
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD12	8	0.12
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD13	8	0.12
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD11	8	0.12
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD12	8	0.12
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD13	8	0.12
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD11	8	0.12
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD12	8	0.12
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD13	8	0.12
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD11	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD12	2	0.12
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD13	2	0.12
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD11	2	0.12
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD12	2	0.12
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD13	2	0.12
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD11	19	0.12
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD12	19	0.12
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD13	19	0.12
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD11	19	0.12
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD12	19	0.12
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD13	19	0.12
(1,2826)	1:1:B:MET:HG2	2:1076:A:LEU:HD21	18	0.11
(1,2826)	1:1:B:MET:HG2	2:1076:A:LEU:HD22	18	0.11
(1,2826)	1:1:B:MET:HG2	2:1076:A:LEU:HD23	18	0.11
(1,2826)	1:1:B:MET:HG3	2:1076:A:LEU:HD21	18	0.11
(1,2826)	1:1:B:MET:HG3	2:1076:A:LEU:HD22	18	0.11
(1,2826)	1:1:B:MET:HG3	2:1076:A:LEU:HD23	18	0.11
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE21	5	0.11
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE22	5	0.11
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE21	5	0.11
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE22	5	0.11
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE21	5	0.11
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE22	5	0.11
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE21	6	0.11
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE22	6	0.11
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE21	6	0.11
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE22	6	0.11
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE21	6	0.11
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE22	6	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD11	3	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD12	3	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD13	3	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD11	3	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD12	3	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD13	3	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD11	5	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD12	5	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD13	5	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD11	5	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD12	5	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD13	5	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD11	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD12	8	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD13	8	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD11	8	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD12	8	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD13	8	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD11	9	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD12	9	0.11
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD13	9	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD11	9	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD12	9	0.11
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD13	9	0.11
(1,2723)	2:1059:A:LEU:HD21	2:1063:A:ILE:HG12	3	0.11
(1,2723)	2:1059:A:LEU:HD21	2:1063:A:ILE:HG13	3	0.11
(1,2723)	2:1059:A:LEU:HD22	2:1063:A:ILE:HG12	3	0.11
(1,2723)	2:1059:A:LEU:HD22	2:1063:A:ILE:HG13	3	0.11
(1,2723)	2:1059:A:LEU:HD23	2:1063:A:ILE:HG12	3	0.11
(1,2723)	2:1059:A:LEU:HD23	2:1063:A:ILE:HG13	3	0.11
(1,2723)	2:1059:A:LEU:HD21	2:1063:A:ILE:HG12	7	0.11
(1,2723)	2:1059:A:LEU:HD21	2:1063:A:ILE:HG13	7	0.11
(1,2723)	2:1059:A:LEU:HD22	2:1063:A:ILE:HG12	7	0.11
(1,2723)	2:1059:A:LEU:HD22	2:1063:A:ILE:HG13	7	0.11
(1,2723)	2:1059:A:LEU:HD23	2:1063:A:ILE:HG12	7	0.11
(1,2723)	2:1059:A:LEU:HD23	2:1063:A:ILE:HG13	7	0.11
(1,2723)	2:1059:A:LEU:HD21	2:1063:A:ILE:HG12	13	0.11
(1,2723)	2:1059:A:LEU:HD21	2:1063:A:ILE:HG13	13	0.11
(1,2723)	2:1059:A:LEU:HD22	2:1063:A:ILE:HG12	13	0.11
(1,2723)	2:1059:A:LEU:HD22	2:1063:A:ILE:HG13	13	0.11
(1,2723)	2:1059:A:LEU:HD23	2:1063:A:ILE:HG12	13	0.11
(1,2723)	2:1059:A:LEU:HD23	2:1063:A:ILE:HG13	13	0.11
(1,2723)	2:1059:A:LEU:HD21	2:1063:A:ILE:HG12	20	0.11
(1,2723)	2:1059:A:LEU:HD21	2:1063:A:ILE:HG13	20	0.11
(1,2723)	2:1059:A:LEU:HD22	2:1063:A:ILE:HG12	20	0.11
(1,2723)	2:1059:A:LEU:HD22	2:1063:A:ILE:HG13	20	0.11
(1,2723)	2:1059:A:LEU:HD23	2:1063:A:ILE:HG12	20	0.11
(1,2723)	2:1059:A:LEU:HD23	2:1063:A:ILE:HG13	20	0.11
(1,2691)	2:1049:A:GLN:HG2	2:1052:A:ALA:HB1	7	0.11
(1,2691)	2:1049:A:GLN:HG2	2:1052:A:ALA:HB2	7	0.11
(1,2691)	2:1049:A:GLN:HG2	2:1052:A:ALA:HB3	7	0.11
(1,2691)	2:1049:A:GLN:HG3	2:1052:A:ALA:HB1	7	0.11
(1,2691)	2:1049:A:GLN:HG3	2:1052:A:ALA:HB2	7	0.11
(1,2691)	2:1049:A:GLN:HG3	2:1052:A:ALA:HB3	7	0.11
(1,2691)	2:1049:A:GLN:HG2	2:1052:A:ALA:HB1	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2691)	2:1049:A:GLN:HG2	2:1052:A:ALA:HB2	11	0.11
(1,2691)	2:1049:A:GLN:HG2	2:1052:A:ALA:HB3	11	0.11
(1,2691)	2:1049:A:GLN:HG3	2:1052:A:ALA:HB1	11	0.11
(1,2691)	2:1049:A:GLN:HG3	2:1052:A:ALA:HB2	11	0.11
(1,2691)	2:1049:A:GLN:HG3	2:1052:A:ALA:HB3	11	0.11
(1,2691)	2:1049:A:GLN:HG2	2:1052:A:ALA:HB1	12	0.11
(1,2691)	2:1049:A:GLN:HG2	2:1052:A:ALA:HB2	12	0.11
(1,2691)	2:1049:A:GLN:HG2	2:1052:A:ALA:HB3	12	0.11
(1,2691)	2:1049:A:GLN:HG3	2:1052:A:ALA:HB1	12	0.11
(1,2691)	2:1049:A:GLN:HG3	2:1052:A:ALA:HB2	12	0.11
(1,2691)	2:1049:A:GLN:HG3	2:1052:A:ALA:HB3	12	0.11
(1,2587)	2:1035:A:SER:H	2:1036:A:ARG:HD2	15	0.11
(1,2587)	2:1035:A:SER:H	2:1036:A:ARG:HD3	15	0.11
(1,2563)	2:1032:A:GLN:HG2	2:1035:A:SER:HB2	11	0.11
(1,2563)	2:1032:A:GLN:HG2	2:1035:A:SER:HB3	11	0.11
(1,2563)	2:1032:A:GLN:HG3	2:1035:A:SER:HB2	11	0.11
(1,2563)	2:1032:A:GLN:HG3	2:1035:A:SER:HB3	11	0.11
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE21	4	0.11
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE22	4	0.11
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE21	4	0.11
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE22	4	0.11
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE21	4	0.11
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE22	4	0.11
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE21	6	0.11
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE22	6	0.11
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE21	6	0.11
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE22	6	0.11
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE21	6	0.11
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE22	6	0.11
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE21	8	0.11
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE22	8	0.11
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE21	8	0.11
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE22	8	0.11
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE21	8	0.11
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE22	8	0.11
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE21	10	0.11
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE22	10	0.11
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE21	10	0.11
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE22	10	0.11
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE21	10	0.11
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE22	10	0.11
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE21	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE22	14	0.11
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE21	14	0.11
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE22	14	0.11
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE21	14	0.11
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE22	14	0.11
(1,2466)	2:1009:A:LEU:HD21	2:1024:A:GLY:HA2	4	0.11
(1,2466)	2:1009:A:LEU:HD21	2:1024:A:GLY:HA3	4	0.11
(1,2466)	2:1009:A:LEU:HD22	2:1024:A:GLY:HA2	4	0.11
(1,2466)	2:1009:A:LEU:HD22	2:1024:A:GLY:HA3	4	0.11
(1,2466)	2:1009:A:LEU:HD23	2:1024:A:GLY:HA2	4	0.11
(1,2466)	2:1009:A:LEU:HD23	2:1024:A:GLY:HA3	4	0.11
(1,2466)	2:1009:A:LEU:HD21	2:1024:A:GLY:HA2	14	0.11
(1,2466)	2:1009:A:LEU:HD21	2:1024:A:GLY:HA3	14	0.11
(1,2466)	2:1009:A:LEU:HD22	2:1024:A:GLY:HA2	14	0.11
(1,2466)	2:1009:A:LEU:HD22	2:1024:A:GLY:HA3	14	0.11
(1,2466)	2:1009:A:LEU:HD23	2:1024:A:GLY:HA2	14	0.11
(1,2466)	2:1009:A:LEU:HD23	2:1024:A:GLY:HA3	14	0.11
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD11	1	0.11
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD12	1	0.11
(1,2440)	2:1006:A:GLN:HG2	2:1014:A:ILE:HD13	1	0.11
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD11	1	0.11
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD12	1	0.11
(1,2440)	2:1006:A:GLN:HG3	2:1014:A:ILE:HD13	1	0.11
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	2	0.11
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	2	0.11
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	2	0.11
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	2	0.11
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	2	0.11
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	2	0.11
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	5	0.11
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	5	0.11
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	5	0.11
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	5	0.11
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	5	0.11
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	5	0.11
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	7	0.11
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	7	0.11
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	7	0.11
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	7	0.11
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	7	0.11
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	7	0.11
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	15	0.11
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	15	0.11
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	15	0.11
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	15	0.11
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	15	0.11
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE21	16	0.11
(1,2410)	2:1004:A:ILE:HG21	2:1006:A:GLN:HE22	16	0.11
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE21	16	0.11
(1,2410)	2:1004:A:ILE:HG22	2:1006:A:GLN:HE22	16	0.11
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE21	16	0.11
(1,2410)	2:1004:A:ILE:HG23	2:1006:A:GLN:HE22	16	0.11
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD21	11	0.11
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD22	11	0.11
(1,2376)	2:1000:A:GLN:HG2	2:1001:A:LEU:HD23	11	0.11
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD21	11	0.11
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD22	11	0.11
(1,2376)	2:1000:A:GLN:HG3	2:1001:A:LEU:HD23	11	0.11
(1,2283)	1:29:B:GLN:H	1:29:B:GLN:HB2	3	0.11
(1,2283)	1:29:B:GLN:H	1:29:B:GLN:HB3	3	0.11
(1,2272)	1:26:B:LEU:HD21	2:1072:A:ASP:HB2	7	0.11
(1,2272)	1:26:B:LEU:HD21	2:1072:A:ASP:HB3	7	0.11
(1,2272)	1:26:B:LEU:HD22	2:1072:A:ASP:HB2	7	0.11
(1,2272)	1:26:B:LEU:HD22	2:1072:A:ASP:HB3	7	0.11
(1,2272)	1:26:B:LEU:HD23	2:1072:A:ASP:HB2	7	0.11
(1,2272)	1:26:B:LEU:HD23	2:1072:A:ASP:HB3	7	0.11
(1,2272)	1:26:B:LEU:HD21	2:1072:A:ASP:HB2	17	0.11
(1,2272)	1:26:B:LEU:HD21	2:1072:A:ASP:HB3	17	0.11
(1,2272)	1:26:B:LEU:HD22	2:1072:A:ASP:HB2	17	0.11
(1,2272)	1:26:B:LEU:HD22	2:1072:A:ASP:HB3	17	0.11
(1,2272)	1:26:B:LEU:HD23	2:1072:A:ASP:HB2	17	0.11
(1,2272)	1:26:B:LEU:HD23	2:1072:A:ASP:HB3	17	0.11
(1,2272)	1:26:B:LEU:HD21	2:1072:A:ASP:HB2	19	0.11
(1,2272)	1:26:B:LEU:HD21	2:1072:A:ASP:HB3	19	0.11
(1,2272)	1:26:B:LEU:HD22	2:1072:A:ASP:HB2	19	0.11
(1,2272)	1:26:B:LEU:HD22	2:1072:A:ASP:HB3	19	0.11
(1,2272)	1:26:B:LEU:HD23	2:1072:A:ASP:HB2	19	0.11
(1,2272)	1:26:B:LEU:HD23	2:1072:A:ASP:HB3	19	0.11
(1,2252)	1:20:B:LEU:HD11	2:1084:A:GLU:HG2	13	0.11
(1,2252)	1:20:B:LEU:HD11	2:1084:A:GLU:HG3	13	0.11
(1,2252)	1:20:B:LEU:HD12	2:1084:A:GLU:HG2	13	0.11
(1,2252)	1:20:B:LEU:HD12	2:1084:A:GLU:HG3	13	0.11
(1,2252)	1:20:B:LEU:HD13	2:1084:A:GLU:HG2	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2252)	1:20:B:LEU:HD13	2:1084:A:GLU:HG3	13	0.11
(1,2252)	1:20:B:LEU:HD11	2:1084:A:GLU:HG2	14	0.11
(1,2252)	1:20:B:LEU:HD11	2:1084:A:GLU:HG3	14	0.11
(1,2252)	1:20:B:LEU:HD12	2:1084:A:GLU:HG2	14	0.11
(1,2252)	1:20:B:LEU:HD12	2:1084:A:GLU:HG3	14	0.11
(1,2252)	1:20:B:LEU:HD13	2:1084:A:GLU:HG2	14	0.11
(1,2252)	1:20:B:LEU:HD13	2:1084:A:GLU:HG3	14	0.11
(1,2252)	1:20:B:LEU:HD11	2:1084:A:GLU:HG2	20	0.11
(1,2252)	1:20:B:LEU:HD11	2:1084:A:GLU:HG3	20	0.11
(1,2252)	1:20:B:LEU:HD12	2:1084:A:GLU:HG2	20	0.11
(1,2252)	1:20:B:LEU:HD12	2:1084:A:GLU:HG3	20	0.11
(1,2252)	1:20:B:LEU:HD13	2:1084:A:GLU:HG2	20	0.11
(1,2252)	1:20:B:LEU:HD13	2:1084:A:GLU:HG3	20	0.11
(1,2208)	1:16:B:ARG:HG2	1:20:B:LEU:HD11	10	0.11
(1,2208)	1:16:B:ARG:HG2	1:20:B:LEU:HD12	10	0.11
(1,2208)	1:16:B:ARG:HG2	1:20:B:LEU:HD13	10	0.11
(1,2208)	1:16:B:ARG:HG3	1:20:B:LEU:HD11	10	0.11
(1,2208)	1:16:B:ARG:HG3	1:20:B:LEU:HD12	10	0.11
(1,2208)	1:16:B:ARG:HG3	1:20:B:LEU:HD13	10	0.11
(1,2208)	1:16:B:ARG:HG2	1:20:B:LEU:HD11	17	0.11
(1,2208)	1:16:B:ARG:HG2	1:20:B:LEU:HD12	17	0.11
(1,2208)	1:16:B:ARG:HG2	1:20:B:LEU:HD13	17	0.11
(1,2208)	1:16:B:ARG:HG3	1:20:B:LEU:HD11	17	0.11
(1,2208)	1:16:B:ARG:HG3	1:20:B:LEU:HD12	17	0.11
(1,2208)	1:16:B:ARG:HG3	1:20:B:LEU:HD13	17	0.11
(1,2208)	1:16:B:ARG:HG2	1:20:B:LEU:HD11	20	0.11
(1,2208)	1:16:B:ARG:HG2	1:20:B:LEU:HD12	20	0.11
(1,2208)	1:16:B:ARG:HG2	1:20:B:LEU:HD13	20	0.11
(1,2208)	1:16:B:ARG:HG3	1:20:B:LEU:HD11	20	0.11
(1,2208)	1:16:B:ARG:HG3	1:20:B:LEU:HD12	20	0.11
(1,2208)	1:16:B:ARG:HG3	1:20:B:LEU:HD13	20	0.11
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD21	5	0.11
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD22	5	0.11
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD23	5	0.11
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD21	5	0.11
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD22	5	0.11
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD23	5	0.11
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD21	11	0.11
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD22	11	0.11
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD23	11	0.11
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD21	11	0.11
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD22	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD23	11	0.11
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD21	13	0.11
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD22	13	0.11
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD23	13	0.11
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD21	13	0.11
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD22	13	0.11
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD23	13	0.11
(1,2099)	1:26:B:LEU:HD11	2:1071:A:PHE:HD1	11	0.11
(1,2099)	1:26:B:LEU:HD11	2:1071:A:PHE:HD2	11	0.11
(1,2099)	1:26:B:LEU:HD12	2:1071:A:PHE:HD1	11	0.11
(1,2099)	1:26:B:LEU:HD12	2:1071:A:PHE:HD2	11	0.11
(1,2099)	1:26:B:LEU:HD13	2:1071:A:PHE:HD1	11	0.11
(1,2099)	1:26:B:LEU:HD13	2:1071:A:PHE:HD2	11	0.11
(1,1975)	1:17:B:LEU:HD11	2:1079:A:ILE:HA	5	0.11
(1,1975)	1:17:B:LEU:HD12	2:1079:A:ILE:HA	5	0.11
(1,1975)	1:17:B:LEU:HD13	2:1079:A:ILE:HA	5	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD21	3	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD22	3	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD23	3	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD21	3	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD22	3	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD23	3	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD21	3	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD22	3	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD23	3	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD21	6	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD22	6	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD23	6	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD21	6	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD22	6	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD23	6	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD21	6	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD22	6	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD23	6	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD21	7	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD22	7	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD23	7	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD21	7	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD22	7	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD23	7	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD21	7	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD22	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD23	7	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD21	10	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD22	10	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD23	10	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD21	10	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD22	10	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD23	10	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD21	10	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD22	10	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD23	10	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD21	18	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD22	18	0.11
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD23	18	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD21	18	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD22	18	0.11
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD23	18	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD21	18	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD22	18	0.11
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD23	18	0.11
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD11	2	0.11
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD12	2	0.11
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD13	2	0.11
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD11	2	0.11
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD12	2	0.11
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD13	2	0.11
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD11	2	0.11
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD12	2	0.11
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD13	2	0.11
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD11	16	0.11
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD12	16	0.11
(1,1800)	2:1037:A:ILE:HG21	2:1045:A:ILE:HD13	16	0.11
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD11	16	0.11
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD12	16	0.11
(1,1800)	2:1037:A:ILE:HG22	2:1045:A:ILE:HD13	16	0.11
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD11	16	0.11
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD12	16	0.11
(1,1800)	2:1037:A:ILE:HG23	2:1045:A:ILE:HD13	16	0.11
(1,1776)	2:1000:A:GLN:HB2	2:1040:A:ILE:HG21	11	0.11
(1,1776)	2:1000:A:GLN:HB2	2:1040:A:ILE:HG22	11	0.11
(1,1776)	2:1000:A:GLN:HB2	2:1040:A:ILE:HG23	11	0.11
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG21	10	0.11
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG22	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG23	10	0.11
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG21	10	0.11
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG22	10	0.11
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG23	10	0.11
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG21	10	0.11
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG22	10	0.11
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG23	10	0.11
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG21	15	0.11
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG22	15	0.11
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG23	15	0.11
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG21	15	0.11
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG22	15	0.11
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG23	15	0.11
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG21	15	0.11
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG22	15	0.11
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG23	15	0.11
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG21	17	0.11
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG22	17	0.11
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG23	17	0.11
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG21	17	0.11
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG22	17	0.11
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG23	17	0.11
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG21	17	0.11
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG22	17	0.11
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG23	17	0.11
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD11	6	0.11
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD12	6	0.11
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD13	6	0.11
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD11	6	0.11
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD12	6	0.11
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD13	6	0.11
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD11	6	0.11
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD12	6	0.11
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD13	6	0.11
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD11	12	0.11
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD12	12	0.11
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD13	12	0.11
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD11	12	0.11
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD12	12	0.11
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD13	12	0.11
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD11	12	0.11
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD12	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD13	12	0.11
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD11	17	0.11
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD12	17	0.11
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD13	17	0.11
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD11	17	0.11
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD12	17	0.11
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD13	17	0.11
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD11	17	0.11
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD12	17	0.11
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD13	17	0.11
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD11	5	0.11
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD12	5	0.11
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD13	5	0.11
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD11	5	0.11
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD12	5	0.11
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD13	5	0.11
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD11	5	0.11
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD12	5	0.11
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD13	5	0.11
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB2	6	0.11
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB3	6	0.11
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB2	6	0.11
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB3	6	0.11
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB2	6	0.11
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB3	6	0.11
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB2	9	0.11
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB3	9	0.11
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB2	9	0.11
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB3	9	0.11
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB2	9	0.11
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB3	9	0.11
(1,1500)	2:1007:A:THR:HG21	2:1010:A:LYS:H	10	0.11
(1,1500)	2:1007:A:THR:HG22	2:1010:A:LYS:H	10	0.11
(1,1500)	2:1007:A:THR:HG23	2:1010:A:LYS:H	10	0.11
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD21	1	0.11
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD22	1	0.11
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD23	1	0.11
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD21	1	0.11
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD22	1	0.11
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD23	1	0.11
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD21	1	0.11
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD22	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD23	1	0.11
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD21	5	0.11
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD22	5	0.11
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD23	5	0.11
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD21	5	0.11
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD22	5	0.11
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD23	5	0.11
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD21	5	0.11
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD22	5	0.11
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD23	5	0.11
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD21	11	0.11
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD22	11	0.11
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD23	11	0.11
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD21	11	0.11
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD22	11	0.11
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD23	11	0.11
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD21	11	0.11
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD22	11	0.11
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD23	11	0.11
(1,1405)	2:997:A:ILE:HG21	2:1063:A:ILE:HD11	8	0.11
(1,1405)	2:997:A:ILE:HG21	2:1063:A:ILE:HD12	8	0.11
(1,1405)	2:997:A:ILE:HG21	2:1063:A:ILE:HD13	8	0.11
(1,1405)	2:997:A:ILE:HG22	2:1063:A:ILE:HD11	8	0.11
(1,1405)	2:997:A:ILE:HG22	2:1063:A:ILE:HD12	8	0.11
(1,1405)	2:997:A:ILE:HG22	2:1063:A:ILE:HD13	8	0.11
(1,1405)	2:997:A:ILE:HG23	2:1063:A:ILE:HD11	8	0.11
(1,1405)	2:997:A:ILE:HG23	2:1063:A:ILE:HD12	8	0.11
(1,1405)	2:997:A:ILE:HG23	2:1063:A:ILE:HD13	8	0.11
(1,1354)	2:988:A:GLN:HA	2:988:A:GLN:HG2	17	0.11
(1,1354)	2:988:A:GLN:HA	2:988:A:GLN:HG3	17	0.11
(1,1344)	2:986:A:ILE:HG21	2:988:A:GLN:HG2	15	0.11
(1,1344)	2:986:A:ILE:HG21	2:988:A:GLN:HG3	15	0.11
(1,1344)	2:986:A:ILE:HG22	2:988:A:GLN:HG2	15	0.11
(1,1344)	2:986:A:ILE:HG22	2:988:A:GLN:HG3	15	0.11
(1,1344)	2:986:A:ILE:HG23	2:988:A:GLN:HG2	15	0.11
(1,1344)	2:986:A:ILE:HG23	2:988:A:GLN:HG3	15	0.11
(1,1344)	2:986:A:ILE:HG21	2:988:A:GLN:HG2	20	0.11
(1,1344)	2:986:A:ILE:HG21	2:988:A:GLN:HG3	20	0.11
(1,1344)	2:986:A:ILE:HG22	2:988:A:GLN:HG2	20	0.11
(1,1344)	2:986:A:ILE:HG22	2:988:A:GLN:HG3	20	0.11
(1,1344)	2:986:A:ILE:HG23	2:988:A:GLN:HG2	20	0.11
(1,1344)	2:986:A:ILE:HG23	2:988:A:GLN:HG3	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1324)	1:20:B:LEU:HD11	2:1079:A:ILE:HD11	14	0.11
(1,1324)	1:20:B:LEU:HD11	2:1079:A:ILE:HD12	14	0.11
(1,1324)	1:20:B:LEU:HD11	2:1079:A:ILE:HD13	14	0.11
(1,1324)	1:20:B:LEU:HD12	2:1079:A:ILE:HD11	14	0.11
(1,1324)	1:20:B:LEU:HD12	2:1079:A:ILE:HD12	14	0.11
(1,1324)	1:20:B:LEU:HD12	2:1079:A:ILE:HD13	14	0.11
(1,1324)	1:20:B:LEU:HD13	2:1079:A:ILE:HD11	14	0.11
(1,1324)	1:20:B:LEU:HD13	2:1079:A:ILE:HD12	14	0.11
(1,1324)	1:20:B:LEU:HD13	2:1079:A:ILE:HD13	14	0.11
(1,1324)	1:20:B:LEU:HD11	2:1079:A:ILE:HD11	18	0.11
(1,1324)	1:20:B:LEU:HD11	2:1079:A:ILE:HD12	18	0.11
(1,1324)	1:20:B:LEU:HD11	2:1079:A:ILE:HD13	18	0.11
(1,1324)	1:20:B:LEU:HD12	2:1079:A:ILE:HD11	18	0.11
(1,1324)	1:20:B:LEU:HD12	2:1079:A:ILE:HD12	18	0.11
(1,1324)	1:20:B:LEU:HD12	2:1079:A:ILE:HD13	18	0.11
(1,1324)	1:20:B:LEU:HD13	2:1079:A:ILE:HD11	18	0.11
(1,1324)	1:20:B:LEU:HD13	2:1079:A:ILE:HD12	18	0.11
(1,1324)	1:20:B:LEU:HD13	2:1079:A:ILE:HD13	18	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	1	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	1	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	1	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	1	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	1	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	1	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	1	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	1	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	1	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	2	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	2	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	2	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	2	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	2	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	2	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	2	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	2	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	2	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	5	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	5	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	5	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	5	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	5	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	5	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	5	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	5	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	6	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	6	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	6	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	6	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	6	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	6	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	6	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	6	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	6	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	7	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	7	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	7	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	7	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	7	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	7	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	7	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	7	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	7	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	8	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	8	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	8	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	8	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	8	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	8	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	8	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	8	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	8	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	14	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	14	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	14	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	14	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	14	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	14	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	14	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	14	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	14	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	15	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	15	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	15	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	15	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	15	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	15	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	15	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	15	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	16	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	16	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	16	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	16	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	16	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	16	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	16	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	16	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	16	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	17	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	17	0.11
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	17	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	17	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	17	0.11
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	17	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	17	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	17	0.11
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	17	0.11
(1,1276)	1:18:B:LEU:HD11	1:22:B:LYS:HD2	14	0.11
(1,1276)	1:18:B:LEU:HD11	1:22:B:LYS:HD3	14	0.11
(1,1276)	1:18:B:LEU:HD12	1:22:B:LYS:HD2	14	0.11
(1,1276)	1:18:B:LEU:HD12	1:22:B:LYS:HD3	14	0.11
(1,1276)	1:18:B:LEU:HD13	1:22:B:LYS:HD2	14	0.11
(1,1276)	1:18:B:LEU:HD13	1:22:B:LYS:HD3	14	0.11
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD11	13	0.11
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD12	13	0.11
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD13	13	0.11
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD11	13	0.11
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD12	13	0.11
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD13	13	0.11
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD11	13	0.11
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD12	13	0.11
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD13	13	0.11
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD11	18	0.11
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD12	18	0.11
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD13	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD11	18	0.11
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD12	18	0.11
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD13	18	0.11
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD11	18	0.11
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD12	18	0.11
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD13	18	0.11
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD11	19	0.11
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD12	19	0.11
(1,1256)	1:17:B:LEU:HD11	1:18:B:LEU:HD13	19	0.11
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD11	19	0.11
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD12	19	0.11
(1,1256)	1:17:B:LEU:HD12	1:18:B:LEU:HD13	19	0.11
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD11	19	0.11
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD12	19	0.11
(1,1256)	1:17:B:LEU:HD13	1:18:B:LEU:HD13	19	0.11
(1,1204)	1:11:B:LEU:HD11	2:1064:A:ILE:HD11	7	0.11
(1,1204)	1:11:B:LEU:HD11	2:1064:A:ILE:HD12	7	0.11
(1,1204)	1:11:B:LEU:HD11	2:1064:A:ILE:HD13	7	0.11
(1,1204)	1:11:B:LEU:HD12	2:1064:A:ILE:HD11	7	0.11
(1,1204)	1:11:B:LEU:HD12	2:1064:A:ILE:HD12	7	0.11
(1,1204)	1:11:B:LEU:HD12	2:1064:A:ILE:HD13	7	0.11
(1,1204)	1:11:B:LEU:HD13	2:1064:A:ILE:HD11	7	0.11
(1,1204)	1:11:B:LEU:HD13	2:1064:A:ILE:HD12	7	0.11
(1,1204)	1:11:B:LEU:HD13	2:1064:A:ILE:HD13	7	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD11	4	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD12	4	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD13	4	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD11	4	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD12	4	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD13	4	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD11	7	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD12	7	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD13	7	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD11	7	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD12	7	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD13	7	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD11	8	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD12	8	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD13	8	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD11	8	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD12	8	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD13	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD11	11	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD12	11	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD13	11	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD11	11	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD12	11	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD13	11	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD11	13	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD12	13	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD13	13	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD11	13	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD12	13	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD13	13	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD11	16	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD12	16	0.11
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD13	16	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD11	16	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD12	16	0.11
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD13	16	0.11
(1,1169)	1:3:B:ASN:HB2	1:7:B:THR:HG21	11	0.11
(1,1169)	1:3:B:ASN:HB2	1:7:B:THR:HG22	11	0.11
(1,1169)	1:3:B:ASN:HB2	1:7:B:THR:HG23	11	0.11
(1,1169)	1:3:B:ASN:HB3	1:7:B:THR:HG21	11	0.11
(1,1169)	1:3:B:ASN:HB3	1:7:B:THR:HG22	11	0.11
(1,1169)	1:3:B:ASN:HB3	1:7:B:THR:HG23	11	0.11
(1,1169)	1:3:B:ASN:HB2	1:7:B:THR:HG21	19	0.11
(1,1169)	1:3:B:ASN:HB2	1:7:B:THR:HG22	19	0.11
(1,1169)	1:3:B:ASN:HB2	1:7:B:THR:HG23	19	0.11
(1,1169)	1:3:B:ASN:HB3	1:7:B:THR:HG21	19	0.11
(1,1169)	1:3:B:ASN:HB3	1:7:B:THR:HG22	19	0.11
(1,1169)	1:3:B:ASN:HB3	1:7:B:THR:HG23	19	0.11
(1,938)	1:7:B:THR:H	2:1068:A:LEU:HD11	7	0.11
(1,938)	1:7:B:THR:H	2:1068:A:LEU:HD12	7	0.11
(1,938)	1:7:B:THR:H	2:1068:A:LEU:HD13	7	0.11
(1,838)	2:1004:A:ILE:HG21	2:1032:A:GLN:HE22	12	0.11
(1,838)	2:1004:A:ILE:HG22	2:1032:A:GLN:HE22	12	0.11
(1,838)	2:1004:A:ILE:HG23	2:1032:A:GLN:HE22	12	0.11
(1,661)	2:1066:A:ALA:H	2:1069:A:LEU:HD11	14	0.11
(1,661)	2:1066:A:ALA:H	2:1069:A:LEU:HD12	14	0.11
(1,661)	2:1066:A:ALA:H	2:1069:A:LEU:HD13	14	0.11
(1,242)	2:1014:A:ILE:H	2:1056:A:ILE:HD11	12	0.11
(1,242)	2:1014:A:ILE:H	2:1056:A:ILE:HD12	12	0.11
(1,242)	2:1014:A:ILE:H	2:1056:A:ILE:HD13	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	2:1001:A:LEU:H	2:1059:A:LEU:HD11	19	0.11
(1,96)	2:1001:A:LEU:H	2:1059:A:LEU:HD12	19	0.11
(1,96)	2:1001:A:LEU:H	2:1059:A:LEU:HD13	19	0.11
(1,2819)	2:1083:A:MET:HG2	2:1084:A:GLU:H	18	0.1
(1,2819)	2:1083:A:MET:HG3	2:1084:A:GLU:H	18	0.1
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE21	1	0.1
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE22	1	0.1
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE21	1	0.1
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE22	1	0.1
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE21	1	0.1
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE22	1	0.1
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE21	8	0.1
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE22	8	0.1
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE21	8	0.1
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE22	8	0.1
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE21	8	0.1
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE22	8	0.1
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE21	10	0.1
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE22	10	0.1
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE21	10	0.1
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE22	10	0.1
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE21	10	0.1
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE22	10	0.1
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE21	11	0.1
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE22	11	0.1
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE21	11	0.1
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE22	11	0.1
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE21	11	0.1
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE22	11	0.1
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE21	20	0.1
(1,2779)	2:1076:A:LEU:HD21	2:1077:A:GLN:HE22	20	0.1
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE21	20	0.1
(1,2779)	2:1076:A:LEU:HD22	2:1077:A:GLN:HE22	20	0.1
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE21	20	0.1
(1,2779)	2:1076:A:LEU:HD23	2:1077:A:GLN:HE22	20	0.1
(1,2768)	2:1072:A:ASP:HB2	2:1076:A:LEU:H	11	0.1
(1,2768)	2:1072:A:ASP:HB3	2:1076:A:LEU:H	11	0.1
(1,2768)	2:1072:A:ASP:HB2	2:1076:A:LEU:H	19	0.1
(1,2768)	2:1072:A:ASP:HB3	2:1076:A:LEU:H	19	0.1
(1,2763)	2:1070:A:GLN:HG2	2:1071:A:PHE:H	20	0.1
(1,2763)	2:1070:A:GLN:HG3	2:1071:A:PHE:H	20	0.1
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD11	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD12	12	0.1
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD13	12	0.1
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD11	12	0.1
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD12	12	0.1
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD13	12	0.1
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD11	14	0.1
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD12	14	0.1
(1,2740)	2:1065:A:ASN:HD21	2:1068:A:LEU:HD13	14	0.1
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD11	14	0.1
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD12	14	0.1
(1,2740)	2:1065:A:ASN:HD22	2:1068:A:LEU:HD13	14	0.1
(1,2723)	2:1059:A:LEU:HD21	2:1063:A:ILE:HG12	5	0.1
(1,2723)	2:1059:A:LEU:HD21	2:1063:A:ILE:HG13	5	0.1
(1,2723)	2:1059:A:LEU:HD22	2:1063:A:ILE:HG12	5	0.1
(1,2723)	2:1059:A:LEU:HD22	2:1063:A:ILE:HG13	5	0.1
(1,2723)	2:1059:A:LEU:HD23	2:1063:A:ILE:HG12	5	0.1
(1,2723)	2:1059:A:LEU:HD23	2:1063:A:ILE:HG13	5	0.1
(1,2711)	2:1056:A:ILE:HG21	2:1057:A:CYS:HB2	20	0.1
(1,2711)	2:1056:A:ILE:HG21	2:1057:A:CYS:HB3	20	0.1
(1,2711)	2:1056:A:ILE:HG22	2:1057:A:CYS:HB2	20	0.1
(1,2711)	2:1056:A:ILE:HG22	2:1057:A:CYS:HB3	20	0.1
(1,2711)	2:1056:A:ILE:HG23	2:1057:A:CYS:HB2	20	0.1
(1,2711)	2:1056:A:ILE:HG23	2:1057:A:CYS:HB3	20	0.1
(1,2611)	2:1036:A:ARG:HD2	2:1039:A:GLU:H	16	0.1
(1,2611)	2:1036:A:ARG:HD3	2:1039:A:GLU:H	16	0.1
(1,2587)	2:1035:A:SER:H	2:1036:A:ARG:HD2	16	0.1
(1,2587)	2:1035:A:SER:H	2:1036:A:ARG:HD3	16	0.1
(1,2573)	2:1034:A:GLN:HB2	2:1035:A:SER:HB2	20	0.1
(1,2573)	2:1034:A:GLN:HB2	2:1035:A:SER:HB3	20	0.1
(1,2573)	2:1034:A:GLN:HB3	2:1035:A:SER:HB2	20	0.1
(1,2573)	2:1034:A:GLN:HB3	2:1035:A:SER:HB3	20	0.1
(1,2552)	2:1031:A:LEU:HD21	2:1034:A:GLN:HE21	4	0.1
(1,2552)	2:1031:A:LEU:HD21	2:1034:A:GLN:HE22	4	0.1
(1,2552)	2:1031:A:LEU:HD22	2:1034:A:GLN:HE21	4	0.1
(1,2552)	2:1031:A:LEU:HD22	2:1034:A:GLN:HE22	4	0.1
(1,2552)	2:1031:A:LEU:HD23	2:1034:A:GLN:HE21	4	0.1
(1,2552)	2:1031:A:LEU:HD23	2:1034:A:GLN:HE22	4	0.1
(1,2552)	2:1031:A:LEU:HD21	2:1034:A:GLN:HE21	15	0.1
(1,2552)	2:1031:A:LEU:HD21	2:1034:A:GLN:HE22	15	0.1
(1,2552)	2:1031:A:LEU:HD22	2:1034:A:GLN:HE21	15	0.1
(1,2552)	2:1031:A:LEU:HD22	2:1034:A:GLN:HE22	15	0.1
(1,2552)	2:1031:A:LEU:HD23	2:1034:A:GLN:HE21	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2552)	2:1031:A:LEU:HD23	2:1034:A:GLN:HE22	15	0.1
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE21	7	0.1
(1,2543)	2:1029:A:LEU:HD21	2:1032:A:GLN:HE22	7	0.1
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE21	7	0.1
(1,2543)	2:1029:A:LEU:HD22	2:1032:A:GLN:HE22	7	0.1
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE21	7	0.1
(1,2543)	2:1029:A:LEU:HD23	2:1032:A:GLN:HE22	7	0.1
(1,2377)	2:1000:A:GLN:HG2	2:1004:A:ILE:HD11	3	0.1
(1,2377)	2:1000:A:GLN:HG2	2:1004:A:ILE:HD12	3	0.1
(1,2377)	2:1000:A:GLN:HG2	2:1004:A:ILE:HD13	3	0.1
(1,2377)	2:1000:A:GLN:HG3	2:1004:A:ILE:HD11	3	0.1
(1,2377)	2:1000:A:GLN:HG3	2:1004:A:ILE:HD12	3	0.1
(1,2377)	2:1000:A:GLN:HG3	2:1004:A:ILE:HD13	3	0.1
(1,2314)	2:990:A:TYR:HD1	2:1013:A:ARG:HB2	12	0.1
(1,2314)	2:990:A:TYR:HD1	2:1013:A:ARG:HB3	12	0.1
(1,2314)	2:990:A:TYR:HD2	2:1013:A:ARG:HB2	12	0.1
(1,2314)	2:990:A:TYR:HD2	2:1013:A:ARG:HB3	12	0.1
(1,2306)	2:988:A:GLN:HE21	2:989:A:GLU:H	9	0.1
(1,2306)	2:988:A:GLN:HE22	2:989:A:GLU:H	9	0.1
(1,2296)	2:986:A:ILE:HG21	2:988:A:GLN:HE21	18	0.1
(1,2296)	2:986:A:ILE:HG21	2:988:A:GLN:HE22	18	0.1
(1,2296)	2:986:A:ILE:HG22	2:988:A:GLN:HE21	18	0.1
(1,2296)	2:986:A:ILE:HG22	2:988:A:GLN:HE22	18	0.1
(1,2296)	2:986:A:ILE:HG23	2:988:A:GLN:HE21	18	0.1
(1,2296)	2:986:A:ILE:HG23	2:988:A:GLN:HE22	18	0.1
(1,2252)	1:20:B:LEU:HD11	2:1084:A:GLU:HG2	19	0.1
(1,2252)	1:20:B:LEU:HD11	2:1084:A:GLU:HG3	19	0.1
(1,2252)	1:20:B:LEU:HD12	2:1084:A:GLU:HG2	19	0.1
(1,2252)	1:20:B:LEU:HD12	2:1084:A:GLU:HG3	19	0.1
(1,2252)	1:20:B:LEU:HD13	2:1084:A:GLU:HG2	19	0.1
(1,2252)	1:20:B:LEU:HD13	2:1084:A:GLU:HG3	19	0.1
(1,2242)	1:19:B:GLU:HG2	1:20:B:LEU:HD21	16	0.1
(1,2242)	1:19:B:GLU:HG2	1:20:B:LEU:HD22	16	0.1
(1,2242)	1:19:B:GLU:HG2	1:20:B:LEU:HD23	16	0.1
(1,2242)	1:19:B:GLU:HG3	1:20:B:LEU:HD21	16	0.1
(1,2242)	1:19:B:GLU:HG3	1:20:B:LEU:HD22	16	0.1
(1,2242)	1:19:B:GLU:HG3	1:20:B:LEU:HD23	16	0.1
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD21	1	0.1
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD22	1	0.1
(1,2130)	1:3:B:ASN:HD21	2:1069:A:LEU:HD23	1	0.1
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD21	1	0.1
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD22	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2130)	1:3:B:ASN:HD22	2:1069:A:LEU:HD23	1	0.1
(1,2127)	1:3:B:ASN:HA	1:3:B:ASN:HD21	14	0.1
(1,2127)	1:3:B:ASN:HA	1:3:B:ASN:HD22	14	0.1
(1,2105)	1:28:B:ARG:HD2	2:1071:A:PHE:HD1	10	0.1
(1,2105)	1:28:B:ARG:HD2	2:1071:A:PHE:HD2	10	0.1
(1,2105)	1:28:B:ARG:HD3	2:1071:A:PHE:HD1	10	0.1
(1,2105)	1:28:B:ARG:HD3	2:1071:A:PHE:HD2	10	0.1
(1,2086)	1:20:B:LEU:HD11	2:1083:A:MET:HB2	10	0.1
(1,2086)	1:20:B:LEU:HD12	2:1083:A:MET:HB2	10	0.1
(1,2086)	1:20:B:LEU:HD13	2:1083:A:MET:HB2	10	0.1
(1,2086)	1:20:B:LEU:HD11	2:1083:A:MET:HB2	20	0.1
(1,2086)	1:20:B:LEU:HD12	2:1083:A:MET:HB2	20	0.1
(1,2086)	1:20:B:LEU:HD13	2:1083:A:MET:HB2	20	0.1
(1,2013)	1:20:B:LEU:HD11	2:1079:A:ILE:HG21	9	0.1
(1,2013)	1:20:B:LEU:HD11	2:1079:A:ILE:HG22	9	0.1
(1,2013)	1:20:B:LEU:HD11	2:1079:A:ILE:HG23	9	0.1
(1,2013)	1:20:B:LEU:HD12	2:1079:A:ILE:HG21	9	0.1
(1,2013)	1:20:B:LEU:HD12	2:1079:A:ILE:HG22	9	0.1
(1,2013)	1:20:B:LEU:HD12	2:1079:A:ILE:HG23	9	0.1
(1,2013)	1:20:B:LEU:HD13	2:1079:A:ILE:HG21	9	0.1
(1,2013)	1:20:B:LEU:HD13	2:1079:A:ILE:HG22	9	0.1
(1,2013)	1:20:B:LEU:HD13	2:1079:A:ILE:HG23	9	0.1
(1,1983)	1:17:B:LEU:HB2	2:1079:A:ILE:HG21	5	0.1
(1,1983)	1:17:B:LEU:HB2	2:1079:A:ILE:HG22	5	0.1
(1,1983)	1:17:B:LEU:HB2	2:1079:A:ILE:HG23	5	0.1
(1,1983)	1:17:B:LEU:HB3	2:1079:A:ILE:HG21	5	0.1
(1,1983)	1:17:B:LEU:HB3	2:1079:A:ILE:HG22	5	0.1
(1,1983)	1:17:B:LEU:HB3	2:1079:A:ILE:HG23	5	0.1
(1,1975)	1:17:B:LEU:HD11	2:1079:A:ILE:HA	11	0.1
(1,1975)	1:17:B:LEU:HD12	2:1079:A:ILE:HA	11	0.1
(1,1975)	1:17:B:LEU:HD13	2:1079:A:ILE:HA	11	0.1
(1,1886)	2:1059:A:LEU:HD11	2:1062:A:CYS:HB2	11	0.1
(1,1886)	2:1059:A:LEU:HD11	2:1062:A:CYS:HB3	11	0.1
(1,1886)	2:1059:A:LEU:HD12	2:1062:A:CYS:HB2	11	0.1
(1,1886)	2:1059:A:LEU:HD12	2:1062:A:CYS:HB3	11	0.1
(1,1886)	2:1059:A:LEU:HD13	2:1062:A:CYS:HB2	11	0.1
(1,1886)	2:1059:A:LEU:HD13	2:1062:A:CYS:HB3	11	0.1
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD21	4	0.1
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD22	4	0.1
(1,1868)	2:1056:A:ILE:HD11	2:1059:A:LEU:HD23	4	0.1
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD21	4	0.1
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD22	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1868)	2:1056:A:ILE:HD12	2:1059:A:LEU:HD23	4	0.1
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD21	4	0.1
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD22	4	0.1
(1,1868)	2:1056:A:ILE:HD13	2:1059:A:LEU:HD23	4	0.1
(1,1863)	2:1048:A:GLN:HG2	2:1052:A:ALA:HB1	3	0.1
(1,1863)	2:1048:A:GLN:HG2	2:1052:A:ALA:HB2	3	0.1
(1,1863)	2:1048:A:GLN:HG2	2:1052:A:ALA:HB3	3	0.1
(1,1863)	2:1048:A:GLN:HG3	2:1052:A:ALA:HB1	3	0.1
(1,1863)	2:1048:A:GLN:HG3	2:1052:A:ALA:HB2	3	0.1
(1,1863)	2:1048:A:GLN:HG3	2:1052:A:ALA:HB3	3	0.1
(1,1819)	2:1047:A:ILE:HA	2:1047:A:ILE:HD11	11	0.1
(1,1819)	2:1047:A:ILE:HA	2:1047:A:ILE:HD12	11	0.1
(1,1819)	2:1047:A:ILE:HA	2:1047:A:ILE:HD13	11	0.1
(1,1819)	2:1047:A:ILE:HA	2:1047:A:ILE:HD11	16	0.1
(1,1819)	2:1047:A:ILE:HA	2:1047:A:ILE:HD12	16	0.1
(1,1819)	2:1047:A:ILE:HA	2:1047:A:ILE:HD13	16	0.1
(1,1819)	2:1047:A:ILE:HA	2:1047:A:ILE:HD11	18	0.1
(1,1819)	2:1047:A:ILE:HA	2:1047:A:ILE:HD12	18	0.1
(1,1819)	2:1047:A:ILE:HA	2:1047:A:ILE:HD13	18	0.1
(1,1804)	2:1045:A:ILE:HD11	2:1063:A:ILE:HA	3	0.1
(1,1804)	2:1045:A:ILE:HD12	2:1063:A:ILE:HA	3	0.1
(1,1804)	2:1045:A:ILE:HD13	2:1063:A:ILE:HA	3	0.1
(1,1799)	2:1045:A:ILE:HD11	2:1063:A:ILE:HD11	13	0.1
(1,1799)	2:1045:A:ILE:HD11	2:1063:A:ILE:HD12	13	0.1
(1,1799)	2:1045:A:ILE:HD11	2:1063:A:ILE:HD13	13	0.1
(1,1799)	2:1045:A:ILE:HD12	2:1063:A:ILE:HD11	13	0.1
(1,1799)	2:1045:A:ILE:HD12	2:1063:A:ILE:HD12	13	0.1
(1,1799)	2:1045:A:ILE:HD12	2:1063:A:ILE:HD13	13	0.1
(1,1799)	2:1045:A:ILE:HD13	2:1063:A:ILE:HD11	13	0.1
(1,1799)	2:1045:A:ILE:HD13	2:1063:A:ILE:HD12	13	0.1
(1,1799)	2:1045:A:ILE:HD13	2:1063:A:ILE:HD13	13	0.1
(1,1776)	2:1000:A:GLN:HB2	2:1040:A:ILE:HG21	6	0.1
(1,1776)	2:1000:A:GLN:HB2	2:1040:A:ILE:HG22	6	0.1
(1,1776)	2:1000:A:GLN:HB2	2:1040:A:ILE:HG23	6	0.1
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG21	8	0.1
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG22	8	0.1
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG23	8	0.1
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG21	8	0.1
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG22	8	0.1
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG23	8	0.1
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG21	8	0.1
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG22	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG23	8	0.1
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG21	9	0.1
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG22	9	0.1
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG23	9	0.1
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG21	9	0.1
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG22	9	0.1
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG23	9	0.1
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG21	9	0.1
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG22	9	0.1
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG23	9	0.1
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG21	11	0.1
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG22	11	0.1
(1,1771)	2:1004:A:ILE:HG21	2:1040:A:ILE:HG23	11	0.1
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG21	11	0.1
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG22	11	0.1
(1,1771)	2:1004:A:ILE:HG22	2:1040:A:ILE:HG23	11	0.1
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG21	11	0.1
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG22	11	0.1
(1,1771)	2:1004:A:ILE:HG23	2:1040:A:ILE:HG23	11	0.1
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD11	4	0.1
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD12	4	0.1
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD13	4	0.1
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD11	4	0.1
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD12	4	0.1
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD13	4	0.1
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD11	4	0.1
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD12	4	0.1
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD13	4	0.1
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD11	10	0.1
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD12	10	0.1
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD13	10	0.1
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD11	10	0.1
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD12	10	0.1
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD13	10	0.1
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD11	10	0.1
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD12	10	0.1
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD13	10	0.1
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD11	13	0.1
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD12	13	0.1
(1,1765)	2:1004:A:ILE:HG21	2:1040:A:ILE:HD13	13	0.1
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD11	13	0.1
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD12	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1765)	2:1004:A:ILE:HG22	2:1040:A:ILE:HD13	13	0.1
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD11	13	0.1
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD12	13	0.1
(1,1765)	2:1004:A:ILE:HG23	2:1040:A:ILE:HD13	13	0.1
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD11	12	0.1
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD12	12	0.1
(1,1723)	2:1004:A:ILE:HD11	2:1033:A:LEU:HD13	12	0.1
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD11	12	0.1
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD12	12	0.1
(1,1723)	2:1004:A:ILE:HD12	2:1033:A:LEU:HD13	12	0.1
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD11	12	0.1
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD12	12	0.1
(1,1723)	2:1004:A:ILE:HD13	2:1033:A:LEU:HD13	12	0.1
(1,1622)	2:1014:A:ILE:HG21	2:1056:A:ILE:HG21	19	0.1
(1,1622)	2:1014:A:ILE:HG21	2:1056:A:ILE:HG22	19	0.1
(1,1622)	2:1014:A:ILE:HG21	2:1056:A:ILE:HG23	19	0.1
(1,1622)	2:1014:A:ILE:HG22	2:1056:A:ILE:HG21	19	0.1
(1,1622)	2:1014:A:ILE:HG22	2:1056:A:ILE:HG22	19	0.1
(1,1622)	2:1014:A:ILE:HG22	2:1056:A:ILE:HG23	19	0.1
(1,1622)	2:1014:A:ILE:HG23	2:1056:A:ILE:HG21	19	0.1
(1,1622)	2:1014:A:ILE:HG23	2:1056:A:ILE:HG22	19	0.1
(1,1622)	2:1014:A:ILE:HG23	2:1056:A:ILE:HG23	19	0.1
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB2	10	0.1
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB3	10	0.1
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB2	10	0.1
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB3	10	0.1
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB2	10	0.1
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB3	10	0.1
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB2	17	0.1
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB3	17	0.1
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB2	17	0.1
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB3	17	0.1
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB2	17	0.1
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB3	17	0.1
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB2	18	0.1
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB3	18	0.1
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB2	18	0.1
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB3	18	0.1
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB2	18	0.1
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB3	18	0.1
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB2	19	0.1
(1,1573)	2:1011:A:ILE:HG21	2:1012:A:ASP:HB3	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB2	19	0.1
(1,1573)	2:1011:A:ILE:HG22	2:1012:A:ASP:HB3	19	0.1
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB2	19	0.1
(1,1573)	2:1011:A:ILE:HG23	2:1012:A:ASP:HB3	19	0.1
(1,1564)	2:1011:A:ILE:H	2:1011:A:ILE:HD11	13	0.1
(1,1564)	2:1011:A:ILE:H	2:1011:A:ILE:HD12	13	0.1
(1,1564)	2:1011:A:ILE:H	2:1011:A:ILE:HD13	13	0.1
(1,1525)	2:1008:A:ILE:HD11	2:1009:A:LEU:HD21	14	0.1
(1,1525)	2:1008:A:ILE:HD11	2:1009:A:LEU:HD22	14	0.1
(1,1525)	2:1008:A:ILE:HD11	2:1009:A:LEU:HD23	14	0.1
(1,1525)	2:1008:A:ILE:HD12	2:1009:A:LEU:HD21	14	0.1
(1,1525)	2:1008:A:ILE:HD12	2:1009:A:LEU:HD22	14	0.1
(1,1525)	2:1008:A:ILE:HD12	2:1009:A:LEU:HD23	14	0.1
(1,1525)	2:1008:A:ILE:HD13	2:1009:A:LEU:HD21	14	0.1
(1,1525)	2:1008:A:ILE:HD13	2:1009:A:LEU:HD22	14	0.1
(1,1525)	2:1008:A:ILE:HD13	2:1009:A:LEU:HD23	14	0.1
(1,1500)	2:1007:A:THR:HG21	2:1010:A:LYS:H	11	0.1
(1,1500)	2:1007:A:THR:HG22	2:1010:A:LYS:H	11	0.1
(1,1500)	2:1007:A:THR:HG23	2:1010:A:LYS:H	11	0.1
(1,1500)	2:1007:A:THR:HG21	2:1010:A:LYS:H	14	0.1
(1,1500)	2:1007:A:THR:HG22	2:1010:A:LYS:H	14	0.1
(1,1500)	2:1007:A:THR:HG23	2:1010:A:LYS:H	14	0.1
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD21	14	0.1
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD22	14	0.1
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD23	14	0.1
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD21	14	0.1
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD22	14	0.1
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD23	14	0.1
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD21	14	0.1
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD22	14	0.1
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD23	14	0.1
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD21	19	0.1
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD22	19	0.1
(1,1475)	2:1004:A:ILE:HG21	2:1033:A:LEU:HD23	19	0.1
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD21	19	0.1
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD22	19	0.1
(1,1475)	2:1004:A:ILE:HG22	2:1033:A:LEU:HD23	19	0.1
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD21	19	0.1
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD22	19	0.1
(1,1475)	2:1004:A:ILE:HG23	2:1033:A:LEU:HD23	19	0.1
(1,1473)	2:1004:A:ILE:HD11	2:1041:A:PHE:HD1	5	0.1
(1,1473)	2:1004:A:ILE:HD11	2:1041:A:PHE:HD2	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1473)	2:1004:A:ILE:HD12	2:1041:A:PHE:HD1	5	0.1
(1,1473)	2:1004:A:ILE:HD12	2:1041:A:PHE:HD2	5	0.1
(1,1473)	2:1004:A:ILE:HD13	2:1041:A:PHE:HD1	5	0.1
(1,1473)	2:1004:A:ILE:HD13	2:1041:A:PHE:HD2	5	0.1
(1,1473)	2:1004:A:ILE:HD11	2:1041:A:PHE:HD1	12	0.1
(1,1473)	2:1004:A:ILE:HD11	2:1041:A:PHE:HD2	12	0.1
(1,1473)	2:1004:A:ILE:HD12	2:1041:A:PHE:HD1	12	0.1
(1,1473)	2:1004:A:ILE:HD12	2:1041:A:PHE:HD2	12	0.1
(1,1473)	2:1004:A:ILE:HD13	2:1041:A:PHE:HD1	12	0.1
(1,1473)	2:1004:A:ILE:HD13	2:1041:A:PHE:HD2	12	0.1
(1,1414)	2:997:A:ILE:HG21	2:1001:A:LEU:H	3	0.1
(1,1414)	2:997:A:ILE:HG22	2:1001:A:LEU:H	3	0.1
(1,1414)	2:997:A:ILE:HG23	2:1001:A:LEU:H	3	0.1
(1,1405)	2:997:A:ILE:HG21	2:1063:A:ILE:HD11	14	0.1
(1,1405)	2:997:A:ILE:HG21	2:1063:A:ILE:HD12	14	0.1
(1,1405)	2:997:A:ILE:HG21	2:1063:A:ILE:HD13	14	0.1
(1,1405)	2:997:A:ILE:HG22	2:1063:A:ILE:HD11	14	0.1
(1,1405)	2:997:A:ILE:HG22	2:1063:A:ILE:HD12	14	0.1
(1,1405)	2:997:A:ILE:HG22	2:1063:A:ILE:HD13	14	0.1
(1,1405)	2:997:A:ILE:HG23	2:1063:A:ILE:HD11	14	0.1
(1,1405)	2:997:A:ILE:HG23	2:1063:A:ILE:HD12	14	0.1
(1,1405)	2:997:A:ILE:HG23	2:1063:A:ILE:HD13	14	0.1
(1,1344)	2:986:A:ILE:HG21	2:988:A:GLN:HG2	17	0.1
(1,1344)	2:986:A:ILE:HG21	2:988:A:GLN:HG3	17	0.1
(1,1344)	2:986:A:ILE:HG22	2:988:A:GLN:HG2	17	0.1
(1,1344)	2:986:A:ILE:HG22	2:988:A:GLN:HG3	17	0.1
(1,1344)	2:986:A:ILE:HG23	2:988:A:GLN:HG2	17	0.1
(1,1344)	2:986:A:ILE:HG23	2:988:A:GLN:HG3	17	0.1
(1,1341)	2:986:A:ILE:HB	2:986:A:ILE:HD11	16	0.1
(1,1341)	2:986:A:ILE:HB	2:986:A:ILE:HD12	16	0.1
(1,1341)	2:986:A:ILE:HB	2:986:A:ILE:HD13	16	0.1
(1,1337)	2:985:A:VAL:HG21	2:986:A:ILE:HA	13	0.1
(1,1337)	2:985:A:VAL:HG22	2:986:A:ILE:HA	13	0.1
(1,1337)	2:985:A:VAL:HG23	2:986:A:ILE:HA	13	0.1
(1,1331)	2:984:A:SER:HB2	2:985:A:VAL:HG11	8	0.1
(1,1331)	2:984:A:SER:HB2	2:985:A:VAL:HG12	8	0.1
(1,1331)	2:984:A:SER:HB2	2:985:A:VAL:HG13	8	0.1
(1,1331)	2:984:A:SER:HB3	2:985:A:VAL:HG11	8	0.1
(1,1331)	2:984:A:SER:HB3	2:985:A:VAL:HG12	8	0.1
(1,1331)	2:984:A:SER:HB3	2:985:A:VAL:HG13	8	0.1
(1,1331)	2:984:A:SER:HB2	2:985:A:VAL:HG11	15	0.1
(1,1331)	2:984:A:SER:HB2	2:985:A:VAL:HG12	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1331)	2:984:A:SER:HB2	2:985:A:VAL:HG13	15	0.1
(1,1331)	2:984:A:SER:HB3	2:985:A:VAL:HG11	15	0.1
(1,1331)	2:984:A:SER:HB3	2:985:A:VAL:HG12	15	0.1
(1,1331)	2:984:A:SER:HB3	2:985:A:VAL:HG13	15	0.1
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	13	0.1
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	13	0.1
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	13	0.1
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	13	0.1
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	13	0.1
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	13	0.1
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	13	0.1
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	13	0.1
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	13	0.1
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD21	18	0.1
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD22	18	0.1
(1,1317)	1:11:B:LEU:HD11	1:18:B:LEU:HD23	18	0.1
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD21	18	0.1
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD22	18	0.1
(1,1317)	1:11:B:LEU:HD12	1:18:B:LEU:HD23	18	0.1
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD21	18	0.1
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD22	18	0.1
(1,1317)	1:11:B:LEU:HD13	1:18:B:LEU:HD23	18	0.1
(1,1316)	1:11:B:LEU:HD11	1:14:B:ARG:HG2	9	0.1
(1,1316)	1:11:B:LEU:HD11	1:14:B:ARG:HG3	9	0.1
(1,1316)	1:11:B:LEU:HD12	1:14:B:ARG:HG2	9	0.1
(1,1316)	1:11:B:LEU:HD12	1:14:B:ARG:HG3	9	0.1
(1,1316)	1:11:B:LEU:HD13	1:14:B:ARG:HG2	9	0.1
(1,1316)	1:11:B:LEU:HD13	1:14:B:ARG:HG3	9	0.1
(1,1296)	1:24:B:ALA:HB1	1:26:B:LEU:HD11	4	0.1
(1,1296)	1:24:B:ALA:HB1	1:26:B:LEU:HD12	4	0.1
(1,1296)	1:24:B:ALA:HB1	1:26:B:LEU:HD13	4	0.1
(1,1296)	1:24:B:ALA:HB2	1:26:B:LEU:HD11	4	0.1
(1,1296)	1:24:B:ALA:HB2	1:26:B:LEU:HD12	4	0.1
(1,1296)	1:24:B:ALA:HB2	1:26:B:LEU:HD13	4	0.1
(1,1296)	1:24:B:ALA:HB3	1:26:B:LEU:HD11	4	0.1
(1,1296)	1:24:B:ALA:HB3	1:26:B:LEU:HD12	4	0.1
(1,1296)	1:24:B:ALA:HB3	1:26:B:LEU:HD13	4	0.1
(1,1276)	1:18:B:LEU:HD11	1:22:B:LYS:HD2	11	0.1
(1,1276)	1:18:B:LEU:HD11	1:22:B:LYS:HD3	11	0.1
(1,1276)	1:18:B:LEU:HD12	1:22:B:LYS:HD2	11	0.1
(1,1276)	1:18:B:LEU:HD12	1:22:B:LYS:HD3	11	0.1
(1,1276)	1:18:B:LEU:HD13	1:22:B:LYS:HD2	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:18:B:LEU:HD13	1:22:B:LYS:HD3	11	0.1
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD11	5	0.1
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD12	5	0.1
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD13	5	0.1
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD11	5	0.1
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD12	5	0.1
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD13	5	0.1
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD11	12	0.1
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD12	12	0.1
(1,1173)	1:27:B:SER:HB2	2:1079:A:ILE:HD13	12	0.1
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD11	12	0.1
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD12	12	0.1
(1,1173)	1:27:B:SER:HB3	2:1079:A:ILE:HD13	12	0.1
(1,1169)	1:3:B:ASN:HB2	1:7:B:THR:HG21	4	0.1
(1,1169)	1:3:B:ASN:HB2	1:7:B:THR:HG22	4	0.1
(1,1169)	1:3:B:ASN:HB2	1:7:B:THR:HG23	4	0.1
(1,1169)	1:3:B:ASN:HB3	1:7:B:THR:HG21	4	0.1
(1,1169)	1:3:B:ASN:HB3	1:7:B:THR:HG22	4	0.1
(1,1169)	1:3:B:ASN:HB3	1:7:B:THR:HG23	4	0.1
(1,938)	1:7:B:THR:H	2:1068:A:LEU:HD11	11	0.1
(1,938)	1:7:B:THR:H	2:1068:A:LEU:HD12	11	0.1
(1,938)	1:7:B:THR:H	2:1068:A:LEU:HD13	11	0.1
(1,938)	1:7:B:THR:H	2:1068:A:LEU:HD11	17	0.1
(1,938)	1:7:B:THR:H	2:1068:A:LEU:HD12	17	0.1
(1,938)	1:7:B:THR:H	2:1068:A:LEU:HD13	17	0.1
(1,838)	2:1004:A:ILE:HG21	2:1032:A:GLN:HE22	13	0.1
(1,838)	2:1004:A:ILE:HG22	2:1032:A:GLN:HE22	13	0.1
(1,838)	2:1004:A:ILE:HG23	2:1032:A:GLN:HE22	13	0.1
(1,838)	2:1004:A:ILE:HG21	2:1032:A:GLN:HE22	15	0.1
(1,838)	2:1004:A:ILE:HG22	2:1032:A:GLN:HE22	15	0.1
(1,838)	2:1004:A:ILE:HG23	2:1032:A:GLN:HE22	15	0.1
(1,838)	2:1004:A:ILE:HG21	2:1032:A:GLN:HE22	19	0.1
(1,838)	2:1004:A:ILE:HG22	2:1032:A:GLN:HE22	19	0.1
(1,838)	2:1004:A:ILE:HG23	2:1032:A:GLN:HE22	19	0.1
(1,729)	2:1076:A:LEU:H	2:1076:A:LEU:HD21	11	0.1
(1,729)	2:1076:A:LEU:H	2:1076:A:LEU:HD22	11	0.1
(1,729)	2:1076:A:LEU:H	2:1076:A:LEU:HD23	11	0.1
(1,403)	2:1035:A:SER:H	2:1050:A:LEU:HD11	16	0.1
(1,403)	2:1035:A:SER:H	2:1050:A:LEU:HD12	16	0.1
(1,403)	2:1035:A:SER:H	2:1050:A:LEU:HD13	16	0.1
(1,242)	2:1014:A:ILE:H	2:1056:A:ILE:HD11	18	0.1
(1,242)	2:1014:A:ILE:H	2:1056:A:ILE:HD12	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	2:1014:A:ILE:H	2:1056:A:ILE:HD13	18	0.1

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

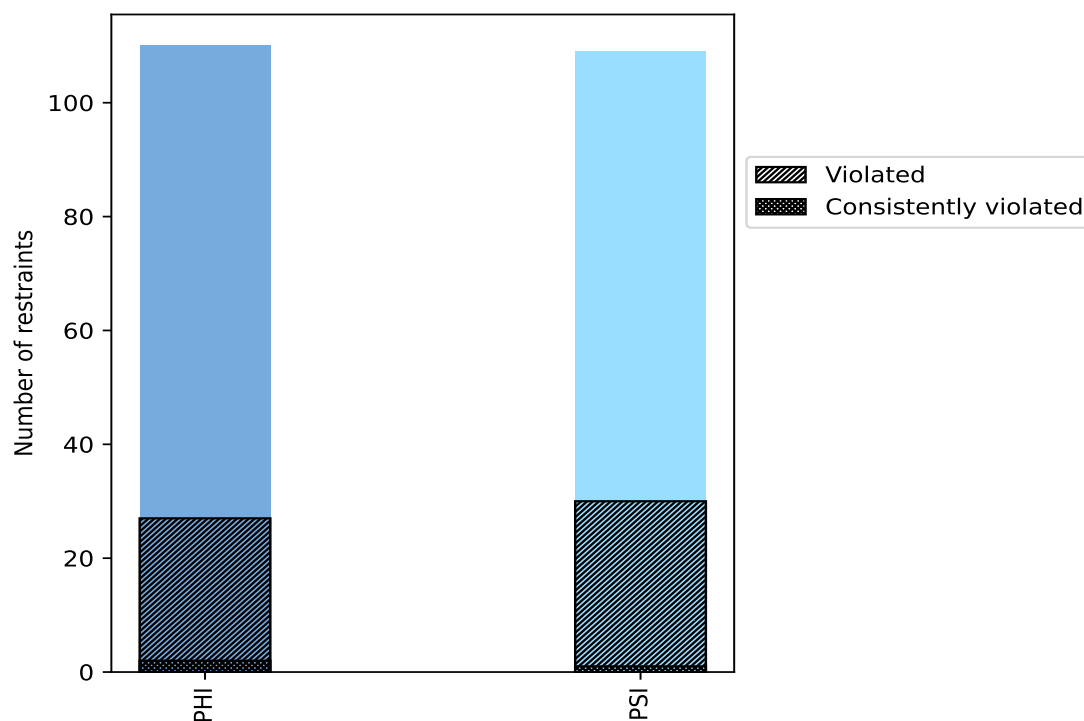
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	110	50.2	27	24.5	12.3	2	1.8	0.9
PSI	109	49.8	30	27.5	13.7	1	0.9	0.5
Total	219	100.0	57	26.0	26.0	3	1.4	1.4

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

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



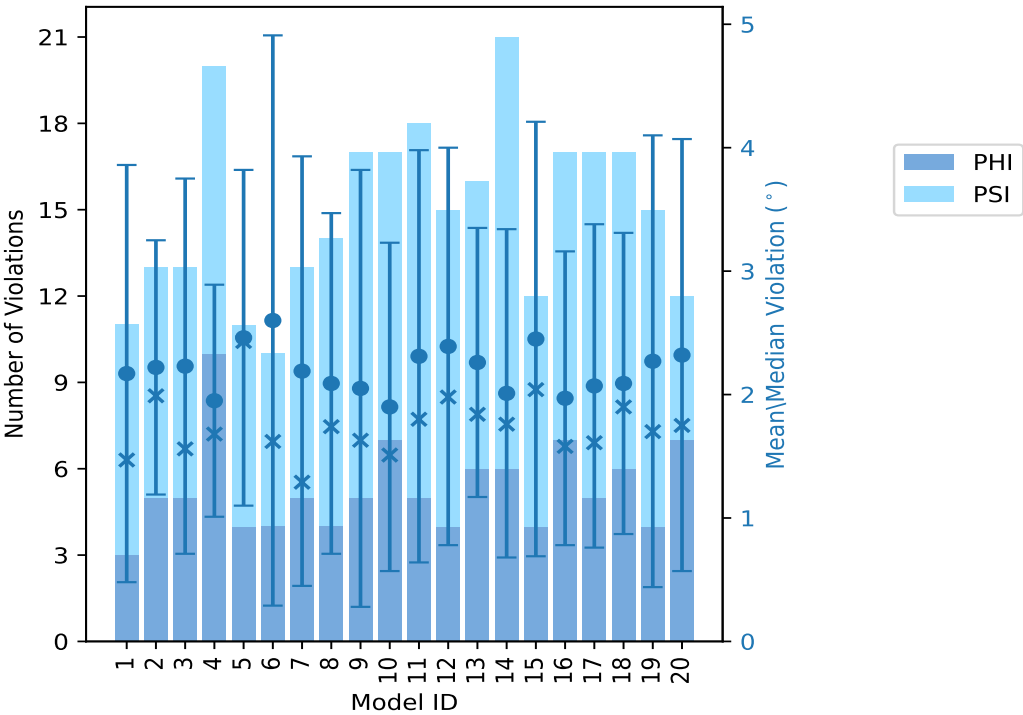
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	3	8	11	2.17	7.22	1.69	1.47
2	5	8	13	2.22	5.28	1.03	1.99
3	5	8	13	2.23	6.91	1.52	1.56
4	10	10	20	1.95	4.35	0.94	1.68
5	4	7	11	2.46	6.08	1.36	2.43
6	4	6	10	2.6	9.16	2.31	1.62
7	5	8	13	2.19	7.64	1.74	1.29
8	4	10	14	2.09	6.67	1.38	1.74
9	5	12	17	2.05	8.87	1.77	1.63
10	7	10	17	1.9	6.78	1.33	1.51
11	5	13	18	2.31	8.26	1.67	1.8
12	4	11	15	2.39	7.9	1.61	1.98
13	6	10	16	2.26	5.58	1.09	1.84
14	6	15	21	2.01	7.47	1.33	1.76
15	4	8	12	2.45	7.81	1.76	2.04
16	7	10	17	1.97	6.18	1.19	1.58
17	5	12	17	2.07	6.5	1.31	1.61
18	6	11	17	2.09	6.62	1.22	1.9
19	4	11	15	2.27	8.55	1.83	1.7
20	7	5	12	2.32	7.75	1.75	1.75

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
13	8	21	1	5.0
2	3	5	2	10.0
4	2	6	3	15.0
1	1	2	4	20.0
2	0	2	5	25.0
0	1	1	6	30.0
2	2	4	7	35.0
0	3	3	8	40.0
1	3	4	9	45.0
0	0	0	10	50.0
0	1	1	11	55.0

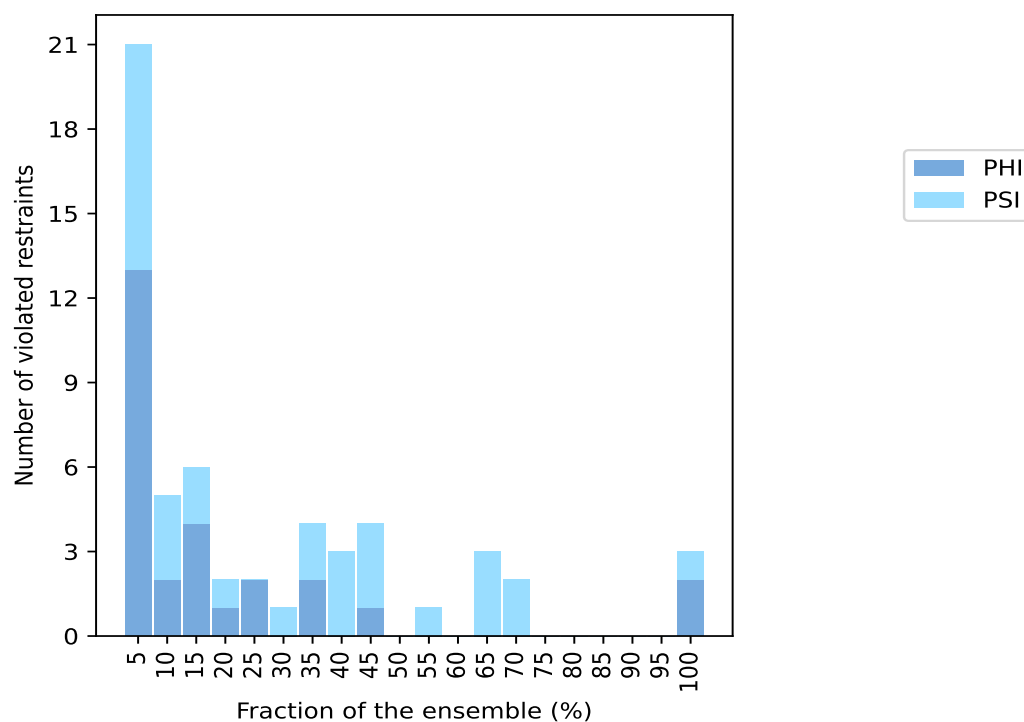
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	3	3	13	65.0
0	2	2	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
2	1	3	20	100.0

¹ Number of models with violations

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

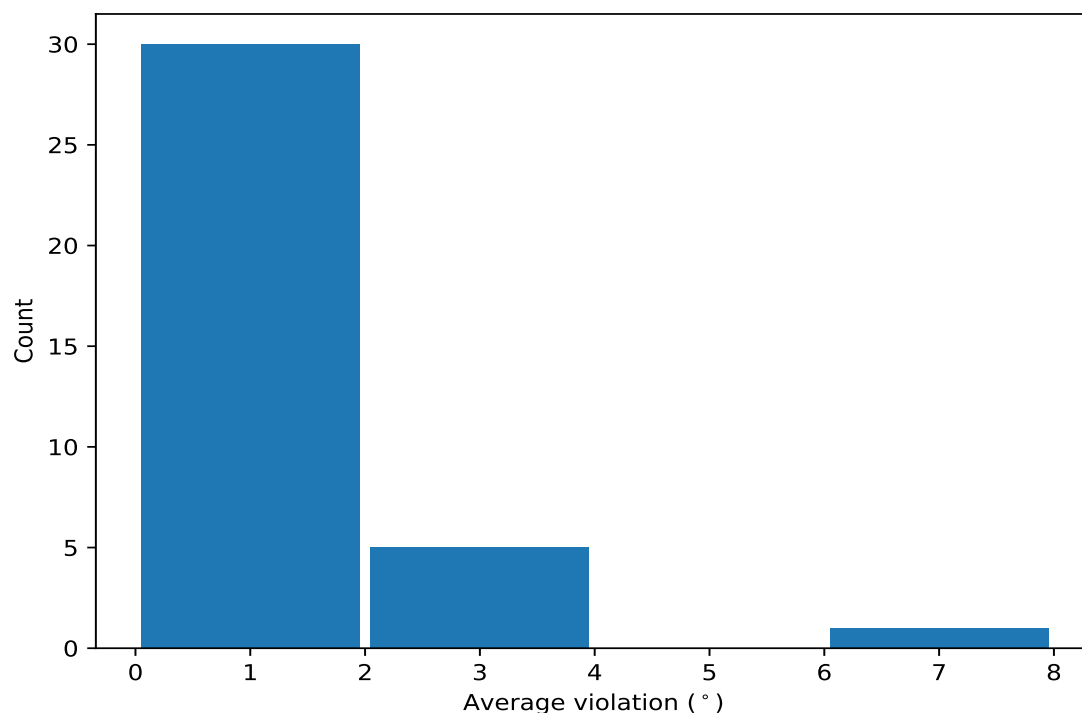


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints ⓘ

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Medi
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	20	7.08	1.2	7.06
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	20	2.93	0.55	3.07
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	20	2.59	0.56	2.46
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	14	1.62	0.39	1.64
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	14	1.59	0.47	1.39
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	13	2.25	0.92	1.9
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	13	1.9	0.49	2.03
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	13	1.57	0.48	1.41
(1,166)	2:1056:A:ILE:N	2:1056:A:ILE:CA	2:1056:A:ILE:C	2:1057:A:CYS:N	11	2.06	0.84	1.81
(1,59)	2:997:A:ILE:C	2:998:A:GLU:N	2:998:A:GLU:CA	2:998:A:GLU:C	9	1.88	0.4	1.8
(1,202)	2:1074:A:ASP:N	2:1074:A:ASP:CA	2:1074:A:ASP:C	2:1075:A:SER:N	9	1.83	0.52	1.61
(1,62)	2:999:A:GLU:N	2:999:A:GLU:CA	2:999:A:GLU:C	2:1000:A:GLN:N	9	1.78	0.48	1.91
(1,4)	1:4:B:ASN:N	1:4:B:ASN:CA	1:4:B:ASN:C	1:5:B:GLU:N	9	1.67	0.32	1.67
(1,98)	2:1018:A:ASP:N	2:1018:A:ASP:CA	2:1018:A:ASP:C	2:1019:A:ASN:N	8	2.05	0.59	2.02
(1,204)	2:1075:A:SER:N	2:1075:A:SER:CA	2:1075:A:SER:C	2:1076:A:LEU:N	8	1.71	0.69	1.44
(1,18)	1:12:B:ALA:N	1:12:B:ALA:CA	1:12:B:ALA:C	1:13:B:GLU:N	8	1.38	0.28	1.23
(1,65)	2:1000:A:GLN:C	2:1001:A:LEU:N	2:1001:A:LEU:CA	2:1001:A:LEU:C	7	1.87	0.59	1.85
(1,106)	2:1023:A:LEU:N	2:1023:A:LEU:CA	2:1023:A:LEU:C	2:1024:A:GLY:N	7	1.68	0.22	1.69
(1,133)	2:1038:A:ASN:C	2:1039:A:GLU:N	2:1039:A:GLU:CA	2:1039:A:GLU:C	7	1.53	0.46	1.42
(1,132)	2:1038:A:ASN:N	2:1038:A:ASN:CA	2:1038:A:ASN:C	2:1039:A:GLU:N	7	1.43	0.53	1.1

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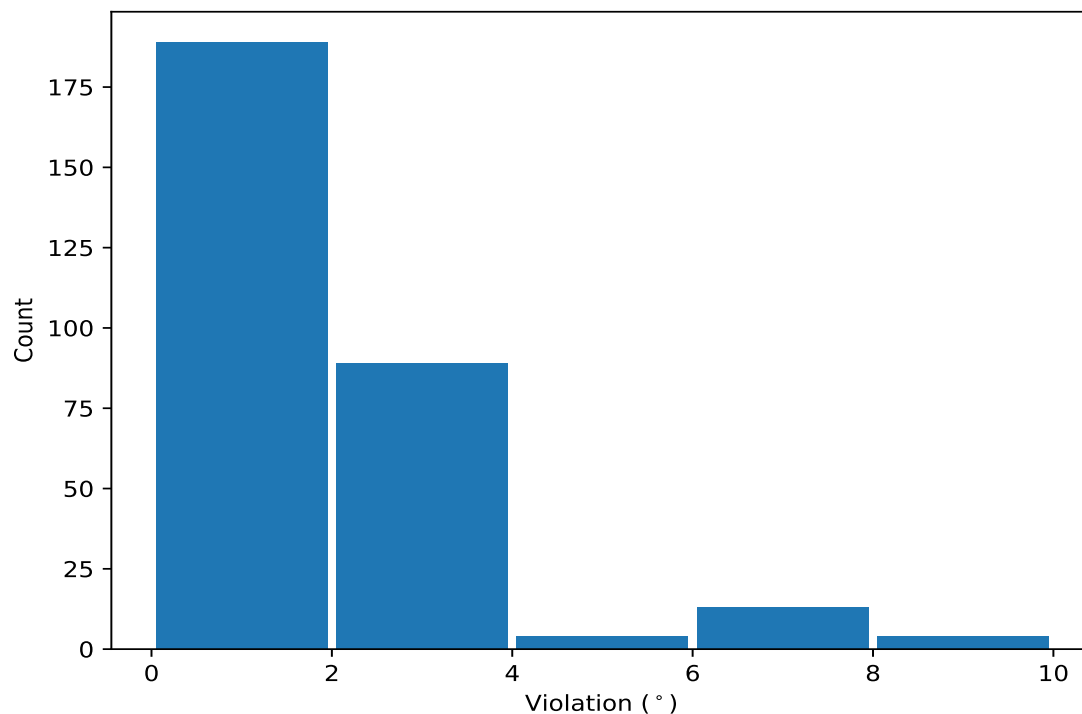
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,26)	1:16:B:ARG:N	1:16:B:ARG:CA	1:16:B:ARG:C	1:17:B:LEU:N	6	1.42	0.2	1.42
(1,77)	2:1006:A:GLN:C	2:1007:A:THR:N	2:1007:A:THR:CA	2:1007:A:THR:C	5	1.64	0.23	1.61
(1,173)	2:1059:A:LEU:C	2:1060:A:GLU:N	2:1060:A:GLU:CA	2:1060:A:GLU:C	5	1.51	0.55	1.29
(1,198)	2:1072:A:ASP:N	2:1072:A:ASP:CA	2:1072:A:ASP:C	2:1073:A:ALA:N	4	1.44	0.27	1.4
(1,169)	2:1057:A:CYS:C	2:1058:A:GLN:N	2:1058:A:GLN:CA	2:1058:A:GLN:C	4	1.2	0.1	1.18
(1,147)	2:1045:A:ILE:C	2:1046:A:SER:N	2:1046:A:SER:CA	2:1046:A:SER:C	3	1.95	0.05	1.92
(1,194)	2:1070:A:GLN:N	2:1070:A:GLN:CA	2:1070:A:GLN:C	2:1071:A:PHE:N	3	1.42	0.15	1.46
(1,217)	2:1081:A:LYS:C	2:1082:A:SER:N	2:1082:A:SER:CA	2:1082:A:SER:C	3	1.37	0.2	1.43
(1,85)	2:1010:A:LYS:C	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	3	1.13	0.12	1.05
(1,103)	2:1021:A:PHE:C	2:1022:A:GLU:N	2:1022:A:GLU:CA	2:1022:A:GLU:C	3	1.08	0.06	1.05
(1,142)	2:1043:A:VAL:N	2:1043:A:VAL:CA	2:1043:A:VAL:C	2:1044:A:ASP:N	3	1.07	0.07	1.05
(1,71)	2:1003:A:ASP:C	2:1004:A:ILE:N	2:1004:A:ILE:CA	2:1004:A:ILE:C	2	1.84	0.26	1.84
(1,8)	1:6:B:LEU:N	1:6:B:LEU:CA	1:6:B:LEU:C	1:7:B:THR:N	2	1.63	0.38	1.63
(1,196)	2:1071:A:PHE:N	2:1071:A:PHE:CA	2:1071:A:PHE:C	2:1072:A:ASP:N	2	1.52	0.46	1.52
(1,63)	2:999:A:GLU:C	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2	1.36	0.01	1.36
(1,192)	2:1069:A:LEU:N	2:1069:A:LEU:CA	2:1069:A:LEU:C	2:1070:A:GLN:N	2	1.3	0.04	1.3

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	6	9.16
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	9	8.87
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	19	8.55
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	11	8.26
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	12	7.9
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	15	7.81
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	20	7.75
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	7	7.64
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	14	7.47
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	1	7.22
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	3	6.91
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	10	6.78
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	8	6.67
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	18	6.62
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	17	6.5
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	16	6.18
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	5	6.08
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	13	5.58
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	2	5.28
(1,52)	2:994:A:GLN:N	2:994:A:GLN:CA	2:994:A:GLN:C	2:995:A:GLY:N	4	4.35
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	11	4.14
(1,166)	2:1056:A:ILE:N	2:1056:A:ILE:CA	2:1056:A:ILE:C	2:1057:A:CYS:N	4	3.87
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	5	3.57
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	12	3.52
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	15	3.5
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	17	3.47
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	19	3.44
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	6	3.42
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	11	3.42
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	7	3.41
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	20	3.41
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	3	3.38
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	1	3.35
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	4	3.34
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	13	3.25
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	10	3.22
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	12	3.2
(1,166)	2:1056:A:ILE:N	2:1056:A:ILE:CA	2:1056:A:ILE:C	2:1057:A:CYS:N	19	3.14
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	13	3.08
(1,204)	2:1075:A:SER:N	2:1075:A:SER:CA	2:1075:A:SER:C	2:1076:A:LEU:N	11	3.07
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	15	3.07
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	9	3.06
(1,98)	2:1018:A:ASP:N	2:1018:A:ASP:CA	2:1018:A:ASP:C	2:1019:A:ASN:N	14	3.01
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	3	3.0
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	6	2.99
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	16	2.98
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	8	2.97

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	13	2.87
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	16	2.87
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	14	2.82
(1,98)	2:1018:A:ASP:N	2:1018:A:ASP:CA	2:1018:A:ASP:C	2:1019:A:ASN:N	13	2.74
(1,62)	2:999:A:GLU:N	2:999:A:GLU:CA	2:999:A:GLU:C	2:1000:A:GLN:N	4	2.74
(1,202)	2:1074:A:ASP:N	2:1074:A:ASP:CA	2:1074:A:ASP:C	2:1075:A:SER:N	19	2.73
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	17	2.72
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	7	2.72
(1,132)	2:1038:A:ASN:N	2:1038:A:ASN:CA	2:1038:A:ASN:C	2:1039:A:GLU:N	2	2.64
(1,65)	2:1000:A:GLN:C	2:1001:A:LEU:N	2:1001:A:LEU:CA	2:1001:A:LEU:C	13	2.64
(1,166)	2:1056:A:ILE:N	2:1056:A:ILE:CA	2:1056:A:ILE:C	2:1057:A:CYS:N	5	2.63
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	5	2.61
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	4	2.57
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	17	2.57
(1,133)	2:1038:A:ASN:C	2:1039:A:GLU:N	2:1039:A:GLU:CA	2:1039:A:GLU:C	2	2.56
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	2	2.56
(1,59)	2:997:A:ILE:C	2:998:A:GLU:N	2:998:A:GLU:CA	2:998:A:GLU:C	17	2.56
(1,173)	2:1059:A:LEU:C	2:1060:A:GLU:N	2:1060:A:GLU:CA	2:1060:A:GLU:C	20	2.55
(1,202)	2:1074:A:ASP:N	2:1074:A:ASP:CA	2:1074:A:ASP:C	2:1075:A:SER:N	7	2.54
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	2	2.54
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	18	2.53
(1,59)	2:997:A:ILE:C	2:998:A:GLU:N	2:998:A:GLU:CA	2:998:A:GLU:C	5	2.53
(1,199)	2:1072:A:ASP:C	2:1073:A:ALA:N	2:1073:A:ALA:CA	2:1073:A:ALA:C	11	2.49
(1,166)	2:1056:A:ILE:N	2:1056:A:ILE:CA	2:1056:A:ILE:C	2:1057:A:CYS:N	17	2.49
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	11	2.47
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	3	2.46
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	8	2.46
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2	2.44
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	5	2.43
(1,65)	2:1000:A:GLN:C	2:1001:A:LEU:N	2:1001:A:LEU:CA	2:1001:A:LEU:C	12	2.42
(1,65)	2:1000:A:GLN:C	2:1001:A:LEU:N	2:1001:A:LEU:CA	2:1001:A:LEU:C	18	2.41
(1,98)	2:1018:A:ASP:N	2:1018:A:ASP:CA	2:1018:A:ASP:C	2:1019:A:ASN:N	7	2.39
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	13	2.38
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	18	2.35
(1,204)	2:1075:A:SER:N	2:1075:A:SER:CA	2:1075:A:SER:C	2:1076:A:LEU:N	12	2.33
(1,3)	1:3:B:ASN:C	1:4:B:ASN:N	1:4:B:ASN:CA	1:4:B:ASN:C	9	2.31
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	18	2.26
(1,202)	2:1074:A:ASP:N	2:1074:A:ASP:CA	2:1074:A:ASP:C	2:1075:A:SER:N	8	2.25
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	10	2.25
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	14	2.24
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	12	2.24
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	18	2.23
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	14	2.22
(1,4)	1:4:B:ASN:N	1:4:B:ASN:CA	1:4:B:ASN:C	1:5:B:GLU:N	4	2.18
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	15	2.15
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	16	2.13
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	5	2.13
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	6	2.11
(1,71)	2:1003:A:ASP:C	2:1004:A:ILE:N	2:1004:A:ILE:CA	2:1004:A:ILE:C	20	2.1
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	3	2.1
(1,204)	2:1075:A:SER:N	2:1075:A:SER:CA	2:1075:A:SER:C	2:1076:A:LEU:N	14	2.09

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,98)	2:1018:A:ASP:N	2:1018:A:ASP:CA	2:1018:A:ASP:C	2:1019:A:ASN:N	18	2.09
(1,62)	2:999:A:GLU:N	2:999:A:GLU:CA	2:999:A:GLU:C	2:1000:A:GLN:N	18	2.08
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	9	2.07
(1,4)	1:4:B:ASN:N	1:4:B:ASN:CA	1:4:B:ASN:C	1:5:B:GLU:N	15	2.07
(1,166)	2:1056:A:ILE:N	2:1056:A:ILE:CA	2:1056:A:ILE:C	2:1057:A:CYS:N	15	2.05
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	12	2.05
(1,106)	2:1023:A:LEU:N	2:1023:A:LEU:CA	2:1023:A:LEU:C	2:1024:A:GLY:N	14	2.03
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	11	2.03
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	20	2.03
(1,147)	2:1045:A:ILE:C	2:1046:A:SER:N	2:1046:A:SER:CA	2:1046:A:SER:C	15	2.02
(1,62)	2:999:A:GLU:N	2:999:A:GLU:CA	2:999:A:GLU:C	2:1000:A:GLN:N	11	2.01
(1,8)	1:6:B:LEU:N	1:6:B:LEU:CA	1:6:B:LEU:C	1:7:B:THR:N	19	2.01
(1,196)	2:1071:A:PHE:N	2:1071:A:PHE:CA	2:1071:A:PHE:C	2:1072:A:ASP:N	16	1.99
(1,62)	2:999:A:GLU:N	2:999:A:GLU:CA	2:999:A:GLU:C	2:1000:A:GLN:N	8	1.99
(1,59)	2:997:A:ILE:C	2:998:A:GLU:N	2:998:A:GLU:CA	2:998:A:GLU:C	14	1.99
(1,57)	2:996:A:GLU:C	2:997:A:ILE:N	2:997:A:ILE:CA	2:997:A:ILE:C	2	1.99
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	12	1.98
(1,189)	2:1067:A:GLN:C	2:1068:A:LEU:N	2:1068:A:LEU:CA	2:1068:A:LEU:C	10	1.97
(1,77)	2:1006:A:GLN:C	2:1007:A:THR:N	2:1007:A:THR:CA	2:1007:A:THR:C	19	1.97
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	10	1.97
(1,98)	2:1018:A:ASP:N	2:1018:A:ASP:CA	2:1018:A:ASP:C	2:1019:A:ASN:N	4	1.96
(1,147)	2:1045:A:ILE:C	2:1046:A:SER:N	2:1046:A:SER:CA	2:1046:A:SER:C	20	1.92
(1,62)	2:999:A:GLU:N	2:999:A:GLU:CA	2:999:A:GLU:C	2:1000:A:GLN:N	2	1.91
(1,147)	2:1045:A:ILE:C	2:1046:A:SER:N	2:1046:A:SER:CA	2:1046:A:SER:C	13	1.9
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	18	1.9
(1,59)	2:997:A:ILE:C	2:998:A:GLU:N	2:998:A:GLU:CA	2:998:A:GLU:C	8	1.89
(1,18)	1:12:B:ALA:N	1:12:B:ALA:CA	1:12:B:ALA:C	1:13:B:GLU:N	17	1.89
(1,4)	1:4:B:ASN:N	1:4:B:ASN:CA	1:4:B:ASN:C	1:5:B:GLU:N	16	1.89
(1,65)	2:1000:A:GLN:C	2:1001:A:LEU:N	2:1001:A:LEU:CA	2:1001:A:LEU:C	16	1.85
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	14	1.83
(1,198)	2:1072:A:ASP:N	2:1072:A:ASP:CA	2:1072:A:ASP:C	2:1073:A:ALA:N	9	1.82
(1,106)	2:1023:A:LEU:N	2:1023:A:LEU:CA	2:1023:A:LEU:C	2:1024:A:GLY:N	11	1.82
(1,166)	2:1056:A:ILE:N	2:1056:A:ILE:CA	2:1056:A:ILE:C	2:1057:A:CYS:N	16	1.81
(1,77)	2:1006:A:GLN:C	2:1007:A:THR:N	2:1007:A:THR:CA	2:1007:A:THR:C	4	1.81
(1,59)	2:997:A:ILE:C	2:998:A:GLU:N	2:998:A:GLU:CA	2:998:A:GLU:C	4	1.8
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	17	1.8
(1,160)	2:1052:A:ALA:N	2:1052:A:ALA:CA	2:1052:A:ALA:C	2:1053:A:HIS:N	18	1.79
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	14	1.79
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	13	1.78
(1,4)	1:4:B:ASN:N	1:4:B:ASN:CA	1:4:B:ASN:C	1:5:B:GLU:N	12	1.78
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	11	1.77
(1,106)	2:1023:A:LEU:N	2:1023:A:LEU:CA	2:1023:A:LEU:C	2:1024:A:GLY:N	8	1.76
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	14	1.76
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	19	1.75
(1,26)	1:16:B:ARG:N	1:16:B:ARG:CA	1:16:B:ARG:C	1:17:B:LEU:N	1	1.75
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	8	1.73
(1,53)	2:994:A:GLN:C	2:995:A:GLY:N	2:995:A:GLY:CA	2:995:A:GLY:C	4	1.73
(1,18)	1:12:B:ALA:N	1:12:B:ALA:CA	1:12:B:ALA:C	1:13:B:GLU:N	2	1.73
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	9	1.72
(1,55)	2:995:A:GLY:C	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	1	1.72
(1,204)	2:1075:A:SER:N	2:1075:A:SER:CA	2:1075:A:SER:C	2:1076:A:LEU:N	19	1.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,202)	2:1074:A:ASP:N	2:1074:A:ASP:CA	2:1074:A:ASP:C	2:1075:A:SER:N	18	1.7
(1,106)	2:1023:A:LEU:N	2:1023:A:LEU:CA	2:1023:A:LEU:C	2:1024:A:GLY:N	9	1.69
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	9	1.68
(1,4)	1:4:B:ASN:N	1:4:B:ASN:CA	1:4:B:ASN:C	1:5:B:GLU:N	1	1.67
(1,106)	2:1023:A:LEU:N	2:1023:A:LEU:CA	2:1023:A:LEU:C	2:1024:A:GLY:N	7	1.66
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	5	1.65
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	6	1.65
(1,133)	2:1038:A:ASN:C	2:1039:A:GLU:N	2:1039:A:GLU:CA	2:1039:A:GLU:C	9	1.63
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	14	1.63
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	15	1.63
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	4	1.62
(1,202)	2:1074:A:ASP:N	2:1074:A:ASP:CA	2:1074:A:ASP:C	2:1075:A:SER:N	11	1.61
(1,132)	2:1038:A:ASN:N	2:1038:A:ASN:CA	2:1038:A:ASN:C	2:1039:A:GLU:N	13	1.61
(1,77)	2:1006:A:GLN:C	2:1007:A:THR:N	2:1007:A:THR:CA	2:1007:A:THR:C	17	1.61
(1,59)	2:997:A:ILE:C	2:998:A:GLU:N	2:998:A:GLU:CA	2:998:A:GLU:C	12	1.61
(1,217)	2:1081:A:LYS:C	2:1082:A:SER:N	2:1082:A:SER:CA	2:1082:A:SER:C	6	1.58
(1,202)	2:1074:A:ASP:N	2:1074:A:ASP:CA	2:1074:A:ASP:C	2:1075:A:SER:N	4	1.58
(1,198)	2:1072:A:ASP:N	2:1072:A:ASP:CA	2:1072:A:ASP:C	2:1073:A:ALA:N	10	1.58
(1,194)	2:1070:A:GLN:N	2:1070:A:GLN:CA	2:1070:A:GLN:C	2:1071:A:PHE:N	20	1.58
(1,59)	2:997:A:ILE:C	2:998:A:GLU:N	2:998:A:GLU:CA	2:998:A:GLU:C	16	1.58
(1,71)	2:1003:A:ASP:C	2:1004:A:ILE:N	2:1004:A:ILE:CA	2:1004:A:ILE:C	2	1.57
(1,59)	2:997:A:ILE:C	2:998:A:GLU:N	2:998:A:GLU:CA	2:998:A:GLU:C	3	1.57
(1,173)	2:1059:A:LEU:C	2:1060:A:GLU:N	2:1060:A:GLU:CA	2:1060:A:GLU:C	10	1.56
(1,166)	2:1056:A:ILE:N	2:1056:A:ILE:CA	2:1056:A:ILE:C	2:1057:A:CYS:N	3	1.56
(1,202)	2:1074:A:ASP:N	2:1074:A:ASP:CA	2:1074:A:ASP:C	2:1075:A:SER:N	12	1.55
(1,106)	2:1023:A:LEU:N	2:1023:A:LEU:CA	2:1023:A:LEU:C	2:1024:A:GLY:N	4	1.54
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	6	1.54
(1,65)	2:1000:A:GLN:C	2:1001:A:LEU:N	2:1001:A:LEU:CA	2:1001:A:LEU:C	3	1.54
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	10	1.54
(1,26)	1:16:B:ARG:N	1:16:B:ARG:CA	1:16:B:ARG:C	1:17:B:LEU:N	12	1.52
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	16	1.51
(1,45)	2:989:A:GLU:C	2:990:A:TYR:N	2:990:A:TYR:CA	2:990:A:TYR:C	10	1.51
(1,133)	2:1038:A:ASN:C	2:1039:A:GLU:N	2:1039:A:GLU:CA	2:1039:A:GLU:C	13	1.5
(1,26)	1:16:B:ARG:N	1:16:B:ARG:CA	1:16:B:ARG:C	1:17:B:LEU:N	8	1.5
(1,18)	1:12:B:ALA:N	1:12:B:ALA:CA	1:12:B:ALA:C	1:13:B:GLU:N	10	1.5
(1,202)	2:1074:A:ASP:N	2:1074:A:ASP:CA	2:1074:A:ASP:C	2:1075:A:SER:N	3	1.49
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	17	1.47
(1,62)	2:999:A:GLU:N	2:999:A:GLU:CA	2:999:A:GLU:C	2:1000:A:GLN:N	1	1.47
(1,4)	1:4:B:ASN:N	1:4:B:ASN:CA	1:4:B:ASN:C	1:5:B:GLU:N	8	1.47
(1,194)	2:1070:A:GLN:N	2:1070:A:GLN:CA	2:1070:A:GLN:C	2:1071:A:PHE:N	1	1.46
(1,132)	2:1038:A:ASN:N	2:1038:A:ASN:CA	2:1038:A:ASN:C	2:1039:A:GLU:N	19	1.46
(1,98)	2:1018:A:ASP:N	2:1018:A:ASP:CA	2:1018:A:ASP:C	2:1019:A:ASN:N	9	1.46
(1,77)	2:1006:A:GLN:C	2:1007:A:THR:N	2:1007:A:THR:CA	2:1007:A:THR:C	20	1.46
(1,98)	2:1018:A:ASP:N	2:1018:A:ASP:CA	2:1018:A:ASP:C	2:1019:A:ASN:N	20	1.45
(1,157)	2:1050:A:LEU:C	2:1051:A:PHE:N	2:1051:A:PHE:CA	2:1051:A:PHE:C	18	1.44
(1,217)	2:1081:A:LYS:C	2:1082:A:SER:N	2:1082:A:SER:CA	2:1082:A:SER:C	9	1.43
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	13	1.43
(1,133)	2:1038:A:ASN:C	2:1039:A:GLU:N	2:1039:A:GLU:CA	2:1039:A:GLU:C	14	1.42
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	15	1.42
(1,62)	2:999:A:GLU:N	2:999:A:GLU:CA	2:999:A:GLU:C	2:1000:A:GLN:N	16	1.42
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	18	1.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,75)	2:1005:A:TRP:C	2:1006:A:GLN:N	2:1006:A:GLN:CA	2:1006:A:GLN:C	20	1.41
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	9	1.41
(1,4)	1:4:B:ASN:N	1:4:B:ASN:CA	1:4:B:ASN:C	1:5:B:GLU:N	13	1.41
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	3	1.4
(1,166)	2:1056:A:ILE:N	2:1056:A:ILE:CA	2:1056:A:ILE:C	2:1057:A:CYS:N	13	1.39
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	1	1.39
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	12	1.39
(1,63)	2:999:A:GLU:C	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	4	1.38
(1,143)	2:1043:A:VAL:C	2:1044:A:ASP:N	2:1044:A:ASP:CA	2:1044:A:ASP:C	1	1.37
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	1	1.37
(1,59)	2:997:A:ILE:C	2:998:A:GLU:N	2:998:A:GLU:CA	2:998:A:GLU:C	13	1.37
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	19	1.36
(1,150)	2:1047:A:ILE:N	2:1047:A:ILE:CA	2:1047:A:ILE:C	2:1048:A:GLN:N	11	1.35
(1,77)	2:1006:A:GLN:C	2:1007:A:THR:N	2:1007:A:THR:CA	2:1007:A:THR:C	3	1.35
(1,63)	2:999:A:GLU:C	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	16	1.35
(1,169)	2:1057:A:CYS:C	2:1058:A:GLN:N	2:1058:A:GLN:CA	2:1058:A:GLN:C	16	1.34
(1,26)	1:16:B:ARG:N	1:16:B:ARG:CA	1:16:B:ARG:C	1:17:B:LEU:N	14	1.34
(1,192)	2:1069:A:LEU:N	2:1069:A:LEU:CA	2:1069:A:LEU:C	2:1070:A:GLN:N	12	1.33
(1,133)	2:1038:A:ASN:C	2:1039:A:GLU:N	2:1039:A:GLU:CA	2:1039:A:GLU:C	18	1.31
(1,4)	1:4:B:ASN:N	1:4:B:ASN:CA	1:4:B:ASN:C	1:5:B:GLU:N	10	1.31
(1,123)	2:1033:A:LEU:C	2:1034:A:GLN:N	2:1034:A:GLN:CA	2:1034:A:GLN:C	6	1.3
(1,85)	2:1010:A:LYS:C	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	14	1.3
(1,173)	2:1059:A:LEU:C	2:1060:A:GLU:N	2:1060:A:GLU:CA	2:1060:A:GLU:C	5	1.29
(1,166)	2:1056:A:ILE:N	2:1056:A:ILE:CA	2:1056:A:ILE:C	2:1057:A:CYS:N	14	1.29
(1,98)	2:1018:A:ASP:N	2:1018:A:ASP:CA	2:1018:A:ASP:C	2:1019:A:ASN:N	10	1.29
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	7	1.29
(1,58)	2:997:A:ILE:N	2:997:A:ILE:CA	2:997:A:ILE:C	2:998:A:GLU:N	14	1.29
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	11	1.29
(1,118)	2:1031:A:LEU:N	2:1031:A:LEU:CA	2:1031:A:LEU:C	2:1032:A:GLN:N	19	1.28
(1,106)	2:1023:A:LEU:N	2:1023:A:LEU:CA	2:1023:A:LEU:C	2:1024:A:GLY:N	10	1.28
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	2	1.28
(1,128)	2:1036:A:ARG:N	2:1036:A:ARG:CA	2:1036:A:ARG:C	2:1037:A:ILE:N	15	1.27
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	16	1.27
(1,205)	2:1075:A:SER:C	2:1076:A:LEU:N	2:1076:A:LEU:CA	2:1076:A:LEU:C	11	1.26
(1,192)	2:1069:A:LEU:N	2:1069:A:LEU:CA	2:1069:A:LEU:C	2:1070:A:GLN:N	9	1.26
(1,169)	2:1057:A:CYS:C	2:1058:A:GLN:N	2:1058:A:GLN:CA	2:1058:A:GLN:C	8	1.25
(1,8)	1:6:B:LEU:N	1:6:B:LEU:CA	1:6:B:LEU:C	1:7:B:THR:N	2	1.25
(1,26)	1:16:B:ARG:N	1:16:B:ARG:CA	1:16:B:ARG:C	1:17:B:LEU:N	10	1.24
(1,4)	1:4:B:ASN:N	1:4:B:ASN:CA	1:4:B:ASN:C	1:5:B:GLU:N	7	1.24
(1,133)	2:1038:A:ASN:C	2:1039:A:GLU:N	2:1039:A:GLU:CA	2:1039:A:GLU:C	15	1.23
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	18	1.23
(1,18)	1:12:B:ALA:N	1:12:B:ALA:CA	1:12:B:ALA:C	1:13:B:GLU:N	11	1.23
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	8	1.22
(1,18)	1:12:B:ALA:N	1:12:B:ALA:CA	1:12:B:ALA:C	1:13:B:GLU:N	7	1.22
(1,198)	2:1072:A:ASP:N	2:1072:A:ASP:CA	2:1072:A:ASP:C	2:1073:A:ALA:N	17	1.21
(1,194)	2:1070:A:GLN:N	2:1070:A:GLN:CA	2:1070:A:GLN:C	2:1071:A:PHE:N	14	1.21
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	19	1.21
(1,62)	2:999:A:GLU:N	2:999:A:GLU:CA	2:999:A:GLU:C	2:1000:A:GLN:N	17	1.21
(1,166)	2:1056:A:ILE:N	2:1056:A:ILE:CA	2:1056:A:ILE:C	2:1057:A:CYS:N	11	1.2
(1,46)	2:990:A:TYR:N	2:990:A:TYR:CA	2:990:A:TYR:C	2:991:A:ALA:N	19	1.2
(1,166)	2:1056:A:ILE:N	2:1056:A:ILE:CA	2:1056:A:ILE:C	2:1057:A:CYS:N	10	1.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,60)	2:998:A:GLU:N	2:998:A:GLU:CA	2:998:A:GLU:C	2:999:A:GLU:N	17	1.19
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	13	1.19
(1,64)	2:1000:A:GLN:N	2:1000:A:GLN:CA	2:1000:A:GLN:C	2:1001:A:LEU:N	9	1.18
(1,204)	2:1075:A:SER:N	2:1075:A:SER:CA	2:1075:A:SER:C	2:1076:A:LEU:N	17	1.17
(1,198)	2:1072:A:ASP:N	2:1072:A:ASP:CA	2:1072:A:ASP:C	2:1073:A:ALA:N	20	1.17
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	6	1.17
(1,18)	1:12:B:ALA:N	1:12:B:ALA:CA	1:12:B:ALA:C	1:13:B:GLU:N	19	1.17
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	4	1.17
(1,142)	2:1043:A:VAL:N	2:1043:A:VAL:CA	2:1043:A:VAL:C	2:1044:A:ASP:N	11	1.16
(1,103)	2:1021:A:PHE:C	2:1022:A:GLU:N	2:1022:A:GLU:CA	2:1022:A:GLU:C	7	1.16
(1,62)	2:999:A:GLU:N	2:999:A:GLU:CA	2:999:A:GLU:C	2:1000:A:GLN:N	15	1.16
(1,18)	1:12:B:ALA:N	1:12:B:ALA:CA	1:12:B:ALA:C	1:13:B:GLU:N	14	1.16
(1,26)	1:16:B:ARG:N	1:16:B:ARG:CA	1:16:B:ARG:C	1:17:B:LEU:N	16	1.15
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	17	1.14
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	2	1.13
(1,204)	2:1075:A:SER:N	2:1075:A:SER:CA	2:1075:A:SER:C	2:1076:A:LEU:N	3	1.12
(1,204)	2:1075:A:SER:N	2:1075:A:SER:CA	2:1075:A:SER:C	2:1076:A:LEU:N	5	1.12
(1,169)	2:1057:A:CYS:C	2:1058:A:GLN:N	2:1058:A:GLN:CA	2:1058:A:GLN:C	7	1.12
(1,65)	2:1000:A:GLN:C	2:1001:A:LEU:N	2:1001:A:LEU:CA	2:1001:A:LEU:C	4	1.12
(1,56)	2:996:A:GLU:N	2:996:A:GLU:CA	2:996:A:GLU:C	2:997:A:ILE:N	1	1.12
(1,18)	1:12:B:ALA:N	1:12:B:ALA:CA	1:12:B:ALA:C	1:13:B:GLU:N	9	1.12
(1,144)	2:1044:A:ASP:N	2:1044:A:ASP:CA	2:1044:A:ASP:C	2:1045:A:ILE:N	14	1.11
(1,129)	2:1036:A:ARG:C	2:1037:A:ILE:N	2:1037:A:ILE:CA	2:1037:A:ILE:C	4	1.11
(1,65)	2:1000:A:GLN:C	2:1001:A:LEU:N	2:1001:A:LEU:CA	2:1001:A:LEU:C	14	1.11
(1,217)	2:1081:A:LYS:C	2:1082:A:SER:N	2:1082:A:SER:CA	2:1082:A:SER:C	4	1.1
(1,173)	2:1059:A:LEU:C	2:1060:A:GLU:N	2:1060:A:GLU:CA	2:1060:A:GLU:C	17	1.1
(1,132)	2:1038:A:ASN:N	2:1038:A:ASN:CA	2:1038:A:ASN:C	2:1039:A:GLU:N	18	1.1
(1,132)	2:1038:A:ASN:N	2:1038:A:ASN:CA	2:1038:A:ASN:C	2:1039:A:GLU:N	9	1.09
(1,132)	2:1038:A:ASN:N	2:1038:A:ASN:CA	2:1038:A:ASN:C	2:1039:A:GLU:N	17	1.09
(1,169)	2:1057:A:CYS:C	2:1058:A:GLN:N	2:1058:A:GLN:CA	2:1058:A:GLN:C	18	1.08
(1,173)	2:1059:A:LEU:C	2:1060:A:GLU:N	2:1060:A:GLU:CA	2:1060:A:GLU:C	16	1.07
(1,109)	2:1026:A:HIS:C	2:1027:A:SER:N	2:1027:A:SER:CA	2:1027:A:SER:C	7	1.07
(1,204)	2:1075:A:SER:N	2:1075:A:SER:CA	2:1075:A:SER:C	2:1076:A:LEU:N	9	1.06
(1,202)	2:1074:A:ASP:N	2:1074:A:ASP:CA	2:1074:A:ASP:C	2:1075:A:SER:N	5	1.06
(1,196)	2:1071:A:PHE:N	2:1071:A:PHE:CA	2:1071:A:PHE:C	2:1072:A:ASP:N	12	1.06
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	8	1.06
(1,12)	1:8:B:SER:N	1:8:B:SER:CA	1:8:B:SER:C	1:9:B:LEU:N	16	1.06
(1,142)	2:1043:A:VAL:N	2:1043:A:VAL:CA	2:1043:A:VAL:C	2:1044:A:ASP:N	6	1.05
(1,133)	2:1038:A:ASN:C	2:1039:A:GLU:N	2:1039:A:GLU:CA	2:1039:A:GLU:C	4	1.05
(1,132)	2:1038:A:ASN:N	2:1038:A:ASN:CA	2:1038:A:ASN:C	2:1039:A:GLU:N	3	1.05
(1,103)	2:1021:A:PHE:C	2:1022:A:GLU:N	2:1022:A:GLU:CA	2:1022:A:GLU:C	19	1.05
(1,85)	2:1010:A:LYS:C	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	4	1.05
(1,85)	2:1010:A:LYS:C	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	10	1.04
(1,103)	2:1021:A:PHE:C	2:1022:A:GLU:N	2:1022:A:GLU:CA	2:1022:A:GLU:C	10	1.02
(1,86)	2:1011:A:ILE:N	2:1011:A:ILE:CA	2:1011:A:ILE:C	2:1012:A:ASP:N	8	1.02
(1,74)	2:1005:A:TRP:N	2:1005:A:TRP:CA	2:1005:A:TRP:C	2:1006:A:GLN:N	7	1.01
(1,47)	2:990:A:TYR:C	2:991:A:ALA:N	2:991:A:ALA:CA	2:991:A:ALA:C	11	1.01
(1,142)	2:1043:A:VAL:N	2:1043:A:VAL:CA	2:1043:A:VAL:C	2:1044:A:ASP:N	20	1.0