



Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 11:38 AM EST

PDB ID : 2FO8
BMRB ID : 6876
Title : Solution structure of the Trypanosoma cruzi cysteine protease inhibitor chagasin
Authors : Salmon, D.; do Aido-Machado, R.; de Lima, A.A.P.; Scharfstein, J.; Oschkinat, H.; Pires, J.R.
Deposited on : 2006-01-13

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

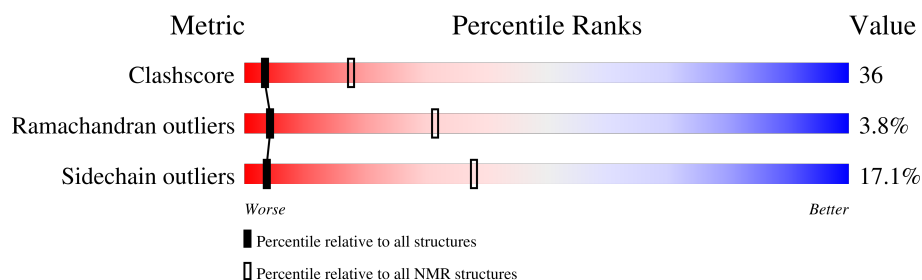
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

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	A	111	

2 Ensemble composition and analysis

This entry contains 15 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:58, A:69-A:110 (98)	0.52	12

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

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

The models can be grouped into 2 clusters and 7 single-model clusters were found.

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

3 Entry composition

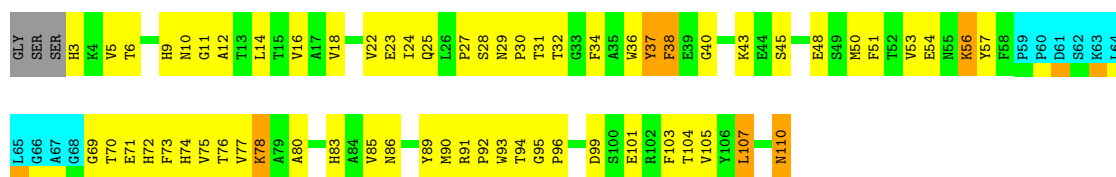
There is only 1 type of molecule in this entry. The entry contains 1644 atoms, of which 807 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Chagasin.

Mol	Chain	Residues	Atoms						Trace
1	A	108	Total	C	H	N	O	S	0
			1644	534	807	142	159	2	

There are 2 discrepancies between the modelled and reference sequences:

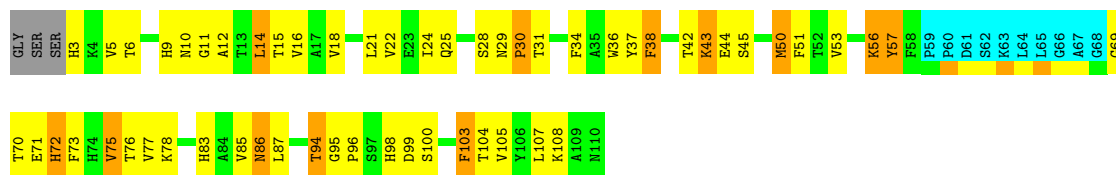
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	cloning artifact	UNP Q966X9
A	1	SER	-	cloning artifact	UNP Q966X9



4.2.3 Score per residue for model 3

- Molecule 1: Chagasin

Chain A: 38% 40% 11% 9% .



4.2.4 Score per residue for model 4

- Molecule 1: Chagasin

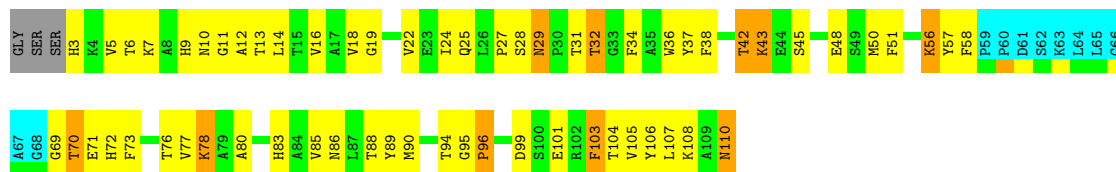
Chain A: 29% 53% 6% 9% .



4.2.5 Score per residue for model 5

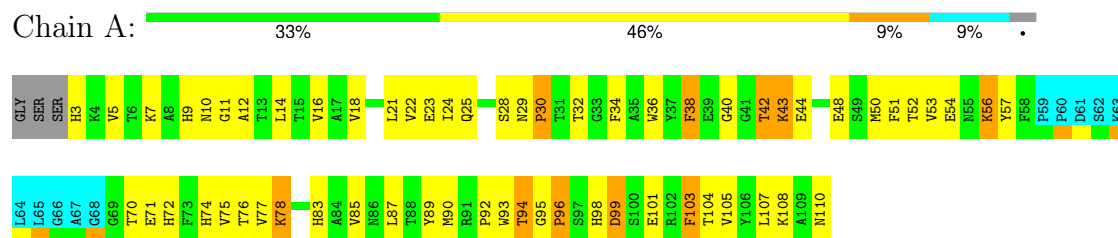
- Molecule 1: Chagasin

Chain A: 33% 46% 9% 9% .



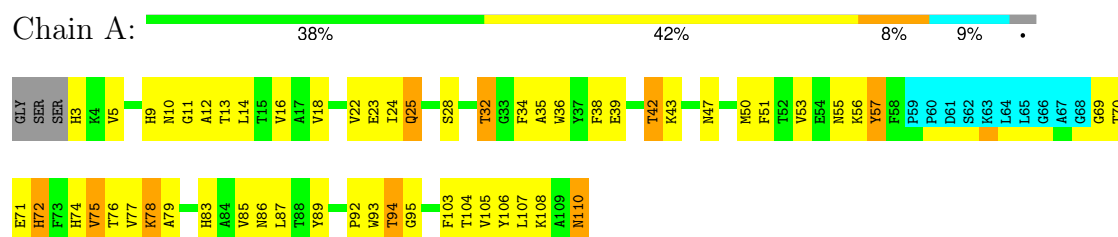
4.2.6 Score per residue for model 6

- Molecule 1: Chagasin



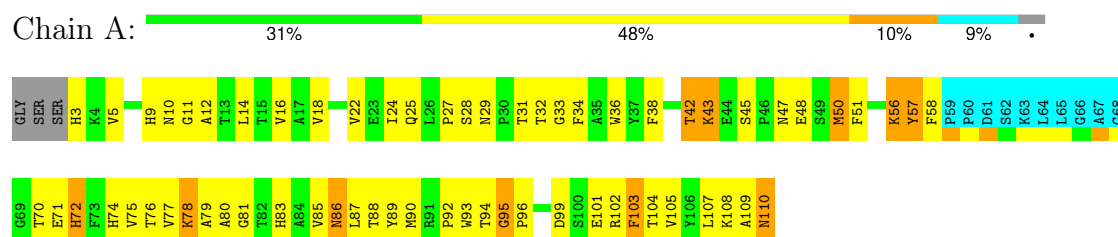
4.2.7 Score per residue for model 7

- Molecule 1: Chagasin



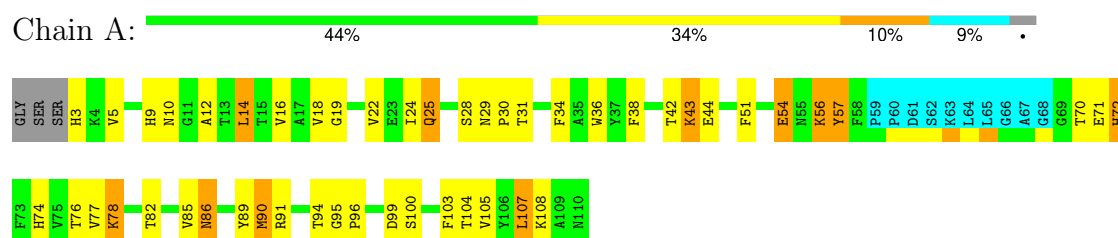
4.2.8 Score per residue for model 8

- Molecule 1: Chagasin



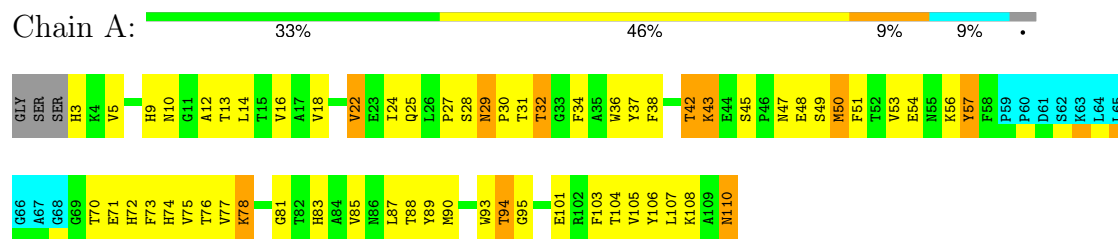
4.2.9 Score per residue for model 9

- Molecule 1: Chagasin



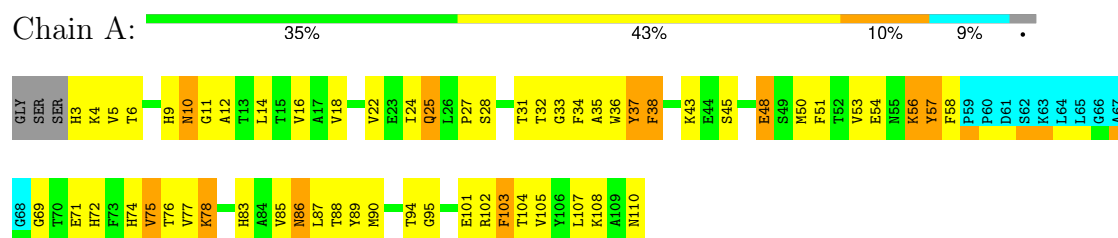
4.2.10 Score per residue for model 10

- Molecule 1: Chagasin



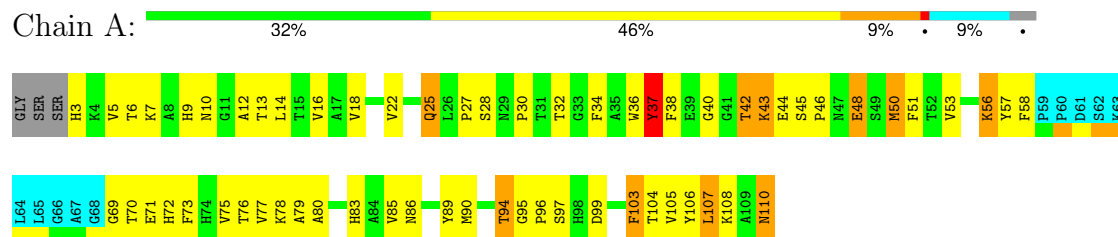
4.2.11 Score per residue for model 11

- Molecule 1: Chagasin



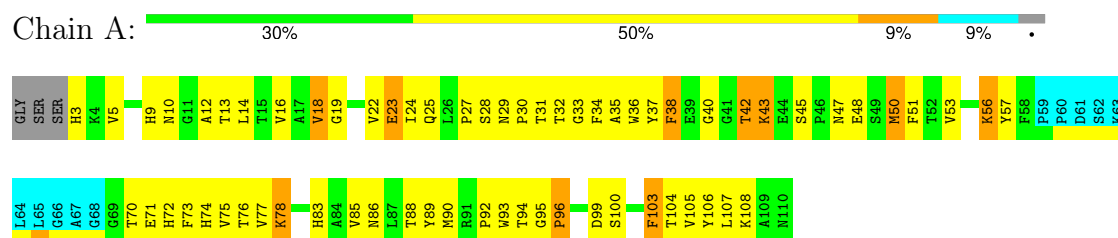
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Chagasin



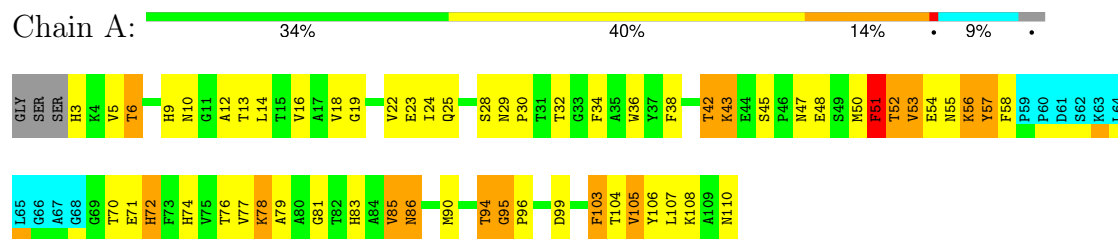
4.2.13 Score per residue for model 13

- Molecule 1: Chagasin



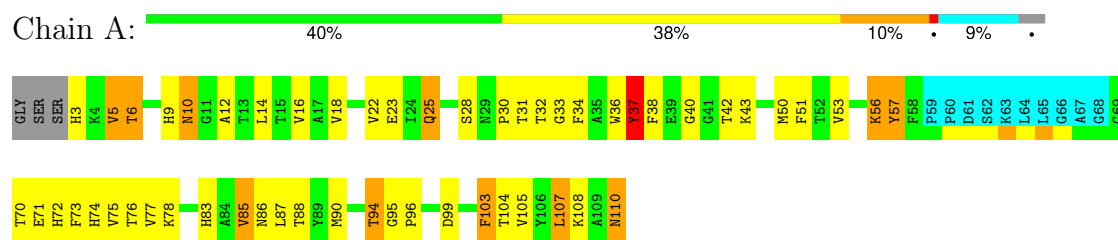
4.2.14 Score per residue for model 14

- Molecule 1: Chagasin



4.2.15 Score per residue for model 15

- Molecule 1: Chagasin



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CNS	refinement	1.1
ARIA	refinement	1.2

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	1096
Number of shifts mapped to atoms	1084
Number of unparsed shifts	0
Number of shifts with mapping errors	12
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

6 Model quality

6.1 Standard geometry

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	A	0.48±0.06	1±1/795 (0.1± 0.2%)	0.55±0.02	0±0/1083 (0.0± 0.0%)
All	All	0.48	11/11925 (0.1%)	0.55	0/16245 (0.0%)

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	A	0.0±0.0	0.1±0.3
All	All	0	2

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	57	TYR	CE2-CZ	-6.02	1.30	1.38	9	3
1	A	57	TYR	CE1-CZ	5.97	1.46	1.38	9	3
1	A	51	PHE	CE1-CZ	5.60	1.48	1.37	14	1
1	A	37	TYR	CE2-CZ	5.51	1.45	1.38	11	1
1	A	37	TYR	CE1-CZ	-5.43	1.31	1.38	15	2
1	A	58	PHE	CE2-CZ	5.25	1.47	1.37	12	1

There are no bond-angle outliers.

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	A	37	TYR	Sidechain	1
1	A	51	PHE	Sidechain	1

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	771	738	731	54±5
All	All	11565	11070	10965	805

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ALA:HB3	1:A:105:VAL:HG23	0.89	1.44	10	14
1:A:5:VAL:HG21	1:A:105:VAL:HG11	0.85	1.48	9	13
1:A:96:PRO:HB2	1:A:99:ASP:HB3	0.84	1.47	15	10
1:A:3:HIS:HB3	1:A:22:VAL:HG22	0.84	1.50	7	15
1:A:5:VAL:HG13	1:A:9:HIS:ND1	0.82	1.89	15	1
1:A:5:VAL:HG21	1:A:105:VAL:HG21	0.77	1.53	15	10
1:A:57:TYR:HB3	1:A:71:GLU:HG2	0.74	1.59	3	2
1:A:45:SER:HB2	1:A:53:VAL:HB	0.74	1.59	12	1
1:A:51:PHE:HB3	1:A:76:THR:O	0.74	1.82	9	14
1:A:45:SER:HB2	1:A:52:THR:HG23	0.73	1.59	14	1
1:A:57:TYR:HA	1:A:71:GLU:HA	0.72	1.61	7	14
1:A:5:VAL:HG11	1:A:103:PHE:CZ	0.72	2.20	7	14
1:A:85:VAL:O	1:A:104:THR:HA	0.71	1.85	11	15
1:A:34:PHE:HB2	1:A:89:TYR:CE2	0.71	2.21	8	5
1:A:9:HIS:HA	1:A:12:ALA:HB2	0.71	1.60	15	6
1:A:16:VAL:HG22	1:A:108:LYS:O	0.70	1.87	12	14
1:A:53:VAL:HB	1:A:75:VAL:HB	0.69	1.64	7	1
1:A:5:VAL:HG13	1:A:9:HIS:HB2	0.68	1.64	3	14
1:A:45:SER:HB3	1:A:53:VAL:HB	0.68	1.66	1	2
1:A:54:GLU:HG3	1:A:74:HIS:HB2	0.67	1.67	1	5
1:A:37:TYR:HA	1:A:73:PHE:HZ	0.67	1.49	2	8
1:A:56:LYS:HD3	1:A:72:HIS:HB2	0.66	1.67	11	8
1:A:37:TYR:CE1	1:A:40:GLY:HA2	0.66	2.25	13	2
1:A:34:PHE:HA	1:A:90:MET:C	0.66	2.10	9	8
1:A:89:TYR:HB3	1:A:101:GLU:HB3	0.66	1.65	6	6
1:A:103:PHE:CZ	1:A:105:VAL:HB	0.66	2.26	14	2
1:A:14:LEU:O	1:A:107:LEU:HA	0.66	1.90	3	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:TYR:CD1	1:A:40:GLY:HA2	0.66	2.26	2	4
1:A:78:LYS:O	1:A:78:LYS:HG2	0.65	1.91	8	5
1:A:56:LYS:HD2	1:A:72:HIS:HB2	0.65	1.67	12	2
1:A:45:SER:HB2	1:A:53:VAL:CG2	0.65	2.22	2	3
1:A:10:ASN:ND2	1:A:103:PHE:HA	0.63	2.08	7	15
1:A:48:GLU:OE1	1:A:50:MET:HG2	0.63	1.93	14	2
1:A:5:VAL:HG11	1:A:103:PHE:HZ	0.63	1.51	2	11
1:A:28:SER:HA	1:A:36:TRP:CD1	0.63	2.29	8	15
1:A:45:SER:HB3	1:A:48:GLU:HB3	0.62	1.70	4	3
1:A:23:GLU:HB2	1:A:74:HIS:CD2	0.62	2.29	14	7
1:A:83:HIS:ND1	1:A:85:VAL:HG22	0.62	2.09	15	13
1:A:103:PHE:CZ	1:A:105:VAL:HG12	0.62	2.29	15	1
1:A:3:HIS:NE2	1:A:107:LEU:HD13	0.61	2.11	10	1
1:A:34:PHE:CD2	1:A:90:MET:HA	0.61	2.31	6	1
1:A:50:MET:HG2	1:A:51:PHE:HD1	0.60	1.56	4	4
1:A:18:VAL:HG21	1:A:78:LYS:HA	0.60	1.73	6	1
1:A:18:VAL:HG12	1:A:19:GLY:H	0.60	1.55	9	2
1:A:94:THR:HG23	1:A:95:GLY:H	0.60	1.57	7	11
1:A:37:TYR:HA	1:A:73:PHE:CZ	0.60	2.32	4	7
1:A:5:VAL:HG13	1:A:9:HIS:CG	0.60	2.32	15	1
1:A:43:LYS:HE3	1:A:43:LYS:H	0.59	1.57	12	1
1:A:88:THR:HG22	1:A:90:MET:HG3	0.59	1.74	11	2
1:A:96:PRO:HB2	1:A:99:ASP:HB2	0.59	1.74	9	1
1:A:51:PHE:O	1:A:52:THR:HB	0.59	1.97	14	1
1:A:9:HIS:C	1:A:9:HIS:CD2	0.59	2.74	15	1
1:A:18:VAL:HG12	1:A:22:VAL:HG21	0.59	1.74	4	12
1:A:7:LYS:HD3	1:A:29:ASN:HD21	0.58	1.58	6	1
1:A:103:PHE:HZ	1:A:105:VAL:HG12	0.58	1.58	15	1
1:A:83:HIS:HB3	1:A:107:LEU:HG	0.58	1.75	7	4
1:A:38:PHE:HA	1:A:87:LEU:HD23	0.58	1.76	11	6
1:A:106:TYR:O	1:A:107:LEU:HD12	0.57	1.99	14	1
1:A:80:ALA:HA	1:A:110:ASN:HB3	0.57	1.76	12	3
1:A:10:ASN:HD22	1:A:103:PHE:HA	0.57	1.58	7	6
1:A:90:MET:HB3	1:A:95:GLY:HA3	0.57	1.76	10	4
1:A:57:TYR:HB3	1:A:71:GLU:CB	0.57	2.29	7	1
1:A:12:ALA:CB	1:A:105:VAL:HG23	0.57	2.27	8	1
1:A:9:HIS:CD2	1:A:103:PHE:CE2	0.57	2.93	15	1
1:A:43:LYS:O	1:A:43:LYS:HD2	0.56	2.00	13	5
1:A:5:VAL:HG22	1:A:9:HIS:CG	0.56	2.35	10	14
1:A:10:ASN:HA	1:A:103:PHE:CD2	0.56	2.36	12	11
1:A:51:PHE:CE2	1:A:76:THR:HG22	0.56	2.36	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:VAL:HG13	1:A:107:LEU:HD12	0.56	1.77	9	2
1:A:9:HIS:CD2	1:A:103:PHE:CD2	0.56	2.93	15	1
1:A:56:LYS:CD	1:A:72:HIS:HB2	0.55	2.31	2	3
1:A:35:ALA:O	1:A:89:TYR:HA	0.55	2.00	13	2
1:A:83:HIS:HD1	1:A:85:VAL:HG22	0.55	1.62	13	3
1:A:51:PHE:CB	1:A:77:VAL:HA	0.55	2.32	2	12
1:A:54:GLU:HB3	1:A:74:HIS:HB2	0.55	1.78	14	1
1:A:5:VAL:HB	1:A:24:ILE:HD13	0.54	1.79	9	8
1:A:96:PRO:HB2	1:A:99:ASP:CB	0.54	2.31	12	5
1:A:38:PHE:HB2	1:A:42:THR:O	0.54	2.03	7	9
1:A:18:VAL:HG12	1:A:22:VAL:CG2	0.54	2.31	5	7
1:A:57:TYR:CB	1:A:71:GLU:HA	0.54	2.33	4	1
1:A:85:VAL:HG23	1:A:105:VAL:HG12	0.54	1.79	14	1
1:A:18:VAL:HG22	1:A:110:ASN:C	0.54	2.23	11	6
1:A:56:LYS:HE2	1:A:74:HIS:CE1	0.54	2.38	6	2
1:A:51:PHE:HB3	1:A:77:VAL:HA	0.54	1.78	6	12
1:A:28:SER:HA	1:A:36:TRP:HD1	0.53	1.61	9	7
1:A:79:ALA:O	1:A:110:ASN:HA	0.53	2.03	7	4
1:A:34:PHE:HA	1:A:91:ARG:N	0.53	2.18	9	1
1:A:29:ASN:O	1:A:31:THR:HG22	0.53	2.03	9	1
1:A:43:LYS:HE3	1:A:43:LYS:N	0.53	2.19	12	1
1:A:18:VAL:HB	1:A:77:VAL:O	0.53	2.02	14	1
1:A:53:VAL:HG22	1:A:75:VAL:HG12	0.53	1.80	13	2
1:A:13:THR:HA	1:A:106:TYR:O	0.53	2.02	10	7
1:A:45:SER:HB2	1:A:48:GLU:HB3	0.53	1.77	10	1
1:A:50:MET:HG3	1:A:51:PHE:HD1	0.52	1.63	5	1
1:A:105:VAL:HG22	1:A:107:LEU:HG	0.52	1.80	8	2
1:A:85:VAL:CG1	1:A:105:VAL:HG12	0.52	2.35	9	1
1:A:70:THR:HG22	1:A:72:HIS:NE2	0.52	2.19	5	1
1:A:3:HIS:CD2	1:A:16:VAL:HG11	0.52	2.39	5	10
1:A:53:VAL:HA	1:A:75:VAL:HA	0.52	1.81	7	2
1:A:83:HIS:CE1	1:A:85:VAL:HG22	0.52	2.39	1	5
1:A:37:TYR:HE1	1:A:90:MET:CE	0.52	2.18	4	2
1:A:28:SER:OG	1:A:71:GLU:HG3	0.52	2.05	3	1
1:A:5:VAL:HG13	1:A:9:HIS:CE1	0.51	2.40	15	1
1:A:88:THR:HA	1:A:102:ARG:HG3	0.51	1.82	1	2
1:A:45:SER:HB2	1:A:53:VAL:HG23	0.51	1.82	4	2
1:A:43:LYS:HB3	1:A:73:PHE:HE2	0.51	1.66	3	1
1:A:103:PHE:HZ	1:A:105:VAL:HB	0.51	1.62	14	1
1:A:19:GLY:HA2	1:A:78:LYS:HB3	0.51	1.82	14	2
1:A:38:PHE:CD2	1:A:43:LYS:HA	0.51	2.41	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ILE:HD12	1:A:105:VAL:HG11	0.51	1.82	7	4
1:A:37:TYR:HE1	1:A:90:MET:HE2	0.51	1.66	13	2
1:A:25:GLN:HG3	1:A:72:HIS:CE1	0.51	2.41	11	4
1:A:34:PHE:CE2	1:A:100:SER:HA	0.51	2.40	3	1
1:A:73:PHE:CE2	1:A:87:LEU:HD22	0.51	2.41	10	1
1:A:92:PRO:HG2	1:A:93:TRP:CE3	0.50	2.41	4	6
1:A:34:PHE:HA	1:A:90:MET:O	0.50	2.06	12	5
1:A:50:MET:HG2	1:A:51:PHE:CD1	0.50	2.41	13	1
1:A:86:ASN:HA	1:A:103:PHE:O	0.50	2.05	11	3
1:A:18:VAL:HG22	1:A:22:VAL:HG21	0.50	1.82	13	1
1:A:90:MET:HB3	1:A:95:GLY:CA	0.50	2.35	15	2
1:A:52:THR:O	1:A:53:VAL:HG13	0.50	2.06	14	1
1:A:18:VAL:CG2	1:A:78:LYS:HA	0.49	2.37	5	6
1:A:87:LEU:HG	1:A:103:PHE:CE1	0.49	2.42	15	1
1:A:5:VAL:CG2	1:A:105:VAL:HG21	0.49	2.36	14	6
1:A:30:PRO:HA	1:A:89:TYR:OH	0.49	2.07	4	4
1:A:24:ILE:HG21	1:A:85:VAL:HG11	0.49	1.84	8	3
1:A:27:PRO:HA	1:A:69:GLY:O	0.49	2.07	1	3
1:A:32:THR:HG23	1:A:34:PHE:HD1	0.49	1.67	7	3
1:A:101:GLU:HG2	1:A:102:ARG:H	0.49	1.67	1	2
1:A:78:LYS:HB2	1:A:78:LYS:NZ	0.49	2.22	5	1
1:A:48:GLU:HG2	1:A:51:PHE:HB2	0.49	1.85	6	1
1:A:37:TYR:OH	1:A:90:MET:C	0.49	2.51	12	1
1:A:54:GLU:CG	1:A:74:HIS:HB2	0.48	2.38	6	3
1:A:27:PRO:HG2	1:A:29:ASN:OD1	0.48	2.08	4	5
1:A:56:LYS:HB3	1:A:56:LYS:NZ	0.48	2.22	9	2
1:A:31:THR:HG23	1:A:89:TYR:CE2	0.48	2.43	11	6
1:A:48:GLU:HA	1:A:51:PHE:O	0.48	2.08	12	2
1:A:14:LEU:HB2	1:A:107:LEU:HD23	0.48	1.85	2	1
1:A:3:HIS:HB2	1:A:16:VAL:HB	0.48	1.86	7	2
1:A:34:PHE:HB2	1:A:89:TYR:CD2	0.48	2.43	8	2
1:A:45:SER:O	1:A:48:GLU:HG2	0.48	2.08	5	2
1:A:57:TYR:HB3	1:A:71:GLU:CG	0.48	2.33	3	1
1:A:78:LYS:O	1:A:78:LYS:HD3	0.48	2.09	5	2
1:A:40:GLY:HA3	1:A:90:MET:CE	0.48	2.39	6	1
1:A:50:MET:SD	1:A:50:MET:N	0.47	2.87	10	6
1:A:9:HIS:NE2	1:A:103:PHE:CD2	0.47	2.82	15	1
1:A:6:THR:C	1:A:9:HIS:ND1	0.47	2.68	15	1
1:A:16:VAL:HG11	1:A:107:LEU:HD13	0.47	1.85	1	3
1:A:40:GLY:HA3	1:A:90:MET:HE1	0.47	1.87	6	1
1:A:25:GLN:HA	1:A:72:HIS:HA	0.47	1.87	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:THR:HG22	1:A:33:GLY:H	0.47	1.69	8	2
1:A:47:ASN:ND2	1:A:81:GLY:HA3	0.47	2.24	14	2
1:A:105:VAL:HG22	1:A:107:LEU:HD13	0.47	1.86	14	1
1:A:18:VAL:HG22	1:A:110:ASN:O	0.47	2.09	6	2
1:A:5:VAL:HG13	1:A:9:HIS:CB	0.47	2.40	14	2
1:A:52:THR:HG23	1:A:52:THR:O	0.47	2.10	14	1
1:A:9:HIS:O	1:A:105:VAL:HG23	0.47	2.10	14	1
1:A:110:ASN:HD22	1:A:110:ASN:N	0.47	2.07	10	5
1:A:28:SER:HB2	1:A:71:GLU:HG3	0.47	1.87	5	2
1:A:15:THR:HG23	1:A:108:LYS:HB3	0.46	1.86	3	1
1:A:45:SER:OG	1:A:53:VAL:HB	0.46	2.10	3	1
1:A:22:VAL:HG12	1:A:75:VAL:HG22	0.46	1.87	10	1
1:A:54:GLU:HB3	1:A:74:HIS:CB	0.46	2.40	14	1
1:A:9:HIS:CD2	1:A:10:ASN:N	0.46	2.84	15	1
1:A:36:TRP:CZ3	1:A:103:PHE:HB3	0.46	2.45	15	1
1:A:57:TYR:HB3	1:A:71:GLU:HB3	0.46	1.86	7	2
1:A:56:LYS:O	1:A:56:LYS:HG2	0.46	2.09	15	5
1:A:56:LYS:O	1:A:56:LYS:HD3	0.46	2.09	12	1
1:A:12:ALA:HB3	1:A:105:VAL:CG2	0.46	2.41	14	1
1:A:75:VAL:HG11	1:A:83:HIS:HE2	0.46	1.71	15	1
1:A:3:HIS:NE2	1:A:107:LEU:HD22	0.46	2.26	1	1
1:A:92:PRO:HG2	1:A:93:TRP:CZ3	0.46	2.46	2	4
1:A:24:ILE:HD11	1:A:107:LEU:CD2	0.46	2.40	13	2
1:A:37:TYR:CE1	1:A:90:MET:HE2	0.46	2.46	13	1
1:A:37:TYR:HH	1:A:90:MET:C	0.45	2.12	12	1
1:A:75:VAL:HG11	1:A:83:HIS:NE2	0.45	2.26	3	2
1:A:53:VAL:HB	1:A:75:VAL:HG12	0.45	1.89	6	2
1:A:80:ALA:HA	1:A:110:ASN:CB	0.45	2.41	8	1
1:A:43:LYS:N	1:A:43:LYS:HD3	0.45	2.26	9	1
1:A:82:THR:HG23	1:A:108:LYS:HD2	0.45	1.89	1	1
1:A:83:HIS:HB2	1:A:109:ALA:HB2	0.45	1.88	8	1
1:A:45:SER:HB2	1:A:52:THR:CG2	0.45	2.35	14	1
1:A:48:GLU:HB2	1:A:51:PHE:O	0.45	2.11	4	2
1:A:52:THR:HB	1:A:77:VAL:HB	0.45	1.87	14	1
1:A:3:HIS:HB3	1:A:22:VAL:CG2	0.45	2.41	3	1
1:A:34:PHE:CE1	1:A:96:PRO:HD2	0.45	2.47	4	1
1:A:96:PRO:CB	1:A:99:ASP:HB3	0.45	2.40	2	1
1:A:75:VAL:HG21	1:A:83:HIS:NE2	0.45	2.27	12	1
1:A:94:THR:HG23	1:A:95:GLY:N	0.44	2.27	10	6
1:A:16:VAL:CG1	1:A:107:LEU:HB2	0.44	2.42	9	3
1:A:36:TRP:HZ3	1:A:103:PHE:N	0.44	2.10	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:ASN:N	1:A:86:ASN:HD22	0.44	2.10	3	4
1:A:22:VAL:O	1:A:75:VAL:HG22	0.44	2.13	6	2
1:A:46:PRO:HD2	1:A:83:HIS:CD2	0.44	2.47	12	1
1:A:87:LEU:H	1:A:103:PHE:HD1	0.44	1.55	15	1
1:A:53:VAL:HG13	1:A:75:VAL:HG12	0.44	1.89	13	2
1:A:37:TYR:OH	1:A:90:MET:HB2	0.44	2.12	12	2
1:A:35:ALA:HA	1:A:89:TYR:CE1	0.44	2.48	7	1
1:A:5:VAL:HB	1:A:24:ILE:CD1	0.44	2.42	4	2
1:A:53:VAL:CG2	1:A:75:VAL:HG12	0.44	2.42	12	2
1:A:37:TYR:OH	1:A:92:PRO:HA	0.44	2.13	13	1
1:A:48:GLU:HG3	1:A:51:PHE:H	0.44	1.73	6	1
1:A:56:LYS:HD2	1:A:74:HIS:CD2	0.44	2.47	8	1
1:A:5:VAL:CG2	1:A:107:LEU:HD11	0.44	2.43	10	1
1:A:5:VAL:HG22	1:A:9:HIS:CB	0.44	2.43	15	1
1:A:37:TYR:O	1:A:88:THR:N	0.43	2.51	1	4
1:A:72:HIS:CD2	1:A:72:HIS:N	0.43	2.87	4	7
1:A:93:TRP:CD1	1:A:94:THR:HG22	0.43	2.49	10	1
1:A:53:VAL:HG23	1:A:75:VAL:HG12	0.43	1.88	12	1
1:A:88:THR:HG22	1:A:90:MET:CG	0.43	2.43	15	2
1:A:16:VAL:HG13	1:A:107:LEU:HB2	0.43	1.91	15	2
1:A:16:VAL:CG2	1:A:109:ALA:HA	0.43	2.43	8	1
1:A:83:HIS:O	1:A:107:LEU:HD13	0.43	2.14	12	1
1:A:5:VAL:HB	1:A:24:ILE:HA	0.43	1.91	8	1
1:A:22:VAL:O	1:A:75:VAL:HB	0.43	2.13	8	1
1:A:47:ASN:HD21	1:A:81:GLY:HA3	0.43	1.74	10	1
1:A:6:THR:O	1:A:9:HIS:HB2	0.42	2.14	14	1
1:A:9:HIS:C	1:A:11:GLY:N	0.42	2.72	8	7
1:A:48:GLU:O	1:A:48:GLU:HG3	0.42	2.14	2	1
1:A:22:VAL:HG12	1:A:75:VAL:HG13	0.42	1.90	3	1
1:A:34:PHE:CD1	1:A:34:PHE:N	0.42	2.87	6	1
1:A:87:LEU:O	1:A:102:ARG:HG3	0.42	2.14	11	1
1:A:85:VAL:HB	1:A:103:PHE:CZ	0.42	2.49	15	1
1:A:103:PHE:CG	1:A:104:THR:N	0.42	2.87	15	1
1:A:5:VAL:HG22	1:A:9:HIS:CD2	0.42	2.50	9	2
1:A:101:GLU:HG2	1:A:102:ARG:N	0.42	2.30	1	1
1:A:53:VAL:HG23	1:A:75:VAL:HB	0.42	1.91	3	1
1:A:107:LEU:H	1:A:107:LEU:HD13	0.42	1.75	9	2
1:A:31:THR:CG2	1:A:89:TYR:CE2	0.42	3.03	11	1
1:A:48:GLU:HG3	1:A:77:VAL:HG23	0.42	1.90	14	1
1:A:54:GLU:O	1:A:74:HIS:HB2	0.42	2.15	10	1
1:A:107:LEU:HD13	1:A:107:LEU:H	0.42	1.75	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:PHE:CZ	1:A:99:ASP:HB3	0.41	2.50	6	1
1:A:105:VAL:HG13	1:A:107:LEU:HD13	0.41	1.90	14	1
1:A:91:ARG:H	1:A:95:GLY:HA2	0.41	1.75	2	1
1:A:32:THR:HG22	1:A:33:GLY:N	0.41	2.30	13	1
1:A:34:PHE:CD1	1:A:91:ARG:HG3	0.41	2.50	1	1
1:A:70:THR:HB	1:A:72:HIS:NE2	0.41	2.30	1	1
1:A:78:LYS:HG2	1:A:78:LYS:O	0.41	2.16	7	1
1:A:3:HIS:NE2	1:A:107:LEU:HG	0.41	2.31	12	1
1:A:7:LYS:HB2	1:A:27:PRO:HG3	0.41	1.91	12	1
1:A:7:LYS:HB2	1:A:27:PRO:HD3	0.41	1.92	5	1
1:A:34:PHE:CE2	1:A:99:ASP:HB3	0.41	2.51	6	1
1:A:37:TYR:OH	1:A:90:MET:O	0.41	2.36	12	1
1:A:90:MET:HG2	1:A:100:SER:CB	0.41	2.45	13	1
1:A:85:VAL:HB	1:A:103:PHE:CE1	0.41	2.51	15	1
1:A:35:ALA:HA	1:A:89:TYR:HE1	0.40	1.76	11	1
1:A:21:LEU:HG	1:A:22:VAL:N	0.40	2.31	6	1
1:A:85:VAL:CG2	1:A:105:VAL:HG12	0.40	2.46	14	1
1:A:32:THR:HG23	1:A:34:PHE:CD1	0.40	2.50	5	1
1:A:14:LEU:N	1:A:14:LEU:HD23	0.40	2.32	15	1
1:A:5:VAL:CG1	1:A:6:THR:N	0.40	2.85	14	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	A	96/111 (86%)	76±3 (79±3%)	17±3 (17±3%)	4±1 (4±1%)	4	31
All	All	1440/1665 (86%)	1138 (79%)	248 (17%)	54 (4%)	4	31

All 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	94	THR	11
1	A	32	THR	10

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Mol	Chain	Res	Type	Models (Total)
1	A	30	PRO	4
1	A	50	MET	4
1	A	38	PHE	3
1	A	47	ASN	3
1	A	96	PRO	3
1	A	95	GLY	3
1	A	49	SER	2
1	A	18	VAL	2
1	A	98	HIS	2
1	A	33	GLY	2
1	A	80	ALA	1
1	A	70	THR	1
1	A	100	SER	1
1	A	97	SER	1
1	A	52	THR	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	82/91 (90%)	68±2 (83±3%)	14±2 (17±3%)	4	38
All	All	1230/1365 (90%)	1020 (83%)	210 (17%)	4	38

All 42 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	25	GLN	15
1	A	43	LYS	15
1	A	56	LYS	15
1	A	78	LYS	15
1	A	70	THR	13
1	A	86	ASN	12
1	A	103	PHE	10
1	A	42	THR	10
1	A	6	THR	9
1	A	72	HIS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	110	ASN	8
1	A	38	PHE	6
1	A	57	TYR	6
1	A	29	ASN	6
1	A	50	MET	6
1	A	75	VAL	4
1	A	37	TYR	4
1	A	107	LEU	4
1	A	44	GLU	4
1	A	54	GLU	3
1	A	82	THR	3
1	A	31	THR	3
1	A	14	LEU	3
1	A	55	ASN	3
1	A	48	GLU	3
1	A	4	LYS	2
1	A	89	TYR	2
1	A	10	ASN	2
1	A	85	VAL	2
1	A	21	LEU	1
1	A	58	PHE	1
1	A	52	THR	1
1	A	96	PRO	1
1	A	99	ASP	1
1	A	39	GLU	1
1	A	90	MET	1
1	A	22	VAL	1
1	A	23	GLU	1
1	A	51	PHE	1
1	A	53	VAL	1
1	A	105	VAL	1
1	A	5	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 77% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	1096
Number of shifts mapped to atoms	1084
Number of unparsed shifts	0
Number of shifts with mapping errors	12
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	13

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 12 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	SER	H	8.639	0.02	1
1	A	1	SER	HA	4.493	0.02	1
1	A	1	SER	HB2	3.735	0.02	2
1	A	1	SER	CA	58.102	0.1	1
1	A	1	SER	CB	63.956	0.1	1
1	A	1	SER	N	116.438	0.05	1
1	A	2	SER	H	8.337	0.02	1
1	A	2	SER	HA	4.63	0.02	1
1	A	2	SER	HB2	3.727	0.02	2
1	A	2	SER	CA	57.837	0.1	1
1	A	2	SER	CB	64.314	0.1	1
1	A	2	SER	N	117.467	0.05	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	109	0.14 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	99	0.09 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	102	-0.56 ± 0.28	Should be applied

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 77%, i.e. 992 atoms were assigned a chemical shift out of a possible 1294. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	388/488 (80%)	198/199 (99%)	98/196 (50%)	92/93 (99%)
Sidechain	529/638 (83%)	348/417 (83%)	172/202 (85%)	9/19 (47%)
Aromatic	75/168 (45%)	41/82 (50%)	32/72 (44%)	2/14 (14%)
Overall	992/1294 (77%)	587/698 (84%)	302/470 (64%)	103/126 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1084 atoms were assigned a chemical shift out of a possible 1410. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	424/536 (79%)	217/219 (99%)	107/216 (50%)	100/101 (99%)
Sidechain	585/706 (83%)	384/462 (83%)	192/224 (86%)	9/20 (45%)
Aromatic	75/168 (45%)	41/82 (50%)	32/72 (44%)	2/14 (14%)
Overall	1084/1410 (77%)	642/763 (84%)	331/512 (65%)	111/135 (82%)

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	89	TYR	HB3	0.04	0.93 – 4.76	-7.3
1	A	26	LEU	HD21	-1.27	-0.65 – 2.13	-7.2
1	A	26	LEU	HD22	-1.27	-0.65 – 2.13	-7.2

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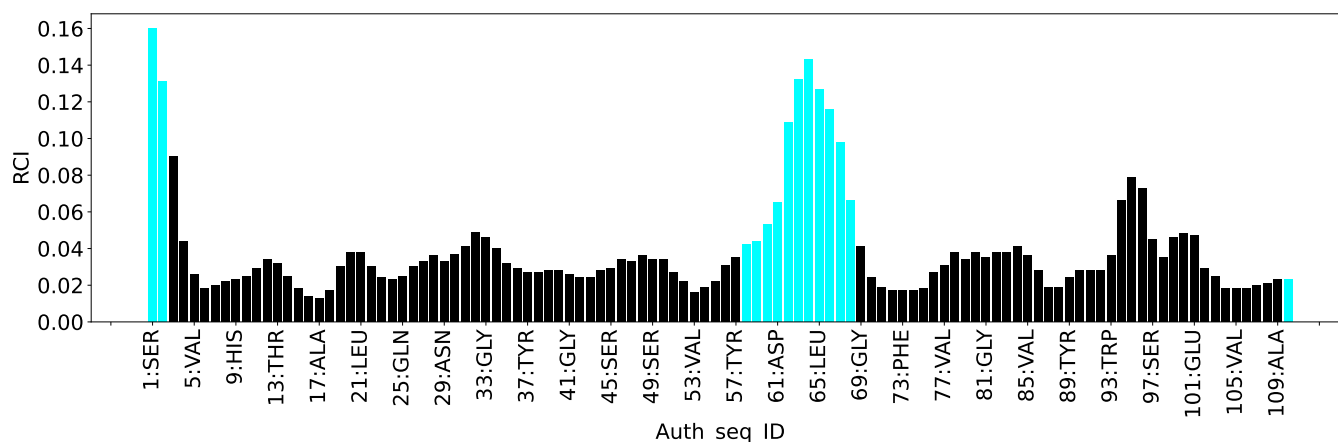
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	26	LEU	HD23	-1.27	-0.65 – 2.13	-7.2
1	A	91	ARG	HB3	0.04	0.43 – 3.11	-6.5
1	A	91	ARG	HG3	-0.13	0.15 – 2.94	-6.0
1	A	34	PHE	HB3	0.75	1.03 – 4.85	-5.8
1	A	87	LEU	HD21	-0.81	-0.65 – 2.13	-5.5
1	A	87	LEU	HD22	-0.81	-0.65 – 2.13	-5.5
1	A	87	LEU	HD23	-0.81	-0.65 – 2.13	-5.5
1	A	26	LEU	HD11	-0.65	-0.61 – 2.12	-5.2
1	A	26	LEU	HD12	-0.65	-0.61 – 2.12	-5.2
1	A	26	LEU	HD13	-0.65	-0.61 – 2.12	-5.2

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2770
Intra-residue ($ i-j =0$)	868
Sequential ($ i-j =1$)	566
Medium range ($ i-j >1$ and $ i-j <5$)	257
Long range ($ i-j \geq 5$)	1003
Inter-chain	0
Hydrogen bond restraints	76
Disulfide bond restraints	0
Total dihedral-angle restraints	103
Number of unmapped restraints	30
Number of restraints per residue	25.9
Number of long range restraints per residue ¹	9.6

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)	56.2	0.2
0.2-0.5 (Medium)	48.8	0.5
>0.5 (Large)	42.4	5.44

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)	23.2	9.73
10.0-20.0 (Medium)	0.1	17.22
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

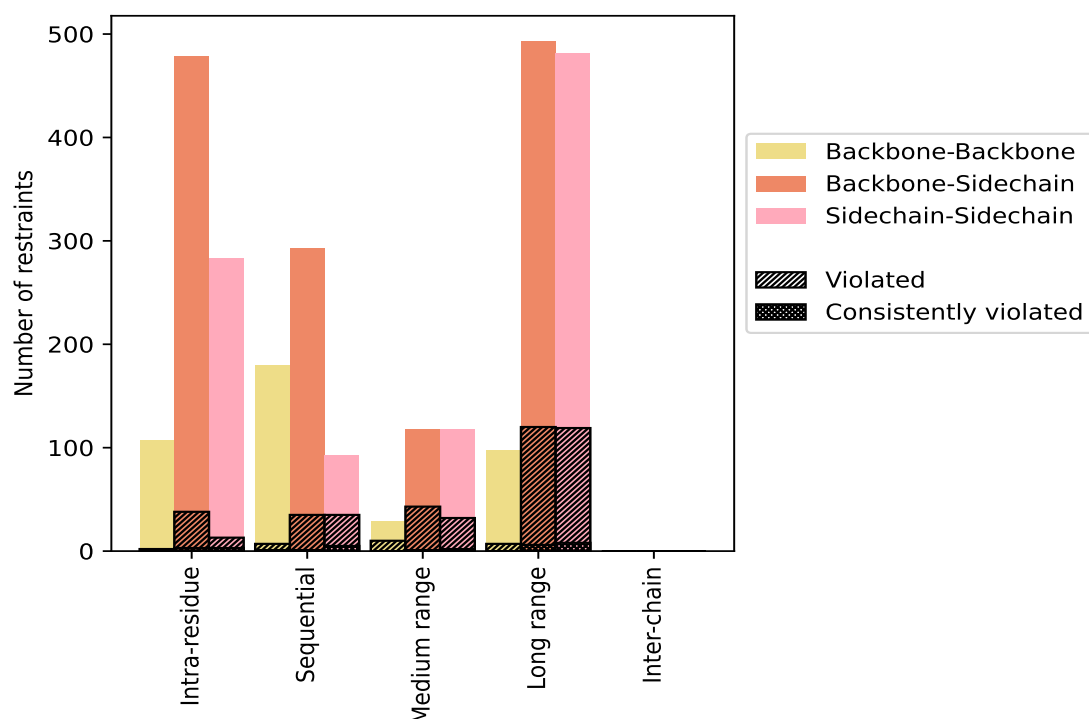
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	868	31.3	53	6.1	1.9	6	0.7	0.2
Backbone-Backbone	107	3.9	2	1.9	0.1	0	0.0	0.0
Backbone-Sidechain	478	17.3	38	7.9	1.4	3	0.6	0.1
Sidechain-Sidechain	283	10.2	13	4.6	0.5	3	1.1	0.1
Sequential ($i-j =1$)	566	20.4	77	13.6	2.8	7	1.2	0.3
Backbone-Backbone	180	6.5	7	3.9	0.3	1	0.6	0.0
Backbone-Sidechain	293	10.6	35	11.9	1.3	1	0.3	0.0
Sidechain-Sidechain	93	3.4	35	37.6	1.3	5	5.4	0.2
Medium range ($i-j >1$ & $i-j <5$)	257	9.3	82	31.9	3.0	2	0.8	0.1
Backbone-Backbone	29	1.0	10	34.5	0.4	0	0.0	0.0
Backbone-Sidechain	110	4.0	40	36.4	1.4	0	0.0	0.0
Sidechain-Sidechain	118	4.3	32	27.1	1.2	2	1.7	0.1
Long range ($i-j \geq 5$)	1003	36.2	238	23.7	8.6	14	1.4	0.5
Backbone-Backbone	97	3.5	7	7.2	0.3	0	0.0	0.0
Backbone-Sidechain	425	15.3	112	26.4	4.0	6	1.4	0.2
Sidechain-Sidechain	481	17.4	119	24.7	4.3	8	1.7	0.3
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	76	2.7	11	14.5	0.4	1	1.3	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2770	100.0	461	16.6	16.6	30	1.1	1.1
Backbone-Backbone	413	14.9	26	6.3	0.9	1	0.2	0.0
Backbone-Sidechain	1382	49.9	236	17.1	8.5	11	0.8	0.4
Sidechain-Sidechain	975	35.2	199	20.4	7.2	18	1.8	0.6

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	16	21	21	79	0	137	0.43	2.66	0.45	0.24
2	21	20	21	74	0	136	0.42	2.36	0.42	0.26
3	19	36	22	93	0	170	0.48	2.23	0.48	0.28
4	20	21	21	74	0	136	0.43	3.35	0.45	0.25
5	16	24	28	75	0	143	0.4	2.58	0.42	0.25
6	17	22	24	74	0	137	0.38	2.05	0.41	0.21
7	23	31	33	86	0	173	0.47	3.25	0.49	0.24
8	24	38	33	97	0	192	0.54	5.26	0.61	0.29
9	19	25	31	72	0	147	0.46	3.07	0.5	0.25
10	16	27	25	72	0	140	0.45	2.94	0.47	0.25

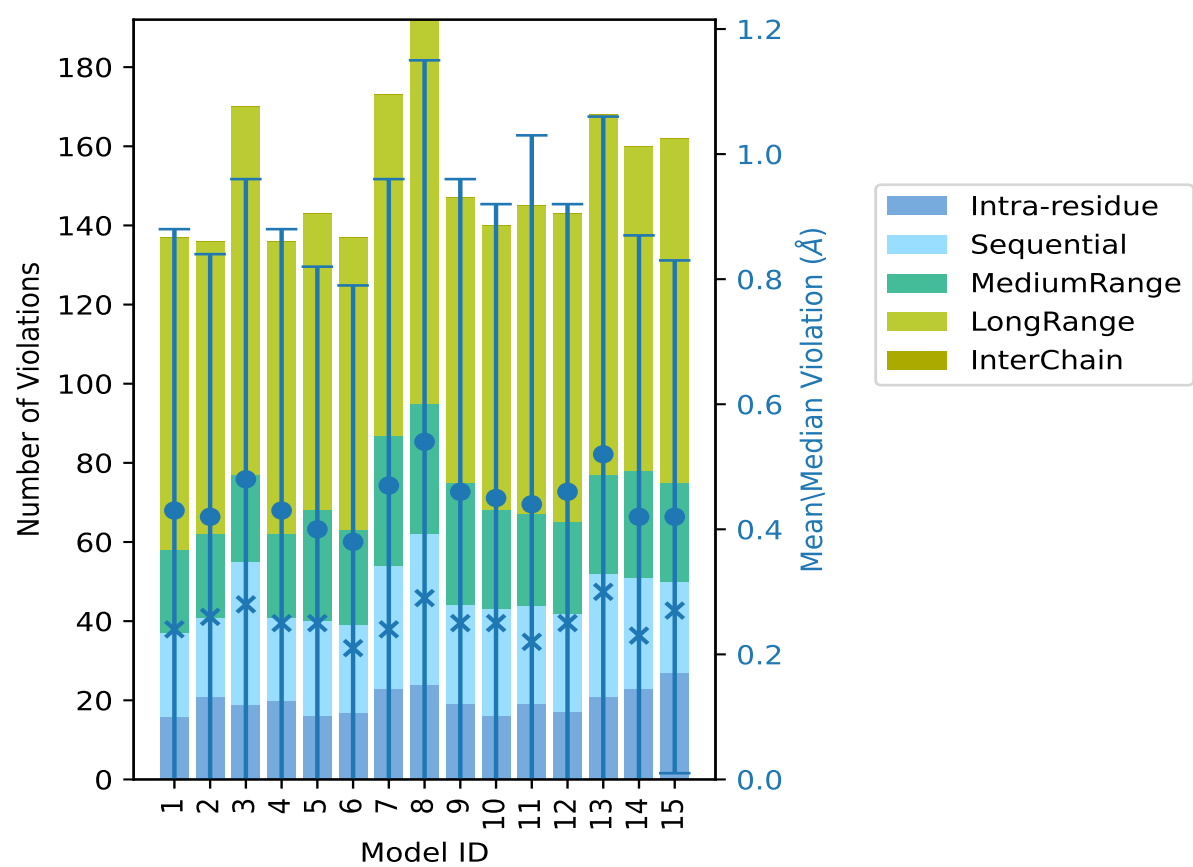
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	19	25	23	78	0	145	0.44	5.44	0.59	0.22
12	17	25	23	78	0	143	0.46	3.03	0.46	0.25
13	21	31	25	91	0	168	0.52	3.44	0.54	0.3
14	23	28	27	82	0	160	0.42	2.63	0.45	0.23
15	27	23	25	87	0	162	0.42	2.39	0.41	0.27

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

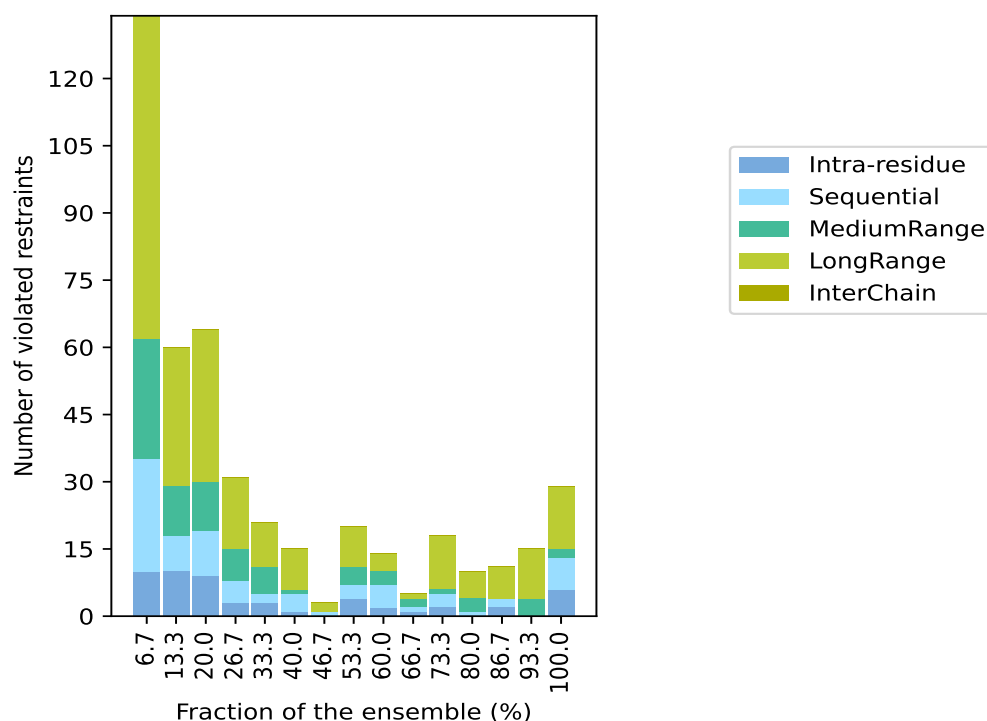
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2244(IR:815, SQ:489, MR:175, LR:765, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
10	25	27	72	0	134	1	6.7
10	8	11	31	0	60	2	13.3
9	10	11	34	0	64	3	20.0
3	5	7	16	0	31	4	26.7
3	2	6	10	0	21	5	33.3
1	4	1	9	0	15	6	40.0
0	1	0	2	0	3	7	46.7
4	3	4	9	0	20	8	53.3
2	5	3	4	0	14	9	60.0
1	1	2	1	0	5	10	66.7
2	3	1	12	0	18	11	73.3
0	1	3	6	0	10	12	80.0
2	2	0	7	0	11	13	86.7
0	0	4	11	0	15	14	93.3
6	7	2	14	0	29	15	100.0

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

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

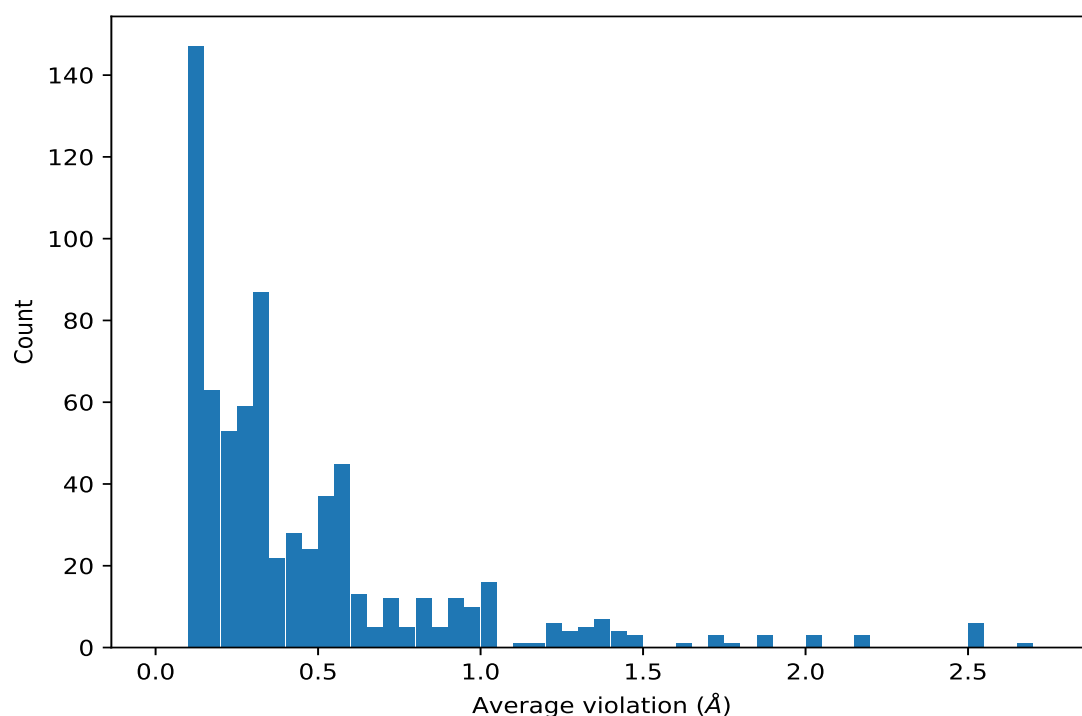
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	15	2.67	0.49	2.63
(1,2330)	1:70:A:THR:HG21	1:57:A:TYR:HB2	15	1.4	0.39	1.46
(1,2330)	1:70:A:THR:HG22	1:57:A:TYR:HB2	15	1.4	0.39	1.46
(1,2330)	1:70:A:THR:HG23	1:57:A:TYR:HB2	15	1.4	0.39	1.46
(1,2330)	1:56:A:LYS:HG3	1:57:A:TYR:HB2	15	1.4	0.39	1.46
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	15	1.34	0.06	1.36
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	15	1.29	0.24	1.38
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	15	1.29	0.24	1.38
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	15	1.29	0.24	1.38
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	15	1.04	0.09	1.0
(1,2288)	1:24:A:ILE:HG13	1:45:A:SER:HA	15	0.97	0.29	0.98
(1,2288)	1:64:A:LEU:HB3	1:60:A:PRO:HD3	15	0.97	0.29	0.98
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	15	0.93	0.2	0.99
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	15	0.93	0.2	0.99
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	15	0.93	0.2	0.99
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	15	0.8	0.57	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	15	0.66	0.06	0.68
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	15	0.6	0.04	0.61
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	15	0.57	0.26	0.47
(1,2351)	1:23:A:GLU:HB3	1:24:A:ILE:H	15	0.57	0.26	0.47
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	15	0.53	0.59	0.25
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	15	0.53	0.59	0.25
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	15	0.53	0.59	0.25
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	15	0.49	0.57	0.37
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	15	0.49	0.57	0.37
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	15	0.49	0.57	0.37
(1,2390)	1:75:A:VAL:HG21	1:51:A:PHE:HB3	15	0.4	0.33	0.36
(1,2390)	1:75:A:VAL:HG22	1:51:A:PHE:HB3	15	0.4	0.33	0.36
(1,2390)	1:75:A:VAL:HG23	1:51:A:PHE:HB3	15	0.4	0.33	0.36
(1,2390)	1:75:A:VAL:HG21	1:83:A:HIS:HB3	15	0.4	0.33	0.36
(1,2390)	1:75:A:VAL:HG22	1:83:A:HIS:HB3	15	0.4	0.33	0.36
(1,2390)	1:75:A:VAL:HG23	1:83:A:HIS:HB3	15	0.4	0.33	0.36
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	15	0.39	0.22	0.29
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	15	0.35	0.1	0.36
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	15	0.35	0.1	0.36
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	15	0.35	0.1	0.36
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	15	0.35	0.4	0.16
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	15	0.35	0.4	0.16
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	15	0.35	0.4	0.16
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	15	0.3	0.07	0.31
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	15	0.29	0.05	0.29
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	15	0.29	0.05	0.29
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	15	0.29	0.05	0.29
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	15	0.29	0.06	0.27
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	15	0.22	0.04	0.22
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	15	0.22	0.01	0.22
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	15	0.22	0.04	0.23
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	15	0.21	0.03	0.21
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	15	0.21	0.07	0.17
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	15	0.19	0.04	0.19
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	15	0.16	0.02	0.16
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	15	0.16	0.03	0.15
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	15	0.16	0.03	0.15
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	15	0.11	0.01	0.11
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	14	1.61	0.42	1.74
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	14	1.14	0.29	1.25
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	14	0.54	0.24	0.48
(1,2276)	1:75:A:VAL:HB	1:46:A:PRO:HD3	14	0.53	0.1	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2276)	1:27:A:PRO:HG2	1:29:A:ASN:HB3	14	0.53	0.1	0.52
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	14	0.53	0.31	0.44
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	14	0.5	0.15	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	14	0.48	0.08	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	14	0.48	0.08	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	14	0.48	0.08	0.51
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	14	0.29	0.21	0.24
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	14	0.29	0.21	0.24
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	14	0.29	0.21	0.24
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	14	0.24	0.02	0.24
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	14	0.24	0.02	0.24
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	14	0.24	0.02	0.24
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	14	0.23	0.02	0.24
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	14	0.23	0.02	0.24
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	14	0.23	0.02	0.24
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	14	0.22	0.04	0.21
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	14	0.19	0.06	0.18
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	14	0.18	0.04	0.18
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	14	0.18	0.04	0.18
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	14	0.18	0.04	0.18
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	14	0.17	0.04	0.18
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	14	0.15	0.05	0.12
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	14	0.15	0.05	0.12
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	14	0.15	0.05	0.12
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	13	0.71	0.44	1.02
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	13	0.71	0.44	1.02
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	13	0.71	0.44	1.02
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	13	0.58	0.34	0.59
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	13	0.58	0.34	0.59
(1,2363)	1:53:A:VAL:HA	1:75:A:VAL:HG21	13	0.51	0.19	0.57
(1,2363)	1:53:A:VAL:HA	1:75:A:VAL:HG22	13	0.51	0.19	0.57
(1,2363)	1:53:A:VAL:HA	1:75:A:VAL:HG23	13	0.51	0.19	0.57
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG21	13	0.51	0.19	0.57
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG22	13	0.51	0.19	0.57
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG23	13	0.51	0.19	0.57
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	13	0.4	0.16	0.43
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	13	0.3	0.11	0.3
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	13	0.22	0.04	0.23
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	13	0.21	0.05	0.22
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	13	0.21	0.05	0.22
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	13	0.21	0.05	0.22
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	13	0.17	0.01	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	13	0.17	0.03	0.18
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	13	0.17	0.03	0.18
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	13	0.17	0.03	0.18
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	13	0.15	0.04	0.13
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	13	0.12	0.01	0.11
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	13	0.12	0.01	0.11
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	13	0.12	0.01	0.11
(1,1897)	1:36:A:TRP:HD1	1:57:A:TYR:HB2	12	1.33	0.43	1.45
(2,19)	1:63:A:LYS:HD3	1:65:A:LEU:HA	12	0.98	0.68	1.27
(1,1752)	1:56:A:LYS:HB3	1:72:A:HIS:HB3	12	0.89	0.51	1.05
(1,2321)	1:44:A:GLU:HG3	1:46:A:PRO:HD2	12	0.7	0.47	0.59
(1,2258)	1:18:A:VAL:HG11	1:21:A:LEU:HA	12	0.58	0.06	0.59
(1,2258)	1:18:A:VAL:HG12	1:21:A:LEU:HA	12	0.58	0.06	0.59
(1,2258)	1:18:A:VAL:HG13	1:21:A:LEU:HA	12	0.58	0.06	0.59
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE1	12	0.36	0.12	0.34
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE2	12	0.36	0.12	0.34
(1,2232)	1:12:A:ALA:HB1	1:106:A:TYR:HA	12	0.34	0.11	0.32
(1,2232)	1:12:A:ALA:HB2	1:106:A:TYR:HA	12	0.34	0.11	0.32
(1,2232)	1:12:A:ALA:HB3	1:106:A:TYR:HA	12	0.34	0.11	0.32
(1,2164)	1:38:A:PHE:HA	1:38:A:PHE:HZ	12	0.28	0.07	0.29
(1,2164)	1:43:A:LYS:HA	1:38:A:PHE:HZ	12	0.28	0.07	0.29
(1,1535)	1:90:A:MET:HE1	1:92:A:PRO:HA	12	0.2	0.07	0.18
(1,1535)	1:90:A:MET:HE2	1:92:A:PRO:HA	12	0.2	0.07	0.18
(1,1535)	1:90:A:MET:HE3	1:92:A:PRO:HA	12	0.2	0.07	0.18
(1,2306)	1:48:A:GLU:HA	1:47:A:ASN:HA	12	0.19	0.04	0.19
(1,963)	1:107:A:LEU:HB3	1:16:A:VAL:H	11	1.43	0.16	1.47
(1,1642)	1:67:A:ALA:HB1	1:60:A:PRO:HG2	11	0.64	0.44	0.7
(1,1642)	1:67:A:ALA:HB2	1:60:A:PRO:HG2	11	0.64	0.44	0.7
(1,1642)	1:67:A:ALA:HB3	1:60:A:PRO:HG2	11	0.64	0.44	0.7
(1,1543)	1:14:A:LEU:HB2	1:14:A:LEU:H	11	0.6	0.05	0.62
(1,304)	1:61:A:ASP:HB3	1:62:A:SER:HA	11	0.47	0.55	0.17
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD11	11	0.43	0.26	0.39
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD12	11	0.43	0.26	0.39
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD13	11	0.43	0.26	0.39
(1,2131)	1:37:A:TYR:H	1:90:A:MET:HG2	11	0.36	0.13	0.34
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG11	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG12	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG13	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG11	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG12	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG13	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG11	11	0.35	0.12	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG12	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG13	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG21	1:82:A:THR:HG21	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG21	1:82:A:THR:HG22	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG21	1:82:A:THR:HG23	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG22	1:82:A:THR:HG21	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG22	1:82:A:THR:HG22	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG22	1:82:A:THR:HG23	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG23	1:82:A:THR:HG21	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG23	1:82:A:THR:HG22	11	0.35	0.12	0.37
(1,2446)	1:16:A:VAL:HG23	1:82:A:THR:HG23	11	0.35	0.12	0.37
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD1	11	0.32	0.38	0.17
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD2	11	0.32	0.38	0.17
(1,661)	1:91:A:ARG:HB3	1:90:A:MET:HB2	11	0.32	0.29	0.16
(1,2413)	1:31:A:THR:HG21	1:89:A:TYR:HB3	11	0.27	0.19	0.19
(1,2413)	1:31:A:THR:HG22	1:89:A:TYR:HB3	11	0.27	0.19	0.19
(1,2413)	1:31:A:THR:HG23	1:89:A:TYR:HB3	11	0.27	0.19	0.19
(1,1430)	1:82:A:THR:HG21	1:110:A:ASN:HD21	11	0.26	0.3	0.13
(1,1430)	1:82:A:THR:HG22	1:110:A:ASN:HD21	11	0.26	0.3	0.13
(1,1430)	1:82:A:THR:HG23	1:110:A:ASN:HD21	11	0.26	0.3	0.13
(1,2329)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	11	0.25	0.13	0.25
(2,107)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	11	0.25	0.13	0.25
(1,205)	1:56:A:LYS:HD3	1:72:A:HIS:HE1	11	0.22	0.06	0.22
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG11	11	0.16	0.03	0.15
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG12	11	0.16	0.03	0.15
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG13	11	0.16	0.03	0.15
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG11	11	0.16	0.03	0.15
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG12	11	0.16	0.03	0.15
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG13	11	0.16	0.03	0.15
(3,43)	1:105:A:VAL:H	1:85:A:VAL:O	11	0.16	0.05	0.15
(2,148)	1:29:A:ASN:HD22	1:10:A:ASN:HB2	11	0.15	0.04	0.15
(1,1869)	1:83:A:HIS:HE1	1:87:A:LEU:HG	11	0.14	0.03	0.14
(1,1763)	1:86:A:ASN:HA	1:36:A:TRP:HZ3	11	0.14	0.02	0.14
(3,73)	1:12:A:ALA:H	1:9:A:HIS:O	11	0.13	0.02	0.12
(3,70)	1:11:A:GLY:N	1:8:A:ALA:O	11	0.12	0.01	0.11
(1,878)	1:63:A:LYS:HD3	1:61:A:ASP:HB3	10	0.98	0.63	0.96
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD1	10	0.78	0.39	0.86
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD2	10	0.78	0.39	0.86
(1,722)	1:4:A:LYS:HD3	1:4:A:LYS:HE3	10	0.52	0.01	0.52
(1,2420)	1:30:A:PRO:HA	1:34:A:PHE:HB2	10	0.34	0.13	0.36
(1,1415)	1:31:A:THR:HG21	1:36:A:TRP:HD1	10	0.16	0.04	0.16
(1,1415)	1:31:A:THR:HG22	1:36:A:TRP:HD1	10	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1415)	1:31:A:THR:HG23	1:36:A:TRP:HD1	10	0.16	0.04	0.16
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD21	9	1.72	2.0	0.51
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD22	9	1.72	2.0	0.51
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD23	9	1.72	2.0	0.51
(1,480)	1:78:A:LYS:HB2	1:77:A:VAL:HA	9	1.25	0.03	1.25
(2,129)	1:66:A:GLY:H	1:68:A:GLY:HA3	9	0.57	0.37	0.56
(1,1833)	1:69:A:GLY:HA3	1:58:A:PHE:HB2	9	0.46	0.24	0.41
(2,80)	1:56:A:LYS:HD3	1:55:A:ASN:HB2	9	0.39	0.44	0.17
(1,341)	1:78:A:LYS:HB3	1:78:A:LYS:HA	9	0.34	0.06	0.36
(1,1259)	1:4:A:LYS:HB3	1:3:A:HIS:HB3	9	0.32	0.26	0.16
(1,730)	1:7:A:LYS:HA	1:7:A:LYS:HD3	9	0.28	0.38	0.15
(1,2274)	1:54:A:GLU:HB3	1:74:A:HIS:HB3	9	0.27	0.14	0.21
(1,2274)	1:27:A:PRO:HG3	1:29:A:ASN:HB3	9	0.27	0.14	0.21
(1,2301)	1:16:A:VAL:HG11	1:18:A:VAL:HA	9	0.23	0.1	0.21
(1,2301)	1:16:A:VAL:HG12	1:18:A:VAL:HA	9	0.23	0.1	0.21
(1,2301)	1:16:A:VAL:HG13	1:18:A:VAL:HA	9	0.23	0.1	0.21
(1,1853)	1:34:A:PHE:HA	1:90:A:MET:HG2	9	0.22	0.07	0.18
(1,677)	1:26:A:LEU:HG	1:27:A:PRO:HG2	9	0.14	0.05	0.12
(1,1339)	1:87:A:LEU:HG	1:38:A:PHE:H	9	0.13	0.01	0.13
(1,746)	1:70:A:THR:HG21	1:71:A:GLU:H	9	0.13	0.03	0.11
(1,746)	1:70:A:THR:HG22	1:71:A:GLU:H	9	0.13	0.03	0.11
(1,746)	1:70:A:THR:HG23	1:71:A:GLU:H	9	0.13	0.03	0.11
(1,173)	1:43:A:LYS:HB3	1:38:A:PHE:HZ	8	1.01	0.67	1.45
(1,1997)	1:61:A:ASP:H	1:60:A:PRO:HG2	8	0.55	0.4	0.48
(1,1059)	1:78:A:LYS:HD3	1:50:A:MET:HG3	8	0.4	0.21	0.39
(1,2532)	1:5:A:VAL:H	1:23:A:GLU:HB2	8	0.38	0.15	0.4
(1,1955)	1:23:A:GLU:H	1:23:A:GLU:HG3	8	0.38	0.23	0.31
(1,2453)	1:31:A:THR:HG21	1:36:A:TRP:HZ2	8	0.34	0.17	0.28
(1,2453)	1:31:A:THR:HG22	1:36:A:TRP:HZ2	8	0.34	0.17	0.28
(1,2453)	1:31:A:THR:HG23	1:36:A:TRP:HZ2	8	0.34	0.17	0.28
(1,2522)	1:52:A:THR:HG21	1:48:A:GLU:HB3	8	0.33	0.18	0.3
(1,2522)	1:52:A:THR:HG22	1:48:A:GLU:HB3	8	0.33	0.18	0.3
(1,2522)	1:52:A:THR:HG23	1:48:A:GLU:HB3	8	0.33	0.18	0.3
(1,2522)	1:52:A:THR:HG21	1:54:A:GLU:HB2	8	0.33	0.18	0.3
(1,2522)	1:52:A:THR:HG22	1:54:A:GLU:HB2	8	0.33	0.18	0.3
(1,2522)	1:52:A:THR:HG23	1:54:A:GLU:HB2	8	0.33	0.18	0.3
(1,852)	1:14:A:LEU:HD11	1:14:A:LEU:H	8	0.33	0.14	0.3
(1,852)	1:14:A:LEU:HD12	1:14:A:LEU:H	8	0.33	0.14	0.3
(1,852)	1:14:A:LEU:HD13	1:14:A:LEU:H	8	0.33	0.14	0.3
(1,1588)	1:70:A:THR:HB	1:58:A:PHE:HB2	8	0.31	0.3	0.15
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG21	8	0.3	0.29	0.18
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG22	8	0.3	0.29	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG23	8	0.3	0.29	0.18
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG21	8	0.3	0.29	0.18
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG22	8	0.3	0.29	0.18
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG23	8	0.3	0.29	0.18
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG21	8	0.3	0.29	0.18
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG22	8	0.3	0.29	0.18
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG23	8	0.3	0.29	0.18
(1,912)	1:91:A:ARG:HB3	1:91:A:ARG:HD3	8	0.26	0.02	0.26
(1,809)	1:65:A:LEU:HA	1:66:A:GLY:H	8	0.2	0.01	0.2
(1,2360)	1:106:A:TYR:HD1	1:106:A:TYR:H	8	0.2	0.04	0.22
(1,2360)	1:106:A:TYR:HD2	1:106:A:TYR:H	8	0.2	0.04	0.22
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD1	8	0.2	0.06	0.17
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD2	8	0.2	0.06	0.17
(1,488)	1:75:A:VAL:HG11	1:45:A:SER:HA	8	0.18	0.06	0.17
(1,488)	1:75:A:VAL:HG12	1:45:A:SER:HA	8	0.18	0.06	0.17
(1,488)	1:75:A:VAL:HG13	1:45:A:SER:HA	8	0.18	0.06	0.17
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG21	8	0.15	0.05	0.14
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG22	8	0.15	0.05	0.14
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG23	8	0.15	0.05	0.14
(2,41)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	8	0.15	0.05	0.13
(1,2320)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	8	0.15	0.05	0.13
(1,2320)	1:38:A:PHE:HB3	1:40:A:GLY:HA2	8	0.15	0.05	0.13
(1,350)	1:7:A:LYS:HD3	1:28:A:SER:HA	8	0.14	0.02	0.14
(1,303)	1:36:A:TRP:HB2	1:26:A:LEU:HA	8	0.14	0.03	0.12
(1,368)	1:30:A:PRO:HG3	1:69:A:GLY:HA2	7	0.83	0.4	0.84
(1,734)	1:108:A:LYS:HG3	1:109:A:ALA:H	7	0.42	0.12	0.41
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD1	7	0.29	0.12	0.36
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD2	7	0.29	0.12	0.36
(2,140)	1:52:A:THR:H	1:50:A:MET:HG3	6	1.76	0.02	1.76
(1,1554)	1:44:A:GLU:HG3	1:43:A:LYS:HA	6	0.77	0.05	0.78
(1,1654)	1:42:A:THR:HA	1:43:A:LYS:HD3	6	0.77	0.25	0.83
(1,1559)	1:101:A:GLU:HG3	1:36:A:TRP:HH2	6	0.72	0.23	0.64
(1,2335)	1:53:A:VAL:HG11	1:54:A:GLU:HG3	6	0.56	0.29	0.5
(1,2335)	1:53:A:VAL:HG12	1:54:A:GLU:HG3	6	0.56	0.29	0.5
(1,2335)	1:53:A:VAL:HG13	1:54:A:GLU:HG3	6	0.56	0.29	0.5
(1,2335)	1:78:A:LYS:HG3	1:50:A:MET:HG2	6	0.56	0.29	0.5
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD1	6	0.47	0.19	0.5
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD2	6	0.47	0.19	0.5
(1,401)	1:64:A:LEU:HD21	1:64:A:LEU:HA	6	0.46	0.01	0.46
(1,401)	1:64:A:LEU:HD22	1:64:A:LEU:HA	6	0.46	0.01	0.46
(1,401)	1:64:A:LEU:HD23	1:64:A:LEU:HA	6	0.46	0.01	0.46
(1,1854)	1:50:A:MET:HG3	1:77:A:VAL:HA	6	0.46	0.16	0.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2193)	1:77:A:VAL:HG11	1:83:A:HIS:HE1	6	0.34	0.08	0.36
(1,2193)	1:77:A:VAL:HG12	1:83:A:HIS:HE1	6	0.34	0.08	0.36
(1,2193)	1:77:A:VAL:HG13	1:83:A:HIS:HE1	6	0.34	0.08	0.36
(1,2452)	1:18:A:VAL:HG11	1:110:A:ASN:HD22	6	0.33	0.1	0.35
(1,2452)	1:18:A:VAL:HG12	1:110:A:ASN:HD22	6	0.33	0.1	0.35
(1,2452)	1:18:A:VAL:HG13	1:110:A:ASN:HD22	6	0.33	0.1	0.35
(1,2452)	1:105:A:VAL:HG11	1:106:A:TYR:HD1	6	0.33	0.1	0.35
(1,2452)	1:105:A:VAL:HG11	1:106:A:TYR:HD2	6	0.33	0.1	0.35
(1,2452)	1:105:A:VAL:HG12	1:106:A:TYR:HD1	6	0.33	0.1	0.35
(1,2452)	1:105:A:VAL:HG12	1:106:A:TYR:HD2	6	0.33	0.1	0.35
(1,2452)	1:105:A:VAL:HG13	1:106:A:TYR:HD1	6	0.33	0.1	0.35
(1,2452)	1:105:A:VAL:HG13	1:106:A:TYR:HD2	6	0.33	0.1	0.35
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD1	6	0.23	0.08	0.26
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD2	6	0.23	0.08	0.26
(1,1615)	1:60:A:PRO:HA	1:66:A:GLY:HA3	6	0.21	0.06	0.21
(1,604)	1:25:A:GLN:HB2	1:73:A:PHE:HB2	6	0.13	0.02	0.13
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG21	6	0.12	0.02	0.12
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG22	6	0.12	0.02	0.12
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG23	6	0.12	0.02	0.12
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG21	6	0.12	0.02	0.12
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG22	6	0.12	0.02	0.12
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG23	6	0.12	0.02	0.12
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG21	6	0.12	0.02	0.12
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG22	6	0.12	0.02	0.12
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG23	6	0.12	0.02	0.12
(1,1834)	1:24:A:ILE:HD11	1:106:A:TYR:H	6	0.12	0.01	0.12
(1,1834)	1:24:A:ILE:HD12	1:106:A:TYR:H	6	0.12	0.01	0.12
(1,1834)	1:24:A:ILE:HD13	1:106:A:TYR:H	6	0.12	0.01	0.12
(1,1722)	1:64:A:LEU:HB3	1:66:A:GLY:HA2	5	0.87	0.57	1.15
(1,1088)	1:63:A:LYS:HD3	1:65:A:LEU:H	5	0.74	0.13	0.74
(1,721)	1:64:A:LEU:HB3	1:65:A:LEU:H	5	0.73	0.32	0.82
(1,1730)	1:56:A:LYS:HD3	1:74:A:HIS:HA	5	0.63	0.63	0.19
(1,1563)	1:26:A:LEU:HD11	1:10:A:ASN:HA	5	0.55	0.37	0.76
(1,1563)	1:26:A:LEU:HD12	1:10:A:ASN:HA	5	0.55	0.37	0.76
(1,1563)	1:26:A:LEU:HD13	1:10:A:ASN:HA	5	0.55	0.37	0.76
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB1	5	0.53	0.58	0.17
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB2	5	0.53	0.58	0.17
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB3	5	0.53	0.58	0.17
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB1	5	0.53	0.58	0.17
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB2	5	0.53	0.58	0.17
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB3	5	0.53	0.58	0.17
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB1	5	0.53	0.58	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB2	5	0.53	0.58	0.17
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB3	5	0.53	0.58	0.17
(1,2486)	1:16:A:VAL:HB	1:110:A:ASN:HD21	5	0.42	0.17	0.38
(1,2486)	1:85:A:VAL:HB	1:38:A:PHE:HD1	5	0.42	0.17	0.38
(1,2486)	1:85:A:VAL:HB	1:38:A:PHE:HD2	5	0.42	0.17	0.38
(1,1433)	1:46:A:PRO:HB3	1:48:A:GLU:H	5	0.42	0.21	0.46
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB1	5	0.39	0.43	0.15
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB2	5	0.39	0.43	0.15
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB3	5	0.39	0.43	0.15
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB1	5	0.39	0.43	0.15
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB2	5	0.39	0.43	0.15
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB3	5	0.39	0.43	0.15
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB1	5	0.39	0.43	0.15
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB2	5	0.39	0.43	0.15
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB3	5	0.39	0.43	0.15
(1,1011)	1:63:A:LYS:HD3	1:63:A:LYS:H	5	0.33	0.18	0.3
(1,2523)	1:36:A:TRP:HB3	1:36:A:TRP:HZ2	5	0.3	0.01	0.3
(2,101)	1:47:A:ASN:HB3	1:48:A:GLU:HB3	5	0.29	0.17	0.22
(1,841)	1:43:A:LYS:HG3	1:38:A:PHE:HD1	5	0.27	0.09	0.29
(1,841)	1:43:A:LYS:HG3	1:38:A:PHE:HD2	5	0.27	0.09	0.29
(2,114)	1:90:A:MET:HE1	1:37:A:TYR:HA	5	0.26	0.03	0.27
(2,114)	1:90:A:MET:HE2	1:37:A:TYR:HA	5	0.26	0.03	0.27
(2,114)	1:90:A:MET:HE3	1:37:A:TYR:HA	5	0.26	0.03	0.27
(1,2283)	1:65:A:LEU:HG	1:28:A:SER:HB2	5	0.23	0.1	0.23
(1,2283)	1:65:A:LEU:HG	1:30:A:PRO:HD3	5	0.23	0.1	0.23
(1,1630)	1:60:A:PRO:HA	1:66:A:GLY:HA2	5	0.23	0.07	0.26
(1,1314)	1:60:A:PRO:HB2	1:62:A:SER:H	5	0.17	0.05	0.17
(1,2379)	1:38:A:PHE:HB3	1:38:A:PHE:H	5	0.17	0.03	0.15
(1,2357)	1:85:A:VAL:HB	1:85:A:VAL:H	5	0.15	0.04	0.16
(1,1303)	1:104:A:THR:HG21	1:11:A:GLY:H	5	0.13	0.03	0.12
(1,1303)	1:104:A:THR:HG22	1:11:A:GLY:H	5	0.13	0.03	0.12
(1,1303)	1:104:A:THR:HG23	1:11:A:GLY:H	5	0.13	0.03	0.12
(3,59)	1:90:A:MET:H	1:35:A:ALA:O	5	0.13	0.01	0.13
(1,1747)	1:87:A:LEU:HD21	1:104:A:THR:HA	5	0.12	0.01	0.12
(1,1747)	1:87:A:LEU:HD22	1:104:A:THR:HA	5	0.12	0.01	0.12
(1,1747)	1:87:A:LEU:HD23	1:104:A:THR:HA	5	0.12	0.01	0.12
(1,1525)	1:26:A:LEU:HD11	1:7:A:LYS:HD3	4	1.46	0.55	1.76
(1,1525)	1:26:A:LEU:HD12	1:7:A:LYS:HD3	4	1.46	0.55	1.76
(1,1525)	1:26:A:LEU:HD13	1:7:A:LYS:HD3	4	1.46	0.55	1.76
(1,2177)	1:34:A:PHE:HB3	1:37:A:TYR:HE1	4	1.3	0.59	1.54
(1,2177)	1:34:A:PHE:HB3	1:37:A:TYR:HE2	4	1.3	0.59	1.54
(1,2177)	1:54:A:GLU:HG3	1:74:A:HIS:HD2	4	1.3	0.59	1.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,269)	1:26:A:LEU:HD21	1:57:A:TYR:HD1	4	1.22	0.66	1.48
(1,269)	1:26:A:LEU:HD21	1:57:A:TYR:HD2	4	1.22	0.66	1.48
(1,269)	1:26:A:LEU:HD22	1:57:A:TYR:HD1	4	1.22	0.66	1.48
(1,269)	1:26:A:LEU:HD22	1:57:A:TYR:HD2	4	1.22	0.66	1.48
(1,269)	1:26:A:LEU:HD23	1:57:A:TYR:HD1	4	1.22	0.66	1.48
(1,269)	1:26:A:LEU:HD23	1:57:A:TYR:HD2	4	1.22	0.66	1.48
(1,223)	1:4:A:LYS:HG3	1:3:A:HIS:HE1	4	0.74	0.39	0.86
(1,1702)	1:64:A:LEU:HD11	1:61:A:ASP:HB3	4	0.72	0.23	0.64
(1,1702)	1:64:A:LEU:HD12	1:61:A:ASP:HB3	4	0.72	0.23	0.64
(1,1702)	1:64:A:LEU:HD13	1:61:A:ASP:HB3	4	0.72	0.23	0.64
(1,1238)	1:53:A:VAL:HG11	1:52:A:THR:H	4	0.66	0.17	0.74
(1,1238)	1:53:A:VAL:HG12	1:52:A:THR:H	4	0.66	0.17	0.74
(1,1238)	1:53:A:VAL:HG13	1:52:A:THR:H	4	0.66	0.17	0.74
(1,570)	1:30:A:PRO:HD2	1:28:A:SER:HB2	4	0.6	0.2	0.65
(1,1540)	1:18:A:VAL:HG11	1:3:A:HIS:HB2	4	0.55	0.34	0.57
(1,1540)	1:18:A:VAL:HG12	1:3:A:HIS:HB2	4	0.55	0.34	0.57
(1,1540)	1:18:A:VAL:HG13	1:3:A:HIS:HB2	4	0.55	0.34	0.57
(1,472)	1:65:A:LEU:HG	1:28:A:SER:HB3	4	0.48	0.57	0.16
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD21	4	0.43	0.18	0.48
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD22	4	0.43	0.18	0.48
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD23	4	0.43	0.18	0.48
(1,1673)	1:42:A:THR:HB	1:39:A:GLU:HG3	4	0.35	0.17	0.35
(1,1847)	1:55:A:ASN:HA	1:56:A:LYS:HG3	4	0.34	0.11	0.36
(1,1357)	1:25:A:GLN:HE22	1:71:A:GLU:H	4	0.34	0.08	0.35
(1,512)	1:100:A:SER:HB3	1:89:A:TYR:HD1	4	0.32	0.13	0.32
(1,512)	1:100:A:SER:HB3	1:89:A:TYR:HD2	4	0.32	0.13	0.32
(2,75)	1:107:A:LEU:HB3	1:83:A:HIS:HB2	4	0.3	0.13	0.28
(1,1947)	1:64:A:LEU:H	1:64:A:LEU:HB3	4	0.28	0.02	0.3
(1,1858)	1:80:A:ALA:HA	1:110:A:ASN:HB3	4	0.28	0.11	0.26
(1,1225)	1:101:A:GLU:HG3	1:10:A:ASN:HD22	4	0.24	0.06	0.24
(2,103)	1:48:A:GLU:HA	1:50:A:MET:HA	4	0.2	0.08	0.2
(1,2293)	1:31:A:THR:HG21	1:29:A:ASN:HB3	4	0.16	0.03	0.16
(1,2293)	1:31:A:THR:HG22	1:29:A:ASN:HB3	4	0.16	0.03	0.16
(1,2293)	1:31:A:THR:HG23	1:29:A:ASN:HB3	4	0.16	0.03	0.16
(1,2293)	1:21:A:LEU:HG	1:74:A:HIS:HB3	4	0.16	0.03	0.16
(1,1668)	1:78:A:LYS:HB2	1:78:A:LYS:HE3	4	0.14	0.03	0.13
(1,1209)	1:42:A:THR:HG21	1:44:A:GLU:H	4	0.13	0.03	0.12
(1,1209)	1:42:A:THR:HG22	1:44:A:GLU:H	4	0.13	0.03	0.12
(1,1209)	1:42:A:THR:HG23	1:44:A:GLU:H	4	0.13	0.03	0.12
(1,752)	1:22:A:VAL:HG21	1:23:A:GLU:H	4	0.13	0.04	0.11
(1,752)	1:22:A:VAL:HG22	1:23:A:GLU:H	4	0.13	0.04	0.11
(1,752)	1:22:A:VAL:HG23	1:23:A:GLU:H	4	0.13	0.04	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1029)	1:6:A:THR:HG21	1:27:A:PRO:HG3	4	0.13	0.01	0.12
(1,1029)	1:6:A:THR:HG22	1:27:A:PRO:HG3	4	0.13	0.01	0.12
(1,1029)	1:6:A:THR:HG23	1:27:A:PRO:HG3	4	0.13	0.01	0.12
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB1	4	0.13	0.02	0.12
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB2	4	0.13	0.02	0.12
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB3	4	0.13	0.02	0.12
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG21	4	0.12	0.02	0.12
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG22	4	0.12	0.02	0.12
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG23	4	0.12	0.02	0.12
(2,82)	1:5:A:VAL:HG11	1:106:A:TYR:H	4	0.12	0.02	0.12
(2,82)	1:5:A:VAL:HG12	1:106:A:TYR:H	4	0.12	0.02	0.12
(2,82)	1:5:A:VAL:HG13	1:106:A:TYR:H	4	0.12	0.02	0.12
(1,2023)	1:19:A:GLY:H	1:22:A:VAL:HB	4	0.12	0.01	0.12
(1,1886)	1:38:A:PHE:HZ	1:85:A:VAL:HB	4	0.12	0.01	0.12
(1,720)	1:25:A:GLN:HG2	1:26:A:LEU:H	4	0.12	0.01	0.12
(1,1784)	1:42:A:THR:HA	1:38:A:PHE:HB3	4	0.11	0.01	0.11
(1,1547)	1:26:A:LEU:HD21	1:73:A:PHE:HD1	3	2.51	0.03	2.52
(1,1547)	1:26:A:LEU:HD21	1:73:A:PHE:HD2	3	2.51	0.03	2.52
(1,1547)	1:26:A:LEU:HD22	1:73:A:PHE:HD1	3	2.51	0.03	2.52
(1,1547)	1:26:A:LEU:HD22	1:73:A:PHE:HD2	3	2.51	0.03	2.52
(1,1547)	1:26:A:LEU:HD23	1:73:A:PHE:HD1	3	2.51	0.03	2.52
(1,1547)	1:26:A:LEU:HD23	1:73:A:PHE:HD2	3	2.51	0.03	2.52
(1,2058)	1:81:A:GLY:H	1:18:A:VAL:HG11	3	2.16	0.07	2.18
(1,2058)	1:81:A:GLY:H	1:18:A:VAL:HG12	3	2.16	0.07	2.18
(1,2058)	1:81:A:GLY:H	1:18:A:VAL:HG13	3	2.16	0.07	2.18
(2,98)	1:80:A:ALA:HA	1:18:A:VAL:HG11	3	2.0	0.09	2.04
(2,98)	1:80:A:ALA:HA	1:18:A:VAL:HG12	3	2.0	0.09	2.04
(2,98)	1:80:A:ALA:HA	1:18:A:VAL:HG13	3	2.0	0.09	2.04
(1,65)	1:26:A:LEU:HD11	1:7:A:LYS:HB2	3	1.85	0.02	1.87
(1,65)	1:26:A:LEU:HD12	1:7:A:LYS:HB2	3	1.85	0.02	1.87
(1,65)	1:26:A:LEU:HD13	1:7:A:LYS:HB2	3	1.85	0.02	1.87
(1,769)	1:26:A:LEU:HD11	1:36:A:TRP:HZ2	3	1.44	0.02	1.44
(1,769)	1:26:A:LEU:HD12	1:36:A:TRP:HZ2	3	1.44	0.02	1.44
(1,769)	1:26:A:LEU:HD13	1:36:A:TRP:HZ2	3	1.44	0.02	1.44
(1,897)	1:45:A:SER:HB3	1:53:A:VAL:HG11	3	1.36	0.19	1.4
(1,897)	1:45:A:SER:HB3	1:53:A:VAL:HG12	3	1.36	0.19	1.4
(1,897)	1:45:A:SER:HB3	1:53:A:VAL:HG13	3	1.36	0.19	1.4
(1,1865)	1:24:A:ILE:HG21	1:26:A:LEU:HD21	3	1.03	0.08	1.06
(1,1865)	1:24:A:ILE:HG21	1:26:A:LEU:HD22	3	1.03	0.08	1.06
(1,1865)	1:24:A:ILE:HG21	1:26:A:LEU:HD23	3	1.03	0.08	1.06
(1,1865)	1:24:A:ILE:HG22	1:26:A:LEU:HD21	3	1.03	0.08	1.06
(1,1865)	1:24:A:ILE:HG22	1:26:A:LEU:HD22	3	1.03	0.08	1.06

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1865)	1:24:A:ILE:HG22	1:26:A:LEU:HD23	3	1.03	0.08	1.06
(1,1865)	1:24:A:ILE:HG23	1:26:A:LEU:HD21	3	1.03	0.08	1.06
(1,1865)	1:24:A:ILE:HG23	1:26:A:LEU:HD22	3	1.03	0.08	1.06
(1,1865)	1:24:A:ILE:HG23	1:26:A:LEU:HD23	3	1.03	0.08	1.06
(1,1626)	1:7:A:LYS:HA	1:26:A:LEU:HD11	3	1.0	0.02	1.01
(1,1626)	1:7:A:LYS:HA	1:26:A:LEU:HD12	3	1.0	0.02	1.01
(1,1626)	1:7:A:LYS:HA	1:26:A:LEU:HD13	3	1.0	0.02	1.01
(1,1018)	1:27:A:PRO:HD2	1:26:A:LEU:HD11	3	0.98	0.04	0.96
(1,1018)	1:27:A:PRO:HD2	1:26:A:LEU:HD12	3	0.98	0.04	0.96
(1,1018)	1:27:A:PRO:HD2	1:26:A:LEU:HD13	3	0.98	0.04	0.96
(1,1071)	1:26:A:LEU:HD11	1:7:A:LYS:HG3	3	0.97	0.03	0.95
(1,1071)	1:26:A:LEU:HD12	1:7:A:LYS:HG3	3	0.97	0.03	0.95
(1,1071)	1:26:A:LEU:HD13	1:7:A:LYS:HG3	3	0.97	0.03	0.95
(1,1202)	1:26:A:LEU:HD11	1:7:A:LYS:HB3	3	0.9	0.02	0.91
(1,1202)	1:26:A:LEU:HD12	1:7:A:LYS:HB3	3	0.9	0.02	0.91
(1,1202)	1:26:A:LEU:HD13	1:7:A:LYS:HB3	3	0.9	0.02	0.91
(1,1534)	1:26:A:LEU:HD11	1:26:A:LEU:HA	3	0.89	0.01	0.89
(1,1534)	1:26:A:LEU:HD12	1:26:A:LEU:HA	3	0.89	0.01	0.89
(1,1534)	1:26:A:LEU:HD13	1:26:A:LEU:HA	3	0.89	0.01	0.89
(1,1536)	1:87:A:LEU:HD11	1:26:A:LEU:HD21	3	0.83	0.02	0.83
(1,1536)	1:87:A:LEU:HD11	1:26:A:LEU:HD22	3	0.83	0.02	0.83
(1,1536)	1:87:A:LEU:HD11	1:26:A:LEU:HD23	3	0.83	0.02	0.83
(1,1536)	1:87:A:LEU:HD12	1:26:A:LEU:HD21	3	0.83	0.02	0.83
(1,1536)	1:87:A:LEU:HD12	1:26:A:LEU:HD22	3	0.83	0.02	0.83
(1,1536)	1:87:A:LEU:HD12	1:26:A:LEU:HD23	3	0.83	0.02	0.83
(1,1536)	1:87:A:LEU:HD13	1:26:A:LEU:HD21	3	0.83	0.02	0.83
(1,1536)	1:87:A:LEU:HD13	1:26:A:LEU:HD22	3	0.83	0.02	0.83
(1,1536)	1:87:A:LEU:HD13	1:26:A:LEU:HD23	3	0.83	0.02	0.83
(1,628)	1:65:A:LEU:HG	1:60:A:PRO:HB3	3	0.73	0.4	0.77
(1,628)	1:65:A:LEU:HB3	1:60:A:PRO:HB3	3	0.73	0.4	0.77
(1,2039)	1:45:A:SER:H	1:53:A:VAL:HG11	3	0.63	0.11	0.69
(1,2039)	1:45:A:SER:H	1:53:A:VAL:HG12	3	0.63	0.11	0.69
(1,2039)	1:45:A:SER:H	1:53:A:VAL:HG13	3	0.63	0.11	0.69
(1,1046)	1:109:A:ALA:HA	1:18:A:VAL:HG11	3	0.62	0.06	0.59
(1,1046)	1:109:A:ALA:HA	1:18:A:VAL:HG12	3	0.62	0.06	0.59
(1,1046)	1:109:A:ALA:HA	1:18:A:VAL:HG13	3	0.62	0.06	0.59
(1,1494)	1:26:A:LEU:HD21	1:26:A:LEU:HB2	3	0.6	0.01	0.6
(1,1494)	1:26:A:LEU:HD22	1:26:A:LEU:HB2	3	0.6	0.01	0.6
(1,1494)	1:26:A:LEU:HD23	1:26:A:LEU:HB2	3	0.6	0.01	0.6
(1,1027)	1:27:A:PRO:HD3	1:26:A:LEU:HD11	3	0.6	0.01	0.6
(1,1027)	1:27:A:PRO:HD3	1:26:A:LEU:HD12	3	0.6	0.01	0.6
(1,1027)	1:27:A:PRO:HD3	1:26:A:LEU:HD13	3	0.6	0.01	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1801)	1:27:A:PRO:HG3	1:26:A:LEU:HD11	3	0.58	0.03	0.57
(1,1801)	1:27:A:PRO:HG3	1:26:A:LEU:HD12	3	0.58	0.03	0.57
(1,1801)	1:27:A:PRO:HG3	1:26:A:LEU:HD13	3	0.58	0.03	0.57
(1,2442)	1:42:A:THR:HB	1:44:A:GLU:H	3	0.56	0.15	0.47
(1,2442)	1:47:A:ASN:HA	1:49:A:SER:H	3	0.56	0.15	0.47
(1,1734)	1:26:A:LEU:HD11	1:6:A:THR:HG21	3	0.55	0.02	0.55
(1,1734)	1:26:A:LEU:HD11	1:6:A:THR:HG22	3	0.55	0.02	0.55
(1,1734)	1:26:A:LEU:HD11	1:6:A:THR:HG23	3	0.55	0.02	0.55
(1,1734)	1:26:A:LEU:HD12	1:6:A:THR:HG21	3	0.55	0.02	0.55
(1,1734)	1:26:A:LEU:HD12	1:6:A:THR:HG22	3	0.55	0.02	0.55
(1,1734)	1:26:A:LEU:HD12	1:6:A:THR:HG23	3	0.55	0.02	0.55
(1,1734)	1:26:A:LEU:HD13	1:6:A:THR:HG21	3	0.55	0.02	0.55
(1,1734)	1:26:A:LEU:HD13	1:6:A:THR:HG22	3	0.55	0.02	0.55
(1,1734)	1:26:A:LEU:HD13	1:6:A:THR:HG23	3	0.55	0.02	0.55
(2,113)	1:91:A:ARG:HG3	1:92:A:PRO:HG2	3	0.54	0.14	0.45
(1,1034)	1:108:A:LYS:HB2	1:110:A:ASN:HD22	3	0.52	0.08	0.51
(1,822)	1:18:A:VAL:HG11	1:18:A:VAL:H	3	0.5	0.03	0.48
(1,822)	1:18:A:VAL:HG12	1:18:A:VAL:H	3	0.5	0.03	0.48
(1,822)	1:18:A:VAL:HG13	1:18:A:VAL:H	3	0.5	0.03	0.48
(1,597)	1:78:A:LYS:HD3	1:78:A:LYS:HE3	3	0.5	0.03	0.52
(1,1318)	1:26:A:LEU:HD11	1:25:A:GLN:HE22	3	0.46	0.04	0.44
(1,1318)	1:26:A:LEU:HD12	1:25:A:GLN:HE22	3	0.46	0.04	0.44
(1,1318)	1:26:A:LEU:HD13	1:25:A:GLN:HE22	3	0.46	0.04	0.44
(1,2340)	1:65:A:LEU:HD11	1:60:A:PRO:HG3	3	0.46	0.06	0.46
(1,2340)	1:65:A:LEU:HD12	1:60:A:PRO:HG3	3	0.46	0.06	0.46
(1,2340)	1:65:A:LEU:HD13	1:60:A:PRO:HG3	3	0.46	0.06	0.46
(1,2340)	1:75:A:VAL:HG11	1:22:A:VAL:HB	3	0.46	0.06	0.46
(1,2340)	1:75:A:VAL:HG12	1:22:A:VAL:HB	3	0.46	0.06	0.46
(1,2340)	1:75:A:VAL:HG13	1:22:A:VAL:HB	3	0.46	0.06	0.46
(1,1704)	1:26:A:LEU:HD11	1:6:A:THR:HA	3	0.44	0.08	0.48
(1,1704)	1:26:A:LEU:HD12	1:6:A:THR:HA	3	0.44	0.08	0.48
(1,1704)	1:26:A:LEU:HD13	1:6:A:THR:HA	3	0.44	0.08	0.48
(1,1970)	1:19:A:GLY:H	1:18:A:VAL:HG11	3	0.43	0.18	0.56
(1,1970)	1:19:A:GLY:H	1:18:A:VAL:HG12	3	0.43	0.18	0.56
(1,1970)	1:19:A:GLY:H	1:18:A:VAL:HG13	3	0.43	0.18	0.56
(1,1550)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	3	0.42	0.06	0.46
(1,658)	1:94:A:THR:HG21	1:90:A:MET:HB2	3	0.37	0.14	0.39
(1,658)	1:94:A:THR:HG22	1:90:A:MET:HB2	3	0.37	0.14	0.39
(1,658)	1:94:A:THR:HG23	1:90:A:MET:HB2	3	0.37	0.14	0.39
(1,2387)	1:96:A:PRO:HG3	1:95:A:GLY:HA2	3	0.37	0.05	0.37
(1,2387)	1:60:A:PRO:HB2	1:66:A:GLY:HA2	3	0.37	0.05	0.37
(1,1892)	1:38:A:PHE:HE1	1:53:A:VAL:HG11	3	0.35	0.32	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1892)	1:38:A:PHE:HE1	1:53:A:VAL:HG12	3	0.35	0.32	0.15
(1,1892)	1:38:A:PHE:HE1	1:53:A:VAL:HG13	3	0.35	0.32	0.15
(1,1892)	1:38:A:PHE:HE2	1:53:A:VAL:HG11	3	0.35	0.32	0.15
(1,1892)	1:38:A:PHE:HE2	1:53:A:VAL:HG12	3	0.35	0.32	0.15
(1,1892)	1:38:A:PHE:HE2	1:53:A:VAL:HG13	3	0.35	0.32	0.15
(1,1252)	1:26:A:LEU:HD11	1:7:A:LYS:H	3	0.34	0.03	0.35
(1,1252)	1:26:A:LEU:HD12	1:7:A:LYS:H	3	0.34	0.03	0.35
(1,1252)	1:26:A:LEU:HD13	1:7:A:LYS:H	3	0.34	0.03	0.35
(1,471)	1:92:A:PRO:HG2	1:33:A:GLY:HA2	3	0.33	0.16	0.25
(1,1624)	1:45:A:SER:HA	1:53:A:VAL:HG11	3	0.32	0.07	0.31
(1,1624)	1:45:A:SER:HA	1:53:A:VAL:HG12	3	0.32	0.07	0.31
(1,1624)	1:45:A:SER:HA	1:53:A:VAL:HG13	3	0.32	0.07	0.31
(1,608)	1:88:A:THR:HG21	1:90:A:MET:HG3	3	0.3	0.12	0.36
(1,608)	1:88:A:THR:HG22	1:90:A:MET:HG3	3	0.3	0.12	0.36
(1,608)	1:88:A:THR:HG23	1:90:A:MET:HG3	3	0.3	0.12	0.36
(1,1774)	1:24:A:ILE:HD11	1:26:A:LEU:HD21	3	0.3	0.07	0.32
(1,1774)	1:24:A:ILE:HD11	1:26:A:LEU:HD22	3	0.3	0.07	0.32
(1,1774)	1:24:A:ILE:HD11	1:26:A:LEU:HD23	3	0.3	0.07	0.32
(1,1774)	1:24:A:ILE:HD12	1:26:A:LEU:HD21	3	0.3	0.07	0.32
(1,1774)	1:24:A:ILE:HD12	1:26:A:LEU:HD22	3	0.3	0.07	0.32
(1,1774)	1:24:A:ILE:HD12	1:26:A:LEU:HD23	3	0.3	0.07	0.32
(1,1774)	1:24:A:ILE:HD13	1:26:A:LEU:HD21	3	0.3	0.07	0.32
(1,1774)	1:24:A:ILE:HD13	1:26:A:LEU:HD22	3	0.3	0.07	0.32
(1,1774)	1:24:A:ILE:HD13	1:26:A:LEU:HD23	3	0.3	0.07	0.32
(1,842)	1:49:A:SER:HB3	1:49:A:SER:H	3	0.29	0.07	0.29
(1,1428)	1:56:A:LYS:HD3	1:57:A:TYR:HD1	3	0.27	0.21	0.12
(1,1428)	1:56:A:LYS:HD3	1:57:A:TYR:HD2	3	0.27	0.21	0.12
(1,504)	1:91:A:ARG:HB2	1:96:A:PRO:HB2	3	0.23	0.02	0.22
(1,1517)	1:4:A:LYS:HB3	1:4:A:LYS:HA	3	0.22	0.0	0.22
(1,1221)	1:55:A:ASN:HD22	1:56:A:LYS:H	3	0.2	0.05	0.21
(1,2018)	1:67:A:ALA:H	1:65:A:LEU:HA	3	0.2	0.04	0.18
(1,2044)	1:70:A:THR:H	1:72:A:HIS:HD2	3	0.17	0.08	0.12
(2,152)	1:69:A:GLY:H	1:29:A:ASN:HA	3	0.16	0.03	0.15
(1,528)	1:70:A:THR:HB	1:58:A:PHE:HA	3	0.16	0.08	0.1
(1,61)	1:26:A:LEU:HD11	1:25:A:GLN:HB3	3	0.15	0.01	0.15
(1,61)	1:26:A:LEU:HD12	1:25:A:GLN:HB3	3	0.15	0.01	0.15
(1,61)	1:26:A:LEU:HD13	1:25:A:GLN:HB3	3	0.15	0.01	0.15
(1,745)	1:37:A:TYR:HB2	1:37:A:TYR:HD1	3	0.15	0.01	0.15
(1,745)	1:37:A:TYR:HB2	1:37:A:TYR:HD2	3	0.15	0.01	0.15
(1,1308)	1:87:A:LEU:HB2	1:89:A:TYR:H	3	0.15	0.04	0.12
(1,2072)	1:29:A:ASN:HD22	1:31:A:THR:HG21	3	0.14	0.02	0.14
(1,2072)	1:29:A:ASN:HD22	1:31:A:THR:HG22	3	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2072)	1:29:A:ASN:HD22	1:31:A:THR:HG23	3	0.14	0.02	0.14
(1,1785)	1:27:A:PRO:HG2	1:26:A:LEU:HD11	3	0.14	0.04	0.11
(1,1785)	1:27:A:PRO:HG2	1:26:A:LEU:HD12	3	0.14	0.04	0.11
(1,1785)	1:27:A:PRO:HG2	1:26:A:LEU:HD13	3	0.14	0.04	0.11
(1,294)	1:51:A:PHE:HB3	1:78:A:LYS:HA	3	0.14	0.01	0.13
(1,1613)	1:29:A:ASN:HB3	1:31:A:THR:HG21	3	0.14	0.05	0.1
(1,1613)	1:29:A:ASN:HB3	1:31:A:THR:HG22	3	0.14	0.05	0.1
(1,1613)	1:29:A:ASN:HB3	1:31:A:THR:HG23	3	0.14	0.05	0.1
(1,172)	1:27:A:PRO:HG3	1:36:A:TRP:HZ2	3	0.13	0.02	0.12
(1,694)	1:76:A:THR:HA	1:22:A:VAL:H	3	0.13	0.01	0.14
(1,668)	1:105:A:VAL:HG21	1:12:A:ALA:HB1	3	0.13	0.01	0.13
(1,668)	1:105:A:VAL:HG21	1:12:A:ALA:HB2	3	0.13	0.01	0.13
(1,668)	1:105:A:VAL:HG21	1:12:A:ALA:HB3	3	0.13	0.01	0.13
(1,668)	1:105:A:VAL:HG22	1:12:A:ALA:HB1	3	0.13	0.01	0.13
(1,668)	1:105:A:VAL:HG22	1:12:A:ALA:HB2	3	0.13	0.01	0.13
(1,668)	1:105:A:VAL:HG22	1:12:A:ALA:HB3	3	0.13	0.01	0.13
(1,668)	1:105:A:VAL:HG23	1:12:A:ALA:HB1	3	0.13	0.01	0.13
(1,668)	1:105:A:VAL:HG23	1:12:A:ALA:HB2	3	0.13	0.01	0.13
(1,668)	1:105:A:VAL:HG23	1:12:A:ALA:HB3	3	0.13	0.01	0.13
(1,2263)	1:24:A:ILE:HD11	1:106:A:TYR:HA	3	0.13	0.01	0.13
(1,2263)	1:24:A:ILE:HD12	1:106:A:TYR:HA	3	0.13	0.01	0.13
(1,2263)	1:24:A:ILE:HD13	1:106:A:TYR:HA	3	0.13	0.01	0.13
(1,119)	1:102:A:ARG:HA	1:36:A:TRP:HZ3	3	0.12	0.0	0.12
(1,886)	1:6:A:THR:HG21	1:25:A:GLN:H	3	0.12	0.01	0.12
(1,886)	1:6:A:THR:HG22	1:25:A:GLN:H	3	0.12	0.01	0.12
(1,886)	1:6:A:THR:HG23	1:25:A:GLN:H	3	0.12	0.01	0.12
(1,1426)	1:6:A:THR:HG21	1:72:A:HIS:HE1	3	0.12	0.02	0.11
(1,1426)	1:6:A:THR:HG22	1:72:A:HIS:HE1	3	0.12	0.02	0.11
(1,1426)	1:6:A:THR:HG23	1:72:A:HIS:HE1	3	0.12	0.02	0.11
(1,175)	1:27:A:PRO:HG2	1:36:A:TRP:HD1	3	0.12	0.0	0.12
(1,306)	1:47:A:ASN:HB3	1:47:A:ASN:HA	3	0.11	0.01	0.11
(3,51)	1:101:A:GLU:H	1:89:A:TYR:O	3	0.11	0.01	0.11
(1,126)	1:25:A:GLN:HA	1:72:A:HIS:HE1	3	0.11	0.0	0.11
(1,1934)	1:78:A:LYS:H	1:78:A:LYS:HD3	2	1.16	0.23	1.16
(1,207)	1:56:A:LYS:HD3	1:74:A:HIS:HD2	2	1.03	0.34	1.03
(1,1596)	1:78:A:LYS:HD3	1:78:A:LYS:HA	2	1.02	0.07	1.02
(1,1124)	1:21:A:LEU:HD11	1:51:A:PHE:HD1	2	0.94	0.83	0.94
(1,1124)	1:21:A:LEU:HD11	1:51:A:PHE:HD2	2	0.94	0.83	0.94
(1,1124)	1:21:A:LEU:HD12	1:51:A:PHE:HD1	2	0.94	0.83	0.94
(1,1124)	1:21:A:LEU:HD12	1:51:A:PHE:HD2	2	0.94	0.83	0.94
(1,1124)	1:21:A:LEU:HD13	1:51:A:PHE:HD1	2	0.94	0.83	0.94
(1,1124)	1:21:A:LEU:HD13	1:51:A:PHE:HD2	2	0.94	0.83	0.94

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1829)	1:10:A:ASN:HA	1:7:A:LYS:HD3	2	0.8	0.65	0.8
(2,76)	1:46:A:PRO:HD3	1:48:A:GLU:HB3	2	0.77	0.67	0.77
(1,1762)	1:14:A:LEU:HD11	1:16:A:VAL:H	2	0.62	0.16	0.62
(1,1762)	1:14:A:LEU:HD12	1:16:A:VAL:H	2	0.62	0.16	0.62
(1,1762)	1:14:A:LEU:HD13	1:16:A:VAL:H	2	0.62	0.16	0.62
(1,215)	1:53:A:VAL:HG11	1:38:A:PHE:HZ	2	0.6	0.44	0.6
(1,215)	1:53:A:VAL:HG12	1:38:A:PHE:HZ	2	0.6	0.44	0.6
(1,215)	1:53:A:VAL:HG13	1:38:A:PHE:HZ	2	0.6	0.44	0.6
(1,2370)	1:25:A:GLN:HB3	1:26:A:LEU:H	2	0.52	0.2	0.52
(1,2370)	1:78:A:LYS:HD3	1:78:A:LYS:H	2	0.52	0.2	0.52
(1,359)	1:108:A:LYS:HD3	1:15:A:THR:HA	2	0.52	0.07	0.52
(2,50)	1:57:A:TYR:HB3	1:58:A:PHE:HD1	2	0.5	0.06	0.5
(2,50)	1:57:A:TYR:HB3	1:58:A:PHE:HD2	2	0.5	0.06	0.5
(1,1633)	1:69:A:GLY:HA2	1:60:A:PRO:HG3	2	0.5	0.06	0.5
(1,2529)	1:28:A:SER:HB3	1:71:A:GLU:HB3	2	0.5	0.14	0.5
(1,733)	1:99:A:ASP:HB3	1:99:A:ASP:H	2	0.43	0.17	0.43
(2,151)	1:52:A:THR:H	1:45:A:SER:HB3	2	0.4	0.07	0.4
(1,1391)	1:81:A:GLY:HA3	1:47:A:ASN:HD22	2	0.36	0.09	0.36
(1,448)	1:71:A:GLU:HG2	1:57:A:TYR:HB3	2	0.35	0.13	0.35
(1,1680)	1:41:A:GLY:HA3	1:37:A:TYR:HB2	2	0.34	0.18	0.34
(1,489)	1:65:A:LEU:HD11	1:30:A:PRO:HD3	2	0.34	0.07	0.34
(1,489)	1:65:A:LEU:HD12	1:30:A:PRO:HD3	2	0.34	0.07	0.34
(1,489)	1:65:A:LEU:HD13	1:30:A:PRO:HD3	2	0.34	0.07	0.34
(1,1458)	1:75:A:VAL:HG21	1:52:A:THR:H	2	0.31	0.1	0.31
(1,1458)	1:75:A:VAL:HG22	1:52:A:THR:H	2	0.31	0.1	0.31
(1,1458)	1:75:A:VAL:HG23	1:52:A:THR:H	2	0.31	0.1	0.31
(1,2231)	1:63:A:LYS:HD3	1:64:A:LEU:HA	2	0.31	0.07	0.31
(1,2231)	1:92:A:PRO:HB3	1:91:A:ARG:HA	2	0.31	0.07	0.31
(1,1074)	1:18:A:VAL:HG11	1:79:A:ALA:H	2	0.24	0.08	0.24
(1,1074)	1:18:A:VAL:HG12	1:79:A:ALA:H	2	0.24	0.08	0.24
(1,1074)	1:18:A:VAL:HG13	1:79:A:ALA:H	2	0.24	0.08	0.24
(1,1097)	1:37:A:TYR:HB3	1:42:A:THR:H	2	0.24	0.12	0.24
(1,349)	1:102:A:ARG:HG3	1:88:A:THR:HA	2	0.23	0.03	0.23
(1,2333)	1:5:A:VAL:HG21	1:3:A:HIS:HB3	2	0.23	0.06	0.23
(1,2333)	1:5:A:VAL:HG22	1:3:A:HIS:HB3	2	0.23	0.06	0.23
(1,2333)	1:5:A:VAL:HG23	1:3:A:HIS:HB3	2	0.23	0.06	0.23
(1,2435)	1:90:A:MET:HB2	1:37:A:TYR:HD1	2	0.2	0.06	0.2
(1,2435)	1:90:A:MET:HB2	1:37:A:TYR:HD2	2	0.2	0.06	0.2
(1,946)	1:34:A:PHE:HD1	1:34:A:PHE:H	2	0.2	0.02	0.2
(1,946)	1:34:A:PHE:HD2	1:34:A:PHE:H	2	0.2	0.02	0.2
(2,145)	1:40:A:GLY:H	1:43:A:LYS:HB3	2	0.19	0.04	0.19
(1,1165)	1:65:A:LEU:H	1:66:A:GLY:H	2	0.18	0.05	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1852)	1:87:A:LEU:HD11	1:10:A:ASN:HA	2	0.18	0.07	0.18
(1,1852)	1:87:A:LEU:HD12	1:10:A:ASN:HA	2	0.18	0.07	0.18
(1,1852)	1:87:A:LEU:HD13	1:10:A:ASN:HA	2	0.18	0.07	0.18
(2,142)	1:50:A:MET:H	1:52:A:THR:HB	2	0.18	0.04	0.18
(1,2403)	1:36:A:TRP:HB2	1:57:A:TYR:HD1	2	0.18	0.04	0.18
(1,2403)	1:36:A:TRP:HB2	1:57:A:TYR:HD2	2	0.18	0.04	0.18
(1,2403)	1:91:A:ARG:HD3	1:93:A:TRP:HH2	2	0.18	0.04	0.18
(1,1154)	1:56:A:LYS:HG3	1:56:A:LYS:H	2	0.16	0.06	0.16
(1,2006)	1:58:A:PHE:H	1:58:A:PHE:HD1	2	0.16	0.02	0.16
(1,2006)	1:58:A:PHE:H	1:58:A:PHE:HD2	2	0.16	0.02	0.16
(1,802)	1:64:A:LEU:HD11	1:65:A:LEU:H	2	0.16	0.01	0.16
(1,802)	1:64:A:LEU:HD12	1:65:A:LEU:H	2	0.16	0.01	0.16
(1,802)	1:64:A:LEU:HD13	1:65:A:LEU:H	2	0.16	0.01	0.16
(1,2149)	1:26:A:LEU:HD11	1:85:A:VAL:HG11	2	0.16	0.06	0.16
(1,2149)	1:26:A:LEU:HD11	1:85:A:VAL:HG12	2	0.16	0.06	0.16
(1,2149)	1:26:A:LEU:HD11	1:85:A:VAL:HG13	2	0.16	0.06	0.16
(1,2149)	1:26:A:LEU:HD12	1:85:A:VAL:HG11	2	0.16	0.06	0.16
(1,2149)	1:26:A:LEU:HD12	1:85:A:VAL:HG12	2	0.16	0.06	0.16
(1,2149)	1:26:A:LEU:HD12	1:85:A:VAL:HG13	2	0.16	0.06	0.16
(1,2149)	1:26:A:LEU:HD13	1:85:A:VAL:HG11	2	0.16	0.06	0.16
(1,2149)	1:26:A:LEU:HD13	1:85:A:VAL:HG12	2	0.16	0.06	0.16
(1,2149)	1:26:A:LEU:HD13	1:85:A:VAL:HG13	2	0.16	0.06	0.16
(1,2424)	1:35:A:ALA:HB1	1:71:A:GLU:HB3	2	0.16	0.04	0.16
(1,2424)	1:35:A:ALA:HB2	1:71:A:GLU:HB3	2	0.16	0.04	0.16
(1,2424)	1:35:A:ALA:HB3	1:71:A:GLU:HB3	2	0.16	0.04	0.16
(1,1767)	1:7:A:LYS:HA	1:24:A:ILE:HG21	2	0.15	0.01	0.15
(1,1767)	1:7:A:LYS:HA	1:24:A:ILE:HG22	2	0.15	0.01	0.15
(1,1767)	1:7:A:LYS:HA	1:24:A:ILE:HG23	2	0.15	0.01	0.15
(1,255)	1:26:A:LEU:HB3	1:36:A:TRP:HH2	2	0.15	0.0	0.15
(2,131)	1:65:A:LEU:H	1:62:A:SER:HA	2	0.15	0.03	0.15
(1,1631)	1:10:A:ASN:HB2	1:36:A:TRP:HH2	2	0.15	0.02	0.15
(1,1066)	1:58:A:PHE:HD1	1:57:A:TYR:H	2	0.14	0.0	0.14
(1,1066)	1:58:A:PHE:HD2	1:57:A:TYR:H	2	0.14	0.0	0.14
(1,2135)	1:70:A:THR:H	1:59:A:PRO:HG3	2	0.14	0.03	0.14
(2,96)	1:103:A:PHE:HB2	1:26:A:LEU:HA	2	0.14	0.0	0.14
(1,133)	1:90:A:MET:HA	1:34:A:PHE:HD1	2	0.13	0.02	0.13
(1,133)	1:90:A:MET:HA	1:34:A:PHE:HD2	2	0.13	0.02	0.13
(1,393)	1:82:A:THR:HG21	1:109:A:ALA:HA	2	0.12	0.02	0.12
(1,393)	1:82:A:THR:HG22	1:109:A:ALA:HA	2	0.12	0.02	0.12
(1,393)	1:82:A:THR:HG23	1:109:A:ALA:HA	2	0.12	0.02	0.12
(1,1662)	1:41:A:GLY:HA2	1:90:A:MET:HE1	2	0.12	0.01	0.12
(1,1662)	1:41:A:GLY:HA2	1:90:A:MET:HE2	2	0.12	0.01	0.12

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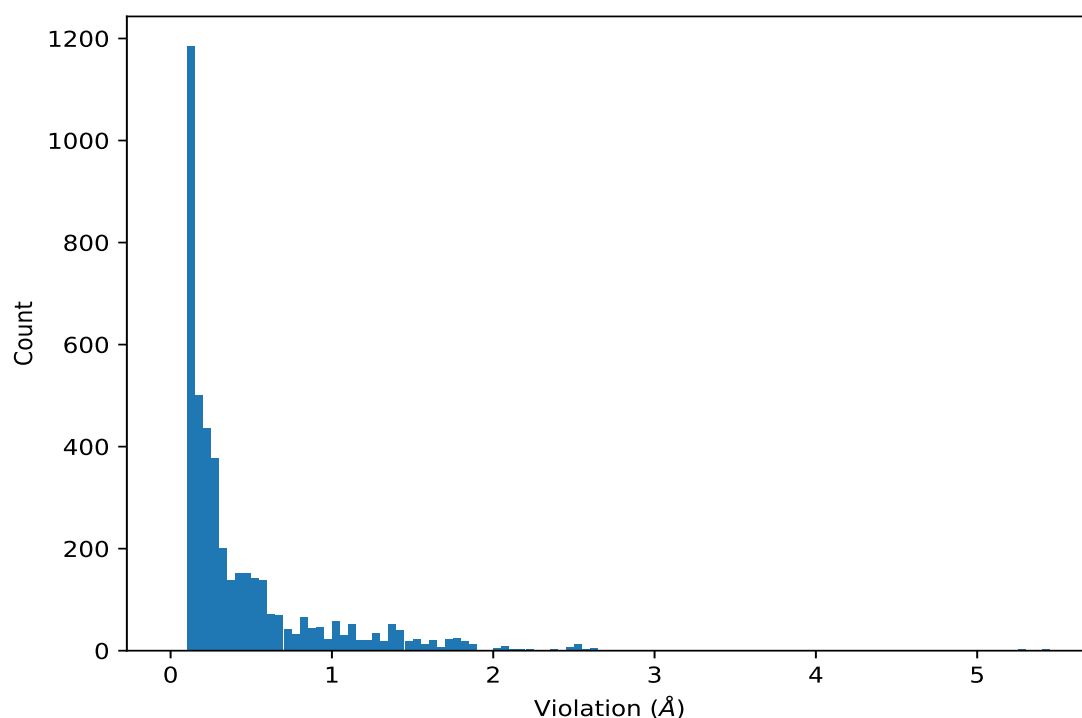
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1662)	1:41:A:GLY:HA2	1:90:A:MET:HE3	2	0.12	0.01	0.12
(1,1803)	1:26:A:LEU:HD21	1:25:A:GLN:HB3	2	0.12	0.02	0.12
(1,1803)	1:26:A:LEU:HD22	1:25:A:GLN:HB3	2	0.12	0.02	0.12
(1,1803)	1:26:A:LEU:HD23	1:25:A:GLN:HB3	2	0.12	0.02	0.12
(1,2130)	1:47:A:ASN:HD21	1:110:A:ASN:HA	2	0.12	0.02	0.12
(1,772)	1:102:A:ARG:HA	1:102:A:ARG:H	2	0.12	0.02	0.12
(1,1885)	1:38:A:PHE:HZ	1:45:A:SER:HA	2	0.12	0.02	0.12
(1,120)	1:13:A:THR:HA	1:106:A:TYR:HE1	2	0.12	0.0	0.12
(1,120)	1:13:A:THR:HA	1:106:A:TYR:HE2	2	0.12	0.0	0.12
(1,1036)	1:16:A:VAL:HB	1:108:A:LYS:H	2	0.12	0.01	0.12
(1,1818)	1:108:A:LYS:HD3	1:108:A:LYS:H	2	0.12	0.02	0.12
(1,687)	1:22:A:VAL:HG11	1:3:A:HIS:HD2	2	0.11	0.01	0.11
(1,687)	1:22:A:VAL:HG12	1:3:A:HIS:HD2	2	0.11	0.01	0.11
(1,687)	1:22:A:VAL:HG13	1:3:A:HIS:HD2	2	0.11	0.01	0.11
(1,723)	1:54:A:GLU:HA	1:55:A:ASN:H	2	0.11	0.0	0.11
(1,1015)	1:10:A:ASN:HB2	1:10:A:ASN:HD21	2	0.11	0.0	0.11
(1,1792)	1:16:A:VAL:HA	1:3:A:HIS:HE1	2	0.11	0.01	0.11
(1,2279)	1:59:A:PRO:HB3	1:59:A:PRO:HD2	2	0.11	0.0	0.11
(2,51)	1:35:A:ALA:HA	1:31:A:THR:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD21	11	5.44
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD22	11	5.44
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD23	11	5.44
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD21	8	5.26
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD22	8	5.26
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD23	8	5.26
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	13	3.44
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	4	3.35
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	7	3.25
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	9	3.07
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	12	3.03
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	10	2.94
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	1	2.66
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	14	2.63
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	9	2.61
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	9	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	9	2.61
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	5	2.58
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	8	2.56
(1,1547)	1:26:A:LEU:HD21	1:73:A:PHE:HD1	7	2.54
(1,1547)	1:26:A:LEU:HD21	1:73:A:PHE:HD2	7	2.54
(1,1547)	1:26:A:LEU:HD22	1:73:A:PHE:HD1	7	2.54
(1,1547)	1:26:A:LEU:HD22	1:73:A:PHE:HD2	7	2.54
(1,1547)	1:26:A:LEU:HD23	1:73:A:PHE:HD1	7	2.54
(1,1547)	1:26:A:LEU:HD23	1:73:A:PHE:HD2	7	2.54
(1,1547)	1:26:A:LEU:HD21	1:73:A:PHE:HD1	8	2.52
(1,1547)	1:26:A:LEU:HD21	1:73:A:PHE:HD2	8	2.52
(1,1547)	1:26:A:LEU:HD22	1:73:A:PHE:HD1	8	2.52
(1,1547)	1:26:A:LEU:HD22	1:73:A:PHE:HD2	8	2.52
(1,1547)	1:26:A:LEU:HD23	1:73:A:PHE:HD1	8	2.52
(1,1547)	1:26:A:LEU:HD23	1:73:A:PHE:HD2	8	2.52
(1,1547)	1:26:A:LEU:HD21	1:73:A:PHE:HD1	13	2.46
(1,1547)	1:26:A:LEU:HD21	1:73:A:PHE:HD2	13	2.46
(1,1547)	1:26:A:LEU:HD22	1:73:A:PHE:HD1	13	2.46
(1,1547)	1:26:A:LEU:HD22	1:73:A:PHE:HD2	13	2.46
(1,1547)	1:26:A:LEU:HD23	1:73:A:PHE:HD1	13	2.46
(1,1547)	1:26:A:LEU:HD23	1:73:A:PHE:HD2	13	2.46
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	15	2.39
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	2	2.36
(1,2058)	1:81:A:GLY:H	1:18:A:VAL:HG11	3	2.23
(1,2058)	1:81:A:GLY:H	1:18:A:VAL:HG12	3	2.23
(1,2058)	1:81:A:GLY:H	1:18:A:VAL:HG13	3	2.23
(1,2058)	1:81:A:GLY:H	1:18:A:VAL:HG11	9	2.18
(1,2058)	1:81:A:GLY:H	1:18:A:VAL:HG12	9	2.18
(1,2058)	1:81:A:GLY:H	1:18:A:VAL:HG13	9	2.18
(3,3)	1:76:A:THR:H	1:52:A:THR:O	14	2.14
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	11	2.13
(2,98)	1:80:A:ALA:HA	1:18:A:VAL:HG11	9	2.08
(2,98)	1:80:A:ALA:HA	1:18:A:VAL:HG12	9	2.08
(2,98)	1:80:A:ALA:HA	1:18:A:VAL:HG13	9	2.08
(1,1980)	1:76:A:THR:H	1:21:A:LEU:HD11	3	2.08
(1,1980)	1:76:A:THR:H	1:21:A:LEU:HD12	3	2.08
(1,1980)	1:76:A:THR:H	1:21:A:LEU:HD13	3	2.08
(1,2058)	1:81:A:GLY:H	1:18:A:VAL:HG11	13	2.06
(1,2058)	1:81:A:GLY:H	1:18:A:VAL:HG12	13	2.06
(1,2058)	1:81:A:GLY:H	1:18:A:VAL:HG13	13	2.06
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	6	2.05
(2,98)	1:80:A:ALA:HA	1:18:A:VAL:HG11	3	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:80:A:ALA:HA	1:18:A:VAL:HG12	3	2.04
(2,98)	1:80:A:ALA:HA	1:18:A:VAL:HG13	3	2.04
(3,4)	1:76:A:THR:N	1:52:A:THR:O	14	1.96
(1,2330)	1:56:A:LYS:HG3	1:57:A:TYR:HB2	2	1.92
(2,98)	1:80:A:ALA:HA	1:18:A:VAL:HG11	13	1.88
(2,98)	1:80:A:ALA:HA	1:18:A:VAL:HG12	13	1.88
(2,98)	1:80:A:ALA:HA	1:18:A:VAL:HG13	13	1.88
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	13	1.88
(2,19)	1:63:A:LYS:HD3	1:65:A:LEU:HA	5	1.87
(1,65)	1:26:A:LEU:HD11	1:7:A:LYS:HB2	7	1.87
(1,65)	1:26:A:LEU:HD12	1:7:A:LYS:HB2	7	1.87
(1,65)	1:26:A:LEU:HD13	1:7:A:LYS:HB2	7	1.87
(1,65)	1:26:A:LEU:HD11	1:7:A:LYS:HB2	8	1.87
(1,65)	1:26:A:LEU:HD12	1:7:A:LYS:HB2	8	1.87
(1,65)	1:26:A:LEU:HD13	1:7:A:LYS:HB2	8	1.87
(1,2330)	1:56:A:LYS:HG3	1:57:A:TYR:HB2	9	1.86
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	12	1.85
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	2	1.83
(1,2177)	1:54:A:GLU:HG3	1:74:A:HIS:HD2	3	1.82
(1,65)	1:26:A:LEU:HD11	1:7:A:LYS:HB2	13	1.82
(1,65)	1:26:A:LEU:HD12	1:7:A:LYS:HB2	13	1.82
(1,65)	1:26:A:LEU:HD13	1:7:A:LYS:HB2	13	1.82
(1,1525)	1:26:A:LEU:HD11	1:7:A:LYS:HD3	8	1.81
(1,1525)	1:26:A:LEU:HD12	1:7:A:LYS:HD3	8	1.81
(1,1525)	1:26:A:LEU:HD13	1:7:A:LYS:HD3	8	1.81
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	13	1.81
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	13	1.81
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	13	1.81
(1,269)	1:26:A:LEU:HD21	1:57:A:TYR:HD1	7	1.81
(1,269)	1:26:A:LEU:HD21	1:57:A:TYR:HD2	7	1.81
(1,269)	1:26:A:LEU:HD22	1:57:A:TYR:HD1	7	1.81
(1,269)	1:26:A:LEU:HD22	1:57:A:TYR:HD2	7	1.81
(1,269)	1:26:A:LEU:HD23	1:57:A:TYR:HD1	7	1.81
(1,269)	1:26:A:LEU:HD23	1:57:A:TYR:HD2	7	1.81
(2,140)	1:52:A:THR:H	1:50:A:MET:HG3	8	1.8
(1,2330)	1:56:A:LYS:HG3	1:57:A:TYR:HB2	11	1.8
(1,1897)	1:36:A:TRP:HD1	1:57:A:TYR:HB2	9	1.79
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD21	13	1.79
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD22	13	1.79
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD23	13	1.79
(1,1525)	1:26:A:LEU:HD11	1:7:A:LYS:HD3	13	1.79
(1,1525)	1:26:A:LEU:HD12	1:7:A:LYS:HD3	13	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1525)	1:26:A:LEU:HD13	1:7:A:LYS:HD3	13	1.79
(1,878)	1:63:A:LYS:HD3	1:61:A:ASP:HB3	7	1.79
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	5	1.78
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	10	1.78
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	14	1.78
(1,878)	1:63:A:LYS:HD3	1:61:A:ASP:HB3	3	1.78
(2,140)	1:52:A:THR:H	1:50:A:MET:HG3	3	1.77
(2,19)	1:63:A:LYS:HD3	1:65:A:LEU:HA	10	1.77
(1,1124)	1:21:A:LEU:HD11	1:51:A:PHE:HD1	3	1.77
(1,1124)	1:21:A:LEU:HD11	1:51:A:PHE:HD2	3	1.77
(1,1124)	1:21:A:LEU:HD12	1:51:A:PHE:HD1	3	1.77
(1,1124)	1:21:A:LEU:HD12	1:51:A:PHE:HD2	3	1.77
(1,1124)	1:21:A:LEU:HD13	1:51:A:PHE:HD1	3	1.77
(1,1124)	1:21:A:LEU:HD13	1:51:A:PHE:HD2	3	1.77
(2,140)	1:52:A:THR:H	1:50:A:MET:HG3	4	1.76
(2,140)	1:52:A:THR:H	1:50:A:MET:HG3	12	1.75
(2,140)	1:52:A:THR:H	1:50:A:MET:HG3	13	1.75
(1,878)	1:63:A:LYS:HD3	1:61:A:ASP:HB3	14	1.75
(2,140)	1:52:A:THR:H	1:50:A:MET:HG3	10	1.74
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	4	1.74
(1,1897)	1:36:A:TRP:HD1	1:57:A:TYR:HB2	6	1.74
(1,493)	1:75:A:VAL:HG21	1:77:A:VAL:HA	8	1.74
(1,493)	1:75:A:VAL:HG22	1:77:A:VAL:HA	8	1.74
(1,493)	1:75:A:VAL:HG23	1:77:A:VAL:HA	8	1.74
(2,110)	1:14:A:LEU:HD11	1:9:A:HIS:HD2	15	1.73
(2,110)	1:14:A:LEU:HD12	1:9:A:HIS:HD2	15	1.73
(2,110)	1:14:A:LEU:HD13	1:9:A:HIS:HD2	15	1.73
(2,19)	1:63:A:LYS:HD3	1:65:A:LEU:HA	15	1.73
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	8	1.73
(1,1897)	1:36:A:TRP:HD1	1:57:A:TYR:HB2	13	1.73
(1,1525)	1:26:A:LEU:HD11	1:7:A:LYS:HD3	7	1.73
(1,1525)	1:26:A:LEU:HD12	1:7:A:LYS:HD3	7	1.73
(1,1525)	1:26:A:LEU:HD13	1:7:A:LYS:HD3	7	1.73
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	1	1.72
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	15	1.72
(1,1249)	1:104:A:THR:HB	1:86:A:ASN:HD22	11	1.71
(1,993)	1:75:A:VAL:HG21	1:77:A:VAL:H	8	1.71
(1,993)	1:75:A:VAL:HG22	1:77:A:VAL:H	8	1.71
(1,993)	1:75:A:VAL:HG23	1:77:A:VAL:H	8	1.71
(1,143)	1:5:A:VAL:HA	1:9:A:HIS:HE1	15	1.71
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	9	1.69
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	9	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	9	1.69
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	2	1.68
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	11	1.68
(1,2177)	1:54:A:GLU:HG3	1:74:A:HIS:HD2	10	1.66
(1,2515)	1:40:A:GLY:HA3	1:100:A:SER:HB2	3	1.65
(1,2330)	1:70:A:THR:HG21	1:57:A:TYR:HB2	1	1.65
(1,2330)	1:70:A:THR:HG22	1:57:A:TYR:HB2	1	1.65
(1,2330)	1:70:A:THR:HG23	1:57:A:TYR:HB2	1	1.65
(1,1730)	1:56:A:LYS:HD3	1:74:A:HIS:HA	1	1.65
(1,963)	1:107:A:LEU:HB3	1:16:A:VAL:H	6	1.65
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	3	1.65
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	3	1.65
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	3	1.65
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB1	11	1.65
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB2	11	1.65
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB3	11	1.65
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB1	11	1.65
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB2	11	1.65
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB3	11	1.65
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB1	11	1.65
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB2	11	1.65
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB3	11	1.65
(1,2288)	1:24:A:ILE:HG13	1:45:A:SER:HA	5	1.64
(1,173)	1:43:A:LYS:HB3	1:38:A:PHE:HZ	11	1.64
(1,2330)	1:56:A:LYS:HG3	1:57:A:TYR:HB2	6	1.61
(1,2390)	1:75:A:VAL:HG21	1:83:A:HIS:HB3	8	1.59
(1,2390)	1:75:A:VAL:HG22	1:83:A:HIS:HB3	8	1.59
(1,2390)	1:75:A:VAL:HG23	1:83:A:HIS:HB3	8	1.59
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	6	1.59
(1,963)	1:107:A:LEU:HB3	1:16:A:VAL:H	4	1.59
(1,1897)	1:36:A:TRP:HD1	1:57:A:TYR:HB2	10	1.58
(1,1897)	1:36:A:TRP:HD1	1:57:A:TYR:HB2	11	1.57
(1,963)	1:107:A:LEU:HB3	1:16:A:VAL:H	13	1.57
(1,897)	1:45:A:SER:HB3	1:53:A:VAL:HG11	13	1.57
(1,897)	1:45:A:SER:HB3	1:53:A:VAL:HG12	13	1.57
(1,897)	1:45:A:SER:HB3	1:53:A:VAL:HG13	13	1.57
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	11	1.56
(1,304)	1:61:A:ASP:HB3	1:62:A:SER:HA	5	1.56
(1,963)	1:107:A:LEU:HB3	1:16:A:VAL:H	5	1.54
(1,173)	1:43:A:LYS:HB3	1:38:A:PHE:HZ	1	1.54
(1,173)	1:43:A:LYS:HB3	1:38:A:PHE:HZ	2	1.54
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	3	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	7	1.53
(1,1788)	1:75:A:VAL:HG11	1:87:A:LEU:HD11	8	1.52
(1,1788)	1:75:A:VAL:HG11	1:87:A:LEU:HD12	8	1.52
(1,1788)	1:75:A:VAL:HG11	1:87:A:LEU:HD13	8	1.52
(1,1788)	1:75:A:VAL:HG12	1:87:A:LEU:HD11	8	1.52
(1,1788)	1:75:A:VAL:HG12	1:87:A:LEU:HD12	8	1.52
(1,1788)	1:75:A:VAL:HG12	1:87:A:LEU:HD13	8	1.52
(1,1788)	1:75:A:VAL:HG13	1:87:A:LEU:HD11	8	1.52
(1,1788)	1:75:A:VAL:HG13	1:87:A:LEU:HD12	8	1.52
(1,1788)	1:75:A:VAL:HG13	1:87:A:LEU:HD13	8	1.52
(1,304)	1:61:A:ASP:HB3	1:62:A:SER:HA	12	1.52
(1,269)	1:26:A:LEU:HD21	1:57:A:TYR:HD1	13	1.52
(1,269)	1:26:A:LEU:HD21	1:57:A:TYR:HD2	13	1.52
(1,269)	1:26:A:LEU:HD22	1:57:A:TYR:HD1	13	1.52
(1,269)	1:26:A:LEU:HD22	1:57:A:TYR:HD2	13	1.52
(1,269)	1:26:A:LEU:HD23	1:57:A:TYR:HD1	13	1.52
(1,269)	1:26:A:LEU:HD23	1:57:A:TYR:HD2	13	1.52
(1,1722)	1:64:A:LEU:HB3	1:66:A:GLY:HA2	10	1.51
(1,368)	1:30:A:PRO:HG3	1:69:A:GLY:HA2	6	1.5
(1,1087)	1:75:A:VAL:HG11	1:38:A:PHE:HE1	8	1.49
(1,1087)	1:75:A:VAL:HG11	1:38:A:PHE:HE2	8	1.49
(1,1087)	1:75:A:VAL:HG12	1:38:A:PHE:HE1	8	1.49
(1,1087)	1:75:A:VAL:HG12	1:38:A:PHE:HE2	8	1.49
(1,1087)	1:75:A:VAL:HG13	1:38:A:PHE:HE1	8	1.49
(1,1087)	1:75:A:VAL:HG13	1:38:A:PHE:HE2	8	1.49
(1,963)	1:107:A:LEU:HB3	1:16:A:VAL:H	7	1.49
(1,2330)	1:56:A:LYS:HG3	1:57:A:TYR:HB2	15	1.48
(1,1897)	1:36:A:TRP:HD1	1:57:A:TYR:HB2	12	1.47
(1,963)	1:107:A:LEU:HB3	1:16:A:VAL:H	1	1.47
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	15	1.47
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	15	1.47
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	15	1.47
(1,2330)	1:56:A:LYS:HG3	1:57:A:TYR:HB2	3	1.46
(1,2330)	1:56:A:LYS:HG3	1:57:A:TYR:HB2	12	1.46
(1,769)	1:26:A:LEU:HD11	1:36:A:TRP:HZ2	7	1.46
(1,769)	1:26:A:LEU:HD12	1:36:A:TRP:HZ2	7	1.46
(1,769)	1:26:A:LEU:HD13	1:36:A:TRP:HZ2	7	1.46
(1,472)	1:65:A:LEU:HG	1:28:A:SER:HB3	3	1.46
(1,1829)	1:10:A:ASN:HA	1:7:A:LYS:HD3	6	1.45
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	14	1.45
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	14	1.45
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	14	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,269)	1:26:A:LEU:HD21	1:57:A:TYR:HD1	8	1.45
(1,269)	1:26:A:LEU:HD21	1:57:A:TYR:HD2	8	1.45
(1,269)	1:26:A:LEU:HD22	1:57:A:TYR:HD1	8	1.45
(1,269)	1:26:A:LEU:HD22	1:57:A:TYR:HD2	8	1.45
(1,269)	1:26:A:LEU:HD23	1:57:A:TYR:HD1	8	1.45
(1,269)	1:26:A:LEU:HD23	1:57:A:TYR:HD2	8	1.45
(1,173)	1:43:A:LYS:HB3	1:38:A:PHE:HZ	4	1.45
(1,173)	1:43:A:LYS:HB3	1:38:A:PHE:HZ	15	1.45
(2,76)	1:46:A:PRO:HD3	1:48:A:GLU:HB3	14	1.44
(1,2330)	1:70:A:THR:HG21	1:57:A:TYR:HB2	7	1.44
(1,2330)	1:70:A:THR:HG22	1:57:A:TYR:HB2	7	1.44
(1,2330)	1:70:A:THR:HG23	1:57:A:TYR:HB2	7	1.44
(1,963)	1:107:A:LEU:HB3	1:16:A:VAL:H	11	1.44
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	12	1.44
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	12	1.44
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	12	1.44
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	13	1.44
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	13	1.44
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	13	1.44
(1,769)	1:26:A:LEU:HD11	1:36:A:TRP:HZ2	8	1.44
(1,769)	1:26:A:LEU:HD12	1:36:A:TRP:HZ2	8	1.44
(1,769)	1:26:A:LEU:HD13	1:36:A:TRP:HZ2	8	1.44
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD1	1	1.43
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD2	1	1.43
(1,1897)	1:36:A:TRP:HD1	1:57:A:TYR:HB2	15	1.43
(1,1752)	1:56:A:LYS:HB3	1:72:A:HIS:HB3	7	1.43
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	7	1.43
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	7	1.43
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	7	1.43
(1,769)	1:26:A:LEU:HD11	1:36:A:TRP:HZ2	13	1.42
(1,769)	1:26:A:LEU:HD12	1:36:A:TRP:HZ2	13	1.42
(1,769)	1:26:A:LEU:HD13	1:36:A:TRP:HZ2	13	1.42
(1,2330)	1:56:A:LYS:HG3	1:57:A:TYR:HB2	8	1.41
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	5	1.41
(1,2177)	1:34:A:PHE:HB3	1:37:A:TYR:HE1	8	1.41
(1,2177)	1:34:A:PHE:HB3	1:37:A:TYR:HE2	8	1.41
(2,19)	1:63:A:LYS:HD3	1:65:A:LEU:HA	8	1.4
(2,19)	1:63:A:LYS:HD3	1:65:A:LEU:HA	14	1.4
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	12	1.4
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	13	1.4
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	6	1.4
(1,963)	1:107:A:LEU:HB3	1:16:A:VAL:H	9	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,897)	1:45:A:SER:HB3	1:53:A:VAL:HG11	4	1.4
(1,897)	1:45:A:SER:HB3	1:53:A:VAL:HG12	4	1.4
(1,897)	1:45:A:SER:HB3	1:53:A:VAL:HG13	4	1.4
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	2	1.4
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	2	1.4
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	2	1.4
(2,129)	1:66:A:GLY:H	1:68:A:GLY:HA3	8	1.39
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	14	1.39
(1,1934)	1:78:A:LYS:H	1:78:A:LYS:HD3	8	1.39
(1,1752)	1:56:A:LYS:HB3	1:72:A:HIS:HB3	8	1.39
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	15	1.39
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	6	1.39
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	6	1.39
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	6	1.39
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	7	1.38
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	9	1.38
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	10	1.38
(1,1877)	1:51:A:PHE:HD1	1:75:A:VAL:HG21	8	1.38
(1,1877)	1:51:A:PHE:HD1	1:75:A:VAL:HG22	8	1.38
(1,1877)	1:51:A:PHE:HD1	1:75:A:VAL:HG23	8	1.38
(1,1877)	1:51:A:PHE:HD2	1:75:A:VAL:HG21	8	1.38
(1,1877)	1:51:A:PHE:HD2	1:75:A:VAL:HG22	8	1.38
(1,1877)	1:51:A:PHE:HD2	1:75:A:VAL:HG23	8	1.38
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	5	1.38
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	5	1.38
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	5	1.38
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	3	1.37
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	3	1.37
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	3	1.37
(1,1897)	1:36:A:TRP:HD1	1:57:A:TYR:HB2	2	1.37
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	3	1.37
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	3	1.37
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	3	1.37
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	8	1.37
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	8	1.37
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	8	1.37
(1,207)	1:56:A:LYS:HD3	1:74:A:HIS:HD2	1	1.37
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	5	1.36
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	6	1.36
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	3	1.35
(1,1752)	1:56:A:LYS:HB3	1:72:A:HIS:HB3	1	1.35
(1,1752)	1:56:A:LYS:HB3	1:72:A:HIS:HB3	4	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	1	1.35
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	1	1.35
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	1	1.35
(1,730)	1:7:A:LYS:HA	1:7:A:LYS:HD3	6	1.35
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	15	1.34
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	13	1.34
(1,454)	1:59:A:PRO:HG3	1:28:A:SER:HB2	3	1.34
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	8	1.33
(1,2330)	1:70:A:THR:HG21	1:57:A:TYR:HB2	14	1.33
(1,2330)	1:70:A:THR:HG22	1:57:A:TYR:HB2	14	1.33
(1,2330)	1:70:A:THR:HG23	1:57:A:TYR:HB2	14	1.33
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD1	9	1.33
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD2	9	1.33
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	14	1.33
(2,19)	1:63:A:LYS:HD3	1:65:A:LEU:HA	7	1.32
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	2	1.31
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	15	1.31
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	8	1.31
(1,878)	1:63:A:LYS:HD3	1:61:A:ASP:HB3	8	1.31
(1,2321)	1:44:A:GLU:HG3	1:46:A:PRO:HD2	9	1.3
(1,2321)	1:44:A:GLU:HG3	1:46:A:PRO:HD2	12	1.3
(1,1752)	1:56:A:LYS:HB3	1:72:A:HIS:HB3	3	1.3
(1,1722)	1:64:A:LEU:HB3	1:66:A:GLY:HA2	7	1.3
(1,1997)	1:61:A:ASP:H	1:60:A:PRO:HG2	12	1.29
(1,480)	1:78:A:LYS:HB2	1:77:A:VAL:HA	14	1.29
(1,1887)	1:38:A:PHE:HZ	1:85:A:VAL:HG11	9	1.28
(1,1887)	1:38:A:PHE:HZ	1:85:A:VAL:HG12	9	1.28
(1,1887)	1:38:A:PHE:HZ	1:85:A:VAL:HG13	9	1.28
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD21	2	1.28
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD22	2	1.28
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD23	2	1.28
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	10	1.28
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	10	1.28
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	10	1.28
(1,480)	1:78:A:LYS:HB2	1:77:A:VAL:HA	2	1.28
(2,80)	1:56:A:LYS:HD3	1:55:A:ASN:HB2	10	1.27
(1,2330)	1:56:A:LYS:HG3	1:57:A:TYR:HB2	10	1.27
(1,1897)	1:36:A:TRP:HD1	1:57:A:TYR:HB2	8	1.27
(1,1816)	1:48:A:GLU:HB3	1:45:A:SER:HA	14	1.27
(1,963)	1:107:A:LEU:HB3	1:16:A:VAL:H	12	1.27
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	4	1.27
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	10	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2288)	1:24:A:ILE:HG13	1:45:A:SER:HA	10	1.26
(1,480)	1:78:A:LYS:HB2	1:77:A:VAL:HA	11	1.26
(3,1)	1:52:A:THR:H	1:76:A:THR:O	14	1.25
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB1	8	1.25
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB2	8	1.25
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB3	8	1.25
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB1	8	1.25
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB2	8	1.25
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB3	8	1.25
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB1	8	1.25
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB2	8	1.25
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB3	8	1.25
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	1	1.25
(1,480)	1:78:A:LYS:HB2	1:77:A:VAL:HA	1	1.25
(1,480)	1:78:A:LYS:HB2	1:77:A:VAL:HA	3	1.25
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	1	1.24
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	4	1.24
(1,2528)	1:87:A:LEU:HB2	1:38:A:PHE:HB2	11	1.24
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	11	1.24
(1,480)	1:78:A:LYS:HB2	1:77:A:VAL:HA	7	1.24
(1,480)	1:78:A:LYS:HB2	1:77:A:VAL:HA	8	1.24
(1,480)	1:78:A:LYS:HB2	1:77:A:VAL:HA	10	1.24
(2,19)	1:63:A:LYS:HD3	1:65:A:LEU:HA	3	1.23
(1,2321)	1:44:A:GLU:HG3	1:46:A:PRO:HD2	1	1.23
(1,2288)	1:24:A:ILE:HG13	1:45:A:SER:HA	15	1.23
(1,1642)	1:67:A:ALA:HB1	1:60:A:PRO:HG2	10	1.23
(1,1642)	1:67:A:ALA:HB2	1:60:A:PRO:HG2	10	1.23
(1,1642)	1:67:A:ALA:HB3	1:60:A:PRO:HG2	10	1.23
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	12	1.23
(1,2330)	1:56:A:LYS:HG3	1:57:A:TYR:HB2	13	1.22
(1,2321)	1:44:A:GLU:HG3	1:46:A:PRO:HD2	6	1.22
(1,1752)	1:56:A:LYS:HB3	1:72:A:HIS:HB3	14	1.22
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD1	1	1.22
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD2	1	1.22
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	12	1.21
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	11	1.2
(1,628)	1:65:A:LEU:HB3	1:60:A:PRO:HB3	5	1.2
(1,1642)	1:67:A:ALA:HB1	1:60:A:PRO:HG2	4	1.19
(1,1642)	1:67:A:ALA:HB2	1:60:A:PRO:HG2	4	1.19
(1,1642)	1:67:A:ALA:HB3	1:60:A:PRO:HG2	4	1.19
(1,963)	1:107:A:LEU:HB3	1:16:A:VAL:H	15	1.19
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	4	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	4	1.19
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	4	1.19
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	14	1.18
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	4	1.18
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	5	1.18
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	5	1.18
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	5	1.18
(1,1821)	1:38:A:PHE:HA	1:86:A:ASN:HB3	11	1.17
(1,480)	1:78:A:LYS:HB2	1:77:A:VAL:HA	13	1.17
(1,1430)	1:82:A:THR:HG21	1:110:A:ASN:HD21	12	1.16
(1,1430)	1:82:A:THR:HG22	1:110:A:ASN:HD21	12	1.16
(1,1430)	1:82:A:THR:HG23	1:110:A:ASN:HD21	12	1.16
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	7	1.16
(1,368)	1:30:A:PRO:HG3	1:69:A:GLY:HA2	4	1.16
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	7	1.15
(1,1722)	1:64:A:LEU:HB3	1:66:A:GLY:HA2	11	1.15
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	6	1.15
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	6	1.15
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	6	1.15
(1,963)	1:107:A:LEU:HB3	1:16:A:VAL:H	3	1.15
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	9	1.14
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	9	1.14
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	9	1.14
(2,80)	1:56:A:LYS:HD3	1:55:A:ASN:HB2	1	1.14
(1,2288)	1:24:A:ILE:HG13	1:45:A:SER:HA	2	1.14
(1,2288)	1:24:A:ILE:HG13	1:45:A:SER:HA	13	1.14
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	4	1.14
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	4	1.14
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	4	1.14
(1,87)	1:9:A:HIS:HB3	1:104:A:THR:H	15	1.14
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	15	1.13
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	7	1.13
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	7	1.13
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	7	1.13
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	8	1.12
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD1	13	1.12
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD2	13	1.12
(1,897)	1:45:A:SER:HB3	1:53:A:VAL:HG11	2	1.12
(1,897)	1:45:A:SER:HB3	1:53:A:VAL:HG12	2	1.12
(1,897)	1:45:A:SER:HB3	1:53:A:VAL:HG13	2	1.12
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	2	1.12
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	2	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1865)	1:24:A:ILE:HG21	1:26:A:LEU:HD21	8	1.11
(1,1865)	1:24:A:ILE:HG21	1:26:A:LEU:HD22	8	1.11
(1,1865)	1:24:A:ILE:HG21	1:26:A:LEU:HD23	8	1.11
(1,1865)	1:24:A:ILE:HG22	1:26:A:LEU:HD21	8	1.11
(1,1865)	1:24:A:ILE:HG22	1:26:A:LEU:HD22	8	1.11
(1,1865)	1:24:A:ILE:HG22	1:26:A:LEU:HD23	8	1.11
(1,1865)	1:24:A:ILE:HG23	1:26:A:LEU:HD21	8	1.11
(1,1865)	1:24:A:ILE:HG23	1:26:A:LEU:HD22	8	1.11
(1,1865)	1:24:A:ILE:HG23	1:26:A:LEU:HD23	8	1.11
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	15	1.11
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	15	1.11
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	15	1.11
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	3	1.11
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	3	1.11
(1,2321)	1:44:A:GLU:HG3	1:46:A:PRO:HD2	8	1.1
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	3	1.1
(1,1730)	1:56:A:LYS:HD3	1:74:A:HIS:HA	12	1.1
(1,1642)	1:67:A:ALA:HB1	1:60:A:PRO:HG2	9	1.1
(1,1642)	1:67:A:ALA:HB2	1:60:A:PRO:HG2	9	1.1
(1,1642)	1:67:A:ALA:HB3	1:60:A:PRO:HG2	9	1.1
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	1	1.1
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	1	1.1
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	1	1.1
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	2	1.1
(1,223)	1:4:A:LYS:HG3	1:3:A:HIS:HE1	11	1.09
(1,223)	1:4:A:LYS:HG3	1:3:A:HIS:HE1	12	1.09
(1,1702)	1:64:A:LEU:HD11	1:61:A:ASP:HB3	5	1.08
(1,1702)	1:64:A:LEU:HD12	1:61:A:ASP:HB3	5	1.08
(1,1702)	1:64:A:LEU:HD13	1:61:A:ASP:HB3	5	1.08
(1,1642)	1:67:A:ALA:HB1	1:60:A:PRO:HG2	14	1.08
(1,1642)	1:67:A:ALA:HB2	1:60:A:PRO:HG2	14	1.08
(1,1642)	1:67:A:ALA:HB3	1:60:A:PRO:HG2	14	1.08
(1,1596)	1:78:A:LYS:HD3	1:78:A:LYS:HA	8	1.08
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	10	1.08
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	10	1.08
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	10	1.08
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	12	1.08
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	12	1.08
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	12	1.08
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	7	1.08
(1,1997)	1:61:A:ASP:H	1:60:A:PRO:HG2	10	1.07
(1,1897)	1:36:A:TRP:HD1	1:57:A:TYR:HB2	3	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1865)	1:24:A:ILE:HG21	1:26:A:LEU:HD21	13	1.06
(1,1865)	1:24:A:ILE:HG21	1:26:A:LEU:HD22	13	1.06
(1,1865)	1:24:A:ILE:HG21	1:26:A:LEU:HD23	13	1.06
(1,1865)	1:24:A:ILE:HG22	1:26:A:LEU:HD21	13	1.06
(1,1865)	1:24:A:ILE:HG22	1:26:A:LEU:HD22	13	1.06
(1,1865)	1:24:A:ILE:HG22	1:26:A:LEU:HD23	13	1.06
(1,1865)	1:24:A:ILE:HG23	1:26:A:LEU:HD21	13	1.06
(1,1865)	1:24:A:ILE:HG23	1:26:A:LEU:HD22	13	1.06
(1,1865)	1:24:A:ILE:HG23	1:26:A:LEU:HD23	13	1.06
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	8	1.06
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	8	1.06
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	8	1.06
(1,368)	1:30:A:PRO:HG3	1:69:A:GLY:HA2	12	1.05
(1,1654)	1:42:A:THR:HA	1:43:A:LYS:HD3	5	1.04
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	12	1.04
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	12	1.04
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	12	1.04
(1,1018)	1:27:A:PRO:HD2	1:26:A:LEU:HD11	7	1.04
(1,1018)	1:27:A:PRO:HD2	1:26:A:LEU:HD12	7	1.04
(1,1018)	1:27:A:PRO:HD2	1:26:A:LEU:HD13	7	1.04
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	5	1.04
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	5	1.04
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	5	1.04
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	9	1.04
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	9	1.04
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	9	1.04
(1,215)	1:53:A:VAL:HG11	1:38:A:PHE:HZ	3	1.04
(1,215)	1:53:A:VAL:HG12	1:38:A:PHE:HZ	3	1.04
(1,215)	1:53:A:VAL:HG13	1:38:A:PHE:HZ	3	1.04
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG21	3	1.03
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG22	3	1.03
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG23	3	1.03
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG21	3	1.03
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG22	3	1.03
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG23	3	1.03
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG21	3	1.03
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG22	3	1.03
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG23	3	1.03
(1,1588)	1:70:A:THR:HB	1:58:A:PHE:HB2	9	1.03
(1,1559)	1:101:A:GLU:HG3	1:36:A:TRP:HH2	1	1.03
(1,1559)	1:101:A:GLU:HG3	1:36:A:TRP:HH2	4	1.03
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD1	10	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD2	10	1.03
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD1	12	1.03
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD2	12	1.03
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	3	1.03
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	10	1.02
(1,1654)	1:42:A:THR:HA	1:43:A:LYS:HD3	10	1.02
(1,1626)	1:7:A:LYS:HA	1:26:A:LEU:HD11	7	1.02
(1,1626)	1:7:A:LYS:HA	1:26:A:LEU:HD12	7	1.02
(1,1626)	1:7:A:LYS:HA	1:26:A:LEU:HD13	7	1.02
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	8	1.02
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	8	1.02
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	8	1.02
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	10	1.02
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	10	1.02
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	10	1.02
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	9	1.02
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	9	1.02
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	9	1.02
(1,2288)	1:24:A:ILE:HG13	1:45:A:SER:HA	9	1.01
(1,2288)	1:24:A:ILE:HG13	1:45:A:SER:HA	12	1.01
(1,1626)	1:7:A:LYS:HA	1:26:A:LEU:HD11	8	1.01
(1,1626)	1:7:A:LYS:HA	1:26:A:LEU:HD12	8	1.01
(1,1626)	1:7:A:LYS:HA	1:26:A:LEU:HD13	8	1.01
(1,1071)	1:26:A:LEU:HD11	1:7:A:LYS:HG3	13	1.01
(1,1071)	1:26:A:LEU:HD12	1:7:A:LYS:HG3	13	1.01
(1,1071)	1:26:A:LEU:HD13	1:7:A:LYS:HG3	13	1.01
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	1	1.0
(1,721)	1:64:A:LEU:HB3	1:65:A:LEU:H	3	1.0
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	6	0.99
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	12	0.99
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	3	0.99
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	3	0.99
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	3	0.99
(1,878)	1:63:A:LYS:HD3	1:61:A:ASP:HB3	12	0.99
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	14	0.98
(1,2288)	1:64:A:LEU:HB3	1:60:A:PRO:HD3	4	0.98
(1,1626)	1:7:A:LYS:HA	1:26:A:LEU:HD11	13	0.98
(1,1626)	1:7:A:LYS:HA	1:26:A:LEU:HD12	13	0.98
(1,1626)	1:7:A:LYS:HA	1:26:A:LEU:HD13	13	0.98
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	2	0.97
(1,1833)	1:69:A:GLY:HA3	1:58:A:PHE:HB2	9	0.97
(1,721)	1:64:A:LEU:HB3	1:65:A:LEU:H	7	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	5	0.96
(1,2288)	1:24:A:ILE:HG13	1:45:A:SER:HA	1	0.96
(1,1797)	1:38:A:PHE:HA	1:85:A:VAL:HG11	9	0.96
(1,1797)	1:38:A:PHE:HA	1:85:A:VAL:HG12	9	0.96
(1,1797)	1:38:A:PHE:HA	1:85:A:VAL:HG13	9	0.96
(1,1018)	1:27:A:PRO:HD2	1:26:A:LEU:HD11	8	0.96
(1,1018)	1:27:A:PRO:HD2	1:26:A:LEU:HD12	8	0.96
(1,1018)	1:27:A:PRO:HD2	1:26:A:LEU:HD13	8	0.96
(1,2335)	1:53:A:VAL:HG11	1:54:A:GLU:HG3	14	0.95
(1,2335)	1:53:A:VAL:HG12	1:54:A:GLU:HG3	14	0.95
(1,2335)	1:53:A:VAL:HG13	1:54:A:GLU:HG3	14	0.95
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	13	0.95
(1,2288)	1:64:A:LEU:HB3	1:60:A:PRO:HD3	14	0.95
(1,1596)	1:78:A:LYS:HD3	1:78:A:LYS:HA	2	0.95
(1,1071)	1:26:A:LEU:HD11	1:7:A:LYS:HG3	7	0.95
(1,1071)	1:26:A:LEU:HD12	1:7:A:LYS:HG3	7	0.95
(1,1071)	1:26:A:LEU:HD13	1:7:A:LYS:HG3	7	0.95
(1,1018)	1:27:A:PRO:HD2	1:26:A:LEU:HD11	13	0.95
(1,1018)	1:27:A:PRO:HD2	1:26:A:LEU:HD12	13	0.95
(1,1018)	1:27:A:PRO:HD2	1:26:A:LEU:HD13	13	0.95
(1,1540)	1:18:A:VAL:HG11	1:3:A:HIS:HB2	13	0.94
(1,1540)	1:18:A:VAL:HG12	1:3:A:HIS:HB2	13	0.94
(1,1540)	1:18:A:VAL:HG13	1:3:A:HIS:HB2	13	0.94
(1,1071)	1:26:A:LEU:HD11	1:7:A:LYS:HG3	8	0.94
(1,1071)	1:26:A:LEU:HD12	1:7:A:LYS:HG3	8	0.94
(1,1071)	1:26:A:LEU:HD13	1:7:A:LYS:HG3	8	0.94
(1,1865)	1:24:A:ILE:HG21	1:26:A:LEU:HD21	7	0.93
(1,1865)	1:24:A:ILE:HG21	1:26:A:LEU:HD22	7	0.93
(1,1865)	1:24:A:ILE:HG21	1:26:A:LEU:HD23	7	0.93
(1,1865)	1:24:A:ILE:HG22	1:26:A:LEU:HD21	7	0.93
(1,1865)	1:24:A:ILE:HG22	1:26:A:LEU:HD22	7	0.93
(1,1865)	1:24:A:ILE:HG22	1:26:A:LEU:HD23	7	0.93
(1,1865)	1:24:A:ILE:HG23	1:26:A:LEU:HD21	7	0.93
(1,1865)	1:24:A:ILE:HG23	1:26:A:LEU:HD22	7	0.93
(1,1865)	1:24:A:ILE:HG23	1:26:A:LEU:HD23	7	0.93
(1,2335)	1:78:A:LYS:HG3	1:50:A:MET:HG2	10	0.92
(1,1934)	1:78:A:LYS:H	1:78:A:LYS:HD3	2	0.92
(1,878)	1:63:A:LYS:HD3	1:61:A:ASP:HB3	10	0.92
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	12	0.92
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	8	0.91
(1,1563)	1:26:A:LEU:HD11	1:10:A:ASN:HA	8	0.91
(1,1563)	1:26:A:LEU:HD12	1:10:A:ASN:HA	8	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1563)	1:26:A:LEU:HD13	1:10:A:ASN:HA	8	0.91
(1,1202)	1:26:A:LEU:HD11	1:7:A:LYS:HB3	7	0.91
(1,1202)	1:26:A:LEU:HD12	1:7:A:LYS:HB3	7	0.91
(1,1202)	1:26:A:LEU:HD13	1:7:A:LYS:HB3	7	0.91
(1,1202)	1:26:A:LEU:HD11	1:7:A:LYS:HB3	8	0.91
(1,1202)	1:26:A:LEU:HD12	1:7:A:LYS:HB3	8	0.91
(1,1202)	1:26:A:LEU:HD13	1:7:A:LYS:HB3	8	0.91
(1,1088)	1:63:A:LYS:HD3	1:65:A:LEU:H	7	0.91
(1,2315)	1:81:A:GLY:HA2	1:108:A:LYS:HA	9	0.9
(1,1534)	1:26:A:LEU:HD11	1:26:A:LEU:HA	7	0.9
(1,1534)	1:26:A:LEU:HD12	1:26:A:LEU:HA	7	0.9
(1,1534)	1:26:A:LEU:HD13	1:26:A:LEU:HA	7	0.9
(1,2386)	1:54:A:GLU:HA	1:55:A:ASN:HB3	10	0.89
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	6	0.89
(1,1534)	1:26:A:LEU:HD11	1:26:A:LEU:HA	8	0.89
(1,1534)	1:26:A:LEU:HD12	1:26:A:LEU:HA	8	0.89
(1,1534)	1:26:A:LEU:HD13	1:26:A:LEU:HA	8	0.89
(1,1955)	1:23:A:GLU:H	1:23:A:GLU:HG3	13	0.88
(1,1874)	1:38:A:PHE:HD1	1:85:A:VAL:HG11	9	0.88
(1,1874)	1:38:A:PHE:HD1	1:85:A:VAL:HG12	9	0.88
(1,1874)	1:38:A:PHE:HD1	1:85:A:VAL:HG13	9	0.88
(1,1874)	1:38:A:PHE:HD2	1:85:A:VAL:HG11	9	0.88
(1,1874)	1:38:A:PHE:HD2	1:85:A:VAL:HG12	9	0.88
(1,1874)	1:38:A:PHE:HD2	1:85:A:VAL:HG13	9	0.88
(1,1752)	1:56:A:LYS:HB3	1:72:A:HIS:HB3	5	0.88
(1,1563)	1:26:A:LEU:HD11	1:10:A:ASN:HA	7	0.88
(1,1563)	1:26:A:LEU:HD12	1:10:A:ASN:HA	7	0.88
(1,1563)	1:26:A:LEU:HD13	1:10:A:ASN:HA	7	0.88
(1,1534)	1:26:A:LEU:HD11	1:26:A:LEU:HA	13	0.88
(1,1534)	1:26:A:LEU:HD12	1:26:A:LEU:HA	13	0.88
(1,1534)	1:26:A:LEU:HD13	1:26:A:LEU:HA	13	0.88
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	7	0.88
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	7	0.88
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	7	0.88
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	14	0.88
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	14	0.88
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	14	0.88
(1,304)	1:61:A:ASP:HB3	1:62:A:SER:HA	15	0.88
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	13	0.87
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	13	0.87
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	13	0.87
(1,1202)	1:26:A:LEU:HD11	1:7:A:LYS:HB3	13	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1202)	1:26:A:LEU:HD12	1:7:A:LYS:HB3	13	0.87
(1,1202)	1:26:A:LEU:HD13	1:7:A:LYS:HB3	13	0.87
(1,1554)	1:44:A:GLU:HG3	1:43:A:LYS:HA	12	0.86
(1,1536)	1:87:A:LEU:HD11	1:26:A:LEU:HD21	13	0.86
(1,1536)	1:87:A:LEU:HD11	1:26:A:LEU:HD22	13	0.86
(1,1536)	1:87:A:LEU:HD11	1:26:A:LEU:HD23	13	0.86
(1,1536)	1:87:A:LEU:HD12	1:26:A:LEU:HD21	13	0.86
(1,1536)	1:87:A:LEU:HD12	1:26:A:LEU:HD22	13	0.86
(1,1536)	1:87:A:LEU:HD12	1:26:A:LEU:HD23	13	0.86
(1,1536)	1:87:A:LEU:HD13	1:26:A:LEU:HD21	13	0.86
(1,1536)	1:87:A:LEU:HD13	1:26:A:LEU:HD22	13	0.86
(1,1536)	1:87:A:LEU:HD13	1:26:A:LEU:HD23	13	0.86
(1,661)	1:91:A:ARG:HB3	1:90:A:MET:HB2	5	0.86
(1,661)	1:91:A:ARG:HB3	1:90:A:MET:HB2	11	0.86
(2,129)	1:66:A:GLY:H	1:68:A:GLY:HA3	2	0.85
(1,1752)	1:56:A:LYS:HB3	1:72:A:HIS:HB3	12	0.85
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	9	0.85
(1,2330)	1:70:A:THR:HG21	1:57:A:TYR:HB2	4	0.84
(1,2330)	1:70:A:THR:HG22	1:57:A:TYR:HB2	4	0.84
(1,2330)	1:70:A:THR:HG23	1:57:A:TYR:HB2	4	0.84
(1,1654)	1:42:A:THR:HA	1:43:A:LYS:HD3	13	0.84
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	13	0.84
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	13	0.84
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	13	0.84
(1,1088)	1:63:A:LYS:HD3	1:65:A:LEU:H	14	0.84
(1,368)	1:30:A:PRO:HG3	1:69:A:GLY:HA2	7	0.84
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	2	0.83
(1,1536)	1:87:A:LEU:HD11	1:26:A:LEU:HD21	7	0.83
(1,1536)	1:87:A:LEU:HD11	1:26:A:LEU:HD22	7	0.83
(1,1536)	1:87:A:LEU:HD11	1:26:A:LEU:HD23	7	0.83
(1,1536)	1:87:A:LEU:HD12	1:26:A:LEU:HD21	7	0.83
(1,1536)	1:87:A:LEU:HD12	1:26:A:LEU:HD22	7	0.83
(1,1536)	1:87:A:LEU:HD12	1:26:A:LEU:HD23	7	0.83
(1,1536)	1:87:A:LEU:HD13	1:26:A:LEU:HD21	7	0.83
(1,1536)	1:87:A:LEU:HD13	1:26:A:LEU:HD22	7	0.83
(1,1536)	1:87:A:LEU:HD13	1:26:A:LEU:HD23	7	0.83
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	14	0.83
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	14	0.83
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	14	0.83
(1,2321)	1:44:A:GLU:HG3	1:46:A:PRO:HD2	3	0.82
(1,2288)	1:64:A:LEU:HB3	1:60:A:PRO:HD3	7	0.82
(1,1654)	1:42:A:THR:HA	1:43:A:LYS:HD3	8	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1642)	1:67:A:ALA:HB1	1:60:A:PRO:HG2	6	0.82
(1,1642)	1:67:A:ALA:HB2	1:60:A:PRO:HG2	6	0.82
(1,1642)	1:67:A:ALA:HB3	1:60:A:PRO:HG2	6	0.82
(1,1540)	1:18:A:VAL:HG11	1:3:A:HIS:HB2	9	0.82
(1,1540)	1:18:A:VAL:HG12	1:3:A:HIS:HB2	9	0.82
(1,1540)	1:18:A:VAL:HG13	1:3:A:HIS:HB2	9	0.82
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	4	0.82
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	4	0.82
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	4	0.82
(1,721)	1:64:A:LEU:HB3	1:65:A:LEU:H	10	0.82
(1,570)	1:30:A:PRO:HD2	1:28:A:SER:HB2	7	0.82
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	4	0.82
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	4	0.82
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	15	0.81
(1,1536)	1:87:A:LEU:HD11	1:26:A:LEU:HD21	8	0.81
(1,1536)	1:87:A:LEU:HD11	1:26:A:LEU:HD22	8	0.81
(1,1536)	1:87:A:LEU:HD11	1:26:A:LEU:HD23	8	0.81
(1,1536)	1:87:A:LEU:HD12	1:26:A:LEU:HD21	8	0.81
(1,1536)	1:87:A:LEU:HD12	1:26:A:LEU:HD22	8	0.81
(1,1536)	1:87:A:LEU:HD12	1:26:A:LEU:HD23	8	0.81
(1,1536)	1:87:A:LEU:HD13	1:26:A:LEU:HD21	8	0.81
(1,1536)	1:87:A:LEU:HD13	1:26:A:LEU:HD22	8	0.81
(1,1536)	1:87:A:LEU:HD13	1:26:A:LEU:HD23	8	0.81
(1,1892)	1:38:A:PHE:HE1	1:53:A:VAL:HG11	3	0.8
(1,1892)	1:38:A:PHE:HE1	1:53:A:VAL:HG12	3	0.8
(1,1892)	1:38:A:PHE:HE1	1:53:A:VAL:HG13	3	0.8
(1,1892)	1:38:A:PHE:HE2	1:53:A:VAL:HG11	3	0.8
(1,1892)	1:38:A:PHE:HE2	1:53:A:VAL:HG12	3	0.8
(1,1892)	1:38:A:PHE:HE2	1:53:A:VAL:HG13	3	0.8
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	1	0.8
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	11	0.8
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	11	0.8
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	11	0.8
(1,1238)	1:53:A:VAL:HG11	1:52:A:THR:H	13	0.8
(1,1238)	1:53:A:VAL:HG12	1:52:A:THR:H	13	0.8
(1,1238)	1:53:A:VAL:HG13	1:52:A:THR:H	13	0.8
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	14	0.8
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	14	0.8
(1,2127)	1:73:A:PHE:H	1:85:A:VAL:HG11	9	0.79
(1,2127)	1:73:A:PHE:H	1:85:A:VAL:HG12	9	0.79
(1,2127)	1:73:A:PHE:H	1:85:A:VAL:HG13	9	0.79
(1,1554)	1:44:A:GLU:HG3	1:43:A:LYS:HA	1	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1554)	1:44:A:GLU:HG3	1:43:A:LYS:HA	6	0.79
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	4	0.78
(1,1554)	1:44:A:GLU:HG3	1:43:A:LYS:HA	9	0.78
(2,129)	1:66:A:GLY:H	1:68:A:GLY:HA3	3	0.77
(1,2442)	1:42:A:THR:HB	1:44:A:GLU:H	1	0.77
(1,1762)	1:14:A:LEU:HD11	1:16:A:VAL:H	10	0.77
(1,1762)	1:14:A:LEU:HD12	1:16:A:VAL:H	10	0.77
(1,1762)	1:14:A:LEU:HD13	1:16:A:VAL:H	10	0.77
(1,1059)	1:78:A:LYS:HD3	1:50:A:MET:HG3	8	0.77
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	11	0.77
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	11	0.77
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	11	0.77
(1,848)	1:23:A:GLU:HA	1:21:A:LEU:HD11	3	0.77
(1,848)	1:23:A:GLU:HA	1:21:A:LEU:HD12	3	0.77
(1,848)	1:23:A:GLU:HA	1:21:A:LEU:HD13	3	0.77
(1,628)	1:65:A:LEU:HG	1:60:A:PRO:HB3	2	0.77
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	1	0.76
(1,1563)	1:26:A:LEU:HD11	1:10:A:ASN:HA	13	0.76
(1,1563)	1:26:A:LEU:HD12	1:10:A:ASN:HA	13	0.76
(1,1563)	1:26:A:LEU:HD13	1:10:A:ASN:HA	13	0.76
(1,1259)	1:4:A:LYS:HB3	1:3:A:HIS:HB3	3	0.76
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	11	0.76
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	11	0.76
(1,2413)	1:31:A:THR:HG21	1:89:A:TYR:HB3	2	0.75
(1,2413)	1:31:A:THR:HG22	1:89:A:TYR:HB3	2	0.75
(1,2413)	1:31:A:THR:HG23	1:89:A:TYR:HB3	2	0.75
(1,1833)	1:69:A:GLY:HA3	1:58:A:PHE:HB2	12	0.75
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	5	0.75
(1,721)	1:64:A:LEU:HB3	1:65:A:LEU:H	11	0.75
(1,1702)	1:64:A:LEU:HD11	1:61:A:ASP:HB3	15	0.74
(1,1702)	1:64:A:LEU:HD12	1:61:A:ASP:HB3	15	0.74
(1,1702)	1:64:A:LEU:HD13	1:61:A:ASP:HB3	15	0.74
(1,1238)	1:53:A:VAL:HG11	1:52:A:THR:H	2	0.74
(1,1238)	1:53:A:VAL:HG12	1:52:A:THR:H	2	0.74
(1,1238)	1:53:A:VAL:HG13	1:52:A:THR:H	2	0.74
(1,1238)	1:53:A:VAL:HG11	1:52:A:THR:H	4	0.74
(1,1238)	1:53:A:VAL:HG12	1:52:A:THR:H	4	0.74
(1,1238)	1:53:A:VAL:HG13	1:52:A:THR:H	4	0.74
(1,1088)	1:63:A:LYS:HD3	1:65:A:LEU:H	3	0.74
(1,1040)	1:9:A:HIS:HB2	1:6:A:THR:H	15	0.74
(2,113)	1:91:A:ARG:HG3	1:92:A:PRO:HG2	10	0.73
(1,2370)	1:25:A:GLN:HB3	1:26:A:LEU:H	8	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	7	0.72
(1,2039)	1:45:A:SER:H	1:53:A:VAL:HG11	4	0.72
(1,2039)	1:45:A:SER:H	1:53:A:VAL:HG12	4	0.72
(1,2039)	1:45:A:SER:H	1:53:A:VAL:HG13	4	0.72
(1,1554)	1:44:A:GLU:HG3	1:43:A:LYS:HA	3	0.72
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD11	6	0.72
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD12	6	0.72
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD13	6	0.72
(1,2486)	1:16:A:VAL:HB	1:110:A:ASN:HD21	11	0.71
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG21	12	0.71
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG22	12	0.71
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG23	12	0.71
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	11	0.71
(1,1672)	1:75:A:VAL:HG21	1:22:A:VAL:H	8	0.71
(1,1672)	1:75:A:VAL:HG22	1:22:A:VAL:H	8	0.71
(1,1672)	1:75:A:VAL:HG23	1:22:A:VAL:H	8	0.71
(1,1046)	1:109:A:ALA:HA	1:18:A:VAL:HG11	3	0.71
(1,1046)	1:109:A:ALA:HA	1:18:A:VAL:HG12	3	0.71
(1,1046)	1:109:A:ALA:HA	1:18:A:VAL:HG13	3	0.71
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD11	7	0.71
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD12	7	0.71
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD13	7	0.71
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD11	15	0.71
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD12	15	0.71
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD13	15	0.71
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	5	0.71
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	6	0.71
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	10	0.71
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	15	0.71
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	15	0.71
(1,2377)	1:7:A:LYS:HA	1:103:A:PHE:HD1	15	0.7
(1,2377)	1:7:A:LYS:HA	1:103:A:PHE:HD2	15	0.7
(1,2288)	1:24:A:ILE:HG13	1:45:A:SER:HA	11	0.7
(1,2258)	1:18:A:VAL:HG11	1:21:A:LEU:HA	1	0.7
(1,2258)	1:18:A:VAL:HG12	1:21:A:LEU:HA	1	0.7
(1,2258)	1:18:A:VAL:HG13	1:21:A:LEU:HA	1	0.7
(1,1642)	1:67:A:ALA:HB1	1:60:A:PRO:HG2	12	0.7
(1,1642)	1:67:A:ALA:HB2	1:60:A:PRO:HG2	12	0.7
(1,1642)	1:67:A:ALA:HB3	1:60:A:PRO:HG2	12	0.7
(1,1554)	1:44:A:GLU:HG3	1:43:A:LYS:HA	8	0.7
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD11	5	0.7
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD12	5	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD13	5	0.7
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	3	0.7
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	4	0.7
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	13	0.7
(1,570)	1:30:A:PRO:HD2	1:28:A:SER:HB2	12	0.7
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	3	0.69
(1,2276)	1:27:A:PRO:HG2	1:29:A:ASN:HB3	11	0.69
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	5	0.69
(1,2039)	1:45:A:SER:H	1:53:A:VAL:HG11	13	0.69
(1,2039)	1:45:A:SER:H	1:53:A:VAL:HG12	13	0.69
(1,2039)	1:45:A:SER:H	1:53:A:VAL:HG13	13	0.69
(1,1897)	1:36:A:TRP:HD1	1:57:A:TYR:HB2	7	0.69
(1,1259)	1:4:A:LYS:HB3	1:3:A:HIS:HB3	14	0.69
(1,1088)	1:63:A:LYS:HD3	1:65:A:LEU:H	15	0.69
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD1	4	0.69
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD2	4	0.69
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD11	8	0.69
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD12	8	0.69
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD13	8	0.69
(1,207)	1:56:A:LYS:HD3	1:74:A:HIS:HD2	12	0.69
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD1	4	0.69
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD2	4	0.69
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD1	12	0.68
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD2	12	0.68
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	14	0.68
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG21	2	0.68
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG22	2	0.68
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG23	2	0.68
(1,1559)	1:101:A:GLU:HG3	1:36:A:TRP:HH2	15	0.68
(1,852)	1:14:A:LEU:HD11	1:14:A:LEU:H	10	0.68
(1,852)	1:14:A:LEU:HD12	1:14:A:LEU:H	10	0.68
(1,852)	1:14:A:LEU:HD13	1:14:A:LEU:H	10	0.68
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	1	0.68
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	15	0.68
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	9	0.67
(1,2276)	1:27:A:PRO:HG2	1:29:A:ASN:HB3	12	0.67
(1,2260)	1:21:A:LEU:HD11	1:23:A:GLU:HA	3	0.67
(1,2260)	1:21:A:LEU:HD12	1:23:A:GLU:HA	3	0.67
(1,2260)	1:21:A:LEU:HD13	1:23:A:GLU:HA	3	0.67
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG21	5	0.66
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG22	5	0.66
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG23	5	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2276)	1:27:A:PRO:HG2	1:29:A:ASN:HB3	3	0.66
(1,1543)	1:14:A:LEU:HB2	1:14:A:LEU:H	14	0.66
(1,1011)	1:63:A:LYS:HD3	1:63:A:LYS:H	7	0.66
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	12	0.65
(1,2522)	1:52:A:THR:HG21	1:54:A:GLU:HB2	11	0.65
(1,2522)	1:52:A:THR:HG22	1:54:A:GLU:HB2	11	0.65
(1,2522)	1:52:A:THR:HG23	1:54:A:GLU:HB2	11	0.65
(1,2063)	1:47:A:ASN:H	1:48:A:GLU:HB3	14	0.65
(1,1623)	1:28:A:SER:HB2	1:71:A:GLU:HG3	3	0.65
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	2	0.65
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	2	0.65
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	2	0.65
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	8	0.65
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	9	0.65
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD1	8	0.65
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD2	8	0.65
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE1	7	0.64
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE2	7	0.64
(1,2529)	1:28:A:SER:HB3	1:71:A:GLU:HB3	11	0.64
(1,2288)	1:24:A:ILE:HG13	1:45:A:SER:HA	8	0.64
(1,1676)	1:47:A:ASN:HA	1:48:A:GLU:HB3	14	0.64
(1,1543)	1:14:A:LEU:HB2	1:14:A:LEU:H	8	0.64
(1,1433)	1:46:A:PRO:HB3	1:48:A:GLU:H	15	0.64
(1,854)	1:85:A:VAL:HG11	1:86:A:ASN:HD22	9	0.64
(1,854)	1:85:A:VAL:HG12	1:86:A:ASN:HD22	9	0.64
(1,854)	1:85:A:VAL:HG13	1:86:A:ASN:HD22	9	0.64
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	11	0.64
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	14	0.64
(1,661)	1:91:A:ARG:HB3	1:90:A:MET:HB2	7	0.64
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	14	0.64
(2,101)	1:47:A:ASN:HB3	1:48:A:GLU:HB3	15	0.63
(1,2532)	1:5:A:VAL:H	1:23:A:GLU:HB2	13	0.63
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG21	10	0.63
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG22	10	0.63
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG23	10	0.63
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG21	15	0.63
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG22	15	0.63
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG23	15	0.63
(1,2203)	1:85:A:VAL:HG21	1:83:A:HIS:HD2	9	0.63
(1,2203)	1:85:A:VAL:HG22	1:83:A:HIS:HD2	9	0.63
(1,2203)	1:85:A:VAL:HG23	1:83:A:HIS:HD2	9	0.63
(1,2131)	1:37:A:TYR:H	1:90:A:MET:HG2	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1543)	1:14:A:LEU:HB2	1:14:A:LEU:H	3	0.63
(1,1543)	1:14:A:LEU:HB2	1:14:A:LEU:H	9	0.63
(1,1433)	1:46:A:PRO:HB3	1:48:A:GLU:H	8	0.63
(1,1401)	1:85:A:VAL:HG21	1:83:A:HIS:HD2	9	0.63
(1,1401)	1:85:A:VAL:HG22	1:83:A:HIS:HD2	9	0.63
(1,1401)	1:85:A:VAL:HG23	1:83:A:HIS:HD2	9	0.63
(1,223)	1:4:A:LYS:HG3	1:3:A:HIS:HE1	14	0.63
(1,8)	1:85:A:VAL:HG21	1:107:A:LEU:H	9	0.63
(1,8)	1:85:A:VAL:HG22	1:107:A:LEU:H	9	0.63
(1,8)	1:85:A:VAL:HG23	1:107:A:LEU:H	9	0.63
(1,2288)	1:64:A:LEU:HB3	1:60:A:PRO:HD3	6	0.62
(1,2258)	1:18:A:VAL:HG11	1:21:A:LEU:HA	2	0.62
(1,2258)	1:18:A:VAL:HG12	1:21:A:LEU:HA	2	0.62
(1,2258)	1:18:A:VAL:HG13	1:21:A:LEU:HA	2	0.62
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	14	0.62
(1,1854)	1:50:A:MET:HG3	1:77:A:VAL:HA	12	0.62
(1,1801)	1:27:A:PRO:HG3	1:26:A:LEU:HD11	7	0.62
(1,1801)	1:27:A:PRO:HG3	1:26:A:LEU:HD12	7	0.62
(1,1801)	1:27:A:PRO:HG3	1:26:A:LEU:HD13	7	0.62
(1,1543)	1:14:A:LEU:HB2	1:14:A:LEU:H	5	0.62
(1,1543)	1:14:A:LEU:HB2	1:14:A:LEU:H	6	0.62
(1,1543)	1:14:A:LEU:HB2	1:14:A:LEU:H	7	0.62
(1,1494)	1:26:A:LEU:HD21	1:26:A:LEU:HB2	13	0.62
(1,1494)	1:26:A:LEU:HD22	1:26:A:LEU:HB2	13	0.62
(1,1494)	1:26:A:LEU:HD23	1:26:A:LEU:HB2	13	0.62
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	3	0.62
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	7	0.62
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	10	0.62
(1,1034)	1:108:A:LYS:HB2	1:110:A:ASN:HD22	6	0.62
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	12	0.62
(1,2276)	1:27:A:PRO:HG2	1:29:A:ASN:HB3	15	0.61
(1,2258)	1:18:A:VAL:HG11	1:21:A:LEU:HA	8	0.61
(1,2258)	1:18:A:VAL:HG12	1:21:A:LEU:HA	8	0.61
(1,2258)	1:18:A:VAL:HG13	1:21:A:LEU:HA	8	0.61
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	4	0.61
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	2	0.61
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	4	0.61
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	5	0.61
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	6	0.61
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	9	0.61
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	12	0.61
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	13	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1027)	1:27:A:PRO:HD3	1:26:A:LEU:HD11	7	0.61
(1,1027)	1:27:A:PRO:HD3	1:26:A:LEU:HD12	7	0.61
(1,1027)	1:27:A:PRO:HD3	1:26:A:LEU:HD13	7	0.61
(1,734)	1:108:A:LYS:HG3	1:109:A:ALA:H	7	0.61
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG21	13	0.6
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG22	13	0.6
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG23	13	0.6
(1,2258)	1:18:A:VAL:HG11	1:21:A:LEU:HA	12	0.6
(1,2258)	1:18:A:VAL:HG12	1:21:A:LEU:HA	12	0.6
(1,2258)	1:18:A:VAL:HG13	1:21:A:LEU:HA	12	0.6
(1,2185)	1:43:A:LYS:HD3	1:73:A:PHE:HD1	14	0.6
(1,2185)	1:43:A:LYS:HD3	1:73:A:PHE:HD2	14	0.6
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	4	0.6
(1,1543)	1:14:A:LEU:HB2	1:14:A:LEU:H	12	0.6
(1,1494)	1:26:A:LEU:HD21	1:26:A:LEU:HB2	8	0.6
(1,1494)	1:26:A:LEU:HD22	1:26:A:LEU:HB2	8	0.6
(1,1494)	1:26:A:LEU:HD23	1:26:A:LEU:HB2	8	0.6
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	14	0.6
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	15	0.6
(1,1027)	1:27:A:PRO:HD3	1:26:A:LEU:HD11	8	0.6
(1,1027)	1:27:A:PRO:HD3	1:26:A:LEU:HD12	8	0.6
(1,1027)	1:27:A:PRO:HD3	1:26:A:LEU:HD13	8	0.6
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD21	3	0.6
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD22	3	0.6
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD23	3	0.6
(1,733)	1:99:A:ASP:HB3	1:99:A:ASP:H	9	0.6
(1,570)	1:30:A:PRO:HD2	1:28:A:SER:HB2	9	0.6
(1,2453)	1:31:A:THR:HG21	1:36:A:TRP:HZ2	2	0.59
(1,2453)	1:31:A:THR:HG22	1:36:A:TRP:HZ2	2	0.59
(1,2453)	1:31:A:THR:HG23	1:36:A:TRP:HZ2	2	0.59
(1,2258)	1:18:A:VAL:HG11	1:21:A:LEU:HA	5	0.59
(1,2258)	1:18:A:VAL:HG12	1:21:A:LEU:HA	5	0.59
(1,2258)	1:18:A:VAL:HG13	1:21:A:LEU:HA	5	0.59
(1,2258)	1:18:A:VAL:HG11	1:21:A:LEU:HA	10	0.59
(1,2258)	1:18:A:VAL:HG12	1:21:A:LEU:HA	10	0.59
(1,2258)	1:18:A:VAL:HG13	1:21:A:LEU:HA	10	0.59
(1,2258)	1:18:A:VAL:HG11	1:21:A:LEU:HA	15	0.59
(1,2258)	1:18:A:VAL:HG12	1:21:A:LEU:HA	15	0.59
(1,2258)	1:18:A:VAL:HG13	1:21:A:LEU:HA	15	0.59
(1,2232)	1:12:A:ALA:HB1	1:106:A:TYR:HA	14	0.59
(1,2232)	1:12:A:ALA:HB2	1:106:A:TYR:HA	14	0.59
(1,2232)	1:12:A:ALA:HB3	1:106:A:TYR:HA	14	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1997)	1:61:A:ASP:H	1:60:A:PRO:HG2	4	0.59
(1,1559)	1:101:A:GLU:HG3	1:36:A:TRP:HH2	7	0.59
(1,1494)	1:26:A:LEU:HD21	1:26:A:LEU:HB2	7	0.59
(1,1494)	1:26:A:LEU:HD22	1:26:A:LEU:HB2	7	0.59
(1,1494)	1:26:A:LEU:HD23	1:26:A:LEU:HB2	7	0.59
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	1	0.59
(1,1259)	1:4:A:LYS:HB3	1:3:A:HIS:HB3	12	0.59
(1,1059)	1:78:A:LYS:HD3	1:50:A:MET:HG3	10	0.59
(1,1046)	1:109:A:ALA:HA	1:18:A:VAL:HG11	9	0.59
(1,1046)	1:109:A:ALA:HA	1:18:A:VAL:HG12	9	0.59
(1,1046)	1:109:A:ALA:HA	1:18:A:VAL:HG13	9	0.59
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD21	1	0.59
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD22	1	0.59
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD23	1	0.59
(1,359)	1:108:A:LYS:HD3	1:15:A:THR:HA	7	0.59
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	13	0.59
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	13	0.59
(2,129)	1:66:A:GLY:H	1:68:A:GLY:HA3	1	0.58
(1,2276)	1:27:A:PRO:HG2	1:29:A:ASN:HB3	7	0.58
(1,2258)	1:18:A:VAL:HG11	1:21:A:LEU:HA	7	0.58
(1,2258)	1:18:A:VAL:HG12	1:21:A:LEU:HA	7	0.58
(1,2258)	1:18:A:VAL:HG13	1:21:A:LEU:HA	7	0.58
(1,1734)	1:26:A:LEU:HD11	1:6:A:THR:HG21	8	0.58
(1,1734)	1:26:A:LEU:HD11	1:6:A:THR:HG22	8	0.58
(1,1734)	1:26:A:LEU:HD11	1:6:A:THR:HG23	8	0.58
(1,1734)	1:26:A:LEU:HD12	1:6:A:THR:HG21	8	0.58
(1,1734)	1:26:A:LEU:HD12	1:6:A:THR:HG22	8	0.58
(1,1734)	1:26:A:LEU:HD12	1:6:A:THR:HG23	8	0.58
(1,1734)	1:26:A:LEU:HD13	1:6:A:THR:HG21	8	0.58
(1,1734)	1:26:A:LEU:HD13	1:6:A:THR:HG22	8	0.58
(1,1734)	1:26:A:LEU:HD13	1:6:A:THR:HG23	8	0.58
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	2	0.58
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	2	0.58
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	2	0.58
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	11	0.58
(1,1027)	1:27:A:PRO:HD3	1:26:A:LEU:HD11	13	0.58
(1,1027)	1:27:A:PRO:HD3	1:26:A:LEU:HD12	13	0.58
(1,1027)	1:27:A:PRO:HD3	1:26:A:LEU:HD13	13	0.58
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG21	6	0.57
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG22	6	0.57
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG23	6	0.57
(1,1801)	1:27:A:PRO:HG3	1:26:A:LEU:HD11	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1801)	1:27:A:PRO:HG3	1:26:A:LEU:HD12	8	0.57
(1,1801)	1:27:A:PRO:HG3	1:26:A:LEU:HD13	8	0.57
(1,1543)	1:14:A:LEU:HB2	1:14:A:LEU:H	15	0.57
(1,1428)	1:56:A:LYS:HD3	1:57:A:TYR:HD1	1	0.57
(1,1428)	1:56:A:LYS:HD3	1:57:A:TYR:HD2	1	0.57
(1,1046)	1:109:A:ALA:HA	1:18:A:VAL:HG11	13	0.57
(1,1046)	1:109:A:ALA:HA	1:18:A:VAL:HG12	13	0.57
(1,1046)	1:109:A:ALA:HA	1:18:A:VAL:HG13	13	0.57
(2,129)	1:66:A:GLY:H	1:68:A:GLY:HA3	7	0.56
(2,112)	1:46:A:PRO:HD2	1:48:A:GLU:HB3	14	0.56
(2,50)	1:57:A:TYR:HB3	1:58:A:PHE:HD1	5	0.56
(2,50)	1:57:A:TYR:HB3	1:58:A:PHE:HD2	5	0.56
(1,2410)	1:77:A:VAL:HG11	1:47:A:ASN:HB3	15	0.56
(1,2410)	1:77:A:VAL:HG12	1:47:A:ASN:HB3	15	0.56
(1,2410)	1:77:A:VAL:HG13	1:47:A:ASN:HB3	15	0.56
(1,2258)	1:18:A:VAL:HG11	1:21:A:LEU:HA	6	0.56
(1,2258)	1:18:A:VAL:HG12	1:21:A:LEU:HA	6	0.56
(1,2258)	1:18:A:VAL:HG13	1:21:A:LEU:HA	6	0.56
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	12	0.56
(1,1970)	1:19:A:GLY:H	1:18:A:VAL:HG11	9	0.56
(1,1970)	1:19:A:GLY:H	1:18:A:VAL:HG12	9	0.56
(1,1970)	1:19:A:GLY:H	1:18:A:VAL:HG13	9	0.56
(1,1970)	1:19:A:GLY:H	1:18:A:VAL:HG11	13	0.56
(1,1970)	1:19:A:GLY:H	1:18:A:VAL:HG12	13	0.56
(1,1970)	1:19:A:GLY:H	1:18:A:VAL:HG13	13	0.56
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	3	0.56
(1,1633)	1:69:A:GLY:HA2	1:60:A:PRO:HG3	5	0.56
(1,1532)	1:50:A:MET:HE1	1:78:A:LYS:HD3	8	0.56
(1,1532)	1:50:A:MET:HE2	1:78:A:LYS:HD3	8	0.56
(1,1532)	1:50:A:MET:HE3	1:78:A:LYS:HD3	8	0.56
(1,734)	1:108:A:LYS:HG3	1:109:A:ALA:H	8	0.56
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	2	0.56
(1,471)	1:92:A:PRO:HG2	1:33:A:GLY:HA2	13	0.56
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG21	4	0.55
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG22	4	0.55
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG23	4	0.55
(1,2276)	1:75:A:VAL:HB	1:46:A:PRO:HD3	1	0.55
(1,2258)	1:18:A:VAL:HG11	1:21:A:LEU:HA	4	0.55
(1,2258)	1:18:A:VAL:HG12	1:21:A:LEU:HA	4	0.55
(1,2258)	1:18:A:VAL:HG13	1:21:A:LEU:HA	4	0.55
(1,1997)	1:61:A:ASP:H	1:60:A:PRO:HG2	14	0.55
(1,1955)	1:23:A:GLU:H	1:23:A:GLU:HG3	15	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	2	0.55
(1,1734)	1:26:A:LEU:HD11	1:6:A:THR:HG21	7	0.55
(1,1734)	1:26:A:LEU:HD11	1:6:A:THR:HG22	7	0.55
(1,1734)	1:26:A:LEU:HD11	1:6:A:THR:HG23	7	0.55
(1,1734)	1:26:A:LEU:HD12	1:6:A:THR:HG21	7	0.55
(1,1734)	1:26:A:LEU:HD12	1:6:A:THR:HG22	7	0.55
(1,1734)	1:26:A:LEU:HD12	1:6:A:THR:HG23	7	0.55
(1,1734)	1:26:A:LEU:HD13	1:6:A:THR:HG21	7	0.55
(1,1734)	1:26:A:LEU:HD13	1:6:A:THR:HG22	7	0.55
(1,1734)	1:26:A:LEU:HD13	1:6:A:THR:HG23	7	0.55
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	6	0.55
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	6	0.55
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	6	0.55
(1,1702)	1:64:A:LEU:HD11	1:61:A:ASP:HB3	1	0.55
(1,1702)	1:64:A:LEU:HD12	1:61:A:ASP:HB3	1	0.55
(1,1702)	1:64:A:LEU:HD13	1:61:A:ASP:HB3	1	0.55
(1,1673)	1:42:A:THR:HB	1:39:A:GLU:HG3	3	0.55
(2,94)	1:65:A:LEU:HG	1:60:A:PRO:HD3	5	0.54
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	1	0.54
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	15	0.54
(1,2522)	1:52:A:THR:HG21	1:54:A:GLU:HB2	9	0.54
(1,2522)	1:52:A:THR:HG22	1:54:A:GLU:HB2	9	0.54
(1,2522)	1:52:A:THR:HG23	1:54:A:GLU:HB2	9	0.54
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG11	13	0.54
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG12	13	0.54
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG13	13	0.54
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG11	13	0.54
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG12	13	0.54
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG13	13	0.54
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG11	13	0.54
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG12	13	0.54
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG13	13	0.54
(1,2276)	1:75:A:VAL:HB	1:46:A:PRO:HD3	6	0.54
(1,1833)	1:69:A:GLY:HA3	1:58:A:PHE:HB2	4	0.54
(1,1801)	1:27:A:PRO:HG3	1:26:A:LEU:HD11	13	0.54
(1,1801)	1:27:A:PRO:HG3	1:26:A:LEU:HD12	13	0.54
(1,1801)	1:27:A:PRO:HG3	1:26:A:LEU:HD13	13	0.54
(1,822)	1:18:A:VAL:HG11	1:18:A:VAL:H	9	0.54
(1,822)	1:18:A:VAL:HG12	1:18:A:VAL:H	9	0.54
(1,822)	1:18:A:VAL:HG13	1:18:A:VAL:H	9	0.54
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB1	13	0.54
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB2	13	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB3	13	0.54
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB1	13	0.54
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB2	13	0.54
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB3	13	0.54
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB1	13	0.54
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB2	13	0.54
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB3	13	0.54
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	12	0.54
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	12	0.54
(1,2453)	1:31:A:THR:HG21	1:36:A:TRP:HZ2	14	0.53
(1,2453)	1:31:A:THR:HG22	1:36:A:TRP:HZ2	14	0.53
(1,2453)	1:31:A:THR:HG23	1:36:A:TRP:HZ2	14	0.53
(1,2340)	1:75:A:VAL:HG11	1:22:A:VAL:HB	15	0.53
(1,2340)	1:75:A:VAL:HG12	1:22:A:VAL:HB	15	0.53
(1,2340)	1:75:A:VAL:HG13	1:22:A:VAL:HB	15	0.53
(1,2335)	1:53:A:VAL:HG11	1:54:A:GLU:HG3	8	0.53
(1,2335)	1:53:A:VAL:HG12	1:54:A:GLU:HG3	8	0.53
(1,2335)	1:53:A:VAL:HG13	1:54:A:GLU:HG3	8	0.53
(1,2274)	1:27:A:PRO:HG3	1:29:A:ASN:HB3	7	0.53
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	10	0.53
(1,1734)	1:26:A:LEU:HD11	1:6:A:THR:HG21	13	0.53
(1,1734)	1:26:A:LEU:HD11	1:6:A:THR:HG22	13	0.53
(1,1734)	1:26:A:LEU:HD11	1:6:A:THR:HG23	13	0.53
(1,1734)	1:26:A:LEU:HD12	1:6:A:THR:HG21	13	0.53
(1,1734)	1:26:A:LEU:HD12	1:6:A:THR:HG22	13	0.53
(1,1734)	1:26:A:LEU:HD12	1:6:A:THR:HG23	13	0.53
(1,1734)	1:26:A:LEU:HD13	1:6:A:THR:HG21	13	0.53
(1,1734)	1:26:A:LEU:HD13	1:6:A:THR:HG22	13	0.53
(1,1734)	1:26:A:LEU:HD13	1:6:A:THR:HG23	13	0.53
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	11	0.53
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	11	0.53
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	11	0.53
(1,1559)	1:101:A:GLU:HG3	1:36:A:TRP:HH2	9	0.53
(1,1088)	1:63:A:LYS:HD3	1:65:A:LEU:H	10	0.53
(1,658)	1:94:A:THR:HG21	1:90:A:MET:HB2	11	0.53
(1,658)	1:94:A:THR:HG22	1:90:A:MET:HB2	11	0.53
(1,658)	1:94:A:THR:HG23	1:90:A:MET:HB2	11	0.53
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	10	0.52
(1,2453)	1:31:A:THR:HG21	1:36:A:TRP:HZ2	3	0.52
(1,2453)	1:31:A:THR:HG22	1:36:A:TRP:HZ2	3	0.52
(1,2453)	1:31:A:THR:HG23	1:36:A:TRP:HZ2	3	0.52
(1,2420)	1:30:A:PRO:HA	1:34:A:PHE:HB2	7	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	13	0.52
(1,1854)	1:50:A:MET:HG3	1:77:A:VAL:HA	10	0.52
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	7	0.52
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	7	0.52
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	7	0.52
(1,1680)	1:41:A:GLY:HA3	1:37:A:TYR:HB2	9	0.52
(1,722)	1:4:A:LYS:HD3	1:4:A:LYS:HE3	6	0.52
(1,722)	1:4:A:LYS:HD3	1:4:A:LYS:HE3	7	0.52
(1,722)	1:4:A:LYS:HD3	1:4:A:LYS:HE3	8	0.52
(1,722)	1:4:A:LYS:HD3	1:4:A:LYS:HE3	12	0.52
(1,722)	1:4:A:LYS:HD3	1:4:A:LYS:HE3	13	0.52
(1,597)	1:78:A:LYS:HD3	1:78:A:LYS:HE3	12	0.52
(1,597)	1:78:A:LYS:HD3	1:78:A:LYS:HE3	13	0.52
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	2	0.52
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	11	0.52
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	15	0.52
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD1	12	0.52
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD2	12	0.52
(2,107)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	4	0.51
(1,2486)	1:16:A:VAL:HB	1:110:A:ASN:HD21	13	0.51
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG21	9	0.51
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG22	9	0.51
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG23	9	0.51
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	1	0.51
(1,2329)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	4	0.51
(1,2131)	1:37:A:TYR:H	1:90:A:MET:HG2	6	0.51
(1,2084)	1:69:A:GLY:H	1:60:A:PRO:HG3	8	0.51
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	7	0.51
(1,1854)	1:50:A:MET:HG3	1:77:A:VAL:HA	4	0.51
(1,1854)	1:50:A:MET:HG3	1:77:A:VAL:HA	8	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	3	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	3	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	3	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	4	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	4	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	4	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	5	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	5	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	5	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	9	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	9	0.51
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	9	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1704)	1:26:A:LEU:HD11	1:6:A:THR:HA	8	0.51
(1,1704)	1:26:A:LEU:HD12	1:6:A:THR:HA	8	0.51
(1,1704)	1:26:A:LEU:HD13	1:6:A:THR:HA	8	0.51
(1,1702)	1:64:A:LEU:HD11	1:61:A:ASP:HB3	2	0.51
(1,1702)	1:64:A:LEU:HD12	1:61:A:ASP:HB3	2	0.51
(1,1702)	1:64:A:LEU:HD13	1:61:A:ASP:HB3	2	0.51
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD21	3	0.51
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD22	3	0.51
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD23	3	0.51
(1,1588)	1:70:A:THR:HB	1:58:A:PHE:HB2	12	0.51
(1,1543)	1:14:A:LEU:HB2	1:14:A:LEU:H	4	0.51
(1,1525)	1:26:A:LEU:HD11	1:7:A:LYS:HD3	6	0.51
(1,1525)	1:26:A:LEU:HD12	1:7:A:LYS:HD3	6	0.51
(1,1525)	1:26:A:LEU:HD13	1:7:A:LYS:HD3	6	0.51
(1,1318)	1:26:A:LEU:HD11	1:25:A:GLN:HE22	7	0.51
(1,1318)	1:26:A:LEU:HD12	1:25:A:GLN:HE22	7	0.51
(1,1318)	1:26:A:LEU:HD13	1:25:A:GLN:HE22	7	0.51
(1,1059)	1:78:A:LYS:HD3	1:50:A:MET:HG3	13	0.51
(1,1034)	1:108:A:LYS:HB2	1:110:A:ASN:HD22	13	0.51
(1,722)	1:4:A:LYS:HD3	1:4:A:LYS:HE3	2	0.51
(1,722)	1:4:A:LYS:HD3	1:4:A:LYS:HE3	3	0.51
(1,722)	1:4:A:LYS:HD3	1:4:A:LYS:HE3	4	0.51
(1,722)	1:4:A:LYS:HD3	1:4:A:LYS:HE3	5	0.51
(1,722)	1:4:A:LYS:HD3	1:4:A:LYS:HE3	14	0.51
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	6	0.5
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG21	14	0.5
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG22	14	0.5
(1,2363)	1:74:A:HIS:HA	1:75:A:VAL:HG23	14	0.5
(1,2131)	1:37:A:TYR:H	1:90:A:MET:HG2	11	0.5
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	1	0.5
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	1	0.5
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	1	0.5
(1,821)	1:28:A:SER:HB3	1:29:A:ASN:H	3	0.5
(2,75)	1:107:A:LEU:HB3	1:83:A:HIS:HB2	12	0.49
(1,2420)	1:30:A:PRO:HA	1:34:A:PHE:HB2	8	0.49
(1,2276)	1:27:A:PRO:HG2	1:29:A:ASN:HB3	14	0.49
(1,1847)	1:55:A:ASN:HA	1:56:A:LYS:HG3	10	0.49
(1,1752)	1:56:A:LYS:HB3	1:72:A:HIS:HB3	9	0.49
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	13	0.49
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	13	0.49
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	13	0.49
(1,1654)	1:42:A:THR:HA	1:43:A:LYS:HD3	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1059)	1:78:A:LYS:HD3	1:50:A:MET:HG3	3	0.49
(1,878)	1:63:A:LYS:HD3	1:61:A:ASP:HB3	5	0.49
(1,718)	1:96:A:PRO:HA	1:96:A:PRO:HB2	7	0.49
(1,368)	1:30:A:PRO:HG3	1:69:A:GLY:HA2	13	0.49
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD1	13	0.49
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD2	13	0.49
(1,144)	1:12:A:ALA:HA	1:9:A:HIS:HD2	15	0.49
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	2	0.48
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	4	0.48
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE1	14	0.48
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE2	14	0.48
(1,2413)	1:31:A:THR:HG21	1:89:A:TYR:HB3	14	0.48
(1,2413)	1:31:A:THR:HG22	1:89:A:TYR:HB3	14	0.48
(1,2413)	1:31:A:THR:HG23	1:89:A:TYR:HB3	14	0.48
(1,2390)	1:75:A:VAL:HG21	1:83:A:HIS:HB3	10	0.48
(1,2390)	1:75:A:VAL:HG22	1:83:A:HIS:HB3	10	0.48
(1,2390)	1:75:A:VAL:HG23	1:83:A:HIS:HB3	10	0.48
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	9	0.48
(1,2335)	1:53:A:VAL:HG11	1:54:A:GLU:HG3	15	0.48
(1,2335)	1:53:A:VAL:HG12	1:54:A:GLU:HG3	15	0.48
(1,2335)	1:53:A:VAL:HG13	1:54:A:GLU:HG3	15	0.48
(1,2276)	1:27:A:PRO:HG2	1:29:A:ASN:HB3	8	0.48
(1,2276)	1:27:A:PRO:HG2	1:29:A:ASN:HB3	13	0.48
(1,2274)	1:54:A:GLU:HB3	1:74:A:HIS:HB3	4	0.48
(1,2258)	1:18:A:VAL:HG11	1:21:A:LEU:HA	11	0.48
(1,2258)	1:18:A:VAL:HG12	1:21:A:LEU:HA	11	0.48
(1,2258)	1:18:A:VAL:HG13	1:21:A:LEU:HA	11	0.48
(1,2232)	1:12:A:ALA:HB1	1:106:A:TYR:HA	9	0.48
(1,2232)	1:12:A:ALA:HB2	1:106:A:TYR:HA	9	0.48
(1,2232)	1:12:A:ALA:HB3	1:106:A:TYR:HA	9	0.48
(1,2039)	1:45:A:SER:H	1:53:A:VAL:HG11	2	0.48
(1,2039)	1:45:A:SER:H	1:53:A:VAL:HG12	2	0.48
(1,2039)	1:45:A:SER:H	1:53:A:VAL:HG13	2	0.48
(1,1708)	1:64:A:LEU:HB3	1:61:A:ASP:HB3	11	0.48
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	12	0.48
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	12	0.48
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	12	0.48
(1,1704)	1:26:A:LEU:HD11	1:6:A:THR:HA	7	0.48
(1,1704)	1:26:A:LEU:HD12	1:6:A:THR:HA	7	0.48
(1,1704)	1:26:A:LEU:HD13	1:6:A:THR:HA	7	0.48
(1,1559)	1:101:A:GLU:HG3	1:36:A:TRP:HH2	14	0.48
(1,1543)	1:14:A:LEU:HB2	1:14:A:LEU:H	11	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1430)	1:82:A:THR:HG21	1:110:A:ASN:HD21	1	0.48
(1,1430)	1:82:A:THR:HG22	1:110:A:ASN:HD21	1	0.48
(1,1430)	1:82:A:THR:HG23	1:110:A:ASN:HD21	1	0.48
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD1	14	0.48
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD2	14	0.48
(1,822)	1:18:A:VAL:HG11	1:18:A:VAL:H	3	0.48
(1,822)	1:18:A:VAL:HG12	1:18:A:VAL:H	3	0.48
(1,822)	1:18:A:VAL:HG13	1:18:A:VAL:H	3	0.48
(1,822)	1:18:A:VAL:HG11	1:18:A:VAL:H	13	0.48
(1,822)	1:18:A:VAL:HG12	1:18:A:VAL:H	13	0.48
(1,822)	1:18:A:VAL:HG13	1:18:A:VAL:H	13	0.48
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	10	0.48
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	10	0.48
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	10	0.48
(1,448)	1:71:A:GLU:HG2	1:57:A:TYR:HB3	3	0.48
(1,401)	1:64:A:LEU:HD21	1:64:A:LEU:HA	1	0.48
(1,401)	1:64:A:LEU:HD22	1:64:A:LEU:HA	1	0.48
(1,401)	1:64:A:LEU:HD23	1:64:A:LEU:HA	1	0.48
(2,151)	1:52:A:THR:H	1:45:A:SER:HB3	3	0.47
(1,2532)	1:5:A:VAL:H	1:23:A:GLU:HB2	15	0.47
(1,2442)	1:47:A:ASN:HA	1:49:A:SER:H	4	0.47
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	2	0.47
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	11	0.47
(1,1854)	1:50:A:MET:HG3	1:77:A:VAL:HA	3	0.47
(1,1830)	1:28:A:SER:HB2	1:71:A:GLU:HB3	3	0.47
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	15	0.47
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	15	0.47
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	15	0.47
(1,1673)	1:42:A:THR:HB	1:39:A:GLU:HG3	8	0.47
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	5	0.47
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	5	0.47
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	5	0.47
(1,1550)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	4	0.47
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD1	6	0.47
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD2	6	0.47
(1,512)	1:100:A:SER:HB3	1:89:A:TYR:HD1	3	0.47
(1,512)	1:100:A:SER:HB3	1:89:A:TYR:HD2	3	0.47
(1,401)	1:64:A:LEU:HD21	1:64:A:LEU:HA	5	0.47
(1,401)	1:64:A:LEU:HD22	1:64:A:LEU:HA	5	0.47
(1,401)	1:64:A:LEU:HD23	1:64:A:LEU:HA	5	0.47
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	15	0.46
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG11	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG12	3	0.46
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG13	3	0.46
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG11	3	0.46
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG12	3	0.46
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG13	3	0.46
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG11	3	0.46
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG12	3	0.46
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG13	3	0.46
(1,2390)	1:75:A:VAL:HG21	1:83:A:HIS:HB3	2	0.46
(1,2390)	1:75:A:VAL:HG22	1:83:A:HIS:HB3	2	0.46
(1,2390)	1:75:A:VAL:HG23	1:83:A:HIS:HB3	2	0.46
(1,2340)	1:75:A:VAL:HG11	1:22:A:VAL:HB	5	0.46
(1,2340)	1:75:A:VAL:HG12	1:22:A:VAL:HB	5	0.46
(1,2340)	1:75:A:VAL:HG13	1:22:A:VAL:HB	5	0.46
(1,2276)	1:27:A:PRO:HG2	1:29:A:ASN:HB3	4	0.46
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	13	0.46
(1,1762)	1:14:A:LEU:HD11	1:16:A:VAL:H	2	0.46
(1,1762)	1:14:A:LEU:HD12	1:16:A:VAL:H	2	0.46
(1,1762)	1:14:A:LEU:HD13	1:16:A:VAL:H	2	0.46
(1,1550)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	15	0.46
(1,1433)	1:46:A:PRO:HB3	1:48:A:GLU:H	4	0.46
(1,401)	1:64:A:LEU:HD21	1:64:A:LEU:HA	4	0.46
(1,401)	1:64:A:LEU:HD22	1:64:A:LEU:HA	4	0.46
(1,401)	1:64:A:LEU:HD23	1:64:A:LEU:HA	4	0.46
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	7	0.46
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	7	0.46
(2,113)	1:91:A:ARG:HG3	1:92:A:PRO:HG2	5	0.45
(2,50)	1:57:A:TYR:HB3	1:58:A:PHE:HD1	9	0.45
(2,50)	1:57:A:TYR:HB3	1:58:A:PHE:HD2	9	0.45
(1,2532)	1:5:A:VAL:H	1:23:A:GLU:HB2	2	0.45
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG11	11	0.45
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG12	11	0.45
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG13	11	0.45
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG11	11	0.45
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG12	11	0.45
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG13	11	0.45
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG11	11	0.45
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG12	11	0.45
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG13	11	0.45
(1,2288)	1:64:A:LEU:HB3	1:60:A:PRO:HD3	3	0.45
(1,2232)	1:12:A:ALA:HB1	1:106:A:TYR:HA	12	0.45
(1,2232)	1:12:A:ALA:HB2	1:106:A:TYR:HA	12	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2232)	1:12:A:ALA:HB3	1:106:A:TYR:HA	12	0.45
(1,1955)	1:23:A:GLU:H	1:23:A:GLU:HG3	2	0.45
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	1	0.45
(1,1833)	1:69:A:GLY:HA3	1:58:A:PHE:HB2	1	0.45
(1,1391)	1:81:A:GLY:HA3	1:47:A:ASN:HD22	10	0.45
(1,1377)	1:24:A:ILE:HG21	1:25:A:GLN:HE22	9	0.45
(1,1377)	1:24:A:ILE:HG22	1:25:A:GLN:HE22	9	0.45
(1,1377)	1:24:A:ILE:HG23	1:25:A:GLN:HE22	9	0.45
(1,597)	1:78:A:LYS:HD3	1:78:A:LYS:HE3	8	0.45
(1,401)	1:64:A:LEU:HD21	1:64:A:LEU:HA	14	0.45
(1,401)	1:64:A:LEU:HD22	1:64:A:LEU:HA	14	0.45
(1,401)	1:64:A:LEU:HD23	1:64:A:LEU:HA	14	0.45
(1,401)	1:64:A:LEU:HD21	1:64:A:LEU:HA	15	0.45
(1,401)	1:64:A:LEU:HD22	1:64:A:LEU:HA	15	0.45
(1,401)	1:64:A:LEU:HD23	1:64:A:LEU:HA	15	0.45
(1,359)	1:108:A:LYS:HD3	1:15:A:THR:HA	5	0.45
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE1	10	0.44
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE2	10	0.44
(1,2446)	1:16:A:VAL:HG21	1:82:A:THR:HG21	2	0.44
(1,2446)	1:16:A:VAL:HG21	1:82:A:THR:HG22	2	0.44
(1,2446)	1:16:A:VAL:HG21	1:82:A:THR:HG23	2	0.44
(1,2446)	1:16:A:VAL:HG22	1:82:A:THR:HG21	2	0.44
(1,2446)	1:16:A:VAL:HG22	1:82:A:THR:HG22	2	0.44
(1,2446)	1:16:A:VAL:HG22	1:82:A:THR:HG23	2	0.44
(1,2446)	1:16:A:VAL:HG23	1:82:A:THR:HG21	2	0.44
(1,2446)	1:16:A:VAL:HG23	1:82:A:THR:HG22	2	0.44
(1,2446)	1:16:A:VAL:HG23	1:82:A:THR:HG23	2	0.44
(1,2420)	1:30:A:PRO:HA	1:34:A:PHE:HB2	1	0.44
(1,2390)	1:75:A:VAL:HG21	1:83:A:HIS:HB3	9	0.44
(1,2390)	1:75:A:VAL:HG22	1:83:A:HIS:HB3	9	0.44
(1,2390)	1:75:A:VAL:HG23	1:83:A:HIS:HB3	9	0.44
(1,2258)	1:18:A:VAL:HG11	1:21:A:LEU:HA	14	0.44
(1,2258)	1:18:A:VAL:HG12	1:21:A:LEU:HA	14	0.44
(1,2258)	1:18:A:VAL:HG13	1:21:A:LEU:HA	14	0.44
(1,1858)	1:80:A:ALA:HA	1:110:A:ASN:HB3	12	0.44
(1,1633)	1:69:A:GLY:HA2	1:60:A:PRO:HG3	8	0.44
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	4	0.44
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	4	0.44
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	4	0.44
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	6	0.44
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	6	0.44
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1479)	1:59:A:PRO:HG3	1:59:A:PRO:HD2	8	0.44
(1,1357)	1:25:A:GLN:HE22	1:71:A:GLU:H	14	0.44
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD1	15	0.44
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD2	15	0.44
(1,1318)	1:26:A:LEU:HD11	1:25:A:GLN:HE22	8	0.44
(1,1318)	1:26:A:LEU:HD12	1:25:A:GLN:HE22	8	0.44
(1,1318)	1:26:A:LEU:HD13	1:25:A:GLN:HE22	8	0.44
(1,401)	1:64:A:LEU:HD21	1:64:A:LEU:HA	2	0.44
(1,401)	1:64:A:LEU:HD22	1:64:A:LEU:HA	2	0.44
(1,401)	1:64:A:LEU:HD23	1:64:A:LEU:HA	2	0.44
(2,113)	1:91:A:ARG:HG3	1:92:A:PRO:HG2	1	0.43
(1,2532)	1:5:A:VAL:H	1:23:A:GLU:HB2	11	0.43
(1,2442)	1:42:A:THR:HB	1:44:A:GLU:H	15	0.43
(1,2387)	1:60:A:PRO:HB2	1:66:A:GLY:HA2	10	0.43
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	8	0.43
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	11	0.43
(1,1318)	1:26:A:LEU:HD11	1:25:A:GLN:HE22	13	0.43
(1,1318)	1:26:A:LEU:HD12	1:25:A:GLN:HE22	13	0.43
(1,1318)	1:26:A:LEU:HD13	1:25:A:GLN:HE22	13	0.43
(1,734)	1:108:A:LYS:HG3	1:109:A:ALA:H	12	0.43
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	3	0.43
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	5	0.43
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG21	11	0.42
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG22	11	0.42
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG23	11	0.42
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG21	11	0.42
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG22	11	0.42
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG23	11	0.42
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG21	11	0.42
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG22	11	0.42
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG23	11	0.42
(2,107)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	7	0.42
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE1	5	0.42
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE2	5	0.42
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE1	8	0.42
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE2	8	0.42
(1,2522)	1:52:A:THR:HG21	1:48:A:GLU:HB3	4	0.42
(1,2522)	1:52:A:THR:HG22	1:48:A:GLU:HB3	4	0.42
(1,2522)	1:52:A:THR:HG23	1:48:A:GLU:HB3	4	0.42
(1,2452)	1:105:A:VAL:HG11	1:106:A:TYR:HD1	3	0.42
(1,2452)	1:105:A:VAL:HG11	1:106:A:TYR:HD2	3	0.42
(1,2452)	1:105:A:VAL:HG12	1:106:A:TYR:HD1	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2452)	1:105:A:VAL:HG12	1:106:A:TYR:HD2	3	0.42
(1,2452)	1:105:A:VAL:HG13	1:106:A:TYR:HD1	3	0.42
(1,2452)	1:105:A:VAL:HG13	1:106:A:TYR:HD2	3	0.42
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG11	9	0.42
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG12	9	0.42
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG13	9	0.42
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG11	9	0.42
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG12	9	0.42
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG13	9	0.42
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG11	9	0.42
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG12	9	0.42
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG13	9	0.42
(1,2420)	1:30:A:PRO:HA	1:34:A:PHE:HB2	12	0.42
(1,2329)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	7	0.42
(1,2301)	1:16:A:VAL:HG11	1:18:A:VAL:HA	2	0.42
(1,2301)	1:16:A:VAL:HG12	1:18:A:VAL:HA	2	0.42
(1,2301)	1:16:A:VAL:HG13	1:18:A:VAL:HA	2	0.42
(1,2276)	1:27:A:PRO:HG2	1:29:A:ASN:HB3	5	0.42
(1,2193)	1:77:A:VAL:HG11	1:83:A:HIS:HE1	7	0.42
(1,2193)	1:77:A:VAL:HG12	1:83:A:HIS:HE1	7	0.42
(1,2193)	1:77:A:VAL:HG13	1:83:A:HIS:HE1	7	0.42
(1,2164)	1:38:A:PHE:HA	1:38:A:PHE:HZ	15	0.42
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	9	0.42
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD21	15	0.42
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD22	15	0.42
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD23	15	0.42
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	3	0.42
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	3	0.42
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	3	0.42
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	8	0.42
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	8	0.42
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	8	0.42
(1,1034)	1:108:A:LYS:HB2	1:110:A:ASN:HD22	9	0.42
(1,512)	1:100:A:SER:HB3	1:89:A:TYR:HD1	15	0.42
(1,512)	1:100:A:SER:HB3	1:89:A:TYR:HD2	15	0.42
(1,450)	1:60:A:PRO:HB3	1:66:A:GLY:HA2	3	0.42
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	7	0.41
(2,71)	1:22:A:VAL:HB	1:21:A:LEU:HD11	3	0.41
(2,71)	1:22:A:VAL:HB	1:21:A:LEU:HD12	3	0.41
(2,71)	1:22:A:VAL:HB	1:21:A:LEU:HD13	3	0.41
(1,2420)	1:30:A:PRO:HA	1:34:A:PHE:HB2	13	0.41
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1833)	1:69:A:GLY:HA3	1:58:A:PHE:HB2	14	0.41
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	15	0.41
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	7	0.41
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	7	0.41
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	7	0.41
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	10	0.41
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	10	0.41
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	10	0.41
(1,1458)	1:75:A:VAL:HG21	1:52:A:THR:H	8	0.41
(1,1458)	1:75:A:VAL:HG22	1:52:A:THR:H	8	0.41
(1,1458)	1:75:A:VAL:HG23	1:52:A:THR:H	8	0.41
(1,878)	1:63:A:LYS:HD3	1:61:A:ASP:HB3	15	0.41
(1,734)	1:108:A:LYS:HG3	1:109:A:ALA:H	4	0.41
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	6	0.41
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	6	0.41
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	6	0.41
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	8	0.41
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	8	0.41
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	8	0.41
(1,608)	1:88:A:THR:HG21	1:90:A:MET:HG3	11	0.41
(1,608)	1:88:A:THR:HG22	1:90:A:MET:HG3	11	0.41
(1,608)	1:88:A:THR:HG23	1:90:A:MET:HG3	11	0.41
(1,489)	1:65:A:LEU:HD11	1:30:A:PRO:HD3	8	0.41
(1,489)	1:65:A:LEU:HD12	1:30:A:PRO:HD3	8	0.41
(1,489)	1:65:A:LEU:HD13	1:30:A:PRO:HD3	8	0.41
(1,368)	1:30:A:PRO:HG3	1:69:A:GLY:HA2	15	0.41
(1,341)	1:78:A:LYS:HB3	1:78:A:LYS:HA	13	0.41
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	10	0.4
(1,2452)	1:105:A:VAL:HG11	1:106:A:TYR:HD1	9	0.4
(1,2452)	1:105:A:VAL:HG11	1:106:A:TYR:HD2	9	0.4
(1,2452)	1:105:A:VAL:HG12	1:106:A:TYR:HD1	9	0.4
(1,2452)	1:105:A:VAL:HG12	1:106:A:TYR:HD2	9	0.4
(1,2452)	1:105:A:VAL:HG13	1:106:A:TYR:HD1	9	0.4
(1,2452)	1:105:A:VAL:HG13	1:106:A:TYR:HD2	9	0.4
(1,2351)	1:23:A:GLU:HB3	1:24:A:ILE:H	5	0.4
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	10	0.4
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	1	0.4
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	10	0.4
(1,1997)	1:61:A:ASP:H	1:60:A:PRO:HG2	8	0.4
(1,1624)	1:45:A:SER:HA	1:53:A:VAL:HG11	2	0.4
(1,1624)	1:45:A:SER:HA	1:53:A:VAL:HG12	2	0.4
(1,1624)	1:45:A:SER:HA	1:53:A:VAL:HG13	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	14	0.39
(1,2193)	1:77:A:VAL:HG11	1:83:A:HIS:HE1	11	0.39
(1,2193)	1:77:A:VAL:HG12	1:83:A:HIS:HE1	11	0.39
(1,2193)	1:77:A:VAL:HG13	1:83:A:HIS:HE1	11	0.39
(1,1955)	1:23:A:GLU:H	1:23:A:GLU:HG3	6	0.39
(1,1654)	1:42:A:THR:HA	1:43:A:LYS:HD3	11	0.39
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD1	12	0.39
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD2	12	0.39
(1,874)	1:85:A:VAL:HG21	1:85:A:VAL:H	9	0.39
(1,874)	1:85:A:VAL:HG22	1:85:A:VAL:H	9	0.39
(1,874)	1:85:A:VAL:HG23	1:85:A:VAL:H	9	0.39
(1,841)	1:43:A:LYS:HG3	1:38:A:PHE:HD1	10	0.39
(1,841)	1:43:A:LYS:HG3	1:38:A:PHE:HD2	10	0.39
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD11	2	0.39
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD12	2	0.39
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD13	2	0.39
(1,658)	1:94:A:THR:HG21	1:90:A:MET:HB2	7	0.39
(1,658)	1:94:A:THR:HG22	1:90:A:MET:HB2	7	0.39
(1,658)	1:94:A:THR:HG23	1:90:A:MET:HB2	7	0.39
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	2	0.39
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	2	0.39
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	2	0.39
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	1	0.39
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	2	0.38
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	2	0.38
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	2	0.38
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	7	0.38
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE1	12	0.38
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE2	12	0.38
(1,2486)	1:85:A:VAL:HB	1:38:A:PHE:HD1	3	0.38
(1,2486)	1:85:A:VAL:HB	1:38:A:PHE:HD2	3	0.38
(1,2390)	1:75:A:VAL:HG21	1:83:A:HIS:HB3	6	0.38
(1,2390)	1:75:A:VAL:HG22	1:83:A:HIS:HB3	6	0.38
(1,2390)	1:75:A:VAL:HG23	1:83:A:HIS:HB3	6	0.38
(1,2390)	1:75:A:VAL:HG21	1:83:A:HIS:HB3	12	0.38
(1,2390)	1:75:A:VAL:HG22	1:83:A:HIS:HB3	12	0.38
(1,2390)	1:75:A:VAL:HG23	1:83:A:HIS:HB3	12	0.38
(1,2390)	1:75:A:VAL:HG21	1:83:A:HIS:HB3	15	0.38
(1,2390)	1:75:A:VAL:HG22	1:83:A:HIS:HB3	15	0.38
(1,2390)	1:75:A:VAL:HG23	1:83:A:HIS:HB3	15	0.38
(1,2340)	1:65:A:LEU:HD11	1:60:A:PRO:HG3	2	0.38
(1,2340)	1:65:A:LEU:HD12	1:60:A:PRO:HG3	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2340)	1:65:A:LEU:HD13	1:60:A:PRO:HG3	2	0.38
(1,2276)	1:27:A:PRO:HG2	1:29:A:ASN:HB3	2	0.38
(1,2276)	1:27:A:PRO:HG2	1:29:A:ASN:HB3	10	0.38
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	8	0.38
(1,2232)	1:12:A:ALA:HB1	1:106:A:TYR:HA	15	0.38
(1,2232)	1:12:A:ALA:HB2	1:106:A:TYR:HA	15	0.38
(1,2232)	1:12:A:ALA:HB3	1:106:A:TYR:HA	15	0.38
(1,2231)	1:92:A:PRO:HB3	1:91:A:ARG:HA	2	0.38
(1,2209)	1:58:A:PHE:HB3	1:69:A:GLY:HA3	6	0.38
(1,2193)	1:77:A:VAL:HG11	1:83:A:HIS:HE1	1	0.38
(1,2193)	1:77:A:VAL:HG12	1:83:A:HIS:HE1	1	0.38
(1,2193)	1:77:A:VAL:HG13	1:83:A:HIS:HE1	1	0.38
(1,2131)	1:37:A:TYR:H	1:90:A:MET:HG2	8	0.38
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	3	0.38
(1,1252)	1:26:A:LEU:HD11	1:7:A:LYS:H	7	0.38
(1,1252)	1:26:A:LEU:HD12	1:7:A:LYS:H	7	0.38
(1,1252)	1:26:A:LEU:HD13	1:7:A:LYS:H	7	0.38
(1,842)	1:49:A:SER:HB3	1:49:A:SER:H	15	0.38
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	3	0.38
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	3	0.38
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	3	0.38
(1,341)	1:78:A:LYS:HB3	1:78:A:LYS:HA	8	0.38
(1,138)	1:9:A:HIS:HA	1:9:A:HIS:HE1	15	0.38
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	1	0.37
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	11	0.37
(1,2532)	1:5:A:VAL:H	1:23:A:GLU:HB2	14	0.37
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG11	15	0.37
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG12	15	0.37
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG13	15	0.37
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG11	15	0.37
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG12	15	0.37
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG13	15	0.37
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG11	15	0.37
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG12	15	0.37
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG13	15	0.37
(1,2387)	1:96:A:PRO:HG3	1:95:A:GLY:HA2	8	0.37
(1,2164)	1:38:A:PHE:HA	1:38:A:PHE:HZ	2	0.37
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	5	0.37
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	6	0.37
(1,1774)	1:24:A:ILE:HD11	1:26:A:LEU:HD21	8	0.37
(1,1774)	1:24:A:ILE:HD11	1:26:A:LEU:HD22	8	0.37
(1,1774)	1:24:A:ILE:HD11	1:26:A:LEU:HD23	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	1:24:A:ILE:HD12	1:26:A:LEU:HD21	8	0.37
(1,1774)	1:24:A:ILE:HD12	1:26:A:LEU:HD22	8	0.37
(1,1774)	1:24:A:ILE:HD12	1:26:A:LEU:HD23	8	0.37
(1,1774)	1:24:A:ILE:HD13	1:26:A:LEU:HD21	8	0.37
(1,1774)	1:24:A:ILE:HD13	1:26:A:LEU:HD22	8	0.37
(1,1774)	1:24:A:ILE:HD13	1:26:A:LEU:HD23	8	0.37
(1,1238)	1:53:A:VAL:HG11	1:52:A:THR:H	3	0.37
(1,1238)	1:53:A:VAL:HG12	1:52:A:THR:H	3	0.37
(1,1238)	1:53:A:VAL:HG13	1:52:A:THR:H	3	0.37
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD21	13	0.37
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD22	13	0.37
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD23	13	0.37
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	4	0.37
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	4	0.37
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	4	0.37
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	5	0.37
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	5	0.37
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	5	0.37
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	13	0.37
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	13	0.37
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	13	0.37
(1,563)	1:9:A:HIS:HB3	1:105:A:VAL:HA	15	0.37
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	8	0.37
(1,341)	1:78:A:LYS:HB3	1:78:A:LYS:HA	7	0.37
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	8	0.36
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	12	0.36
(2,19)	1:63:A:LYS:HD3	1:65:A:LEU:HA	4	0.36
(1,2529)	1:28:A:SER:HB3	1:71:A:GLU:HB3	8	0.36
(1,2390)	1:75:A:VAL:HG21	1:83:A:HIS:HB3	5	0.36
(1,2390)	1:75:A:VAL:HG22	1:83:A:HIS:HB3	5	0.36
(1,2390)	1:75:A:VAL:HG23	1:83:A:HIS:HB3	5	0.36
(1,2321)	1:44:A:GLU:HG3	1:46:A:PRO:HD2	14	0.36
(1,2283)	1:65:A:LEU:HG	1:28:A:SER:HB2	4	0.36
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	10	0.36
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	13	0.36
(1,2164)	1:38:A:PHE:HA	1:38:A:PHE:HZ	3	0.36
(1,1847)	1:55:A:ASN:HA	1:56:A:LYS:HG3	15	0.36
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	12	0.36
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	12	0.36
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	12	0.36
(1,1357)	1:25:A:GLN:HE22	1:71:A:GLU:H	3	0.36
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD1	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD2	2	0.36
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD1	4	0.36
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD2	4	0.36
(1,1097)	1:37:A:TYR:HB3	1:42:A:THR:H	2	0.36
(1,734)	1:108:A:LYS:HG3	1:109:A:ALA:H	9	0.36
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	7	0.36
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	7	0.36
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	7	0.36
(1,608)	1:88:A:THR:HG21	1:90:A:MET:HG3	5	0.36
(1,608)	1:88:A:THR:HG22	1:90:A:MET:HG3	5	0.36
(1,608)	1:88:A:THR:HG23	1:90:A:MET:HG3	5	0.36
(1,341)	1:78:A:LYS:HB3	1:78:A:LYS:HA	10	0.36
(1,341)	1:78:A:LYS:HB3	1:78:A:LYS:HA	11	0.36
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	9	0.35
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	9	0.35
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	9	0.35
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	11	0.35
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	11	0.35
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	11	0.35
(2,56)	1:83:A:HIS:HB2	1:47:A:ASN:HD21	15	0.35
(1,2532)	1:5:A:VAL:H	1:23:A:GLU:HB2	6	0.35
(1,2452)	1:18:A:VAL:HG11	1:110:A:ASN:HD22	11	0.35
(1,2452)	1:18:A:VAL:HG12	1:110:A:ASN:HD22	11	0.35
(1,2452)	1:18:A:VAL:HG13	1:110:A:ASN:HD22	11	0.35
(1,2452)	1:105:A:VAL:HG11	1:106:A:TYR:HD1	13	0.35
(1,2452)	1:105:A:VAL:HG11	1:106:A:TYR:HD2	13	0.35
(1,2452)	1:105:A:VAL:HG12	1:106:A:TYR:HD1	13	0.35
(1,2452)	1:105:A:VAL:HG12	1:106:A:TYR:HD2	13	0.35
(1,2452)	1:105:A:VAL:HG13	1:106:A:TYR:HD1	13	0.35
(1,2452)	1:105:A:VAL:HG13	1:106:A:TYR:HD2	13	0.35
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	3	0.35
(1,2351)	1:23:A:GLU:HB3	1:24:A:ILE:H	4	0.35
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	10	0.35
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	12	0.35
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	3	0.35
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	4	0.35
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	9	0.35
(1,2193)	1:77:A:VAL:HG11	1:83:A:HIS:HE1	15	0.35
(1,2193)	1:77:A:VAL:HG12	1:83:A:HIS:HE1	15	0.35
(1,2193)	1:77:A:VAL:HG13	1:83:A:HIS:HE1	15	0.35
(1,2131)	1:37:A:TYR:H	1:90:A:MET:HG2	2	0.35
(1,1847)	1:55:A:ASN:HA	1:56:A:LYS:HG3	13	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	9	0.35
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	9	0.35
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	9	0.35
(1,1252)	1:26:A:LEU:HD11	1:7:A:LYS:H	8	0.35
(1,1252)	1:26:A:LEU:HD12	1:7:A:LYS:H	8	0.35
(1,1252)	1:26:A:LEU:HD13	1:7:A:LYS:H	8	0.35
(1,1011)	1:63:A:LYS:HD3	1:63:A:LYS:H	15	0.35
(1,852)	1:14:A:LEU:HD11	1:14:A:LEU:H	8	0.35
(1,852)	1:14:A:LEU:HD12	1:14:A:LEU:H	8	0.35
(1,852)	1:14:A:LEU:HD13	1:14:A:LEU:H	8	0.35
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	11	0.35
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	11	0.35
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	11	0.35
(1,368)	1:30:A:PRO:HG3	1:69:A:GLY:HA2	1	0.35
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD1	10	0.35
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD2	10	0.35
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	13	0.34
(2,129)	1:66:A:GLY:H	1:68:A:GLY:HA3	6	0.34
(2,75)	1:107:A:LEU:HB3	1:83:A:HIS:HB2	15	0.34
(1,2301)	1:16:A:VAL:HG11	1:18:A:VAL:HA	14	0.34
(1,2301)	1:16:A:VAL:HG12	1:18:A:VAL:HA	14	0.34
(1,2301)	1:16:A:VAL:HG13	1:18:A:VAL:HA	14	0.34
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	12	0.34
(1,2131)	1:37:A:TYR:H	1:90:A:MET:HG2	13	0.34
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	7	0.34
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	1	0.34
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	1	0.34
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	1	0.34
(1,1558)	1:75:A:VAL:HG21	1:76:A:THR:H	8	0.34
(1,1558)	1:75:A:VAL:HG22	1:76:A:THR:H	8	0.34
(1,1558)	1:75:A:VAL:HG23	1:76:A:THR:H	8	0.34
(1,1550)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	11	0.34
(1,1357)	1:25:A:GLN:HE22	1:71:A:GLU:H	13	0.34
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	1	0.34
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	1	0.34
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	1	0.34
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	6	0.34
(1,341)	1:78:A:LYS:HB3	1:78:A:LYS:HA	1	0.34
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	13	0.33
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	14	0.33
(1,2452)	1:18:A:VAL:HG11	1:110:A:ASN:HD22	1	0.33
(1,2452)	1:18:A:VAL:HG12	1:110:A:ASN:HD22	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2452)	1:18:A:VAL:HG13	1:110:A:ASN:HD22	1	0.33
(1,2232)	1:12:A:ALA:HB1	1:106:A:TYR:HA	4	0.33
(1,2232)	1:12:A:ALA:HB2	1:106:A:TYR:HA	4	0.33
(1,2232)	1:12:A:ALA:HB3	1:106:A:TYR:HA	4	0.33
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	8	0.33
(1,1853)	1:34:A:PHE:HA	1:90:A:MET:HG2	9	0.33
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	14	0.33
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	14	0.33
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	14	0.33
(1,1588)	1:70:A:THR:HB	1:58:A:PHE:HB2	5	0.33
(1,1540)	1:18:A:VAL:HG11	1:3:A:HIS:HB2	3	0.33
(1,1540)	1:18:A:VAL:HG12	1:3:A:HIS:HB2	3	0.33
(1,1540)	1:18:A:VAL:HG13	1:3:A:HIS:HB2	3	0.33
(1,341)	1:78:A:LYS:HB3	1:78:A:LYS:HA	3	0.33
(2,151)	1:52:A:THR:H	1:45:A:SER:HB3	10	0.32
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	9	0.32
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	11	0.32
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	5	0.32
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	5	0.32
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	5	0.32
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD1	7	0.32
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD2	7	0.32
(1,2522)	1:52:A:THR:HG21	1:48:A:GLU:HB3	1	0.32
(1,2522)	1:52:A:THR:HG22	1:48:A:GLU:HB3	1	0.32
(1,2522)	1:52:A:THR:HG23	1:48:A:GLU:HB3	1	0.32
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG11	5	0.32
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG12	5	0.32
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG13	5	0.32
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG11	5	0.32
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG12	5	0.32
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG13	5	0.32
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG11	5	0.32
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG12	5	0.32
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG13	5	0.32
(1,2370)	1:78:A:LYS:HD3	1:78:A:LYS:H	2	0.32
(1,2232)	1:12:A:ALA:HB1	1:106:A:TYR:HA	5	0.32
(1,2232)	1:12:A:ALA:HB2	1:106:A:TYR:HA	5	0.32
(1,2232)	1:12:A:ALA:HB3	1:106:A:TYR:HA	5	0.32
(1,2232)	1:12:A:ALA:HB1	1:106:A:TYR:HA	6	0.32
(1,2232)	1:12:A:ALA:HB2	1:106:A:TYR:HA	6	0.32
(1,2232)	1:12:A:ALA:HB3	1:106:A:TYR:HA	6	0.32
(1,2232)	1:12:A:ALA:HB1	1:106:A:TYR:HA	13	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2232)	1:12:A:ALA:HB2	1:106:A:TYR:HA	13	0.32
(1,2232)	1:12:A:ALA:HB3	1:106:A:TYR:HA	13	0.32
(1,2177)	1:34:A:PHE:HB3	1:37:A:TYR:HE1	15	0.32
(1,2177)	1:34:A:PHE:HB3	1:37:A:TYR:HE2	15	0.32
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD1	4	0.32
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD2	4	0.32
(1,2118)	1:29:A:ASN:HD22	1:28:A:SER:HB3	3	0.32
(1,1774)	1:24:A:ILE:HD11	1:26:A:LEU:HD21	13	0.32
(1,1774)	1:24:A:ILE:HD11	1:26:A:LEU:HD22	13	0.32
(1,1774)	1:24:A:ILE:HD11	1:26:A:LEU:HD23	13	0.32
(1,1774)	1:24:A:ILE:HD12	1:26:A:LEU:HD21	13	0.32
(1,1774)	1:24:A:ILE:HD12	1:26:A:LEU:HD22	13	0.32
(1,1774)	1:24:A:ILE:HD12	1:26:A:LEU:HD23	13	0.32
(1,1774)	1:24:A:ILE:HD13	1:26:A:LEU:HD21	13	0.32
(1,1774)	1:24:A:ILE:HD13	1:26:A:LEU:HD22	13	0.32
(1,1774)	1:24:A:ILE:HD13	1:26:A:LEU:HD23	13	0.32
(1,1704)	1:26:A:LEU:HD11	1:6:A:THR:HA	13	0.32
(1,1704)	1:26:A:LEU:HD12	1:6:A:THR:HA	13	0.32
(1,1704)	1:26:A:LEU:HD13	1:6:A:THR:HA	13	0.32
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	10	0.32
(1,1225)	1:101:A:GLU:HG3	1:10:A:ASN:HD22	14	0.32
(1,1074)	1:18:A:VAL:HG11	1:79:A:ALA:H	3	0.32
(1,1074)	1:18:A:VAL:HG12	1:79:A:ALA:H	3	0.32
(1,1074)	1:18:A:VAL:HG13	1:79:A:ALA:H	3	0.32
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	9	0.32
(1,650)	1:64:A:LEU:HD11	1:63:A:LYS:HD3	2	0.32
(1,650)	1:64:A:LEU:HD12	1:63:A:LYS:HD3	2	0.32
(1,650)	1:64:A:LEU:HD13	1:63:A:LYS:HD3	2	0.32
(1,535)	1:60:A:PRO:HD3	1:59:A:PRO:HA	8	0.32
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	13	0.32
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	12	0.32
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	12	0.32
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	12	0.32
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	15	0.32
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	15	0.32
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	15	0.32
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	4	0.31
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	10	0.31
(2,107)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	9	0.31
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	8	0.31
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	8	0.31
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	13	0.31
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	13	0.31
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	13	0.31
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE1	13	0.31
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE2	13	0.31
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE1	15	0.31
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE2	15	0.31
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	3	0.31
(1,2523)	1:36:A:TRP:HB3	1:36:A:TRP:HZ2	7	0.31
(1,2420)	1:30:A:PRO:HA	1:34:A:PHE:HB2	10	0.31
(1,2413)	1:31:A:THR:HG21	1:89:A:TYR:HB3	3	0.31
(1,2413)	1:31:A:THR:HG22	1:89:A:TYR:HB3	3	0.31
(1,2413)	1:31:A:THR:HG23	1:89:A:TYR:HB3	3	0.31
(1,2351)	1:48:A:GLU:HB3	1:48:A:GLU:H	13	0.31
(1,2335)	1:53:A:VAL:HG11	1:54:A:GLU:HG3	5	0.31
(1,2335)	1:53:A:VAL:HG12	1:54:A:GLU:HG3	5	0.31
(1,2335)	1:53:A:VAL:HG13	1:54:A:GLU:HG3	5	0.31
(1,2330)	1:70:A:THR:HG21	1:57:A:TYR:HB2	5	0.31
(1,2330)	1:70:A:THR:HG22	1:57:A:TYR:HB2	5	0.31
(1,2330)	1:70:A:THR:HG23	1:57:A:TYR:HB2	5	0.31
(1,2329)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	9	0.31
(1,2283)	1:65:A:LEU:HG	1:28:A:SER:HB2	6	0.31
(1,2274)	1:27:A:PRO:HG3	1:29:A:ASN:HB3	10	0.31
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	7	0.31
(1,2164)	1:38:A:PHE:HA	1:38:A:PHE:HZ	1	0.31
(1,2164)	1:38:A:PHE:HA	1:38:A:PHE:HZ	4	0.31
(1,2131)	1:37:A:TYR:H	1:90:A:MET:HG2	4	0.31
(1,1897)	1:36:A:TRP:HD1	1:57:A:TYR:HB2	14	0.31
(1,1853)	1:34:A:PHE:HA	1:90:A:MET:HG2	6	0.31
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	8	0.31
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	8	0.31
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	8	0.31
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD21	12	0.31
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD22	12	0.31
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD23	12	0.31
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	12	0.31
(1,1624)	1:45:A:SER:HA	1:53:A:VAL:HG11	4	0.31
(1,1624)	1:45:A:SER:HA	1:53:A:VAL:HG12	4	0.31
(1,1624)	1:45:A:SER:HA	1:53:A:VAL:HG13	4	0.31
(1,852)	1:14:A:LEU:HD11	1:14:A:LEU:H	2	0.31
(1,852)	1:14:A:LEU:HD12	1:14:A:LEU:H	2	0.31
(1,852)	1:14:A:LEU:HD13	1:14:A:LEU:H	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,841)	1:43:A:LYS:HG3	1:38:A:PHE:HD1	13	0.31
(1,841)	1:43:A:LYS:HG3	1:38:A:PHE:HD2	13	0.31
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	11	0.31
(2,114)	1:90:A:MET:HE1	1:37:A:TYR:HA	15	0.3
(2,114)	1:90:A:MET:HE2	1:37:A:TYR:HA	15	0.3
(2,114)	1:90:A:MET:HE3	1:37:A:TYR:HA	15	0.3
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	15	0.3
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	15	0.3
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	15	0.3
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	8	0.3
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	13	0.3
(1,2523)	1:36:A:TRP:HB3	1:36:A:TRP:HZ2	4	0.3
(1,2523)	1:36:A:TRP:HB3	1:36:A:TRP:HZ2	5	0.3
(1,2523)	1:36:A:TRP:HB3	1:36:A:TRP:HZ2	14	0.3
(1,2387)	1:60:A:PRO:HB2	1:66:A:GLY:HA2	11	0.3
(1,2274)	1:54:A:GLU:HB3	1:74:A:HIS:HB3	5	0.3
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	7	0.3
(1,2232)	1:12:A:ALA:HB1	1:106:A:TYR:HA	1	0.3
(1,2232)	1:12:A:ALA:HB2	1:106:A:TYR:HA	1	0.3
(1,2232)	1:12:A:ALA:HB3	1:106:A:TYR:HA	1	0.3
(1,2105)	1:8:A:ALA:H	1:9:A:HIS:HB2	15	0.3
(1,1947)	1:64:A:LEU:H	1:64:A:LEU:HB3	7	0.3
(1,1947)	1:64:A:LEU:H	1:64:A:LEU:HB3	10	0.3
(1,1853)	1:34:A:PHE:HA	1:90:A:MET:HG2	2	0.3
(1,1833)	1:69:A:GLY:HA3	1:58:A:PHE:HB2	5	0.3
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	13	0.3
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	13	0.3
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	13	0.3
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	15	0.3
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	15	0.3
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	15	0.3
(1,1535)	1:90:A:MET:HE1	1:92:A:PRO:HA	15	0.3
(1,1535)	1:90:A:MET:HE2	1:92:A:PRO:HA	15	0.3
(1,1535)	1:90:A:MET:HE3	1:92:A:PRO:HA	15	0.3
(1,1252)	1:26:A:LEU:HD11	1:7:A:LYS:H	13	0.3
(1,1252)	1:26:A:LEU:HD12	1:7:A:LYS:H	13	0.3
(1,1252)	1:26:A:LEU:HD13	1:7:A:LYS:H	13	0.3
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD1	3	0.3
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD2	3	0.3
(1,1011)	1:63:A:LYS:HD3	1:63:A:LYS:H	14	0.3
(1,852)	1:14:A:LEU:HD11	1:14:A:LEU:H	5	0.3
(1,852)	1:14:A:LEU:HD12	1:14:A:LEU:H	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,852)	1:14:A:LEU:HD13	1:14:A:LEU:H	5	0.3
(1,852)	1:14:A:LEU:HD11	1:14:A:LEU:H	6	0.3
(1,852)	1:14:A:LEU:HD12	1:14:A:LEU:H	6	0.3
(1,852)	1:14:A:LEU:HD13	1:14:A:LEU:H	6	0.3
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	10	0.3
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	15	0.3
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	15	0.3
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	15	0.3
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	14	0.3
(1,205)	1:56:A:LYS:HD3	1:72:A:HIS:HE1	15	0.3
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	5	0.29
(2,103)	1:48:A:GLU:HA	1:50:A:MET:HA	6	0.29
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	3	0.29
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	3	0.29
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	3	0.29
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	6	0.29
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	6	0.29
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	6	0.29
(1,2523)	1:36:A:TRP:HB3	1:36:A:TRP:HZ2	1	0.29
(1,2453)	1:31:A:THR:HG21	1:36:A:TRP:HZ2	5	0.29
(1,2453)	1:31:A:THR:HG22	1:36:A:TRP:HZ2	5	0.29
(1,2453)	1:31:A:THR:HG23	1:36:A:TRP:HZ2	5	0.29
(1,2420)	1:30:A:PRO:HA	1:34:A:PHE:HB2	5	0.29
(1,2413)	1:31:A:THR:HG21	1:89:A:TYR:HB3	8	0.29
(1,2413)	1:31:A:THR:HG22	1:89:A:TYR:HB3	8	0.29
(1,2413)	1:31:A:THR:HG23	1:89:A:TYR:HB3	8	0.29
(1,2390)	1:75:A:VAL:HG21	1:51:A:PHE:HB3	3	0.29
(1,2390)	1:75:A:VAL:HG22	1:51:A:PHE:HB3	3	0.29
(1,2390)	1:75:A:VAL:HG23	1:51:A:PHE:HB3	3	0.29
(1,2321)	1:44:A:GLU:HG3	1:46:A:PRO:HD2	10	0.29
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	15	0.29
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	15	0.29
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	15	0.29
(1,2205)	1:72:A:HIS:HB3	1:26:A:LEU:HA	14	0.29
(1,2164)	1:38:A:PHE:HA	1:38:A:PHE:HZ	11	0.29
(1,2164)	1:43:A:LYS:HA	1:38:A:PHE:HZ	13	0.29
(1,1947)	1:64:A:LEU:H	1:64:A:LEU:HB3	3	0.29
(1,1858)	1:80:A:ALA:HA	1:110:A:ASN:HB3	2	0.29
(1,1833)	1:69:A:GLY:HA3	1:58:A:PHE:HB2	6	0.29
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	13	0.29
(1,1630)	1:60:A:PRO:HA	1:66:A:GLY:HA2	5	0.29
(1,1615)	1:60:A:PRO:HA	1:66:A:GLY:HA3	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1059)	1:78:A:LYS:HD3	1:50:A:MET:HG3	2	0.29
(1,912)	1:91:A:ARG:HB3	1:91:A:ARG:HD3	3	0.29
(1,852)	1:14:A:LEU:HD11	1:14:A:LEU:H	7	0.29
(1,852)	1:14:A:LEU:HD12	1:14:A:LEU:H	7	0.29
(1,852)	1:14:A:LEU:HD13	1:14:A:LEU:H	7	0.29
(1,842)	1:49:A:SER:HB3	1:49:A:SER:H	10	0.29
(1,841)	1:43:A:LYS:HG3	1:38:A:PHE:HD1	5	0.29
(1,841)	1:43:A:LYS:HG3	1:38:A:PHE:HD2	5	0.29
(1,734)	1:108:A:LYS:HG3	1:109:A:ALA:H	5	0.29
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	13	0.29
(1,205)	1:56:A:LYS:HD3	1:72:A:HIS:HE1	2	0.29
(1,205)	1:56:A:LYS:HD3	1:72:A:HIS:HE1	11	0.29
(1,43)	1:87:A:LEU:HD21	1:85:A:VAL:HG11	9	0.29
(1,43)	1:87:A:LEU:HD21	1:85:A:VAL:HG12	9	0.29
(1,43)	1:87:A:LEU:HD21	1:85:A:VAL:HG13	9	0.29
(1,43)	1:87:A:LEU:HD22	1:85:A:VAL:HG11	9	0.29
(1,43)	1:87:A:LEU:HD22	1:85:A:VAL:HG12	9	0.29
(1,43)	1:87:A:LEU:HD22	1:85:A:VAL:HG13	9	0.29
(1,43)	1:87:A:LEU:HD23	1:85:A:VAL:HG11	9	0.29
(1,43)	1:87:A:LEU:HD23	1:85:A:VAL:HG12	9	0.29
(1,43)	1:87:A:LEU:HD23	1:85:A:VAL:HG13	9	0.29
(2,114)	1:90:A:MET:HE1	1:37:A:TYR:HA	4	0.28
(2,114)	1:90:A:MET:HE2	1:37:A:TYR:HA	4	0.28
(2,114)	1:90:A:MET:HE3	1:37:A:TYR:HA	4	0.28
(2,107)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	8	0.28
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD1	6	0.28
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD2	6	0.28
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE1	6	0.28
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE2	6	0.28
(2,18)	1:30:A:PRO:HB2	1:28:A:SER:HB3	12	0.28
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	1	0.28
(1,2333)	1:5:A:VAL:HG21	1:3:A:HIS:HB3	15	0.28
(1,2333)	1:5:A:VAL:HG22	1:3:A:HIS:HB3	15	0.28
(1,2333)	1:5:A:VAL:HG23	1:3:A:HIS:HB3	15	0.28
(1,2329)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	8	0.28
(1,2321)	1:44:A:GLU:HG3	1:46:A:PRO:HD2	13	0.28
(1,2301)	1:16:A:VAL:HG11	1:18:A:VAL:HA	9	0.28
(1,2301)	1:16:A:VAL:HG12	1:18:A:VAL:HA	9	0.28
(1,2301)	1:16:A:VAL:HG13	1:18:A:VAL:HA	9	0.28
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD1	14	0.28
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD2	14	0.28
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD1	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD2	15	0.28
(1,2044)	1:70:A:THR:H	1:72:A:HIS:HD2	5	0.28
(1,1945)	1:48:A:GLU:H	1:48:A:GLU:HB3	14	0.28
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	6	0.28
(1,1642)	1:67:A:ALA:HB1	1:60:A:PRO:HG2	15	0.28
(1,1642)	1:67:A:ALA:HB2	1:60:A:PRO:HG2	15	0.28
(1,1642)	1:67:A:ALA:HB3	1:60:A:PRO:HG2	15	0.28
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB1	11	0.28
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB2	11	0.28
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB3	11	0.28
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB1	11	0.28
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB2	11	0.28
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB3	11	0.28
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB1	11	0.28
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB2	11	0.28
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB3	11	0.28
(1,1535)	1:90:A:MET:HE1	1:92:A:PRO:HA	4	0.28
(1,1535)	1:90:A:MET:HE2	1:92:A:PRO:HA	4	0.28
(1,1535)	1:90:A:MET:HE3	1:92:A:PRO:HA	4	0.28
(1,1535)	1:90:A:MET:HE1	1:92:A:PRO:HA	8	0.28
(1,1535)	1:90:A:MET:HE2	1:92:A:PRO:HA	8	0.28
(1,1535)	1:90:A:MET:HE3	1:92:A:PRO:HA	8	0.28
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	4	0.28
(1,939)	1:76:A:THR:HB	1:52:A:THR:H	14	0.28
(1,912)	1:91:A:ARG:HB3	1:91:A:ARG:HD3	11	0.28
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	15	0.28
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	1	0.28
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	1	0.28
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	1	0.28
(1,570)	1:30:A:PRO:HD2	1:28:A:SER:HB2	14	0.28
(1,488)	1:75:A:VAL:HG11	1:45:A:SER:HA	8	0.28
(1,488)	1:75:A:VAL:HG12	1:45:A:SER:HA	8	0.28
(1,488)	1:75:A:VAL:HG13	1:45:A:SER:HA	8	0.28
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	10	0.28
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	9	0.27
(2,129)	1:66:A:GLY:H	1:68:A:GLY:HA3	5	0.27
(2,114)	1:90:A:MET:HE1	1:37:A:TYR:HA	13	0.27
(2,114)	1:90:A:MET:HE2	1:37:A:TYR:HA	13	0.27
(2,114)	1:90:A:MET:HE3	1:37:A:TYR:HA	13	0.27
(2,107)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	5	0.27
(2,101)	1:47:A:ASN:HB3	1:48:A:GLU:HB3	12	0.27
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	4	0.27
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	4	0.27
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE1	9	0.27
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE2	9	0.27
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	2	0.27
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	12	0.27
(1,2522)	1:52:A:THR:HG21	1:48:A:GLU:HB3	2	0.27
(1,2522)	1:52:A:THR:HG22	1:48:A:GLU:HB3	2	0.27
(1,2522)	1:52:A:THR:HG23	1:48:A:GLU:HB3	2	0.27
(1,2453)	1:31:A:THR:HG21	1:36:A:TRP:HZ2	15	0.27
(1,2453)	1:31:A:THR:HG22	1:36:A:TRP:HZ2	15	0.27
(1,2453)	1:31:A:THR:HG23	1:36:A:TRP:HZ2	15	0.27
(1,2435)	1:90:A:MET:HB2	1:37:A:TYR:HD1	10	0.27
(1,2435)	1:90:A:MET:HB2	1:37:A:TYR:HD2	10	0.27
(1,2390)	1:75:A:VAL:HG21	1:83:A:HIS:HB3	4	0.27
(1,2390)	1:75:A:VAL:HG22	1:83:A:HIS:HB3	4	0.27
(1,2390)	1:75:A:VAL:HG23	1:83:A:HIS:HB3	4	0.27
(1,2390)	1:75:A:VAL:HG21	1:83:A:HIS:HB3	13	0.27
(1,2390)	1:75:A:VAL:HG22	1:83:A:HIS:HB3	13	0.27
(1,2390)	1:75:A:VAL:HG23	1:83:A:HIS:HB3	13	0.27
(1,2363)	1:53:A:VAL:HA	1:75:A:VAL:HG21	11	0.27
(1,2363)	1:53:A:VAL:HA	1:75:A:VAL:HG22	11	0.27
(1,2363)	1:53:A:VAL:HA	1:75:A:VAL:HG23	11	0.27
(1,2329)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	5	0.27
(1,2193)	1:77:A:VAL:HG11	1:83:A:HIS:HE1	8	0.27
(1,2193)	1:77:A:VAL:HG12	1:83:A:HIS:HE1	8	0.27
(1,2193)	1:77:A:VAL:HG13	1:83:A:HIS:HE1	8	0.27
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	15	0.27
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	10	0.27
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	12	0.27
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	9	0.27
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	9	0.27
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	9	0.27
(1,1860)	1:69:A:GLY:HA3	1:60:A:PRO:HG3	8	0.27
(1,1722)	1:64:A:LEU:HB3	1:66:A:GLY:HA2	3	0.27
(1,1630)	1:60:A:PRO:HA	1:66:A:GLY:HA2	1	0.27
(1,1615)	1:60:A:PRO:HA	1:66:A:GLY:HA3	9	0.27
(1,1391)	1:81:A:GLY:HA3	1:47:A:ASN:HD22	5	0.27
(1,1225)	1:101:A:GLU:HG3	1:10:A:ASN:HD22	7	0.27
(1,912)	1:91:A:ARG:HB3	1:91:A:ARG:HD3	2	0.27
(1,912)	1:91:A:ARG:HB3	1:91:A:ARG:HD3	15	0.27
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	5	0.27
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	5	0.27
(1,528)	1:70:A:THR:HB	1:58:A:PHE:HA	11	0.27
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	2	0.27
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	2	0.27
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	2	0.27
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	11	0.27
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	11	0.27
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	11	0.27
(1,341)	1:78:A:LYS:HB3	1:78:A:LYS:HA	14	0.27
(3,43)	1:105:A:VAL:H	1:85:A:VAL:O	9	0.26
(3,43)	1:105:A:VAL:H	1:85:A:VAL:O	15	0.26
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	2	0.26
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	5	0.26
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	13	0.26
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	2	0.26
(2,103)	1:48:A:GLU:HA	1:50:A:MET:HA	14	0.26
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	1	0.26
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	1	0.26
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	1	0.26
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	1	0.26
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	12	0.26
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	12	0.26
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	12	0.26
(2,41)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	11	0.26
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	7	0.26
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	9	0.26
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	7	0.26
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	10	0.26
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	10	0.26
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	10	0.26
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	14	0.26
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	14	0.26
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	14	0.26
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG11	1	0.26
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG12	1	0.26
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG13	1	0.26
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG11	1	0.26
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG12	1	0.26
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG13	1	0.26
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG11	1	0.26
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG12	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG13	1	0.26
(1,2321)	1:44:A:GLU:HG3	1:46:A:PRO:HD2	7	0.26
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	3	0.26
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	15	0.26
(1,2164)	1:43:A:LYS:HA	1:38:A:PHE:HZ	5	0.26
(1,2131)	1:37:A:TYR:H	1:90:A:MET:HG2	12	0.26
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	5	0.26
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	5	0.26
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	5	0.26
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	11	0.26
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	11	0.26
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	11	0.26
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	5	0.26
(1,2018)	1:67:A:ALA:H	1:65:A:LEU:HA	8	0.26
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	1	0.26
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	1	0.26
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	1	0.26
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	12	0.26
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	12	0.26
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	12	0.26
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	13	0.26
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	13	0.26
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	13	0.26
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB1	10	0.26
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB2	10	0.26
(1,1707)	1:107:A:LEU:HB2	1:12:A:ALA:HB3	10	0.26
(1,1630)	1:60:A:PRO:HA	1:66:A:GLY:HA2	8	0.26
(1,1535)	1:90:A:MET:HE1	1:92:A:PRO:HA	13	0.26
(1,1535)	1:90:A:MET:HE2	1:92:A:PRO:HA	13	0.26
(1,1535)	1:90:A:MET:HE3	1:92:A:PRO:HA	13	0.26
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	2	0.26
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	10	0.26
(1,1314)	1:60:A:PRO:HB2	1:62:A:SER:H	8	0.26
(1,1221)	1:55:A:ASN:HD22	1:56:A:LYS:H	15	0.26
(1,733)	1:99:A:ASP:HB3	1:99:A:ASP:H	6	0.26
(1,677)	1:26:A:LEU:HG	1:27:A:PRO:HG2	7	0.26
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	12	0.26
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	12	0.26
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	12	0.26
(1,504)	1:91:A:ARG:HB2	1:96:A:PRO:HB2	2	0.26
(1,489)	1:65:A:LEU:HD11	1:30:A:PRO:HD3	11	0.26
(1,489)	1:65:A:LEU:HD12	1:30:A:PRO:HD3	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,489)	1:65:A:LEU:HD13	1:30:A:PRO:HD3	11	0.26
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	13	0.26
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	13	0.26
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	13	0.26
(1,349)	1:102:A:ARG:HG3	1:88:A:THR:HA	1	0.26
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	10	0.25
(2,129)	1:66:A:GLY:H	1:68:A:GLY:HA3	11	0.25
(2,107)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	12	0.25
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	5	0.25
(1,2521)	1:26:A:LEU:HG	1:7:A:LYS:HB2	6	0.25
(1,2486)	1:16:A:VAL:HB	1:110:A:ASN:HD21	1	0.25
(1,2486)	1:85:A:VAL:HB	1:38:A:PHE:HD1	6	0.25
(1,2486)	1:85:A:VAL:HB	1:38:A:PHE:HD2	6	0.25
(1,2453)	1:31:A:THR:HG21	1:36:A:TRP:HZ2	10	0.25
(1,2453)	1:31:A:THR:HG22	1:36:A:TRP:HZ2	10	0.25
(1,2453)	1:31:A:THR:HG23	1:36:A:TRP:HZ2	10	0.25
(1,2390)	1:75:A:VAL:HG21	1:51:A:PHE:HB3	1	0.25
(1,2390)	1:75:A:VAL:HG22	1:51:A:PHE:HB3	1	0.25
(1,2390)	1:75:A:VAL:HG23	1:51:A:PHE:HB3	1	0.25
(1,2360)	1:106:A:TYR:HD1	1:106:A:TYR:H	8	0.25
(1,2360)	1:106:A:TYR:HD2	1:106:A:TYR:H	8	0.25
(1,2329)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	12	0.25
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	1	0.25
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	1	0.25
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	1	0.25
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	7	0.25
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	7	0.25
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	7	0.25
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD1	9	0.25
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD2	9	0.25
(1,2131)	1:37:A:TYR:H	1:90:A:MET:HG2	14	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	2	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	2	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	2	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	3	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	3	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	3	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	4	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	4	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	4	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	8	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	8	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	9	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	9	0.25
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	9	0.25
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	14	0.25
(1,1893)	1:38:A:PHE:HE1	1:85:A:VAL:HG11	9	0.25
(1,1893)	1:38:A:PHE:HE1	1:85:A:VAL:HG12	9	0.25
(1,1893)	1:38:A:PHE:HE1	1:85:A:VAL:HG13	9	0.25
(1,1893)	1:38:A:PHE:HE2	1:85:A:VAL:HG11	9	0.25
(1,1893)	1:38:A:PHE:HE2	1:85:A:VAL:HG12	9	0.25
(1,1893)	1:38:A:PHE:HE2	1:85:A:VAL:HG13	9	0.25
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	11	0.25
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	11	0.25
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	11	0.25
(1,1853)	1:34:A:PHE:HA	1:90:A:MET:HG2	12	0.25
(1,1852)	1:87:A:LEU:HD11	1:10:A:ASN:HA	15	0.25
(1,1852)	1:87:A:LEU:HD12	1:10:A:ASN:HA	15	0.25
(1,1852)	1:87:A:LEU:HD13	1:10:A:ASN:HA	15	0.25
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD21	5	0.25
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD22	5	0.25
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD23	5	0.25
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	5	0.25
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	6	0.25
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	8	0.25
(1,922)	1:100:A:SER:HA	1:90:A:MET:HG3	6	0.25
(1,912)	1:91:A:ARG:HB3	1:91:A:ARG:HD3	4	0.25
(1,912)	1:91:A:ARG:HB3	1:91:A:ARG:HD3	14	0.25
(1,734)	1:108:A:LYS:HG3	1:109:A:ALA:H	10	0.25
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	14	0.25
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	2	0.25
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	2	0.25
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	2	0.25
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	4	0.25
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	4	0.25
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	4	0.25
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	14	0.25
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	14	0.25
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	14	0.25
(1,532)	1:30:A:PRO:HD2	1:28:A:SER:HA	10	0.25
(1,471)	1:92:A:PRO:HG2	1:33:A:GLY:HA2	9	0.25
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	10	0.25
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	10	0.25
(1,205)	1:56:A:LYS:HD3	1:72:A:HIS:HE1	6	0.25
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	7	0.24
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	12	0.24
(2,148)	1:29:A:ASN:HD22	1:10:A:ASN:HB2	11	0.24
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	12	0.24
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	3	0.24
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	5	0.24
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	10	0.24
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	10	0.24
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	10	0.24
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	10	0.24
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	14	0.24
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	14	0.24
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	14	0.24
(2,23)	1:77:A:VAL:HG11	1:46:A:PRO:HD3	8	0.24
(2,23)	1:77:A:VAL:HG12	1:46:A:PRO:HD3	8	0.24
(2,23)	1:77:A:VAL:HG13	1:46:A:PRO:HD3	8	0.24
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	6	0.24
(1,2522)	1:52:A:THR:HG21	1:48:A:GLU:HB3	7	0.24
(1,2522)	1:52:A:THR:HG22	1:48:A:GLU:HB3	7	0.24
(1,2522)	1:52:A:THR:HG23	1:48:A:GLU:HB3	7	0.24
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	12	0.24
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	12	0.24
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	12	0.24
(1,2390)	1:75:A:VAL:HG21	1:83:A:HIS:HB3	14	0.24
(1,2390)	1:75:A:VAL:HG22	1:83:A:HIS:HB3	14	0.24
(1,2390)	1:75:A:VAL:HG23	1:83:A:HIS:HB3	14	0.24
(1,2360)	1:106:A:TYR:HD1	1:106:A:TYR:H	2	0.24
(1,2360)	1:106:A:TYR:HD2	1:106:A:TYR:H	2	0.24
(1,2306)	1:48:A:GLU:HA	1:47:A:ASN:HA	2	0.24
(1,2306)	1:48:A:GLU:HA	1:47:A:ASN:HA	3	0.24
(1,2306)	1:48:A:GLU:HA	1:47:A:ASN:HA	13	0.24
(1,2301)	1:16:A:VAL:HG11	1:18:A:VAL:HA	10	0.24
(1,2301)	1:16:A:VAL:HG12	1:18:A:VAL:HA	10	0.24
(1,2301)	1:16:A:VAL:HG13	1:18:A:VAL:HA	10	0.24
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	10	0.24
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	10	0.24
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	10	0.24
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	11	0.24
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	11	0.24
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2232)	1:12:A:ALA:HB1	1:106:A:TYR:HA	3	0.24
(1,2232)	1:12:A:ALA:HB2	1:106:A:TYR:HA	3	0.24
(1,2232)	1:12:A:ALA:HB3	1:106:A:TYR:HA	3	0.24
(1,2231)	1:63:A:LYS:HD3	1:64:A:LEU:HA	1	0.24
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	10	0.24
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	10	0.24
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	10	0.24
(1,1947)	1:64:A:LEU:H	1:64:A:LEU:HB3	11	0.24
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	2	0.24
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	2	0.24
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	2	0.24
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	5	0.24
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	5	0.24
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	5	0.24
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	7	0.24
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	7	0.24
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	7	0.24
(1,1858)	1:80:A:ALA:HA	1:110:A:ASN:HB3	5	0.24
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG21	1	0.24
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG22	1	0.24
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG23	1	0.24
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	3	0.24
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	14	0.24
(1,1677)	1:55:A:ASN:HA	1:56:A:LYS:HD3	1	0.24
(1,1624)	1:45:A:SER:HA	1:53:A:VAL:HG11	13	0.24
(1,1624)	1:45:A:SER:HA	1:53:A:VAL:HG12	13	0.24
(1,1624)	1:45:A:SER:HA	1:53:A:VAL:HG13	13	0.24
(1,1615)	1:60:A:PRO:HA	1:66:A:GLY:HA3	14	0.24
(1,1535)	1:90:A:MET:HE1	1:92:A:PRO:HA	12	0.24
(1,1535)	1:90:A:MET:HE2	1:92:A:PRO:HA	12	0.24
(1,1535)	1:90:A:MET:HE3	1:92:A:PRO:HA	12	0.24
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	1	0.24
(1,1165)	1:65:A:LEU:H	1:66:A:GLY:H	11	0.24
(1,1059)	1:78:A:LYS:HD3	1:50:A:MET:HG3	4	0.24
(1,488)	1:75:A:VAL:HG11	1:45:A:SER:HA	7	0.24
(1,488)	1:75:A:VAL:HG12	1:45:A:SER:HA	7	0.24
(1,488)	1:75:A:VAL:HG13	1:45:A:SER:HA	7	0.24
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	4	0.24
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	4	0.24
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	4	0.24
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	7	0.24
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	7	0.24
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	6	0.24
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	13	0.24
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	15	0.24
(1,295)	1:51:A:PHE:HB3	1:52:A:THR:HB	6	0.24
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	5	0.24
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	4	0.23
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	11	0.23
(2,145)	1:40:A:GLY:H	1:43:A:LYS:HB3	7	0.23
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	8	0.23
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	3	0.23
(2,114)	1:90:A:MET:HE1	1:37:A:TYR:HA	12	0.23
(2,114)	1:90:A:MET:HE2	1:37:A:TYR:HA	12	0.23
(2,114)	1:90:A:MET:HE3	1:37:A:TYR:HA	12	0.23
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	9	0.23
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	12	0.23
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	14	0.23
(2,54)	1:52:A:THR:HA	1:45:A:SER:H	14	0.23
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD1	8	0.23
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD2	8	0.23
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE1	1	0.23
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE2	1	0.23
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG11	10	0.23
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG12	10	0.23
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG13	10	0.23
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG11	10	0.23
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG12	10	0.23
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG13	10	0.23
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG11	10	0.23
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG12	10	0.23
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG13	10	0.23
(1,2360)	1:106:A:TYR:HD1	1:106:A:TYR:H	3	0.23
(1,2360)	1:106:A:TYR:HD2	1:106:A:TYR:H	3	0.23
(1,2360)	1:106:A:TYR:HD1	1:106:A:TYR:H	6	0.23
(1,2360)	1:106:A:TYR:HD2	1:106:A:TYR:H	6	0.23
(1,2320)	1:38:A:PHE:HB3	1:40:A:GLY:HA2	11	0.23
(1,2284)	1:25:A:GLN:HB3	1:27:A:PRO:HD3	5	0.23
(1,2283)	1:65:A:LEU:HG	1:30:A:PRO:HD3	10	0.23
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	2	0.23
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	2	0.23
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	2	0.23
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	14	0.23
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	14	0.23
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	15	0.23
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	1	0.23
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	12	0.23
(1,1955)	1:23:A:GLU:H	1:23:A:GLU:HG3	1	0.23
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	4	0.23
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	4	0.23
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	4	0.23
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	10	0.23
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	10	0.23
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	10	0.23
(1,1833)	1:69:A:GLY:HA3	1:58:A:PHE:HB2	15	0.23
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	8	0.23
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	9	0.23
(1,1673)	1:42:A:THR:HB	1:39:A:GLU:HG3	6	0.23
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	13	0.23
(1,1415)	1:31:A:THR:HG21	1:36:A:TRP:HD1	9	0.23
(1,1415)	1:31:A:THR:HG22	1:36:A:TRP:HD1	9	0.23
(1,1415)	1:31:A:THR:HG23	1:36:A:TRP:HD1	9	0.23
(1,1154)	1:56:A:LYS:HG3	1:56:A:LYS:H	10	0.23
(1,919)	1:75:A:VAL:HG11	1:75:A:VAL:H	8	0.23
(1,919)	1:75:A:VAL:HG12	1:75:A:VAL:H	8	0.23
(1,919)	1:75:A:VAL:HG13	1:75:A:VAL:H	8	0.23
(1,912)	1:91:A:ARG:HB3	1:91:A:ARG:HD3	7	0.23
(1,912)	1:91:A:ARG:HB3	1:91:A:ARG:HD3	8	0.23
(1,887)	1:75:A:VAL:HG11	1:46:A:PRO:HD3	8	0.23
(1,887)	1:75:A:VAL:HG12	1:46:A:PRO:HD3	8	0.23
(1,887)	1:75:A:VAL:HG13	1:46:A:PRO:HD3	8	0.23
(1,841)	1:43:A:LYS:HG3	1:38:A:PHE:HD1	8	0.23
(1,841)	1:43:A:LYS:HG3	1:38:A:PHE:HD2	8	0.23
(1,730)	1:7:A:LYS:HA	1:7:A:LYS:HD3	8	0.23
(1,628)	1:65:A:LEU:HG	1:60:A:PRO:HB3	1	0.23
(1,488)	1:75:A:VAL:HG11	1:45:A:SER:HA	3	0.23
(1,488)	1:75:A:VAL:HG12	1:45:A:SER:HA	3	0.23
(1,488)	1:75:A:VAL:HG13	1:45:A:SER:HA	3	0.23
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	8	0.23
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	8	0.23
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	8	0.23
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	3	0.23
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	4	0.23
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	10	0.23
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	3	0.23
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	9	0.23
(1,205)	1:56:A:LYS:HD3	1:72:A:HIS:HE1	12	0.23
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	14	0.22
(2,142)	1:50:A:MET:H	1:52:A:THR:HB	6	0.22
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	2	0.22
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	15	0.22
(2,101)	1:47:A:ASN:HB3	1:48:A:GLU:HB3	3	0.22
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	10	0.22
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	10	0.22
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	10	0.22
(2,75)	1:107:A:LEU:HB3	1:83:A:HIS:HB2	9	0.22
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	11	0.22
(1,2413)	1:31:A:THR:HG21	1:89:A:TYR:HB3	15	0.22
(1,2413)	1:31:A:THR:HG22	1:89:A:TYR:HB3	15	0.22
(1,2413)	1:31:A:THR:HG23	1:89:A:TYR:HB3	15	0.22
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG11	8	0.22
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG12	8	0.22
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG13	8	0.22
(1,2403)	1:36:A:TRP:HB2	1:57:A:TYR:HD1	12	0.22
(1,2403)	1:36:A:TRP:HB2	1:57:A:TYR:HD2	12	0.22
(1,2379)	1:38:A:PHE:HB3	1:38:A:PHE:H	12	0.22
(1,2360)	1:106:A:TYR:HD1	1:106:A:TYR:H	1	0.22
(1,2360)	1:106:A:TYR:HD2	1:106:A:TYR:H	1	0.22
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	8	0.22
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	8	0.22
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	8	0.22
(1,2164)	1:43:A:LYS:HA	1:38:A:PHE:HZ	6	0.22
(1,2149)	1:26:A:LEU:HD11	1:85:A:VAL:HG11	15	0.22
(1,2149)	1:26:A:LEU:HD11	1:85:A:VAL:HG12	15	0.22
(1,2149)	1:26:A:LEU:HD11	1:85:A:VAL:HG13	15	0.22
(1,2149)	1:26:A:LEU:HD12	1:85:A:VAL:HG11	15	0.22
(1,2149)	1:26:A:LEU:HD12	1:85:A:VAL:HG12	15	0.22
(1,2149)	1:26:A:LEU:HD12	1:85:A:VAL:HG13	15	0.22
(1,2149)	1:26:A:LEU:HD13	1:85:A:VAL:HG11	15	0.22
(1,2149)	1:26:A:LEU:HD13	1:85:A:VAL:HG12	15	0.22
(1,2149)	1:26:A:LEU:HD13	1:85:A:VAL:HG13	15	0.22
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	1	0.22
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	1	0.22
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	1	0.22
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	6	0.22
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	6	0.22
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	3	0.22
(1,2055)	1:71:A:GLU:H	1:28:A:SER:HB2	3	0.22
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	3	0.22
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	4	0.22
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	5	0.22
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	6	0.22
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	7	0.22
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	11	0.22
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	14	0.22
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	15	0.22
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	8	0.22
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	8	0.22
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	8	0.22
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	14	0.22
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	14	0.22
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	14	0.22
(1,1630)	1:60:A:PRO:HA	1:66:A:GLY:HA2	15	0.22
(1,1517)	1:4:A:LYS:HB3	1:4:A:LYS:HA	3	0.22
(1,1517)	1:4:A:LYS:HB3	1:4:A:LYS:HA	12	0.22
(1,1517)	1:4:A:LYS:HB3	1:4:A:LYS:HA	14	0.22
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	9	0.22
(1,1357)	1:25:A:GLN:HE22	1:71:A:GLU:H	9	0.22
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD1	13	0.22
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD2	13	0.22
(1,1332)	1:60:A:PRO:HB2	1:61:A:ASP:H	5	0.22
(1,1225)	1:101:A:GLU:HG3	1:10:A:ASN:HD22	15	0.22
(1,1011)	1:63:A:LYS:HD3	1:63:A:LYS:H	5	0.22
(1,852)	1:14:A:LEU:HD11	1:14:A:LEU:H	15	0.22
(1,852)	1:14:A:LEU:HD12	1:14:A:LEU:H	15	0.22
(1,852)	1:14:A:LEU:HD13	1:14:A:LEU:H	15	0.22
(1,809)	1:65:A:LEU:HA	1:66:A:GLY:H	3	0.22
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	7	0.22
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	7	0.22
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	7	0.22
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	14	0.22
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	14	0.22
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	14	0.22
(1,512)	1:100:A:SER:HB3	1:89:A:TYR:HD1	11	0.22
(1,512)	1:100:A:SER:HB3	1:89:A:TYR:HD2	11	0.22
(1,504)	1:91:A:ARG:HB2	1:96:A:PRO:HB2	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,472)	1:65:A:LEU:HG	1:28:A:SER:HB3	12	0.22
(1,448)	1:71:A:GLU:HG2	1:57:A:TYR:HB3	15	0.22
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	6	0.22
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	6	0.22
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	6	0.22
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	2	0.22
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	12	0.22
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	7	0.22
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	12	0.22
(1,205)	1:56:A:LYS:HD3	1:72:A:HIS:HE1	5	0.22
(3,15)	1:70:A:THR:H	1:58:A:PHE:O	5	0.21
(2,152)	1:69:A:GLY:H	1:29:A:ASN:HA	13	0.21
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	14	0.21
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	14	0.21
(2,114)	1:90:A:MET:HE1	1:37:A:TYR:HA	2	0.21
(2,114)	1:90:A:MET:HE2	1:37:A:TYR:HA	2	0.21
(2,114)	1:90:A:MET:HE3	1:37:A:TYR:HA	2	0.21
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	8	0.21
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD1	2	0.21
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD2	2	0.21
(2,87)	1:15:A:THR:HG21	1:3:A:HIS:HB2	7	0.21
(2,87)	1:15:A:THR:HG22	1:3:A:HIS:HB2	7	0.21
(2,87)	1:15:A:THR:HG23	1:3:A:HIS:HB2	7	0.21
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	13	0.21
(2,41)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	7	0.21
(2,11)	1:5:A:VAL:HB	1:105:A:VAL:H	4	0.21
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	2	0.21
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	6	0.21
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	8	0.21
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	14	0.21
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	2	0.21
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	2	0.21
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	2	0.21
(1,2420)	1:30:A:PRO:HA	1:34:A:PHE:HB2	11	0.21
(1,2357)	1:85:A:VAL:HB	1:85:A:VAL:H	9	0.21
(1,2320)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	7	0.21
(1,2301)	1:16:A:VAL:HG11	1:18:A:VAL:HA	15	0.21
(1,2301)	1:16:A:VAL:HG12	1:18:A:VAL:HA	15	0.21
(1,2301)	1:16:A:VAL:HG13	1:18:A:VAL:HA	15	0.21
(1,2274)	1:54:A:GLU:HB3	1:74:A:HIS:HB3	2	0.21
(1,2274)	1:54:A:GLU:HB3	1:74:A:HIS:HB3	11	0.21
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	4	0.21
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	4	0.21
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	4	0.21
(1,2131)	1:37:A:TYR:H	1:90:A:MET:HG2	15	0.21
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	7	0.21
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	7	0.21
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	7	0.21
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	1	0.21
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	4	0.21
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	8	0.21
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	13	0.21
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	8	0.21
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	9	0.21
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	10	0.21
(1,1955)	1:23:A:GLU:H	1:23:A:GLU:HG3	11	0.21
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	3	0.21
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	3	0.21
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	3	0.21
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD11	6	0.21
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD12	6	0.21
(1,1870)	1:9:A:HIS:HE1	1:24:A:ILE:HD13	6	0.21
(1,1774)	1:24:A:ILE:HD11	1:26:A:LEU:HD21	7	0.21
(1,1774)	1:24:A:ILE:HD11	1:26:A:LEU:HD22	7	0.21
(1,1774)	1:24:A:ILE:HD11	1:26:A:LEU:HD23	7	0.21
(1,1774)	1:24:A:ILE:HD12	1:26:A:LEU:HD21	7	0.21
(1,1774)	1:24:A:ILE:HD12	1:26:A:LEU:HD22	7	0.21
(1,1774)	1:24:A:ILE:HD12	1:26:A:LEU:HD23	7	0.21
(1,1774)	1:24:A:ILE:HD13	1:26:A:LEU:HD21	7	0.21
(1,1774)	1:24:A:ILE:HD13	1:26:A:LEU:HD22	7	0.21
(1,1774)	1:24:A:ILE:HD13	1:26:A:LEU:HD23	7	0.21
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG21	11	0.21
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG22	11	0.21
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG23	11	0.21
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD21	7	0.21
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD22	7	0.21
(1,1693)	1:27:A:PRO:HB3	1:65:A:LEU:HD23	7	0.21
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	14	0.21
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	14	0.21
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	14	0.21
(1,1613)	1:29:A:ASN:HB3	1:31:A:THR:HG21	9	0.21
(1,1613)	1:29:A:ASN:HB3	1:31:A:THR:HG22	9	0.21
(1,1613)	1:29:A:ASN:HB3	1:31:A:THR:HG23	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1458)	1:75:A:VAL:HG21	1:52:A:THR:H	14	0.21
(1,1458)	1:75:A:VAL:HG22	1:52:A:THR:H	14	0.21
(1,1458)	1:75:A:VAL:HG23	1:52:A:THR:H	14	0.21
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	5	0.21
(1,1308)	1:87:A:LEU:HB2	1:89:A:TYR:H	12	0.21
(1,1221)	1:55:A:ASN:HD22	1:56:A:LYS:H	3	0.21
(1,946)	1:34:A:PHE:HD1	1:34:A:PHE:H	10	0.21
(1,946)	1:34:A:PHE:HD2	1:34:A:PHE:H	10	0.21
(1,809)	1:65:A:LEU:HA	1:66:A:GLY:H	14	0.21
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	12	0.21
(1,730)	1:7:A:LYS:HA	1:7:A:LYS:HD3	9	0.21
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	8	0.21
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	8	0.21
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	8	0.21
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	3	0.21
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	3	0.21
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	3	0.21
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	6	0.21
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	7	0.21
(1,205)	1:56:A:LYS:HD3	1:72:A:HIS:HE1	9	0.21
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	14	0.2
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	8	0.2
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	15	0.2
(2,148)	1:29:A:ASN:HD22	1:10:A:ASN:HB2	6	0.2
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG21	12	0.2
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG22	12	0.2
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG23	12	0.2
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG21	12	0.2
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG22	12	0.2
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG23	12	0.2
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG21	12	0.2
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG22	12	0.2
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG23	12	0.2
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	6	0.2
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	7	0.2
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	11	0.2
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	13	0.2
(2,101)	1:47:A:ASN:HB3	1:48:A:GLU:HB3	11	0.2
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD1	6	0.2
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD2	6	0.2
(2,80)	1:56:A:LYS:HD3	1:55:A:ASN:HB2	12	0.2
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	7	0.2
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	12	0.2
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	9	0.2
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	13	0.2
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	15	0.2
(1,2532)	1:5:A:VAL:H	1:23:A:GLU:HB2	7	0.2
(1,2306)	1:48:A:GLU:HA	1:47:A:ASN:HA	9	0.2
(1,2306)	1:48:A:GLU:HA	1:47:A:ASN:HA	11	0.2
(1,2306)	1:48:A:GLU:HA	1:47:A:ASN:HA	12	0.2
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	9	0.2
(1,2193)	1:77:A:VAL:HG11	1:83:A:HIS:HE1	3	0.2
(1,2193)	1:77:A:VAL:HG12	1:83:A:HIS:HE1	3	0.2
(1,2193)	1:77:A:VAL:HG13	1:83:A:HIS:HE1	3	0.2
(1,2164)	1:43:A:LYS:HA	1:38:A:PHE:HZ	8	0.2
(1,2164)	1:43:A:LYS:HA	1:38:A:PHE:HZ	10	0.2
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	2	0.2
(1,1997)	1:61:A:ASP:H	1:60:A:PRO:HG2	9	0.2
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	2	0.2
(1,1962)	1:29:A:ASN:H	1:28:A:SER:HA	13	0.2
(1,1785)	1:27:A:PRO:HG2	1:26:A:LEU:HD11	7	0.2
(1,1785)	1:27:A:PRO:HG2	1:26:A:LEU:HD12	7	0.2
(1,1785)	1:27:A:PRO:HG2	1:26:A:LEU:HD13	7	0.2
(1,1642)	1:67:A:ALA:HB1	1:60:A:PRO:HG2	3	0.2
(1,1642)	1:67:A:ALA:HB2	1:60:A:PRO:HG2	3	0.2
(1,1642)	1:67:A:ALA:HB3	1:60:A:PRO:HG2	3	0.2
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	10	0.2
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	10	0.2
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	10	0.2
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	3	0.2
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	14	0.2
(1,1415)	1:31:A:THR:HG21	1:36:A:TRP:HD1	5	0.2
(1,1415)	1:31:A:THR:HG22	1:36:A:TRP:HD1	5	0.2
(1,1415)	1:31:A:THR:HG23	1:36:A:TRP:HD1	5	0.2
(1,1415)	1:31:A:THR:HG21	1:36:A:TRP:HD1	10	0.2
(1,1415)	1:31:A:THR:HG22	1:36:A:TRP:HD1	10	0.2
(1,1415)	1:31:A:THR:HG23	1:36:A:TRP:HD1	10	0.2
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	13	0.2
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	13	0.2
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	13	0.2
(1,842)	1:49:A:SER:HB3	1:49:A:SER:H	7	0.2
(1,809)	1:65:A:LEU:HA	1:66:A:GLY:H	4	0.2
(1,809)	1:65:A:LEU:HA	1:66:A:GLY:H	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,809)	1:65:A:LEU:HA	1:66:A:GLY:H	7	0.2
(1,809)	1:65:A:LEU:HA	1:66:A:GLY:H	8	0.2
(1,809)	1:65:A:LEU:HA	1:66:A:GLY:H	9	0.2
(1,809)	1:65:A:LEU:HA	1:66:A:GLY:H	12	0.2
(1,752)	1:22:A:VAL:HG21	1:23:A:GLU:H	8	0.2
(1,752)	1:22:A:VAL:HG22	1:23:A:GLU:H	8	0.2
(1,752)	1:22:A:VAL:HG23	1:23:A:GLU:H	8	0.2
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	10	0.2
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	10	0.2
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	10	0.2
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	12	0.2
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	12	0.2
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	12	0.2
(1,504)	1:91:A:ARG:HB2	1:96:A:PRO:HB2	7	0.2
(1,349)	1:102:A:ARG:HG3	1:88:A:THR:HA	8	0.2
(1,341)	1:78:A:LYS:HB3	1:78:A:LYS:HA	2	0.2
(1,304)	1:61:A:ASP:HB3	1:62:A:SER:HA	10	0.2
(1,178)	1:85:A:VAL:HB	1:105:A:VAL:H	9	0.2
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	9	0.19
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	3	0.19
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD1	10	0.19
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD2	10	0.19
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	2	0.19
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	2	0.19
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	2	0.19
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE1	3	0.19
(2,40)	1:86:A:ASN:HD22	1:38:A:PHE:HE2	3	0.19
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	1	0.19
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	13	0.19
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	15	0.19
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	4	0.19
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	4	0.19
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	4	0.19
(1,2424)	1:35:A:ALA:HB1	1:71:A:GLU:HB3	11	0.19
(1,2424)	1:35:A:ALA:HB2	1:71:A:GLU:HB3	11	0.19
(1,2424)	1:35:A:ALA:HB3	1:71:A:GLU:HB3	11	0.19
(1,2420)	1:30:A:PRO:HA	1:34:A:PHE:HB2	14	0.19
(1,2413)	1:31:A:THR:HG21	1:89:A:TYR:HB3	4	0.19
(1,2413)	1:31:A:THR:HG22	1:89:A:TYR:HB3	4	0.19
(1,2413)	1:31:A:THR:HG23	1:89:A:TYR:HB3	4	0.19
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG11	2	0.19
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG12	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG13	2	0.19
(1,2360)	1:106:A:TYR:HD1	1:106:A:TYR:H	4	0.19
(1,2360)	1:106:A:TYR:HD2	1:106:A:TYR:H	4	0.19
(1,2301)	1:16:A:VAL:HG11	1:18:A:VAL:HA	13	0.19
(1,2301)	1:16:A:VAL:HG12	1:18:A:VAL:HA	13	0.19
(1,2301)	1:16:A:VAL:HG13	1:18:A:VAL:HA	13	0.19
(1,2293)	1:31:A:THR:HG21	1:29:A:ASN:HB3	8	0.19
(1,2293)	1:31:A:THR:HG22	1:29:A:ASN:HB3	8	0.19
(1,2293)	1:31:A:THR:HG23	1:29:A:ASN:HB3	8	0.19
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	5	0.19
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	5	0.19
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	5	0.19
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	12	0.19
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	12	0.19
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	12	0.19
(1,2232)	1:12:A:ALA:HB1	1:106:A:TYR:HA	7	0.19
(1,2232)	1:12:A:ALA:HB2	1:106:A:TYR:HA	7	0.19
(1,2232)	1:12:A:ALA:HB3	1:106:A:TYR:HA	7	0.19
(1,2232)	1:12:A:ALA:HB1	1:106:A:TYR:HA	11	0.19
(1,2232)	1:12:A:ALA:HB2	1:106:A:TYR:HA	11	0.19
(1,2232)	1:12:A:ALA:HB3	1:106:A:TYR:HA	11	0.19
(1,2192)	1:84:A:ALA:HB1	1:83:A:HIS:HE1	8	0.19
(1,2192)	1:84:A:ALA:HB2	1:83:A:HIS:HE1	8	0.19
(1,2192)	1:84:A:ALA:HB3	1:83:A:HIS:HE1	8	0.19
(1,2131)	1:37:A:TYR:H	1:90:A:MET:HG2	7	0.19
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	12	0.19
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	12	0.19
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	12	0.19
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG21	13	0.19
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG22	13	0.19
(1,2095)	1:11:A:GLY:H	1:5:A:VAL:HG23	13	0.19
(1,1869)	1:83:A:HIS:HE1	1:87:A:LEU:HG	4	0.19
(1,1730)	1:56:A:LYS:HD3	1:74:A:HIS:HA	10	0.19
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	7	0.19
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	7	0.19
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	7	0.19
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	12	0.19
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	12	0.19
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	12	0.19
(1,1541)	1:90:A:MET:HE1	1:88:A:THR:HB	9	0.19
(1,1541)	1:90:A:MET:HE2	1:88:A:THR:HB	9	0.19
(1,1541)	1:90:A:MET:HE3	1:88:A:THR:HB	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1535)	1:90:A:MET:HE1	1:92:A:PRO:HA	11	0.19
(1,1535)	1:90:A:MET:HE2	1:92:A:PRO:HA	11	0.19
(1,1535)	1:90:A:MET:HE3	1:92:A:PRO:HA	11	0.19
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	15	0.19
(1,1433)	1:46:A:PRO:HB3	1:48:A:GLU:H	13	0.19
(1,1209)	1:42:A:THR:HG21	1:44:A:GLU:H	7	0.19
(1,1209)	1:42:A:THR:HG22	1:44:A:GLU:H	7	0.19
(1,1209)	1:42:A:THR:HG23	1:44:A:GLU:H	7	0.19
(1,878)	1:63:A:LYS:HD3	1:61:A:ASP:HB3	1	0.19
(1,807)	1:78:A:LYS:HA	1:18:A:VAL:HG11	3	0.19
(1,807)	1:78:A:LYS:HA	1:18:A:VAL:HG12	3	0.19
(1,807)	1:78:A:LYS:HA	1:18:A:VAL:HG13	3	0.19
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	2	0.19
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	4	0.19
(1,661)	1:91:A:ARG:HB3	1:90:A:MET:HB2	15	0.19
(1,658)	1:94:A:THR:HG21	1:90:A:MET:HB2	5	0.19
(1,658)	1:94:A:THR:HG22	1:90:A:MET:HB2	5	0.19
(1,658)	1:94:A:THR:HG23	1:90:A:MET:HB2	5	0.19
(1,471)	1:92:A:PRO:HG2	1:33:A:GLY:HA2	15	0.19
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	7	0.19
(1,303)	1:36:A:TRP:HB2	1:26:A:LEU:HA	13	0.19
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	2	0.19
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	2	0.19
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	2	0.19
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	8	0.19
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	13	0.19
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	3	0.19
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	4	0.19
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	8	0.19
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	2	0.18
(3,43)	1:105:A:VAL:H	1:85:A:VAL:O	10	0.18
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	1	0.18
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	6	0.18
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	10	0.18
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	15	0.18
(2,131)	1:65:A:LEU:H	1:62:A:SER:HA	15	0.18
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG21	5	0.18
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG22	5	0.18
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG23	5	0.18
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG21	5	0.18
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG22	5	0.18
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG23	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG21	5	0.18
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG22	5	0.18
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG23	5	0.18
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	4	0.18
(2,80)	1:56:A:LYS:HD3	1:55:A:ASN:HB2	4	0.18
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	11	0.18
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	9	0.18
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	9	0.18
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	9	0.18
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	13	0.18
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	13	0.18
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	13	0.18
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG11	12	0.18
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG12	12	0.18
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG13	12	0.18
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG11	12	0.18
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG12	12	0.18
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG13	12	0.18
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG11	12	0.18
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG12	12	0.18
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG13	12	0.18
(1,2413)	1:31:A:THR:HG21	1:89:A:TYR:HB3	10	0.18
(1,2413)	1:31:A:THR:HG22	1:89:A:TYR:HB3	10	0.18
(1,2413)	1:31:A:THR:HG23	1:89:A:TYR:HB3	10	0.18
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG11	4	0.18
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG12	4	0.18
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG13	4	0.18
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG11	6	0.18
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG12	6	0.18
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG13	6	0.18
(1,2321)	1:44:A:GLU:HG3	1:46:A:PRO:HD2	5	0.18
(1,2306)	1:48:A:GLU:HA	1:47:A:ASN:HA	10	0.18
(1,2301)	1:16:A:VAL:HG11	1:18:A:VAL:HA	3	0.18
(1,2301)	1:16:A:VAL:HG12	1:18:A:VAL:HA	3	0.18
(1,2301)	1:16:A:VAL:HG13	1:18:A:VAL:HA	3	0.18
(1,2294)	1:52:A:THR:HG21	1:76:A:THR:HB	6	0.18
(1,2294)	1:52:A:THR:HG22	1:76:A:THR:HB	6	0.18
(1,2294)	1:52:A:THR:HG23	1:76:A:THR:HB	6	0.18
(1,2208)	1:51:A:PHE:HB2	1:78:A:LYS:HA	14	0.18
(1,2018)	1:67:A:ALA:H	1:65:A:LEU:HA	11	0.18
(1,2006)	1:58:A:PHE:H	1:58:A:PHE:HD1	12	0.18
(1,2006)	1:58:A:PHE:H	1:58:A:PHE:HD2	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1869)	1:83:A:HIS:HE1	1:87:A:LEU:HG	2	0.18
(1,1853)	1:34:A:PHE:HA	1:90:A:MET:HG2	4	0.18
(1,1853)	1:34:A:PHE:HA	1:90:A:MET:HG2	8	0.18
(1,1833)	1:69:A:GLY:HA3	1:58:A:PHE:HB2	8	0.18
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG21	4	0.18
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG22	4	0.18
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG23	4	0.18
(1,1668)	1:78:A:LYS:HB2	1:78:A:LYS:HE3	9	0.18
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	1	0.18
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	1	0.18
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	1	0.18
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	3	0.18
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	3	0.18
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	3	0.18
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	8	0.18
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	8	0.18
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	8	0.18
(1,1615)	1:60:A:PRO:HA	1:66:A:GLY:HA3	6	0.18
(1,1535)	1:90:A:MET:HE1	1:92:A:PRO:HA	6	0.18
(1,1535)	1:90:A:MET:HE2	1:92:A:PRO:HA	6	0.18
(1,1535)	1:90:A:MET:HE3	1:92:A:PRO:HA	6	0.18
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	11	0.18
(1,1430)	1:82:A:THR:HG21	1:110:A:ASN:HD21	10	0.18
(1,1430)	1:82:A:THR:HG22	1:110:A:ASN:HD21	10	0.18
(1,1430)	1:82:A:THR:HG23	1:110:A:ASN:HD21	10	0.18
(1,1314)	1:60:A:PRO:HB2	1:62:A:SER:H	9	0.18
(1,1303)	1:104:A:THR:HG21	1:11:A:GLY:H	14	0.18
(1,1303)	1:104:A:THR:HG22	1:11:A:GLY:H	14	0.18
(1,1303)	1:104:A:THR:HG23	1:11:A:GLY:H	14	0.18
(1,987)	1:21:A:LEU:HD11	1:22:A:VAL:H	3	0.18
(1,987)	1:21:A:LEU:HD12	1:22:A:VAL:H	3	0.18
(1,987)	1:21:A:LEU:HD13	1:22:A:VAL:H	3	0.18
(1,946)	1:34:A:PHE:HD1	1:34:A:PHE:H	5	0.18
(1,946)	1:34:A:PHE:HD2	1:34:A:PHE:H	5	0.18
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	5	0.18
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	7	0.18
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	10	0.18
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	15	0.18
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD11	12	0.18
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD12	12	0.18
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD13	12	0.18
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD11	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD12	14	0.18
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD13	14	0.18
(1,746)	1:70:A:THR:HG21	1:71:A:GLU:H	11	0.18
(1,746)	1:70:A:THR:HG22	1:71:A:GLU:H	11	0.18
(1,746)	1:70:A:THR:HG23	1:71:A:GLU:H	11	0.18
(1,677)	1:26:A:LEU:HG	1:27:A:PRO:HG2	8	0.18
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	6	0.18
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	6	0.18
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	6	0.18
(1,664)	1:18:A:VAL:HG11	1:16:A:VAL:HB	11	0.18
(1,664)	1:18:A:VAL:HG12	1:16:A:VAL:HB	11	0.18
(1,664)	1:18:A:VAL:HG13	1:16:A:VAL:HB	11	0.18
(1,488)	1:75:A:VAL:HG11	1:45:A:SER:HA	1	0.18
(1,488)	1:75:A:VAL:HG12	1:45:A:SER:HA	1	0.18
(1,488)	1:75:A:VAL:HG13	1:45:A:SER:HA	1	0.18
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	1	0.18
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	1	0.18
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	1	0.18
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	1	0.18
(1,304)	1:61:A:ASP:HB3	1:62:A:SER:HA	11	0.18
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	2	0.18
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	11	0.18
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	15	0.18
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	13	0.18
(1,205)	1:56:A:LYS:HD3	1:72:A:HIS:HE1	4	0.18
(1,176)	1:85:A:VAL:HB	1:103:A:PHE:HE1	9	0.18
(1,176)	1:85:A:VAL:HB	1:103:A:PHE:HE2	9	0.18
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	6	0.17
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	7	0.17
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	13	0.17
(2,148)	1:29:A:ASN:HD22	1:10:A:ASN:HB2	7	0.17
(2,148)	1:29:A:ASN:HD22	1:10:A:ASN:HB2	12	0.17
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	1	0.17
(2,133)	1:43:A:LYS:H	1:44:A:GLU:HB2	6	0.17
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG21	8	0.17
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG22	8	0.17
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG23	8	0.17
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG21	8	0.17
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG22	8	0.17
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG23	8	0.17
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG21	8	0.17
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG22	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG23	8	0.17
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	2	0.17
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD1	13	0.17
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD2	13	0.17
(2,89)	1:48:A:GLU:HA	1:52:A:THR:HG21	6	0.17
(2,89)	1:48:A:GLU:HA	1:52:A:THR:HG22	6	0.17
(2,89)	1:48:A:GLU:HA	1:52:A:THR:HG23	6	0.17
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	1	0.17
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	1	0.17
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	1	0.17
(2,80)	1:56:A:LYS:HD3	1:55:A:ASN:HB2	3	0.17
(2,67)	1:32:A:THR:HG21	1:100:A:SER:HA	11	0.17
(2,67)	1:32:A:THR:HG22	1:100:A:SER:HA	11	0.17
(2,67)	1:32:A:THR:HG23	1:100:A:SER:HA	11	0.17
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	15	0.17
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD1	5	0.17
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD2	5	0.17
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD1	14	0.17
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD2	14	0.17
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	1	0.17
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	1	0.17
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	1	0.17
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	5	0.17
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	5	0.17
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	5	0.17
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	6	0.17
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	6	0.17
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	6	0.17
(1,2357)	1:85:A:VAL:HB	1:85:A:VAL:H	14	0.17
(1,2333)	1:5:A:VAL:HG21	1:3:A:HIS:HB3	10	0.17
(1,2333)	1:5:A:VAL:HG22	1:3:A:HIS:HB3	10	0.17
(1,2333)	1:5:A:VAL:HG23	1:3:A:HIS:HB3	10	0.17
(1,2306)	1:48:A:GLU:HA	1:47:A:ASN:HA	7	0.17
(1,2306)	1:48:A:GLU:HA	1:47:A:ASN:HA	14	0.17
(1,2293)	1:21:A:LEU:HG	1:74:A:HIS:HB3	10	0.17
(1,2164)	1:43:A:LYS:HA	1:38:A:PHE:HZ	12	0.17
(1,2135)	1:70:A:THR:H	1:59:A:PRO:HG3	8	0.17
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB1	7	0.17
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB2	7	0.17
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB3	7	0.17
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	6	0.17
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1997)	1:61:A:ASP:H	1:60:A:PRO:HG2	11	0.17
(1,1970)	1:19:A:GLY:H	1:18:A:VAL:HG11	3	0.17
(1,1970)	1:19:A:GLY:H	1:18:A:VAL:HG12	3	0.17
(1,1970)	1:19:A:GLY:H	1:18:A:VAL:HG13	3	0.17
(1,1869)	1:83:A:HIS:HE1	1:87:A:LEU:HG	8	0.17
(1,1853)	1:34:A:PHE:HA	1:90:A:MET:HG2	10	0.17
(1,1847)	1:55:A:ASN:HA	1:56:A:LYS:HG3	6	0.17
(1,1763)	1:86:A:ASN:HA	1:36:A:TRP:HZ3	8	0.17
(1,1642)	1:67:A:ALA:HB1	1:60:A:PRO:HG2	7	0.17
(1,1642)	1:67:A:ALA:HB2	1:60:A:PRO:HG2	7	0.17
(1,1642)	1:67:A:ALA:HB3	1:60:A:PRO:HG2	7	0.17
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	6	0.17
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	6	0.17
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	6	0.17
(1,1615)	1:60:A:PRO:HA	1:66:A:GLY:HA3	8	0.17
(1,1430)	1:82:A:THR:HG21	1:110:A:ASN:HD21	2	0.17
(1,1430)	1:82:A:THR:HG22	1:110:A:ASN:HD21	2	0.17
(1,1430)	1:82:A:THR:HG23	1:110:A:ASN:HD21	2	0.17
(1,1415)	1:31:A:THR:HG21	1:36:A:TRP:HD1	7	0.17
(1,1415)	1:31:A:THR:HG22	1:36:A:TRP:HD1	7	0.17
(1,1415)	1:31:A:THR:HG23	1:36:A:TRP:HD1	7	0.17
(1,1314)	1:60:A:PRO:HB2	1:62:A:SER:H	1	0.17
(1,1259)	1:4:A:LYS:HB3	1:3:A:HIS:HB3	1	0.17
(1,1233)	1:76:A:THR:HG21	1:51:A:PHE:HE1	14	0.17
(1,1233)	1:76:A:THR:HG21	1:51:A:PHE:HE2	14	0.17
(1,1233)	1:76:A:THR:HG22	1:51:A:PHE:HE1	14	0.17
(1,1233)	1:76:A:THR:HG22	1:51:A:PHE:HE2	14	0.17
(1,1233)	1:76:A:THR:HG23	1:51:A:PHE:HE1	14	0.17
(1,1233)	1:76:A:THR:HG23	1:51:A:PHE:HE2	14	0.17
(1,1225)	1:101:A:GLU:HG3	1:10:A:ASN:HD22	4	0.17
(1,1074)	1:18:A:VAL:HG11	1:79:A:ALA:H	9	0.17
(1,1074)	1:18:A:VAL:HG12	1:79:A:ALA:H	9	0.17
(1,1074)	1:18:A:VAL:HG13	1:79:A:ALA:H	9	0.17
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	11	0.17
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	11	0.17
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	11	0.17
(1,802)	1:64:A:LEU:HD11	1:65:A:LEU:H	7	0.17
(1,802)	1:64:A:LEU:HD12	1:65:A:LEU:H	7	0.17
(1,802)	1:64:A:LEU:HD13	1:65:A:LEU:H	7	0.17
(1,776)	1:96:A:PRO:HB2	1:99:A:ASP:HB2	9	0.17
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	8	0.17
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD11	4	0.17
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD12	4	0.17
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD13	4	0.17
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD11	11	0.17
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD12	11	0.17
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD13	11	0.17
(1,746)	1:70:A:THR:HG21	1:71:A:GLU:H	13	0.17
(1,746)	1:70:A:THR:HG22	1:71:A:GLU:H	13	0.17
(1,746)	1:70:A:THR:HG23	1:71:A:GLU:H	13	0.17
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	6	0.17
(1,730)	1:7:A:LYS:HA	1:7:A:LYS:HD3	14	0.17
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB1	1	0.17
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB2	1	0.17
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB3	1	0.17
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB1	1	0.17
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB2	1	0.17
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB3	1	0.17
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB1	1	0.17
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB2	1	0.17
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB3	1	0.17
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB1	8	0.17
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB2	8	0.17
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB3	8	0.17
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB1	8	0.17
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB2	8	0.17
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB3	8	0.17
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB1	8	0.17
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB2	8	0.17
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB3	8	0.17
(1,604)	1:25:A:GLN:HB2	1:73:A:PHE:HB2	14	0.17
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	5	0.17
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	5	0.17
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	5	0.17
(1,373)	1:31:A:THR:HG21	1:35:A:ALA:HA	14	0.17
(1,373)	1:31:A:THR:HG22	1:35:A:ALA:HA	14	0.17
(1,373)	1:31:A:THR:HG23	1:35:A:ALA:HA	14	0.17
(1,350)	1:7:A:LYS:HD3	1:28:A:SER:HA	10	0.17
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	5	0.17
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	11	0.17
(1,304)	1:61:A:ASP:HB3	1:62:A:SER:HA	4	0.17
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	4	0.17
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	5	0.17
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	5	0.17
(1,61)	1:26:A:LEU:HD11	1:25:A:GLN:HB3	13	0.17
(1,61)	1:26:A:LEU:HD12	1:25:A:GLN:HB3	13	0.17
(1,61)	1:26:A:LEU:HD13	1:25:A:GLN:HB3	13	0.17
(3,73)	1:12:A:ALA:H	1:9:A:HIS:O	1	0.16
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	4	0.16
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	8	0.16
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	10	0.16
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	11	0.16
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	15	0.16
(2,148)	1:29:A:ASN:HD22	1:10:A:ASN:HB2	8	0.16
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG21	1	0.16
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG22	1	0.16
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG23	1	0.16
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG21	1	0.16
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG22	1	0.16
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG23	1	0.16
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG21	1	0.16
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG22	1	0.16
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG23	1	0.16
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD1	15	0.16
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD2	15	0.16
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	5	0.16
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	5	0.16
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	5	0.16
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	12	0.16
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	12	0.16
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	12	0.16
(2,82)	1:5:A:VAL:HG11	1:106:A:TYR:H	14	0.16
(2,82)	1:5:A:VAL:HG12	1:106:A:TYR:H	14	0.16
(2,82)	1:5:A:VAL:HG13	1:106:A:TYR:H	14	0.16
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	9	0.16
(2,19)	1:63:A:LYS:HD3	1:65:A:LEU:HA	6	0.16
(2,19)	1:63:A:LYS:HD3	1:65:A:LEU:HA	11	0.16
(2,19)	1:63:A:LYS:HD3	1:65:A:LEU:HA	12	0.16
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	10	0.16
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	8	0.16
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	8	0.16
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	8	0.16
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	11	0.16
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	11	0.16
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG11	13	0.16
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG12	13	0.16
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG13	13	0.16
(1,2390)	1:75:A:VAL:HG21	1:51:A:PHE:HB3	11	0.16
(1,2390)	1:75:A:VAL:HG22	1:51:A:PHE:HB3	11	0.16
(1,2390)	1:75:A:VAL:HG23	1:51:A:PHE:HB3	11	0.16
(1,2379)	1:38:A:PHE:HB3	1:38:A:PHE:H	4	0.16
(1,2360)	1:106:A:TYR:HD1	1:106:A:TYR:H	14	0.16
(1,2360)	1:106:A:TYR:HD2	1:106:A:TYR:H	14	0.16
(1,2357)	1:85:A:VAL:HB	1:85:A:VAL:H	15	0.16
(1,2350)	1:16:A:VAL:HG11	1:109:A:ALA:HB1	2	0.16
(1,2350)	1:16:A:VAL:HG11	1:109:A:ALA:HB2	2	0.16
(1,2350)	1:16:A:VAL:HG11	1:109:A:ALA:HB3	2	0.16
(1,2350)	1:16:A:VAL:HG12	1:109:A:ALA:HB1	2	0.16
(1,2350)	1:16:A:VAL:HG12	1:109:A:ALA:HB2	2	0.16
(1,2350)	1:16:A:VAL:HG12	1:109:A:ALA:HB3	2	0.16
(1,2350)	1:16:A:VAL:HG13	1:109:A:ALA:HB1	2	0.16
(1,2350)	1:16:A:VAL:HG13	1:109:A:ALA:HB2	2	0.16
(1,2350)	1:16:A:VAL:HG13	1:109:A:ALA:HB3	2	0.16
(1,2335)	1:53:A:VAL:HG11	1:54:A:GLU:HG3	7	0.16
(1,2335)	1:53:A:VAL:HG12	1:54:A:GLU:HG3	7	0.16
(1,2335)	1:53:A:VAL:HG13	1:54:A:GLU:HG3	7	0.16
(1,2274)	1:54:A:GLU:HB3	1:74:A:HIS:HB3	12	0.16
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD1	6	0.16
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD2	6	0.16
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG21	13	0.16
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG22	13	0.16
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG23	13	0.16
(1,2072)	1:29:A:ASN:HD22	1:31:A:THR:HG21	15	0.16
(1,2072)	1:29:A:ASN:HD22	1:31:A:THR:HG22	15	0.16
(1,2072)	1:29:A:ASN:HD22	1:31:A:THR:HG23	15	0.16
(1,2018)	1:67:A:ALA:H	1:65:A:LEU:HA	5	0.16
(1,1955)	1:23:A:GLU:H	1:23:A:GLU:HG3	14	0.16
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	8	0.16
(1,1767)	1:7:A:LYS:HA	1:24:A:ILE:HG21	12	0.16
(1,1767)	1:7:A:LYS:HA	1:24:A:ILE:HG22	12	0.16
(1,1767)	1:7:A:LYS:HA	1:24:A:ILE:HG23	12	0.16
(1,1763)	1:86:A:ASN:HA	1:36:A:TRP:HZ3	10	0.16
(1,1680)	1:41:A:GLY:HA3	1:37:A:TYR:HB2	7	0.16
(1,1631)	1:10:A:ASN:HB2	1:36:A:TRP:HH2	15	0.16
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	2	0.16
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	2	0.16
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	13	0.16
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	13	0.16
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	13	0.16
(1,1535)	1:90:A:MET:HE1	1:92:A:PRO:HA	2	0.16
(1,1535)	1:90:A:MET:HE2	1:92:A:PRO:HA	2	0.16
(1,1535)	1:90:A:MET:HE3	1:92:A:PRO:HA	2	0.16
(1,1535)	1:90:A:MET:HE1	1:92:A:PRO:HA	5	0.16
(1,1535)	1:90:A:MET:HE2	1:92:A:PRO:HA	5	0.16
(1,1535)	1:90:A:MET:HE3	1:92:A:PRO:HA	5	0.16
(1,1433)	1:46:A:PRO:HB3	1:48:A:GLU:H	7	0.16
(1,1415)	1:31:A:THR:HG21	1:36:A:TRP:HD1	2	0.16
(1,1415)	1:31:A:THR:HG22	1:36:A:TRP:HD1	2	0.16
(1,1415)	1:31:A:THR:HG23	1:36:A:TRP:HD1	2	0.16
(1,1415)	1:31:A:THR:HG21	1:36:A:TRP:HD1	4	0.16
(1,1415)	1:31:A:THR:HG22	1:36:A:TRP:HD1	4	0.16
(1,1415)	1:31:A:THR:HG23	1:36:A:TRP:HD1	4	0.16
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD1	9	0.16
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD2	9	0.16
(1,1259)	1:4:A:LYS:HB3	1:3:A:HIS:HB3	6	0.16
(1,1259)	1:4:A:LYS:HB3	1:3:A:HIS:HB3	13	0.16
(1,852)	1:14:A:LEU:HD11	1:14:A:LEU:H	1	0.16
(1,852)	1:14:A:LEU:HD12	1:14:A:LEU:H	1	0.16
(1,852)	1:14:A:LEU:HD13	1:14:A:LEU:H	1	0.16
(1,791)	1:21:A:LEU:HB3	1:21:A:LEU:H	3	0.16
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	3	0.16
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	9	0.16
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	11	0.16
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	14	0.16
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD11	13	0.16
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD12	13	0.16
(1,749)	1:14:A:LEU:HA	1:14:A:LEU:HD13	13	0.16
(1,745)	1:37:A:TYR:HB2	1:37:A:TYR:HD1	12	0.16
(1,745)	1:37:A:TYR:HB2	1:37:A:TYR:HD2	12	0.16
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	5	0.16
(1,661)	1:91:A:ARG:HB3	1:90:A:MET:HB2	13	0.16
(1,661)	1:91:A:ARG:HB3	1:90:A:MET:HB2	14	0.16
(1,512)	1:100:A:SER:HB3	1:89:A:TYR:HD1	2	0.16
(1,512)	1:100:A:SER:HB3	1:89:A:TYR:HD2	2	0.16
(1,488)	1:75:A:VAL:HG11	1:45:A:SER:HA	11	0.16
(1,488)	1:75:A:VAL:HG12	1:45:A:SER:HA	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:75:A:VAL:HG13	1:45:A:SER:HA	11	0.16
(1,339)	1:50:A:MET:HB3	1:50:A:MET:HA	9	0.16
(1,303)	1:36:A:TRP:HB2	1:26:A:LEU:HA	5	0.16
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	10	0.16
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	10	0.16
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	10	0.16
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	11	0.16
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	11	0.16
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	11	0.16
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	14	0.16
(1,173)	1:43:A:LYS:HB3	1:38:A:PHE:HZ	7	0.16
(1,172)	1:27:A:PRO:HG3	1:36:A:TRP:HZ2	7	0.16
(1,139)	1:9:A:HIS:HA	1:9:A:HIS:HD2	15	0.16
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	1	0.16
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	1	0.16
(3,73)	1:12:A:ALA:H	1:9:A:HIS:O	6	0.15
(3,73)	1:12:A:ALA:H	1:9:A:HIS:O	14	0.15
(3,70)	1:11:A:GLY:N	1:8:A:ALA:O	9	0.15
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	1	0.15
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	5	0.15
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	12	0.15
(3,43)	1:105:A:VAL:H	1:85:A:VAL:O	3	0.15
(3,43)	1:105:A:VAL:H	1:85:A:VAL:O	4	0.15
(3,43)	1:105:A:VAL:H	1:85:A:VAL:O	12	0.15
(2,152)	1:69:A:GLY:H	1:29:A:ASN:HA	11	0.15
(2,148)	1:29:A:ASN:HD22	1:10:A:ASN:HB2	15	0.15
(2,145)	1:40:A:GLY:H	1:43:A:LYS:HB3	4	0.15
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	5	0.15
(2,107)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	1	0.15
(2,107)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	6	0.15
(2,102)	1:36:A:TRP:HB3	1:102:A:ARG:HA	15	0.15
(2,101)	1:47:A:ASN:HB3	1:48:A:GLU:HB3	9	0.15
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD1	11	0.15
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD2	11	0.15
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	4	0.15
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	4	0.15
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	4	0.15
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	6	0.15
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	6	0.15
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	6	0.15
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	15	0.15
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	15	0.15
(2,80)	1:56:A:LYS:HD3	1:55:A:ASN:HB2	8	0.15
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	2	0.15
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	4	0.15
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	14	0.15
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD1	9	0.15
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD2	9	0.15
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD1	10	0.15
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD2	10	0.15
(2,41)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	5	0.15
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	10	0.15
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	1	0.15
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	3	0.15
(1,2413)	1:31:A:THR:HG21	1:89:A:TYR:HB3	11	0.15
(1,2413)	1:31:A:THR:HG22	1:89:A:TYR:HB3	11	0.15
(1,2413)	1:31:A:THR:HG23	1:89:A:TYR:HB3	11	0.15
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG11	5	0.15
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG12	5	0.15
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG13	5	0.15
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG11	7	0.15
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG12	7	0.15
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG13	7	0.15
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG11	11	0.15
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG12	11	0.15
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG13	11	0.15
(1,2379)	1:38:A:PHE:HB3	1:38:A:PHE:H	2	0.15
(1,2379)	1:38:A:PHE:HB3	1:38:A:PHE:H	13	0.15
(1,2379)	1:38:A:PHE:HB3	1:38:A:PHE:H	15	0.15
(1,2363)	1:53:A:VAL:HA	1:75:A:VAL:HG21	3	0.15
(1,2363)	1:53:A:VAL:HA	1:75:A:VAL:HG22	3	0.15
(1,2363)	1:53:A:VAL:HA	1:75:A:VAL:HG23	3	0.15
(1,2329)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	1	0.15
(1,2329)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	6	0.15
(1,2320)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	5	0.15
(1,2306)	1:48:A:GLU:HA	1:47:A:ASN:HA	5	0.15
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	3	0.15
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	3	0.15
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	3	0.15
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	11	0.15
(1,2006)	1:58:A:PHE:H	1:58:A:PHE:HD1	9	0.15
(1,2006)	1:58:A:PHE:H	1:58:A:PHE:HD2	9	0.15
(1,1997)	1:61:A:ASP:H	1:60:A:PRO:HG2	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	14	0.15
(1,1892)	1:38:A:PHE:HE1	1:53:A:VAL:HG11	14	0.15
(1,1892)	1:38:A:PHE:HE1	1:53:A:VAL:HG12	14	0.15
(1,1892)	1:38:A:PHE:HE1	1:53:A:VAL:HG13	14	0.15
(1,1892)	1:38:A:PHE:HE2	1:53:A:VAL:HG11	14	0.15
(1,1892)	1:38:A:PHE:HE2	1:53:A:VAL:HG12	14	0.15
(1,1892)	1:38:A:PHE:HE2	1:53:A:VAL:HG13	14	0.15
(1,1869)	1:83:A:HIS:HE1	1:87:A:LEU:HG	10	0.15
(1,1869)	1:83:A:HIS:HE1	1:87:A:LEU:HG	13	0.15
(1,1829)	1:10:A:ASN:HA	1:7:A:LYS:HD3	9	0.15
(1,1778)	1:8:A:ALA:HB1	1:9:A:HIS:HE1	15	0.15
(1,1778)	1:8:A:ALA:HB2	1:9:A:HIS:HE1	15	0.15
(1,1778)	1:8:A:ALA:HB3	1:9:A:HIS:HE1	15	0.15
(1,1763)	1:86:A:ASN:HA	1:36:A:TRP:HZ3	12	0.15
(1,1752)	1:56:A:LYS:HB3	1:72:A:HIS:HB3	13	0.15
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG21	2	0.15
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG22	2	0.15
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG23	2	0.15
(1,1668)	1:78:A:LYS:HB2	1:78:A:LYS:HE3	6	0.15
(1,1642)	1:67:A:ALA:HB1	1:60:A:PRO:HG2	5	0.15
(1,1642)	1:67:A:ALA:HB2	1:60:A:PRO:HG2	5	0.15
(1,1642)	1:67:A:ALA:HB3	1:60:A:PRO:HG2	5	0.15
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB1	1	0.15
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB2	1	0.15
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB3	1	0.15
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB1	1	0.15
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB2	1	0.15
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB3	1	0.15
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB1	1	0.15
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB2	1	0.15
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB3	1	0.15
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB1	3	0.15
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB2	3	0.15
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB3	3	0.15
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB1	3	0.15
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB2	3	0.15
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB3	3	0.15
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB1	3	0.15
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB2	3	0.15
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB3	3	0.15
(1,1588)	1:70:A:THR:HB	1:58:A:PHE:HB2	4	0.15
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1426)	1:6:A:THR:HG21	1:72:A:HIS:HE1	1	0.15
(1,1426)	1:6:A:THR:HG22	1:72:A:HIS:HE1	1	0.15
(1,1426)	1:6:A:THR:HG23	1:72:A:HIS:HE1	1	0.15
(1,1415)	1:31:A:THR:HG21	1:36:A:TRP:HD1	13	0.15
(1,1415)	1:31:A:THR:HG22	1:36:A:TRP:HD1	13	0.15
(1,1415)	1:31:A:THR:HG23	1:36:A:TRP:HD1	13	0.15
(1,1339)	1:87:A:LEU:HG	1:38:A:PHE:H	11	0.15
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD1	8	0.15
(1,1053)	1:39:A:GLU:HG3	1:38:A:PHE:HD2	8	0.15
(1,802)	1:64:A:LEU:HD11	1:65:A:LEU:H	3	0.15
(1,802)	1:64:A:LEU:HD12	1:65:A:LEU:H	3	0.15
(1,802)	1:64:A:LEU:HD13	1:65:A:LEU:H	3	0.15
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD21	12	0.15
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD22	12	0.15
(1,766)	1:65:A:LEU:HA	1:65:A:LEU:HD23	12	0.15
(1,764)	1:110:A:ASN:HB2	1:110:A:ASN:HD22	6	0.15
(1,745)	1:37:A:TYR:HB2	1:37:A:TYR:HD1	2	0.15
(1,745)	1:37:A:TYR:HB2	1:37:A:TYR:HD2	2	0.15
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	3	0.15
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	4	0.15
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	7	0.15
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	8	0.15
(1,730)	1:7:A:LYS:HA	1:7:A:LYS:HD3	15	0.15
(1,423)	1:16:A:VAL:HG21	1:109:A:ALA:HA	8	0.15
(1,423)	1:16:A:VAL:HG22	1:109:A:ALA:HA	8	0.15
(1,423)	1:16:A:VAL:HG23	1:109:A:ALA:HA	8	0.15
(1,350)	1:7:A:LYS:HD3	1:28:A:SER:HA	2	0.15
(1,350)	1:7:A:LYS:HD3	1:28:A:SER:HA	3	0.15
(1,350)	1:7:A:LYS:HD3	1:28:A:SER:HA	4	0.15
(1,304)	1:61:A:ASP:HB3	1:62:A:SER:HA	3	0.15
(1,294)	1:51:A:PHE:HB3	1:78:A:LYS:HA	3	0.15
(1,255)	1:26:A:LEU:HB3	1:36:A:TRP:HH2	4	0.15
(1,255)	1:26:A:LEU:HB3	1:36:A:TRP:HH2	5	0.15
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	4	0.15
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	4	0.15
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	4	0.15
(1,223)	1:4:A:LYS:HG3	1:3:A:HIS:HE1	3	0.15
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	14	0.15
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	15	0.15
(1,215)	1:53:A:VAL:HG11	1:38:A:PHE:HZ	2	0.15
(1,215)	1:53:A:VAL:HG12	1:38:A:PHE:HZ	2	0.15
(1,215)	1:53:A:VAL:HG13	1:38:A:PHE:HZ	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,133)	1:90:A:MET:HA	1:34:A:PHE:HD1	7	0.15
(1,133)	1:90:A:MET:HA	1:34:A:PHE:HD2	7	0.15
(1,84)	1:19:A:GLY:HA2	1:51:A:PHE:HZ	14	0.15
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	8	0.15
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	8	0.15
(1,61)	1:26:A:LEU:HD11	1:25:A:GLN:HB3	7	0.15
(1,61)	1:26:A:LEU:HD12	1:25:A:GLN:HB3	7	0.15
(1,61)	1:26:A:LEU:HD13	1:25:A:GLN:HB3	7	0.15
(3,73)	1:12:A:ALA:H	1:9:A:HIS:O	12	0.14
(3,70)	1:11:A:GLY:N	1:8:A:ALA:O	14	0.14
(3,69)	1:11:A:GLY:H	1:8:A:ALA:O	3	0.14
(3,59)	1:90:A:MET:H	1:35:A:ALA:O	15	0.14
(3,43)	1:105:A:VAL:H	1:85:A:VAL:O	13	0.14
(2,148)	1:29:A:ASN:HD22	1:10:A:ASN:HB2	1	0.14
(2,142)	1:50:A:MET:H	1:52:A:THR:HB	8	0.14
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG21	2	0.14
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG22	2	0.14
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG23	2	0.14
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG21	2	0.14
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG22	2	0.14
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG23	2	0.14
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG21	2	0.14
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG22	2	0.14
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG23	2	0.14
(2,103)	1:48:A:GLU:HA	1:50:A:MET:HA	1	0.14
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD1	7	0.14
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD2	7	0.14
(2,96)	1:103:A:PHE:HB2	1:26:A:LEU:HA	7	0.14
(2,96)	1:103:A:PHE:HB2	1:26:A:LEU:HA	8	0.14
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	11	0.14
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	11	0.14
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	11	0.14
(2,80)	1:56:A:LYS:HD3	1:55:A:ASN:HB2	2	0.14
(2,80)	1:56:A:LYS:HD3	1:55:A:ASN:HB2	14	0.14
(2,80)	1:56:A:LYS:HD3	1:55:A:ASN:HB2	15	0.14
(2,75)	1:107:A:LEU:HB3	1:83:A:HIS:HB2	3	0.14
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	5	0.14
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	6	0.14
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD1	3	0.14
(2,44)	1:38:A:PHE:HB3	1:37:A:TYR:HD2	3	0.14
(2,41)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	6	0.14
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:63:A:LYS:HD3	1:65:A:LEU:HA	9	0.14
(2,14)	1:87:A:LEU:HD21	1:57:A:TYR:HD1	13	0.14
(2,14)	1:87:A:LEU:HD21	1:57:A:TYR:HD2	13	0.14
(2,14)	1:87:A:LEU:HD22	1:57:A:TYR:HD1	13	0.14
(2,14)	1:87:A:LEU:HD22	1:57:A:TYR:HD2	13	0.14
(2,14)	1:87:A:LEU:HD23	1:57:A:TYR:HD1	13	0.14
(2,14)	1:87:A:LEU:HD23	1:57:A:TYR:HD2	13	0.14
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	4	0.14
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	11	0.14
(1,2532)	1:5:A:VAL:H	1:23:A:GLU:HB2	8	0.14
(1,2453)	1:31:A:THR:HG21	1:36:A:TRP:HZ2	11	0.14
(1,2453)	1:31:A:THR:HG22	1:36:A:TRP:HZ2	11	0.14
(1,2453)	1:31:A:THR:HG23	1:36:A:TRP:HZ2	11	0.14
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG11	7	0.14
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG12	7	0.14
(1,2446)	1:16:A:VAL:HG21	1:77:A:VAL:HG13	7	0.14
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG11	7	0.14
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG12	7	0.14
(1,2446)	1:16:A:VAL:HG22	1:77:A:VAL:HG13	7	0.14
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG11	7	0.14
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG12	7	0.14
(1,2446)	1:16:A:VAL:HG23	1:77:A:VAL:HG13	7	0.14
(1,2435)	1:90:A:MET:HB2	1:37:A:TYR:HD1	1	0.14
(1,2435)	1:90:A:MET:HB2	1:37:A:TYR:HD2	1	0.14
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG11	1	0.14
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG12	1	0.14
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG13	1	0.14
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG11	12	0.14
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG12	12	0.14
(1,2408)	1:4:A:LYS:HA	1:5:A:VAL:HG13	12	0.14
(1,2320)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	6	0.14
(1,2293)	1:21:A:LEU:HG	1:74:A:HIS:HB3	3	0.14
(1,2263)	1:24:A:ILE:HD11	1:106:A:TYR:HA	3	0.14
(1,2263)	1:24:A:ILE:HD12	1:106:A:TYR:HA	3	0.14
(1,2263)	1:24:A:ILE:HD13	1:106:A:TYR:HA	3	0.14
(1,2130)	1:47:A:ASN:HD21	1:110:A:ASN:HA	14	0.14
(1,2107)	1:55:A:ASN:H	1:55:A:ASN:HD21	4	0.14
(1,2086)	1:91:A:ARG:H	1:99:A:ASP:HB2	6	0.14
(1,2072)	1:29:A:ASN:HD22	1:31:A:THR:HG21	3	0.14
(1,2072)	1:29:A:ASN:HD22	1:31:A:THR:HG22	3	0.14
(1,2072)	1:29:A:ASN:HD22	1:31:A:THR:HG23	3	0.14
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2056)	1:34:A:PHE:H	1:95:A:GLY:HA2	7	0.14
(1,1955)	1:23:A:GLU:H	1:23:A:GLU:HG3	8	0.14
(1,1949)	1:55:A:ASN:H	1:54:A:GLU:HB3	15	0.14
(1,1885)	1:38:A:PHE:HZ	1:45:A:SER:HA	6	0.14
(1,1869)	1:83:A:HIS:HE1	1:87:A:LEU:HG	6	0.14
(1,1858)	1:80:A:ALA:HA	1:110:A:ASN:HB3	15	0.14
(1,1853)	1:34:A:PHE:HA	1:90:A:MET:HG2	3	0.14
(1,1803)	1:26:A:LEU:HD21	1:25:A:GLN:HB3	7	0.14
(1,1803)	1:26:A:LEU:HD22	1:25:A:GLN:HB3	7	0.14
(1,1803)	1:26:A:LEU:HD23	1:25:A:GLN:HB3	7	0.14
(1,1767)	1:7:A:LYS:HA	1:24:A:ILE:HG21	15	0.14
(1,1767)	1:7:A:LYS:HA	1:24:A:ILE:HG22	15	0.14
(1,1767)	1:7:A:LYS:HA	1:24:A:ILE:HG23	15	0.14
(1,1763)	1:86:A:ASN:HA	1:36:A:TRP:HZ3	2	0.14
(1,1763)	1:86:A:ASN:HA	1:36:A:TRP:HZ3	3	0.14
(1,1763)	1:86:A:ASN:HA	1:36:A:TRP:HZ3	4	0.14
(1,1763)	1:86:A:ASN:HA	1:36:A:TRP:HZ3	7	0.14
(1,1747)	1:87:A:LEU:HD21	1:104:A:THR:HA	1	0.14
(1,1747)	1:87:A:LEU:HD22	1:104:A:THR:HA	1	0.14
(1,1747)	1:87:A:LEU:HD23	1:104:A:THR:HA	1	0.14
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG21	3	0.14
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG22	3	0.14
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG23	3	0.14
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG21	3	0.14
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG22	3	0.14
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG23	3	0.14
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG21	3	0.14
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG22	3	0.14
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG23	3	0.14
(1,1691)	1:42:A:THR:HB	1:43:A:LYS:HB2	7	0.14
(1,1683)	1:92:A:PRO:HA	1:90:A:MET:HB3	9	0.14
(1,1673)	1:42:A:THR:HB	1:39:A:GLU:HG3	14	0.14
(1,1642)	1:67:A:ALA:HB1	1:60:A:PRO:HG2	8	0.14
(1,1642)	1:67:A:ALA:HB2	1:60:A:PRO:HG2	8	0.14
(1,1642)	1:67:A:ALA:HB3	1:60:A:PRO:HG2	8	0.14
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	4	0.14
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	4	0.14
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	4	0.14
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB1	13	0.14
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB2	13	0.14
(1,1617)	1:75:A:VAL:HG21	1:109:A:ALA:HB3	13	0.14
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB1	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB2	13	0.14
(1,1617)	1:75:A:VAL:HG22	1:109:A:ALA:HB3	13	0.14
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB1	13	0.14
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB2	13	0.14
(1,1617)	1:75:A:VAL:HG23	1:109:A:ALA:HB3	13	0.14
(1,1588)	1:70:A:THR:HB	1:58:A:PHE:HB2	14	0.14
(1,1437)	1:83:A:HIS:HB2	1:3:A:HIS:HD2	7	0.14
(1,1339)	1:87:A:LEU:HG	1:38:A:PHE:H	5	0.14
(1,1339)	1:87:A:LEU:HG	1:38:A:PHE:H	7	0.14
(1,1291)	1:103:A:PHE:HE1	1:11:A:GLY:H	15	0.14
(1,1291)	1:103:A:PHE:HE2	1:11:A:GLY:H	15	0.14
(1,1221)	1:55:A:ASN:HD22	1:56:A:LYS:H	6	0.14
(1,1155)	1:53:A:VAL:HB	1:45:A:SER:H	14	0.14
(1,1066)	1:58:A:PHE:HD1	1:57:A:TYR:H	9	0.14
(1,1066)	1:58:A:PHE:HD2	1:57:A:TYR:H	9	0.14
(1,1066)	1:58:A:PHE:HD1	1:57:A:TYR:H	12	0.14
(1,1066)	1:58:A:PHE:HD2	1:57:A:TYR:H	12	0.14
(1,1059)	1:78:A:LYS:HD3	1:50:A:MET:HG3	6	0.14
(1,1059)	1:78:A:LYS:HD3	1:50:A:MET:HG3	12	0.14
(1,1029)	1:6:A:THR:HG21	1:27:A:PRO:HG3	3	0.14
(1,1029)	1:6:A:THR:HG22	1:27:A:PRO:HG3	3	0.14
(1,1029)	1:6:A:THR:HG23	1:27:A:PRO:HG3	3	0.14
(1,1011)	1:63:A:LYS:HD3	1:63:A:LYS:H	11	0.14
(1,1004)	1:85:A:VAL:HG11	1:85:A:VAL:H	9	0.14
(1,1004)	1:85:A:VAL:HG12	1:85:A:VAL:H	9	0.14
(1,1004)	1:85:A:VAL:HG13	1:85:A:VAL:H	9	0.14
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	6	0.14
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	6	0.14
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	6	0.14
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	15	0.14
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	15	0.14
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	15	0.14
(1,886)	1:6:A:THR:HG21	1:25:A:GLN:H	8	0.14
(1,886)	1:6:A:THR:HG22	1:25:A:GLN:H	8	0.14
(1,886)	1:6:A:THR:HG23	1:25:A:GLN:H	8	0.14
(1,772)	1:102:A:ARG:HA	1:102:A:ARG:H	9	0.14
(1,745)	1:37:A:TYR:HB2	1:37:A:TYR:HD1	15	0.14
(1,745)	1:37:A:TYR:HB2	1:37:A:TYR:HD2	15	0.14
(1,720)	1:25:A:GLN:HG2	1:26:A:LEU:H	5	0.14
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	7	0.14
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	7	0.14
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	9	0.14
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	9	0.14
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	9	0.14
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	12	0.14
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	12	0.14
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	12	0.14
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	13	0.14
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	13	0.14
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	13	0.14
(1,694)	1:76:A:THR:HA	1:22:A:VAL:H	13	0.14
(1,694)	1:76:A:THR:HA	1:22:A:VAL:H	14	0.14
(1,677)	1:26:A:LEU:HG	1:27:A:PRO:HG2	10	0.14
(1,668)	1:105:A:VAL:HG21	1:12:A:ALA:HB1	8	0.14
(1,668)	1:105:A:VAL:HG21	1:12:A:ALA:HB2	8	0.14
(1,668)	1:105:A:VAL:HG21	1:12:A:ALA:HB3	8	0.14
(1,668)	1:105:A:VAL:HG22	1:12:A:ALA:HB1	8	0.14
(1,668)	1:105:A:VAL:HG22	1:12:A:ALA:HB2	8	0.14
(1,668)	1:105:A:VAL:HG22	1:12:A:ALA:HB3	8	0.14
(1,668)	1:105:A:VAL:HG23	1:12:A:ALA:HB1	8	0.14
(1,668)	1:105:A:VAL:HG23	1:12:A:ALA:HB2	8	0.14
(1,668)	1:105:A:VAL:HG23	1:12:A:ALA:HB3	8	0.14
(1,661)	1:91:A:ARG:HB3	1:90:A:MET:HB2	9	0.14
(1,604)	1:25:A:GLN:HB2	1:73:A:PHE:HB2	7	0.14
(1,393)	1:82:A:THR:HG21	1:109:A:ALA:HA	1	0.14
(1,393)	1:82:A:THR:HG22	1:109:A:ALA:HA	1	0.14
(1,393)	1:82:A:THR:HG23	1:109:A:ALA:HA	1	0.14
(1,304)	1:61:A:ASP:HB3	1:62:A:SER:HA	9	0.14
(1,303)	1:36:A:TRP:HB2	1:26:A:LEU:HA	3	0.14
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	6	0.14
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	6	0.14
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	6	0.14
(1,222)	1:87:A:LEU:HB2	1:38:A:PHE:HD1	15	0.14
(1,222)	1:87:A:LEU:HB2	1:38:A:PHE:HD2	15	0.14
(1,221)	1:87:A:LEU:HB2	1:103:A:PHE:HD1	15	0.14
(1,221)	1:87:A:LEU:HB2	1:103:A:PHE:HD2	15	0.14
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	2	0.14
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	5	0.14
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	11	0.14
(1,205)	1:56:A:LYS:HD3	1:72:A:HIS:HE1	3	0.14
(1,205)	1:56:A:LYS:HD3	1:72:A:HIS:HE1	13	0.14
(1,205)	1:56:A:LYS:HD3	1:72:A:HIS:HE1	14	0.14
(1,173)	1:43:A:LYS:HB3	1:38:A:PHE:HZ	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:43:A:LYS:HB3	1:38:A:PHE:HZ	14	0.14
(1,61)	1:26:A:LEU:HD11	1:25:A:GLN:HB3	8	0.14
(1,61)	1:26:A:LEU:HD12	1:25:A:GLN:HB3	8	0.14
(1,61)	1:26:A:LEU:HD13	1:25:A:GLN:HB3	8	0.14
(3,73)	1:12:A:ALA:H	1:9:A:HIS:O	3	0.13
(3,70)	1:11:A:GLY:N	1:8:A:ALA:O	15	0.13
(3,59)	1:90:A:MET:H	1:35:A:ALA:O	2	0.13
(3,59)	1:90:A:MET:H	1:35:A:ALA:O	12	0.13
(3,43)	1:105:A:VAL:H	1:85:A:VAL:O	7	0.13
(2,157)	1:110:A:ASN:H	1:22:A:VAL:HB	3	0.13
(2,152)	1:69:A:GLY:H	1:29:A:ASN:HA	15	0.13
(2,148)	1:29:A:ASN:HD22	1:10:A:ASN:HB2	5	0.13
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	7	0.13
(2,129)	1:66:A:GLY:H	1:68:A:GLY:HA3	4	0.13
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG21	15	0.13
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG22	15	0.13
(2,111)	1:67:A:ALA:HB1	1:70:A:THR:HG23	15	0.13
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG21	15	0.13
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG22	15	0.13
(2,111)	1:67:A:ALA:HB2	1:70:A:THR:HG23	15	0.13
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG21	15	0.13
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG22	15	0.13
(2,111)	1:67:A:ALA:HB3	1:70:A:THR:HG23	15	0.13
(2,107)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	10	0.13
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	3	0.13
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	10	0.13
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	3	0.13
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	7	0.13
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	14	0.13
(1,2453)	1:31:A:THR:HG21	1:36:A:TRP:HZ2	1	0.13
(1,2453)	1:31:A:THR:HG22	1:36:A:TRP:HZ2	1	0.13
(1,2453)	1:31:A:THR:HG23	1:36:A:TRP:HZ2	1	0.13
(1,2429)	1:52:A:THR:HG21	1:51:A:PHE:HB3	6	0.13
(1,2429)	1:52:A:THR:HG22	1:51:A:PHE:HB3	6	0.13
(1,2429)	1:52:A:THR:HG23	1:51:A:PHE:HB3	6	0.13
(1,2413)	1:31:A:THR:HG21	1:89:A:TYR:HB3	5	0.13
(1,2413)	1:31:A:THR:HG22	1:89:A:TYR:HB3	5	0.13
(1,2413)	1:31:A:THR:HG23	1:89:A:TYR:HB3	5	0.13
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG11	14	0.13
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG12	14	0.13
(1,2408)	1:21:A:LEU:HA	1:22:A:VAL:HG13	14	0.13
(1,2403)	1:91:A:ARG:HD3	1:93:A:TRP:HH2	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2363)	1:53:A:VAL:HA	1:75:A:VAL:HG21	1	0.13
(1,2363)	1:53:A:VAL:HA	1:75:A:VAL:HG22	1	0.13
(1,2363)	1:53:A:VAL:HA	1:75:A:VAL:HG23	1	0.13
(1,2329)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	10	0.13
(1,2283)	1:65:A:LEU:HG	1:28:A:SER:HB2	9	0.13
(1,2274)	1:54:A:GLU:HB3	1:74:A:HIS:HB3	1	0.13
(1,2274)	1:54:A:GLU:HB3	1:74:A:HIS:HB3	13	0.13
(1,2263)	1:24:A:ILE:HD11	1:106:A:TYR:HA	1	0.13
(1,2263)	1:24:A:ILE:HD12	1:106:A:TYR:HA	1	0.13
(1,2263)	1:24:A:ILE:HD13	1:106:A:TYR:HA	1	0.13
(1,2070)	1:25:A:GLN:HE22	1:7:A:LYS:HD3	2	0.13
(1,2023)	1:19:A:GLY:H	1:22:A:VAL:HB	7	0.13
(1,2023)	1:19:A:GLY:H	1:22:A:VAL:HB	9	0.13
(1,1896)	1:36:A:TRP:HD1	1:28:A:SER:HB3	1	0.13
(1,1886)	1:38:A:PHE:HZ	1:85:A:VAL:HB	7	0.13
(1,1886)	1:38:A:PHE:HZ	1:85:A:VAL:HB	14	0.13
(1,1869)	1:83:A:HIS:HE1	1:87:A:LEU:HG	5	0.13
(1,1834)	1:24:A:ILE:HD11	1:106:A:TYR:H	8	0.13
(1,1834)	1:24:A:ILE:HD12	1:106:A:TYR:H	8	0.13
(1,1834)	1:24:A:ILE:HD13	1:106:A:TYR:H	8	0.13
(1,1818)	1:108:A:LYS:HD3	1:108:A:LYS:H	7	0.13
(1,1763)	1:86:A:ASN:HA	1:36:A:TRP:HZ3	14	0.13
(1,1761)	1:46:A:PRO:HD3	1:53:A:VAL:HG11	3	0.13
(1,1761)	1:46:A:PRO:HD3	1:53:A:VAL:HG12	3	0.13
(1,1761)	1:46:A:PRO:HD3	1:53:A:VAL:HG13	3	0.13
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG21	8	0.13
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG22	8	0.13
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG23	8	0.13
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG21	13	0.13
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG22	13	0.13
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG23	13	0.13
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG21	13	0.13
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG22	13	0.13
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG23	13	0.13
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG21	13	0.13
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG22	13	0.13
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG23	13	0.13
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG21	15	0.13
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG22	15	0.13
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG23	15	0.13
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG21	15	0.13
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG22	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG23	15	0.13
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG21	15	0.13
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG22	15	0.13
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG23	15	0.13
(1,1662)	1:41:A:GLY:HA2	1:90:A:MET:HE1	12	0.13
(1,1662)	1:41:A:GLY:HA2	1:90:A:MET:HE2	12	0.13
(1,1662)	1:41:A:GLY:HA2	1:90:A:MET:HE3	12	0.13
(1,1631)	1:10:A:ASN:HB2	1:36:A:TRP:HH2	11	0.13
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	5	0.13
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	5	0.13
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	5	0.13
(1,1535)	1:90:A:MET:HE1	1:92:A:PRO:HA	7	0.13
(1,1535)	1:90:A:MET:HE2	1:92:A:PRO:HA	7	0.13
(1,1535)	1:90:A:MET:HE3	1:92:A:PRO:HA	7	0.13
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	3	0.13
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	10	0.13
(1,1430)	1:82:A:THR:HG21	1:110:A:ASN:HD21	4	0.13
(1,1430)	1:82:A:THR:HG22	1:110:A:ASN:HD21	4	0.13
(1,1430)	1:82:A:THR:HG23	1:110:A:ASN:HD21	4	0.13
(1,1430)	1:82:A:THR:HG21	1:110:A:ASN:HD21	5	0.13
(1,1430)	1:82:A:THR:HG22	1:110:A:ASN:HD21	5	0.13
(1,1430)	1:82:A:THR:HG23	1:110:A:ASN:HD21	5	0.13
(1,1430)	1:82:A:THR:HG21	1:110:A:ASN:HD21	8	0.13
(1,1430)	1:82:A:THR:HG22	1:110:A:ASN:HD21	8	0.13
(1,1430)	1:82:A:THR:HG23	1:110:A:ASN:HD21	8	0.13
(1,1339)	1:87:A:LEU:HG	1:38:A:PHE:H	1	0.13
(1,1339)	1:87:A:LEU:HG	1:38:A:PHE:H	9	0.13
(1,1303)	1:104:A:THR:HG21	1:11:A:GLY:H	15	0.13
(1,1303)	1:104:A:THR:HG22	1:11:A:GLY:H	15	0.13
(1,1303)	1:104:A:THR:HG23	1:11:A:GLY:H	15	0.13
(1,1298)	1:62:A:SER:H	1:63:A:LYS:H	1	0.13
(1,1165)	1:65:A:LEU:H	1:66:A:GLY:H	15	0.13
(1,1097)	1:37:A:TYR:HB3	1:42:A:THR:H	12	0.13
(1,1036)	1:16:A:VAL:HB	1:108:A:LYS:H	14	0.13
(1,1029)	1:6:A:THR:HG21	1:27:A:PRO:HG3	9	0.13
(1,1029)	1:6:A:THR:HG22	1:27:A:PRO:HG3	9	0.13
(1,1029)	1:6:A:THR:HG23	1:27:A:PRO:HG3	9	0.13
(1,990)	1:10:A:ASN:HB2	1:103:A:PHE:HD1	15	0.13
(1,990)	1:10:A:ASN:HB2	1:103:A:PHE:HD2	15	0.13
(1,940)	1:16:A:VAL:HG21	1:108:A:LYS:HG3	2	0.13
(1,940)	1:16:A:VAL:HG22	1:108:A:LYS:HG3	2	0.13
(1,940)	1:16:A:VAL:HG23	1:108:A:LYS:HG3	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:63:A:LYS:HD3	1:61:A:ASP:HB3	9	0.13
(1,841)	1:43:A:LYS:HG3	1:38:A:PHE:HD1	6	0.13
(1,841)	1:43:A:LYS:HG3	1:38:A:PHE:HD2	6	0.13
(1,746)	1:70:A:THR:HG21	1:71:A:GLU:H	10	0.13
(1,746)	1:70:A:THR:HG22	1:71:A:GLU:H	10	0.13
(1,746)	1:70:A:THR:HG23	1:71:A:GLU:H	10	0.13
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	1	0.13
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	6	0.13
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	6	0.13
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	6	0.13
(1,677)	1:26:A:LEU:HG	1:27:A:PRO:HG2	13	0.13
(1,668)	1:105:A:VAL:HG21	1:12:A:ALA:HB1	2	0.13
(1,668)	1:105:A:VAL:HG21	1:12:A:ALA:HB2	2	0.13
(1,668)	1:105:A:VAL:HG21	1:12:A:ALA:HB3	2	0.13
(1,668)	1:105:A:VAL:HG22	1:12:A:ALA:HB1	2	0.13
(1,668)	1:105:A:VAL:HG22	1:12:A:ALA:HB2	2	0.13
(1,668)	1:105:A:VAL:HG22	1:12:A:ALA:HB3	2	0.13
(1,668)	1:105:A:VAL:HG23	1:12:A:ALA:HB1	2	0.13
(1,668)	1:105:A:VAL:HG23	1:12:A:ALA:HB2	2	0.13
(1,668)	1:105:A:VAL:HG23	1:12:A:ALA:HB3	2	0.13
(1,661)	1:91:A:ARG:HB3	1:90:A:MET:HB2	1	0.13
(1,661)	1:91:A:ARG:HB3	1:90:A:MET:HB2	3	0.13
(1,626)	1:85:A:VAL:HG21	1:106:A:TYR:HB2	15	0.13
(1,626)	1:85:A:VAL:HG22	1:106:A:TYR:HB2	15	0.13
(1,626)	1:85:A:VAL:HG23	1:106:A:TYR:HB2	15	0.13
(1,608)	1:88:A:THR:HG21	1:90:A:MET:HG3	13	0.13
(1,608)	1:88:A:THR:HG22	1:90:A:MET:HG3	13	0.13
(1,608)	1:88:A:THR:HG23	1:90:A:MET:HG3	13	0.13
(1,604)	1:25:A:GLN:HB2	1:73:A:PHE:HB2	9	0.13
(1,604)	1:25:A:GLN:HB2	1:73:A:PHE:HB2	13	0.13
(1,595)	1:7:A:LYS:HD3	1:29:A:ASN:HB2	9	0.13
(1,488)	1:75:A:VAL:HG11	1:45:A:SER:HA	13	0.13
(1,488)	1:75:A:VAL:HG12	1:45:A:SER:HA	13	0.13
(1,488)	1:75:A:VAL:HG13	1:45:A:SER:HA	13	0.13
(1,350)	1:7:A:LYS:HD3	1:28:A:SER:HA	7	0.13
(1,303)	1:36:A:TRP:HB2	1:26:A:LEU:HA	14	0.13
(1,294)	1:51:A:PHE:HB3	1:78:A:LYS:HA	1	0.13
(1,294)	1:51:A:PHE:HB3	1:78:A:LYS:HA	11	0.13
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	1	0.13
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	10	0.13
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	12	0.13
(1,119)	1:102:A:ARG:HA	1:36:A:TRP:HZ3	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,116)	1:109:A:ALA:HA	1:83:A:HIS:HD2	6	0.13
(3,73)	1:12:A:ALA:H	1:9:A:HIS:O	5	0.12
(3,70)	1:11:A:GLY:N	1:8:A:ALA:O	2	0.12
(3,59)	1:90:A:MET:H	1:35:A:ALA:O	13	0.12
(3,51)	1:101:A:GLU:H	1:89:A:TYR:O	9	0.12
(3,43)	1:105:A:VAL:H	1:85:A:VAL:O	5	0.12
(2,148)	1:29:A:ASN:HD22	1:10:A:ASN:HB2	14	0.12
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	11	0.12
(2,131)	1:65:A:LEU:H	1:62:A:SER:HA	1	0.12
(2,107)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	2	0.12
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD1	5	0.12
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD2	5	0.12
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	14	0.12
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	14	0.12
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	14	0.12
(2,82)	1:5:A:VAL:HG11	1:106:A:TYR:H	7	0.12
(2,82)	1:5:A:VAL:HG12	1:106:A:TYR:H	7	0.12
(2,82)	1:5:A:VAL:HG13	1:106:A:TYR:H	7	0.12
(2,45)	1:71:A:GLU:HG2	1:58:A:PHE:HD1	12	0.12
(2,45)	1:71:A:GLU:HG2	1:58:A:PHE:HD2	12	0.12
(2,41)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	13	0.12
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	4	0.12
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	5	0.12
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	7	0.12
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	7	0.12
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	7	0.12
(1,2424)	1:35:A:ALA:HB1	1:71:A:GLU:HB3	8	0.12
(1,2424)	1:35:A:ALA:HB2	1:71:A:GLU:HB3	8	0.12
(1,2424)	1:35:A:ALA:HB3	1:71:A:GLU:HB3	8	0.12
(1,2420)	1:30:A:PRO:HA	1:34:A:PHE:HB2	6	0.12
(1,2393)	1:87:A:LEU:HB3	1:36:A:TRP:HZ3	12	0.12
(1,2357)	1:85:A:VAL:HB	1:85:A:VAL:H	8	0.12
(1,2329)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	2	0.12
(1,2321)	1:44:A:GLU:HG3	1:46:A:PRO:HD2	15	0.12
(1,2320)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	13	0.12
(1,2306)	1:48:A:GLU:HA	1:47:A:ASN:HA	1	0.12
(1,2306)	1:48:A:GLU:HA	1:47:A:ASN:HA	6	0.12
(1,2293)	1:21:A:LEU:HG	1:74:A:HIS:HB3	15	0.12
(1,2283)	1:65:A:LEU:HG	1:30:A:PRO:HD3	14	0.12
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	9	0.12
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	9	0.12
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2176)	1:71:A:GLU:HG2	1:58:A:PHE:HD1	12	0.12
(1,2176)	1:71:A:GLU:HG2	1:58:A:PHE:HD2	12	0.12
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG21	15	0.12
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG22	15	0.12
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG23	15	0.12
(1,2072)	1:29:A:ASN:HD22	1:31:A:THR:HG21	11	0.12
(1,2072)	1:29:A:ASN:HD22	1:31:A:THR:HG22	11	0.12
(1,2072)	1:29:A:ASN:HD22	1:31:A:THR:HG23	11	0.12
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB1	8	0.12
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB2	8	0.12
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB3	8	0.12
(1,2044)	1:70:A:THR:H	1:72:A:HIS:HD2	4	0.12
(1,2023)	1:19:A:GLY:H	1:22:A:VAL:HB	13	0.12
(1,1985)	1:33:A:GLY:H	1:32:A:THR:HG21	8	0.12
(1,1985)	1:33:A:GLY:H	1:32:A:THR:HG22	8	0.12
(1,1985)	1:33:A:GLY:H	1:32:A:THR:HG23	8	0.12
(1,1921)	1:89:A:TYR:HE1	1:31:A:THR:HG21	9	0.12
(1,1921)	1:89:A:TYR:HE1	1:31:A:THR:HG22	9	0.12
(1,1921)	1:89:A:TYR:HE1	1:31:A:THR:HG23	9	0.12
(1,1921)	1:89:A:TYR:HE2	1:31:A:THR:HG21	9	0.12
(1,1921)	1:89:A:TYR:HE2	1:31:A:THR:HG22	9	0.12
(1,1921)	1:89:A:TYR:HE2	1:31:A:THR:HG23	9	0.12
(1,1886)	1:38:A:PHE:HZ	1:85:A:VAL:HB	6	0.12
(1,1873)	1:38:A:PHE:HD1	1:53:A:VAL:HG11	3	0.12
(1,1873)	1:38:A:PHE:HD1	1:53:A:VAL:HG12	3	0.12
(1,1873)	1:38:A:PHE:HD1	1:53:A:VAL:HG13	3	0.12
(1,1873)	1:38:A:PHE:HD2	1:53:A:VAL:HG11	3	0.12
(1,1873)	1:38:A:PHE:HD2	1:53:A:VAL:HG12	3	0.12
(1,1873)	1:38:A:PHE:HD2	1:53:A:VAL:HG13	3	0.12
(1,1854)	1:50:A:MET:HG3	1:77:A:VAL:HA	13	0.12
(1,1853)	1:34:A:PHE:HA	1:90:A:MET:HG2	7	0.12
(1,1834)	1:24:A:ILE:HD11	1:106:A:TYR:H	1	0.12
(1,1834)	1:24:A:ILE:HD12	1:106:A:TYR:H	1	0.12
(1,1834)	1:24:A:ILE:HD13	1:106:A:TYR:H	1	0.12
(1,1834)	1:24:A:ILE:HD11	1:106:A:TYR:H	4	0.12
(1,1834)	1:24:A:ILE:HD12	1:106:A:TYR:H	4	0.12
(1,1834)	1:24:A:ILE:HD13	1:106:A:TYR:H	4	0.12
(1,1834)	1:24:A:ILE:HD11	1:106:A:TYR:H	11	0.12
(1,1834)	1:24:A:ILE:HD12	1:106:A:TYR:H	11	0.12
(1,1834)	1:24:A:ILE:HD13	1:106:A:TYR:H	11	0.12
(1,1792)	1:16:A:VAL:HA	1:3:A:HIS:HE1	12	0.12
(1,1784)	1:42:A:THR:HA	1:38:A:PHE:HB3	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1752)	1:56:A:LYS:HB3	1:72:A:HIS:HB3	2	0.12
(1,1747)	1:87:A:LEU:HD21	1:104:A:THR:HA	5	0.12
(1,1747)	1:87:A:LEU:HD22	1:104:A:THR:HA	5	0.12
(1,1747)	1:87:A:LEU:HD23	1:104:A:THR:HA	5	0.12
(1,1747)	1:87:A:LEU:HD21	1:104:A:THR:HA	7	0.12
(1,1747)	1:87:A:LEU:HD22	1:104:A:THR:HA	7	0.12
(1,1747)	1:87:A:LEU:HD23	1:104:A:THR:HA	7	0.12
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG21	6	0.12
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG22	6	0.12
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG23	6	0.12
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG21	6	0.12
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG22	6	0.12
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG23	6	0.12
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG21	6	0.12
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG22	6	0.12
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG23	6	0.12
(1,1662)	1:41:A:GLY:HA2	1:90:A:MET:HE1	2	0.12
(1,1662)	1:41:A:GLY:HA2	1:90:A:MET:HE2	2	0.12
(1,1662)	1:41:A:GLY:HA2	1:90:A:MET:HE3	2	0.12
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	11	0.12
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	11	0.12
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	11	0.12
(1,1581)	1:107:A:LEU:HB2	1:16:A:VAL:HG11	3	0.12
(1,1581)	1:107:A:LEU:HB2	1:16:A:VAL:HG12	3	0.12
(1,1581)	1:107:A:LEU:HB2	1:16:A:VAL:HG13	3	0.12
(1,1540)	1:18:A:VAL:HG11	1:3:A:HIS:HB2	10	0.12
(1,1540)	1:18:A:VAL:HG12	1:3:A:HIS:HB2	10	0.12
(1,1540)	1:18:A:VAL:HG13	1:3:A:HIS:HB2	10	0.12
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	2	0.12
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	7	0.12
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	14	0.12
(1,1430)	1:82:A:THR:HG21	1:110:A:ASN:HD21	7	0.12
(1,1430)	1:82:A:THR:HG22	1:110:A:ASN:HD21	7	0.12
(1,1430)	1:82:A:THR:HG23	1:110:A:ASN:HD21	7	0.12
(1,1430)	1:82:A:THR:HG21	1:110:A:ASN:HD21	13	0.12
(1,1430)	1:82:A:THR:HG22	1:110:A:ASN:HD21	13	0.12
(1,1430)	1:82:A:THR:HG23	1:110:A:ASN:HD21	13	0.12
(1,1428)	1:56:A:LYS:HD3	1:57:A:TYR:HD1	9	0.12
(1,1428)	1:56:A:LYS:HD3	1:57:A:TYR:HD2	9	0.12
(1,1415)	1:31:A:THR:HG21	1:36:A:TRP:HD1	6	0.12
(1,1415)	1:31:A:THR:HG22	1:36:A:TRP:HD1	6	0.12
(1,1415)	1:31:A:THR:HG23	1:36:A:TRP:HD1	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1415)	1:31:A:THR:HG21	1:36:A:TRP:HD1	8	0.12
(1,1415)	1:31:A:THR:HG22	1:36:A:TRP:HD1	8	0.12
(1,1415)	1:31:A:THR:HG23	1:36:A:TRP:HD1	8	0.12
(1,1339)	1:87:A:LEU:HG	1:38:A:PHE:H	3	0.12
(1,1339)	1:87:A:LEU:HG	1:38:A:PHE:H	10	0.12
(1,1339)	1:87:A:LEU:HG	1:38:A:PHE:H	14	0.12
(1,1314)	1:60:A:PRO:HB2	1:62:A:SER:H	12	0.12
(1,1308)	1:87:A:LEU:HB2	1:89:A:TYR:H	4	0.12
(1,1303)	1:104:A:THR:HG21	1:11:A:GLY:H	6	0.12
(1,1303)	1:104:A:THR:HG22	1:11:A:GLY:H	6	0.12
(1,1303)	1:104:A:THR:HG23	1:11:A:GLY:H	6	0.12
(1,1209)	1:42:A:THR:HG21	1:44:A:GLU:H	5	0.12
(1,1209)	1:42:A:THR:HG22	1:44:A:GLU:H	5	0.12
(1,1209)	1:42:A:THR:HG23	1:44:A:GLU:H	5	0.12
(1,1209)	1:42:A:THR:HG21	1:44:A:GLU:H	9	0.12
(1,1209)	1:42:A:THR:HG22	1:44:A:GLU:H	9	0.12
(1,1209)	1:42:A:THR:HG23	1:44:A:GLU:H	9	0.12
(1,1090)	1:70:A:THR:HG21	1:26:A:LEU:H	11	0.12
(1,1090)	1:70:A:THR:HG22	1:26:A:LEU:H	11	0.12
(1,1090)	1:70:A:THR:HG23	1:26:A:LEU:H	11	0.12
(1,1029)	1:6:A:THR:HG21	1:27:A:PRO:HG3	2	0.12
(1,1029)	1:6:A:THR:HG22	1:27:A:PRO:HG3	2	0.12
(1,1029)	1:6:A:THR:HG23	1:27:A:PRO:HG3	2	0.12
(1,1029)	1:6:A:THR:HG21	1:27:A:PRO:HG3	5	0.12
(1,1029)	1:6:A:THR:HG22	1:27:A:PRO:HG3	5	0.12
(1,1029)	1:6:A:THR:HG23	1:27:A:PRO:HG3	5	0.12
(1,994)	1:9:A:HIS:HB2	1:9:A:HIS:H	15	0.12
(1,886)	1:6:A:THR:HG21	1:25:A:GLN:H	9	0.12
(1,886)	1:6:A:THR:HG22	1:25:A:GLN:H	9	0.12
(1,886)	1:6:A:THR:HG23	1:25:A:GLN:H	9	0.12
(1,856)	1:52:A:THR:HB	1:53:A:VAL:H	14	0.12
(1,763)	1:33:A:GLY:HA3	1:33:A:GLY:H	1	0.12
(1,752)	1:22:A:VAL:HG21	1:23:A:GLU:H	2	0.12
(1,752)	1:22:A:VAL:HG22	1:23:A:GLU:H	2	0.12
(1,752)	1:22:A:VAL:HG23	1:23:A:GLU:H	2	0.12
(1,746)	1:70:A:THR:HG21	1:71:A:GLU:H	7	0.12
(1,746)	1:70:A:THR:HG22	1:71:A:GLU:H	7	0.12
(1,746)	1:70:A:THR:HG23	1:71:A:GLU:H	7	0.12
(1,731)	1:56:A:LYS:HD3	1:56:A:LYS:HE3	2	0.12
(1,720)	1:25:A:GLN:HG2	1:26:A:LEU:H	4	0.12
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	11	0.12
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	11	0.12
(1,687)	1:22:A:VAL:HG11	1:3:A:HIS:HD2	15	0.12
(1,687)	1:22:A:VAL:HG12	1:3:A:HIS:HD2	15	0.12
(1,687)	1:22:A:VAL:HG13	1:3:A:HIS:HD2	15	0.12
(1,677)	1:26:A:LEU:HG	1:27:A:PRO:HG2	5	0.12
(1,665)	1:91:A:ARG:HB3	1:92:A:PRO:HG2	8	0.12
(1,661)	1:91:A:ARG:HB3	1:90:A:MET:HB2	4	0.12
(1,661)	1:91:A:ARG:HB3	1:90:A:MET:HB2	10	0.12
(1,350)	1:7:A:LYS:HD3	1:28:A:SER:HA	13	0.12
(1,350)	1:7:A:LYS:HD3	1:28:A:SER:HA	14	0.12
(1,306)	1:47:A:ASN:HB3	1:47:A:ASN:HA	14	0.12
(1,303)	1:36:A:TRP:HB2	1:26:A:LEU:HA	6	0.12
(1,303)	1:36:A:TRP:HB2	1:26:A:LEU:HA	8	0.12
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	1	0.12
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	1	0.12
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	1	0.12
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	3	0.12
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	3	0.12
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	3	0.12
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	8	0.12
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	8	0.12
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	8	0.12
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	9	0.12
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	9	0.12
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	9	0.12
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	12	0.12
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	12	0.12
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	12	0.12
(1,175)	1:27:A:PRO:HG2	1:36:A:TRP:HD1	3	0.12
(1,175)	1:27:A:PRO:HG2	1:36:A:TRP:HD1	5	0.12
(1,175)	1:27:A:PRO:HG2	1:36:A:TRP:HD1	11	0.12
(1,172)	1:27:A:PRO:HG3	1:36:A:TRP:HZ2	4	0.12
(1,172)	1:27:A:PRO:HG3	1:36:A:TRP:HZ2	12	0.12
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD1	3	0.12
(1,171)	1:50:A:MET:HG2	1:51:A:PHE:HD2	3	0.12
(1,120)	1:13:A:THR:HA	1:106:A:TYR:HE1	8	0.12
(1,120)	1:13:A:THR:HA	1:106:A:TYR:HE2	8	0.12
(1,120)	1:13:A:THR:HA	1:106:A:TYR:HE1	14	0.12
(1,120)	1:13:A:THR:HA	1:106:A:TYR:HE2	14	0.12
(1,119)	1:102:A:ARG:HA	1:36:A:TRP:HZ3	11	0.12
(1,119)	1:102:A:ARG:HA	1:36:A:TRP:HZ3	12	0.12
(3,73)	1:12:A:ALA:H	1:9:A:HIS:O	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,73)	1:12:A:ALA:H	1:9:A:HIS:O	4	0.11
(3,73)	1:12:A:ALA:H	1:9:A:HIS:O	8	0.11
(3,70)	1:11:A:GLY:N	1:8:A:ALA:O	4	0.11
(3,70)	1:11:A:GLY:N	1:8:A:ALA:O	5	0.11
(3,70)	1:11:A:GLY:N	1:8:A:ALA:O	6	0.11
(3,70)	1:11:A:GLY:N	1:8:A:ALA:O	7	0.11
(3,70)	1:11:A:GLY:N	1:8:A:ALA:O	8	0.11
(3,70)	1:11:A:GLY:N	1:8:A:ALA:O	10	0.11
(3,70)	1:11:A:GLY:N	1:8:A:ALA:O	13	0.11
(3,59)	1:90:A:MET:H	1:35:A:ALA:O	14	0.11
(3,51)	1:101:A:GLU:H	1:89:A:TYR:O	7	0.11
(3,49)	1:87:A:LEU:H	1:103:A:PHE:O	15	0.11
(3,43)	1:105:A:VAL:H	1:85:A:VAL:O	1	0.11
(3,43)	1:105:A:VAL:H	1:85:A:VAL:O	2	0.11
(2,148)	1:29:A:ASN:HD22	1:10:A:ASN:HB2	4	0.11
(2,148)	1:29:A:ASN:HD22	1:10:A:ASN:HB2	13	0.11
(2,138)	1:7:A:LYS:H	1:25:A:GLN:HG2	11	0.11
(2,107)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	3	0.11
(2,106)	1:72:A:HIS:HB3	1:24:A:ILE:HA	11	0.11
(2,92)	1:20:A:GLU:HB2	1:22:A:VAL:HA	9	0.11
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	7	0.11
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	7	0.11
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	7	0.11
(2,82)	1:5:A:VAL:HG11	1:106:A:TYR:H	5	0.11
(2,82)	1:5:A:VAL:HG12	1:106:A:TYR:H	5	0.11
(2,82)	1:5:A:VAL:HG13	1:106:A:TYR:H	5	0.11
(2,82)	1:5:A:VAL:HG11	1:106:A:TYR:H	6	0.11
(2,82)	1:5:A:VAL:HG12	1:106:A:TYR:H	6	0.11
(2,82)	1:5:A:VAL:HG13	1:106:A:TYR:H	6	0.11
(2,63)	1:27:A:PRO:HB3	1:70:A:THR:H	8	0.11
(2,51)	1:35:A:ALA:HA	1:31:A:THR:H	2	0.11
(2,41)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	12	0.11
(2,41)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	14	0.11
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	11	0.11
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	12	0.11
(1,2452)	1:18:A:VAL:HG11	1:110:A:ASN:HD22	15	0.11
(1,2452)	1:18:A:VAL:HG12	1:110:A:ASN:HD22	15	0.11
(1,2452)	1:18:A:VAL:HG13	1:110:A:ASN:HD22	15	0.11
(1,2413)	1:31:A:THR:HG21	1:89:A:TYR:HB3	1	0.11
(1,2413)	1:31:A:THR:HG22	1:89:A:TYR:HB3	1	0.11
(1,2413)	1:31:A:THR:HG23	1:89:A:TYR:HB3	1	0.11
(1,2413)	1:31:A:THR:HG21	1:89:A:TYR:HB3	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2413)	1:31:A:THR:HG22	1:89:A:TYR:HB3	6	0.11
(1,2413)	1:31:A:THR:HG23	1:89:A:TYR:HB3	6	0.11
(1,2360)	1:106:A:TYR:HD1	1:106:A:TYR:H	9	0.11
(1,2360)	1:106:A:TYR:HD2	1:106:A:TYR:H	9	0.11
(1,2357)	1:85:A:VAL:HB	1:85:A:VAL:H	12	0.11
(1,2329)	1:108:A:LYS:HG3	1:83:A:HIS:HB2	3	0.11
(1,2320)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	12	0.11
(1,2320)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	14	0.11
(1,2301)	1:16:A:VAL:HG11	1:18:A:VAL:HA	1	0.11
(1,2301)	1:16:A:VAL:HG12	1:18:A:VAL:HA	1	0.11
(1,2301)	1:16:A:VAL:HG13	1:18:A:VAL:HA	1	0.11
(1,2301)	1:16:A:VAL:HG11	1:18:A:VAL:HA	5	0.11
(1,2301)	1:16:A:VAL:HG12	1:18:A:VAL:HA	5	0.11
(1,2301)	1:16:A:VAL:HG13	1:18:A:VAL:HA	5	0.11
(1,2279)	1:59:A:PRO:HB3	1:59:A:PRO:HD2	1	0.11
(1,2263)	1:24:A:ILE:HD11	1:106:A:TYR:HA	14	0.11
(1,2263)	1:24:A:ILE:HD12	1:106:A:TYR:HA	14	0.11
(1,2263)	1:24:A:ILE:HD13	1:106:A:TYR:HA	14	0.11
(1,2254)	1:77:A:VAL:HG21	1:110:A:ASN:HA	13	0.11
(1,2254)	1:77:A:VAL:HG22	1:110:A:ASN:HA	13	0.11
(1,2254)	1:77:A:VAL:HG23	1:110:A:ASN:HA	13	0.11
(1,2135)	1:70:A:THR:H	1:59:A:PRO:HG3	11	0.11
(1,2130)	1:47:A:ASN:HD21	1:110:A:ASN:HA	6	0.11
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG21	2	0.11
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG22	2	0.11
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG23	2	0.11
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG21	4	0.11
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG22	4	0.11
(1,2116)	1:53:A:VAL:H	1:75:A:VAL:HG23	4	0.11
(1,2087)	1:75:A:VAL:H	1:77:A:VAL:H	8	0.11
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB1	10	0.11
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB2	10	0.11
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB3	10	0.11
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB1	13	0.11
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB2	13	0.11
(1,2066)	1:41:A:GLY:H	1:35:A:ALA:HB3	13	0.11
(1,2060)	1:6:A:THR:H	1:105:A:VAL:HB	15	0.11
(1,2043)	1:66:A:GLY:H	1:65:A:LEU:HB3	7	0.11
(1,2023)	1:19:A:GLY:H	1:22:A:VAL:HB	3	0.11
(1,1892)	1:38:A:PHE:HE1	1:53:A:VAL:HG11	15	0.11
(1,1892)	1:38:A:PHE:HE1	1:53:A:VAL:HG12	15	0.11
(1,1892)	1:38:A:PHE:HE1	1:53:A:VAL:HG13	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1892)	1:38:A:PHE:HE2	1:53:A:VAL:HG11	15	0.11
(1,1892)	1:38:A:PHE:HE2	1:53:A:VAL:HG12	15	0.11
(1,1892)	1:38:A:PHE:HE2	1:53:A:VAL:HG13	15	0.11
(1,1869)	1:83:A:HIS:HE1	1:87:A:LEU:HG	7	0.11
(1,1869)	1:83:A:HIS:HE1	1:87:A:LEU:HG	11	0.11
(1,1869)	1:83:A:HIS:HE1	1:87:A:LEU:HG	14	0.11
(1,1852)	1:87:A:LEU:HD11	1:10:A:ASN:HA	5	0.11
(1,1852)	1:87:A:LEU:HD12	1:10:A:ASN:HA	5	0.11
(1,1852)	1:87:A:LEU:HD13	1:10:A:ASN:HA	5	0.11
(1,1834)	1:24:A:ILE:HD11	1:106:A:TYR:H	9	0.11
(1,1834)	1:24:A:ILE:HD12	1:106:A:TYR:H	9	0.11
(1,1834)	1:24:A:ILE:HD13	1:106:A:TYR:H	9	0.11
(1,1803)	1:26:A:LEU:HD21	1:25:A:GLN:HB3	8	0.11
(1,1803)	1:26:A:LEU:HD22	1:25:A:GLN:HB3	8	0.11
(1,1803)	1:26:A:LEU:HD23	1:25:A:GLN:HB3	8	0.11
(1,1785)	1:27:A:PRO:HG2	1:26:A:LEU:HD11	8	0.11
(1,1785)	1:27:A:PRO:HG2	1:26:A:LEU:HD12	8	0.11
(1,1785)	1:27:A:PRO:HG2	1:26:A:LEU:HD13	8	0.11
(1,1785)	1:27:A:PRO:HG2	1:26:A:LEU:HD11	13	0.11
(1,1785)	1:27:A:PRO:HG2	1:26:A:LEU:HD12	13	0.11
(1,1785)	1:27:A:PRO:HG2	1:26:A:LEU:HD13	13	0.11
(1,1784)	1:42:A:THR:HA	1:38:A:PHE:HB3	1	0.11
(1,1784)	1:42:A:THR:HA	1:38:A:PHE:HB3	12	0.11
(1,1763)	1:86:A:ASN:HA	1:36:A:TRP:HZ3	5	0.11
(1,1763)	1:86:A:ASN:HA	1:36:A:TRP:HZ3	6	0.11
(1,1752)	1:56:A:LYS:HB3	1:72:A:HIS:HB3	6	0.11
(1,1747)	1:87:A:LEU:HD21	1:104:A:THR:HA	6	0.11
(1,1747)	1:87:A:LEU:HD22	1:104:A:THR:HA	6	0.11
(1,1747)	1:87:A:LEU:HD23	1:104:A:THR:HA	6	0.11
(1,1730)	1:56:A:LYS:HD3	1:74:A:HIS:HA	5	0.11
(1,1730)	1:56:A:LYS:HD3	1:74:A:HIS:HA	14	0.11
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG21	7	0.11
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG22	7	0.11
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG23	7	0.11
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG21	14	0.11
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG22	14	0.11
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG23	14	0.11
(1,1722)	1:64:A:LEU:HB3	1:66:A:GLY:HA2	8	0.11
(1,1668)	1:78:A:LYS:HB2	1:78:A:LYS:HE3	10	0.11
(1,1668)	1:78:A:LYS:HB2	1:78:A:LYS:HE3	15	0.11
(1,1627)	1:24:A:ILE:HD11	1:73:A:PHE:HB3	11	0.11
(1,1627)	1:24:A:ILE:HD12	1:73:A:PHE:HB3	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1627)	1:24:A:ILE:HD13	1:73:A:PHE:HB3	11	0.11
(1,1615)	1:60:A:PRO:HA	1:66:A:GLY:HA3	11	0.11
(1,1597)	1:16:A:VAL:HG21	1:108:A:LYS:HB2	2	0.11
(1,1597)	1:16:A:VAL:HG22	1:108:A:LYS:HB2	2	0.11
(1,1597)	1:16:A:VAL:HG23	1:108:A:LYS:HB2	2	0.11
(1,1588)	1:70:A:THR:HB	1:58:A:PHE:HB2	6	0.11
(1,1563)	1:26:A:LEU:HD11	1:10:A:ASN:HA	5	0.11
(1,1563)	1:26:A:LEU:HD12	1:10:A:ASN:HA	5	0.11
(1,1563)	1:26:A:LEU:HD13	1:10:A:ASN:HA	5	0.11
(1,1563)	1:26:A:LEU:HD11	1:10:A:ASN:HA	10	0.11
(1,1563)	1:26:A:LEU:HD12	1:10:A:ASN:HA	10	0.11
(1,1563)	1:26:A:LEU:HD13	1:10:A:ASN:HA	10	0.11
(1,1535)	1:90:A:MET:HE1	1:92:A:PRO:HA	9	0.11
(1,1535)	1:90:A:MET:HE2	1:92:A:PRO:HA	9	0.11
(1,1535)	1:90:A:MET:HE3	1:92:A:PRO:HA	9	0.11
(1,1535)	1:90:A:MET:HE1	1:92:A:PRO:HA	10	0.11
(1,1535)	1:90:A:MET:HE2	1:92:A:PRO:HA	10	0.11
(1,1535)	1:90:A:MET:HE3	1:92:A:PRO:HA	10	0.11
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	1	0.11
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	4	0.11
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	5	0.11
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	6	0.11
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	9	0.11
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	11	0.11
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	12	0.11
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	13	0.11
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	15	0.11
(1,1462)	1:6:A:THR:HA	1:103:A:PHE:HE1	15	0.11
(1,1462)	1:6:A:THR:HA	1:103:A:PHE:HE2	15	0.11
(1,1430)	1:82:A:THR:HG21	1:110:A:ASN:HD21	9	0.11
(1,1430)	1:82:A:THR:HG22	1:110:A:ASN:HD21	9	0.11
(1,1430)	1:82:A:THR:HG23	1:110:A:ASN:HD21	9	0.11
(1,1430)	1:82:A:THR:HG21	1:110:A:ASN:HD21	15	0.11
(1,1430)	1:82:A:THR:HG22	1:110:A:ASN:HD21	15	0.11
(1,1430)	1:82:A:THR:HG23	1:110:A:ASN:HD21	15	0.11
(1,1428)	1:56:A:LYS:HD3	1:57:A:TYR:HD1	11	0.11
(1,1428)	1:56:A:LYS:HD3	1:57:A:TYR:HD2	11	0.11
(1,1426)	1:6:A:THR:HG21	1:72:A:HIS:HE1	4	0.11
(1,1426)	1:6:A:THR:HG22	1:72:A:HIS:HE1	4	0.11
(1,1426)	1:6:A:THR:HG23	1:72:A:HIS:HE1	4	0.11
(1,1426)	1:6:A:THR:HG21	1:72:A:HIS:HE1	14	0.11
(1,1426)	1:6:A:THR:HG22	1:72:A:HIS:HE1	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1426)	1:6:A:THR:HG23	1:72:A:HIS:HE1	14	0.11
(1,1339)	1:87:A:LEU:HG	1:38:A:PHE:H	6	0.11
(1,1314)	1:60:A:PRO:HB2	1:62:A:SER:H	6	0.11
(1,1308)	1:87:A:LEU:HB2	1:89:A:TYR:H	2	0.11
(1,1303)	1:104:A:THR:HG21	1:11:A:GLY:H	11	0.11
(1,1303)	1:104:A:THR:HG22	1:11:A:GLY:H	11	0.11
(1,1303)	1:104:A:THR:HG23	1:11:A:GLY:H	11	0.11
(1,1303)	1:104:A:THR:HG21	1:11:A:GLY:H	13	0.11
(1,1303)	1:104:A:THR:HG22	1:11:A:GLY:H	13	0.11
(1,1303)	1:104:A:THR:HG23	1:11:A:GLY:H	13	0.11
(1,1259)	1:4:A:LYS:HB3	1:3:A:HIS:HB3	5	0.11
(1,1259)	1:4:A:LYS:HB3	1:3:A:HIS:HB3	11	0.11
(1,1124)	1:21:A:LEU:HD11	1:51:A:PHE:HD1	10	0.11
(1,1124)	1:21:A:LEU:HD11	1:51:A:PHE:HD2	10	0.11
(1,1124)	1:21:A:LEU:HD12	1:51:A:PHE:HD1	10	0.11
(1,1124)	1:21:A:LEU:HD12	1:51:A:PHE:HD2	10	0.11
(1,1124)	1:21:A:LEU:HD13	1:51:A:PHE:HD1	10	0.11
(1,1124)	1:21:A:LEU:HD13	1:51:A:PHE:HD2	10	0.11
(1,1036)	1:16:A:VAL:HB	1:108:A:LYS:H	12	0.11
(1,1015)	1:10:A:ASN:HB2	1:10:A:ASN:HD21	11	0.11
(1,1015)	1:10:A:ASN:HB2	1:10:A:ASN:HD21	15	0.11
(1,886)	1:6:A:THR:HG21	1:25:A:GLN:H	10	0.11
(1,886)	1:6:A:THR:HG22	1:25:A:GLN:H	10	0.11
(1,886)	1:6:A:THR:HG23	1:25:A:GLN:H	10	0.11
(1,746)	1:70:A:THR:HG21	1:71:A:GLU:H	2	0.11
(1,746)	1:70:A:THR:HG22	1:71:A:GLU:H	2	0.11
(1,746)	1:70:A:THR:HG23	1:71:A:GLU:H	2	0.11
(1,746)	1:70:A:THR:HG21	1:71:A:GLU:H	3	0.11
(1,746)	1:70:A:THR:HG22	1:71:A:GLU:H	3	0.11
(1,746)	1:70:A:THR:HG23	1:71:A:GLU:H	3	0.11
(1,746)	1:70:A:THR:HG21	1:71:A:GLU:H	8	0.11
(1,746)	1:70:A:THR:HG22	1:71:A:GLU:H	8	0.11
(1,746)	1:70:A:THR:HG23	1:71:A:GLU:H	8	0.11
(1,746)	1:70:A:THR:HG21	1:71:A:GLU:H	12	0.11
(1,746)	1:70:A:THR:HG22	1:71:A:GLU:H	12	0.11
(1,746)	1:70:A:THR:HG23	1:71:A:GLU:H	12	0.11
(1,730)	1:7:A:LYS:HA	1:7:A:LYS:HD3	10	0.11
(1,730)	1:7:A:LYS:HA	1:7:A:LYS:HD3	13	0.11
(1,723)	1:54:A:GLU:HA	1:55:A:ASN:H	6	0.11
(1,723)	1:54:A:GLU:HA	1:55:A:ASN:H	14	0.11
(1,721)	1:64:A:LEU:HB3	1:65:A:LEU:H	15	0.11
(1,720)	1:25:A:GLN:HG2	1:26:A:LEU:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	3	0.11
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	3	0.11
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	3	0.11
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	4	0.11
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	4	0.11
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	4	0.11
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	5	0.11
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	5	0.11
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	5	0.11
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	8	0.11
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	8	0.11
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	8	0.11
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	10	0.11
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	10	0.11
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	10	0.11
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	14	0.11
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	14	0.11
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	14	0.11
(1,717)	1:17:A:ALA:HB1	1:17:A:ALA:H	15	0.11
(1,717)	1:17:A:ALA:HB2	1:17:A:ALA:H	15	0.11
(1,717)	1:17:A:ALA:HB3	1:17:A:ALA:H	15	0.11
(1,694)	1:76:A:THR:HA	1:22:A:VAL:H	4	0.11
(1,677)	1:26:A:LEU:HG	1:27:A:PRO:HG2	2	0.11
(1,668)	1:105:A:VAL:HG21	1:12:A:ALA:HB1	10	0.11
(1,668)	1:105:A:VAL:HG21	1:12:A:ALA:HB2	10	0.11
(1,668)	1:105:A:VAL:HG21	1:12:A:ALA:HB3	10	0.11
(1,668)	1:105:A:VAL:HG22	1:12:A:ALA:HB1	10	0.11
(1,668)	1:105:A:VAL:HG22	1:12:A:ALA:HB2	10	0.11
(1,668)	1:105:A:VAL:HG22	1:12:A:ALA:HB3	10	0.11
(1,668)	1:105:A:VAL:HG23	1:12:A:ALA:HB1	10	0.11
(1,668)	1:105:A:VAL:HG23	1:12:A:ALA:HB2	10	0.11
(1,668)	1:105:A:VAL:HG23	1:12:A:ALA:HB3	10	0.11
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB1	2	0.11
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB2	2	0.11
(1,652)	1:65:A:LEU:HD11	1:67:A:ALA:HB3	2	0.11
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB1	2	0.11
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB2	2	0.11
(1,652)	1:65:A:LEU:HD12	1:67:A:ALA:HB3	2	0.11
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB1	2	0.11
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB2	2	0.11
(1,652)	1:65:A:LEU:HD13	1:67:A:ALA:HB3	2	0.11
(1,604)	1:25:A:GLN:HB2	1:73:A:PHE:HB2	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:80:A:ALA:HA	1:109:A:ALA:HA	8	0.11
(1,488)	1:75:A:VAL:HG11	1:45:A:SER:HA	10	0.11
(1,488)	1:75:A:VAL:HG12	1:45:A:SER:HA	10	0.11
(1,488)	1:75:A:VAL:HG13	1:45:A:SER:HA	10	0.11
(1,472)	1:65:A:LEU:HG	1:28:A:SER:HB3	1	0.11
(1,472)	1:65:A:LEU:HG	1:28:A:SER:HB3	13	0.11
(1,393)	1:82:A:THR:HG21	1:109:A:ALA:HA	3	0.11
(1,393)	1:82:A:THR:HG22	1:109:A:ALA:HA	3	0.11
(1,393)	1:82:A:THR:HG23	1:109:A:ALA:HA	3	0.11
(1,350)	1:7:A:LYS:HD3	1:28:A:SER:HA	6	0.11
(1,306)	1:47:A:ASN:HB3	1:47:A:ASN:HA	4	0.11
(1,304)	1:61:A:ASP:HB3	1:62:A:SER:HA	7	0.11
(1,304)	1:61:A:ASP:HB3	1:62:A:SER:HA	14	0.11
(1,303)	1:36:A:TRP:HB2	1:26:A:LEU:HA	7	0.11
(1,303)	1:36:A:TRP:HB2	1:26:A:LEU:HA	10	0.11
(1,269)	1:26:A:LEU:HD21	1:57:A:TYR:HD1	1	0.11
(1,269)	1:26:A:LEU:HD21	1:57:A:TYR:HD2	1	0.11
(1,269)	1:26:A:LEU:HD22	1:57:A:TYR:HD1	1	0.11
(1,269)	1:26:A:LEU:HD22	1:57:A:TYR:HD2	1	0.11
(1,269)	1:26:A:LEU:HD23	1:57:A:TYR:HD1	1	0.11
(1,269)	1:26:A:LEU:HD23	1:57:A:TYR:HD2	1	0.11
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	5	0.11
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	5	0.11
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	5	0.11
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	7	0.11
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	7	0.11
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	7	0.11
(1,239)	1:5:A:VAL:HG11	1:104:A:THR:H	13	0.11
(1,239)	1:5:A:VAL:HG12	1:104:A:THR:H	13	0.11
(1,239)	1:5:A:VAL:HG13	1:104:A:THR:H	13	0.11
(1,225)	1:25:A:GLN:HG2	1:74:A:HIS:HD2	9	0.11
(1,216)	1:25:A:GLN:HB2	1:72:A:HIS:HD2	6	0.11
(1,133)	1:90:A:MET:HA	1:34:A:PHE:HD1	10	0.11
(1,133)	1:90:A:MET:HA	1:34:A:PHE:HD2	10	0.11
(1,126)	1:25:A:GLN:HA	1:72:A:HIS:HE1	5	0.11
(1,126)	1:25:A:GLN:HA	1:72:A:HIS:HE1	10	0.11
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE1	10	0.11
(1,79)	1:33:A:GLY:HA2	1:34:A:PHE:HE2	10	0.11
(3,73)	1:12:A:ALA:H	1:9:A:HIS:O	7	0.1
(3,73)	1:12:A:ALA:H	1:9:A:HIS:O	13	0.1
(3,51)	1:101:A:GLU:H	1:89:A:TYR:O	1	0.1
(2,158)	1:50:A:MET:H	1:48:A:GLU:H	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,134)	1:99:A:ASP:H	1:95:A:GLY:HA2	4	0.1
(2,103)	1:48:A:GLU:HA	1:50:A:MET:HA	4	0.1
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD1	3	0.1
(2,99)	1:56:A:LYS:HD3	1:73:A:PHE:HD2	3	0.1
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG11	8	0.1
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG12	8	0.1
(2,84)	1:79:A:ALA:HA	1:18:A:VAL:HG13	8	0.1
(2,76)	1:46:A:PRO:HD3	1:48:A:GLU:HB3	6	0.1
(2,70)	1:17:A:ALA:HB1	1:20:A:GLU:HG3	8	0.1
(2,70)	1:17:A:ALA:HB2	1:20:A:GLU:HG3	8	0.1
(2,70)	1:17:A:ALA:HB3	1:20:A:GLU:HG3	8	0.1
(2,52)	1:30:A:PRO:HG3	1:29:A:ASN:HB2	8	0.1
(2,51)	1:35:A:ALA:HA	1:31:A:THR:H	9	0.1
(2,41)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	10	0.1
(2,26)	1:38:A:PHE:HB3	1:88:A:THR:HB	6	0.1
(2,6)	1:38:A:PHE:HB3	1:102:A:ARG:HE	9	0.1
(1,2534)	1:74:A:HIS:H	1:53:A:VAL:HG11	14	0.1
(1,2534)	1:74:A:HIS:H	1:53:A:VAL:HG12	14	0.1
(1,2534)	1:74:A:HIS:H	1:53:A:VAL:HG13	14	0.1
(1,2522)	1:52:A:THR:HG21	1:48:A:GLU:HB3	10	0.1
(1,2522)	1:52:A:THR:HG22	1:48:A:GLU:HB3	10	0.1
(1,2522)	1:52:A:THR:HG23	1:48:A:GLU:HB3	10	0.1
(1,2522)	1:52:A:THR:HG21	1:54:A:GLU:HB2	13	0.1
(1,2522)	1:52:A:THR:HG22	1:54:A:GLU:HB2	13	0.1
(1,2522)	1:52:A:THR:HG23	1:54:A:GLU:HB2	13	0.1
(1,2468)	1:12:A:ALA:HB1	1:104:A:THR:H	3	0.1
(1,2468)	1:12:A:ALA:HB2	1:104:A:THR:H	3	0.1
(1,2468)	1:12:A:ALA:HB3	1:104:A:THR:H	3	0.1
(1,2390)	1:75:A:VAL:HG21	1:51:A:PHE:HB3	7	0.1
(1,2390)	1:75:A:VAL:HG22	1:51:A:PHE:HB3	7	0.1
(1,2390)	1:75:A:VAL:HG23	1:51:A:PHE:HB3	7	0.1
(1,2320)	1:92:A:PRO:HD3	1:95:A:GLY:HA2	10	0.1
(1,2297)	1:35:A:ALA:HB1	1:59:A:PRO:HD3	9	0.1
(1,2297)	1:35:A:ALA:HB2	1:59:A:PRO:HD3	9	0.1
(1,2297)	1:35:A:ALA:HB3	1:59:A:PRO:HD3	9	0.1
(1,2279)	1:59:A:PRO:HB3	1:59:A:PRO:HD2	11	0.1
(1,2236)	1:7:A:LYS:HG3	1:26:A:LEU:HA	6	0.1
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD1	3	0.1
(1,2155)	1:11:A:GLY:HA2	1:106:A:TYR:HD2	3	0.1
(1,2149)	1:26:A:LEU:HD11	1:85:A:VAL:HG11	12	0.1
(1,2149)	1:26:A:LEU:HD11	1:85:A:VAL:HG12	12	0.1
(1,2149)	1:26:A:LEU:HD11	1:85:A:VAL:HG13	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2149)	1:26:A:LEU:HD12	1:85:A:VAL:HG11	12	0.1
(1,2149)	1:26:A:LEU:HD12	1:85:A:VAL:HG12	12	0.1
(1,2149)	1:26:A:LEU:HD12	1:85:A:VAL:HG13	12	0.1
(1,2149)	1:26:A:LEU:HD13	1:85:A:VAL:HG11	12	0.1
(1,2149)	1:26:A:LEU:HD13	1:85:A:VAL:HG12	12	0.1
(1,2149)	1:26:A:LEU:HD13	1:85:A:VAL:HG13	12	0.1
(1,2080)	1:97:A:SER:H	1:100:A:SER:H	9	0.1
(1,2044)	1:70:A:THR:H	1:72:A:HIS:HD2	7	0.1
(1,1972)	1:79:A:ALA:H	1:78:A:LYS:H	13	0.1
(1,1886)	1:38:A:PHE:HZ	1:85:A:VAL:HB	10	0.1
(1,1885)	1:38:A:PHE:HZ	1:45:A:SER:HA	3	0.1
(1,1869)	1:83:A:HIS:HE1	1:87:A:LEU:HG	12	0.1
(1,1857)	1:48:A:GLU:HG3	1:49:A:SER:HA	14	0.1
(1,1834)	1:24:A:ILE:HD11	1:106:A:TYR:H	2	0.1
(1,1834)	1:24:A:ILE:HD12	1:106:A:TYR:H	2	0.1
(1,1834)	1:24:A:ILE:HD13	1:106:A:TYR:H	2	0.1
(1,1818)	1:108:A:LYS:HD3	1:108:A:LYS:H	5	0.1
(1,1808)	1:87:A:LEU:HD21	1:39:A:GLU:HA	2	0.1
(1,1808)	1:87:A:LEU:HD22	1:39:A:GLU:HA	2	0.1
(1,1808)	1:87:A:LEU:HD23	1:39:A:GLU:HA	2	0.1
(1,1792)	1:16:A:VAL:HA	1:3:A:HIS:HE1	3	0.1
(1,1784)	1:42:A:THR:HA	1:38:A:PHE:HB3	15	0.1
(1,1763)	1:86:A:ASN:HA	1:36:A:TRP:HZ3	1	0.1
(1,1747)	1:87:A:LEU:HD21	1:104:A:THR:HA	14	0.1
(1,1747)	1:87:A:LEU:HD22	1:104:A:THR:HA	14	0.1
(1,1747)	1:87:A:LEU:HD23	1:104:A:THR:HA	14	0.1
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG21	5	0.1
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG22	5	0.1
(1,1723)	1:27:A:PRO:HG3	1:70:A:THR:HG23	5	0.1
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG21	1	0.1
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG22	1	0.1
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG23	1	0.1
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG21	1	0.1
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG22	1	0.1
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG23	1	0.1
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG21	1	0.1
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG22	1	0.1
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG23	1	0.1
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG21	4	0.1
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG22	4	0.1
(1,1694)	1:8:A:ALA:HB1	1:105:A:VAL:HG23	4	0.1
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG21	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG22	4	0.1
(1,1694)	1:8:A:ALA:HB2	1:105:A:VAL:HG23	4	0.1
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG21	4	0.1
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG22	4	0.1
(1,1694)	1:8:A:ALA:HB3	1:105:A:VAL:HG23	4	0.1
(1,1632)	1:50:A:MET:HE1	1:77:A:VAL:HA	6	0.1
(1,1632)	1:50:A:MET:HE2	1:77:A:VAL:HA	6	0.1
(1,1632)	1:50:A:MET:HE3	1:77:A:VAL:HA	6	0.1
(1,1630)	1:60:A:PRO:HA	1:66:A:GLY:HA2	11	0.1
(1,1613)	1:29:A:ASN:HB3	1:31:A:THR:HG21	2	0.1
(1,1613)	1:29:A:ASN:HB3	1:31:A:THR:HG22	2	0.1
(1,1613)	1:29:A:ASN:HB3	1:31:A:THR:HG23	2	0.1
(1,1613)	1:29:A:ASN:HB3	1:31:A:THR:HG21	14	0.1
(1,1613)	1:29:A:ASN:HB3	1:31:A:THR:HG22	14	0.1
(1,1613)	1:29:A:ASN:HB3	1:31:A:THR:HG23	14	0.1
(1,1588)	1:70:A:THR:HB	1:58:A:PHE:HB2	7	0.1
(1,1588)	1:70:A:THR:HB	1:58:A:PHE:HB2	8	0.1
(1,1482)	1:27:A:PRO:HB3	1:27:A:PRO:HG2	8	0.1
(1,1415)	1:31:A:THR:HG21	1:36:A:TRP:HD1	14	0.1
(1,1415)	1:31:A:THR:HG22	1:36:A:TRP:HD1	14	0.1
(1,1415)	1:31:A:THR:HG23	1:36:A:TRP:HD1	14	0.1
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD1	11	0.1
(1,1348)	1:91:A:ARG:HA	1:37:A:TYR:HD2	11	0.1
(1,1259)	1:4:A:LYS:HB3	1:3:A:HIS:HB3	15	0.1
(1,1209)	1:42:A:THR:HG21	1:44:A:GLU:H	14	0.1
(1,1209)	1:42:A:THR:HG22	1:44:A:GLU:H	14	0.1
(1,1209)	1:42:A:THR:HG23	1:44:A:GLU:H	14	0.1
(1,1154)	1:56:A:LYS:HG3	1:56:A:LYS:H	13	0.1
(1,772)	1:102:A:ARG:HA	1:102:A:ARG:H	7	0.1
(1,752)	1:22:A:VAL:HG21	1:23:A:GLU:H	7	0.1
(1,752)	1:22:A:VAL:HG22	1:23:A:GLU:H	7	0.1
(1,752)	1:22:A:VAL:HG23	1:23:A:GLU:H	7	0.1
(1,752)	1:22:A:VAL:HG21	1:23:A:GLU:H	11	0.1
(1,752)	1:22:A:VAL:HG22	1:23:A:GLU:H	11	0.1
(1,752)	1:22:A:VAL:HG23	1:23:A:GLU:H	11	0.1
(1,746)	1:70:A:THR:HG21	1:71:A:GLU:H	9	0.1
(1,746)	1:70:A:THR:HG22	1:71:A:GLU:H	9	0.1
(1,746)	1:70:A:THR:HG23	1:71:A:GLU:H	9	0.1
(1,736)	1:17:A:ALA:HB1	1:18:A:VAL:H	7	0.1
(1,736)	1:17:A:ALA:HB2	1:18:A:VAL:H	7	0.1
(1,736)	1:17:A:ALA:HB3	1:18:A:VAL:H	7	0.1
(1,730)	1:7:A:LYS:HA	1:7:A:LYS:HD3	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,730)	1:7:A:LYS:HA	1:7:A:LYS:HD3	7	0.1
(1,720)	1:25:A:GLN:HG2	1:26:A:LEU:H	15	0.1
(1,687)	1:22:A:VAL:HG11	1:3:A:HIS:HD2	14	0.1
(1,687)	1:22:A:VAL:HG12	1:3:A:HIS:HD2	14	0.1
(1,687)	1:22:A:VAL:HG13	1:3:A:HIS:HD2	14	0.1
(1,677)	1:26:A:LEU:HG	1:27:A:PRO:HG2	3	0.1
(1,677)	1:26:A:LEU:HG	1:27:A:PRO:HG2	11	0.1
(1,677)	1:26:A:LEU:HG	1:27:A:PRO:HG2	12	0.1
(1,604)	1:25:A:GLN:HB2	1:73:A:PHE:HB2	4	0.1
(1,528)	1:70:A:THR:HB	1:58:A:PHE:HA	1	0.1
(1,528)	1:70:A:THR:HB	1:58:A:PHE:HA	2	0.1
(1,488)	1:75:A:VAL:HG11	1:45:A:SER:HA	4	0.1
(1,488)	1:75:A:VAL:HG12	1:45:A:SER:HA	4	0.1
(1,488)	1:75:A:VAL:HG13	1:45:A:SER:HA	4	0.1
(1,306)	1:47:A:ASN:HB3	1:47:A:ASN:HA	13	0.1
(1,304)	1:61:A:ASP:HB3	1:62:A:SER:HA	13	0.1
(1,298)	1:83:A:HIS:HB2	1:81:A:GLY:HA3	9	0.1
(1,230)	1:56:A:LYS:HG3	1:74:A:HIS:HE1	1	0.1
(1,179)	1:50:A:MET:HE1	1:51:A:PHE:HZ	14	0.1
(1,179)	1:50:A:MET:HE2	1:51:A:PHE:HZ	14	0.1
(1,179)	1:50:A:MET:HE3	1:51:A:PHE:HZ	14	0.1
(1,170)	1:103:A:PHE:HB2	1:105:A:VAL:H	9	0.1
(1,126)	1:25:A:GLN:HA	1:72:A:HIS:HE1	8	0.1

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

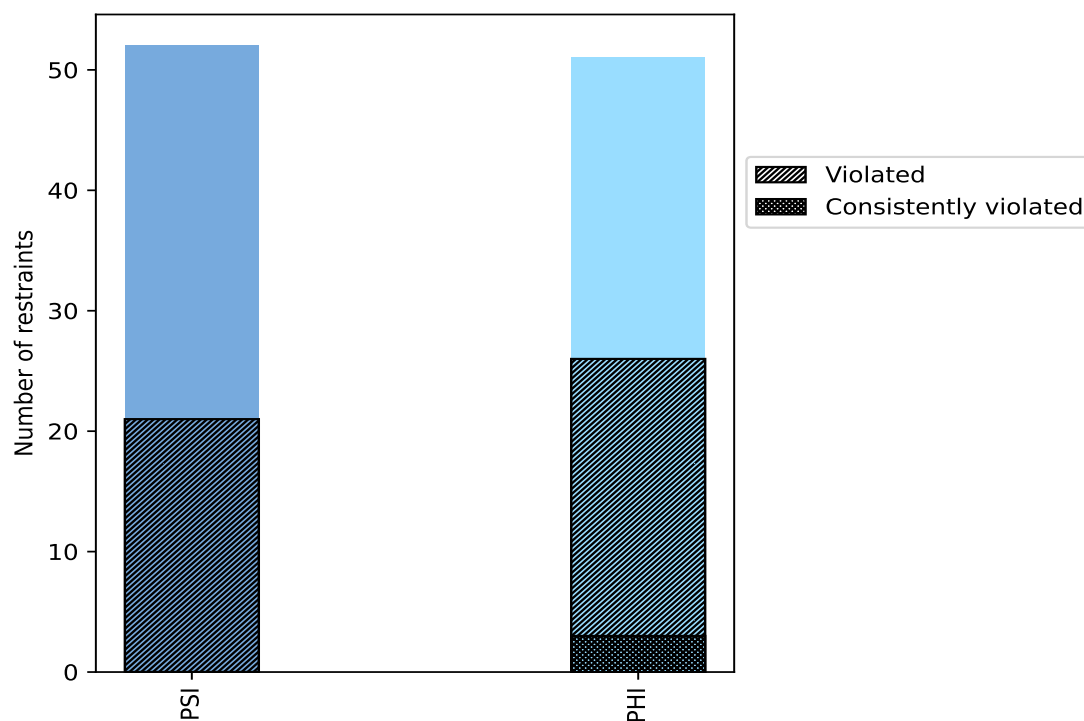
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	52	50.5	21	40.4	20.4	0	0.0	0.0
PHI	51	49.5	26	51.0	25.2	3	5.9	2.9
Total	103	100.0	47	45.6	45.6	3	2.9	2.9

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](#)



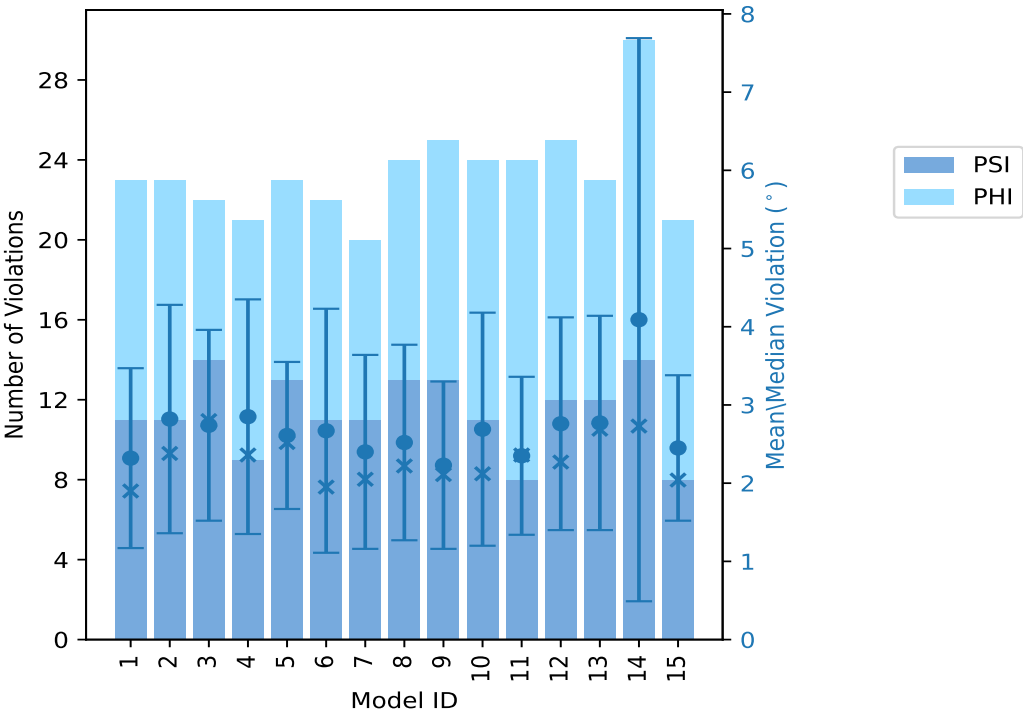
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	11	12	23	2.32	5.64	1.15	1.9
2	11	12	23	2.82	7.04	1.46	2.38
3	14	8	22	2.74	6.14	1.22	2.8
4	9	12	21	2.85	7.08	1.5	2.36
5	13	10	23	2.61	4.32	0.94	2.52
6	11	11	22	2.67	6.61	1.56	1.95
7	11	9	20	2.4	6.56	1.24	2.05
8	13	11	24	2.52	4.79	1.25	2.22
9	13	12	25	2.23	5.34	1.07	2.11
10	11	13	24	2.69	7.83	1.49	2.12
11	8	16	24	2.35	4.47	1.01	2.36
12	12	13	25	2.76	5.82	1.36	2.27
13	12	11	23	2.77	5.6	1.37	2.69
14	14	16	30	4.09	17.22	3.6	2.73
15	8	13	21	2.45	4.38	0.93	2.04

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

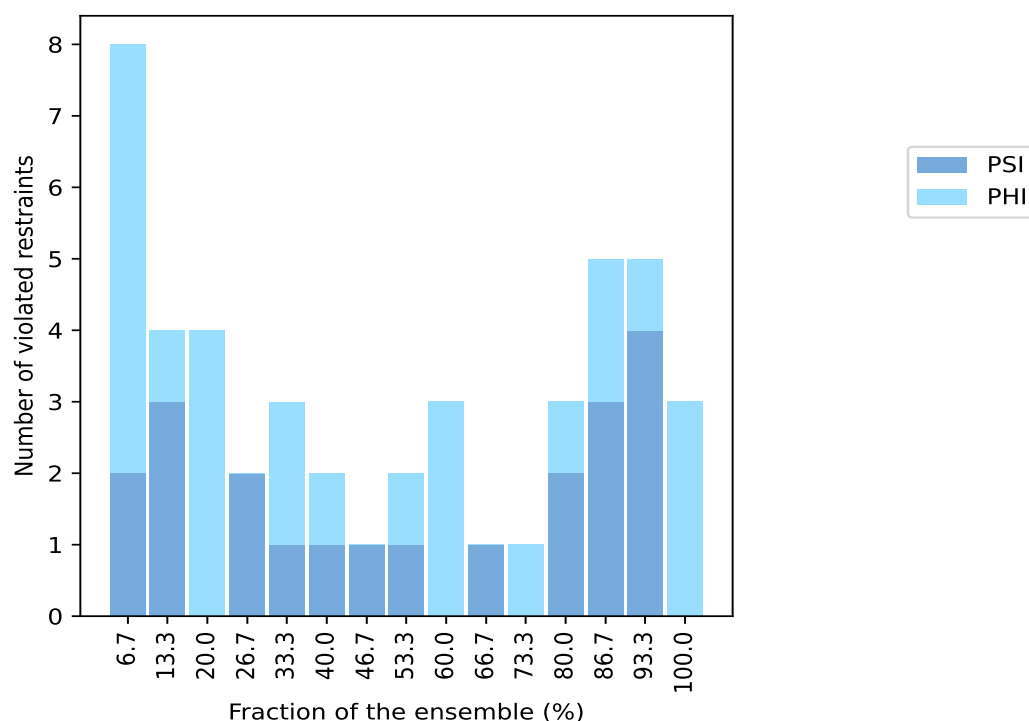
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

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

¹ Number of models with violations

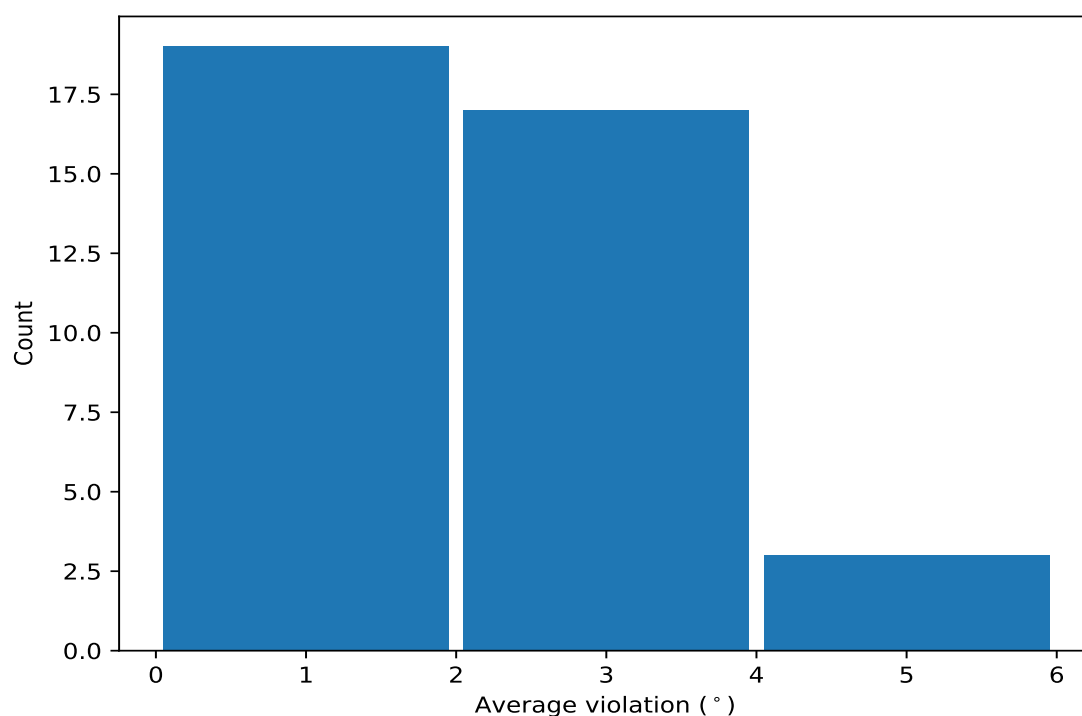
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	15	3.78	0.86	3.86
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	15	3.22	0.78	3.24
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	15	2.43	0.65	2.36
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	14	4.74	2.62	4.86
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	14	4.74	0.88	4.99
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	14	3.19	1.03	3.13
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	14	2.49	1.04	2.19
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	14	2.25	0.69	2.34
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	13	3.89	2.29	3.8
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	13	2.85	1.41	2.46
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	13	2.73	0.76	2.58
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	13	2.5	0.77	2.68
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	13	2.35	0.7	2.52
(1,10)	1:14:A:LEU:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	12	2.79	1.31	2.09
(1,67)	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1:25:A:GLN:N	12	2.53	0.82	2.4
(1,94)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:LEU:N	12	1.61	0.29	1.61
(1,33)	1:74:A:HIS:C	1:75:A:VAL:N	1:75:A:VAL:CA	1:75:A:VAL:C	11	2.22	0.76	2.02
(1,80)	1:58:A:PHE:N	1:58:A:PHE:CA	1:58:A:PHE:C	1:59:A:PRO:N	10	4.32	1.99	4.15
(1,50)	1:107:A:LEU:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	9	1.93	0.63	1.73
(1,13)	1:20:A:GLU:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	9	1.86	0.62	1.88
(1,39)	1:82:A:THR:C	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	9	1.85	0.67	1.62

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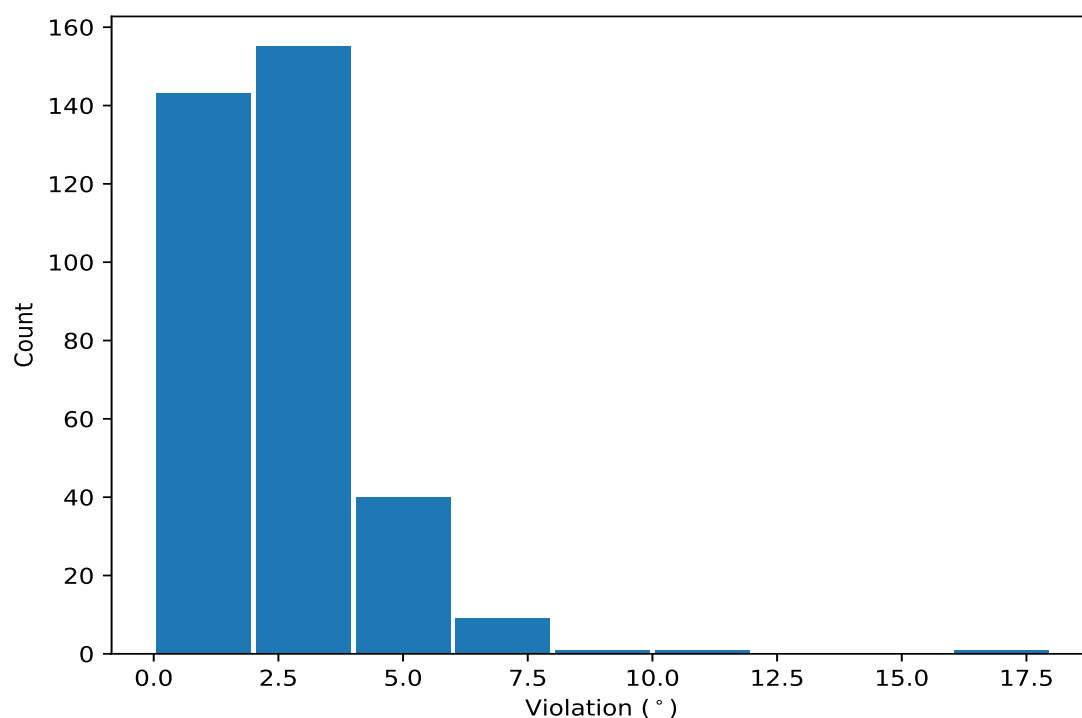
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,32)	1:73:A:PHE:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	8	1.99	0.51	1.93
(1,86)	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	1:77:A:VAL:N	8	1.63	0.79	1.34
(1,93)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:ASN:N	7	1.59	0.62	1.28
(1,36)	1:78:A:LYS:C	1:79:A:ALA:N	1:79:A:ALA:CA	1:79:A:ALA:C	6	2.0	0.73	1.82
(1,91)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ALA:N	6	1.8	0.59	1.7
(1,100)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	5	3.07	2.33	1.66
(1,45)	1:102:A:ARG:C	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:C	5	1.7	0.42	1.64
(1,15)	1:22:A:VAL:C	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	5	1.67	0.34	1.66
(1,73)	1:51:A:PHE:N	1:51:A:PHE:CA	1:51:A:PHE:C	1:52:A:THR:N	4	3.6	2.62	2.6
(1,81)	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	1:72:A:HIS:N	4	1.8	0.46	1.6
(1,29)	1:70:A:THR:C	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	3	1.79	0.78	1.49
(1,25)	1:54:A:GLU:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	3	1.37	0.29	1.23
(1,47)	1:104:A:THR:C	1:105:A:VAL:N	1:105:A:VAL:CA	1:105:A:VAL:C	3	1.27	0.06	1.28
(1,48)	1:105:A:VAL:C	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	3	1.22	0.2	1.1
(1,88)	1:79:A:ALA:N	1:79:A:ALA:CA	1:79:A:ALA:C	1:80:A:ALA:N	2	1.71	0.56	1.71
(1,41)	1:84:A:ALA:C	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	2	1.34	0.3	1.34
(1,59)	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	1:14:A:LEU:N	2	1.32	0.08	1.32
(1,78)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:TYR:N	2	1.11	0.02	1.11

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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 (°)
(1,22)	1:51:A:PHE:C	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	14	17.22
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	14	11.12
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	14	9.73
(1,73)	1:51:A:PHE:N	1:51:A:PHE:CA	1:51:A:PHE:C	1:52:A:THR:N	14	7.99
(1,80)	1:58:A:PHE:N	1:58:A:PHE:CA	1:58:A:PHE:C	1:59:A:PRO:N	10	7.83
(1,100)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	14	7.58
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	4	7.08
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	2	7.04
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	14	6.66
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	6	6.61
(1,80)	1:58:A:PHE:N	1:58:A:PHE:CA	1:58:A:PHE:C	1:59:A:PRO:N	7	6.56
(1,80)	1:58:A:PHE:N	1:58:A:PHE:CA	1:58:A:PHE:C	1:59:A:PRO:N	3	6.14
(1,10)	1:14:A:LEU:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	14	5.83
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	12	5.82
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	4	5.76
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	1	5.64
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	13	5.6
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	13	5.55
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	2	5.43
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	9	5.34
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	10	5.32

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	12	5.29
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	6	5.29
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	4	5.27
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	14	5.2
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	13	5.16
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	12	5.14
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	12	5.06
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	6	5.02
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	14	4.94
(1,80)	1:58:A:PHE:N	1:58:A:PHE:CA	1:58:A:PHE:C	1:59:A:PRO:N	2	4.91
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	8	4.79
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	8	4.78
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	14	4.77
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	6	4.66
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	2	4.58
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	3	4.58
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	8	4.54
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	11	4.47
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	1	4.44
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	15	4.38
(1,80)	1:58:A:PHE:N	1:58:A:PHE:CA	1:58:A:PHE:C	1:59:A:PRO:N	12	4.35
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	6	4.35
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	5	4.32
(1,10)	1:14:A:LEU:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	8	4.3
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	3	4.25
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	5	4.17
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	1	4.13
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	5	4.07
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	10	4.05
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	4	4.02
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	9	4.0
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	7	3.97
(1,80)	1:58:A:PHE:N	1:58:A:PHE:CA	1:58:A:PHE:C	1:59:A:PRO:N	15	3.95
(1,67)	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1:25:A:GLN:N	10	3.94
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	15	3.89
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	8	3.86
(1,10)	1:14:A:LEU:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	11	3.84
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	14	3.83
(1,4)	1:6:A:THR:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	15	3.83
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	10	3.82
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	2	3.82
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	13	3.81
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	4	3.8
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	5	3.8
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	13	3.77
(1,24)	1:53:A:VAL:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	14	3.76
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	5	3.75
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	7	3.75
(1,80)	1:58:A:PHE:N	1:58:A:PHE:CA	1:58:A:PHE:C	1:59:A:PRO:N	13	3.71
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	8	3.69
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	11	3.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	3	3.65
(1,86)	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	1:77:A:VAL:N	14	3.64
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1	3.62
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	3	3.54
(1,67)	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1:25:A:GLN:N	13	3.52
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	15	3.48
(1,10)	1:14:A:LEU:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	9	3.48
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	11	3.47
(1,33)	1:74:A:HIS:C	1:75:A:VAL:N	1:75:A:VAL:CA	1:75:A:VAL:C	6	3.44
(1,67)	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1:25:A:GLN:N	8	3.42
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	4	3.41
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	7	3.41
(1,10)	1:14:A:LEU:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	13	3.41
(1,67)	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1:25:A:GLN:N	3	3.39
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	11	3.39
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	10	3.38
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	13	3.38
(1,39)	1:82:A:THR:C	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	9	3.37
(1,36)	1:78:A:LYS:C	1:79:A:ALA:N	1:79:A:ALA:CA	1:79:A:ALA:C	1	3.34
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	12	3.29
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	11	3.26
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	8	3.26
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	5	3.26
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	3	3.26
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	6	3.26
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	12	3.24
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	5	3.22
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	2	3.21
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	3	3.17
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	10	3.15
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	10	3.15
(1,50)	1:107:A:LEU:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	9	3.11
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	11	3.11
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	12	3.11
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	12	3.1
(1,33)	1:74:A:HIS:C	1:75:A:VAL:N	1:75:A:VAL:CA	1:75:A:VAL:C	11	3.1
(1,33)	1:74:A:HIS:C	1:75:A:VAL:N	1:75:A:VAL:CA	1:75:A:VAL:C	15	3.07
(1,13)	1:20:A:GLU:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	12	3.07
(1,54)	1:6:A:THR:N	1:6:A:THR:CA	1:6:A:THR:C	1:7:A:LYS:N	2	3.06
(1,100)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	9	3.05
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	2	3.05
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	5	3.04
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	9	3.02
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	2	3.01
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	8	3.01
(1,73)	1:51:A:PHE:N	1:51:A:PHE:CA	1:51:A:PHE:C	1:52:A:THR:N	5	2.97
(1,93)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:ASN:N	3	2.93
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	6	2.93
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	13	2.93
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	14	2.92
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	10	2.89

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	11	2.88
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	3	2.87
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	7	2.86
(1,29)	1:70:A:THR:C	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	3	2.86
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	14	2.85
(1,33)	1:74:A:HIS:C	1:75:A:VAL:N	1:75:A:VAL:CA	1:75:A:VAL:C	13	2.82
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	12	2.78
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	3	2.75
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	11	2.74
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	5	2.74
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	1	2.7
(1,32)	1:73:A:PHE:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	13	2.69
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	9	2.68
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	6	2.67
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	10	2.65
(1,13)	1:20:A:GLU:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1	2.64
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	9	2.62
(1,50)	1:107:A:LEU:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	15	2.62
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	14	2.61
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	5	2.6
(1,91)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ALA:N	9	2.58
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	15	2.58
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	7	2.58
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	4	2.57
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	1	2.57
(1,81)	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	1:72:A:HIS:N	7	2.56
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	11	2.56
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	8	2.54
(1,32)	1:73:A:PHE:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	2	2.53
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	8	2.52
(1,80)	1:58:A:PHE:N	1:58:A:PHE:CA	1:58:A:PHE:C	1:59:A:PRO:N	4	2.52
(1,67)	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1:25:A:GLN:N	5	2.52
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	15	2.5
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	6	2.5
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	4	2.5
(1,36)	1:78:A:LYS:C	1:79:A:ALA:N	1:79:A:ALA:CA	1:79:A:ALA:C	4	2.5
(1,91)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ALA:N	8	2.49
(1,67)	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1:25:A:GLN:N	14	2.49
(1,32)	1:73:A:PHE:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	11	2.48
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	2	2.47
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	3	2.46
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	9	2.45
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	5	2.45
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	12	2.4
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	10	2.38
(1,33)	1:74:A:HIS:C	1:75:A:VAL:N	1:75:A:VAL:CA	1:75:A:VAL:C	2	2.38
(1,39)	1:82:A:THR:C	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	2	2.36
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	2	2.36
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	4	2.36
(1,67)	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1:25:A:GLN:N	15	2.31
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	4	2.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	2	2.28
(1,88)	1:79:A:ALA:N	1:79:A:ALA:CA	1:79:A:ALA:C	1:80:A:ALA:N	12	2.27
(1,45)	1:102:A:ARG:C	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:C	7	2.25
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	2	2.25
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	12	2.25
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	13	2.24
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	11	2.23
(1,73)	1:51:A:PHE:N	1:51:A:PHE:CA	1:51:A:PHE:C	1:52:A:THR:N	3	2.23
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	1	2.22
(1,50)	1:107:A:LEU:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	12	2.22
(1,32)	1:73:A:PHE:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	9	2.21
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	10	2.2
(1,50)	1:107:A:LEU:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	14	2.19
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	7	2.18
(1,10)	1:14:A:LEU:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	3	2.16
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	1	2.15
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	6	2.14
(1,94)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:LEU:N	2	2.13
(1,94)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:LEU:N	4	2.11
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	9	2.11
(1,45)	1:102:A:ARG:C	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:C	3	2.1
(1,15)	1:22:A:VAL:C	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	4	2.09
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	7	2.08
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	13	2.07
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	4	2.05
(1,91)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ALA:N	10	2.04
(1,39)	1:82:A:THR:C	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	15	2.04
(1,39)	1:82:A:THR:C	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	5	2.03
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	15	2.03
(1,10)	1:14:A:LEU:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	12	2.03
(1,67)	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1:25:A:GLN:N	7	2.02
(1,67)	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1:25:A:GLN:N	12	2.02
(1,33)	1:74:A:HIS:C	1:75:A:VAL:N	1:75:A:VAL:CA	1:75:A:VAL:C	7	2.02
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	15	1.99
(1,15)	1:22:A:VAL:C	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	5	1.99
(1,80)	1:58:A:PHE:N	1:58:A:PHE:CA	1:58:A:PHE:C	1:59:A:PRO:N	5	1.98
(1,33)	1:74:A:HIS:C	1:75:A:VAL:N	1:75:A:VAL:CA	1:75:A:VAL:C	8	1.96
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	10	1.95
(1,13)	1:20:A:GLU:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	14	1.95
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	4	1.93
(1,67)	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1:25:A:GLN:N	1	1.93
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	10	1.93
(1,93)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:ASN:N	5	1.92
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	13	1.91
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	11	1.91
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1	1.9
(1,13)	1:20:A:GLU:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	8	1.89
(1,10)	1:14:A:LEU:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	15	1.89
(1,13)	1:20:A:GLU:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	13	1.88
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	15	1.85
(1,10)	1:14:A:LEU:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	10	1.85

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	8	1.84
(1,36)	1:78:A:LYS:C	1:79:A:ALA:N	1:79:A:ALA:CA	1:79:A:ALA:C	7	1.84
(1,40)	1:83:A:HIS:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	9	1.79
(1,36)	1:78:A:LYS:C	1:79:A:ALA:N	1:79:A:ALA:CA	1:79:A:ALA:C	10	1.79
(1,2)	1:4:A:LYS:C	1:5:A:VAL:N	1:5:A:VAL:CA	1:5:A:VAL:C	10	1.78
(1,86)	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	1:77:A:VAL:N	15	1.77
(1,81)	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	1:72:A:HIS:N	14	1.77
(1,25)	1:54:A:GLU:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	10	1.77
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	6	1.76
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	6	1.75
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	15	1.75
(1,94)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:LEU:N	5	1.74
(1,94)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:LEU:N	8	1.74
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	5	1.73
(1,50)	1:107:A:LEU:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	4	1.73
(1,50)	1:107:A:LEU:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	13	1.73
(1,94)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:LEU:N	11	1.71
(1,10)	1:14:A:LEU:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	6	1.71
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	7	1.69
(1,33)	1:74:A:HIS:C	1:75:A:VAL:N	1:75:A:VAL:CA	1:75:A:VAL:C	12	1.69
(1,100)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	12	1.66
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	9	1.66
(1,15)	1:22:A:VAL:C	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	10	1.66
(1,32)	1:73:A:PHE:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	4	1.65
(1,93)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:ASN:N	2	1.64
(1,45)	1:102:A:ARG:C	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:C	1	1.64
(1,41)	1:84:A:ALA:C	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1	1.64
(1,13)	1:20:A:GLU:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	11	1.64
(1,9)	1:13:A:THR:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	14	1.64
(1,94)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:LEU:N	3	1.63
(1,67)	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1:25:A:GLN:N	6	1.62
(1,39)	1:82:A:THR:C	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1	1.62
(1,94)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:LEU:N	1	1.59
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	7	1.58
(1,38)	1:81:A:GLY:C	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	1	1.57
(1,100)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	15	1.56
(1,10)	1:14:A:LEU:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	4	1.56
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	4	1.55
(1,39)	1:82:A:THR:C	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	6	1.55
(1,33)	1:74:A:HIS:C	1:75:A:VAL:N	1:75:A:VAL:CA	1:75:A:VAL:C	10	1.55
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	12	1.53
(1,51)	1:108:A:LYS:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	1	1.53
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	7	1.52
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	14	1.52
(1,50)	1:107:A:LEU:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	6	1.52
(1,100)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	1	1.51
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	11	1.5
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	2	1.5
(1,48)	1:105:A:VAL:C	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	15	1.5
(1,39)	1:82:A:THR:C	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	14	1.5
(1,94)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:LEU:N	12	1.49

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,29)	1:70:A:THR:C	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	5	1.49
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	9	1.48
(1,32)	1:73:A:PHE:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	12	1.47
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	5	1.46
(1,86)	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	1:77:A:VAL:N	9	1.46
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	7	1.46
(1,44)	1:87:A:LEU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	7	1.46
(1,32)	1:73:A:PHE:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	14	1.46
(1,13)	1:20:A:GLU:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	5	1.46
(1,10)	1:14:A:LEU:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	2	1.46
(1,81)	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	1:72:A:HIS:N	11	1.44
(1,81)	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	1:72:A:HIS:N	13	1.41
(1,59)	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	1:14:A:LEU:N	8	1.41
(1,94)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:LEU:N	14	1.4
(1,32)	1:73:A:PHE:C	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	15	1.4
(1,15)	1:22:A:VAL:C	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	12	1.4
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	8	1.39
(1,86)	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	1:77:A:VAL:N	13	1.39
(1,91)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ALA:N	6	1.36
(1,87)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ALA:N	3	1.35
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	3	1.35
(1,47)	1:104:A:THR:C	1:105:A:VAL:N	1:105:A:VAL:CA	1:105:A:VAL:C	8	1.34
(1,92)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:VAL:N	9	1.3
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	1	1.3
(1,36)	1:78:A:LYS:C	1:79:A:ALA:N	1:79:A:ALA:CA	1:79:A:ALA:C	8	1.3
(1,94)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:LEU:N	13	1.29
(1,86)	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	1:77:A:VAL:N	10	1.29
(1,80)	1:58:A:PHE:N	1:58:A:PHE:CA	1:58:A:PHE:C	1:59:A:PRO:N	1	1.29
(1,93)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:ASN:N	14	1.28
(1,84)	1:74:A:HIS:N	1:74:A:HIS:CA	1:74:A:HIS:C	1:75:A:VAL:N	3	1.28
(1,47)	1:104:A:THR:C	1:105:A:VAL:N	1:105:A:VAL:CA	1:105:A:VAL:C	11	1.28
(1,60)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	6	1.27
(1,86)	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	1:77:A:VAL:N	5	1.26
(1,45)	1:102:A:ARG:C	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:C	11	1.25
(1,33)	1:74:A:HIS:C	1:75:A:VAL:N	1:75:A:VAL:CA	1:75:A:VAL:C	1	1.25
(1,94)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:LEU:N	9	1.24
(1,59)	1:13:A:THR:N	1:13:A:THR:CA	1:13:A:THR:C	1:14:A:LEU:N	10	1.24
(1,50)	1:107:A:LEU:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	11	1.24
(1,45)	1:102:A:ARG:C	1:103:A:PHE:N	1:103:A:PHE:CA	1:103:A:PHE:C	14	1.24
(1,25)	1:54:A:GLU:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	12	1.23
(1,36)	1:78:A:LYS:C	1:79:A:ALA:N	1:79:A:ALA:CA	1:79:A:ALA:C	11	1.21
(1,94)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:LEU:N	6	1.2
(1,67)	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1:25:A:GLN:N	2	1.2
(1,15)	1:22:A:VAL:C	1:23:A:GLU:N	1:23:A:GLU:CA	1:23:A:GLU:C	9	1.2
(1,86)	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	1:77:A:VAL:N	3	1.19
(1,73)	1:51:A:PHE:N	1:51:A:PHE:CA	1:51:A:PHE:C	1:52:A:THR:N	9	1.19
(1,47)	1:104:A:THR:C	1:105:A:VAL:N	1:105:A:VAL:CA	1:105:A:VAL:C	14	1.19
(1,91)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ALA:N	14	1.18
(1,34)	1:75:A:VAL:C	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	9	1.18
(1,93)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:ASN:N	1	1.17
(1,91)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ALA:N	3	1.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,43)	1:86:A:ASN:C	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	8	1.17
(1,98)	1:104:A:THR:N	1:104:A:THR:CA	1:104:A:THR:C	1:105:A:VAL:N	9	1.16
(1,89)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:THR:N	13	1.16
(1,39)	1:82:A:THR:C	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	13	1.16
(1,88)	1:79:A:ALA:N	1:79:A:ALA:CA	1:79:A:ALA:C	1:80:A:ALA:N	7	1.15
(1,78)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:TYR:N	14	1.13
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:VAL:N	15	1.13
(1,93)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:ASN:N	8	1.12
(1,13)	1:20:A:GLU:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	4	1.12
(1,57)	1:9:A:HIS:N	1:9:A:HIS:CA	1:9:A:HIS:C	1:10:A:ASN:N	12	1.1
(1,48)	1:105:A:VAL:C	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	6	1.1
(1,25)	1:54:A:GLU:C	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	2	1.1
(1,78)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:TYR:N	8	1.09
(1,33)	1:74:A:HIS:C	1:75:A:VAL:N	1:75:A:VAL:CA	1:75:A:VAL:C	9	1.09
(1,93)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:ASN:N	13	1.07
(1,48)	1:105:A:VAL:C	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	9	1.06
(1,13)	1:20:A:GLU:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	7	1.05
(1,41)	1:84:A:ALA:C	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	11	1.04
(1,39)	1:82:A:THR:C	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	10	1.04
(1,86)	1:76:A:THR:N	1:76:A:THR:CA	1:76:A:THR:C	1:77:A:VAL:N	6	1.02
(1,29)	1:70:A:THR:C	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	11	1.02
(1,50)	1:107:A:LEU:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	2	1.01
(1,23)	1:52:A:THR:C	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	8	1.01