



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 01:23 AM UTC

PDB ID : 2L75 / pdb_00002l75
BMRB ID : 17344
Title : Solution structure of CHD4-PHD2 in complex with H3K9me3
Authors : Mansfield, R.E.; Kwan, A.H.; Mackay, J.P.
Deposited on : 2010-12-02

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

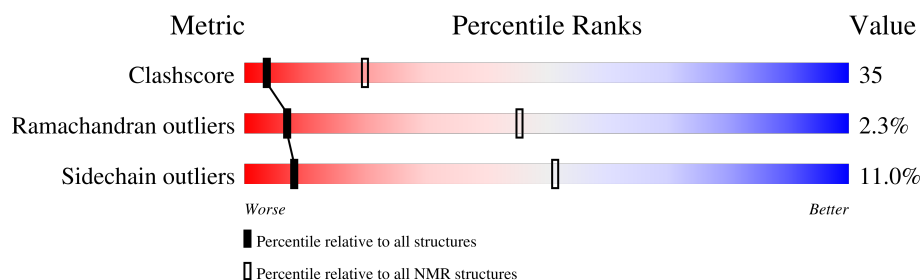
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	61	
2	B	14	

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:89-A:135, B:145-B:151 (54)	0.39	8

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

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

The models can be grouped into 5 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1033 atoms, of which 510 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Chromodomain-helicase-DNA-binding protein 4.

Mol	Chain	Residues	Atoms						Trace
1	A	56	Total	C	H	N	O	S	0
			838	268	406	76	78	10	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	GLY	-	expression tag	UNP Q14839
A	83	PRO	-	expression tag	UNP Q14839
A	84	LEU	-	expression tag	UNP Q14839
A	85	GLY	-	expression tag	UNP Q14839
A	86	SER	-	expression tag	UNP Q14839

- Molecule 2 is a protein called 14-meric peptide from 1Histone H3.1.

Mol	Chain	Residues	Atoms					Trace
2	B	11	Total	C	H	N	O	0
			193	53	104	20	16	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	157	TYR	-	SEE REMARK 999	UNP P68431

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

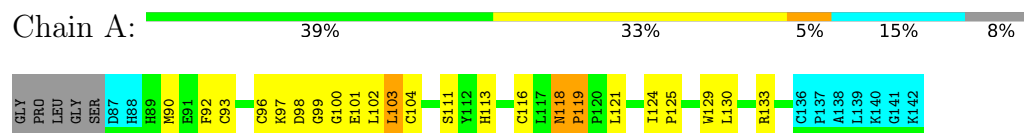
Mol	Chain	Residues	Atoms	
3	A	2	Total	Zn
			2	2

4 Residue-property plots [i](#)

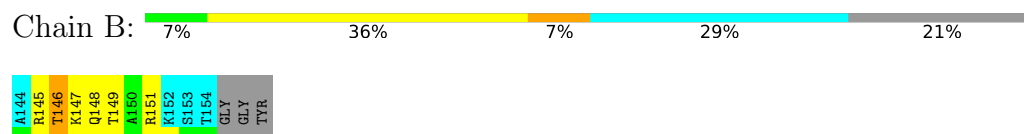
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



- Molecule 2: 14-meric peptide from 1Histone H3.1

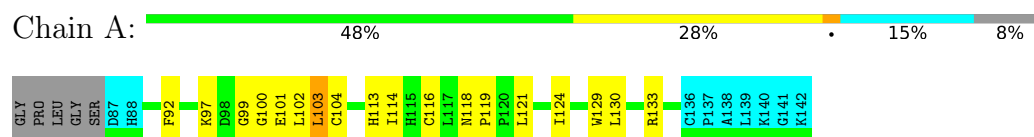


4.2 Scores per residue for each member of the ensemble

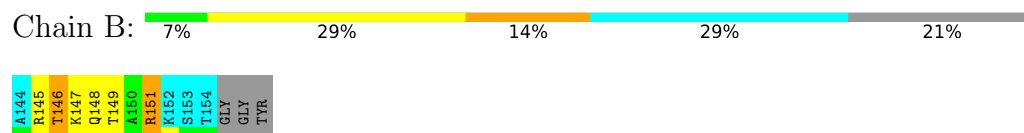
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

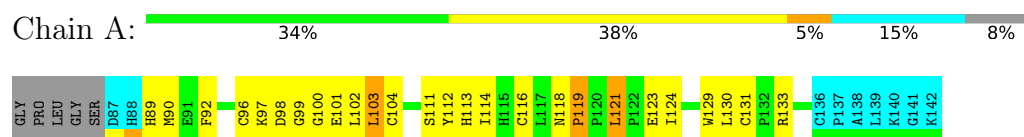


- Molecule 2: 14-meric peptide from 1Histone H3.1

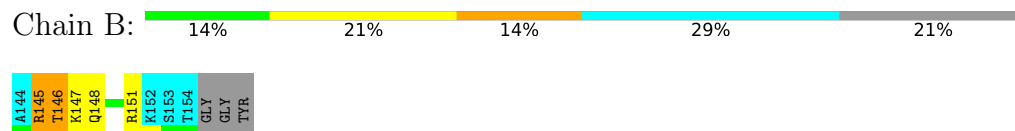


4.2.2 Score per residue for model 2

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

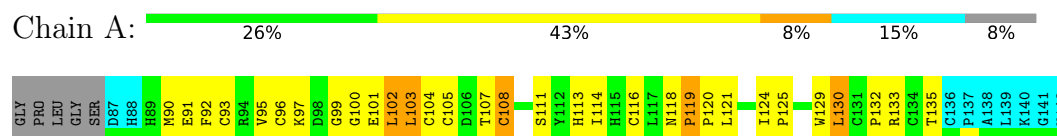


- Molecule 2: 14-meric peptide from 1Histone H3.1

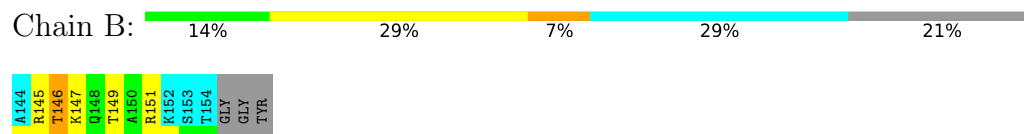


4.2.3 Score per residue for model 3

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

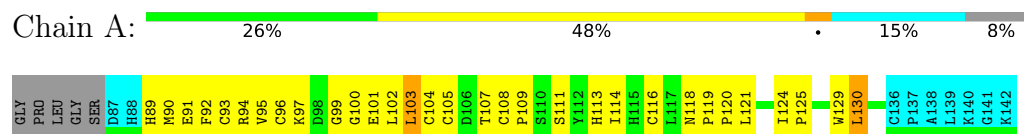


- Molecule 2: 14-meric peptide from 1Histone H3.1

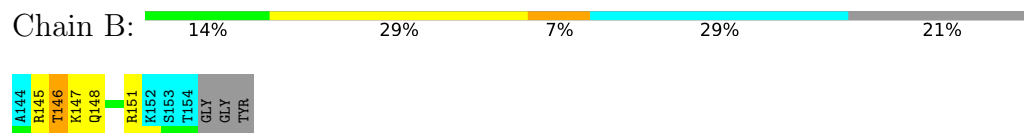


4.2.4 Score per residue for model 4

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

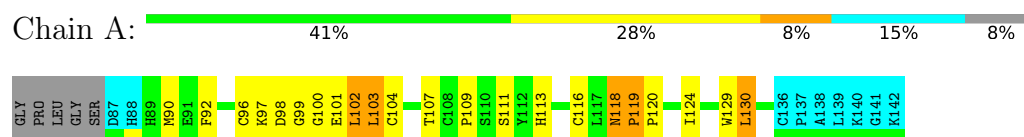


- Molecule 2: 14-meric peptide from 1Histone H3.1

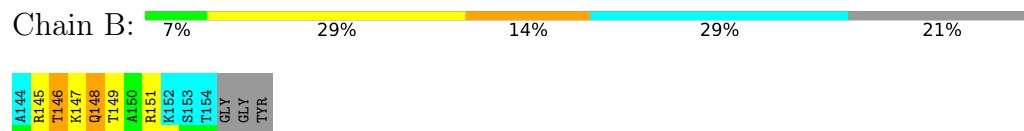


4.2.5 Score per residue for model 5

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

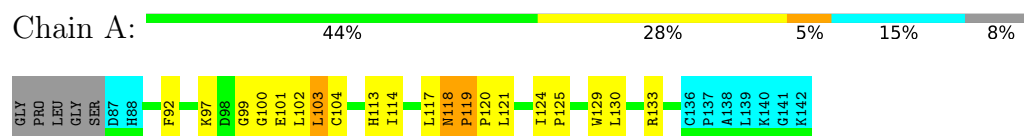


- Molecule 2: 14-meric peptide from 1Histone H3.1

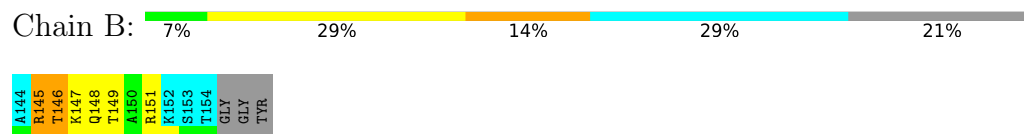


4.2.6 Score per residue for model 6

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



- Molecule 2: 14-meric peptide from 1Histone H3.1

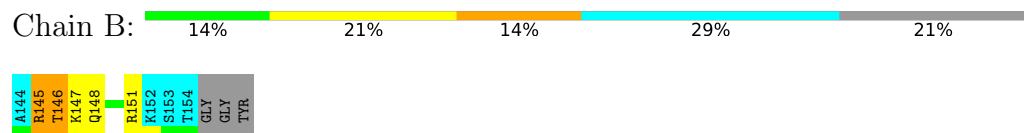


4.2.7 Score per residue for model 7

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

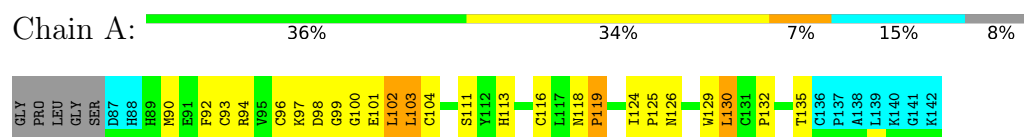


- Molecule 2: 14-meric peptide from 1Histone H3.1

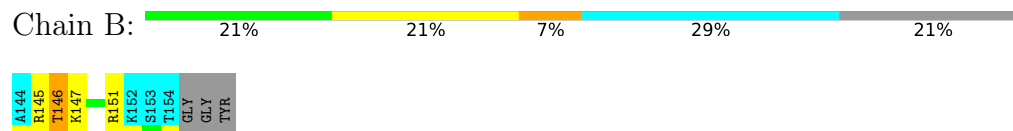


4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

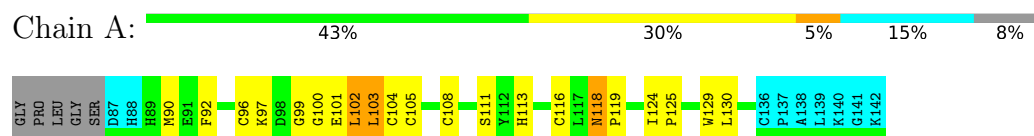


- Molecule 2: 14-meric peptide from 1Histone H3.1

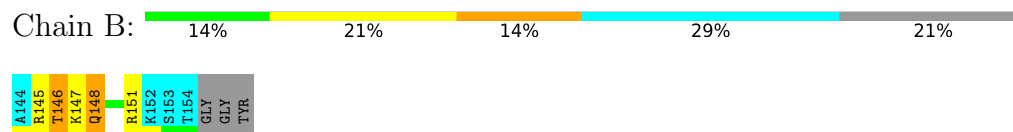


4.2.9 Score per residue for model 9

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

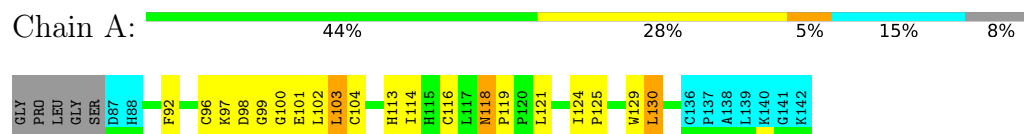


- Molecule 2: 14-meric peptide from 1Histone H3.1

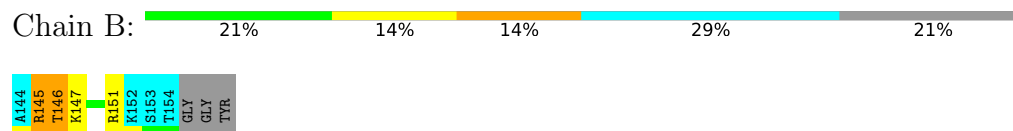


4.2.10 Score per residue for model 10

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

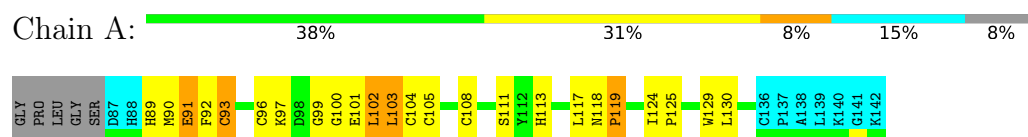


- Molecule 2: 14-meric peptide from 1Histone H3.1

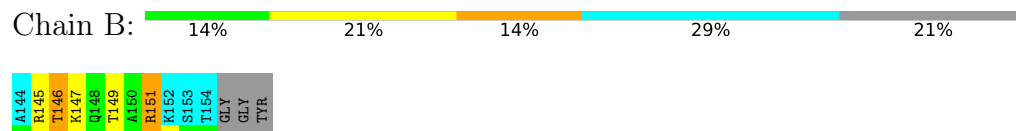


4.2.11 Score per residue for model 11

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

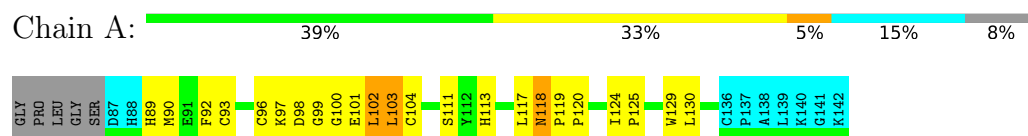


- Molecule 2: 14-meric peptide from 1Histone H3.1

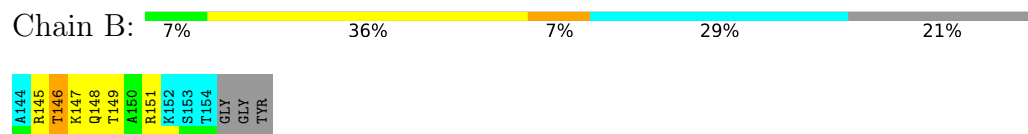


4.2.12 Score per residue for model 12

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

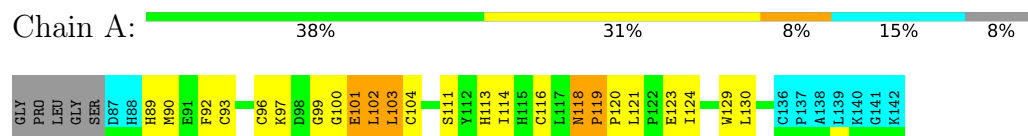


- Molecule 2: 14-meric peptide from 1Histone H3.1

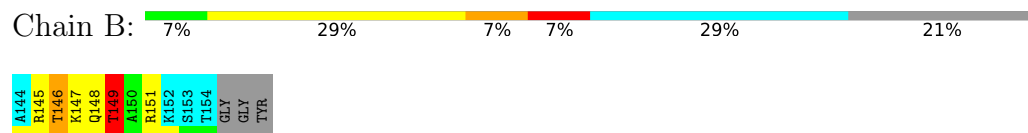


4.2.13 Score per residue for model 13

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

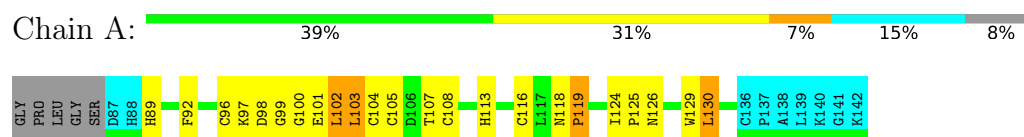


- Molecule 2: 14-meric peptide from 1Histone H3.1

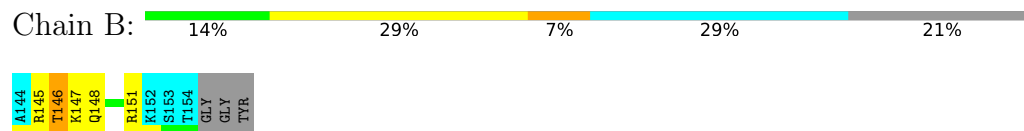


4.2.14 Score per residue for model 14

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

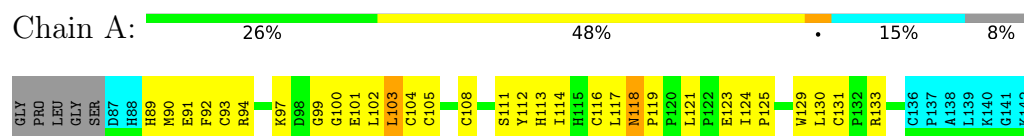


- Molecule 2: 14-meric peptide from 1Histone H3.1

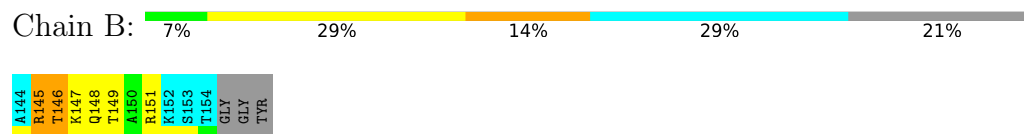


4.2.15 Score per residue for model 15

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

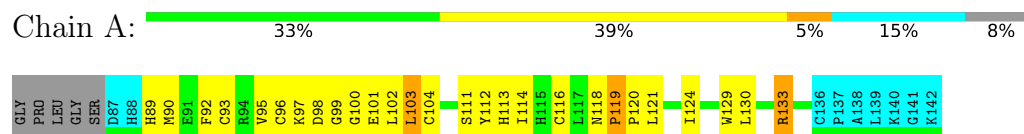


- Molecule 2: 14-meric peptide from 1Histone H3.1

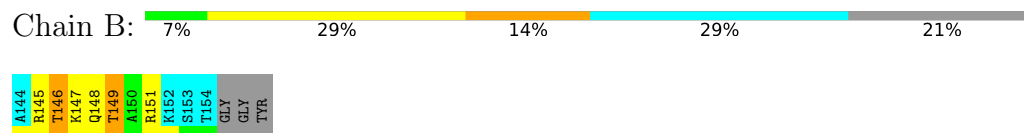


4.2.16 Score per residue for model 16

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

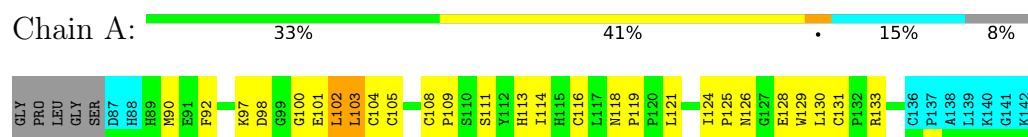


- Molecule 2: 14-meric peptide from 1Histone H3.1

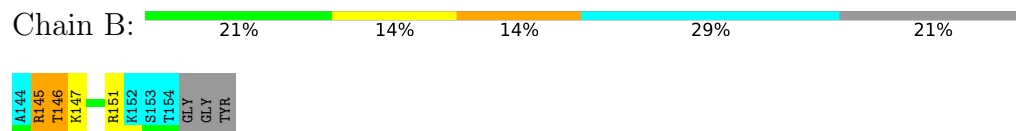


4.2.17 Score per residue for model 17

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

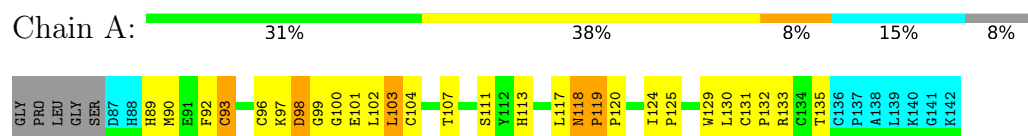


- Molecule 2: 14-meric peptide from 1Histone H3.1

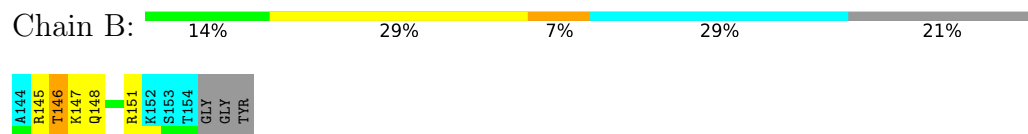


4.2.18 Score per residue for model 18

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

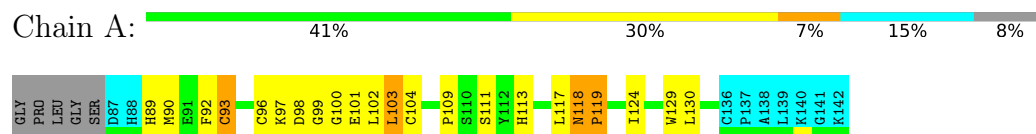


- Molecule 2: 14-meric peptide from 1Histone H3.1

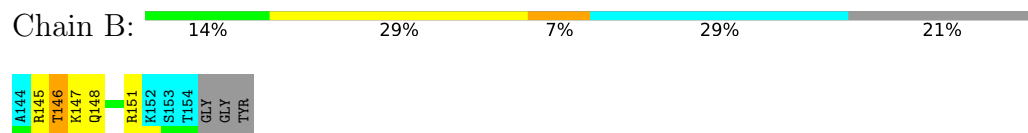


4.2.19 Score per residue for model 19

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4

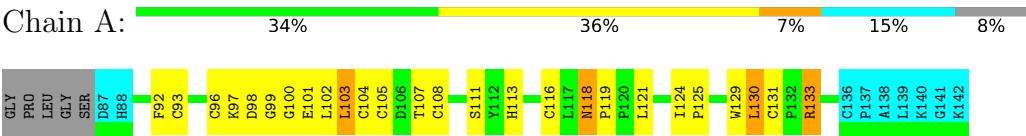


- Molecule 2: 14-meric peptide from 1Histone H3.1

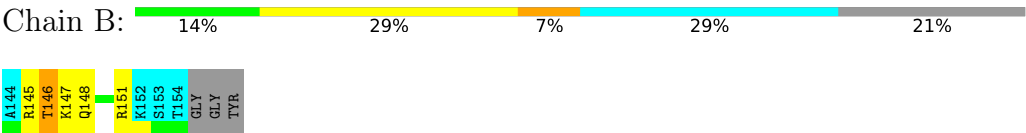


4.2.20 Score per residue for model 20

- Molecule 1: Chromodomain-helicase-DNA-binding protein 4



- Molecule 2: 14-meric peptide from 1Histone H3.1



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	
ARIA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	793
Number of shifts mapped to atoms	741
Number of unparsed shifts	0
Number of shifts with mapping errors	52
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M3L

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	365	337	335	28±4
2	B	59	66	66	13±2
All	All	8520	8060	8020	576

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:CYS:HB2	2:B:145:ARG:HB2	1.01	1.32	3	1
1:A:104:CYS:HB3	2:B:145:ARG:HB3	0.96	1.37	17	13
1:A:118:ASN:HB3	1:A:119:PRO:HD2	0.90	1.42	14	1
1:A:100:GLY:HA2	2:B:151:ARG:HD2	0.89	1.41	12	15
1:A:104:CYS:HB2	2:B:145:ARG:HB3	0.83	1.47	18	5
1:A:101:GLU:HA	2:B:147:LYS:O	0.81	1.76	14	20
2:B:151:ARG:HD3	2:B:151:ARG:H	0.78	1.38	5	18
1:A:99:GLY:H	2:B:151:ARG:HA	0.75	1.40	19	19
1:A:118:ASN:HB2	1:A:119:PRO:HD3	0.74	1.60	3	17
1:A:104:CYS:HB3	2:B:145:ARG:HB2	0.74	1.57	13	1
1:A:104:CYS:SG	2:B:147:LYS:HG3	0.71	2.25	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:HIS:HE1	2:B:147:LYS:HG3	0.70	1.46	12	1
1:A:98:ASP:HB3	2:B:151:ARG:HB2	0.69	1.63	20	2
1:A:90:MET:HB2	1:A:111:SER:HB2	0.69	1.62	17	2
1:A:118:ASN:HB2	1:A:119:PRO:HD2	0.68	1.65	7	1
1:A:103:LEU:HD13	1:A:124:ILE:HG23	0.68	1.66	5	18
1:A:96:CYS:HB2	1:A:98:ASP:OD1	0.67	1.89	16	1
1:A:113:HIS:HB2	1:A:116:CYS:SG	0.67	2.29	15	15
1:A:98:ASP:OD2	2:B:151:ARG:HB2	0.66	1.91	7	1
1:A:102:LEU:O	2:B:146:THR:HA	0.65	1.90	8	19
1:A:92:PHE:HA	1:A:99:GLY:HA2	0.65	1.67	12	18
1:A:99:GLY:N	2:B:151:ARG:HA	0.65	2.07	19	19
1:A:124:ILE:HG13	2:B:146:THR:HG21	0.65	1.67	3	8
1:A:114:ILE:HB	1:A:121:LEU:HB2	0.64	1.70	2	9
1:A:90:MET:HB2	1:A:111:SER:OG	0.63	1.94	8	8
1:A:101:GLU:HG2	2:B:146:THR:HB	0.62	1.69	6	1
1:A:90:MET:HB2	1:A:111:SER:CB	0.62	2.24	17	2
1:A:100:GLY:HA2	2:B:151:ARG:HB2	0.60	1.73	17	1
1:A:104:CYS:CB	2:B:145:ARG:HB3	0.60	2.24	9	1
1:A:89:HIS:CE1	2:B:147:LYS:HG3	0.59	2.32	12	1
1:A:103:LEU:HG	1:A:129:TRP:CE3	0.59	2.33	10	20
1:A:102:LEU:HB3	1:A:111:SER:HB2	0.59	1.73	8	4
2:B:147:LYS:O	2:B:148:GLN:HG2	0.59	1.98	9	4
1:A:124:ILE:CD1	2:B:146:THR:HG21	0.58	2.28	15	20
1:A:93:CYS:HA	1:A:111:SER:O	0.58	1.99	19	9
1:A:100:GLY:N	2:B:151:ARG:HB3	0.57	2.14	10	18
1:A:118:ASN:CG	1:A:119:PRO:HD3	0.57	2.24	8	1
1:A:113:HIS:O	1:A:117:LEU:HG	0.56	1.99	19	5
1:A:101:GLU:HB2	2:B:148:GLN:HE21	0.56	1.60	7	7
1:A:124:ILE:HD12	2:B:146:THR:HG21	0.56	1.78	15	7
1:A:92:PHE:CD1	1:A:97:LYS:HA	0.55	2.36	10	3
1:A:103:LEU:HG	1:A:129:TRP:CD2	0.55	2.36	11	20
1:A:100:GLY:CA	2:B:151:ARG:HB3	0.54	2.32	4	17
1:A:96:CYS:SG	1:A:98:ASP:HB2	0.54	2.43	18	2
1:A:99:GLY:HA3	2:B:149:THR:HG23	0.54	1.80	6	4
1:A:103:LEU:HD11	1:A:125:PRO:HD2	0.54	1.80	20	8
1:A:103:LEU:HD12	2:B:145:ARG:O	0.53	2.03	17	8
1:A:102:LEU:CB	1:A:111:SER:HB2	0.53	2.34	8	1
1:A:124:ILE:CG1	2:B:146:THR:HG21	0.52	2.34	3	6
1:A:118:ASN:HB3	1:A:119:PRO:CD	0.52	2.28	14	1
1:A:100:GLY:O	1:A:102:LEU:HG	0.52	2.04	4	9
1:A:96:CYS:HB2	1:A:98:ASP:HB2	0.52	1.82	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:MET:O	1:A:91:GLU:HG2	0.52	2.04	4	2
1:A:115:HIS:HA	1:A:120:PRO:HB3	0.52	1.82	7	1
1:A:114:ILE:CD1	1:A:123:GLU:HA	0.52	2.35	15	1
1:A:131:CYS:SG	1:A:133:ARG:HB3	0.51	2.45	15	2
1:A:92:PHE:CD2	1:A:97:LYS:HA	0.51	2.41	1	5
1:A:107:THR:HG22	1:A:130:LEU:CD1	0.51	2.35	3	1
1:A:118:ASN:O	1:A:120:PRO:HD3	0.51	2.06	18	7
1:A:102:LEU:HG	1:A:111:SER:HB2	0.50	1.82	11	3
1:A:102:LEU:HG	1:A:111:SER:HB3	0.50	1.83	5	1
1:A:92:PHE:CE2	1:A:97:LYS:HE3	0.50	2.41	13	1
1:A:96:CYS:CB	1:A:98:ASP:HB2	0.50	2.36	7	1
1:A:114:ILE:HD12	1:A:123:GLU:HA	0.50	1.83	15	1
1:A:102:LEU:HB3	1:A:111:SER:HB3	0.49	1.83	17	2
1:A:89:HIS:HB3	1:A:109:PRO:HA	0.49	1.85	19	1
1:A:118:ASN:CB	1:A:119:PRO:HD3	0.49	2.37	5	8
1:A:129:TRP:C	1:A:130:LEU:HG	0.49	2.32	18	1
1:A:105:CYS:HB3	1:A:108:CYS:O	0.49	2.07	20	9
1:A:96:CYS:HB3	1:A:98:ASP:OD1	0.48	2.07	20	3
1:A:89:HIS:HB3	1:A:111:SER:OG	0.48	2.07	4	2
1:A:103:LEU:CD1	1:A:124:ILE:HG23	0.48	2.37	3	10
1:A:96:CYS:HB3	1:A:98:ASP:OD2	0.48	2.08	5	1
1:A:102:LEU:HA	1:A:112:TYR:O	0.48	2.08	16	4
1:A:114:ILE:HD13	1:A:124:ILE:HD13	0.47	1.86	13	1
1:A:118:ASN:O	1:A:119:PRO:C	0.47	2.58	7	2
1:A:132:PRO:HG2	1:A:133:ARG:HH11	0.47	1.69	3	1
1:A:91:GLU:HG3	1:A:92:PHE:HD1	0.47	1.70	3	1
1:A:91:GLU:HG2	1:A:92:PHE:CD2	0.47	2.44	11	1
1:A:90:MET:SD	1:A:94:ARG:HB2	0.47	2.50	4	3
1:A:102:LEU:CB	1:A:111:SER:HB3	0.47	2.39	5	2
1:A:92:PHE:HD1	1:A:97:LYS:HA	0.47	1.68	10	1
1:A:107:THR:HG22	1:A:130:LEU:HD12	0.47	1.86	3	1
1:A:102:LEU:HD22	2:B:147:LYS:HB2	0.46	1.86	9	1
1:A:133:ARG:NE	1:A:133:ARG:HA	0.46	2.26	6	1
1:A:132:PRO:HA	1:A:135:THR:OG1	0.46	2.11	3	3
1:A:90:MET:HG3	1:A:109:PRO:O	0.46	2.10	17	3
1:A:131:CYS:SG	1:A:133:ARG:HB2	0.46	2.49	18	3
1:A:99:GLY:CA	2:B:149:THR:HG23	0.46	2.41	16	1
1:A:90:MET:O	2:B:147:LYS:HE2	0.46	2.11	3	2
2:B:151:ARG:HD3	2:B:151:ARG:N	0.46	2.19	5	4
1:A:98:ASP:HB3	1:A:113:HIS:CE1	0.45	2.46	7	1
1:A:114:ILE:O	1:A:120:PRO:HA	0.45	2.12	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:ASN:HD22	1:A:118:ASN:N	0.45	2.10	13	3
1:A:93:CYS:O	1:A:97:LYS:N	0.45	2.44	13	1
1:A:101:GLU:HB2	2:B:148:GLN:NE2	0.44	2.27	16	1
1:A:125:PRO:HG2	1:A:129:TRP:CD1	0.44	2.47	17	5
1:A:104:CYS:SG	2:B:145:ARG:HD3	0.44	2.53	17	2
1:A:92:PHE:HB2	1:A:97:LYS:C	0.44	2.38	13	4
1:A:92:PHE:HD2	1:A:97:LYS:HA	0.44	1.70	1	2
1:A:93:CYS:HB2	1:A:102:LEU:HD12	0.44	1.88	12	1
1:A:94:ARG:HD3	1:A:112:TYR:OH	0.44	2.13	15	1
1:A:133:ARG:HA	1:A:133:ARG:HE	0.43	1.74	16	1
1:A:107:THR:HG23	1:A:130:LEU:HD21	0.43	1.90	18	1
1:A:89:HIS:HB2	2:B:147:LYS:HD2	0.42	1.91	2	1
1:A:93:CYS:SG	1:A:95:VAL:HB	0.42	2.54	3	3
1:A:107:THR:HG23	1:A:130:LEU:HD11	0.42	1.91	14	5
1:A:103:LEU:HD22	1:A:114:ILE:HG22	0.42	1.92	13	2
1:A:121:LEU:HB3	1:A:123:GLU:O	0.42	2.14	2	1
1:A:89:HIS:CD2	1:A:104:CYS:HA	0.42	2.50	11	2
1:A:100:GLY:O	2:B:148:GLN:HA	0.42	2.14	5	4
1:A:104:CYS:HB3	2:B:145:ARG:CB	0.42	2.45	10	2
1:A:98:ASP:HB2	2:B:151:ARG:HA	0.42	1.91	16	1
1:A:129:TRP:O	1:A:130:LEU:HD13	0.41	2.14	3	3
1:A:101:GLU:CG	2:B:146:THR:HB	0.41	2.43	6	1
1:A:118:ASN:N	1:A:118:ASN:HD22	0.41	2.13	10	2
1:A:133:ARG:HA	1:A:133:ARG:NE	0.41	2.30	1	1
1:A:117:LEU:HD12	1:A:121:LEU:HD12	0.41	1.91	15	1
1:A:101:GLU:HG2	2:B:146:THR:CB	0.41	2.44	6	1
1:A:118:ASN:CB	1:A:119:PRO:HD2	0.41	2.28	14	1
1:A:91:GLU:H	1:A:91:GLU:CD	0.41	2.24	11	1
1:A:100:GLY:HA3	1:A:113:HIS:HE2	0.40	1.76	11	1
1:A:101:GLU:HA	2:B:147:LYS:C	0.40	2.41	9	1
1:A:100:GLY:HA2	2:B:151:ARG:HB3	0.40	1.94	4	1
1:A:96:CYS:O	1:A:97:LYS:HB2	0.40	2.16	11	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	47/61 (77%)	41±1 (86±3%)	6±2 (12±4%)	1±1 (1±1%)	11	57
2	B	7/14 (50%)	4±1 (60±14%)	2±1 (32±13%)	1±1 (8±10%)	1	14
All	All	1080/1500 (72%)	897 (83%)	158 (15%)	25 (2%)	7	45

All 6 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	119	PRO	12
2	B	145	ARG	6
2	B	148	GLN	3
2	B	149	THR	2
1	A	89	HIS	1
1	A	128	GLU	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	44/54 (81%)	40±1 (91±2%)	4±1 (9±2%)	11	56
2	B	6/9 (67%)	5±1 (77±11%)	1±1 (23±11%)	2	27
All	All	1000/1260 (79%)	890 (89%)	110 (11%)	8	51

All 17 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	103	LEU	20
2	B	146	THR	20
1	A	130	LEU	19
1	A	118	ASN	10
1	A	102	LEU	9
2	B	149	THR	6
1	A	121	LEU	4
1	A	98	ASP	4
1	A	89	HIS	4
1	A	126	ASN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	93	CYS	3
2	B	151	ARG	2
1	A	133	ARG	2
1	A	108	CYS	1
1	A	91	GLU	1
1	A	101	GLU	1
1	A	123	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	M3L	B	152	2	10,11,12	0.69±0.03	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	M3L	B	152	2	9,14,16	0.45±0.05	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M3L	B	152	2	-	0±0,9,10,12	-

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 85% for the well-defined parts and 84% 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	793
Number of shifts mapped to atoms	741
Number of unparsed shifts	0
Number of shifts with mapping errors	52
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- No matching atom found in the structure. All 52 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	82	GLY	HA2	3.97	0.005	2
1	A	82	GLY	HA3	3.981	0.005	2
1	A	82	GLY	CA	43.506	0.000	1
1	A	83	PRO	HA	4.48	0.002	1
1	A	83	PRO	HB2	2.304	0.006	2
1	A	83	PRO	HB3	1.945	0.002	2
1	A	83	PRO	HD2	3.57	0.006	2
1	A	83	PRO	HD3	3.57	0.006	2
1	A	83	PRO	HG2	1.989	0.018	2
1	A	83	PRO	HG3	1.989	0.018	2
1	A	83	PRO	C	176.981	0.000	1
1	A	83	PRO	CA	63.144	0.043	1
1	A	83	PRO	CB	32.339	0.020	1
1	A	83	PRO	CD	49.579	0.062	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	83	PRO	CG	27.105	0.048	1
1	A	84	LEU	H	8.507	0.005	1
1	A	84	LEU	HA	4.372	0.004	1
1	A	84	LEU	HB2	1.665	0.003	2
1	A	84	LEU	HB3	1.572	0.004	2
1	A	84	LEU	HD11	0.886	0.012	.
1	A	84	LEU	HD12	0.886	0.012	.
1	A	84	LEU	HD13	0.886	0.012	.
1	A	84	LEU	HD21	0.844	0.004	.
1	A	84	LEU	HD22	0.844	0.004	.
1	A	84	LEU	HD23	0.844	0.004	.
1	A	84	LEU	HG	1.642	0.011	1
1	A	84	LEU	C	177.939	0.000	1
1	A	84	LEU	CA	55.206	0.062	1
1	A	84	LEU	CB	42.459	0.003	1
1	A	84	LEU	CD1	24.855	0.014	2
1	A	84	LEU	CD2	23.461	0.039	2
1	A	84	LEU	CG	27.042	0.053	1
1	A	84	LEU	N	122.453	0.037	1
1	A	85	GLY	H	8.42	0.002	1
1	A	85	GLY	HA2	4.018	0.002	2
1	A	85	GLY	HA3	4.018	0.002	2
1	A	85	GLY	CA	45.177	0.087	1
1	A	85	GLY	N	110.001	0.046	1
1	A	86	SER	H	8.333	0.005	1
1	A	86	SER	HA	4.465	0.022	1
1	A	86	SER	HB2	3.83	0.010	2
1	A	86	SER	HB3	3.745	0.012	2
1	A	86	SER	CA	58.42	0.130	1
1	A	86	SER	CB	63.913	0.094	1
1	A	86	SER	N	116.008	0.051	1
1	B	156	GLY	H	8.175	0.002	1
1	B	156	GLY	HA2	3.857	0.002	2
1	B	156	GLY	HA3	3.857	0.002	2
1	B	157	TYR	H	7.574	0.001	1
1	B	157	TYR	HA	4.379	0.003	1
1	B	157	TYR	HB2	3.056	0.001	2
1	B	157	TYR	HB3	2.843	0.004	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	61	-0.11 ± 0.40	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	54	-0.31 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	54	0.24 ± 0.27	None needed (< 0.5 ppm)
^{15}N	51	-0.73 ± 0.38	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 85%, i.e. 608 atoms were assigned a chemical shift out of a possible 715. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	237/261 (91%)	104/105 (99%)	92/108 (85%)	41/48 (85%)
Sidechain	332/399 (83%)	236/258 (91%)	94/124 (76%)	2/17 (12%)
Aromatic	39/55 (71%)	20/27 (74%)	13/21 (62%)	6/7 (86%)
Overall	608/715 (85%)	360/390 (92%)	199/253 (79%)	49/72 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 722 atoms were assigned a chemical shift out of a possible 857. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	282/320 (88%)	126/129 (98%)	108/132 (82%)	48/59 (81%)
Sidechain	397/474 (84%)	283/307 (92%)	112/148 (76%)	2/19 (11%)
Aromatic	43/63 (68%)	22/31 (71%)	13/23 (57%)	8/9 (89%)
Overall	722/857 (84%)	431/467 (92%)	233/303 (77%)	58/87 (67%)

7.1.4 Statistically unusual chemical shifts [i](#)

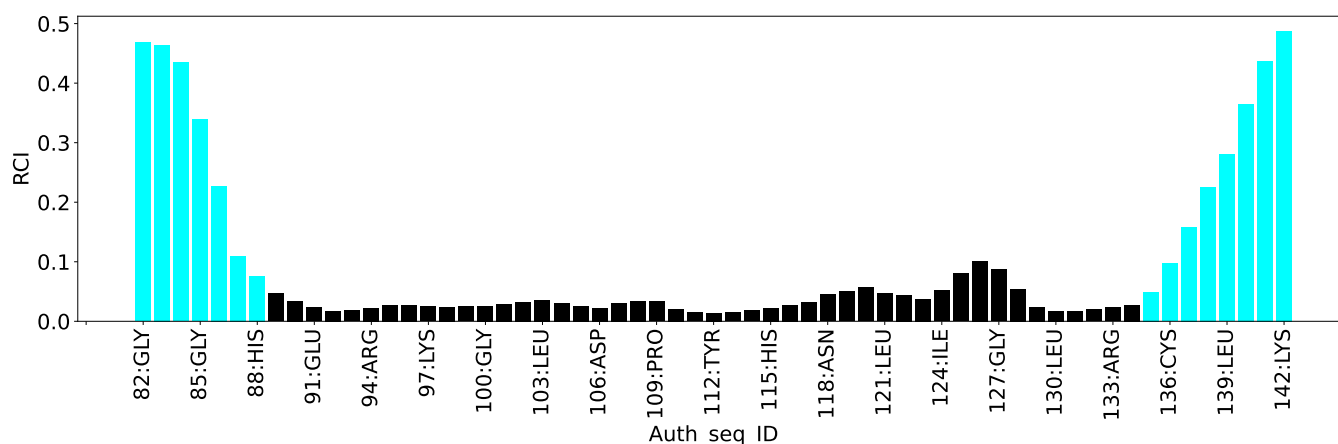
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	103	LEU	HD11	-0.78	-0.61 – 2.12	-5.6
1	A	103	LEU	HD12	-0.78	-0.61 – 2.12	-5.6
1	A	103	LEU	HD13	-0.78	-0.61 – 2.12	-5.6

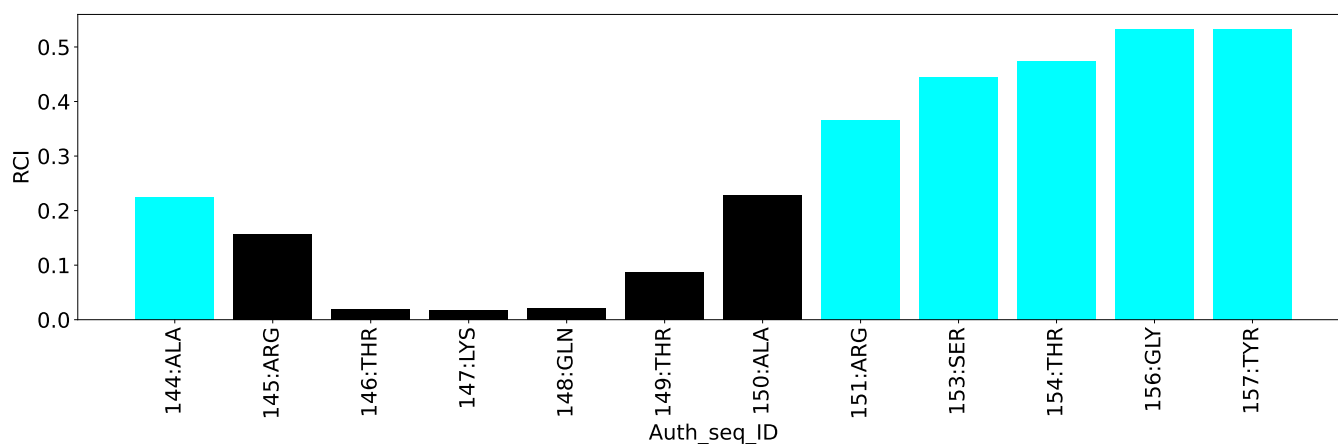
7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



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	1006
Intra-residue ($ i-j =0$)	178
Sequential ($ i-j =1$)	271
Medium range ($ i-j >1$ and $ i-j <5$)	143
Long range ($ i-j \geq 5$)	292
Inter-chain	122
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	11
Number of restraints per residue	13.1
Number of long range restraints per residue ¹	3.8

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)	32.5	0.2
0.2-0.5 (Medium)	52.6	0.5
>0.5 (Large)	81.0	5.3

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

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

9 Distance violation analysis ⓘ

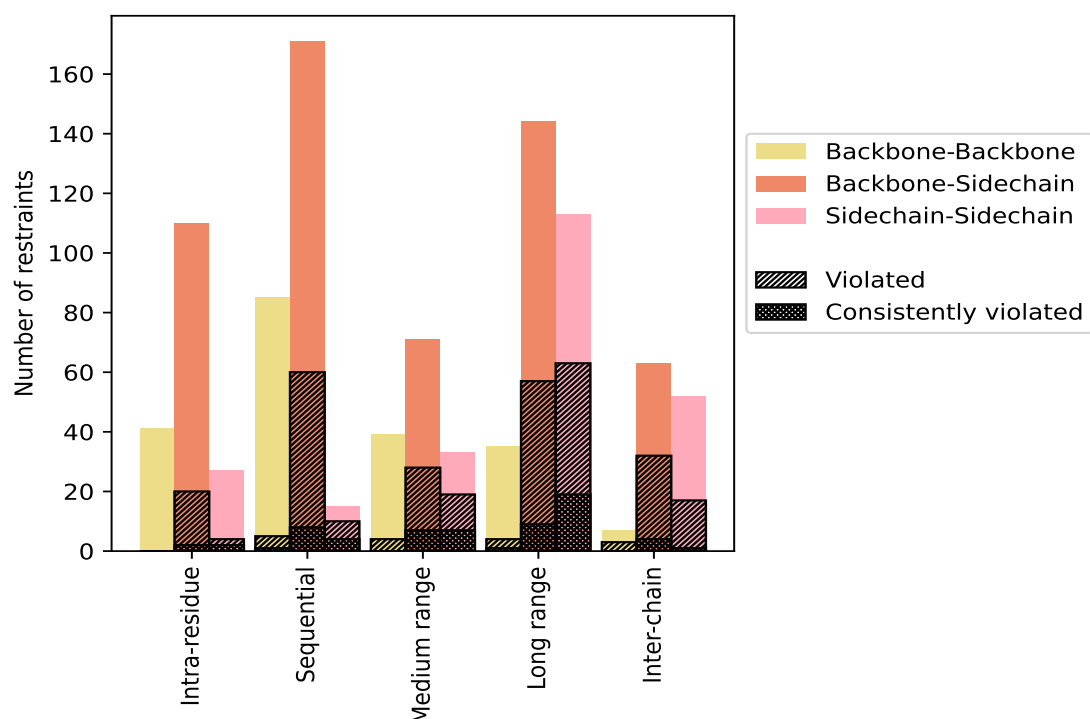
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	178	17.7	24	13.5	2.4	4	2.2	0.4
Backbone-Backbone	41	4.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	110	10.9	20	18.2	2.0	2	1.8	0.2
Sidechain-Sidechain	27	2.7	4	14.8	0.4	2	7.4	0.2
Sequential ($i-j =1$)	271	26.9	75	27.7	7.5	13	4.8	1.3
Backbone-Backbone	85	8.4	5	5.9	0.5	1	1.2	0.1
Backbone-Sidechain	171	17.0	60	35.1	6.0	8	4.7	0.8
Sidechain-Sidechain	15	1.5	10	66.7	1.0	4	26.7	0.4
Medium range ($i-j >1$ & $i-j <5$)	143	14.2	51	35.7	5.1	14	9.8	1.4
Backbone-Backbone	39	3.9	4	10.3	0.4	0	0.0	0.0
Backbone-Sidechain	71	7.1	28	39.4	2.8	7	9.9	0.7
Sidechain-Sidechain	33	3.3	19	57.6	1.9	7	21.2	0.7
Long range ($i-j \geq 5$)	292	29.0	124	42.5	12.3	29	9.9	2.9
Backbone-Backbone	35	3.5	4	11.4	0.4	1	2.9	0.1
Backbone-Sidechain	144	14.3	57	39.6	5.7	9	6.2	0.9
Sidechain-Sidechain	113	11.2	63	55.8	6.3	19	16.8	1.9
Inter-chain	122	12.1	52	42.6	5.2	5	4.1	0.5
Backbone-Backbone	7	0.7	3	42.9	0.3	0	0.0	0.0
Backbone-Sidechain	63	6.3	32	50.8	3.2	4	6.3	0.4
Sidechain-Sidechain	52	5.2	17	32.7	1.7	1	1.9	0.1
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1006	100.0	326	32.4	32.4	65	6.5	6.5
Backbone-Backbone	207	20.6	16	7.7	1.6	2	1.0	0.2
Backbone-Sidechain	559	55.6	197	35.2	19.6	30	5.4	3.0
Sidechain-Sidechain	240	23.9	113	47.1	11.2	33	13.8	3.3

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	14	38	32	76	26	186	0.9	4.0	0.9	0.52
2	15	37	34	78	22	186	1.02	4.79	0.98	0.63
3	11	37	38	66	23	175	0.78	3.63	0.77	0.47
4	9	33	26	62	20	150	0.8	3.82	0.8	0.48
5	12	36	29	66	24	167	0.81	4.18	0.82	0.47
6	14	43	27	68	22	174	0.82	5.06	0.9	0.46
7	11	37	28	61	23	160	0.84	5.3	0.93	0.42
8	9	38	27	56	20	150	0.6	3.15	0.59	0.38
9	12	37	29	62	24	164	0.8	4.11	0.82	0.45
10	10	38	27	60	22	157	0.78	3.84	0.77	0.45

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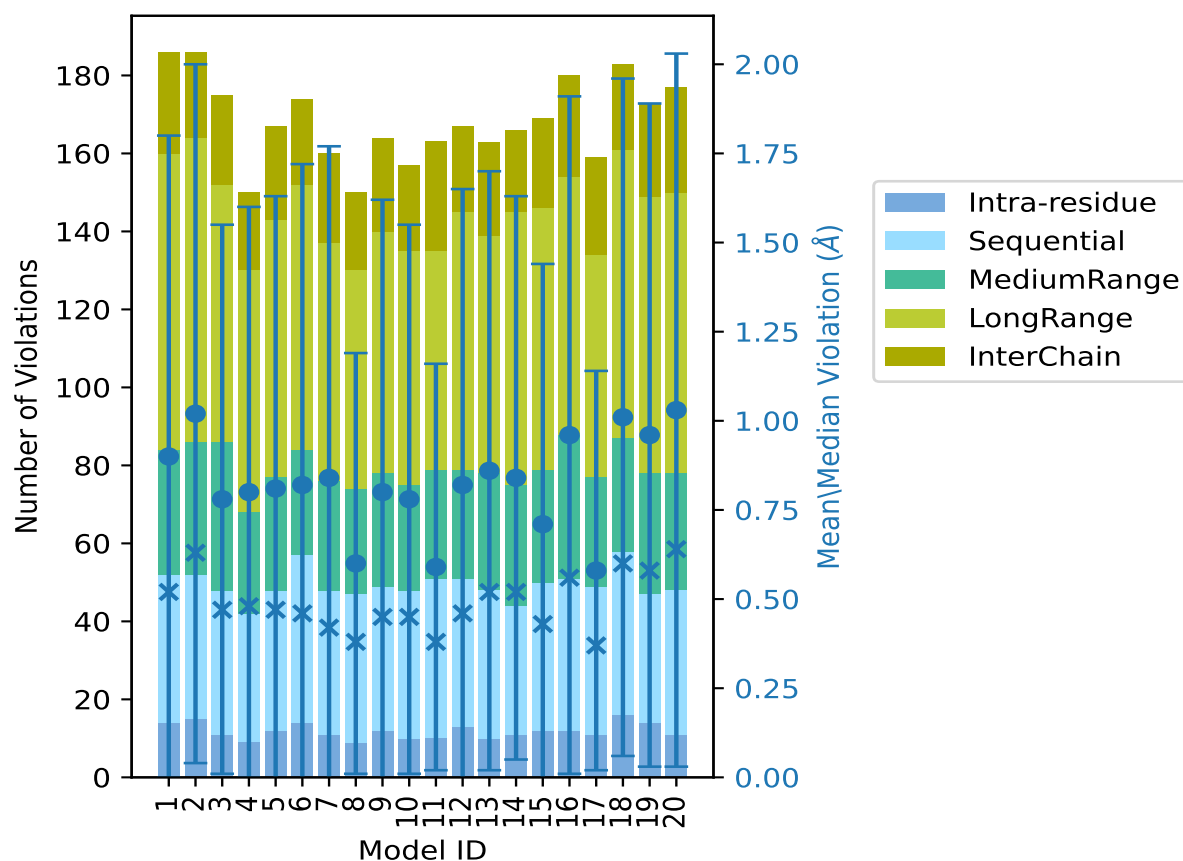
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	10	41	28	56	28	163	0.59	3.15	0.57	0.38
12	13	38	28	66	22	167	0.82	3.98	0.83	0.46
13	10	38	30	61	24	163	0.86	3.74	0.84	0.52
14	11	33	31	70	21	166	0.84	4.1	0.79	0.52
15	12	38	29	67	23	169	0.71	3.76	0.73	0.43
16	12	39	37	66	26	180	0.96	4.34	0.95	0.56
17	11	38	28	57	25	159	0.58	2.86	0.56	0.37
18	16	42	29	74	22	183	1.01	4.06	0.95	0.6
19	14	33	31	71	24	173	0.96	3.98	0.93	0.58
20	11	37	30	72	27	177	1.03	4.91	1.0	0.64

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

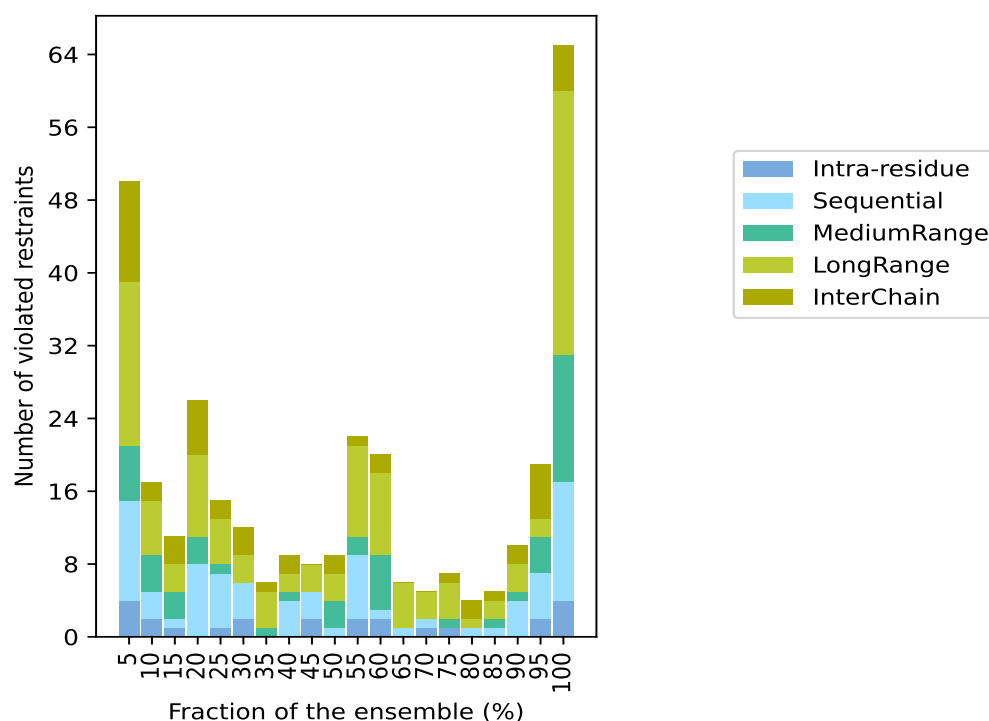
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 680(IR:154, SQ:196, MR:92, LR:168, IC:70) restraints are 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	%
4	11	6	18	11	50	1	5.0
2	3	4	6	2	17	2	10.0
1	1	3	3	3	11	3	15.0
0	8	3	9	6	26	4	20.0
1	6	1	5	2	15	5	25.0
2	4	0	3	3	12	6	30.0
0	0	1	4	1	6	7	35.0
0	4	1	2	2	9	8	40.0
2	3	0	3	0	8	9	45.0
0	1	3	3	2	9	10	50.0
2	7	2	10	1	22	11	55.0
2	1	6	9	2	20	12	60.0
0	1	0	5	0	6	13	65.0
1	1	0	3	0	5	14	70.0
1	0	1	4	1	7	15	75.0
0	1	0	1	2	4	16	80.0
0	1	1	2	1	5	17	85.0
0	4	1	3	2	10	18	90.0
2	5	4	2	6	19	19	95.0
4	13	14	29	5	65	20	100.0

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

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

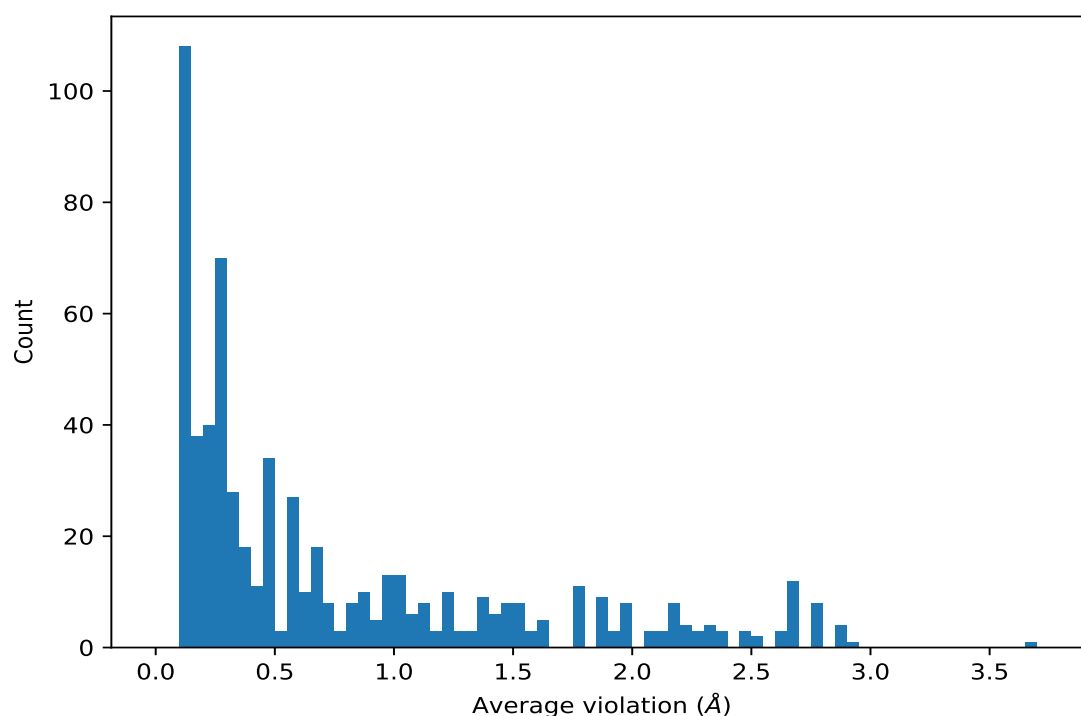
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD12	20	2.89	0.15	2.92
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD11	20	2.89	0.15	2.92
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD13	20	2.89	0.15	2.92
(1,532)	1:103:A:LEU:HD11	1:129:A:TRP:HZ2	20	2.8	0.05	2.82
(1,532)	1:103:A:LEU:HD13	1:129:A:TRP:HZ2	20	2.8	0.05	2.82
(1,532)	1:103:A:LEU:HD12	1:129:A:TRP:HZ2	20	2.8	0.05	2.82
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	20	2.8	1.47	3.77
(1,62)	1:121:A:LEU:HD12	1:103:A:LEU:HD11	20	2.69	1.17	2.14
(1,62)	1:121:A:LEU:HD11	1:103:A:LEU:HD11	20	2.69	1.17	2.14
(1,62)	1:121:A:LEU:HD13	1:103:A:LEU:HD13	20	2.69	1.17	2.14
(1,62)	1:121:A:LEU:HD12	1:103:A:LEU:HD13	20	2.69	1.17	2.14
(1,62)	1:121:A:LEU:HD13	1:103:A:LEU:HD11	20	2.69	1.17	2.14
(1,62)	1:121:A:LEU:HD11	1:103:A:LEU:HD12	20	2.69	1.17	2.14
(1,62)	1:121:A:LEU:HD13	1:103:A:LEU:HD12	20	2.69	1.17	2.14
(1,62)	1:121:A:LEU:HD12	1:103:A:LEU:HD12	20	2.69	1.17	2.14
(1,62)	1:121:A:LEU:HD11	1:103:A:LEU:HD13	20	2.69	1.17	2.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,208)	1:103:A:LEU:HD23	1:104:A:CYS:H	20	2.47	0.07	2.5
(1,208)	1:103:A:LEU:HD22	1:104:A:CYS:H	20	2.47	0.07	2.5
(1,208)	1:103:A:LEU:HD21	1:104:A:CYS:H	20	2.47	0.07	2.5
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD13	20	2.36	1.56	3.7
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD11	20	2.36	1.56	3.7
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD12	20	2.36	1.56	3.7
(1,57)	1:103:A:LEU:HD21	1:104:A:CYS:HB3	20	2.31	0.56	2.02
(1,57)	1:103:A:LEU:HD22	1:104:A:CYS:HB3	20	2.31	0.56	2.02
(1,57)	1:103:A:LEU:HD23	1:104:A:CYS:HB3	20	2.31	0.56	2.02
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD13	20	2.2	1.62	3.58
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD11	20	2.2	1.62	3.58
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD12	20	2.2	1.62	3.58
(1,61)	1:117:A:LEU:HD11	1:103:A:LEU:HD11	20	2.15	0.11	2.17
(1,61)	1:117:A:LEU:HD12	1:103:A:LEU:HD13	20	2.15	0.11	2.17
(1,61)	1:117:A:LEU:HD13	1:103:A:LEU:HD11	20	2.15	0.11	2.17
(1,61)	1:117:A:LEU:HD13	1:103:A:LEU:HD12	20	2.15	0.11	2.17
(1,61)	1:117:A:LEU:HD11	1:103:A:LEU:HD13	20	2.15	0.11	2.17
(1,61)	1:117:A:LEU:HD13	1:103:A:LEU:HD13	20	2.15	0.11	2.17
(1,61)	1:117:A:LEU:HD12	1:103:A:LEU:HD12	20	2.15	0.11	2.17
(1,61)	1:117:A:LEU:HD12	1:103:A:LEU:HD11	20	2.15	0.11	2.17
(1,1)	1:121:A:LEU:HD12	1:124:A:ILE:HG13	20	1.99	1.0	1.55
(1,1)	1:121:A:LEU:HD13	1:124:A:ILE:HG13	20	1.99	1.0	1.55
(1,1)	1:121:A:LEU:HD11	1:130:A:LEU:HB2	20	1.99	1.0	1.55
(1,1)	1:121:A:LEU:HD11	1:124:A:ILE:HG13	20	1.99	1.0	1.55
(1,1)	1:121:A:LEU:HD13	1:130:A:LEU:HB2	20	1.99	1.0	1.55
(1,874)	2:150:B:ALA:HB1	2:151:B:ARG:HD2	20	1.92	0.14	1.94
(1,874)	2:150:B:ALA:HB3	2:151:B:ARG:HD2	20	1.92	0.14	1.94
(1,874)	2:150:B:ALA:HB2	2:151:B:ARG:HD2	20	1.92	0.14	1.94
(1,613)	1:114:A:ILE:HG23	1:103:A:LEU:HD12	20	1.78	0.11	1.78
(1,613)	1:114:A:ILE:HG21	1:103:A:LEU:HD12	20	1.78	0.11	1.78
(1,613)	1:114:A:ILE:HG22	1:103:A:LEU:HD11	20	1.78	0.11	1.78
(1,613)	1:114:A:ILE:HG22	1:103:A:LEU:HD12	20	1.78	0.11	1.78
(1,613)	1:114:A:ILE:HG21	1:103:A:LEU:HD13	20	1.78	0.11	1.78
(1,613)	1:114:A:ILE:HG23	1:103:A:LEU:HD13	20	1.78	0.11	1.78
(1,613)	1:114:A:ILE:HG22	1:103:A:LEU:HD13	20	1.78	0.11	1.78
(1,613)	1:114:A:ILE:HG21	1:103:A:LEU:HD11	20	1.78	0.11	1.78
(1,66)	1:130:A:LEU:HD21	1:128:A:GLU:HB2	20	1.75	0.14	1.74
(1,66)	1:130:A:LEU:HD23	1:128:A:GLU:HB2	20	1.75	0.14	1.74
(1,66)	1:130:A:LEU:HD22	1:128:A:GLU:HB2	20	1.75	0.14	1.74
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM11	20	1.52	0.58	1.65
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM21	20	1.52	0.58	1.65
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM32	20	1.52	0.58	1.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM22	20	1.52	0.58	1.65
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM13	20	1.52	0.58	1.65
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM23	20	1.52	0.58	1.65
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM33	20	1.52	0.58	1.65
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM31	20	1.52	0.58	1.65
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD12	20	1.46	1.1	0.92
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD11	20	1.46	1.1	0.92
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD13	20	1.46	1.1	0.92
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD22	20	1.43	0.32	1.52
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD23	20	1.43	0.32	1.52
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD21	20	1.43	0.32	1.52
(1,696)	1:90:A:MET:HE1	1:92:A:PHE:HD1	20	1.43	1.04	2.12
(1,696)	1:90:A:MET:HE3	1:92:A:PHE:HD1	20	1.43	1.04	2.12
(1,696)	1:90:A:MET:HE2	1:92:A:PHE:HD1	20	1.43	1.04	2.12
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	20	1.38	0.06	1.37
(1,126)	1:103:A:LEU:HD11	1:129:A:TRP:HE1	20	1.37	0.06	1.36
(1,126)	1:103:A:LEU:HD13	1:129:A:TRP:HE1	20	1.37	0.06	1.36
(1,126)	1:103:A:LEU:HD12	1:129:A:TRP:HE1	20	1.37	0.06	1.36
(1,64)	1:121:A:LEU:HD12	1:125:A:PRO:HB2	20	1.32	0.53	1.08
(1,64)	1:121:A:LEU:HD11	1:125:A:PRO:HB2	20	1.32	0.53	1.08
(1,64)	1:121:A:LEU:HD13	1:125:A:PRO:HB2	20	1.32	0.53	1.08
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG21	20	1.23	0.04	1.22
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG22	20	1.23	0.04	1.22
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG23	20	1.23	0.04	1.22
(1,582)	1:103:A:LEU:HD11	1:125:A:PRO:HG3	20	1.22	0.08	1.24
(1,582)	1:103:A:LEU:HD13	1:125:A:PRO:HG3	20	1.22	0.08	1.24
(1,582)	1:103:A:LEU:HD12	1:125:A:PRO:HG3	20	1.22	0.08	1.24
(1,665)	1:103:A:LEU:HD21	1:129:A:TRP:HE3	20	1.19	0.06	1.2
(1,665)	1:103:A:LEU:HD23	1:129:A:TRP:HE3	20	1.19	0.06	1.2
(1,665)	1:103:A:LEU:HD22	1:129:A:TRP:HE3	20	1.19	0.06	1.2
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	20	1.13	0.56	1.43
(1,47)	1:114:A:ILE:HG22	1:121:A:LEU:HB3	20	1.05	0.11	1.08
(1,47)	1:114:A:ILE:HG23	1:121:A:LEU:HB3	20	1.05	0.11	1.08
(1,47)	1:114:A:ILE:HG21	1:121:A:LEU:HB3	20	1.05	0.11	1.08
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD21	20	1.04	0.09	1.03
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD23	20	1.04	0.09	1.03
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD22	20	1.04	0.09	1.03
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	20	0.98	0.24	0.98
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	20	0.97	0.08	0.96
(1,583)	1:103:A:LEU:HD23	1:124:A:ILE:HG21	20	0.89	0.09	0.85
(1,583)	1:103:A:LEU:HD22	1:124:A:ILE:HG21	20	0.89	0.09	0.85
(1,583)	1:103:A:LEU:HD23	1:124:A:ILE:HG23	20	0.89	0.09	0.85

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,583)	1:103:A:LEU:HD21	1:124:A:ILE:HG23	20	0.89	0.09	0.85
(1,583)	1:103:A:LEU:HD21	1:124:A:ILE:HG22	20	0.89	0.09	0.85
(1,583)	1:103:A:LEU:HD22	1:124:A:ILE:HG22	20	0.89	0.09	0.85
(1,583)	1:103:A:LEU:HD23	1:124:A:ILE:HG22	20	0.89	0.09	0.85
(1,583)	1:103:A:LEU:HD22	1:124:A:ILE:HG23	20	0.89	0.09	0.85
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	20	0.87	0.01	0.86
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	20	0.8	0.23	0.75
(1,154)	1:102:A:LEU:HD13	1:94:A:ARG:H	20	0.73	0.29	0.75
(1,154)	1:102:A:LEU:HD11	1:94:A:ARG:H	20	0.73	0.29	0.75
(1,154)	1:102:A:LEU:HD12	1:94:A:ARG:H	20	0.73	0.29	0.75
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	20	0.73	0.18	0.68
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	20	0.73	0.19	0.71
(1,246)	1:114:A:ILE:HD12	1:115:A:HIS:H	20	0.66	0.08	0.7
(1,246)	1:114:A:ILE:HD13	1:115:A:HIS:H	20	0.66	0.08	0.7
(1,246)	1:114:A:ILE:HD11	1:115:A:HIS:H	20	0.66	0.08	0.7
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	20	0.64	0.15	0.66
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD21	20	0.62	0.27	0.72
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD22	20	0.62	0.27	0.72
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD23	20	0.62	0.27	0.72
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE1	20	0.62	0.09	0.6
(1,4)	1:92:A:PHE:H	1:111:A:SER:H	20	0.62	0.09	0.6
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE2	20	0.62	0.09	0.6
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	20	0.6	0.07	0.6
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD11	20	0.58	0.06	0.59
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD12	20	0.58	0.06	0.59
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD13	20	0.58	0.06	0.59
(1,851)	1:114:A:ILE:HG21	1:117:A:LEU:H	20	0.57	0.09	0.56
(1,851)	1:114:A:ILE:HG22	1:117:A:LEU:H	20	0.57	0.09	0.56
(1,851)	1:114:A:ILE:HG23	1:117:A:LEU:H	20	0.57	0.09	0.56
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD22	20	0.55	0.11	0.56
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD21	20	0.55	0.11	0.56
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD23	20	0.55	0.11	0.56
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	20	0.55	0.12	0.52
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	20	0.52	0.03	0.52
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD12	20	0.49	0.12	0.48
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD11	20	0.49	0.12	0.48
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD13	20	0.49	0.12	0.48
(1,571)	1:95:A:VAL:HG22	1:112:A:TYR:HE1	20	0.48	0.06	0.46
(1,571)	1:95:A:VAL:HG23	1:112:A:TYR:HE1	20	0.48	0.06	0.46
(1,571)	1:95:A:VAL:HG21	1:112:A:TYR:HE1	20	0.48	0.06	0.46
(1,247)	1:114:A:ILE:HG23	1:115:A:HIS:H	20	0.46	0.06	0.48
(1,247)	1:114:A:ILE:HG21	1:115:A:HIS:H	20	0.46	0.06	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,247)	1:114:A:ILE:HG22	1:115:A:HIS:H	20	0.46	0.06	0.48
(1,235)	1:95:A:VAL:HG22	1:96:A:CYS:H	20	0.46	0.05	0.48
(1,235)	1:95:A:VAL:HG23	1:96:A:CYS:H	20	0.46	0.05	0.48
(1,235)	1:95:A:VAL:HG21	1:96:A:CYS:H	20	0.46	0.05	0.48
(1,676)	1:117:A:LEU:HD11	1:129:A:TRP:HZ3	20	0.45	0.04	0.45
(1,676)	1:117:A:LEU:HD12	1:129:A:TRP:HZ3	20	0.45	0.04	0.45
(1,676)	1:117:A:LEU:HD13	1:129:A:TRP:HZ3	20	0.45	0.04	0.45
(1,60)	1:117:A:LEU:HD23	1:114:A:ILE:HA	20	0.44	0.08	0.46
(1,60)	1:117:A:LEU:HD21	1:114:A:ILE:HA	20	0.44	0.08	0.46
(1,60)	1:117:A:LEU:HD22	1:114:A:ILE:HA	20	0.44	0.08	0.46
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	20	0.39	0.06	0.38
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	20	0.39	0.07	0.38
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	20	0.36	0.05	0.36
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	20	0.36	0.05	0.36
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	20	0.36	0.05	0.36
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD13	20	0.34	0.03	0.35
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD11	20	0.34	0.03	0.35
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD12	20	0.34	0.03	0.35
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	20	0.34	0.04	0.34
(1,612)	1:103:A:LEU:HD11	1:129:A:TRP:HD1	20	0.34	0.09	0.32
(1,612)	1:103:A:LEU:HD13	1:129:A:TRP:HD1	20	0.34	0.09	0.32
(1,612)	1:103:A:LEU:HD12	1:129:A:TRP:HD1	20	0.34	0.09	0.32
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	20	0.31	0.01	0.32
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	20	0.31	0.01	0.31
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	20	0.31	0.08	0.31
(1,21)	1:93:A:CYS:HB3	1:113:A:HIS:H	20	0.31	0.08	0.31
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	20	0.29	0.07	0.29
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	20	0.29	0.07	0.29
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	20	0.29	0.07	0.29
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	20	0.28	0.07	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	20	0.28	0.07	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	20	0.28	0.07	0.26
(1,46)	1:124:A:ILE:HG21	1:123:A:GLU:HA	20	0.27	0.05	0.28
(1,46)	1:124:A:ILE:HG23	1:123:A:GLU:HA	20	0.27	0.05	0.28
(1,46)	1:124:A:ILE:HG22	1:123:A:GLU:HA	20	0.27	0.05	0.28
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	20	0.26	0.05	0.26
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	20	0.26	0.05	0.26
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG21	20	0.25	0.03	0.25
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG23	20	0.25	0.03	0.25
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG22	20	0.25	0.03	0.25
(1,670)	1:117:A:LEU:HD11	1:129:A:TRP:HH2	20	0.22	0.04	0.22
(1,670)	1:117:A:LEU:HD12	1:129:A:TRP:HH2	20	0.22	0.04	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,670)	1:117:A:LEU:HD13	1:129:A:TRP:HH2	20	0.22	0.04	0.22
(1,876)	2:149:B:THR:HG21	2:147:B:LYS:HE2	19	1.06	0.35	1.06
(1,876)	2:149:B:THR:HG23	2:147:B:LYS:HE2	19	1.06	0.35	1.06
(1,876)	2:149:B:THR:HG22	2:147:B:LYS:HE2	19	1.06	0.35	1.06
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM11	19	1.02	0.5	0.98
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM22	19	1.02	0.5	0.98
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM32	19	1.02	0.5	0.98
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM13	19	1.02	0.5	0.98
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM23	19	1.02	0.5	0.98
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM21	19	1.02	0.5	0.98
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM31	19	1.02	0.5	0.98
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM12	19	1.02	0.5	0.98
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM33	19	1.02	0.5	0.98
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD23	19	0.77	0.13	0.8
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD22	19	0.77	0.13	0.8
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD21	19	0.77	0.13	0.8
(1,68)	1:130:A:LEU:HD23	1:134:A:CYS:HB3	19	0.69	0.07	0.7
(1,68)	1:130:A:LEU:HD22	1:134:A:CYS:HB3	19	0.69	0.07	0.7
(1,68)	1:130:A:LEU:HD21	1:134:A:CYS:HB3	19	0.69	0.07	0.7
(1,585)	1:107:A:THR:HG23	1:130:A:LEU:HD22	19	0.55	0.09	0.53
(1,585)	1:107:A:THR:HG23	1:130:A:LEU:HD21	19	0.55	0.09	0.53
(1,585)	1:107:A:THR:HG21	1:130:A:LEU:HD21	19	0.55	0.09	0.53
(1,585)	1:107:A:THR:HG21	1:130:A:LEU:HD22	19	0.55	0.09	0.53
(1,585)	1:107:A:THR:HG22	1:130:A:LEU:HD21	19	0.55	0.09	0.53
(1,585)	1:107:A:THR:HG23	1:130:A:LEU:HD23	19	0.55	0.09	0.53
(1,585)	1:107:A:THR:HG22	1:130:A:LEU:HD22	19	0.55	0.09	0.53
(1,585)	1:107:A:THR:HG22	1:130:A:LEU:HD23	19	0.55	0.09	0.53
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	19	0.48	0.13	0.52
(1,51)	1:95:A:VAL:HG22	1:96:A:CYS:HB2	19	0.42	0.38	0.23
(1,51)	1:95:A:VAL:HG23	1:96:A:CYS:HB2	19	0.42	0.38	0.23
(1,51)	1:95:A:VAL:HG21	1:96:A:CYS:HB2	19	0.42	0.38	0.23
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	19	0.39	0.11	0.36
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	19	0.39	0.11	0.36
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD13	19	0.36	0.05	0.36
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD12	19	0.36	0.05	0.36
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD11	19	0.36	0.05	0.36
(1,258)	1:107:A:THR:HG23	1:108:A:CYS:H	19	0.35	0.08	0.36
(1,258)	1:107:A:THR:HG21	1:108:A:CYS:H	19	0.35	0.08	0.36
(1,258)	1:107:A:THR:HG22	1:108:A:CYS:H	19	0.35	0.08	0.36
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	19	0.28	0.04	0.28
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD13	19	0.28	0.41	0.18
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD11	19	0.28	0.41	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD12	19	0.28	0.41	0.18
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	19	0.26	0.09	0.25
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	19	0.25	0.07	0.25
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	19	0.25	0.07	0.25
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	19	0.19	0.05	0.18
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	19	0.19	0.05	0.18
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	19	0.19	0.05	0.18
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	19	0.17	0.04	0.17
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	19	0.17	0.03	0.17
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	19	0.17	0.02	0.17
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	19	0.14	0.03	0.13
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	19	0.14	0.03	0.13
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	19	0.14	0.03	0.13
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	19	0.14	0.03	0.13
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	19	0.14	0.03	0.13
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	19	0.14	0.03	0.13
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD21	18	1.88	1.29	2.76
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD22	18	1.88	1.29	2.76
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD23	18	1.88	1.29	2.76
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	18	0.61	0.23	0.67
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	18	0.51	0.24	0.51
(1,655)	1:117:A:LEU:HD21	1:113:A:HIS:HB2	18	0.49	0.19	0.49
(1,655)	1:117:A:LEU:HD22	1:113:A:HIS:HB2	18	0.49	0.19	0.49
(1,655)	1:117:A:LEU:HD23	1:113:A:HIS:HB2	18	0.49	0.19	0.49
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	18	0.38	0.01	0.38
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD21	18	0.27	0.14	0.22
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD22	18	0.27	0.14	0.22
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD23	18	0.27	0.14	0.22
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	18	0.26	0.05	0.28
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	18	0.26	0.05	0.28
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	18	0.26	0.05	0.28
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	18	0.22	0.13	0.16
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	18	0.2	0.04	0.2
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	18	0.2	0.04	0.2
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	18	0.2	0.04	0.2
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	18	0.17	0.02	0.17
(1,550)	1:90:A:MET:HE1	1:92:A:PHE:HE1	17	1.87	1.04	2.4
(1,550)	1:90:A:MET:HE3	1:92:A:PHE:HE1	17	1.87	1.04	2.4
(1,550)	1:90:A:MET:HE2	1:92:A:PHE:HE1	17	1.87	1.04	2.4
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD13	17	1.49	0.97	2.11
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD11	17	1.49	0.97	2.11
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD12	17	1.49	0.97	2.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,344)	1:102:A:LEU:HD13	1:103:A:LEU:H	17	1.23	0.79	1.72
(1,344)	1:102:A:LEU:HD11	1:103:A:LEU:H	17	1.23	0.79	1.72
(1,344)	1:102:A:LEU:HD12	1:103:A:LEU:H	17	1.23	0.79	1.72
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD23	17	0.73	0.44	0.73
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD21	17	0.73	0.44	0.73
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD22	17	0.73	0.44	0.73
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	17	0.15	0.02	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	17	0.15	0.02	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	17	0.15	0.02	0.16
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD13	16	1.63	1.0	2.09
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD11	16	1.63	1.0	2.09
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD12	16	1.63	1.0	2.09
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	16	0.15	0.03	0.15
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	16	0.15	0.03	0.15
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	16	0.15	0.03	0.15
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	16	0.15	0.03	0.15
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	16	0.15	0.03	0.15
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	16	0.15	0.03	0.15
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	16	0.14	0.02	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	16	0.14	0.02	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	16	0.14	0.02	0.13
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	16	0.12	0.02	0.12
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	15	1.36	0.26	1.32
(1,580)	1:90:A:MET:HE1	1:90:A:MET:HG2	15	1.27	0.02	1.28
(1,580)	1:90:A:MET:HE3	1:90:A:MET:HG2	15	1.27	0.02	1.28
(1,580)	1:90:A:MET:HE2	1:90:A:MET:HG2	15	1.27	0.02	1.28
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	15	1.22	0.41	1.35
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	15	0.99	0.17	0.93
(1,578)	1:130:A:LEU:HD12	1:106:A:ASP:HB2	15	0.93	0.87	1.03
(1,578)	1:130:A:LEU:HD11	1:106:A:ASP:HB2	15	0.93	0.87	1.03
(1,578)	1:130:A:LEU:HD13	1:106:A:ASP:HB2	15	0.93	0.87	1.03
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	15	0.18	0.05	0.16
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	15	0.14	0.03	0.13
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	15	0.14	0.03	0.13
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	14	2.32	0.95	2.17
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	14	2.2	0.85	2.52
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	14	0.28	0.12	0.22
(1,65)	1:121:A:LEU:HD22	1:114:A:ILE:HA	14	0.27	0.08	0.25
(1,65)	1:121:A:LEU:HD21	1:114:A:ILE:HA	14	0.27	0.08	0.25
(1,65)	1:121:A:LEU:HD23	1:114:A:ILE:HA	14	0.27	0.08	0.25
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	14	0.24	0.04	0.25
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD21	13	0.84	0.53	0.83

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD22	13	0.84	0.53	0.83
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD23	13	0.84	0.53	0.83
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	13	0.61	0.1	0.62
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD13	13	0.49	0.22	0.47
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD12	13	0.49	0.22	0.47
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD11	13	0.49	0.22	0.47
(1,466)	1:130:A:LEU:HD23	1:135:A:THR:H	13	0.39	0.18	0.42
(1,466)	1:130:A:LEU:HD22	1:135:A:THR:H	13	0.39	0.18	0.42
(1,466)	1:130:A:LEU:HD21	1:135:A:THR:H	13	0.39	0.18	0.42
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	13	0.36	0.14	0.3
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD23	13	0.24	0.09	0.22
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD22	13	0.24	0.09	0.22
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD21	13	0.24	0.09	0.22
(1,95)	1:94:A:ARG:HA	1:92:A:PHE:HD1	12	3.66	0.09	3.68
(1,147)	1:92:A:PHE:HD1	1:94:A:ARG:H	12	2.93	0.1	2.89
(1,689)	1:97:A:LYS:HD3	1:92:A:PHE:HE1	12	2.89	0.56	3.16
(1,691)	1:97:A:LYS:HG3	1:92:A:PHE:HE1	12	2.77	0.21	2.8
(1,685)	1:97:A:LYS:HA	1:92:A:PHE:HD1	12	2.53	0.12	2.52
(1,811)	1:92:A:PHE:HD1	1:97:A:LYS:H	12	2.51	0.1	2.54
(1,697)	1:97:A:LYS:HD2	1:92:A:PHE:HD1	12	2.14	0.55	2.0
(1,768)	1:92:A:PHE:HD1	1:98:A:ASP:H	12	2.12	0.09	2.13
(1,557)	1:97:A:LYS:HD2	1:92:A:PHE:HE1	12	2.11	0.47	2.1
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG21	12	2.06	0.05	2.08
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG22	12	2.06	0.05	2.08
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG23	12	2.06	0.05	2.08
(1,555)	1:94:A:ARG:HA	1:92:A:PHE:HE1	12	1.65	0.11	1.64
(1,42)	1:102:A:LEU:HD12	1:99:A:GLY:HA3	12	0.97	0.45	1.15
(1,42)	1:102:A:LEU:HD11	1:99:A:GLY:HA3	12	0.97	0.45	1.15
(1,42)	1:102:A:LEU:HD13	1:99:A:GLY:HA3	12	0.97	0.45	1.15
(1,522)	1:92:A:PHE:HB2	1:92:A:PHE:HD1	12	0.81	0.01	0.81
(1,796)	1:92:A:PHE:HD1	1:93:A:CYS:H	12	0.6	0.03	0.59
(1,845)	1:115:A:HIS:HB2	1:117:A:LEU:H	12	0.46	0.13	0.47
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD21	12	0.34	0.11	0.35
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD22	12	0.34	0.11	0.35
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD23	12	0.34	0.11	0.35
(1,501)	1:121:A:LEU:HB2	1:123:A:GLU:H	12	0.26	0.1	0.27
(1,785)	1:128:A:GLU:HG3	1:128:A:GLU:H	12	0.17	0.05	0.16
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB1	12	0.16	0.03	0.16
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB2	12	0.16	0.03	0.16
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB3	12	0.16	0.03	0.16
(1,77)	1:95:A:VAL:HB	1:116:A:CYS:HB2	12	0.15	0.02	0.15
(1,533)	1:102:A:LEU:HD12	1:113:A:HIS:HD2	11	2.76	0.19	2.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,533)	1:102:A:LEU:HD13	1:113:A:HIS:HD2	11	2.76	0.19	2.68
(1,533)	1:102:A:LEU:HD11	1:113:A:HIS:HD2	11	2.76	0.19	2.68
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD13	11	2.66	0.17	2.68
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD11	11	2.66	0.17	2.68
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD12	11	2.66	0.17	2.68
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD13	11	2.65	0.09	2.61
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD11	11	2.65	0.09	2.61
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD12	11	2.65	0.09	2.61
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD13	11	1.97	0.03	1.97
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD11	11	1.97	0.03	1.97
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD12	11	1.97	0.03	1.97
(1,41)	1:102:A:LEU:HD13	1:93:A:CYS:HB2	11	1.86	0.23	1.91
(1,41)	1:102:A:LEU:HD11	1:93:A:CYS:HB2	11	1.86	0.23	1.91
(1,41)	1:102:A:LEU:HD12	1:93:A:CYS:HB2	11	1.86	0.23	1.91
(1,674)	1:97:A:LYS:HD3	1:92:A:PHE:HD1	11	1.46	0.63	1.73
(1,375)	1:102:A:LEU:HD12	1:101:A:GLU:H	11	1.15	0.1	1.16
(1,375)	1:102:A:LEU:HD13	1:101:A:GLU:H	11	1.15	0.1	1.16
(1,375)	1:102:A:LEU:HD11	1:101:A:GLU:H	11	1.15	0.1	1.16
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD13	11	1.12	0.2	1.12
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD11	11	1.12	0.2	1.12
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD12	11	1.12	0.2	1.12
(1,394)	1:102:A:LEU:HD12	1:98:A:ASP:H	11	0.98	0.18	1.0
(1,394)	1:102:A:LEU:HD13	1:98:A:ASP:H	11	0.98	0.18	1.0
(1,394)	1:102:A:LEU:HD11	1:98:A:ASP:H	11	0.98	0.18	1.0
(1,761)	1:94:A:ARG:HD2	1:95:A:VAL:H	11	0.9	0.09	0.89
(1,288)	1:102:A:LEU:HD13	1:112:A:TYR:H	11	0.68	0.08	0.69
(1,288)	1:102:A:LEU:HD11	1:112:A:TYR:H	11	0.68	0.08	0.69
(1,288)	1:102:A:LEU:HD12	1:112:A:TYR:H	11	0.68	0.08	0.69
(1,482)	1:115:A:HIS:HB2	1:116:A:CYS:H	11	0.66	0.06	0.66
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM12	11	0.46	0.12	0.47
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM23	11	0.46	0.12	0.47
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM33	11	0.46	0.12	0.47
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM21	11	0.46	0.12	0.47
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM22	11	0.46	0.12	0.47
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM32	11	0.46	0.12	0.47
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG22	11	0.42	0.08	0.44
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG23	11	0.42	0.08	0.44
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG21	11	0.42	0.08	0.44
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG21	11	0.29	0.08	0.3
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG22	11	0.29	0.08	0.3
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG23	11	0.29	0.08	0.3
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD23	11	0.29	0.12	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD21	11	0.29	0.12	0.29
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD22	11	0.29	0.12	0.29
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD13	11	0.28	0.1	0.27
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD11	11	0.28	0.1	0.27
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD12	11	0.28	0.1	0.27
(1,739)	1:130:A:LEU:HD12	1:129:A:TRP:H	11	0.27	0.27	0.19
(1,739)	1:130:A:LEU:HD13	1:129:A:TRP:H	11	0.27	0.27	0.19
(1,739)	1:130:A:LEU:HD11	1:129:A:TRP:H	11	0.27	0.27	0.19
(1,858)	2:148:B:GLN:H	2:147:B:LYS:HB2	11	0.25	0.08	0.29
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG23	11	0.23	0.05	0.24
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG21	11	0.23	0.05	0.24
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG22	11	0.23	0.05	0.24
(1,820)	1:121:A:LEU:HD22	1:121:A:LEU:H	11	0.17	0.04	0.17
(1,820)	1:121:A:LEU:HD21	1:121:A:LEU:H	11	0.17	0.04	0.17
(1,820)	1:121:A:LEU:HD23	1:121:A:LEU:H	11	0.17	0.04	0.17
(1,108)	1:117:A:LEU:HA	1:129:A:TRP:HZ2	11	0.13	0.02	0.14
(1,683)	1:110:A:SER:HB3	1:112:A:TYR:HD1	10	1.62	0.11	1.63
(1,111)	1:102:A:LEU:HA	1:111:A:SER:HB2	10	1.38	0.08	1.41
(1,684)	1:112:A:TYR:HE1	1:110:A:SER:HB3	10	0.85	0.17	0.87
(1,602)	1:137:A:PRO:HD2	1:136:A:CYS:HB2	10	0.63	0.29	0.58
(1,596)	1:97:A:LYS:HB3	1:92:A:PHE:HD1	10	0.38	0.12	0.38
(1,651)	1:114:A:ILE:HG23	1:125:A:PRO:HD2	10	0.21	0.07	0.2
(1,651)	1:114:A:ILE:HG21	1:125:A:PRO:HD2	10	0.21	0.07	0.2
(1,651)	1:114:A:ILE:HG22	1:125:A:PRO:HD2	10	0.21	0.07	0.2
(1,980)	1:101:A:GLU:HG2	2:148:B:GLN:HA	10	0.16	0.07	0.12
(1,980)	1:101:A:GLU:HG3	2:148:B:GLN:HA	10	0.16	0.07	0.12
(1,396)	1:105:A:CYS:H	1:103:A:LEU:H	10	0.15	0.02	0.15
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD2	10	0.14	0.02	0.12
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD3	10	0.14	0.02	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD2	10	0.14	0.02	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD3	10	0.14	0.02	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD2	10	0.14	0.02	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD3	10	0.14	0.02	0.12
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD2	10	0.14	0.02	0.12
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD3	10	0.14	0.02	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD2	10	0.14	0.02	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD3	10	0.14	0.02	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD2	10	0.14	0.02	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD3	10	0.14	0.02	0.12
(1,213)	1:133:A:ARG:H	1:133:A:ARG:HD3	9	1.14	0.42	1.14
(1,403)	1:89:A:HIS:HB2	1:105:A:CYS:H	9	0.93	0.39	1.08
(1,600)	1:111:A:SER:HB2	1:102:A:LEU:HD13	9	0.68	0.54	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,600)	1:111:A:SER:HB2	1:102:A:LEU:HD11	9	0.68	0.54	0.41
(1,600)	1:111:A:SER:HB2	1:102:A:LEU:HD12	9	0.68	0.54	0.41
(1,100)	1:93:A:CYS:HA	1:102:A:LEU:HD22	9	0.67	0.03	0.66
(1,100)	1:93:A:CYS:HA	1:102:A:LEU:HD21	9	0.67	0.03	0.66
(1,100)	1:93:A:CYS:HA	1:102:A:LEU:HD23	9	0.67	0.03	0.66
(1,752)	1:102:A:LEU:HD21	1:103:A:LEU:H	9	0.55	0.05	0.57
(1,752)	1:102:A:LEU:HD23	1:103:A:LEU:H	9	0.55	0.05	0.57
(1,752)	1:102:A:LEU:HD22	1:103:A:LEU:H	9	0.55	0.05	0.57
(1,825)	1:110:A:SER:HB3	1:111:A:SER:H	9	0.45	0.15	0.48
(1,762)	1:91:A:GLU:HG2	1:91:A:GLU:H	9	0.28	0.07	0.29
(1,730)	1:111:A:SER:HB2	1:112:A:TYR:H	9	0.22	0.08	0.22
(1,568)	1:133:A:ARG:HD3	1:112:A:TYR:HE1	8	1.48	0.23	1.5
(1,713)	1:106:A:ASP:HB2	1:107:A:THR:H	8	0.49	0.05	0.48
(1,701)	1:111:A:SER:HB2	1:89:A:HIS:HD2	8	0.38	0.27	0.26
(1,556)	1:91:A:GLU:HG3	1:92:A:PHE:HE1	8	0.36	0.09	0.36
(1,327)	1:132:A:PRO:HD3	1:131:A:CYS:H	8	0.32	0.1	0.34
(1,69)	1:130:A:LEU:HD11	1:128:A:GLU:HB2	8	0.31	0.12	0.28
(1,69)	1:130:A:LEU:HD12	1:128:A:GLU:HB2	8	0.31	0.12	0.28
(1,69)	1:130:A:LEU:HD13	1:128:A:GLU:HB2	8	0.31	0.12	0.28
(1,171)	1:135:A:THR:HG22	1:136:A:CYS:H	8	0.24	0.06	0.26
(1,171)	1:135:A:THR:HG23	1:136:A:CYS:H	8	0.24	0.06	0.26
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD2	8	0.14	0.05	0.12
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD3	8	0.14	0.05	0.12
(1,931)	1:98:A:ASP:H	2:152:B:M3L:HE2	8	0.14	0.02	0.14
(1,76)	1:90:A:MET:HE1	1:110:A:SER:HA	7	0.6	0.26	0.77
(1,76)	1:90:A:MET:HE2	1:110:A:SER:HA	7	0.6	0.26	0.77
(1,76)	1:90:A:MET:HE3	1:110:A:SER:HA	7	0.6	0.26	0.77
(1,534)	1:98:A:ASP:HB3	1:113:A:HIS:HD2	7	0.59	0.41	0.44
(1,509)	1:102:A:LEU:HD23	1:92:A:PHE:H	7	0.32	0.09	0.36
(1,509)	1:102:A:LEU:HD21	1:92:A:PHE:H	7	0.32	0.09	0.36
(1,509)	1:102:A:LEU:HD22	1:92:A:PHE:H	7	0.32	0.09	0.36
(1,754)	1:89:A:HIS:HD2	1:103:A:LEU:H	7	0.21	0.04	0.21
(1,890)	1:91:A:GLU:HA	2:147:B:LYS:HB2	7	0.19	0.04	0.19
(1,529)	1:131:A:CYS:HA	1:129:A:TRP:HZ3	7	0.12	0.01	0.11
(1,782)	1:123:A:GLU:HG2	1:124:A:ILE:H	6	1.02	0.04	1.04
(1,75)	1:135:A:THR:HG22	1:130:A:LEU:HG	6	0.45	0.25	0.48
(1,75)	1:135:A:THR:HG21	1:130:A:LEU:HG	6	0.45	0.25	0.48
(1,75)	1:135:A:THR:HG23	1:130:A:LEU:HG	6	0.45	0.25	0.48
(1,178)	1:97:A:LYS:H	1:97:A:LYS:HD2	6	0.42	0.07	0.41
(1,944)	1:98:A:ASP:HA	2:152:B:M3L:HE3	6	0.29	0.07	0.3
(1,909)	1:98:A:ASP:H	2:152:B:M3L:HM12	6	0.29	0.12	0.29
(1,909)	1:98:A:ASP:H	2:152:B:M3L:HM33	6	0.29	0.12	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,909)	1:98:A:ASP:H	2:152:B:M3L:HM32	6	0.29	0.12	0.29
(1,709)	1:94:A:ARG:HD2	1:94:A:ARG:H	6	0.24	0.19	0.18
(1,821)	1:130:A:LEU:HD13	1:135:A:THR:H	6	0.24	0.08	0.28
(1,821)	1:130:A:LEU:HD12	1:135:A:THR:H	6	0.24	0.08	0.28
(1,821)	1:130:A:LEU:HD11	1:135:A:THR:H	6	0.24	0.08	0.28
(1,234)	1:95:A:VAL:HG12	1:96:A:CYS:H	6	0.24	0.09	0.24
(1,234)	1:95:A:VAL:HG13	1:96:A:CYS:H	6	0.24	0.09	0.24
(1,234)	1:95:A:VAL:HG11	1:96:A:CYS:H	6	0.24	0.09	0.24
(1,805)	1:135:A:THR:HA	1:136:A:CYS:H	6	0.15	0.03	0.16
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG2	6	0.15	0.02	0.15
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG3	6	0.15	0.02	0.15
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG2	6	0.15	0.02	0.15
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG3	6	0.15	0.02	0.15
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG2	6	0.15	0.02	0.15
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG3	6	0.15	0.02	0.15
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG2	6	0.15	0.02	0.15
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG3	6	0.15	0.02	0.15
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG2	6	0.15	0.02	0.15
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG3	6	0.15	0.02	0.15
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG2	6	0.15	0.02	0.15
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG3	6	0.15	0.02	0.15
(1,756)	1:112:A:TYR:HD1	1:95:A:VAL:H	6	0.12	0.02	0.11
(1,85)	1:109:A:PRO:HA	1:108:A:CYS:HB3	6	0.11	0.01	0.11
(1,587)	1:114:A:ILE:HA	1:121:A:LEU:HD12	5	2.29	1.08	2.86
(1,587)	1:114:A:ILE:HA	1:121:A:LEU:HD13	5	2.29	1.08	2.86
(1,587)	1:114:A:ILE:HA	1:121:A:LEU:HD11	5	2.29	1.08	2.86
(1,932)	1:98:A:ASP:H	2:152:B:M3L:HE3	5	0.88	0.09	0.93
(1,576)	1:136:A:CYS:HA	1:137:A:PRO:HD2	5	0.29	0.08	0.33
(1,688)	1:94:A:ARG:HB2	1:112:A:TYR:HD1	5	0.29	0.11	0.26
(1,597)	1:121:A:LEU:HD23	1:129:A:TRP:HD1	5	0.29	0.12	0.29
(1,597)	1:121:A:LEU:HD22	1:129:A:TRP:HD1	5	0.29	0.12	0.29
(1,597)	1:121:A:LEU:HD21	1:129:A:TRP:HD1	5	0.29	0.12	0.29
(1,318)	1:89:A:HIS:HB2	1:90:A:MET:H	5	0.27	0.07	0.32
(1,439)	1:96:A:CYS:HB2	1:97:A:LYS:H	5	0.26	0.04	0.28
(1,738)	1:130:A:LEU:HD21	1:129:A:TRP:H	5	0.23	0.11	0.16
(1,738)	1:130:A:LEU:HD23	1:129:A:TRP:H	5	0.23	0.11	0.16
(1,738)	1:130:A:LEU:HD22	1:129:A:TRP:H	5	0.23	0.11	0.16
(1,239)	1:96:A:CYS:HB2	1:96:A:CYS:H	5	0.23	0.02	0.24
(1,609)	1:132:A:PRO:HD3	1:129:A:TRP:HH2	5	0.19	0.03	0.2
(1,677)	1:112:A:TYR:HB3	1:129:A:TRP:HZ3	5	0.19	0.05	0.2
(1,545)	1:102:A:LEU:HA	1:103:A:LEU:HD23	5	0.18	0.04	0.16
(1,545)	1:102:A:LEU:HA	1:103:A:LEU:HD21	5	0.18	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,545)	1:102:A:LEU:HA	1:103:A:LEU:HD22	5	0.18	0.04	0.16
(1,608)	1:98:A:ASP:HA	1:92:A:PHE:HD1	5	0.14	0.02	0.14
(1,914)	1:101:A:GLU:H	2:148:B:GLN:HG2	5	0.14	0.02	0.14
(1,914)	1:101:A:GLU:H	2:148:B:GLN:HG3	5	0.14	0.02	0.14
(1,365)	1:95:A:VAL:H	1:96:A:CYS:HA	5	0.11	0.01	0.11
(1,127)	1:121:A:LEU:HD11	1:129:A:TRP:HE1	4	1.57	0.15	1.59
(1,127)	1:121:A:LEU:HD13	1:129:A:TRP:HE1	4	1.57	0.15	1.59
(1,872)	2:147:B:LYS:H	2:148:B:GLN:HG2	4	1.55	0.15	1.6
(1,667)	1:129:A:TRP:HZ2	1:121:A:LEU:HD11	4	1.38	0.2	1.48
(1,667)	1:129:A:TRP:HZ2	1:121:A:LEU:HD13	4	1.38	0.2	1.48
(1,667)	1:129:A:TRP:HZ2	1:121:A:LEU:HD12	4	1.38	0.2	1.48
(1,63)	1:121:A:LEU:HD12	1:117:A:LEU:HG	4	0.96	0.41	1.16
(1,63)	1:121:A:LEU:HD11	1:117:A:LEU:HG	4	0.96	0.41	1.16
(1,559)	1:121:A:LEU:HD11	1:129:A:TRP:HD1	4	0.96	0.16	1.04
(1,559)	1:121:A:LEU:HD13	1:129:A:TRP:HD1	4	0.96	0.16	1.04
(1,257)	1:123:A:GLU:H	1:121:A:LEU:HD22	4	0.84	0.08	0.84
(1,257)	1:123:A:GLU:H	1:121:A:LEU:HD23	4	0.84	0.08	0.84
(1,813)	1:133:A:ARG:HD3	1:134:A:CYS:H	4	0.68	0.29	0.81
(1,879)	2:148:B:GLN:HG2	2:147:B:LYS:HA	4	0.66	0.05	0.66
(1,567)	1:94:A:ARG:HD2	1:112:A:TYR:HE1	4	0.54	0.28	0.42
(1,681)	1:94:A:ARG:HD2	1:112:A:TYR:HE1	4	0.43	0.28	0.3
(1,169)	1:137:A:PRO:HD2	1:136:A:CYS:H	4	0.34	0.06	0.36
(1,644)	1:95:A:VAL:HG22	1:94:A:ARG:HD2	4	0.3	0.08	0.26
(1,644)	1:95:A:VAL:HG21	1:94:A:ARG:HD2	4	0.3	0.08	0.26
(1,654)	1:132:A:PRO:HD2	1:117:A:LEU:HD22	4	0.27	0.13	0.26
(1,654)	1:132:A:PRO:HD2	1:117:A:LEU:HD23	4	0.27	0.13	0.26
(1,569)	1:91:A:GLU:HG3	1:92:A:PHE:HD1	4	0.23	0.13	0.22
(1,16)	1:117:A:LEU:HD11	1:114:A:ILE:H	4	0.17	0.06	0.15
(1,16)	1:117:A:LEU:HD13	1:114:A:ILE:H	4	0.17	0.06	0.15
(1,562)	1:112:A:TYR:HE1	1:117:A:LEU:HD21	4	0.16	0.04	0.16
(1,562)	1:112:A:TYR:HE1	1:117:A:LEU:HD23	4	0.16	0.04	0.16
(1,642)	1:105:A:CYS:HA	1:89:A:HIS:HD2	4	0.16	0.02	0.17
(1,487)	1:116:A:CYS:H	1:117:A:LEU:HD11	4	0.16	0.03	0.15
(1,487)	1:116:A:CYS:H	1:117:A:LEU:HD12	4	0.16	0.03	0.15
(1,487)	1:116:A:CYS:H	1:117:A:LEU:HD13	4	0.16	0.03	0.15
(1,625)	1:129:A:TRP:HB3	1:103:A:LEU:HD21	4	0.15	0.03	0.15
(1,625)	1:129:A:TRP:HB3	1:103:A:LEU:HD22	4	0.15	0.03	0.15
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB1	4	0.14	0.04	0.13
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB2	4	0.14	0.04	0.13
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB3	4	0.14	0.04	0.13
(1,915)	1:101:A:GLU:H	2:151:B:ARG:HG2	4	0.14	0.04	0.12
(1,915)	1:101:A:GLU:H	2:151:B:ARG:HG3	4	0.14	0.04	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG21	4	0.14	0.03	0.12
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG22	4	0.14	0.03	0.12
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG23	4	0.14	0.03	0.12
(1,908)	1:101:A:GLU:H	2:151:B:ARG:HD2	4	0.12	0.01	0.12
(1,908)	1:101:A:GLU:H	2:151:B:ARG:HD3	4	0.12	0.01	0.12
(1,977)	1:101:A:GLU:HB2	2:148:B:GLN:HA	4	0.12	0.01	0.12
(1,977)	1:101:A:GLU:HB3	2:148:B:GLN:HA	4	0.12	0.01	0.12
(1,182)	1:118:A:ASN:H	1:117:A:LEU:H	4	0.12	0.01	0.12
(1,925)	1:101:A:GLU:H	2:148:B:GLN:HE22	4	0.12	0.02	0.11
(1,204)	1:101:A:GLU:H	1:101:A:GLU:HB2	3	0.33	0.05	0.36
(1,574)	1:114:A:ILE:HG22	1:122:A:PRO:HD2	3	0.21	0.04	0.23
(1,574)	1:114:A:ILE:HG23	1:122:A:PRO:HD2	3	0.21	0.04	0.23
(1,818)	1:114:A:ILE:HG21	1:121:A:LEU:H	3	0.17	0.02	0.17
(1,818)	1:114:A:ILE:HG23	1:121:A:LEU:H	3	0.17	0.02	0.17
(1,5)	1:115:A:HIS:H	1:117:A:LEU:H	3	0.17	0.01	0.17
(1,558)	1:125:A:PRO:HB3	1:129:A:TRP:HD1	3	0.14	0.02	0.13
(1,464)	1:135:A:THR:H	1:133:A:ARG:HB3	3	0.13	0.01	0.14
(1,606)	1:89:A:HIS:HA	1:88:A:HIS:HE1	3	0.13	0.02	0.12
(1,912)	1:99:A:GLY:H	2:149:B:THR:HG21	3	0.12	0.03	0.11
(1,912)	1:99:A:GLY:H	2:149:B:THR:HG22	3	0.12	0.03	0.11
(1,912)	1:99:A:GLY:H	2:149:B:THR:HG23	3	0.12	0.03	0.11
(1,950)	1:103:A:LEU:HD21	2:146:B:THR:HG21	3	0.12	0.01	0.12
(1,950)	1:103:A:LEU:HD21	2:146:B:THR:HG22	3	0.12	0.01	0.12
(1,950)	1:103:A:LEU:HD21	2:146:B:THR:HG23	3	0.12	0.01	0.12
(1,950)	1:103:A:LEU:HD22	2:146:B:THR:HG21	3	0.12	0.01	0.12
(1,950)	1:103:A:LEU:HD22	2:146:B:THR:HG22	3	0.12	0.01	0.12
(1,950)	1:103:A:LEU:HD22	2:146:B:THR:HG23	3	0.12	0.01	0.12
(1,950)	1:103:A:LEU:HD23	2:146:B:THR:HG21	3	0.12	0.01	0.12
(1,950)	1:103:A:LEU:HD23	2:146:B:THR:HG22	3	0.12	0.01	0.12
(1,950)	1:103:A:LEU:HD23	2:146:B:THR:HG23	3	0.12	0.01	0.12
(1,520)	1:113:A:HIS:H	1:116:A:CYS:HA	3	0.12	0.01	0.12
(1,896)	1:102:A:LEU:HD21	2:147:B:LYS:HE2	3	0.11	0.01	0.11
(1,896)	1:102:A:LEU:HD22	2:147:B:LYS:HE2	3	0.11	0.01	0.11
(1,896)	1:102:A:LEU:HD23	2:147:B:LYS:HE2	3	0.11	0.01	0.11
(1,290)	1:99:A:GLY:H	1:92:A:PHE:HD1	2	0.31	0.11	0.31
(1,290)	1:99:A:GLY:H	1:92:A:PHE:HD2	2	0.31	0.11	0.31
(1,589)	1:134:A:CYS:HA	1:130:A:LEU:HD13	2	0.3	0.01	0.3
(1,74)	1:107:A:THR:HG23	1:130:A:LEU:HG	2	0.26	0.16	0.26
(1,74)	1:107:A:THR:HG21	1:130:A:LEU:HG	2	0.26	0.16	0.26
(1,979)	1:101:A:GLU:HG2	2:146:B:THR:HG21	2	0.26	0.15	0.26
(1,979)	1:101:A:GLU:HG2	2:146:B:THR:HG22	2	0.26	0.15	0.26
(1,979)	1:101:A:GLU:HG2	2:146:B:THR:HG23	2	0.26	0.15	0.26

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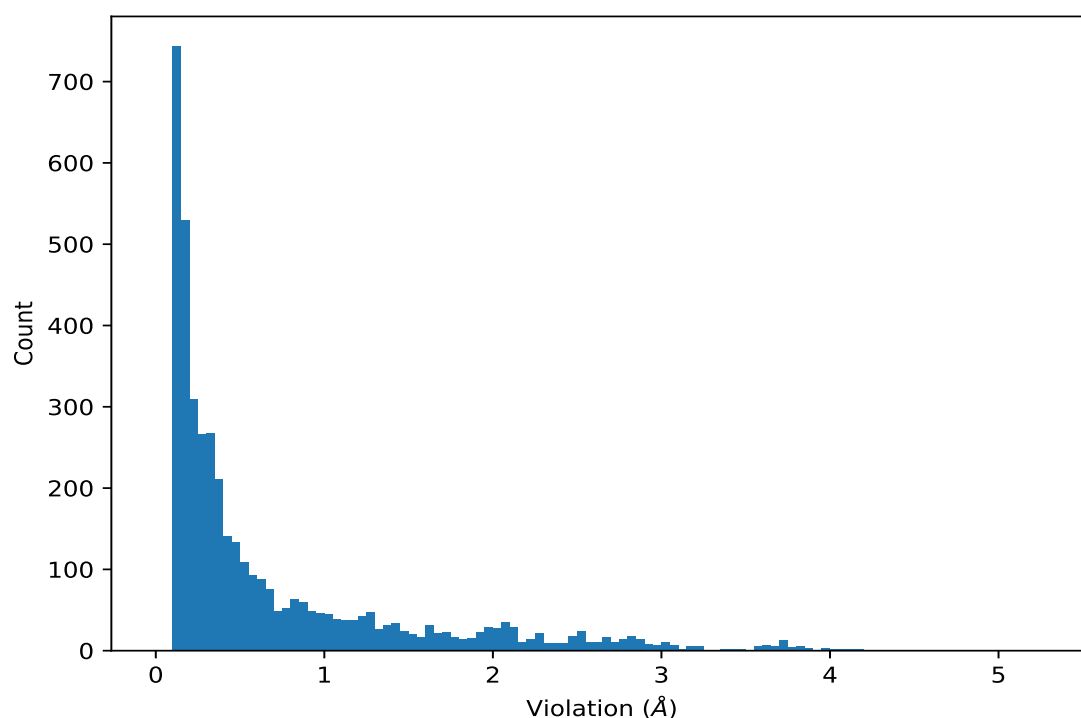
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,979)	1:101:A:GLU:HG3	2:146:B:THR:HG21	2	0.26	0.15	0.26
(1,979)	1:101:A:GLU:HG3	2:146:B:THR:HG22	2	0.26	0.15	0.26
(1,979)	1:101:A:GLU:HG3	2:146:B:THR:HG23	2	0.26	0.15	0.26
(1,861)	2:146:B:THR:H	2:145:B:ARG:HG2	2	0.24	0.12	0.24
(1,185)	1:118:A:ASN:HB2	1:118:A:ASN:H	2	0.24	0.03	0.24
(1,293)	1:99:A:GLY:H	1:98:A:ASP:HB2	2	0.24	0.08	0.24
(1,25)	1:131:A:CYS:HA	1:105:A:CYS:H	2	0.22	0.09	0.22
(1,25)	1:111:A:SER:HB2	1:105:A:CYS:H	2	0.22	0.09	0.22
(1,645)	1:101:A:GLU:HG2	1:114:A:ILE:HD13	2	0.18	0.04	0.18
(1,645)	1:101:A:GLU:HG2	1:114:A:ILE:HD11	2	0.18	0.04	0.18
(1,663)	1:118:A:ASN:HA	1:120:A:PRO:HD2	2	0.17	0.07	0.17
(1,26)	1:131:A:CYS:HB3	1:105:A:CYS:H	2	0.16	0.04	0.16
(1,766)	1:109:A:PRO:HA	1:90:A:MET:H	2	0.12	0.02	0.12
(1,893)	1:103:A:LEU:HD21	2:144:B:ALA:HB1	2	0.12	0.01	0.12
(1,893)	1:103:A:LEU:HD21	2:144:B:ALA:HB2	2	0.12	0.01	0.12
(1,893)	1:103:A:LEU:HD21	2:144:B:ALA:HB3	2	0.12	0.01	0.12
(1,893)	1:103:A:LEU:HD22	2:144:B:ALA:HB1	2	0.12	0.01	0.12
(1,893)	1:103:A:LEU:HD22	2:144:B:ALA:HB2	2	0.12	0.01	0.12
(1,893)	1:103:A:LEU:HD22	2:144:B:ALA:HB3	2	0.12	0.01	0.12
(1,893)	1:103:A:LEU:HD23	2:144:B:ALA:HB1	2	0.12	0.01	0.12
(1,893)	1:103:A:LEU:HD23	2:144:B:ALA:HB2	2	0.12	0.01	0.12
(1,893)	1:103:A:LEU:HD23	2:144:B:ALA:HB3	2	0.12	0.01	0.12
(1,240)	1:93:A:CYS:HA	1:96:A:CYS:H	2	0.12	0.01	0.12
(1,517)	1:117:A:LEU:H	1:117:A:LEU:HD22	2	0.12	0.0	0.12
(1,793)	1:103:A:LEU:HB3	1:104:A:CYS:H	2	0.12	0.0	0.12
(1,729)	1:110:A:SER:HA	1:112:A:TYR: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)
(1,62)	1:121:A:LEU:HD11	1:103:A:LEU:HD12	7	5.3
(1,62)	1:121:A:LEU:HD11	1:103:A:LEU:HD12	6	5.06
(1,62)	1:121:A:LEU:HD13	1:103:A:LEU:HD12	20	4.91
(1,62)	1:121:A:LEU:HD11	1:103:A:LEU:HD11	2	4.79
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	16	4.34
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	5	4.18
(1,1)	1:121:A:LEU:HD13	1:124:A:ILE:HG13	6	4.17
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	9	4.11
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	14	4.1
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	20	4.07
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	18	4.06
(1,1)	1:121:A:LEU:HD11	1:130:A:LEU:HB2	7	4.04
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	1	4.0
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD11	7	3.99
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	12	3.98
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	19	3.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	2	3.91
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD13	20	3.87
(1,1)	1:121:A:LEU:HD13	1:124:A:ILE:HG13	2	3.86
(1,1)	1:121:A:LEU:HD13	1:130:A:LEU:HB2	20	3.86
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD13	10	3.84
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD13	4	3.82
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD13	7	3.82
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD11	16	3.8
(1,95)	1:94:A:ARG:HA	1:92:A:PHE:HD1	2	3.8
(1,95)	1:94:A:ARG:HA	1:92:A:PHE:HD1	5	3.78
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD12	15	3.76
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD11	16	3.76
(1,95)	1:94:A:ARG:HA	1:92:A:PHE:HD1	1	3.76
(1,697)	1:97:A:LYS:HD2	1:92:A:PHE:HD1	13	3.74
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD12	19	3.73
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	12	3.72
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD13	1	3.72
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD13	7	3.72
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD13	20	3.72
(1,95)	1:94:A:ARG:HA	1:92:A:PHE:HD1	13	3.72
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD11	2	3.71
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD12	18	3.71
(1,95)	1:94:A:ARG:HA	1:92:A:PHE:HD1	9	3.71
(1,689)	1:97:A:LYS:HD3	1:92:A:PHE:HE1	13	3.7
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD13	4	3.7
(1,95)	1:94:A:ARG:HA	1:92:A:PHE:HD1	16	3.7
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD12	6	3.69
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD13	10	3.69
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD11	6	3.68
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD12	19	3.68
(1,95)	1:94:A:ARG:HA	1:92:A:PHE:HD1	19	3.66
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD13	1	3.64
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD12	18	3.64
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	3	3.63
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	2	3.63
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD12	15	3.63
(1,95)	1:94:A:ARG:HA	1:92:A:PHE:HD1	18	3.62
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD12	6	3.61
(1,95)	1:94:A:ARG:HA	1:92:A:PHE:HD1	12	3.57
(1,95)	1:94:A:ARG:HA	1:92:A:PHE:HD1	14	3.57
(1,95)	1:94:A:ARG:HA	1:92:A:PHE:HD1	20	3.57
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	1	3.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD13	20	3.55
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD11	2	3.55
(1,95)	1:94:A:ARG:HA	1:92:A:PHE:HD1	3	3.51
(1,557)	1:97:A:LYS:HD2	1:92:A:PHE:HE1	13	3.45
(1,428)	1:130:A:LEU:HD13	1:108:A:CYS:H	18	3.45
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	13	3.41
(1,578)	1:130:A:LEU:HD12	1:106:A:ASP:HB2	18	3.41
(1,689)	1:97:A:LYS:HD3	1:92:A:PHE:HE1	16	3.38
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD11	2	3.38
(1,689)	1:97:A:LYS:HD3	1:92:A:PHE:HE1	18	3.28
(1,689)	1:97:A:LYS:HD3	1:92:A:PHE:HE1	5	3.22
(1,689)	1:97:A:LYS:HD3	1:92:A:PHE:HE1	19	3.22
(1,689)	1:97:A:LYS:HD3	1:92:A:PHE:HE1	20	3.22
(1,57)	1:103:A:LEU:HD21	1:104:A:CYS:HB3	6	3.22
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD22	15	3.21
(1,57)	1:103:A:LEU:HD21	1:104:A:CYS:HB3	4	3.21
(1,691)	1:97:A:LYS:HG3	1:92:A:PHE:HE1	16	3.16
(1,57)	1:103:A:LEU:HD23	1:104:A:CYS:HB3	3	3.16
(1,57)	1:103:A:LEU:HD22	1:104:A:CYS:HB3	18	3.16
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD12	11	3.15
(1,57)	1:103:A:LEU:HD22	1:104:A:CYS:HB3	8	3.15
(1,147)	1:92:A:PHE:HD1	1:94:A:ARG:H	2	3.13
(1,689)	1:97:A:LYS:HD3	1:92:A:PHE:HE1	9	3.1
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD13	18	3.09
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD22	10	3.08
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	19	3.08
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD22	2	3.06
(1,533)	1:102:A:LEU:HD11	1:113:A:HIS:HD2	6	3.06
(1,147)	1:92:A:PHE:HD1	1:94:A:ARG:H	1	3.06
(1,147)	1:92:A:PHE:HD1	1:94:A:ARG:H	9	3.06
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD21	19	3.03
(1,533)	1:102:A:LEU:HD11	1:113:A:HIS:HD2	18	3.03
(1,587)	1:114:A:ILE:HA	1:121:A:LEU:HD11	20	3.02
(1,533)	1:102:A:LEU:HD11	1:113:A:HIS:HD2	19	3.02
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD12	5	3.01
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD13	19	3.01
(1,691)	1:97:A:LYS:HG3	1:92:A:PHE:HE1	5	3.0
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD13	8	3.0
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD12	12	3.0
(1,587)	1:114:A:ILE:HA	1:121:A:LEU:HD12	2	3.0
(1,147)	1:92:A:PHE:HD1	1:94:A:ARG:H	13	3.0
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD11	3	2.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:121:A:LEU:HD11	1:125:A:PRO:HB2	7	2.99
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD21	6	2.98
(1,689)	1:97:A:LYS:HD3	1:92:A:PHE:HE1	14	2.97
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD11	4	2.96
(1,57)	1:103:A:LEU:HD23	1:104:A:CYS:HB3	16	2.96
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	3	2.95
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD12	9	2.94
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD13	10	2.94
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD11	14	2.91
(1,147)	1:92:A:PHE:HD1	1:94:A:ARG:H	18	2.91
(1,691)	1:97:A:LYS:HG3	1:92:A:PHE:HE1	14	2.9
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD23	18	2.9
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD11	16	2.9
(1,147)	1:92:A:PHE:HD1	1:94:A:ARG:H	12	2.9
(1,691)	1:97:A:LYS:HG3	1:92:A:PHE:HE1	9	2.89
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD13	6	2.88
(1,532)	1:103:A:LEU:HD12	1:129:A:TRP:HZ2	10	2.88
(1,147)	1:92:A:PHE:HD1	1:94:A:ARG:H	19	2.88
(1,147)	1:92:A:PHE:HD1	1:94:A:ARG:H	14	2.87
(1,691)	1:97:A:LYS:HG3	1:92:A:PHE:HE1	18	2.86
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD12	17	2.86
(1,587)	1:114:A:ILE:HA	1:121:A:LEU:HD12	6	2.86
(1,532)	1:103:A:LEU:HD12	1:129:A:TRP:HZ2	18	2.86
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD21	1	2.85
(1,532)	1:103:A:LEU:HD11	1:129:A:TRP:HZ2	11	2.85
(1,532)	1:103:A:LEU:HD12	1:129:A:TRP:HZ2	19	2.85
(1,147)	1:92:A:PHE:HD1	1:94:A:ARG:H	5	2.85
(1,147)	1:92:A:PHE:HD1	1:94:A:ARG:H	16	2.85
(1,532)	1:103:A:LEU:HD13	1:129:A:TRP:HZ2	4	2.84
(1,532)	1:103:A:LEU:HD12	1:129:A:TRP:HZ2	15	2.84
(1,147)	1:92:A:PHE:HD1	1:94:A:ARG:H	3	2.84
(1,691)	1:97:A:LYS:HG3	1:92:A:PHE:HE1	20	2.83
(1,533)	1:102:A:LEU:HD13	1:113:A:HIS:HD2	16	2.83
(1,532)	1:103:A:LEU:HD12	1:129:A:TRP:HZ2	7	2.83
(1,532)	1:103:A:LEU:HD12	1:129:A:TRP:HZ2	20	2.83
(1,532)	1:103:A:LEU:HD11	1:129:A:TRP:HZ2	5	2.82
(1,532)	1:103:A:LEU:HD11	1:129:A:TRP:HZ2	9	2.82
(1,532)	1:103:A:LEU:HD11	1:129:A:TRP:HZ2	17	2.82
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD13	20	2.81
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD12	16	2.81
(1,532)	1:103:A:LEU:HD11	1:129:A:TRP:HZ2	12	2.81
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD13	4	2.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD13	7	2.8
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD12	1	2.8
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD13	7	2.8
(1,532)	1:103:A:LEU:HD11	1:129:A:TRP:HZ2	1	2.8
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD13	20	2.79
(1,532)	1:103:A:LEU:HD11	1:129:A:TRP:HZ2	16	2.79
(1,532)	1:103:A:LEU:HD13	1:129:A:TRP:HZ2	14	2.78
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD13	7	2.78
(1,147)	1:92:A:PHE:HD1	1:94:A:ARG:H	20	2.78
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD21	7	2.77
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD23	20	2.77
(1,532)	1:103:A:LEU:HD12	1:129:A:TRP:HZ2	6	2.77
(1,532)	1:103:A:LEU:HD12	1:129:A:TRP:HZ2	8	2.77
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD13	4	2.77
(1,691)	1:97:A:LYS:HG3	1:92:A:PHE:HE1	19	2.76
(1,550)	1:90:A:MET:HE2	1:92:A:PHE:HE1	19	2.75
(1,532)	1:103:A:LEU:HD11	1:129:A:TRP:HZ2	2	2.75
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD13	20	2.75
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD23	16	2.74
(1,691)	1:97:A:LYS:HG3	1:92:A:PHE:HE1	12	2.73
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD13	1	2.73
(1,550)	1:90:A:MET:HE2	1:92:A:PHE:HE1	18	2.73
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD13	16	2.72
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	18	2.71
(1,532)	1:103:A:LEU:HD13	1:129:A:TRP:HZ2	3	2.71
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD11	16	2.71
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD12	19	2.71
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD12	2	2.7
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD13	13	2.69
(1,685)	1:97:A:LYS:HA	1:92:A:PHE:HD1	16	2.68
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD13	10	2.68
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	12	2.68
(1,533)	1:102:A:LEU:HD12	1:113:A:HIS:HD2	10	2.68
(1,533)	1:102:A:LEU:HD12	1:113:A:HIS:HD2	20	2.68
(1,533)	1:102:A:LEU:HD12	1:113:A:HIS:HD2	1	2.67
(1,532)	1:103:A:LEU:HD12	1:129:A:TRP:HZ2	13	2.67
(1,811)	1:92:A:PHE:HD1	1:97:A:LYS:H	12	2.66
(1,811)	1:92:A:PHE:HD1	1:97:A:LYS:H	18	2.66
(1,691)	1:97:A:LYS:HG3	1:92:A:PHE:HE1	2	2.66
(1,685)	1:97:A:LYS:HA	1:92:A:PHE:HD1	12	2.66
(1,685)	1:97:A:LYS:HA	1:92:A:PHE:HD1	18	2.66
(1,550)	1:90:A:MET:HE2	1:92:A:PHE:HE1	5	2.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD11	2	2.65
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	16	2.65
(1,550)	1:90:A:MET:HE3	1:92:A:PHE:HE1	12	2.65
(1,550)	1:90:A:MET:HE3	1:92:A:PHE:HE1	2	2.64
(1,550)	1:90:A:MET:HE1	1:92:A:PHE:HE1	20	2.64
(1,685)	1:97:A:LYS:HA	1:92:A:PHE:HD1	5	2.63
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	5	2.63
(1,533)	1:102:A:LEU:HD12	1:113:A:HIS:HD2	4	2.63
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD12	15	2.62
(1,691)	1:97:A:LYS:HG3	1:92:A:PHE:HE1	1	2.61
(1,533)	1:102:A:LEU:HD12	1:113:A:HIS:HD2	7	2.61
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD13	1	2.61
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD13	10	2.6
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD12	18	2.6
(1,811)	1:92:A:PHE:HD1	1:97:A:LYS:H	13	2.59
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	13	2.58
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD13	4	2.57
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	19	2.57
(1,550)	1:90:A:MET:HE1	1:92:A:PHE:HE1	1	2.57
(1,533)	1:102:A:LEU:HD13	1:113:A:HIS:HD2	2	2.57
(1,811)	1:92:A:PHE:HD1	1:97:A:LYS:H	5	2.55
(1,811)	1:92:A:PHE:HD1	1:97:A:LYS:H	16	2.55
(1,811)	1:92:A:PHE:HD1	1:97:A:LYS:H	19	2.55
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD12	6	2.55
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM13	16	2.54
(1,685)	1:97:A:LYS:HA	1:92:A:PHE:HD1	1	2.54
(1,533)	1:102:A:LEU:HD11	1:113:A:HIS:HD2	15	2.54
(1,811)	1:92:A:PHE:HD1	1:97:A:LYS:H	1	2.53
(1,685)	1:97:A:LYS:HA	1:92:A:PHE:HD1	19	2.53
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD22	4	2.53
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD13	7	2.53
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	20	2.53
(1,208)	1:103:A:LEU:HD22	1:104:A:CYS:H	9	2.53
(1,208)	1:103:A:LEU:HD22	1:104:A:CYS:H	14	2.53
(1,697)	1:97:A:LYS:HD2	1:92:A:PHE:HD1	2	2.52
(1,685)	1:97:A:LYS:HA	1:92:A:PHE:HD1	20	2.52
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD11	2	2.52
(1,352)	1:113:A:HIS:H	1:102:A:LEU:HD12	15	2.52
(1,208)	1:103:A:LEU:HD21	1:104:A:CYS:H	8	2.52
(1,208)	1:103:A:LEU:HD23	1:104:A:CYS:H	15	2.52
(1,685)	1:97:A:LYS:HA	1:92:A:PHE:HD1	9	2.51
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	2	2.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:103:A:LEU:HD23	1:104:A:CYS:H	3	2.51
(1,208)	1:103:A:LEU:HD23	1:104:A:CYS:H	10	2.51
(1,208)	1:103:A:LEU:HD21	1:104:A:CYS:H	17	2.51
(1,208)	1:103:A:LEU:HD22	1:104:A:CYS:H	18	2.51
(1,208)	1:103:A:LEU:HD21	1:104:A:CYS:H	6	2.5
(1,208)	1:103:A:LEU:HD23	1:104:A:CYS:H	12	2.5
(1,617)	1:114:A:ILE:HA	1:103:A:LEU:HD13	15	2.49
(1,550)	1:90:A:MET:HE2	1:92:A:PHE:HE1	14	2.49
(1,208)	1:103:A:LEU:HD21	1:104:A:CYS:H	4	2.49
(1,811)	1:92:A:PHE:HD1	1:97:A:LYS:H	9	2.48
(1,696)	1:90:A:MET:HE2	1:92:A:PHE:HD1	18	2.48
(1,811)	1:92:A:PHE:HD1	1:97:A:LYS:H	2	2.47
(1,691)	1:97:A:LYS:HG3	1:92:A:PHE:HE1	13	2.47
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD13	1	2.47
(1,208)	1:103:A:LEU:HD23	1:104:A:CYS:H	5	2.47
(1,208)	1:103:A:LEU:HD23	1:104:A:CYS:H	11	2.47
(1,208)	1:103:A:LEU:HD23	1:104:A:CYS:H	19	2.47
(1,685)	1:97:A:LYS:HA	1:92:A:PHE:HD1	2	2.46
(1,685)	1:97:A:LYS:HA	1:92:A:PHE:HD1	14	2.46
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	1	2.46
(1,208)	1:103:A:LEU:HD21	1:104:A:CYS:H	7	2.46
(1,811)	1:92:A:PHE:HD1	1:97:A:LYS:H	20	2.45
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	9	2.45
(1,208)	1:103:A:LEU:HD23	1:104:A:CYS:H	1	2.45
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD12	18	2.44
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD13	2	2.44
(1,208)	1:103:A:LEU:HD21	1:104:A:CYS:H	20	2.44
(1,696)	1:90:A:MET:HE2	1:92:A:PHE:HD1	19	2.43
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	14	2.43
(1,685)	1:97:A:LYS:HA	1:92:A:PHE:HD1	13	2.42
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD12	19	2.42
(1,811)	1:92:A:PHE:HD1	1:97:A:LYS:H	14	2.4
(1,550)	1:90:A:MET:HE2	1:92:A:PHE:HE1	3	2.4
(1,691)	1:97:A:LYS:HG3	1:92:A:PHE:HE1	3	2.39
(1,621)	1:113:A:HIS:HB2	1:102:A:LEU:HD12	6	2.39
(1,587)	1:114:A:ILE:HA	1:121:A:LEU:HD12	7	2.38
(1,208)	1:103:A:LEU:HD22	1:104:A:CYS:H	2	2.38
(1,696)	1:90:A:MET:HE3	1:92:A:PHE:HD1	2	2.37
(1,696)	1:90:A:MET:HE3	1:92:A:PHE:HD1	12	2.37
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD11	16	2.37
(1,62)	1:121:A:LEU:HD13	1:103:A:LEU:HD11	5	2.37
(1,696)	1:90:A:MET:HE2	1:92:A:PHE:HD1	5	2.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD13	10	2.34
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD13	7	2.34
(1,697)	1:97:A:LYS:HD2	1:92:A:PHE:HD1	1	2.33
(1,61)	1:117:A:LEU:HD13	1:103:A:LEU:HD12	18	2.32
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD12	20	2.31
(1,208)	1:103:A:LEU:HD22	1:104:A:CYS:H	16	2.31
(1,62)	1:121:A:LEU:HD13	1:103:A:LEU:HD13	3	2.31
(1,550)	1:90:A:MET:HE1	1:92:A:PHE:HE1	13	2.3
(1,550)	1:90:A:MET:HE1	1:92:A:PHE:HE1	16	2.3
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM21	2	2.29
(1,768)	1:92:A:PHE:HD1	1:98:A:ASP:H	12	2.29
(1,696)	1:90:A:MET:HE1	1:92:A:PHE:HD1	20	2.29
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	3	2.29
(1,550)	1:90:A:MET:HE3	1:92:A:PHE:HE1	9	2.29
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD13	20	2.29
(1,689)	1:97:A:LYS:HD3	1:92:A:PHE:HE1	3	2.28
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD13	1	2.28
(1,64)	1:121:A:LEU:HD11	1:125:A:PRO:HB2	6	2.28
(1,61)	1:117:A:LEU:HD11	1:103:A:LEU:HD11	9	2.28
(1,811)	1:92:A:PHE:HD1	1:97:A:LYS:H	3	2.27
(1,768)	1:92:A:PHE:HD1	1:98:A:ASP:H	18	2.26
(1,696)	1:90:A:MET:HE2	1:92:A:PHE:HD1	3	2.26
(1,61)	1:117:A:LEU:HD11	1:103:A:LEU:HD13	10	2.26
(1,61)	1:117:A:LEU:HD12	1:103:A:LEU:HD11	16	2.26
(1,696)	1:90:A:MET:HE1	1:92:A:PHE:HD1	1	2.25
(1,685)	1:97:A:LYS:HA	1:92:A:PHE:HD1	3	2.25
(1,557)	1:97:A:LYS:HD2	1:92:A:PHE:HE1	2	2.25
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD13	4	2.25
(1,208)	1:103:A:LEU:HD22	1:104:A:CYS:H	13	2.25
(1,61)	1:117:A:LEU:HD11	1:103:A:LEU:HD11	1	2.25
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	16	2.24
(1,61)	1:117:A:LEU:HD13	1:103:A:LEU:HD11	5	2.23
(1,61)	1:117:A:LEU:HD13	1:103:A:LEU:HD12	8	2.23
(1,689)	1:97:A:LYS:HD3	1:92:A:PHE:HE1	12	2.22
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	14	2.22
(1,62)	1:121:A:LEU:HD13	1:103:A:LEU:HD12	8	2.22
(1,62)	1:121:A:LEU:HD12	1:103:A:LEU:HD12	19	2.22
(1,57)	1:103:A:LEU:HD23	1:104:A:CYS:HB3	15	2.22
(1,768)	1:92:A:PHE:HD1	1:98:A:ASP:H	19	2.21
(1,674)	1:97:A:LYS:HD3	1:92:A:PHE:HD1	13	2.21
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD12	15	2.21
(1,61)	1:117:A:LEU:HD11	1:103:A:LEU:HD11	17	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:97:A:LYS:HD2	1:92:A:PHE:HE1	16	2.2
(1,557)	1:97:A:LYS:HD2	1:92:A:PHE:HE1	18	2.2
(1,874)	2:150:B:ALA:HB2	2:151:B:ARG:HD2	4	2.19
(1,62)	1:121:A:LEU:HD12	1:103:A:LEU:HD11	1	2.19
(1,61)	1:117:A:LEU:HD12	1:103:A:LEU:HD13	4	2.19
(1,61)	1:117:A:LEU:HD13	1:103:A:LEU:HD11	11	2.19
(1,62)	1:121:A:LEU:HD11	1:103:A:LEU:HD13	14	2.18
(1,41)	1:102:A:LEU:HD11	1:93:A:CYS:HB2	16	2.18
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD12	18	2.17
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD12	19	2.16
(1,768)	1:92:A:PHE:HD1	1:98:A:ASP:H	13	2.15
(1,61)	1:117:A:LEU:HD11	1:103:A:LEU:HD13	7	2.15
(1,41)	1:102:A:LEU:HD13	1:93:A:CYS:HB2	4	2.15
(1,768)	1:92:A:PHE:HD1	1:98:A:ASP:H	5	2.14
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD13	10	2.14
(1,768)	1:92:A:PHE:HD1	1:98:A:ASP:H	2	2.13
(1,768)	1:92:A:PHE:HD1	1:98:A:ASP:H	20	2.13
(1,557)	1:97:A:LYS:HD2	1:92:A:PHE:HE1	19	2.13
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	13	2.13
(1,61)	1:117:A:LEU:HD13	1:103:A:LEU:HD12	6	2.13
(1,61)	1:117:A:LEU:HD11	1:103:A:LEU:HD11	12	2.13
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG21	9	2.12
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG22	9	2.12
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG23	9	2.12
(1,697)	1:97:A:LYS:HD2	1:92:A:PHE:HD1	16	2.12
(1,696)	1:90:A:MET:HE1	1:92:A:PHE:HD1	13	2.12
(1,696)	1:90:A:MET:HE2	1:92:A:PHE:HD1	14	2.12
(1,696)	1:90:A:MET:HE1	1:92:A:PHE:HD1	16	2.12
(1,689)	1:97:A:LYS:HD3	1:92:A:PHE:HE1	1	2.12
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	5	2.12
(1,61)	1:117:A:LEU:HD12	1:103:A:LEU:HD12	19	2.12
(1,557)	1:97:A:LYS:HD2	1:92:A:PHE:HE1	5	2.11
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD11	2	2.11
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG21	12	2.1
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG22	12	2.1
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG23	12	2.1
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG21	16	2.1
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG22	16	2.1
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG23	16	2.1
(1,768)	1:92:A:PHE:HD1	1:98:A:ASP:H	14	2.1
(1,557)	1:97:A:LYS:HD2	1:92:A:PHE:HE1	20	2.1
(1,62)	1:121:A:LEU:HD12	1:103:A:LEU:HD11	9	2.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG21	14	2.09
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG22	14	2.09
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG23	14	2.09
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG21	20	2.09
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG22	20	2.09
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG23	20	2.09
(1,61)	1:117:A:LEU:HD13	1:103:A:LEU:HD13	20	2.09
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG21	19	2.08
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG22	19	2.08
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG23	19	2.08
(1,874)	2:150:B:ALA:HB3	2:151:B:ARG:HD2	5	2.08
(1,874)	2:150:B:ALA:HB2	2:151:B:ARG:HD2	8	2.08
(1,62)	1:121:A:LEU:HD13	1:103:A:LEU:HD12	18	2.08
(1,61)	1:117:A:LEU:HD11	1:103:A:LEU:HD11	3	2.08
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG21	3	2.07
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG22	3	2.07
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG23	3	2.07
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG21	18	2.07
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG22	18	2.07
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG23	18	2.07
(1,874)	2:150:B:ALA:HB2	2:151:B:ARG:HD2	11	2.07
(1,768)	1:92:A:PHE:HD1	1:98:A:ASP:H	3	2.07
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD12	6	2.07
(1,62)	1:121:A:LEU:HD11	1:103:A:LEU:HD12	15	2.07
(1,41)	1:102:A:LEU:HD13	1:93:A:CYS:HB2	7	2.07
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM21	9	2.06
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM33	20	2.06
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG21	13	2.06
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG22	13	2.06
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG23	13	2.06
(1,62)	1:121:A:LEU:HD12	1:103:A:LEU:HD11	16	2.06
(1,57)	1:103:A:LEU:HD23	1:104:A:CYS:HB3	10	2.06
(1,57)	1:103:A:LEU:HD21	1:104:A:CYS:HB3	12	2.06
(1,874)	2:150:B:ALA:HB2	2:151:B:ARG:HD2	17	2.05
(1,57)	1:103:A:LEU:HD21	1:104:A:CYS:HB3	20	2.05
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM13	18	2.04
(1,557)	1:97:A:LYS:HD2	1:92:A:PHE:HE1	9	2.04
(1,62)	1:121:A:LEU:HD12	1:103:A:LEU:HD11	11	2.04
(1,62)	1:121:A:LEU:HD12	1:103:A:LEU:HD12	13	2.04
(1,768)	1:92:A:PHE:HD1	1:98:A:ASP:H	9	2.03
(1,768)	1:92:A:PHE:HD1	1:98:A:ASP:H	16	2.03
(1,697)	1:97:A:LYS:HD2	1:92:A:PHE:HD1	9	2.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,696)	1:90:A:MET:HE3	1:92:A:PHE:HD1	9	2.03
(1,62)	1:121:A:LEU:HD12	1:103:A:LEU:HD11	17	2.03
(1,61)	1:117:A:LEU:HD11	1:103:A:LEU:HD11	2	2.03
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM11	12	2.02
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG21	2	2.02
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG22	2	2.02
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG23	2	2.02
(1,874)	2:150:B:ALA:HB2	2:151:B:ARG:HD2	3	2.02
(1,874)	2:150:B:ALA:HB2	2:151:B:ARG:HD2	6	2.02
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD13	18	2.02
(1,697)	1:97:A:LYS:HD2	1:92:A:PHE:HD1	19	2.01
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD13	1	2.01
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD13	10	2.01
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG21	5	2.0
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG22	5	2.0
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG23	5	2.0
(1,697)	1:97:A:LYS:HD2	1:92:A:PHE:HD1	18	2.0
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD13	4	2.0
(1,613)	1:114:A:ILE:HG22	1:103:A:LEU:HD11	4	2.0
(1,57)	1:103:A:LEU:HD21	1:104:A:CYS:HB3	7	2.0
(1,57)	1:103:A:LEU:HD21	1:104:A:CYS:HB3	11	2.0
(1,557)	1:97:A:LYS:HD2	1:92:A:PHE:HE1	1	1.99
(1,344)	1:102:A:LEU:HD11	1:103:A:LEU:H	16	1.99
(1,64)	1:121:A:LEU:HD13	1:125:A:PRO:HB2	20	1.99
(1,62)	1:121:A:LEU:HD12	1:103:A:LEU:HD11	12	1.99
(1,57)	1:103:A:LEU:HD23	1:104:A:CYS:HB3	14	1.99
(1,876)	2:149:B:THR:HG22	2:147:B:LYS:HE2	8	1.98
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD12	6	1.98
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD12	6	1.98
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM33	13	1.97
(1,874)	2:150:B:ALA:HB3	2:151:B:ARG:HD2	2	1.97
(1,874)	2:150:B:ALA:HB2	2:151:B:ARG:HD2	9	1.97
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD11	2	1.97
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD11	16	1.97
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD13	20	1.97
(1,613)	1:114:A:ILE:HG22	1:103:A:LEU:HD13	10	1.97
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	20	1.97
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD12	15	1.97
(1,61)	1:117:A:LEU:HD12	1:103:A:LEU:HD12	15	1.97
(1,57)	1:103:A:LEU:HD23	1:104:A:CYS:HB3	9	1.97
(1,41)	1:102:A:LEU:HD13	1:93:A:CYS:HB2	1	1.97
(1,41)	1:102:A:LEU:HD13	1:93:A:CYS:HB2	20	1.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:97:A:LYS:HD3	1:92:A:PHE:HD1	16	1.96
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD13	7	1.96
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD12	15	1.96
(1,66)	1:130:A:LEU:HD21	1:128:A:GLU:HB2	2	1.96
(1,62)	1:121:A:LEU:HD11	1:103:A:LEU:HD12	10	1.96
(1,768)	1:92:A:PHE:HD1	1:98:A:ASP:H	1	1.95
(1,61)	1:117:A:LEU:HD11	1:103:A:LEU:HD11	14	1.95
(1,57)	1:103:A:LEU:HD21	1:104:A:CYS:HB3	1	1.95
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG21	1	1.94
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG22	1	1.94
(1,904)	1:92:A:PHE:HD2	2:149:B:THR:HG23	1	1.94
(1,874)	2:150:B:ALA:HB1	2:151:B:ARG:HD2	19	1.94
(1,613)	1:114:A:ILE:HG23	1:103:A:LEU:HD13	8	1.94
(1,344)	1:102:A:LEU:HD13	1:103:A:LEU:H	20	1.94
(1,66)	1:130:A:LEU:HD21	1:128:A:GLU:HB2	12	1.94
(1,66)	1:130:A:LEU:HD22	1:128:A:GLU:HB2	18	1.94
(1,64)	1:121:A:LEU:HD11	1:125:A:PRO:HB2	2	1.94
(1,874)	2:150:B:ALA:HB1	2:151:B:ARG:HD2	18	1.93
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD12	19	1.93
(1,344)	1:102:A:LEU:HD13	1:103:A:LEU:H	7	1.93
(1,66)	1:130:A:LEU:HD22	1:128:A:GLU:HB2	13	1.93
(1,61)	1:117:A:LEU:HD13	1:103:A:LEU:HD13	13	1.93
(1,874)	2:150:B:ALA:HB1	2:151:B:ARG:HD2	10	1.92
(1,689)	1:97:A:LYS:HD3	1:92:A:PHE:HE1	2	1.92
(1,623)	1:102:A:LEU:HA	1:102:A:LEU:HD12	18	1.92
(1,57)	1:103:A:LEU:HD22	1:104:A:CYS:HB3	17	1.92
(1,874)	2:150:B:ALA:HB1	2:151:B:ARG:HD2	13	1.91
(1,697)	1:97:A:LYS:HD2	1:92:A:PHE:HD1	5	1.91
(1,344)	1:102:A:LEU:HD13	1:103:A:LEU:H	1	1.91
(1,66)	1:130:A:LEU:HD22	1:128:A:GLU:HB2	4	1.91
(1,41)	1:102:A:LEU:HD13	1:93:A:CYS:HB2	10	1.91
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM12	16	1.89
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD23	17	1.89
(1,613)	1:114:A:ILE:HG21	1:103:A:LEU:HD13	19	1.88
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD11	18	1.88
(1,270)	1:130:A:LEU:HD12	1:107:A:THR:H	18	1.88
(1,66)	1:130:A:LEU:HD21	1:128:A:GLU:HB2	8	1.88
(1,62)	1:121:A:LEU:HD12	1:103:A:LEU:HD13	4	1.88
(1,57)	1:103:A:LEU:HD21	1:104:A:CYS:HB3	19	1.88
(1,41)	1:102:A:LEU:HD11	1:93:A:CYS:HB2	2	1.88
(1,697)	1:97:A:LYS:HD2	1:92:A:PHE:HD1	20	1.87
(1,57)	1:103:A:LEU:HD21	1:104:A:CYS:HB3	5	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,613)	1:114:A:ILE:HG22	1:103:A:LEU:HD13	18	1.86
(1,344)	1:102:A:LEU:HD12	1:103:A:LEU:H	18	1.86
(1,344)	1:102:A:LEU:HD12	1:103:A:LEU:H	19	1.86
(1,66)	1:130:A:LEU:HD22	1:128:A:GLU:HB2	15	1.86
(1,697)	1:97:A:LYS:HD2	1:92:A:PHE:HD1	12	1.84
(1,613)	1:114:A:ILE:HG23	1:103:A:LEU:HD12	17	1.82
(1,683)	1:110:A:SER:HB3	1:112:A:TYR:HD1	2	1.81
(1,674)	1:97:A:LYS:HD3	1:92:A:PHE:HD1	19	1.81
(1,613)	1:114:A:ILE:HG22	1:103:A:LEU:HD12	11	1.81
(1,613)	1:114:A:ILE:HG22	1:103:A:LEU:HD13	20	1.81
(1,555)	1:94:A:ARG:HA	1:92:A:PHE:HE1	2	1.81
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM31	14	1.8
(1,874)	2:150:B:ALA:HB1	2:151:B:ARG:HD2	14	1.8
(1,674)	1:97:A:LYS:HD3	1:92:A:PHE:HD1	9	1.8
(1,674)	1:97:A:LYS:HD3	1:92:A:PHE:HD1	18	1.8
(1,613)	1:114:A:ILE:HG22	1:103:A:LEU:HD12	5	1.8
(1,613)	1:114:A:ILE:HG22	1:103:A:LEU:HD12	12	1.8
(1,555)	1:94:A:ARG:HA	1:92:A:PHE:HE1	5	1.8
(1,874)	2:150:B:ALA:HB1	2:151:B:ARG:HD2	7	1.79
(1,557)	1:97:A:LYS:HD2	1:92:A:PHE:HE1	14	1.79
(1,876)	2:149:B:THR:HG22	2:147:B:LYS:HE2	14	1.78
(1,874)	2:150:B:ALA:HB1	2:151:B:ARG:HD2	1	1.78
(1,697)	1:97:A:LYS:HD2	1:92:A:PHE:HD1	14	1.78
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD23	16	1.78
(1,568)	1:133:A:ARG:HD3	1:112:A:TYR:HE1	4	1.78
(1,66)	1:130:A:LEU:HD21	1:128:A:GLU:HB2	1	1.78
(1,874)	2:150:B:ALA:HB1	2:151:B:ARG:HD2	16	1.77
(1,57)	1:103:A:LEU:HD22	1:104:A:CYS:HB3	2	1.77
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM11	12	1.76
(1,613)	1:114:A:ILE:HG22	1:103:A:LEU:HD12	16	1.76
(1,555)	1:94:A:ARG:HA	1:92:A:PHE:HE1	1	1.76
(1,613)	1:114:A:ILE:HG21	1:103:A:LEU:HD13	7	1.75
(1,613)	1:114:A:ILE:HG21	1:103:A:LEU:HD12	9	1.75
(1,66)	1:130:A:LEU:HD22	1:128:A:GLU:HB2	17	1.75
(1,613)	1:114:A:ILE:HG21	1:103:A:LEU:HD11	14	1.74
(1,143)	1:130:A:LEU:HD12	1:106:A:ASP:H	18	1.74
(1,127)	1:121:A:LEU:HD11	1:129:A:TRP:HE1	2	1.74
(1,66)	1:130:A:LEU:HD21	1:128:A:GLU:HB2	14	1.74
(1,66)	1:130:A:LEU:HD23	1:128:A:GLU:HB2	19	1.74
(1,674)	1:97:A:LYS:HD3	1:92:A:PHE:HD1	5	1.73
(1,555)	1:94:A:ARG:HA	1:92:A:PHE:HE1	13	1.73
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	18	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,344)	1:102:A:LEU:HD13	1:103:A:LEU:H	4	1.73
(1,344)	1:102:A:LEU:HD12	1:103:A:LEU:H	6	1.73
(1,66)	1:130:A:LEU:HD21	1:128:A:GLU:HB2	20	1.73
(1,874)	2:150:B:ALA:HB3	2:151:B:ARG:HD2	20	1.72
(1,613)	1:114:A:ILE:HG23	1:103:A:LEU:HD12	1	1.72
(1,613)	1:114:A:ILE:HG22	1:103:A:LEU:HD11	3	1.72
(1,344)	1:102:A:LEU:HD11	1:103:A:LEU:H	2	1.72
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD22	11	1.71
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD12	19	1.71
(1,557)	1:97:A:LYS:HD2	1:92:A:PHE:HE1	12	1.71
(1,66)	1:130:A:LEU:HD23	1:128:A:GLU:HB2	9	1.71
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM11	1	1.7
(1,874)	2:150:B:ALA:HB3	2:151:B:ARG:HD2	15	1.7
(1,674)	1:97:A:LYS:HD3	1:92:A:PHE:HD1	20	1.7
(1,41)	1:102:A:LEU:HD12	1:93:A:CYS:HB2	15	1.7
(1,872)	2:147:B:LYS:H	2:148:B:GLN:HG2	6	1.69
(1,683)	1:110:A:SER:HB3	1:112:A:TYR:HD1	13	1.69
(1,333)	1:131:A:CYS:H	1:130:A:LEU:HD13	18	1.69
(1,568)	1:133:A:ARG:HD3	1:112:A:TYR:HE1	16	1.68
(1,683)	1:110:A:SER:HB3	1:112:A:TYR:HD1	4	1.67
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD22	14	1.67
(1,568)	1:133:A:ARG:HD3	1:112:A:TYR:HE1	2	1.67
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM22	19	1.66
(1,874)	2:150:B:ALA:HB3	2:151:B:ARG:HD2	12	1.66
(1,613)	1:114:A:ILE:HG23	1:103:A:LEU:HD13	13	1.66
(1,578)	1:130:A:LEU:HD12	1:106:A:ASP:HB2	13	1.66
(1,555)	1:94:A:ARG:HA	1:92:A:PHE:HE1	9	1.66
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	11	1.66
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	12	1.66
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM13	18	1.65
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM32	3	1.65
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM13	5	1.65
(1,555)	1:94:A:ARG:HA	1:92:A:PHE:HE1	18	1.65
(1,127)	1:121:A:LEU:HD11	1:129:A:TRP:HE1	6	1.65
(1,1)	1:121:A:LEU:HD13	1:124:A:ILE:HG13	5	1.65
(1,1)	1:121:A:LEU:HD12	1:124:A:ILE:HG13	19	1.65
(1,683)	1:110:A:SER:HB3	1:112:A:TYR:HD1	3	1.64
(1,683)	1:110:A:SER:HB3	1:112:A:TYR:HD1	20	1.64
(1,555)	1:94:A:ARG:HA	1:92:A:PHE:HE1	16	1.64
(1,344)	1:102:A:LEU:HD13	1:103:A:LEU:H	10	1.64
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	12	1.64
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	10	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	19	1.64
(1,683)	1:110:A:SER:HB3	1:112:A:TYR:HD1	7	1.63
(1,674)	1:97:A:LYS:HD3	1:92:A:PHE:HD1	14	1.63
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD23	9	1.63
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD22	20	1.63
(1,1)	1:121:A:LEU:HD11	1:124:A:ILE:HG13	15	1.63
(1,872)	2:147:B:LYS:H	2:148:B:GLN:HG2	5	1.62
(1,613)	1:114:A:ILE:HG21	1:103:A:LEU:HD12	2	1.62
(1,613)	1:114:A:ILE:HG21	1:103:A:LEU:HD13	6	1.62
(1,555)	1:94:A:ARG:HA	1:92:A:PHE:HE1	12	1.62
(1,555)	1:94:A:ARG:HA	1:92:A:PHE:HE1	19	1.62
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	9	1.62
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	9	1.62
(1,66)	1:130:A:LEU:HD21	1:128:A:GLU:HB2	6	1.62
(1,66)	1:130:A:LEU:HD21	1:128:A:GLU:HB2	10	1.62
(1,683)	1:110:A:SER:HB3	1:112:A:TYR:HD1	15	1.61
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD21	10	1.61
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	19	1.61
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	3	1.61
(1,66)	1:130:A:LEU:HD23	1:128:A:GLU:HB2	3	1.61
(1,66)	1:130:A:LEU:HD22	1:128:A:GLU:HB2	5	1.61
(1,57)	1:103:A:LEU:HD23	1:104:A:CYS:HB3	13	1.61
(1,613)	1:114:A:ILE:HG22	1:103:A:LEU:HD13	15	1.6
(1,555)	1:94:A:ARG:HA	1:92:A:PHE:HE1	20	1.6
(1,344)	1:102:A:LEU:HD12	1:103:A:LEU:H	15	1.6
(1,683)	1:110:A:SER:HB3	1:112:A:TYR:HD1	19	1.59
(1,872)	2:147:B:LYS:H	2:148:B:GLN:HG2	12	1.58
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	13	1.58
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD21	15	1.58
(1,66)	1:130:A:LEU:HD21	1:128:A:GLU:HB2	7	1.58
(1,66)	1:130:A:LEU:HD23	1:128:A:GLU:HB2	16	1.58
(1,41)	1:102:A:LEU:HD12	1:93:A:CYS:HB2	18	1.58
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD22	12	1.57
(1,41)	1:102:A:LEU:HD12	1:93:A:CYS:HB2	6	1.57
(1,1)	1:121:A:LEU:HD12	1:124:A:ILE:HG13	9	1.57
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD23	18	1.56
(1,213)	1:133:A:ARG:H	1:133:A:ARG:HD3	4	1.56
(1,1)	1:121:A:LEU:HD12	1:124:A:ILE:HG13	17	1.56
(1,600)	1:111:A:SER:HB2	1:102:A:LEU:HD12	17	1.55
(1,534)	1:98:A:ASP:HB3	1:113:A:HIS:HD2	16	1.55
(1,1)	1:121:A:LEU:HD12	1:124:A:ILE:HG13	13	1.55
(1,1)	1:121:A:LEU:HD11	1:124:A:ILE:HG13	14	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM21	9	1.54
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD22	14	1.54
(1,213)	1:133:A:ARG:H	1:133:A:ARG:HD3	6	1.54
(1,66)	1:130:A:LEU:HD21	1:128:A:GLU:HB2	11	1.54
(1,667)	1:129:A:TRP:HZ2	1:121:A:LEU:HD11	2	1.53
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD22	6	1.53
(1,568)	1:133:A:ARG:HD3	1:112:A:TYR:HE1	6	1.53
(1,127)	1:121:A:LEU:HD13	1:129:A:TRP:HE1	20	1.53
(1,126)	1:103:A:LEU:HD12	1:129:A:TRP:HE1	15	1.53
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	16	1.52
(1,213)	1:133:A:ARG:H	1:133:A:ARG:HD3	1	1.52
(1,213)	1:133:A:ARG:H	1:133:A:ARG:HD3	2	1.52
(1,1)	1:121:A:LEU:HD12	1:124:A:ILE:HG13	1	1.52
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD23	4	1.51
(1,1)	1:121:A:LEU:HD12	1:124:A:ILE:HG13	11	1.51
(1,555)	1:94:A:ARG:HA	1:92:A:PHE:HE1	14	1.5
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	11	1.5
(1,41)	1:102:A:LEU:HD12	1:93:A:CYS:HB2	19	1.5
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	10	1.5
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	13	1.5
(1,667)	1:129:A:TRP:HZ2	1:121:A:LEU:HD11	6	1.49
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	11	1.48
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD22	13	1.48
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD22	6	1.48
(1,578)	1:130:A:LEU:HD13	1:106:A:ASP:HB2	17	1.48
(1,111)	1:102:A:LEU:HA	1:111:A:SER:HB2	20	1.48
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	18	1.48
(1,42)	1:102:A:LEU:HD13	1:99:A:GLY:HA3	17	1.48
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	9	1.47
(1,697)	1:97:A:LYS:HD2	1:92:A:PHE:HD1	3	1.47
(1,578)	1:130:A:LEU:HD12	1:106:A:ASP:HB2	8	1.47
(1,568)	1:133:A:ARG:HD3	1:112:A:TYR:HE1	12	1.47
(1,126)	1:103:A:LEU:HD12	1:129:A:TRP:HE1	10	1.47
(1,111)	1:102:A:LEU:HA	1:111:A:SER:HB2	15	1.47
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	13	1.47
(1,94)	1:106:A:ASP:HA	1:130:A:LEU:HD12	18	1.47
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	3	1.46
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	7	1.46
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	10	1.46
(1,683)	1:110:A:SER:HB3	1:112:A:TYR:HD1	11	1.46
(1,667)	1:129:A:TRP:HZ2	1:121:A:LEU:HD13	20	1.46
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	9	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:102:A:LEU:HA	1:111:A:SER:HB2	5	1.45
(1,1)	1:121:A:LEU:HD12	1:124:A:ILE:HG13	16	1.45
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM23	20	1.44
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	1	1.44
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	18	1.44
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD22	11	1.44
(1,126)	1:103:A:LEU:HD12	1:129:A:TRP:HE1	20	1.44
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	6	1.44
(1,1)	1:121:A:LEU:HD13	1:124:A:ILE:HG13	18	1.44
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	6	1.43
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	12	1.43
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD22	3	1.43
(1,555)	1:94:A:ARG:HA	1:92:A:PHE:HE1	3	1.43
(1,126)	1:103:A:LEU:HD11	1:129:A:TRP:HE1	9	1.43
(1,111)	1:102:A:LEU:HA	1:111:A:SER:HB2	17	1.43
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	2	1.43
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	16	1.43
(1,1)	1:121:A:LEU:HD11	1:124:A:ILE:HG13	10	1.43
(1,1)	1:121:A:LEU:HD12	1:124:A:ILE:HG13	12	1.43
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	20	1.42
(1,683)	1:110:A:SER:HB3	1:112:A:TYR:HD1	14	1.42
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD23	18	1.42
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD22	5	1.42
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD13	4	1.42
(1,126)	1:103:A:LEU:HD13	1:129:A:TRP:HE1	4	1.42
(1,111)	1:102:A:LEU:HA	1:111:A:SER:HB2	1	1.42
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	10	1.42
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	17	1.42
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	1	1.42
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	2	1.41
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	17	1.41
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM22	2	1.4
(1,600)	1:111:A:SER:HB2	1:102:A:LEU:HD11	14	1.4
(1,557)	1:97:A:LYS:HD2	1:92:A:PHE:HE1	3	1.4
(1,126)	1:103:A:LEU:HD11	1:129:A:TRP:HE1	5	1.4
(1,111)	1:102:A:LEU:HA	1:111:A:SER:HB2	10	1.4
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD22	2	1.39
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD22	19	1.39
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD13	7	1.39
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	8	1.39
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	19	1.38
(1,568)	1:133:A:ARG:HD3	1:112:A:TYR:HE1	1	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:133:A:ARG:HD3	1:112:A:TYR:HE1	19	1.38
(1,126)	1:103:A:LEU:HD13	1:129:A:TRP:HE1	14	1.38
(1,111)	1:102:A:LEU:HA	1:111:A:SER:HB2	14	1.38
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	4	1.38
(1,126)	1:103:A:LEU:HD11	1:129:A:TRP:HE1	1	1.37
(1,126)	1:103:A:LEU:HD12	1:129:A:TRP:HE1	7	1.37
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	3	1.37
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	8	1.37
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	15	1.37
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	18	1.37
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD22	1	1.36
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	3	1.36
(1,126)	1:103:A:LEU:HD12	1:129:A:TRP:HE1	6	1.36
(1,126)	1:103:A:LEU:HD12	1:129:A:TRP:HE1	18	1.36
(1,665)	1:103:A:LEU:HD22	1:129:A:TRP:HE3	4	1.35
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD23	9	1.35
(1,600)	1:111:A:SER:HB2	1:102:A:LEU:HD11	5	1.35
(1,127)	1:121:A:LEU:HD11	1:129:A:TRP:HE1	7	1.35
(1,126)	1:103:A:LEU:HD11	1:129:A:TRP:HE1	2	1.35
(1,126)	1:103:A:LEU:HD11	1:129:A:TRP:HE1	16	1.35
(1,126)	1:103:A:LEU:HD12	1:129:A:TRP:HE1	19	1.35
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	18	1.35
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	12	1.35
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	19	1.35
(1,1)	1:121:A:LEU:HD13	1:124:A:ILE:HG13	3	1.35
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM33	13	1.34
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	14	1.34
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD13	20	1.34
(1,126)	1:103:A:LEU:HD11	1:129:A:TRP:HE1	12	1.34
(1,126)	1:103:A:LEU:HD11	1:129:A:TRP:HE1	17	1.34
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD23	17	1.33
(1,582)	1:103:A:LEU:HD12	1:125:A:PRO:HG3	18	1.33
(1,126)	1:103:A:LEU:HD12	1:129:A:TRP:HE1	8	1.33
(1,126)	1:103:A:LEU:HD11	1:129:A:TRP:HE1	11	1.33
(1,42)	1:102:A:LEU:HD12	1:99:A:GLY:HA3	13	1.33
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	7	1.33
(1,1)	1:121:A:LEU:HD13	1:124:A:ILE:HG13	8	1.33
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	7	1.32
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	14	1.32
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	5	1.32
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	14	1.32
(1,578)	1:130:A:LEU:HD13	1:106:A:ASP:HB2	5	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:102:A:LEU:HD11	1:101:A:GLU:H	6	1.31
(1,126)	1:103:A:LEU:HD13	1:129:A:TRP:HE1	3	1.31
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	11	1.31
(1,872)	2:147:B:LYS:H	2:148:B:GLN:HG2	13	1.3
(1,582)	1:103:A:LEU:HD11	1:125:A:PRO:HG3	17	1.3
(1,580)	1:90:A:MET:HE1	1:90:A:MET:HG2	13	1.3
(1,580)	1:90:A:MET:HE2	1:90:A:MET:HG2	19	1.3
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	12	1.3
(1,111)	1:102:A:LEU:HA	1:111:A:SER:HB2	4	1.3
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG23	12	1.29
(1,876)	2:149:B:THR:HG22	2:147:B:LYS:HE2	16	1.29
(1,582)	1:103:A:LEU:HD12	1:125:A:PRO:HG3	8	1.29
(1,582)	1:103:A:LEU:HD11	1:125:A:PRO:HG3	9	1.29
(1,582)	1:103:A:LEU:HD11	1:125:A:PRO:HG3	16	1.29
(1,580)	1:90:A:MET:HE3	1:90:A:MET:HG2	3	1.29
(1,580)	1:90:A:MET:HE3	1:90:A:MET:HG2	7	1.29
(1,580)	1:90:A:MET:HE1	1:90:A:MET:HG2	9	1.29
(1,580)	1:90:A:MET:HE2	1:90:A:MET:HG2	18	1.29
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	9	1.29
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG21	19	1.28
(1,582)	1:103:A:LEU:HD11	1:125:A:PRO:HG3	11	1.28
(1,582)	1:103:A:LEU:HD13	1:125:A:PRO:HG3	14	1.28
(1,580)	1:90:A:MET:HE1	1:90:A:MET:HG2	16	1.28
(1,580)	1:90:A:MET:HE1	1:90:A:MET:HG2	20	1.28
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	4	1.28
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	14	1.28
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	10	1.28
(1,111)	1:102:A:LEU:HA	1:111:A:SER:HB2	7	1.28
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	20	1.28
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG23	6	1.27
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG23	11	1.27
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG22	16	1.27
(1,580)	1:90:A:MET:HE3	1:90:A:MET:HG2	11	1.27
(1,375)	1:102:A:LEU:HD12	1:101:A:GLU:H	4	1.27
(1,93)	1:129:A:TRP:HA	1:130:A:LEU:HD23	18	1.27
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	13	1.27
(1,63)	1:121:A:LEU:HD12	1:117:A:LEU:HG	6	1.27
(1,33)	1:94:A:ARG:HB3	1:93:A:CYS:H	20	1.27
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG21	1	1.26
(1,665)	1:103:A:LEU:HD21	1:129:A:TRP:HE3	19	1.26
(1,582)	1:103:A:LEU:HD11	1:125:A:PRO:HG3	5	1.26
(1,582)	1:103:A:LEU:HD12	1:125:A:PRO:HG3	10	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,580)	1:90:A:MET:HE3	1:90:A:MET:HG2	10	1.26
(1,580)	1:90:A:MET:HE3	1:90:A:MET:HG2	12	1.26
(1,126)	1:103:A:LEU:HD12	1:129:A:TRP:HE1	13	1.26
(1,42)	1:102:A:LEU:HD12	1:99:A:GLY:HA3	5	1.26
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG21	14	1.25
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD21	3	1.25
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	11	1.25
(1,580)	1:90:A:MET:HE3	1:90:A:MET:HG2	2	1.25
(1,580)	1:90:A:MET:HE2	1:90:A:MET:HG2	14	1.25
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD11	16	1.25
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	1	1.25
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	19	1.25
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	3	1.25
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	6	1.25
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG23	15	1.24
(1,876)	2:149:B:THR:HG21	2:147:B:LYS:HE2	15	1.24
(1,665)	1:103:A:LEU:HD21	1:129:A:TRP:HE3	11	1.24
(1,665)	1:103:A:LEU:HD21	1:129:A:TRP:HE3	12	1.24
(1,582)	1:103:A:LEU:HD13	1:125:A:PRO:HG3	3	1.24
(1,582)	1:103:A:LEU:HD12	1:125:A:PRO:HG3	7	1.24
(1,582)	1:103:A:LEU:HD12	1:125:A:PRO:HG3	19	1.24
(1,580)	1:90:A:MET:HE1	1:90:A:MET:HG2	1	1.24
(1,580)	1:90:A:MET:HE3	1:90:A:MET:HG2	6	1.24
(1,403)	1:89:A:HIS:HB2	1:105:A:CYS:H	10	1.24
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG22	4	1.23
(1,665)	1:103:A:LEU:HD22	1:129:A:TRP:HE3	20	1.23
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	3	1.23
(1,582)	1:103:A:LEU:HD11	1:125:A:PRO:HG3	1	1.23
(1,403)	1:89:A:HIS:HB2	1:105:A:CYS:H	3	1.23
(1,403)	1:89:A:HIS:HB2	1:105:A:CYS:H	8	1.23
(1,375)	1:102:A:LEU:HD12	1:101:A:GLU:H	1	1.23
(1,47)	1:114:A:ILE:HG21	1:121:A:LEU:HB3	5	1.23
(1,42)	1:102:A:LEU:HD12	1:99:A:GLY:HA3	14	1.23
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG21	3	1.22
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG23	7	1.22
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG21	17	1.22
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD21	10	1.22
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD21	15	1.22
(1,111)	1:102:A:LEU:HA	1:111:A:SER:HB2	2	1.22
(1,63)	1:121:A:LEU:HD11	1:117:A:LEU:HG	20	1.22
(1,42)	1:102:A:LEU:HD11	1:99:A:GLY:HA3	3	1.22
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG21	5	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG23	10	1.21
(1,665)	1:103:A:LEU:HD21	1:129:A:TRP:HE3	3	1.21
(1,665)	1:103:A:LEU:HD23	1:129:A:TRP:HE3	14	1.21
(1,665)	1:103:A:LEU:HD23	1:129:A:TRP:HE3	18	1.21
(1,394)	1:102:A:LEU:HD11	1:98:A:ASP:H	6	1.21
(1,1)	1:121:A:LEU:HD12	1:124:A:ILE:HG13	4	1.21
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG21	18	1.2
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG22	20	1.2
(1,876)	2:149:B:THR:HG23	2:147:B:LYS:HE2	17	1.2
(1,665)	1:103:A:LEU:HD22	1:129:A:TRP:HE3	7	1.2
(1,665)	1:103:A:LEU:HD22	1:129:A:TRP:HE3	8	1.2
(1,665)	1:103:A:LEU:HD23	1:129:A:TRP:HE3	13	1.2
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	9	1.2
(1,64)	1:121:A:LEU:HD13	1:125:A:PRO:HB2	3	1.2
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM31	14	1.19
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG23	9	1.19
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG22	13	1.19
(1,665)	1:103:A:LEU:HD23	1:129:A:TRP:HE3	2	1.19
(1,64)	1:121:A:LEU:HD12	1:125:A:PRO:HB2	1	1.19
(1,394)	1:102:A:LEU:HD11	1:98:A:ASP:H	19	1.18
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	16	1.18
(1,47)	1:114:A:ILE:HG22	1:121:A:LEU:HB3	13	1.18
(1,42)	1:102:A:LEU:HD13	1:99:A:GLY:HA3	8	1.18
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG23	8	1.17
(1,876)	2:149:B:THR:HG23	2:147:B:LYS:HE2	2	1.17
(1,876)	2:149:B:THR:HG21	2:147:B:LYS:HE2	6	1.17
(1,665)	1:103:A:LEU:HD22	1:129:A:TRP:HE3	10	1.17
(1,665)	1:103:A:LEU:HD22	1:129:A:TRP:HE3	15	1.17
(1,665)	1:103:A:LEU:HD22	1:129:A:TRP:HE3	17	1.17
(1,582)	1:103:A:LEU:HD13	1:125:A:PRO:HG3	4	1.17
(1,582)	1:103:A:LEU:HD11	1:125:A:PRO:HG3	12	1.17
(1,403)	1:89:A:HIS:HB2	1:105:A:CYS:H	6	1.17
(1,394)	1:102:A:LEU:HD12	1:98:A:ASP:H	20	1.17
(1,375)	1:102:A:LEU:HD13	1:101:A:GLU:H	2	1.17
(1,375)	1:102:A:LEU:HD13	1:101:A:GLU:H	16	1.17
(1,154)	1:102:A:LEU:HD13	1:94:A:ARG:H	4	1.17
(1,73)	1:107:A:THR:HG23	1:130:A:LEU:HD12	18	1.17
(1,64)	1:121:A:LEU:HD12	1:125:A:PRO:HB2	4	1.17
(1,47)	1:114:A:ILE:HG21	1:121:A:LEU:HB3	15	1.17
(1,882)	2:148:B:GLN:HE22	2:146:B:THR:HG22	2	1.16
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	11	1.16
(1,578)	1:130:A:LEU:HD12	1:106:A:ASP:HB2	1	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,578)	1:130:A:LEU:HD11	1:106:A:ASP:HB2	16	1.16
(1,375)	1:102:A:LEU:HD11	1:101:A:GLU:H	18	1.16
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	8	1.15
(1,665)	1:103:A:LEU:HD23	1:129:A:TRP:HE3	16	1.15
(1,582)	1:103:A:LEU:HD12	1:125:A:PRO:HG3	6	1.15
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	12	1.15
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD21	3	1.15
(1,154)	1:102:A:LEU:HD13	1:94:A:ARG:H	20	1.15
(1,47)	1:114:A:ILE:HG21	1:121:A:LEU:HB3	12	1.15
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	17	1.14
(1,213)	1:133:A:ARG:H	1:133:A:ARG:HD3	16	1.14
(1,64)	1:121:A:LEU:HD13	1:125:A:PRO:HB2	8	1.14
(1,64)	1:121:A:LEU:HD12	1:125:A:PRO:HB2	19	1.14
(1,684)	1:112:A:TYR:HE1	1:110:A:SER:HB3	2	1.13
(1,665)	1:103:A:LEU:HD22	1:129:A:TRP:HE3	6	1.13
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	12	1.13
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD22	10	1.13
(1,582)	1:103:A:LEU:HD12	1:125:A:PRO:HG3	20	1.13
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	3	1.13
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD22	20	1.13
(1,154)	1:102:A:LEU:HD13	1:94:A:ARG:H	7	1.13
(1,876)	2:149:B:THR:HG21	2:147:B:LYS:HE2	1	1.12
(1,582)	1:103:A:LEU:HD12	1:125:A:PRO:HG3	13	1.12
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD13	1	1.12
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD13	10	1.12
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	14	1.12
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD22	4	1.12
(1,51)	1:95:A:VAL:HG21	1:96:A:CYS:HB2	6	1.12
(1,42)	1:102:A:LEU:HD12	1:99:A:GLY:HA3	12	1.12
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	18	1.11
(1,665)	1:103:A:LEU:HD21	1:129:A:TRP:HE3	5	1.11
(1,583)	1:103:A:LEU:HD23	1:124:A:ILE:HG22	15	1.11
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	8	1.11
(1,375)	1:102:A:LEU:HD11	1:101:A:GLU:H	15	1.11
(1,375)	1:102:A:LEU:HD11	1:101:A:GLU:H	19	1.11
(1,47)	1:114:A:ILE:HG21	1:121:A:LEU:HB3	4	1.11
(1,47)	1:114:A:ILE:HG21	1:121:A:LEU:HB3	11	1.11
(1,739)	1:130:A:LEU:HD12	1:129:A:TRP:H	18	1.1
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD13	5	1.1
(1,582)	1:103:A:LEU:HD11	1:125:A:PRO:HG3	2	1.1
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD11	2	1.1
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD22	6	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD23	14	1.1
(1,47)	1:114:A:ILE:HG22	1:121:A:LEU:HB3	8	1.1
(1,47)	1:114:A:ILE:HG23	1:121:A:LEU:HB3	19	1.1
(1,42)	1:102:A:LEU:HD11	1:99:A:GLY:HA3	11	1.1
(1,876)	2:149:B:THR:HG23	2:147:B:LYS:HE2	11	1.09
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	16	1.09
(1,665)	1:103:A:LEU:HD21	1:129:A:TRP:HE3	1	1.09
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD21	10	1.09
(1,63)	1:121:A:LEU:HD12	1:117:A:LEU:HG	2	1.09
(1,42)	1:102:A:LEU:HD13	1:99:A:GLY:HA3	9	1.09
(1,761)	1:94:A:ARG:HD2	1:95:A:VAL:H	14	1.08
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	17	1.08
(1,403)	1:89:A:HIS:HB2	1:105:A:CYS:H	15	1.08
(1,375)	1:102:A:LEU:HD12	1:101:A:GLU:H	10	1.08
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD23	18	1.08
(1,64)	1:121:A:LEU:HD11	1:125:A:PRO:HB2	14	1.08
(1,51)	1:95:A:VAL:HG21	1:96:A:CYS:HB2	18	1.08
(1,47)	1:114:A:ILE:HG22	1:121:A:LEU:HB3	1	1.08
(1,47)	1:114:A:ILE:HG23	1:121:A:LEU:HB3	9	1.08
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	6	1.07
(1,559)	1:121:A:LEU:HD11	1:129:A:TRP:HD1	2	1.07
(1,64)	1:121:A:LEU:HD13	1:125:A:PRO:HB2	5	1.07
(1,64)	1:121:A:LEU:HD12	1:125:A:PRO:HB2	13	1.07
(1,64)	1:121:A:LEU:HD12	1:125:A:PRO:HB2	17	1.07
(1,47)	1:114:A:ILE:HG23	1:121:A:LEU:HB3	14	1.07
(1,876)	2:149:B:THR:HG21	2:147:B:LYS:HE2	13	1.06
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	3	1.06
(1,782)	1:123:A:GLU:HG2	1:124:A:ILE:H	6	1.06
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	2	1.06
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	18	1.06
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD23	2	1.06
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM32	10	1.05
(1,782)	1:123:A:GLU:HG2	1:124:A:ILE:H	20	1.05
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	3	1.05
(1,665)	1:103:A:LEU:HD23	1:129:A:TRP:HE3	9	1.05
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	4	1.05
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD13	3	1.05
(1,582)	1:103:A:LEU:HD12	1:125:A:PRO:HG3	15	1.05
(1,559)	1:121:A:LEU:HD11	1:129:A:TRP:HD1	7	1.05
(1,375)	1:102:A:LEU:HD12	1:101:A:GLU:H	20	1.05
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	20	1.05
(1,64)	1:121:A:LEU:HD11	1:125:A:PRO:HB2	10	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:114:A:ILE:HG21	1:121:A:LEU:HB3	18	1.05
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM23	11	1.04
(1,782)	1:123:A:GLU:HG2	1:124:A:ILE:H	16	1.04
(1,782)	1:123:A:GLU:HG2	1:124:A:ILE:H	17	1.04
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	14	1.04
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	15	1.04
(1,583)	1:103:A:LEU:HD21	1:124:A:ILE:HG23	20	1.04
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD22	7	1.04
(1,47)	1:114:A:ILE:HG21	1:121:A:LEU:HB3	10	1.04
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	13	1.03
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	7	1.03
(1,667)	1:129:A:TRP:HZ2	1:121:A:LEU:HD12	7	1.03
(1,578)	1:130:A:LEU:HD11	1:106:A:ASP:HB2	11	1.03
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	7	1.03
(1,64)	1:121:A:LEU:HD12	1:125:A:PRO:HB2	16	1.03
(1,761)	1:94:A:ARG:HD2	1:95:A:VAL:H	7	1.02
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	19	1.02
(1,559)	1:121:A:LEU:HD11	1:129:A:TRP:HD1	6	1.02
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	20	1.02
(1,394)	1:102:A:LEU:HD12	1:98:A:ASP:H	4	1.02
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD22	8	1.02
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD21	19	1.02
(1,213)	1:133:A:ARG:H	1:133:A:ARG:HD3	14	1.02
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	2	1.02
(1,64)	1:121:A:LEU:HD13	1:125:A:PRO:HB2	18	1.02
(1,51)	1:95:A:VAL:HG21	1:96:A:CYS:HB2	19	1.02
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	6	1.01
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	11	1.01
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD12	19	1.01
(1,583)	1:103:A:LEU:HD23	1:124:A:ILE:HG22	12	1.01
(1,567)	1:94:A:ARG:HD2	1:112:A:TYR:HE1	14	1.01
(1,403)	1:89:A:HIS:HB2	1:105:A:CYS:H	2	1.01
(1,64)	1:121:A:LEU:HD12	1:125:A:PRO:HB2	12	1.01
(1,51)	1:95:A:VAL:HG21	1:96:A:CYS:HB2	11	1.01
(1,51)	1:95:A:VAL:HG22	1:96:A:CYS:HB2	12	1.01
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	11	1.0
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	8	1.0
(1,602)	1:137:A:PRO:HD2	1:136:A:CYS:HB2	2	1.0
(1,583)	1:103:A:LEU:HD21	1:124:A:ILE:HG22	6	1.0
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD12	15	1.0
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	11	1.0
(1,394)	1:102:A:LEU:HD12	1:98:A:ASP:H	7	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:102:A:LEU:HD13	1:98:A:ASP:H	16	1.0
(1,394)	1:102:A:LEU:HD11	1:98:A:ASP:H	18	1.0
(1,154)	1:102:A:LEU:HD11	1:94:A:ARG:H	2	1.0
(1,47)	1:114:A:ILE:HG22	1:121:A:LEU:HB3	17	1.0
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM11	1	0.99
(1,876)	2:149:B:THR:HG23	2:147:B:LYS:HE2	20	0.99
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	1	0.99
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	18	0.99
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD13	8	0.99
(1,568)	1:133:A:ARG:HD3	1:112:A:TYR:HE1	14	0.99
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD23	9	0.99
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD21	12	0.99
(1,154)	1:102:A:LEU:HD13	1:94:A:ARG:H	10	0.99
(1,154)	1:102:A:LEU:HD12	1:94:A:ARG:H	19	0.99
(1,89)	1:110:A:SER:HA	1:90:A:MET:HG2	1	0.99
(1,64)	1:121:A:LEU:HD11	1:125:A:PRO:HB2	15	0.99
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM32	3	0.98
(1,782)	1:123:A:GLU:HG2	1:124:A:ILE:H	14	0.98
(1,684)	1:112:A:TYR:HE1	1:110:A:SER:HB3	20	0.98
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD12	1	0.98
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD23	20	0.98
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	2	0.98
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	19	0.98
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD23	13	0.98
(1,47)	1:114:A:ILE:HG21	1:121:A:LEU:HB3	16	0.98
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM22	19	0.97
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	12	0.97
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	5	0.97
(1,684)	1:112:A:TYR:HE1	1:110:A:SER:HB3	4	0.97
(1,583)	1:103:A:LEU:HD21	1:124:A:ILE:HG23	4	0.97
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	9	0.97
(1,403)	1:89:A:HIS:HB2	1:105:A:CYS:H	4	0.97
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD23	16	0.97
(1,64)	1:121:A:LEU:HD12	1:125:A:PRO:HB2	11	0.97
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	4	0.96
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	19	0.96
(1,684)	1:112:A:TYR:HE1	1:110:A:SER:HB3	13	0.96
(1,583)	1:103:A:LEU:HD22	1:124:A:ILE:HG21	2	0.96
(1,583)	1:103:A:LEU:HD23	1:124:A:ILE:HG22	10	0.96
(1,375)	1:102:A:LEU:HD12	1:101:A:GLU:H	7	0.96
(1,47)	1:114:A:ILE:HG21	1:121:A:LEU:HB3	3	0.96
(1,932)	1:98:A:ASP:H	2:152:B:M3L:HE3	10	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,932)	1:98:A:ASP:H	2:152:B:M3L:HE3	15	0.95
(1,876)	2:149:B:THR:HG21	2:147:B:LYS:HE2	10	0.95
(1,761)	1:94:A:ARG:HD2	1:95:A:VAL:H	1	0.95
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	7	0.95
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	15	0.95
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	17	0.95
(1,257)	1:123:A:GLU:H	1:121:A:LEU:HD22	20	0.95
(1,64)	1:121:A:LEU:HD12	1:125:A:PRO:HB2	9	0.95
(1,782)	1:123:A:GLU:HG2	1:124:A:ILE:H	12	0.94
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	19	0.94
(1,602)	1:137:A:PRO:HD2	1:136:A:CYS:HB2	8	0.94
(1,602)	1:137:A:PRO:HD2	1:136:A:CYS:HB2	15	0.94
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD21	15	0.94
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD12	18	0.94
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD12	19	0.94
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD21	11	0.94
(1,154)	1:102:A:LEU:HD13	1:94:A:ARG:H	1	0.94
(1,47)	1:114:A:ILE:HG23	1:121:A:LEU:HB3	7	0.94
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM22	4	0.93
(1,932)	1:98:A:ASP:H	2:152:B:M3L:HE3	2	0.93
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	11	0.93
(1,761)	1:94:A:ARG:HD2	1:95:A:VAL:H	18	0.93
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	10	0.93
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD11	14	0.93
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD22	2	0.93
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD22	15	0.93
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD23	16	0.93
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	6	0.93
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD21	5	0.93
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD12	3	0.93
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM23	7	0.92
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	10	0.92
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	20	0.92
(1,602)	1:137:A:PRO:HD2	1:136:A:CYS:HB2	18	0.92
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	17	0.92
(1,583)	1:103:A:LEU:HD23	1:124:A:ILE:HG23	3	0.92
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD23	10	0.92
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	15	0.92
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD21	1	0.92
(1,301)	1:129:A:TRP:H	1:103:A:LEU:HD22	17	0.92
(1,813)	1:133:A:ARG:HD3	1:134:A:CYS:H	16	0.91
(1,761)	1:94:A:ARG:HD2	1:95:A:VAL:H	2	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	13	0.91
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD23	1	0.91
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD21	1	0.91
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	8	0.91
(1,154)	1:102:A:LEU:HD11	1:94:A:ARG:H	16	0.91
(1,876)	2:149:B:THR:HG22	2:147:B:LYS:HE2	3	0.9
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	8	0.9
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	19	0.9
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	11	0.9
(1,681)	1:94:A:ARG:HD2	1:112:A:TYR:HE1	14	0.9
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD22	8	0.9
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD11	15	0.9
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD23	10	0.9
(1,47)	1:114:A:ILE:HG23	1:121:A:LEU:HB3	2	0.9
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM11	5	0.89
(1,876)	2:149:B:THR:HG23	2:147:B:LYS:HE2	7	0.89
(1,761)	1:94:A:ARG:HD2	1:95:A:VAL:H	15	0.89
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	4	0.89
(1,684)	1:112:A:TYR:HE1	1:110:A:SER:HB3	7	0.89
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD23	17	0.89
(1,583)	1:103:A:LEU:HD22	1:124:A:ILE:HG21	14	0.89
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	1	0.89
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	16	0.89
(1,394)	1:102:A:LEU:HD11	1:98:A:ASP:H	15	0.89
(1,257)	1:123:A:GLU:H	1:121:A:LEU:HD22	2	0.89
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	16	0.89
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	6	0.88
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD12	13	0.88
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	2	0.88
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	5	0.88
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	6	0.88
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	8	0.88
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD12	15	0.88
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE2	11	0.88
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD13	18	0.87
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	1	0.87
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	4	0.87
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	15	0.87
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	17	0.87
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	20	0.87
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD22	7	0.87
(1,213)	1:133:A:ARG:H	1:133:A:ARG:HD3	12	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,154)	1:102:A:LEU:HD12	1:94:A:ARG:H	15	0.87
(1,154)	1:102:A:LEU:HD12	1:94:A:ARG:H	18	0.87
(1,72)	1:130:A:LEU:HD12	1:107:A:THR:HA	18	0.87
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM21	15	0.86
(1,761)	1:94:A:ARG:HD2	1:95:A:VAL:H	13	0.86
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	18	0.86
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD12	17	0.86
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD22	3	0.86
(1,585)	1:107:A:THR:HG21	1:130:A:LEU:HD21	3	0.86
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	3	0.86
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	7	0.86
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	10	0.86
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	12	0.86
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	13	0.86
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	14	0.86
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	16	0.86
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	18	0.86
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	19	0.86
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	11	0.86
(1,394)	1:102:A:LEU:HD12	1:98:A:ASP:H	1	0.86
(1,394)	1:102:A:LEU:HD13	1:98:A:ASP:H	2	0.86
(1,213)	1:133:A:ARG:H	1:133:A:ARG:HD3	19	0.86
(1,684)	1:112:A:TYR:HE1	1:110:A:SER:HB3	15	0.85
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	9	0.85
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD11	10	0.85
(1,583)	1:103:A:LEU:HD23	1:124:A:ILE:HG23	11	0.85
(1,583)	1:103:A:LEU:HD22	1:124:A:ILE:HG23	18	0.85
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	9	0.85
(1,551)	1:112:A:TYR:HB3	1:112:A:TYR:HD1	11	0.85
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD23	18	0.85
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	13	0.85
(1,47)	1:114:A:ILE:HG23	1:121:A:LEU:HB3	6	0.85
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM11	8	0.84
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	13	0.84
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	7	0.84
(1,813)	1:133:A:ARG:HD3	1:134:A:CYS:H	1	0.84
(1,761)	1:94:A:ARG:HD2	1:95:A:VAL:H	10	0.84
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	11	0.84
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	8	0.84
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD12	4	0.84
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD12	11	0.84
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD12	12	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,583)	1:103:A:LEU:HD21	1:124:A:ILE:HG23	7	0.84
(1,583)	1:103:A:LEU:HD22	1:124:A:ILE:HG22	9	0.84
(1,76)	1:90:A:MET:HE2	1:110:A:SER:HA	8	0.84
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	13	0.83
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	13	0.83
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	8	0.83
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	12	0.83
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD22	19	0.83
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD12	16	0.83
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD23	1	0.83
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	14	0.83
(1,583)	1:103:A:LEU:HD23	1:124:A:ILE:HG21	1	0.83
(1,522)	1:92:A:PHE:HB2	1:92:A:PHE:HD1	12	0.83
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	10	0.83
(1,47)	1:114:A:ILE:HG21	1:121:A:LEU:HB3	20	0.83
(1,932)	1:98:A:ASP:H	2:152:B:M3L:HE3	1	0.82
(1,876)	2:149:B:THR:HG23	2:147:B:LYS:HE2	12	0.82
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD21	13	0.82
(1,583)	1:103:A:LEU:HD21	1:124:A:ILE:HG22	17	0.82
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD21	6	0.82
(1,522)	1:92:A:PHE:HB2	1:92:A:PHE:HD1	2	0.82
(1,522)	1:92:A:PHE:HB2	1:92:A:PHE:HD1	13	0.82
(1,522)	1:92:A:PHE:HB2	1:92:A:PHE:HD1	18	0.82
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	3	0.81
(1,761)	1:94:A:ARG:HD2	1:95:A:VAL:H	17	0.81
(1,701)	1:111:A:SER:HB2	1:89:A:HIS:HD2	4	0.81
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	12	0.81
(1,675)	1:97:A:LYS:HG3	1:92:A:PHE:HD1	4	0.81
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD21	15	0.81
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD22	7	0.81
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD21	9	0.81
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD22	11	0.81
(1,583)	1:103:A:LEU:HD22	1:124:A:ILE:HG23	13	0.81
(1,522)	1:92:A:PHE:HB2	1:92:A:PHE:HD1	9	0.81
(1,522)	1:92:A:PHE:HB2	1:92:A:PHE:HD1	19	0.81
(1,522)	1:92:A:PHE:HB2	1:92:A:PHE:HD1	20	0.81
(1,76)	1:90:A:MET:HE1	1:110:A:SER:HA	5	0.81
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	5	0.8
(1,749)	1:125:A:PRO:HG3	1:129:A:TRP:H	9	0.8
(1,632)	1:125:A:PRO:HD2	1:121:A:LEU:HD12	9	0.8
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	2	0.8
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	15	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD23	5	0.8
(1,583)	1:103:A:LEU:HD21	1:124:A:ILE:HG22	8	0.8
(1,583)	1:103:A:LEU:HD22	1:124:A:ILE:HG23	16	0.8
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD21	19	0.8
(1,522)	1:92:A:PHE:HB2	1:92:A:PHE:HD1	1	0.8
(1,522)	1:92:A:PHE:HB2	1:92:A:PHE:HD1	5	0.8
(1,522)	1:92:A:PHE:HB2	1:92:A:PHE:HD1	14	0.8
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	7	0.8
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	7	0.8
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	20	0.8
(1,76)	1:90:A:MET:HE1	1:110:A:SER:HA	4	0.8
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	7	0.79
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	14	0.79
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD22	14	0.79
(1,583)	1:103:A:LEU:HD23	1:124:A:ILE:HG21	5	0.79
(1,522)	1:92:A:PHE:HB2	1:92:A:PHE:HD1	3	0.79
(1,522)	1:92:A:PHE:HB2	1:92:A:PHE:HD1	16	0.79
(1,494)	1:111:A:SER:H	1:90:A:MET:HG2	2	0.79
(1,75)	1:135:A:THR:HG22	1:130:A:LEU:HG	12	0.79
(1,68)	1:130:A:LEU:HD22	1:134:A:CYS:HB3	16	0.79
(1,813)	1:133:A:ARG:HD3	1:134:A:CYS:H	6	0.78
(1,761)	1:94:A:ARG:HD2	1:95:A:VAL:H	6	0.78
(1,761)	1:94:A:ARG:HD2	1:95:A:VAL:H	16	0.78
(1,701)	1:111:A:SER:HB2	1:89:A:HIS:HD2	2	0.78
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	19	0.78
(1,655)	1:117:A:LEU:HD22	1:113:A:HIS:HB2	17	0.78
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD22	2	0.78
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD21	20	0.78
(1,288)	1:102:A:LEU:HD13	1:112:A:TYR:H	10	0.78
(1,257)	1:123:A:GLU:H	1:121:A:LEU:HD23	6	0.78
(1,68)	1:130:A:LEU:HD23	1:134:A:CYS:HB3	19	0.78
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	9	0.77
(1,655)	1:117:A:LEU:HD21	1:113:A:HIS:HB2	2	0.77
(1,655)	1:117:A:LEU:HD21	1:113:A:HIS:HB2	5	0.77
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD21	2	0.77
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD22	16	0.77
(1,583)	1:103:A:LEU:HD23	1:124:A:ILE:HG23	19	0.77
(1,482)	1:115:A:HIS:HB2	1:116:A:CYS:H	20	0.77
(1,246)	1:114:A:ILE:HD13	1:115:A:HIS:H	4	0.77
(1,76)	1:90:A:MET:HE3	1:110:A:SER:HA	17	0.77
(1,68)	1:130:A:LEU:HD22	1:134:A:CYS:HB3	11	0.77
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	13	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	8	0.76
(1,684)	1:112:A:TYR:HE1	1:110:A:SER:HB3	3	0.76
(1,684)	1:112:A:TYR:HE1	1:110:A:SER:HB3	14	0.76
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	5	0.76
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	20	0.76
(1,288)	1:102:A:LEU:HD11	1:112:A:TYR:H	16	0.76
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM31	10	0.75
(1,851)	1:114:A:ILE:HG23	1:117:A:LEU:H	4	0.75
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	12	0.75
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD23	7	0.75
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	1	0.75
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	17	0.75
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	20	0.75
(1,540)	1:93:A:CYS:HA	1:102:A:LEU:HD12	6	0.75
(1,246)	1:114:A:ILE:HD12	1:115:A:HIS:H	1	0.75
(1,246)	1:114:A:ILE:HD12	1:115:A:HIS:H	14	0.75
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	12	0.75
(1,68)	1:130:A:LEU:HD22	1:134:A:CYS:HB3	6	0.75
(1,68)	1:130:A:LEU:HD21	1:134:A:CYS:HB3	9	0.75
(1,68)	1:130:A:LEU:HD22	1:134:A:CYS:HB3	20	0.75
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	13	0.75
(1,482)	1:115:A:HIS:HB2	1:116:A:CYS:H	16	0.74
(1,257)	1:123:A:GLU:H	1:121:A:LEU:HD23	7	0.74
(1,246)	1:114:A:ILE:HD13	1:115:A:HIS:H	9	0.74
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE2	10	0.74
(1,932)	1:98:A:ASP:H	2:152:B:M3L:HE3	20	0.73
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	9	0.73
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	18	0.73
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD21	7	0.73
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD22	8	0.73
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	13	0.73
(1,288)	1:102:A:LEU:HD13	1:112:A:TYR:H	1	0.73
(1,246)	1:114:A:ILE:HD13	1:115:A:HIS:H	3	0.73
(1,246)	1:114:A:ILE:HD13	1:115:A:HIS:H	13	0.73
(1,246)	1:114:A:ILE:HD12	1:115:A:HIS:H	17	0.73
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD11	5	0.73
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	5	0.73
(1,879)	2:148:B:GLN:HG2	2:147:B:LYS:HA	5	0.72
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	16	0.72
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	17	0.72
(1,655)	1:117:A:LEU:HD23	1:113:A:HIS:HB2	15	0.72
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	6	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:130:A:LEU:HD22	1:134:A:CYS:HB3	7	0.72
(1,68)	1:130:A:LEU:HD21	1:134:A:CYS:HB3	13	0.72
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	14	0.71
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	15	0.71
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	7	0.71
(1,684)	1:112:A:TYR:HE1	1:110:A:SER:HB3	19	0.71
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD23	4	0.71
(1,482)	1:115:A:HIS:HB2	1:116:A:CYS:H	6	0.71
(1,482)	1:115:A:HIS:HB2	1:116:A:CYS:H	14	0.71
(1,246)	1:114:A:ILE:HD11	1:115:A:HIS:H	8	0.71
(1,164)	1:130:A:LEU:H	1:130:A:LEU:HD23	18	0.71
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	9	0.71
(1,100)	1:93:A:CYS:HA	1:102:A:LEU:HD21	14	0.71
(1,68)	1:130:A:LEU:HD23	1:134:A:CYS:HB3	4	0.71
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	3	0.71
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE2	15	0.71
(1,879)	2:148:B:GLN:HG2	2:147:B:LYS:HA	13	0.7
(1,876)	2:149:B:THR:HG22	2:147:B:LYS:HE2	5	0.7
(1,851)	1:114:A:ILE:HG23	1:117:A:LEU:H	10	0.7
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	1	0.7
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	2	0.7
(1,288)	1:102:A:LEU:HD13	1:112:A:TYR:H	7	0.7
(1,288)	1:102:A:LEU:HD12	1:112:A:TYR:H	19	0.7
(1,246)	1:114:A:ILE:HD12	1:115:A:HIS:H	2	0.7
(1,246)	1:114:A:ILE:HD12	1:115:A:HIS:H	11	0.7
(1,100)	1:93:A:CYS:HA	1:102:A:LEU:HD21	9	0.7
(1,68)	1:130:A:LEU:HD23	1:134:A:CYS:HB3	17	0.7
(1,4)	1:92:A:PHE:H	1:111:A:SER:H	8	0.7
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	4	0.69
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	1	0.69
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD22	3	0.69
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD22	11	0.69
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	13	0.69
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	9	0.69
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD22	6	0.69
(1,288)	1:102:A:LEU:HD12	1:112:A:TYR:H	6	0.69
(1,246)	1:114:A:ILE:HD12	1:115:A:HIS:H	7	0.69
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	11	0.69
(1,100)	1:93:A:CYS:HA	1:102:A:LEU:HD22	17	0.69
(1,68)	1:130:A:LEU:HD23	1:134:A:CYS:HB3	5	0.69
(1,68)	1:130:A:LEU:HD22	1:134:A:CYS:HB3	14	0.69
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM13	6	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM12	5	0.68
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD23	8	0.68
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	3	0.68
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	4	0.68
(1,559)	1:121:A:LEU:HD13	1:129:A:TRP:HD1	20	0.68
(1,288)	1:102:A:LEU:HD13	1:112:A:TYR:H	20	0.68
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD12	17	0.68
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD13	8	0.68
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	8	0.68
(1,100)	1:93:A:CYS:HA	1:102:A:LEU:HD23	8	0.68
(1,68)	1:130:A:LEU:HD22	1:134:A:CYS:HB3	12	0.68
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE1	5	0.68
(1,851)	1:114:A:ILE:HG23	1:117:A:LEU:H	15	0.67
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	10	0.67
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	16	0.67
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	20	0.67
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	5	0.67
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	10	0.67
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	5	0.67
(1,288)	1:102:A:LEU:HD13	1:112:A:TYR:H	4	0.67
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD13	18	0.67
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD13	8	0.67
(1,68)	1:130:A:LEU:HD23	1:134:A:CYS:HB3	10	0.67
(1,876)	2:149:B:THR:HG22	2:147:B:LYS:HE2	18	0.66
(1,851)	1:114:A:ILE:HG22	1:117:A:LEU:H	7	0.66
(1,851)	1:114:A:ILE:HG21	1:117:A:LEU:H	17	0.66
(1,851)	1:114:A:ILE:HG23	1:117:A:LEU:H	20	0.66
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	2	0.66
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	5	0.66
(1,709)	1:94:A:ARG:HD2	1:94:A:ARG:H	14	0.66
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	8	0.66
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	14	0.66
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	17	0.66
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD22	19	0.66
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	6	0.66
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	5	0.66
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD23	4	0.66
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD11	9	0.66
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD23	4	0.66
(1,482)	1:115:A:HIS:HB2	1:116:A:CYS:H	3	0.66
(1,482)	1:115:A:HIS:HB2	1:116:A:CYS:H	8	0.66
(1,466)	1:130:A:LEU:HD21	1:135:A:THR:H	15	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,100)	1:93:A:CYS:HA	1:102:A:LEU:HD21	5	0.66
(1,100)	1:93:A:CYS:HA	1:102:A:LEU:HD21	11	0.66
(1,75)	1:135:A:THR:HG23	1:130:A:LEU:HG	20	0.66
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	1	0.66
(1,851)	1:114:A:ILE:HG21	1:117:A:LEU:H	1	0.65
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	9	0.65
(1,845)	1:115:A:HIS:HB2	1:117:A:LEU:H	3	0.65
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	4	0.65
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD21	18	0.65
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	2	0.65
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD22	4	0.65
(1,534)	1:98:A:ASP:HB3	1:113:A:HIS:HD2	19	0.65
(1,288)	1:102:A:LEU:HD11	1:112:A:TYR:H	2	0.65
(1,246)	1:114:A:ILE:HD13	1:115:A:HIS:H	12	0.65
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD11	14	0.65
(1,100)	1:93:A:CYS:HA	1:102:A:LEU:HD22	3	0.65
(1,100)	1:93:A:CYS:HA	1:102:A:LEU:HD23	13	0.65
(1,68)	1:130:A:LEU:HD22	1:134:A:CYS:HB3	2	0.65
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	2	0.65
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE1	20	0.65
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	3	0.64
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	8	0.64
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	2	0.64
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	20	0.64
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	2	0.64
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	11	0.64
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	3	0.64
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	15	0.64
(1,602)	1:137:A:PRO:HD2	1:136:A:CYS:HB2	4	0.64
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	10	0.64
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD11	3	0.64
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD13	5	0.64
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD12	19	0.64
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	6	0.64
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	16	0.64
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD12	8	0.64
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD13	10	0.64
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD13	19	0.64
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	14	0.64
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	20	0.64
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE2	6	0.64
(1,796)	1:92:A:PHE:HD1	1:93:A:CYS:H	9	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:92:A:PHE:HD1	1:93:A:CYS:H	13	0.63
(1,796)	1:92:A:PHE:HD1	1:93:A:CYS:H	20	0.63
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	10	0.63
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD13	8	0.63
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD13	11	0.63
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD11	12	0.63
(1,246)	1:114:A:ILE:HD11	1:115:A:HIS:H	10	0.63
(1,246)	1:114:A:ILE:HD12	1:115:A:HIS:H	16	0.63
(1,246)	1:114:A:ILE:HD11	1:115:A:HIS:H	18	0.63
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD12	9	0.63
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD11	12	0.63
(1,154)	1:102:A:LEU:HD12	1:94:A:ARG:H	6	0.63
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD12	11	0.63
(1,68)	1:130:A:LEU:HD23	1:134:A:CYS:HB3	1	0.63
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	5	0.63
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	9	0.63
(1,879)	2:148:B:GLN:HG2	2:147:B:LYS:HA	12	0.62
(1,851)	1:114:A:ILE:HG22	1:117:A:LEU:H	9	0.62
(1,825)	1:110:A:SER:HB3	1:111:A:SER:H	11	0.62
(1,796)	1:92:A:PHE:HD1	1:93:A:CYS:H	2	0.62
(1,796)	1:92:A:PHE:HD1	1:93:A:CYS:H	5	0.62
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	9	0.62
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	10	0.62
(1,752)	1:102:A:LEU:HD23	1:103:A:LEU:H	14	0.62
(1,585)	1:107:A:THR:HG22	1:130:A:LEU:HD21	8	0.62
(1,482)	1:115:A:HIS:HB2	1:116:A:CYS:H	9	0.62
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD13	11	0.62
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	18	0.62
(1,100)	1:93:A:CYS:HA	1:102:A:LEU:HD23	12	0.62
(1,75)	1:135:A:THR:HG22	1:130:A:LEU:HG	4	0.62
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	14	0.62
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	16	0.62
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM21	13	0.61
(1,876)	2:149:B:THR:HG21	2:147:B:LYS:HE2	4	0.61
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	15	0.61
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	16	0.61
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	1	0.61
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	19	0.61
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD23	17	0.61
(1,612)	1:103:A:LEU:HD12	1:129:A:TRP:HD1	15	0.61
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	16	0.61
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD13	6	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD13	18	0.61
(1,513)	1:120:A:PRO:HB2	1:117:A:LEU:H	18	0.61
(1,466)	1:130:A:LEU:HD21	1:135:A:THR:H	18	0.61
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD11	13	0.61
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	6	0.61
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE1	2	0.61
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE2	7	0.61
(1,947)	1:92:A:PHE:HE1	2:152:B:M3L:HM31	17	0.6
(1,879)	2:148:B:GLN:HG2	2:147:B:LYS:HA	6	0.6
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	2	0.6
(1,851)	1:114:A:ILE:HG21	1:117:A:LEU:H	13	0.6
(1,825)	1:110:A:SER:HB3	1:111:A:SER:H	19	0.6
(1,752)	1:102:A:LEU:HD22	1:103:A:LEU:H	12	0.6
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	5	0.6
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	16	0.6
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	18	0.6
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	8	0.6
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	1	0.6
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD22	20	0.6
(1,585)	1:107:A:THR:HG23	1:130:A:LEU:HD21	2	0.6
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	20	0.6
(1,482)	1:115:A:HIS:HB2	1:116:A:CYS:H	5	0.6
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	17	0.6
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE1	13	0.6
(1,876)	2:149:B:THR:HG23	2:147:B:LYS:HE2	19	0.59
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	6	0.59
(1,851)	1:114:A:ILE:HG23	1:117:A:LEU:H	16	0.59
(1,845)	1:115:A:HIS:HB2	1:117:A:LEU:H	14	0.59
(1,796)	1:92:A:PHE:HD1	1:93:A:CYS:H	1	0.59
(1,796)	1:92:A:PHE:HD1	1:93:A:CYS:H	3	0.59
(1,796)	1:92:A:PHE:HD1	1:93:A:CYS:H	14	0.59
(1,796)	1:92:A:PHE:HD1	1:93:A:CYS:H	16	0.59
(1,796)	1:92:A:PHE:HD1	1:93:A:CYS:H	18	0.59
(1,655)	1:117:A:LEU:HD21	1:113:A:HIS:HB2	1	0.59
(1,596)	1:97:A:LYS:HB3	1:92:A:PHE:HD1	16	0.59
(1,585)	1:107:A:THR:HG22	1:130:A:LEU:HD23	15	0.59
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD11	10	0.59
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD11	17	0.59
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD13	20	0.59
(1,482)	1:115:A:HIS:HB2	1:116:A:CYS:H	2	0.59
(1,482)	1:115:A:HIS:HB2	1:116:A:CYS:H	11	0.59
(1,482)	1:115:A:HIS:HB2	1:116:A:CYS:H	12	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:114:A:ILE:HD13	1:115:A:HIS:H	5	0.59
(1,246)	1:114:A:ILE:HD13	1:115:A:HIS:H	19	0.59
(1,68)	1:130:A:LEU:HD22	1:134:A:CYS:HB3	8	0.59
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	7	0.59
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE1	1	0.59
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE1	19	0.59
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	5	0.58
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	14	0.58
(1,845)	1:115:A:HIS:HB2	1:117:A:LEU:H	2	0.58
(1,752)	1:102:A:LEU:HD21	1:103:A:LEU:H	3	0.58
(1,752)	1:102:A:LEU:HD23	1:103:A:LEU:H	11	0.58
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	15	0.58
(1,585)	1:107:A:THR:HG23	1:130:A:LEU:HD22	1	0.58
(1,585)	1:107:A:THR:HG22	1:130:A:LEU:HD21	12	0.58
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD11	1	0.58
(1,571)	1:95:A:VAL:HG21	1:112:A:TYR:HE1	6	0.58
(1,571)	1:95:A:VAL:HG21	1:112:A:TYR:HE1	11	0.58
(1,288)	1:102:A:LEU:HD12	1:112:A:TYR:H	18	0.58
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	18	0.58
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	19	0.58
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE1	9	0.58
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE1	14	0.58
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE2	17	0.58
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	10	0.57
(1,796)	1:92:A:PHE:HD1	1:93:A:CYS:H	12	0.57
(1,752)	1:102:A:LEU:HD22	1:103:A:LEU:H	13	0.57
(1,713)	1:106:A:ASP:HB2	1:107:A:THR:H	8	0.57
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD22	12	0.57
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD21	14	0.57
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD21	16	0.57
(1,664)	1:118:A:ASN:HD22	1:117:A:LEU:HD22	5	0.57
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	16	0.57
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD21	19	0.57
(1,585)	1:107:A:THR:HG21	1:130:A:LEU:HD21	16	0.57
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD13	13	0.57
(1,466)	1:130:A:LEU:HD22	1:135:A:THR:H	3	0.57
(1,229)	1:114:A:ILE:H	1:102:A:LEU:HD13	3	0.57
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	10	0.57
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD12	5	0.57
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD11	5	0.57
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	20	0.57
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE1	3	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM12	11	0.56
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	15	0.56
(1,845)	1:115:A:HIS:HB2	1:117:A:LEU:H	5	0.56
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	20	0.56
(1,655)	1:117:A:LEU:HD21	1:113:A:HIS:HB2	13	0.56
(1,655)	1:117:A:LEU:HD22	1:113:A:HIS:HB2	16	0.56
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	16	0.56
(1,596)	1:97:A:LYS:HB3	1:92:A:PHE:HD1	5	0.56
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD11	2	0.56
(1,571)	1:95:A:VAL:HG22	1:112:A:TYR:HE1	12	0.56
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	5	0.56
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD12	9	0.56
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	6	0.56
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	8	0.56
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	12	0.56
(1,825)	1:110:A:SER:HB3	1:111:A:SER:H	13	0.55
(1,713)	1:106:A:ASP:HB2	1:107:A:THR:H	13	0.55
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	1	0.55
(1,674)	1:97:A:LYS:HD3	1:92:A:PHE:HD1	3	0.55
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD21	13	0.55
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	1	0.55
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	7	0.55
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD12	4	0.55
(1,571)	1:95:A:VAL:HG22	1:112:A:TYR:HE1	16	0.55
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	11	0.55
(1,556)	1:91:A:GLU:HG3	1:92:A:PHE:HE1	17	0.55
(1,394)	1:102:A:LEU:HD12	1:98:A:ASP:H	10	0.55
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	13	0.55
(1,76)	1:90:A:MET:HE3	1:110:A:SER:HA	15	0.55
(1,60)	1:117:A:LEU:HD21	1:114:A:ILE:HA	11	0.55
(1,60)	1:117:A:LEU:HD22	1:114:A:ILE:HA	18	0.55
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	15	0.55
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE1	18	0.55
(1,851)	1:114:A:ILE:HG21	1:117:A:LEU:H	8	0.54
(1,851)	1:114:A:ILE:HG22	1:117:A:LEU:H	19	0.54
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	18	0.54
(1,655)	1:117:A:LEU:HD23	1:113:A:HIS:HB2	9	0.54
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	9	0.54
(1,585)	1:107:A:THR:HG22	1:130:A:LEU:HD22	10	0.54
(1,585)	1:107:A:THR:HG21	1:130:A:LEU:HD22	17	0.54
(1,571)	1:95:A:VAL:HG23	1:112:A:TYR:HE1	5	0.54
(1,571)	1:95:A:VAL:HG21	1:112:A:TYR:HE1	19	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,466)	1:130:A:LEU:HD23	1:135:A:THR:H	1	0.54
(1,246)	1:114:A:ILE:HD11	1:115:A:HIS:H	15	0.54
(1,246)	1:114:A:ILE:HD13	1:115:A:HIS:H	20	0.54
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	1	0.54
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	8	0.54
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	16	0.54
(1,69)	1:130:A:LEU:HD11	1:128:A:GLU:HB2	3	0.54
(1,68)	1:130:A:LEU:HD21	1:134:A:CYS:HB3	15	0.54
(1,60)	1:117:A:LEU:HD21	1:114:A:ILE:HA	12	0.54
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	11	0.54
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE1	12	0.54
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM22	15	0.53
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM33	17	0.53
(1,851)	1:114:A:ILE:HG22	1:117:A:LEU:H	14	0.53
(1,851)	1:114:A:ILE:HG23	1:117:A:LEU:H	18	0.53
(1,796)	1:92:A:PHE:HD1	1:93:A:CYS:H	19	0.53
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	6	0.53
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD23	7	0.53
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	4	0.53
(1,585)	1:107:A:THR:HG23	1:130:A:LEU:HD21	6	0.53
(1,585)	1:107:A:THR:HG23	1:130:A:LEU:HD23	13	0.53
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD12	16	0.53
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	14	0.53
(1,247)	1:114:A:ILE:HG23	1:115:A:HIS:H	8	0.53
(1,247)	1:114:A:ILE:HG23	1:115:A:HIS:H	13	0.53
(1,247)	1:114:A:ILE:HG23	1:115:A:HIS:H	17	0.53
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	2	0.53
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	6	0.53
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	18	0.53
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	19	0.53
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	19	0.53
(1,68)	1:130:A:LEU:HD22	1:134:A:CYS:HB3	3	0.53
(1,60)	1:117:A:LEU:HD21	1:114:A:ILE:HA	5	0.53
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	4	0.53
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	1	0.53
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM21	15	0.52
(1,851)	1:114:A:ILE:HG22	1:117:A:LEU:H	2	0.52
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	13	0.52
(1,701)	1:111:A:SER:HB2	1:89:A:HIS:HD2	15	0.52
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD23	20	0.52
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	3	0.52
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,602)	1:137:A:PRO:HD2	1:136:A:CYS:HB2	13	0.52
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD11	14	0.52
(1,247)	1:114:A:ILE:HG22	1:115:A:HIS:H	15	0.52
(1,235)	1:95:A:VAL:HG22	1:96:A:CYS:H	1	0.52
(1,235)	1:95:A:VAL:HG23	1:96:A:CYS:H	13	0.52
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	4	0.52
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	9	0.52
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	11	0.52
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	12	0.52
(1,154)	1:102:A:LEU:HD12	1:94:A:ARG:H	8	0.52
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD13	1	0.52
(1,60)	1:117:A:LEU:HD21	1:114:A:ILE:HA	19	0.52
(1,752)	1:102:A:LEU:HD23	1:103:A:LEU:H	9	0.51
(1,676)	1:117:A:LEU:HD13	1:129:A:TRP:HZ3	13	0.51
(1,585)	1:107:A:THR:HG23	1:130:A:LEU:HD21	7	0.51
(1,585)	1:107:A:THR:HG23	1:130:A:LEU:HD23	9	0.51
(1,585)	1:107:A:THR:HG21	1:130:A:LEU:HD21	14	0.51
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD22	17	0.51
(1,247)	1:114:A:ILE:HG23	1:115:A:HIS:H	1	0.51
(1,247)	1:114:A:ILE:HG21	1:115:A:HIS:H	7	0.51
(1,247)	1:114:A:ILE:HG22	1:115:A:HIS:H	10	0.51
(1,247)	1:114:A:ILE:HG22	1:115:A:HIS:H	16	0.51
(1,235)	1:95:A:VAL:HG23	1:96:A:CYS:H	10	0.51
(1,178)	1:97:A:LYS:H	1:97:A:LYS:HD2	2	0.51
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	7	0.51
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	17	0.51
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	20	0.51
(1,154)	1:102:A:LEU:HD12	1:94:A:ARG:H	9	0.51
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD12	12	0.51
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD13	20	0.51
(1,4)	1:92:A:PHE:H	1:111:A:SER:H	4	0.51
(1,4)	1:92:A:PHE:H	1:92:A:PHE:HE1	16	0.51
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	11	0.5
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	3	0.5
(1,752)	1:102:A:LEU:HD22	1:103:A:LEU:H	8	0.5
(1,752)	1:102:A:LEU:HD21	1:103:A:LEU:H	17	0.5
(1,713)	1:106:A:ASP:HB2	1:107:A:THR:H	16	0.5
(1,713)	1:106:A:ASP:HB2	1:107:A:THR:H	18	0.5
(1,676)	1:117:A:LEU:HD11	1:129:A:TRP:HZ3	14	0.5
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD21	2	0.5
(1,655)	1:117:A:LEU:HD21	1:113:A:HIS:HB2	3	0.5
(1,585)	1:107:A:THR:HG23	1:130:A:LEU:HD22	4	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:107:A:THR:HG23	1:130:A:LEU:HD21	20	0.5
(1,571)	1:95:A:VAL:HG22	1:112:A:TYR:HE1	14	0.5
(1,567)	1:94:A:ARG:HD2	1:112:A:TYR:HE1	18	0.5
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD22	6	0.5
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD22	12	0.5
(1,288)	1:102:A:LEU:HD12	1:112:A:TYR:H	15	0.5
(1,247)	1:114:A:ILE:HG21	1:115:A:HIS:H	9	0.5
(1,235)	1:95:A:VAL:HG22	1:96:A:CYS:H	3	0.5
(1,235)	1:95:A:VAL:HG23	1:96:A:CYS:H	8	0.5
(1,178)	1:97:A:LYS:H	1:97:A:LYS:HD2	17	0.5
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	3	0.5
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	4	0.5
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	10	0.5
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD11	17	0.5
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG22	2	0.5
(1,60)	1:117:A:LEU:HD21	1:114:A:ILE:HA	6	0.5
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM12	11	0.49
(1,851)	1:114:A:ILE:HG23	1:117:A:LEU:H	5	0.49
(1,851)	1:114:A:ILE:HG22	1:117:A:LEU:H	6	0.49
(1,825)	1:110:A:SER:HB3	1:111:A:SER:H	2	0.49
(1,684)	1:112:A:TYR:HE1	1:110:A:SER:HB3	11	0.49
(1,676)	1:117:A:LEU:HD11	1:129:A:TRP:HZ3	7	0.49
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD22	5	0.49
(1,466)	1:130:A:LEU:HD23	1:135:A:THR:H	17	0.49
(1,247)	1:114:A:ILE:HG21	1:115:A:HIS:H	14	0.49
(1,235)	1:95:A:VAL:HG22	1:96:A:CYS:H	4	0.49
(1,235)	1:95:A:VAL:HG23	1:96:A:CYS:H	9	0.49
(1,235)	1:95:A:VAL:HG22	1:96:A:CYS:H	16	0.49
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	14	0.49
(1,154)	1:102:A:LEU:HD12	1:94:A:ARG:H	17	0.49
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD12	17	0.49
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	3	0.49
(1,60)	1:117:A:LEU:HD21	1:114:A:ILE:HA	17	0.49
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	11	0.49
(1,851)	1:114:A:ILE:HG23	1:117:A:LEU:H	3	0.48
(1,845)	1:115:A:HIS:HB2	1:117:A:LEU:H	9	0.48
(1,845)	1:115:A:HIS:HB2	1:117:A:LEU:H	11	0.48
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	6	0.48
(1,825)	1:110:A:SER:HB3	1:111:A:SER:H	7	0.48
(1,676)	1:117:A:LEU:HD11	1:129:A:TRP:HZ3	10	0.48
(1,676)	1:117:A:LEU:HD12	1:129:A:TRP:HZ3	16	0.48
(1,676)	1:117:A:LEU:HD13	1:129:A:TRP:HZ3	20	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:97:A:LYS:HD3	1:92:A:PHE:HD1	12	0.48
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD21	6	0.48
(1,655)	1:117:A:LEU:HD22	1:113:A:HIS:HB2	4	0.48
(1,585)	1:107:A:THR:HG22	1:130:A:LEU:HD21	11	0.48
(1,571)	1:95:A:VAL:HG23	1:112:A:TYR:HE1	17	0.48
(1,571)	1:95:A:VAL:HG21	1:112:A:TYR:HE1	18	0.48
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	5	0.48
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	3	0.48
(1,258)	1:107:A:THR:HG22	1:108:A:CYS:H	8	0.48
(1,247)	1:114:A:ILE:HG22	1:115:A:HIS:H	20	0.48
(1,246)	1:114:A:ILE:HD13	1:115:A:HIS:H	6	0.48
(1,235)	1:95:A:VAL:HG22	1:96:A:CYS:H	14	0.48
(1,235)	1:95:A:VAL:HG23	1:96:A:CYS:H	15	0.48
(1,235)	1:95:A:VAL:HG23	1:96:A:CYS:H	17	0.48
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD11	4	0.48
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	17	0.48
(1,60)	1:117:A:LEU:HD23	1:114:A:ILE:HA	1	0.48
(1,60)	1:117:A:LEU:HD23	1:114:A:ILE:HA	3	0.48
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM11	8	0.47
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM33	6	0.47
(1,825)	1:110:A:SER:HB3	1:111:A:SER:H	4	0.47
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	5	0.47
(1,713)	1:106:A:ASP:HB2	1:107:A:THR:H	17	0.47
(1,688)	1:94:A:ARG:HB2	1:112:A:TYR:HD1	20	0.47
(1,676)	1:117:A:LEU:HD12	1:129:A:TRP:HZ3	4	0.47
(1,676)	1:117:A:LEU:HD11	1:129:A:TRP:HZ3	9	0.47
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD22	1	0.47
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD23	16	0.47
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	17	0.47
(1,602)	1:137:A:PRO:HD2	1:136:A:CYS:HB2	16	0.47
(1,597)	1:121:A:LEU:HD23	1:129:A:TRP:HD1	3	0.47
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD12	2	0.47
(1,571)	1:95:A:VAL:HG22	1:112:A:TYR:HE1	3	0.47
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD23	18	0.47
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	9	0.47
(1,154)	1:102:A:LEU:HD11	1:94:A:ARG:H	5	0.47
(1,154)	1:102:A:LEU:HD11	1:94:A:ARG:H	12	0.47
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD11	3	0.47
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD11	14	0.47
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	5	0.47
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD13	2	0.47
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG22	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG23	9	0.47
(1,60)	1:117:A:LEU:HD23	1:114:A:ILE:HA	2	0.47
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	4	0.47
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM12	1	0.46
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	20	0.46
(1,845)	1:115:A:HIS:HB2	1:117:A:LEU:H	6	0.46
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	16	0.46
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	15	0.46
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	12	0.46
(1,752)	1:102:A:LEU:HD23	1:103:A:LEU:H	5	0.46
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	13	0.46
(1,676)	1:117:A:LEU:HD11	1:129:A:TRP:HZ3	17	0.46
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD22	15	0.46
(1,654)	1:132:A:PRO:HD2	1:117:A:LEU:HD23	19	0.46
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	14	0.46
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD12	6	0.46
(1,585)	1:107:A:THR:HG21	1:130:A:LEU:HD22	5	0.46
(1,571)	1:95:A:VAL:HG22	1:112:A:TYR:HE1	1	0.46
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	12	0.46
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD23	13	0.46
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD21	14	0.46
(1,534)	1:98:A:ASP:HB3	1:113:A:HIS:HD2	15	0.46
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD22	5	0.46
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD22	19	0.46
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	15	0.46
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	12	0.46
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	14	0.46
(1,258)	1:107:A:THR:HG22	1:108:A:CYS:H	10	0.46
(1,235)	1:95:A:VAL:HG23	1:96:A:CYS:H	2	0.46
(1,235)	1:95:A:VAL:HG22	1:96:A:CYS:H	7	0.46
(1,235)	1:95:A:VAL:HG21	1:96:A:CYS:H	20	0.46
(1,154)	1:102:A:LEU:HD13	1:94:A:ARG:H	11	0.46
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	2	0.46
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD23	1	0.46
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD21	16	0.46
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD13	11	0.46
(1,60)	1:117:A:LEU:HD21	1:114:A:ILE:HA	4	0.46
(1,60)	1:117:A:LEU:HD23	1:114:A:ILE:HA	15	0.46
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	17	0.46
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	10	0.45
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	10	0.45
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM23	2	0.45
(1,909)	1:98:A:ASP:H	2:152:B:M3L:HM32	13	0.45
(1,845)	1:115:A:HIS:HB2	1:117:A:LEU:H	16	0.45
(1,845)	1:115:A:HIS:HB2	1:117:A:LEU:H	20	0.45
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	11	0.45
(1,676)	1:117:A:LEU:HD11	1:129:A:TRP:HZ3	1	0.45
(1,676)	1:117:A:LEU:HD11	1:129:A:TRP:HZ3	3	0.45
(1,655)	1:117:A:LEU:HD21	1:113:A:HIS:HB2	20	0.45
(1,612)	1:103:A:LEU:HD12	1:129:A:TRP:HD1	10	0.45
(1,612)	1:103:A:LEU:HD12	1:129:A:TRP:HD1	20	0.45
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	7	0.45
(1,585)	1:107:A:THR:HG22	1:130:A:LEU:HD23	19	0.45
(1,571)	1:95:A:VAL:HG22	1:112:A:TYR:HE1	4	0.45
(1,571)	1:95:A:VAL:HG23	1:112:A:TYR:HE1	13	0.45
(1,571)	1:95:A:VAL:HG23	1:112:A:TYR:HE1	15	0.45
(1,501)	1:121:A:LEU:HB2	1:123:A:GLU:H	15	0.45
(1,258)	1:107:A:THR:HG21	1:108:A:CYS:H	16	0.45
(1,178)	1:97:A:LYS:H	1:97:A:LYS:HD2	12	0.45
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD13	7	0.45
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	13	0.45
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD11	12	0.45
(1,60)	1:117:A:LEU:HD23	1:114:A:ILE:HA	8	0.45
(1,60)	1:117:A:LEU:HD21	1:114:A:ILE:HA	16	0.45
(1,21)	1:93:A:CYS:HB3	1:113:A:HIS:H	6	0.45
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	19	0.44
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	19	0.44
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	19	0.44
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	3	0.44
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	17	0.44
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	18	0.44
(1,713)	1:106:A:ASP:HB2	1:107:A:THR:H	1	0.44
(1,713)	1:106:A:ASP:HB2	1:107:A:THR:H	5	0.44
(1,713)	1:106:A:ASP:HB2	1:107:A:THR:H	11	0.44
(1,676)	1:117:A:LEU:HD11	1:129:A:TRP:HZ3	2	0.44
(1,676)	1:117:A:LEU:HD13	1:129:A:TRP:HZ3	8	0.44
(1,644)	1:95:A:VAL:HG21	1:94:A:ARG:HD2	18	0.44
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD12	9	0.44
(1,596)	1:97:A:LYS:HB3	1:92:A:PHE:HD1	20	0.44
(1,571)	1:95:A:VAL:HG22	1:112:A:TYR:HE1	7	0.44
(1,571)	1:95:A:VAL:HG23	1:112:A:TYR:HE1	9	0.44
(1,571)	1:95:A:VAL:HG21	1:112:A:TYR:HE1	20	0.44
(1,534)	1:98:A:ASP:HB3	1:113:A:HIS:HD2	11	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,247)	1:114:A:ILE:HG22	1:115:A:HIS:H	3	0.44
(1,247)	1:114:A:ILE:HG21	1:115:A:HIS:H	19	0.44
(1,235)	1:95:A:VAL:HG23	1:96:A:CYS:H	5	0.44
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD11	5	0.44
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG21	11	0.44
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG22	13	0.44
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG21	17	0.44
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG22	18	0.44
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	8	0.44
(1,18)	1:129:A:TRP:HE3	1:103:A:LEU:H	10	0.44
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	13	0.44
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	6	0.43
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	6	0.43
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	6	0.43
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	6	0.43
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	6	0.43
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	14	0.43
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	13	0.43
(1,781)	1:123:A:GLU:HB2	1:124:A:ILE:H	4	0.43
(1,762)	1:91:A:GLU:HG2	1:91:A:GLU:H	2	0.43
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	1	0.43
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	14	0.43
(1,676)	1:117:A:LEU:HD12	1:129:A:TRP:HZ3	15	0.43
(1,676)	1:117:A:LEU:HD13	1:129:A:TRP:HZ3	18	0.43
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD23	6	0.43
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD21	19	0.43
(1,655)	1:117:A:LEU:HD21	1:113:A:HIS:HB2	8	0.43
(1,600)	1:111:A:SER:HB2	1:102:A:LEU:HD12	9	0.43
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD12	15	0.43
(1,571)	1:95:A:VAL:HG23	1:112:A:TYR:HE1	2	0.43
(1,571)	1:95:A:VAL:HG23	1:112:A:TYR:HE1	10	0.43
(1,247)	1:114:A:ILE:HG22	1:115:A:HIS:H	18	0.43
(1,167)	1:125:A:PRO:HD2	1:124:A:ILE:H	15	0.43
(1,154)	1:102:A:LEU:HD13	1:94:A:ARG:H	3	0.43
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG22	1	0.43
(1,69)	1:130:A:LEU:HD13	1:128:A:GLU:HB2	19	0.43
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	14	0.43
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	12	0.42
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	12	0.42
(1,909)	1:98:A:ASP:H	2:152:B:M3L:HM12	5	0.42
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	18	0.42
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	18	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	18	0.42
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	7	0.42
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	14	0.42
(1,738)	1:130:A:LEU:HD22	1:129:A:TRP:H	18	0.42
(1,676)	1:117:A:LEU:HD13	1:129:A:TRP:HZ3	11	0.42
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD22	12	0.42
(1,588)	1:134:A:CYS:HA	1:130:A:LEU:HD22	12	0.42
(1,577)	1:112:A:TYR:HD1	1:117:A:LEU:HD11	7	0.42
(1,556)	1:91:A:GLU:HG3	1:92:A:PHE:HE1	15	0.42
(1,550)	1:90:A:MET:HE2	1:92:A:PHE:HE1	11	0.42
(1,466)	1:130:A:LEU:HD22	1:135:A:THR:H	7	0.42
(1,466)	1:130:A:LEU:HD23	1:135:A:THR:H	10	0.42
(1,290)	1:99:A:GLY:H	1:92:A:PHE:HD2	17	0.42
(1,258)	1:107:A:THR:HG23	1:108:A:CYS:H	9	0.42
(1,247)	1:114:A:ILE:HG22	1:115:A:HIS:H	5	0.42
(1,154)	1:102:A:LEU:HD11	1:94:A:ARG:H	14	0.42
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	7	0.42
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD12	17	0.42
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD13	13	0.42
(1,74)	1:107:A:THR:HG23	1:130:A:LEU:HG	18	0.42
(1,65)	1:121:A:LEU:HD22	1:114:A:ILE:HA	9	0.42
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	20	0.42
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	11	0.41
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	11	0.41
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	11	0.41
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	17	0.41
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	17	0.41
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	17	0.41
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG22	10	0.41
(1,851)	1:114:A:ILE:HG23	1:117:A:LEU:H	12	0.41
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	2	0.41
(1,600)	1:111:A:SER:HB2	1:102:A:LEU:HD13	3	0.41
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD11	8	0.41
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD11	20	0.41
(1,509)	1:102:A:LEU:HD22	1:92:A:PHE:H	18	0.41
(1,327)	1:132:A:PRO:HD3	1:131:A:CYS:H	6	0.41
(1,327)	1:132:A:PRO:HD3	1:131:A:CYS:H	11	0.41
(1,258)	1:107:A:THR:HG23	1:108:A:CYS:H	1	0.41
(1,247)	1:114:A:ILE:HG21	1:115:A:HIS:H	2	0.41
(1,235)	1:95:A:VAL:HG21	1:96:A:CYS:H	6	0.41
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD13	6	0.41
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD12	9	0.41
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD11	14	0.41
(1,65)	1:121:A:LEU:HD21	1:114:A:ILE:HA	5	0.41
(1,979)	1:101:A:GLU:HG2	2:146:B:THR:HG21	13	0.4
(1,979)	1:101:A:GLU:HG2	2:146:B:THR:HG22	13	0.4
(1,979)	1:101:A:GLU:HG2	2:146:B:THR:HG23	13	0.4
(1,979)	1:101:A:GLU:HG3	2:146:B:THR:HG21	13	0.4
(1,979)	1:101:A:GLU:HG3	2:146:B:THR:HG22	13	0.4
(1,979)	1:101:A:GLU:HG3	2:146:B:THR:HG23	13	0.4
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	7	0.4
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	7	0.4
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	15	0.4
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	15	0.4
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG21	19	0.4
(1,851)	1:114:A:ILE:HG23	1:117:A:LEU:H	11	0.4
(1,845)	1:115:A:HIS:HB2	1:117:A:LEU:H	8	0.4
(1,825)	1:110:A:SER:HB3	1:111:A:SER:H	20	0.4
(1,676)	1:117:A:LEU:HD12	1:129:A:TRP:HZ3	19	0.4
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD22	10	0.4
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	5	0.4
(1,612)	1:103:A:LEU:HD11	1:129:A:TRP:HD1	2	0.4
(1,612)	1:103:A:LEU:HD11	1:129:A:TRP:HD1	9	0.4
(1,600)	1:111:A:SER:HB2	1:102:A:LEU:HD12	8	0.4
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD12	8	0.4
(1,569)	1:91:A:GLU:HG3	1:92:A:PHE:HD1	3	0.4
(1,534)	1:98:A:ASP:HB3	1:113:A:HIS:HD2	20	0.4
(1,466)	1:130:A:LEU:HD22	1:135:A:THR:H	2	0.4
(1,258)	1:107:A:THR:HG23	1:108:A:CYS:H	13	0.4
(1,258)	1:107:A:THR:HG21	1:108:A:CYS:H	14	0.4
(1,247)	1:114:A:ILE:HG22	1:115:A:HIS:H	4	0.4
(1,247)	1:114:A:ILE:HG22	1:115:A:HIS:H	12	0.4
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	12	0.4
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	15	0.4
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD23	2	0.4
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	2	0.4
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	3	0.4
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	5	0.4
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	11	0.4
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	10	0.4
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	3	0.39
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	3	0.39
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	5	0.39
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	8	0.39
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	8	0.39
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	8	0.39
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	9	0.39
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	9	0.39
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	9	0.39
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	4	0.39
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	2	0.39
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	18	0.39
(1,676)	1:117:A:LEU:HD13	1:129:A:TRP:HZ3	5	0.39
(1,676)	1:117:A:LEU:HD11	1:129:A:TRP:HZ3	12	0.39
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD21	9	0.39
(1,655)	1:117:A:LEU:HD22	1:113:A:HIS:HB2	7	0.39
(1,655)	1:117:A:LEU:HD21	1:113:A:HIS:HB2	14	0.39
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	18	0.39
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD21	12	0.39
(1,612)	1:103:A:LEU:HD13	1:129:A:TRP:HD1	4	0.39
(1,602)	1:137:A:PRO:HD2	1:136:A:CYS:HB2	6	0.39
(1,596)	1:97:A:LYS:HB3	1:92:A:PHE:HD1	12	0.39
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD12	10	0.39
(1,534)	1:98:A:ASP:HB3	1:113:A:HIS:HD2	5	0.39
(1,509)	1:102:A:LEU:HD21	1:92:A:PHE:H	2	0.39
(1,509)	1:102:A:LEU:HD21	1:92:A:PHE:H	15	0.39
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	4	0.39
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	20	0.39
(1,169)	1:137:A:PRO:HD2	1:136:A:CYS:H	2	0.39
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD12	16	0.39
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	6	0.39
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD12	8	0.39
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	2	0.39
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	5	0.39
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	20	0.38
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	20	0.38
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	20	0.38
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	14	0.38
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	14	0.38
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	7	0.38
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	7	0.38
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	7	0.38
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	13	0.38
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	13	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	13	0.38
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	6	0.38
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	7	0.38
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	16	0.38
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	16	0.38
(1,681)	1:94:A:ARG:HD2	1:112:A:TYR:HE1	18	0.38
(1,676)	1:117:A:LEU:HD13	1:129:A:TRP:HZ3	6	0.38
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	12	0.38
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD22	11	0.38
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD12	17	0.38
(1,596)	1:97:A:LYS:HB3	1:92:A:PHE:HD1	1	0.38
(1,596)	1:97:A:LYS:HB3	1:92:A:PHE:HD1	14	0.38
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD13	9	0.38
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD13	12	0.38
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD13	19	0.38
(1,550)	1:90:A:MET:HE3	1:92:A:PHE:HE1	10	0.38
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD13	1	0.38
(1,327)	1:132:A:PRO:HD3	1:131:A:CYS:H	18	0.38
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	2	0.38
(1,258)	1:107:A:THR:HG22	1:108:A:CYS:H	12	0.38
(1,247)	1:114:A:ILE:HG22	1:115:A:HIS:H	11	0.38
(1,235)	1:95:A:VAL:HG21	1:96:A:CYS:H	19	0.38
(1,169)	1:137:A:PRO:HD2	1:136:A:CYS:H	15	0.38
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	1	0.38
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	4	0.38
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	8	0.38
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	9	0.38
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	10	0.38
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	12	0.38
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	13	0.38
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	15	0.38
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	17	0.38
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	18	0.38
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	19	0.38
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	20	0.38
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD11	13	0.38
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG22	3	0.38
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	9	0.38
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	19	0.38
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	10	0.37
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	10	0.37
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	16	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	16	0.37
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	3	0.37
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	3	0.37
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	3	0.37
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	6	0.37
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	6	0.37
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	6	0.37
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	15	0.37
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	15	0.37
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	15	0.37
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM22	4	0.37
(1,944)	1:98:A:ASP:HA	2:152:B:M3L:HE3	2	0.37
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	19	0.37
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	19	0.37
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	19	0.37
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	10	0.37
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	10	0.37
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	10	0.37
(1,861)	2:146:B:THR:H	2:145:B:ARG:HG2	10	0.37
(1,848)	1:112:A:TYR:HB2	1:117:A:LEU:H	17	0.37
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	9	0.37
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	15	0.37
(1,688)	1:94:A:ARG:HB2	1:112:A:TYR:HD1	11	0.37
(1,612)	1:103:A:LEU:HD12	1:129:A:TRP:HD1	6	0.37
(1,612)	1:103:A:LEU:HD13	1:129:A:TRP:HD1	14	0.37
(1,602)	1:137:A:PRO:HD2	1:136:A:CYS:HB2	12	0.37
(1,596)	1:97:A:LYS:HB3	1:92:A:PHE:HD1	9	0.37
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD13	13	0.37
(1,576)	1:136:A:CYS:HA	1:137:A:PRO:HD2	2	0.37
(1,571)	1:95:A:VAL:HG23	1:112:A:TYR:HE1	8	0.37
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	1	0.37
(1,556)	1:91:A:GLU:HG3	1:92:A:PHE:HE1	7	0.37
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD21	11	0.37
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD12	8	0.37
(1,235)	1:95:A:VAL:HG22	1:96:A:CYS:H	12	0.37
(1,235)	1:95:A:VAL:HG21	1:96:A:CYS:H	18	0.37
(1,178)	1:97:A:LYS:H	1:97:A:LYS:HD2	13	0.37
(1,115)	1:118:A:ASN:HA	1:119:A:PRO:HB2	16	0.37
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD23	12	0.37
(1,60)	1:117:A:LEU:HD21	1:114:A:ILE:HA	7	0.37
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	3	0.37
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	17	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	3	0.37
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	7	0.37
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	16	0.37
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	4	0.36
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	4	0.36
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	11	0.36
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	11	0.36
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	18	0.36
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	18	0.36
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	4	0.36
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	4	0.36
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	4	0.36
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM13	6	0.36
(1,944)	1:98:A:ASP:HA	2:152:B:M3L:HE3	1	0.36
(1,944)	1:98:A:ASP:HA	2:152:B:M3L:HE3	15	0.36
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	7	0.36
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	7	0.36
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	7	0.36
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	15	0.36
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	15	0.36
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	15	0.36
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	2	0.36
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	2	0.36
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	2	0.36
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	10	0.36
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD23	10	0.36
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD13	4	0.36
(1,556)	1:91:A:GLU:HG3	1:92:A:PHE:HE1	8	0.36
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD11	4	0.36
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD12	6	0.36
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD13	9	0.36
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD12	13	0.36
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD11	16	0.36
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD12	18	0.36
(1,509)	1:102:A:LEU:HD23	1:92:A:PHE:H	6	0.36
(1,501)	1:121:A:LEU:HB2	1:123:A:GLU:H	16	0.36
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	1	0.36
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	10	0.36
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	12	0.36
(1,258)	1:107:A:THR:HG23	1:108:A:CYS:H	6	0.36
(1,258)	1:107:A:THR:HG22	1:108:A:CYS:H	11	0.36
(1,204)	1:101:A:GLU:H	1:101:A:GLU:HB2	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:101:A:GLU:H	1:101:A:GLU:HB2	9	0.36
(1,101)	1:113:A:HIS:HA	1:102:A:LEU:HD13	3	0.36
(1,60)	1:117:A:LEU:HD22	1:114:A:ILE:HA	9	0.36
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	10	0.36
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	1	0.35
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	1	0.35
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	8	0.35
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	8	0.35
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM22	20	0.35
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	14	0.35
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	14	0.35
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	14	0.35
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG23	7	0.35
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	8	0.35
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	20	0.35
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	17	0.35
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD22	2	0.35
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD22	7	0.35
(1,651)	1:114:A:ILE:HG21	1:125:A:PRO:HD2	8	0.35
(1,597)	1:121:A:LEU:HD22	1:129:A:TRP:HD1	5	0.35
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	8	0.35
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD13	11	0.35
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD12	14	0.35
(1,576)	1:136:A:CYS:HA	1:137:A:PRO:HD2	15	0.35
(1,556)	1:91:A:GLU:HG3	1:92:A:PHE:HE1	6	0.35
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD13	2	0.35
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD13	10	0.35
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD11	15	0.35
(1,501)	1:121:A:LEU:HB2	1:123:A:GLU:H	3	0.35
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD22	11	0.35
(1,327)	1:132:A:PRO:HD3	1:131:A:CYS:H	10	0.35
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	3	0.35
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	5	0.35
(1,258)	1:107:A:THR:HG23	1:108:A:CYS:H	18	0.35
(1,235)	1:95:A:VAL:HG21	1:96:A:CYS:H	11	0.35
(1,169)	1:137:A:PRO:HD2	1:136:A:CYS:H	9	0.35
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD23	11	0.35
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG22	16	0.35
(1,46)	1:124:A:ILE:HG22	1:123:A:GLU:HA	8	0.35
(1,46)	1:124:A:ILE:HG23	1:123:A:GLU:HA	20	0.35
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	14	0.34
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	10	0.34
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	10	0.34
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	10	0.34
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	9	0.34
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	9	0.34
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	9	0.34
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	13	0.34
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	13	0.34
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	13	0.34
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	4	0.34
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	4	0.34
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	10	0.34
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	10	0.34
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	8	0.34
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	8	0.34
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	8	0.34
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	1	0.34
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	1	0.34
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	1	0.34
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	16	0.34
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	16	0.34
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	16	0.34
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	20	0.34
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	20	0.34
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	20	0.34
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	1	0.34
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	1	0.34
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG22	15	0.34
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	9	0.34
(1,858)	2:148:B:GLN:H	2:147:B:LYS:HB2	1	0.34
(1,845)	1:115:A:HIS:HB2	1:117:A:LEU:H	12	0.34
(1,674)	1:97:A:LYS:HD3	1:92:A:PHE:HD1	1	0.34
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD23	18	0.34
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD21	14	0.34
(1,633)	1:135:A:THR:HA	1:130:A:LEU:HD21	18	0.34
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD13	10	0.34
(1,567)	1:94:A:ARG:HD2	1:112:A:TYR:HE1	1	0.34
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD12	5	0.34
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD13	17	0.34
(1,509)	1:102:A:LEU:HD23	1:92:A:PHE:H	19	0.34
(1,327)	1:132:A:PRO:HD3	1:131:A:CYS:H	9	0.34
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	13	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	19	0.34
(1,234)	1:95:A:VAL:HG12	1:96:A:CYS:H	19	0.34
(1,178)	1:97:A:LYS:H	1:97:A:LYS:HD2	4	0.34
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD12	1	0.34
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD23	19	0.34
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD12	14	0.34
(1,75)	1:135:A:THR:HG21	1:130:A:LEU:HG	19	0.34
(1,69)	1:130:A:LEU:HD11	1:128:A:GLU:HB2	2	0.34
(1,60)	1:117:A:LEU:HD23	1:114:A:ILE:HA	14	0.34
(1,21)	1:93:A:CYS:HB3	1:113:A:HIS:H	14	0.34
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	15	0.34
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	20	0.33
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	20	0.33
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	6	0.33
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	6	0.33
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	6	0.33
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	9	0.33
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	9	0.33
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	5	0.33
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	5	0.33
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	5	0.33
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	12	0.33
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	12	0.33
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	12	0.33
(1,762)	1:91:A:GLU:HG2	1:91:A:GLU:H	13	0.33
(1,762)	1:91:A:GLU:HG2	1:91:A:GLU:H	17	0.33
(1,701)	1:111:A:SER:HB2	1:89:A:HIS:HD2	10	0.33
(1,671)	1:129:A:TRP:HZ3	1:103:A:LEU:HD22	15	0.33
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD21	13	0.33
(1,612)	1:103:A:LEU:HD11	1:129:A:TRP:HD1	1	0.33
(1,612)	1:103:A:LEU:HD11	1:129:A:TRP:HD1	5	0.33
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD13	3	0.33
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD13	1	0.33
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD11	5	0.33
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD13	17	0.33
(1,576)	1:136:A:CYS:HA	1:137:A:PRO:HD2	9	0.33
(1,569)	1:91:A:GLU:HG3	1:92:A:PHE:HD1	11	0.33
(1,556)	1:91:A:GLU:HG3	1:92:A:PHE:HE1	11	0.33
(1,553)	1:97:A:LYS:HE2	1:92:A:PHE:HE1	7	0.33
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD23	12	0.33
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD12	11	0.33
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD12	20	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	6	0.33
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	13	0.33
(1,327)	1:132:A:PRO:HD3	1:131:A:CYS:H	3	0.33
(1,318)	1:89:A:HIS:HB2	1:90:A:MET:H	3	0.33
(1,318)	1:89:A:HIS:HB2	1:90:A:MET:H	6	0.33
(1,258)	1:107:A:THR:HG22	1:108:A:CYS:H	19	0.33
(1,247)	1:114:A:ILE:HG21	1:115:A:HIS:H	6	0.33
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	3	0.33
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	18	0.33
(1,178)	1:97:A:LYS:H	1:97:A:LYS:HD2	1	0.33
(1,120)	1:114:A:ILE:HB	1:121:A:LEU:HB3	16	0.33
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD23	8	0.33
(1,60)	1:117:A:LEU:HD21	1:114:A:ILE:HA	20	0.33
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	1	0.33
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	5	0.33
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	7	0.33
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	2	0.32
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	2	0.32
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	9	0.32
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	9	0.32
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	14	0.32
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	14	0.32
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	14	0.32
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	8	0.32
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	8	0.32
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	8	0.32
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM32	16	0.32
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	20	0.32
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	20	0.32
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	1	0.32
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	1	0.32
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	1	0.32
(1,909)	1:98:A:ASP:H	2:152:B:M3L:HM33	6	0.32
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	4	0.32
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	4	0.32
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	4	0.32
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	18	0.32
(1,858)	2:148:B:GLN:H	2:147:B:LYS:HB2	7	0.32
(1,821)	1:130:A:LEU:HD12	1:135:A:THR:H	15	0.32
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	19	0.32
(1,730)	1:111:A:SER:HB2	1:112:A:TYR:H	5	0.32
(1,730)	1:111:A:SER:HB2	1:112:A:TYR:H	17	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	9	0.32
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	19	0.32
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD21	20	0.32
(1,655)	1:117:A:LEU:HD23	1:113:A:HIS:HB2	10	0.32
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	11	0.32
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	19	0.32
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG23	7	0.32
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD21	8	0.32
(1,596)	1:97:A:LYS:HB3	1:92:A:PHE:HD1	18	0.32
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD11	3	0.32
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD11	18	0.32
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	10	0.32
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	16	0.32
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	20	0.32
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD13	3	0.32
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD13	12	0.32
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD11	19	0.32
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	3	0.32
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	5	0.32
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	7	0.32
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	8	0.32
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	10	0.32
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	12	0.32
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	16	0.32
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	18	0.32
(1,318)	1:89:A:HIS:HB2	1:90:A:MET:H	10	0.32
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	7	0.32
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	8	0.32
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	16	0.32
(1,293)	1:99:A:GLY:H	1:98:A:ASP:HB2	7	0.32
(1,234)	1:95:A:VAL:HG13	1:96:A:CYS:H	12	0.32
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD23	3	0.32
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD11	10	0.32
(1,65)	1:121:A:LEU:HD21	1:114:A:ILE:HA	13	0.32
(1,46)	1:124:A:ILE:HG23	1:123:A:GLU:HA	4	0.32
(1,46)	1:124:A:ILE:HG22	1:123:A:GLU:HA	6	0.32
(1,42)	1:102:A:LEU:HD12	1:99:A:GLY:HA3	1	0.32
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	18	0.32
(1,980)	1:101:A:GLU:HG2	2:148:B:GLN:HA	5	0.31
(1,980)	1:101:A:GLU:HG3	2:148:B:GLN:HA	5	0.31
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	2	0.31
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	2	0.31
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	4	0.31
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	4	0.31
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	4	0.31
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	18	0.31
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	18	0.31
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	18	0.31
(1,887)	1:98:A:ASP:HA	2:151:B:ARG:HA	17	0.31
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	15	0.31
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	15	0.31
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	17	0.31
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	17	0.31
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG23	6	0.31
(1,858)	2:148:B:GLN:H	2:147:B:LYS:HB2	20	0.31
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	5	0.31
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	3	0.31
(1,730)	1:111:A:SER:HB2	1:112:A:TYR:H	14	0.31
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD21	1	0.31
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD22	9	0.31
(1,612)	1:103:A:LEU:HD13	1:129:A:TRP:HD1	3	0.31
(1,612)	1:103:A:LEU:HD12	1:129:A:TRP:HD1	7	0.31
(1,589)	1:134:A:CYS:HA	1:130:A:LEU:HD13	18	0.31
(1,567)	1:94:A:ARG:HD2	1:112:A:TYR:HE1	7	0.31
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	1	0.31
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	2	0.31
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	3	0.31
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	4	0.31
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	5	0.31
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	6	0.31
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	11	0.31
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	13	0.31
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	14	0.31
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	15	0.31
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	17	0.31
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	18	0.31
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	19	0.31
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	2	0.31
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	4	0.31
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	9	0.31
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	11	0.31
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	14	0.31
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	17	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	19	0.31
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	20	0.31
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	6	0.31
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	14	0.31
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	18	0.31
(1,258)	1:107:A:THR:HG23	1:108:A:CYS:H	2	0.31
(1,258)	1:107:A:THR:HG22	1:108:A:CYS:H	15	0.31
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	6	0.31
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD13	15	0.31
(1,65)	1:121:A:LEU:HD22	1:114:A:ILE:HA	12	0.31
(1,65)	1:121:A:LEU:HD21	1:114:A:ILE:HA	14	0.31
(1,51)	1:95:A:VAL:HG22	1:96:A:CYS:HB2	16	0.31
(1,46)	1:124:A:ILE:HG22	1:123:A:GLU:HA	12	0.31
(1,46)	1:124:A:ILE:HG22	1:123:A:GLU:HA	17	0.31
(1,46)	1:124:A:ILE:HG23	1:123:A:GLU:HA	18	0.31
(1,25)	1:111:A:SER:HB2	1:105:A:CYS:H	15	0.31
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	4	0.31
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	9	0.31
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	12	0.31
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	2	0.3
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	2	0.3
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	2	0.3
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	16	0.3
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	16	0.3
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	16	0.3
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	16	0.3
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	16	0.3
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG21	1	0.3
(1,858)	2:148:B:GLN:H	2:147:B:LYS:HB2	11	0.3
(1,858)	2:148:B:GLN:H	2:147:B:LYS:HB2	18	0.3
(1,825)	1:110:A:SER:HB3	1:111:A:SER:H	3	0.3
(1,762)	1:91:A:GLU:HG2	1:91:A:GLU:H	8	0.3
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	4	0.3
(1,760)	1:112:A:TYR:HB2	1:113:A:HIS:H	15	0.3
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG22	9	0.3
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD23	3	0.3
(1,612)	1:103:A:LEU:HD11	1:129:A:TRP:HD1	16	0.3
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD12	15	0.3
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	18	0.3
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	7	0.3
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	8	0.3
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD13	14	0.3
(1,439)	1:96:A:CYS:HB2	1:97:A:LYS:H	12	0.3
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	15	0.3
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	15	0.3
(1,234)	1:95:A:VAL:HG13	1:96:A:CYS:H	11	0.3
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	4	0.3
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	19	0.3
(1,171)	1:135:A:THR:HG22	1:136:A:CYS:H	1	0.3
(1,171)	1:135:A:THR:HG22	1:136:A:CYS:H	17	0.3
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD21	18	0.3
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD12	11	0.3
(1,65)	1:121:A:LEU:HD21	1:114:A:ILE:HA	8	0.3
(1,60)	1:117:A:LEU:HD23	1:114:A:ILE:HA	10	0.3
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	20	0.29
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	20	0.29
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	20	0.29
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	7	0.29
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	7	0.29
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	7	0.29
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	17	0.29
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	17	0.29
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	17	0.29
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	20	0.29
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	20	0.29
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	20	0.29
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	2	0.29
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	2	0.29
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	19	0.29
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	19	0.29
(1,858)	2:148:B:GLN:H	2:147:B:LYS:HB2	16	0.29
(1,821)	1:130:A:LEU:HD13	1:135:A:THR:H	1	0.29
(1,821)	1:130:A:LEU:HD13	1:135:A:THR:H	8	0.29
(1,762)	1:91:A:GLU:HG2	1:91:A:GLU:H	5	0.29
(1,670)	1:117:A:LEU:HD11	1:129:A:TRP:HH2	14	0.29
(1,654)	1:132:A:PRO:HD2	1:117:A:LEU:HD22	2	0.29
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD21	2	0.29
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG23	13	0.29
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD21	12	0.29
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD23	3	0.29
(1,597)	1:121:A:LEU:HD21	1:129:A:TRP:HD1	19	0.29
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD12	13	0.29
(1,550)	1:90:A:MET:HE3	1:92:A:PHE:HE1	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:129:A:TRP:HB3	1:129:A:TRP:HD1	12	0.29
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD22	3	0.29
(1,501)	1:121:A:LEU:HB2	1:123:A:GLU:H	4	0.29
(1,439)	1:96:A:CYS:HB2	1:97:A:LYS:H	6	0.29
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	19	0.29
(1,338)	1:100:A:GLY:H	1:99:A:GLY:HA3	1	0.29
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	11	0.29
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	17	0.29
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	1	0.29
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	16	0.29
(1,171)	1:135:A:THR:HG22	1:136:A:CYS:H	3	0.29
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD21	4	0.29
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD21	17	0.29
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD23	1	0.29
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD21	6	0.29
(1,46)	1:124:A:ILE:HG22	1:123:A:GLU:HA	9	0.29
(1,46)	1:124:A:ILE:HG21	1:123:A:GLU:HA	14	0.29
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	13	0.29
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	15	0.29
(1,21)	1:93:A:CYS:HB3	1:113:A:HIS:H	18	0.29
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	7	0.28
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	7	0.28
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	7	0.28
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	14	0.28
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	14	0.28
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	14	0.28
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	15	0.28
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	15	0.28
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	15	0.28
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	15	0.28
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	15	0.28
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	15	0.28
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	5	0.28
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	5	0.28
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	9	0.28
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	9	0.28
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	1	0.28
(1,858)	2:148:B:GLN:H	2:147:B:LYS:HB2	17	0.28
(1,741)	1:135:A:THR:HG22	1:131:A:CYS:H	12	0.28
(1,738)	1:130:A:LEU:HD23	1:129:A:TRP:H	8	0.28
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	10	0.28
(1,670)	1:117:A:LEU:HD13	1:129:A:TRP:HH2	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:117:A:LEU:HD12	1:129:A:TRP:HH2	15	0.28
(1,651)	1:114:A:ILE:HG23	1:125:A:PRO:HD2	4	0.28
(1,644)	1:95:A:VAL:HG22	1:94:A:ARG:HD2	7	0.28
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG22	15	0.28
(1,612)	1:103:A:LEU:HD12	1:129:A:TRP:HD1	13	0.28
(1,592)	1:120:A:PRO:HA	1:121:A:LEU:HD13	16	0.28
(1,589)	1:134:A:CYS:HA	1:130:A:LEU:HD13	8	0.28
(1,576)	1:136:A:CYS:HA	1:137:A:PRO:HD2	7	0.28
(1,439)	1:96:A:CYS:HB2	1:97:A:LYS:H	18	0.28
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	11	0.28
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	17	0.28
(1,344)	1:102:A:LEU:HD11	1:103:A:LEU:H	13	0.28
(1,299)	1:129:A:TRP:HE1	1:125:A:PRO:HD2	9	0.28
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	2	0.28
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	20	0.28
(1,171)	1:135:A:THR:HG22	1:136:A:CYS:H	15	0.28
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD13	13	0.28
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD12	15	0.28
(1,69)	1:130:A:LEU:HD11	1:128:A:GLU:HB2	20	0.28
(1,51)	1:95:A:VAL:HG23	1:96:A:CYS:HB2	13	0.28
(1,46)	1:124:A:ILE:HG23	1:123:A:GLU:HA	11	0.28
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	8	0.28
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	1	0.27
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	1	0.27
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	1	0.27
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	18	0.27
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	18	0.27
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	18	0.27
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	18	0.27
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	18	0.27
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	18	0.27
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	7	0.27
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	7	0.27
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	8	0.27
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	8	0.27
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	11	0.27
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	11	0.27
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	19	0.27
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	19	0.27
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	10	0.27
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	10	0.27
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	12	0.27
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	12	0.27
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	12	0.27
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	3	0.27
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	3	0.27
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG23	4	0.27
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG22	8	0.27
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG23	17	0.27
(1,820)	1:121:A:LEU:HD23	1:121:A:LEU:H	16	0.27
(1,754)	1:89:A:HIS:HD2	1:103:A:LEU:H	8	0.27
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	12	0.27
(1,641)	1:115:A:HIS:HA	1:120:A:PRO:HB2	7	0.27
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD23	17	0.27
(1,612)	1:103:A:LEU:HD12	1:129:A:TRP:HD1	8	0.27
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD11	5	0.27
(1,516)	1:117:A:LEU:H	1:117:A:LEU:HD13	7	0.27
(1,501)	1:121:A:LEU:HB2	1:123:A:GLU:H	7	0.27
(1,501)	1:121:A:LEU:HB2	1:123:A:GLU:H	13	0.27
(1,501)	1:121:A:LEU:HB2	1:123:A:GLU:H	14	0.27
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD22	17	0.27
(1,466)	1:130:A:LEU:HD21	1:135:A:THR:H	13	0.27
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	2	0.27
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	20	0.27
(1,258)	1:107:A:THR:HG23	1:108:A:CYS:H	4	0.27
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	5	0.27
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	11	0.27
(1,122)	1:114:A:ILE:HB	1:103:A:LEU:HD12	2	0.27
(1,69)	1:130:A:LEU:HD12	1:128:A:GLU:HB2	9	0.27
(1,60)	1:117:A:LEU:HD21	1:114:A:ILE:HA	13	0.27
(1,46)	1:124:A:ILE:HG21	1:123:A:GLU:HA	2	0.27
(1,46)	1:124:A:ILE:HG23	1:123:A:GLU:HA	3	0.27
(1,16)	1:117:A:LEU:HD11	1:114:A:ILE:H	16	0.27
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	8	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	8	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	8	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	12	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	12	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	12	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	13	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	13	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	13	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	16	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	16	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	16	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	19	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	19	0.26
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	19	0.26
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	15	0.26
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	15	0.26
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	15	0.26
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	17	0.26
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	17	0.26
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	17	0.26
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	4	0.26
(1,909)	1:98:A:ASP:H	2:152:B:M3L:HM12	16	0.26
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG21	3	0.26
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG22	3	0.26
(1,907)	1:124:A:ILE:H	2:146:B:THR:HG23	3	0.26
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	9	0.26
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	9	0.26
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	9	0.26
(1,890)	1:91:A:GLU:HA	2:147:B:LYS:HB2	18	0.26
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	4	0.26
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	4	0.26
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	8	0.26
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	8	0.26
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	18	0.26
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	18	0.26
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG22	16	0.26
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG21	18	0.26
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG22	20	0.26
(1,821)	1:130:A:LEU:HD12	1:135:A:THR:H	3	0.26
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	19	0.26
(1,688)	1:94:A:ARG:HB2	1:112:A:TYR:HD1	14	0.26
(1,677)	1:112:A:TYR:HB3	1:129:A:TRP:HZ3	13	0.26
(1,670)	1:117:A:LEU:HD11	1:129:A:TRP:HH2	7	0.26
(1,670)	1:117:A:LEU:HD13	1:129:A:TRP:HH2	20	0.26
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD22	4	0.26
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG22	12	0.26
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG23	16	0.26
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	12	0.26
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD12	9	0.26
(1,578)	1:130:A:LEU:HD11	1:106:A:ASP:HB2	12	0.26
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	9	0.26
(1,556)	1:91:A:GLU:HG3	1:92:A:PHE:HE1	10	0.26
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD21	5	0.26
(1,466)	1:130:A:LEU:HD21	1:135:A:THR:H	9	0.26
(1,403)	1:89:A:HIS:HB2	1:105:A:CYS:H	14	0.26
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	6	0.26
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	12	0.26
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	5	0.26
(1,258)	1:107:A:THR:HG23	1:108:A:CYS:H	7	0.26
(1,204)	1:101:A:GLU:H	1:101:A:GLU:HB2	13	0.26
(1,185)	1:118:A:ASN:HB2	1:118:A:ASN:H	8	0.26
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	9	0.26
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	15	0.26
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD11	9	0.26
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD11	2	0.26
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD12	16	0.26
(1,69)	1:130:A:LEU:HD11	1:128:A:GLU:HB2	13	0.26
(1,65)	1:121:A:LEU:HD22	1:114:A:ILE:HA	3	0.26
(1,46)	1:124:A:ILE:HG21	1:123:A:GLU:HA	5	0.26
(1,21)	1:93:A:CYS:HB3	1:113:A:HIS:H	12	0.26
(1,13)	1:92:A:PHE:HA	1:99:A:GLY:H	6	0.26
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD2	10	0.25
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD3	10	0.25
(1,980)	1:101:A:GLU:HG2	2:148:B:GLN:HA	9	0.25
(1,980)	1:101:A:GLU:HG3	2:148:B:GLN:HA	9	0.25
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB2	19	0.25
(1,975)	1:101:A:GLU:H	2:151:B:ARG:HB3	19	0.25
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	3	0.25
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	3	0.25
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	13	0.25
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	13	0.25
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	13	0.25
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	20	0.25
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	20	0.25
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	20	0.25
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	10	0.25
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	10	0.25
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	12	0.25
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	12	0.25
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG21	18	0.25
(1,834)	1:120:A:PRO:HB2	1:115:A:HIS:H	7	0.25
(1,785)	1:128:A:GLU:HG3	1:128:A:GLU:H	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,762)	1:91:A:GLU:HG2	1:91:A:GLU:H	19	0.25
(1,739)	1:130:A:LEU:HD12	1:129:A:TRP:H	13	0.25
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	11	0.25
(1,653)	1:103:A:LEU:HD21	1:129:A:TRP:HB2	15	0.25
(1,644)	1:95:A:VAL:HG22	1:94:A:ARG:HD2	1	0.25
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG21	1	0.25
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG22	6	0.25
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG22	10	0.25
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG22	17	0.25
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG23	19	0.25
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD22	11	0.25
(1,612)	1:103:A:LEU:HD12	1:129:A:TRP:HD1	19	0.25
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD11	13	0.25
(1,578)	1:130:A:LEU:HD12	1:106:A:ASP:HB2	2	0.25
(1,578)	1:130:A:LEU:HD12	1:106:A:ASP:HB2	4	0.25
(1,556)	1:91:A:GLU:HG3	1:92:A:PHE:HE1	4	0.25
(1,545)	1:102:A:LEU:HA	1:103:A:LEU:HD22	13	0.25
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD21	10	0.25
(1,258)	1:107:A:THR:HG21	1:108:A:CYS:H	17	0.25
(1,258)	1:107:A:THR:HG23	1:108:A:CYS:H	20	0.25
(1,239)	1:96:A:CYS:HB2	1:96:A:CYS:H	12	0.25
(1,213)	1:133:A:ARG:H	1:133:A:ARG:HD3	15	0.25
(1,69)	1:130:A:LEU:HD11	1:128:A:GLU:HB2	4	0.25
(1,63)	1:121:A:LEU:HD12	1:117:A:LEU:HG	7	0.25
(1,51)	1:95:A:VAL:HG22	1:96:A:CYS:HB2	4	0.25
(1,46)	1:124:A:ILE:HG23	1:123:A:GLU:HA	19	0.25
(1,21)	1:93:A:CYS:HB3	1:113:A:HIS:H	20	0.25
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	13	0.24
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	13	0.24
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	13	0.24
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	13	0.24
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	13	0.24
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	13	0.24
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	17	0.24
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	17	0.24
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	17	0.24
(1,944)	1:98:A:ASP:HA	2:152:B:M3L:HE3	20	0.24
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	2	0.24
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	2	0.24
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	2	0.24
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	4	0.24
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	4	0.24
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	5	0.24
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	5	0.24
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	5	0.24
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	11	0.24
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	11	0.24
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	11	0.24
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	16	0.24
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	16	0.24
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	16	0.24
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	14	0.24
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	14	0.24
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	14	0.24
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	6	0.24
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	6	0.24
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG23	7	0.24
(1,785)	1:128:A:GLU:HG3	1:128:A:GLU:H	6	0.24
(1,754)	1:89:A:HIS:HD2	1:103:A:LEU:H	10	0.24
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	1	0.24
(1,670)	1:117:A:LEU:HD12	1:129:A:TRP:HH2	4	0.24
(1,670)	1:117:A:LEU:HD11	1:129:A:TRP:HH2	17	0.24
(1,663)	1:118:A:ASN:HA	1:120:A:PRO:HD2	14	0.24
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD23	4	0.24
(1,651)	1:114:A:ILE:HG23	1:125:A:PRO:HD2	18	0.24
(1,644)	1:95:A:VAL:HG22	1:94:A:ARG:HD2	14	0.24
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD22	14	0.24
(1,622)	1:91:A:GLU:HA	1:102:A:LEU:HD13	17	0.24
(1,612)	1:103:A:LEU:HD11	1:129:A:TRP:HD1	12	0.24
(1,612)	1:103:A:LEU:HD11	1:129:A:TRP:HD1	17	0.24
(1,612)	1:103:A:LEU:HD12	1:129:A:TRP:HD1	18	0.24
(1,600)	1:111:A:SER:HB2	1:102:A:LEU:HD11	12	0.24
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD11	12	0.24
(1,597)	1:121:A:LEU:HD22	1:129:A:TRP:HD1	13	0.24
(1,574)	1:114:A:ILE:HG23	1:122:A:PRO:HD2	7	0.24
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	18	0.24
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	3	0.24
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	6	0.24
(1,239)	1:96:A:CYS:HB2	1:96:A:CYS:H	11	0.24
(1,239)	1:96:A:CYS:HB2	1:96:A:CYS:H	19	0.24
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	7	0.24
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	14	0.24
(1,171)	1:135:A:THR:HG22	1:136:A:CYS:H	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:90:A:MET:HE1	1:110:A:SER:HA	10	0.24
(1,65)	1:121:A:LEU:HD23	1:114:A:ILE:HA	10	0.24
(1,46)	1:124:A:ILE:HG22	1:123:A:GLU:HA	10	0.24
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	16	0.24
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	9	0.23
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	9	0.23
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	9	0.23
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	17	0.23
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	17	0.23
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	17	0.23
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	19	0.23
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	19	0.23
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	19	0.23
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	1	0.23
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	1	0.23
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	18	0.23
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	18	0.23
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	6	0.23
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	6	0.23
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	6	0.23
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	19	0.23
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	19	0.23
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	19	0.23
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	4	0.23
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	4	0.23
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	4	0.23
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	7	0.23
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	7	0.23
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	7	0.23
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	12	0.23
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG23	10	0.23
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	13	0.23
(1,785)	1:128:A:GLU:HG3	1:128:A:GLU:H	5	0.23
(1,785)	1:128:A:GLU:HG3	1:128:A:GLU:H	16	0.23
(1,763)	1:89:A:HIS:HB3	1:90:A:MET:H	15	0.23
(1,739)	1:130:A:LEU:HD13	1:129:A:TRP:H	5	0.23
(1,739)	1:130:A:LEU:HD11	1:129:A:TRP:H	19	0.23
(1,739)	1:130:A:LEU:HD12	1:129:A:TRP:H	20	0.23
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	3	0.23
(1,670)	1:117:A:LEU:HD11	1:129:A:TRP:HH2	2	0.23
(1,670)	1:117:A:LEU:HD11	1:129:A:TRP:HH2	10	0.23
(1,670)	1:117:A:LEU:HD12	1:129:A:TRP:HH2	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,646)	1:132:A:PRO:HG2	1:117:A:LEU:HD22	17	0.23
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG21	5	0.23
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG21	14	0.23
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG23	18	0.23
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD23	6	0.23
(1,627)	1:111:A:SER:HB2	1:102:A:LEU:HD21	8	0.23
(1,609)	1:132:A:PRO:HD3	1:129:A:TRP:HH2	18	0.23
(1,600)	1:111:A:SER:HB2	1:102:A:LEU:HD11	13	0.23
(1,596)	1:97:A:LYS:HB3	1:92:A:PHE:HD1	2	0.23
(1,574)	1:114:A:ILE:HG22	1:122:A:PRO:HD2	13	0.23
(1,562)	1:112:A:TYR:HE1	1:117:A:LEU:HD21	11	0.23
(1,534)	1:98:A:ASP:HB3	1:113:A:HIS:HD2	6	0.23
(1,501)	1:121:A:LEU:HB2	1:123:A:GLU:H	1	0.23
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD21	2	0.23
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	11	0.23
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	19	0.23
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	8	0.23
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	14	0.23
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	10	0.23
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	11	0.23
(1,169)	1:137:A:PRO:HD2	1:136:A:CYS:H	7	0.23
(1,154)	1:102:A:LEU:HD11	1:94:A:ARG:H	13	0.23
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD13	19	0.23
(1,65)	1:121:A:LEU:HD21	1:114:A:ILE:HA	4	0.23
(1,51)	1:95:A:VAL:HG22	1:96:A:CYS:HB2	1	0.23
(1,51)	1:95:A:VAL:HG23	1:96:A:CYS:HB2	2	0.23
(1,980)	1:101:A:GLU:HG2	2:148:B:GLN:HA	13	0.22
(1,980)	1:101:A:GLU:HG3	2:148:B:GLN:HA	13	0.22
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	1	0.22
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	1	0.22
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	1	0.22
(1,948)	1:92:A:PHE:HD1	2:152:B:M3L:HM23	7	0.22
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	12	0.22
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	12	0.22
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	12	0.22
(1,930)	1:97:A:LYS:H	2:152:B:M3L:HM33	10	0.22
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	4	0.22
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	4	0.22
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	4	0.22
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	6	0.22
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	6	0.22
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,890)	1:91:A:GLU:HA	2:147:B:LYS:HB2	11	0.22
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	13	0.22
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	13	0.22
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG23	8	0.22
(1,820)	1:121:A:LEU:HD21	1:121:A:LEU:H	3	0.22
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	17	0.22
(1,754)	1:89:A:HIS:HD2	1:103:A:LEU:H	2	0.22
(1,730)	1:111:A:SER:HB2	1:112:A:TYR:H	15	0.22
(1,730)	1:111:A:SER:HB2	1:112:A:TYR:H	20	0.22
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	5	0.22
(1,709)	1:94:A:ARG:HD2	1:94:A:ARG:H	7	0.22
(1,696)	1:90:A:MET:HE1	1:92:A:PHE:HD1	15	0.22
(1,681)	1:94:A:ARG:HD2	1:112:A:TYR:HE1	1	0.22
(1,670)	1:117:A:LEU:HD11	1:129:A:TRP:HH2	1	0.22
(1,654)	1:132:A:PRO:HD2	1:117:A:LEU:HD22	1	0.22
(1,651)	1:114:A:ILE:HG23	1:125:A:PRO:HD2	10	0.22
(1,645)	1:101:A:GLU:HG2	1:114:A:ILE:HD11	6	0.22
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG23	4	0.22
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG23	20	0.22
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	6	0.22
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	8	0.22
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD21	9	0.22
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD22	2	0.22
(1,65)	1:121:A:LEU:HD22	1:114:A:ILE:HA	11	0.22
(1,58)	1:103:A:LEU:HD23	1:124:A:ILE:HG12	15	0.22
(1,46)	1:124:A:ILE:HG23	1:123:A:GLU:HA	7	0.22
(1,46)	1:124:A:ILE:HG23	1:123:A:GLU:HA	16	0.22
(1,21)	1:93:A:CYS:HB3	1:95:A:VAL:H	2	0.22
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	1	0.21
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	1	0.21
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	13	0.21
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	13	0.21
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	13	0.21
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	13	0.21
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	13	0.21
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	13	0.21
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB1	3	0.21
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB2	3	0.21
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB3	3	0.21
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB1	17	0.21
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB2	17	0.21
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB3	17	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	5	0.21
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	5	0.21
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	5	0.21
(1,944)	1:98:A:ASP:HA	2:152:B:M3L:HE3	10	0.21
(1,944)	1:98:A:ASP:HA	2:152:B:M3L:HE3	16	0.21
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	11	0.21
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	11	0.21
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	11	0.21
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	1	0.21
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	1	0.21
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	1	0.21
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	7	0.21
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	7	0.21
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	7	0.21
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	5	0.21
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	5	0.21
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	2	0.21
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	8	0.21
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	5	0.21
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	5	0.21
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	5	0.21
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	11	0.21
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	11	0.21
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	11	0.21
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	10	0.21
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	10	0.21
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	10	0.21
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	12	0.21
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	12	0.21
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	12	0.21
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	16	0.21
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	16	0.21
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	16	0.21
(1,890)	1:91:A:GLU:HA	2:147:B:LYS:HB2	1	0.21
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	11	0.21
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	11	0.21
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG22	4	0.21
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG23	15	0.21
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	1	0.21
(1,762)	1:91:A:GLU:HG2	1:91:A:GLU:H	6	0.21
(1,762)	1:91:A:GLU:HG2	1:91:A:GLU:H	20	0.21
(1,754)	1:89:A:HIS:HD2	1:103:A:LEU:H	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,754)	1:89:A:HIS:HD2	1:103:A:LEU:H	6	0.21
(1,698)	1:125:A:PRO:HG3	1:129:A:TRP:HZ2	15	0.21
(1,696)	1:90:A:MET:HE2	1:92:A:PHE:HD1	4	0.21
(1,696)	1:90:A:MET:HE1	1:92:A:PHE:HD1	17	0.21
(1,677)	1:112:A:TYR:HB3	1:129:A:TRP:HZ3	17	0.21
(1,670)	1:117:A:LEU:HD11	1:129:A:TRP:HH2	3	0.21
(1,670)	1:117:A:LEU:HD11	1:129:A:TRP:HH2	9	0.21
(1,670)	1:117:A:LEU:HD13	1:129:A:TRP:HH2	11	0.21
(1,655)	1:117:A:LEU:HD23	1:113:A:HIS:HB2	18	0.21
(1,651)	1:114:A:ILE:HG23	1:125:A:PRO:HD2	11	0.21
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG21	2	0.21
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG23	11	0.21
(1,601)	1:102:A:LEU:HB3	1:111:A:SER:HB2	8	0.21
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	7	0.21
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD12	9	0.21
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD13	11	0.21
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD11	12	0.21
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD21	3	0.21
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD22	13	0.21
(1,439)	1:96:A:CYS:HB2	1:97:A:LYS:H	11	0.21
(1,439)	1:96:A:CYS:HB2	1:97:A:LYS:H	19	0.21
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	12	0.21
(1,318)	1:89:A:HIS:HB2	1:90:A:MET:H	13	0.21
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	6	0.21
(1,258)	1:107:A:THR:HG21	1:108:A:CYS:H	5	0.21
(1,239)	1:96:A:CYS:HB2	1:96:A:CYS:H	6	0.21
(1,239)	1:96:A:CYS:HB2	1:96:A:CYS:H	18	0.21
(1,185)	1:118:A:ASN:HB2	1:118:A:ASN:H	7	0.21
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	8	0.21
(1,181)	1:97:A:LYS:H	1:97:A:LYS:HG3	17	0.21
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	12	0.21
(1,82)	1:132:A:PRO:HA	1:135:A:THR:HG22	15	0.21
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD13	20	0.21
(1,65)	1:121:A:LEU:HD23	1:114:A:ILE:HA	19	0.21
(1,51)	1:95:A:VAL:HG23	1:96:A:CYS:HB2	15	0.21
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	10	0.2
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	10	0.2
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	14	0.2
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	14	0.2
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	14	0.2
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	14	0.2
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB1	10	0.2
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB2	10	0.2
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB3	10	0.2
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	3	0.2
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	3	0.2
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	3	0.2
(1,915)	1:101:A:GLU:H	2:151:B:ARG:HG2	17	0.2
(1,915)	1:101:A:GLU:H	2:151:B:ARG:HG3	17	0.2
(1,898)	1:102:A:LEU:HD11	2:148:B:GLN:HG2	9	0.2
(1,898)	1:102:A:LEU:HD11	2:148:B:GLN:HG3	9	0.2
(1,898)	1:102:A:LEU:HD12	2:148:B:GLN:HG2	9	0.2
(1,898)	1:102:A:LEU:HD12	2:148:B:GLN:HG3	9	0.2
(1,898)	1:102:A:LEU:HD13	2:148:B:GLN:HG2	9	0.2
(1,898)	1:102:A:LEU:HD13	2:148:B:GLN:HG3	9	0.2
(1,820)	1:121:A:LEU:HD21	1:121:A:LEU:H	17	0.2
(1,820)	1:121:A:LEU:HD22	1:121:A:LEU:H	19	0.2
(1,818)	1:114:A:ILE:HG23	1:121:A:LEU:H	15	0.2
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	18	0.2
(1,754)	1:89:A:HIS:HD2	1:103:A:LEU:H	15	0.2
(1,701)	1:111:A:SER:HB2	1:89:A:HIS:HD2	3	0.2
(1,688)	1:94:A:ARG:HB2	1:112:A:TYR:HD1	12	0.2
(1,681)	1:94:A:ARG:HD2	1:112:A:TYR:HE1	7	0.2
(1,677)	1:112:A:TYR:HB3	1:129:A:TRP:HZ3	14	0.2
(1,670)	1:117:A:LEU:HD12	1:129:A:TRP:HH2	19	0.2
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG22	8	0.2
(1,625)	1:129:A:TRP:HB3	1:103:A:LEU:HD21	15	0.2
(1,612)	1:103:A:LEU:HD11	1:129:A:TRP:HD1	11	0.2
(1,609)	1:132:A:PRO:HD3	1:129:A:TRP:HH2	3	0.2
(1,609)	1:132:A:PRO:HD3	1:129:A:TRP:HH2	11	0.2
(1,545)	1:102:A:LEU:HA	1:103:A:LEU:HD21	8	0.2
(1,487)	1:116:A:CYS:H	1:117:A:LEU:HD13	12	0.2
(1,290)	1:99:A:GLY:H	1:92:A:PHE:HD1	16	0.2
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	10	0.2
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	20	0.2
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	18	0.2
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD22	9	0.2
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD23	17	0.2
(1,51)	1:95:A:VAL:HG22	1:96:A:CYS:HB2	3	0.2
(1,51)	1:95:A:VAL:HG23	1:96:A:CYS:HB2	10	0.2
(1,46)	1:124:A:ILE:HG23	1:123:A:GLU:HA	13	0.2
(1,26)	1:131:A:CYS:HB3	1:105:A:CYS:H	15	0.2
(1,21)	1:93:A:CYS:HB3	1:113:A:HIS:H	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	5	0.19
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	5	0.19
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	19	0.19
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	19	0.19
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	19	0.19
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	19	0.19
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	19	0.19
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	19	0.19
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	5	0.19
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	5	0.19
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	5	0.19
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	5	0.19
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	5	0.19
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	5	0.19
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG2	9	0.19
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG3	9	0.19
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG2	9	0.19
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG3	9	0.19
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG2	9	0.19
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG3	9	0.19
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG2	9	0.19
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG3	9	0.19
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG2	9	0.19
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG3	9	0.19
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG2	9	0.19
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG3	9	0.19
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB1	15	0.19
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB2	15	0.19
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB3	15	0.19
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	7	0.19
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	7	0.19
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	7	0.19
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	15	0.19
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	15	0.19
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	15	0.19
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	17	0.19
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	8	0.19
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	8	0.19
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	8	0.19
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	11	0.19
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	11	0.19
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	17	0.19
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	17	0.19
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	17	0.19
(1,890)	1:91:A:GLU:HA	2:147:B:LYS:HB2	17	0.19
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	7	0.19
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	7	0.19
(1,819)	1:117:A:LEU:HD13	1:121:A:LEU:H	3	0.19
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	10	0.19
(1,813)	1:133:A:ARG:HD3	1:134:A:CYS:H	20	0.19
(1,805)	1:135:A:THR:HA	1:136:A:CYS:H	9	0.19
(1,785)	1:128:A:GLU:HG3	1:128:A:GLU:H	7	0.19
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	8	0.19
(1,739)	1:130:A:LEU:HD11	1:129:A:TRP:H	11	0.19
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	6	0.19
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	8	0.19
(1,709)	1:94:A:ARG:HD2	1:94:A:ARG:H	18	0.19
(1,701)	1:111:A:SER:HB2	1:89:A:HIS:HD2	14	0.19
(1,651)	1:114:A:ILE:HG23	1:125:A:PRO:HD2	5	0.19
(1,642)	1:105:A:CYS:HA	1:89:A:HIS:HD2	9	0.19
(1,638)	1:125:A:PRO:HD3	1:124:A:ILE:HG23	3	0.19
(1,635)	1:122:A:PRO:HD2	1:121:A:LEU:HD23	7	0.19
(1,628)	1:91:A:GLU:HA	1:102:A:LEU:HD22	5	0.19
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD13	11	0.19
(1,591)	1:129:A:TRP:HA	1:103:A:LEU:HD21	15	0.19
(1,570)	1:94:A:ARG:HB2	1:112:A:TYR:HE1	17	0.19
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD11	5	0.19
(1,509)	1:102:A:LEU:HD22	1:92:A:PHE:H	10	0.19
(1,501)	1:121:A:LEU:HB2	1:123:A:GLU:H	5	0.19
(1,403)	1:89:A:HIS:HB2	1:105:A:CYS:H	16	0.19
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	13	0.19
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	4	0.19
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	2	0.19
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	5	0.19
(1,234)	1:95:A:VAL:HG12	1:96:A:CYS:H	5	0.19
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	6	0.19
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	16	0.19
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	19	0.19
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	5	0.19
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	14	0.19
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	15	0.19
(1,91)	1:95:A:VAL:HG23	1:116:A:CYS:HA	11	0.19
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD13	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD11	7	0.19
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD13	13	0.19
(1,65)	1:121:A:LEU:HD22	1:114:A:ILE:HA	17	0.19
(1,46)	1:124:A:ILE:HG21	1:123:A:GLU:HA	1	0.19
(1,42)	1:102:A:LEU:HD13	1:99:A:GLY:HA3	16	0.19
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD2	12	0.18
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD3	12	0.18
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD2	12	0.18
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD3	12	0.18
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD2	12	0.18
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD3	12	0.18
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD2	12	0.18
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD3	12	0.18
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD2	12	0.18
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD3	12	0.18
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD2	12	0.18
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD3	12	0.18
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG21	13	0.18
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG22	13	0.18
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG23	13	0.18
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	8	0.18
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	8	0.18
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	8	0.18
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	20	0.18
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	20	0.18
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	20	0.18
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	12	0.18
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	12	0.18
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	15	0.18
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	15	0.18
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	3	0.18
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	5	0.18
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	3	0.18
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	3	0.18
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	3	0.18
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	18	0.18
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	18	0.18
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	18	0.18
(1,858)	2:148:B:GLN:H	2:147:B:LYS:HB2	5	0.18
(1,858)	2:148:B:GLN:H	2:147:B:LYS:HB2	13	0.18
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG21	14	0.18
(1,820)	1:121:A:LEU:HD22	1:121:A:LEU:H	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	17	0.18
(1,762)	1:91:A:GLU:HG2	1:91:A:GLU:H	18	0.18
(1,730)	1:111:A:SER:HB2	1:112:A:TYR:H	1	0.18
(1,730)	1:111:A:SER:HB2	1:112:A:TYR:H	10	0.18
(1,707)	1:90:A:MET:HG2	1:90:A:MET:H	15	0.18
(1,696)	1:90:A:MET:HE3	1:92:A:PHE:HD1	8	0.18
(1,670)	1:117:A:LEU:HD13	1:129:A:TRP:HH2	8	0.18
(1,670)	1:117:A:LEU:HD11	1:129:A:TRP:HH2	12	0.18
(1,670)	1:117:A:LEU:HD13	1:129:A:TRP:HH2	18	0.18
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD21	1	0.18
(1,655)	1:117:A:LEU:HD22	1:113:A:HIS:HB2	6	0.18
(1,655)	1:117:A:LEU:HD22	1:113:A:HIS:HB2	12	0.18
(1,651)	1:114:A:ILE:HG23	1:125:A:PRO:HD2	3	0.18
(1,651)	1:114:A:ILE:HG23	1:125:A:PRO:HD2	12	0.18
(1,642)	1:105:A:CYS:HA	1:89:A:HIS:HD2	17	0.18
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	19	0.18
(1,587)	1:114:A:ILE:HA	1:121:A:LEU:HD13	16	0.18
(1,578)	1:130:A:LEU:HD11	1:106:A:ASP:HB2	3	0.18
(1,543)	1:99:A:GLY:HA3	1:102:A:LEU:HD23	8	0.18
(1,501)	1:121:A:LEU:HB2	1:123:A:GLU:H	10	0.18
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD21	15	0.18
(1,344)	1:102:A:LEU:HD11	1:103:A:LEU:H	5	0.18
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	3	0.18
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	19	0.18
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	13	0.18
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	15	0.18
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	14	0.18
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	1	0.18
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	3	0.18
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	6	0.18
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	7	0.18
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	12	0.18
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD11	17	0.18
(1,77)	1:95:A:VAL:HB	1:116:A:CYS:HB2	1	0.18
(1,77)	1:95:A:VAL:HB	1:116:A:CYS:HB2	10	0.18
(1,77)	1:95:A:VAL:HB	1:116:A:CYS:HB2	13	0.18
(1,76)	1:90:A:MET:HE1	1:110:A:SER:HA	9	0.18
(1,65)	1:121:A:LEU:HD21	1:114:A:ILE:HA	18	0.18
(1,51)	1:95:A:VAL:HG23	1:96:A:CYS:HB2	9	0.18
(1,51)	1:95:A:VAL:HG22	1:96:A:CYS:HB2	14	0.18
(1,16)	1:117:A:LEU:HD13	1:114:A:ILE:H	1	0.18
(1,5)	1:115:A:HIS:H	1:117:A:LEU:H	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD2	13	0.17
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD3	13	0.17
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	6	0.17
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	6	0.17
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	6	0.17
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	6	0.17
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	6	0.17
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	6	0.17
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	11	0.17
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	11	0.17
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	11	0.17
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	11	0.17
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	11	0.17
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	11	0.17
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	12	0.17
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	12	0.17
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	12	0.17
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	12	0.17
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	12	0.17
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	12	0.17
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD2	14	0.17
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD3	14	0.17
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD2	14	0.17
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD3	14	0.17
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD2	14	0.17
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD3	14	0.17
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD2	14	0.17
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD3	14	0.17
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD2	14	0.17
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD3	14	0.17
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD2	14	0.17
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD3	14	0.17
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB1	7	0.17
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB2	7	0.17
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB3	7	0.17
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB1	9	0.17
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB2	9	0.17
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB3	9	0.17
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	11	0.17
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	11	0.17
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	11	0.17
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB1	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB2	18	0.17
(1,954)	1:125:A:PRO:HA	2:144:B:ALA:HB3	18	0.17
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	4	0.17
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	4	0.17
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	4	0.17
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	10	0.17
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	10	0.17
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	10	0.17
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG21	3	0.17
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG22	3	0.17
(1,933)	1:104:A:CYS:H	2:146:B:THR:HG23	3	0.17
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	12	0.17
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	12	0.17
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	12	0.17
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	16	0.17
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	16	0.17
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	20	0.17
(1,914)	1:101:A:GLU:H	2:148:B:GLN:HG2	11	0.17
(1,914)	1:101:A:GLU:H	2:148:B:GLN:HG3	11	0.17
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	5	0.17
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	5	0.17
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	5	0.17
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	15	0.17
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	15	0.17
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	15	0.17
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	16	0.17
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	16	0.17
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	16	0.17
(1,890)	1:91:A:GLU:HA	2:147:B:LYS:HB2	7	0.17
(1,890)	1:91:A:GLU:HA	2:147:B:LYS:HB2	16	0.17
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	14	0.17
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	14	0.17
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	7	0.17
(1,820)	1:121:A:LEU:HD21	1:121:A:LEU:H	11	0.17
(1,818)	1:114:A:ILE:HG21	1:121:A:LEU:H	13	0.17
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	9	0.17
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	12	0.17
(1,805)	1:135:A:THR:HA	1:136:A:CYS:H	6	0.17
(1,805)	1:135:A:THR:HA	1:136:A:CYS:H	14	0.17
(1,785)	1:128:A:GLU:HG3	1:128:A:GLU:H	18	0.17
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	5	0.17
(1,739)	1:130:A:LEU:HD13	1:129:A:TRP:H	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	2	0.17
(1,688)	1:94:A:ARG:HB2	1:112:A:TYR:HD1	5	0.17
(1,609)	1:132:A:PRO:HD3	1:129:A:TRP:HH2	6	0.17
(1,608)	1:98:A:ASP:HA	1:92:A:PHE:HD1	13	0.17
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD13	17	0.17
(1,562)	1:112:A:TYR:HE1	1:117:A:LEU:HD23	3	0.17
(1,558)	1:125:A:PRO:HB3	1:129:A:TRP:HD1	5	0.17
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD12	17	0.17
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD22	20	0.17
(1,487)	1:116:A:CYS:H	1:117:A:LEU:HD12	11	0.17
(1,396)	1:105:A:CYS:H	1:103:A:LEU:H	14	0.17
(1,396)	1:105:A:CYS:H	1:103:A:LEU:H	19	0.17
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	7	0.17
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	18	0.17
(1,318)	1:89:A:HIS:HB2	1:90:A:MET:H	8	0.17
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	1	0.17
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	7	0.17
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	8	0.17
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	15	0.17
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	18	0.17
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	17	0.17
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	5	0.17
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	8	0.17
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	9	0.17
(1,171)	1:135:A:THR:HG23	1:136:A:CYS:H	8	0.17
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	8	0.17
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	13	0.17
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	20	0.17
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD21	6	0.17
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD22	15	0.17
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD11	9	0.17
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD12	11	0.17
(1,77)	1:95:A:VAL:HB	1:116:A:CYS:HB2	4	0.17
(1,5)	1:115:A:HIS:H	1:117:A:LEU:H	16	0.17
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD2	17	0.16
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD3	17	0.16
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	14	0.16
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	14	0.16
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	14	0.16
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	14	0.16
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	14	0.16
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	17	0.16
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	17	0.16
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	17	0.16
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	17	0.16
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	17	0.16
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	17	0.16
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG2	19	0.16
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG3	19	0.16
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG2	19	0.16
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG3	19	0.16
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG2	19	0.16
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG3	19	0.16
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG2	19	0.16
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG3	19	0.16
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG2	19	0.16
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG3	19	0.16
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG2	19	0.16
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG3	19	0.16
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB1	6	0.16
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB2	6	0.16
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB3	6	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	2	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	2	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	2	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	6	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	6	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	6	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	12	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	12	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	12	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	13	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	13	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	13	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	16	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	16	0.16
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	16	0.16
(1,934)	1:98:A:ASP:H	2:152:B:M3L:HD2	16	0.16
(1,934)	1:98:A:ASP:H	2:152:B:M3L:HD3	16	0.16
(1,931)	1:98:A:ASP:H	2:152:B:M3L:HE2	7	0.16
(1,931)	1:98:A:ASP:H	2:152:B:M3L:HE2	12	0.16
(1,931)	1:98:A:ASP:H	2:152:B:M3L:HE2	18	0.16
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	5	0.16
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	5	0.16
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	6	0.16
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	6	0.16
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	6	0.16
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	12	0.16
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	16	0.16
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG21	14	0.16
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG22	14	0.16
(1,916)	1:101:A:GLU:H	2:146:B:THR:HG23	14	0.16
(1,914)	1:101:A:GLU:H	2:148:B:GLN:HG2	3	0.16
(1,914)	1:101:A:GLU:H	2:148:B:GLN:HG3	3	0.16
(1,912)	1:99:A:GLY:H	2:149:B:THR:HG21	9	0.16
(1,912)	1:99:A:GLY:H	2:149:B:THR:HG22	9	0.16
(1,912)	1:99:A:GLY:H	2:149:B:THR:HG23	9	0.16
(1,909)	1:98:A:ASP:H	2:152:B:M3L:HM12	1	0.16
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG2	20	0.16
(1,885)	1:99:A:GLY:H	2:151:B:ARG:HG3	20	0.16
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG21	3	0.16
(1,821)	1:130:A:LEU:HD11	1:135:A:THR:H	17	0.16
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	4	0.16
(1,739)	1:130:A:LEU:HD12	1:129:A:TRP:H	2	0.16
(1,738)	1:130:A:LEU:HD21	1:129:A:TRP:H	1	0.16
(1,738)	1:130:A:LEU:HD22	1:129:A:TRP:H	13	0.16
(1,709)	1:94:A:ARG:HD2	1:94:A:ARG:H	1	0.16
(1,642)	1:105:A:CYS:HA	1:89:A:HIS:HD2	19	0.16
(1,608)	1:98:A:ASP:HA	1:92:A:PHE:HD1	9	0.16
(1,606)	1:89:A:HIS:HA	1:88:A:HIS:HE1	6	0.16
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD12	6	0.16
(1,596)	1:97:A:LYS:HB3	1:92:A:PHE:HD1	19	0.16
(1,550)	1:90:A:MET:HE2	1:92:A:PHE:HE1	4	0.16
(1,550)	1:90:A:MET:HE1	1:92:A:PHE:HE1	15	0.16
(1,545)	1:102:A:LEU:HA	1:103:A:LEU:HD23	5	0.16
(1,509)	1:102:A:LEU:HD23	1:92:A:PHE:H	1	0.16
(1,466)	1:130:A:LEU:HD22	1:135:A:THR:H	11	0.16
(1,396)	1:105:A:CYS:H	1:103:A:LEU:H	16	0.16
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	5	0.16
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	14	0.16
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	15	0.16
(1,344)	1:102:A:LEU:HD12	1:103:A:LEU:H	9	0.16
(1,327)	1:132:A:PRO:HD3	1:131:A:CYS:H	12	0.16
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	14	0.16
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	1	0.16
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	20	0.16
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	7	0.16
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	15	0.16
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	20	0.16
(1,171)	1:135:A:THR:HG23	1:136:A:CYS:H	2	0.16
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	11	0.16
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	17	0.16
(1,135)	1:129:A:TRP:HZ3	1:106:A:ASP:H	13	0.16
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD22	3	0.16
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD22	8	0.16
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD11	10	0.16
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD12	12	0.16
(1,77)	1:95:A:VAL:HB	1:116:A:CYS:HB2	9	0.16
(1,51)	1:95:A:VAL:HG23	1:96:A:CYS:HB2	8	0.16
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	8	0.15
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	8	0.15
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	9	0.15
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	9	0.15
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	18	0.15
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	18	0.15
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	19	0.15
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	19	0.15
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	1	0.15
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	1	0.15
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	1	0.15
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	1	0.15
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	1	0.15
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	1	0.15
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	17	0.15
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	17	0.15
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	17	0.15
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	17	0.15
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	17	0.15
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	17	0.15
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	2	0.15
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	2	0.15
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	2	0.15
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	2	0.15
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	2	0.15
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	3	0.15
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	3	0.15
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	3	0.15
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	3	0.15
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	3	0.15
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	3	0.15
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	16	0.15
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	16	0.15
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	16	0.15
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	16	0.15
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	16	0.15
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	16	0.15
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG2	4	0.15
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG3	4	0.15
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG2	4	0.15
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG3	4	0.15
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG2	4	0.15
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG3	4	0.15
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG2	4	0.15
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG3	4	0.15
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG2	4	0.15
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG3	4	0.15
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG2	4	0.15
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG3	4	0.15
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD2	4	0.15
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD3	4	0.15
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD2	4	0.15
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD3	4	0.15
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD2	4	0.15
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD3	4	0.15
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD2	4	0.15
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD3	4	0.15
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD2	4	0.15
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD3	4	0.15
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD2	4	0.15
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD3	4	0.15
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB1	19	0.15
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB2	19	0.15
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB3	19	0.15
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB1	20	0.15
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB2	20	0.15
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB3	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	1:98:A:ASP:HA	2:152:B:M3L:HB2	11	0.15
(1,939)	1:98:A:ASP:HA	2:152:B:M3L:HB3	11	0.15
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	20	0.15
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	20	0.15
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	20	0.15
(1,931)	1:98:A:ASP:H	2:152:B:M3L:HE2	19	0.15
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	2	0.15
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	2	0.15
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	2	0.15
(1,925)	1:101:A:GLU:H	2:148:B:GLN:HE22	12	0.15
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	2	0.15
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	2	0.15
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	7	0.15
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB1	4	0.15
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB2	4	0.15
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB3	4	0.15
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	1	0.15
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	1	0.15
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	1	0.15
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	13	0.15
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	13	0.15
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	13	0.15
(1,820)	1:121:A:LEU:HD23	1:121:A:LEU:H	4	0.15
(1,818)	1:114:A:ILE:HG21	1:121:A:LEU:H	1	0.15
(1,805)	1:135:A:THR:HA	1:136:A:CYS:H	10	0.15
(1,739)	1:130:A:LEU:HD12	1:129:A:TRP:H	4	0.15
(1,645)	1:101:A:GLU:HG2	1:114:A:ILE:HD13	5	0.15
(1,640)	1:97:A:LYS:HB2	1:94:A:ARG:HA	20	0.15
(1,625)	1:129:A:TRP:HB3	1:103:A:LEU:HD22	4	0.15
(1,625)	1:129:A:TRP:HB3	1:103:A:LEU:HD21	10	0.15
(1,594)	1:129:A:TRP:HH2	1:112:A:TYR:HB3	6	0.15
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD12	14	0.15
(1,574)	1:114:A:ILE:HG22	1:122:A:PRO:HD2	1	0.15
(1,562)	1:112:A:TYR:HE1	1:117:A:LEU:HD21	19	0.15
(1,545)	1:102:A:LEU:HA	1:103:A:LEU:HD22	16	0.15
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD23	9	0.15
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD22	16	0.15
(1,396)	1:105:A:CYS:H	1:103:A:LEU:H	9	0.15
(1,396)	1:105:A:CYS:H	1:103:A:LEU:H	17	0.15
(1,396)	1:105:A:CYS:H	1:103:A:LEU:H	18	0.15
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	8	0.15
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,344)	1:102:A:LEU:HD11	1:103:A:LEU:H	14	0.15
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	10	0.15
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	19	0.15
(1,327)	1:132:A:PRO:HD3	1:131:A:CYS:H	4	0.15
(1,293)	1:99:A:GLY:H	1:98:A:ASP:HB2	17	0.15
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	12	0.15
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	16	0.15
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	11	0.15
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	3	0.15
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	4	0.15
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	2	0.15
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	4	0.15
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	19	0.15
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD21	5	0.15
(1,108)	1:117:A:LEU:HA	1:129:A:TRP:HZ2	5	0.15
(1,108)	1:117:A:LEU:HA	1:129:A:TRP:HZ2	6	0.15
(1,108)	1:117:A:LEU:HA	1:129:A:TRP:HZ2	11	0.15
(1,77)	1:95:A:VAL:HB	1:116:A:CYS:HB2	2	0.15
(1,77)	1:95:A:VAL:HB	1:116:A:CYS:HB2	8	0.15
(1,77)	1:95:A:VAL:HB	1:116:A:CYS:HB2	16	0.15
(1,75)	1:135:A:THR:HG21	1:130:A:LEU:HG	5	0.15
(1,75)	1:135:A:THR:HG22	1:130:A:LEU:HG	14	0.15
(1,51)	1:95:A:VAL:HG22	1:96:A:CYS:HB2	7	0.15
(1,46)	1:124:A:ILE:HG22	1:123:A:GLU:HA	15	0.15
(1,5)	1:115:A:HIS:H	1:117:A:LEU:H	2	0.15
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	5	0.14
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	5	0.14
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	5	0.14
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	5	0.14
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	5	0.14
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	5	0.14
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	8	0.14
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	8	0.14
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	8	0.14
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	8	0.14
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	8	0.14
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	8	0.14
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	11	0.14
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	11	0.14
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	11	0.14
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	11	0.14
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	11	0.14
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	16	0.14
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	16	0.14
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	16	0.14
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	16	0.14
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	16	0.14
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	16	0.14
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	18	0.14
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	18	0.14
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	18	0.14
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	18	0.14
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	18	0.14
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	18	0.14
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG2	15	0.14
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG3	15	0.14
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG2	15	0.14
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG3	15	0.14
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG2	15	0.14
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG3	15	0.14
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG2	15	0.14
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG3	15	0.14
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG2	15	0.14
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG3	15	0.14
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG2	15	0.14
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG3	15	0.14
(1,977)	1:101:A:GLU:HB2	2:148:B:GLN:HA	16	0.14
(1,977)	1:101:A:GLU:HB3	2:148:B:GLN:HA	16	0.14
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB1	14	0.14
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB2	14	0.14
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB3	14	0.14
(1,950)	1:103:A:LEU:HD21	2:146:B:THR:HG21	3	0.14
(1,950)	1:103:A:LEU:HD21	2:146:B:THR:HG22	3	0.14
(1,950)	1:103:A:LEU:HD21	2:146:B:THR:HG23	3	0.14
(1,950)	1:103:A:LEU:HD22	2:146:B:THR:HG21	3	0.14
(1,950)	1:103:A:LEU:HD22	2:146:B:THR:HG22	3	0.14
(1,950)	1:103:A:LEU:HD22	2:146:B:THR:HG23	3	0.14
(1,950)	1:103:A:LEU:HD23	2:146:B:THR:HG21	3	0.14
(1,950)	1:103:A:LEU:HD23	2:146:B:THR:HG22	3	0.14
(1,950)	1:103:A:LEU:HD23	2:146:B:THR:HG23	3	0.14
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	11	0.14
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	11	0.14
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,914)	1:101:A:GLU:H	2:148:B:GLN:HG2	14	0.14
(1,914)	1:101:A:GLU:H	2:148:B:GLN:HG3	14	0.14
(1,908)	1:101:A:GLU:H	2:151:B:ARG:HD2	9	0.14
(1,908)	1:101:A:GLU:H	2:151:B:ARG:HD3	9	0.14
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	3	0.14
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	3	0.14
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	3	0.14
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	14	0.14
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	14	0.14
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	14	0.14
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	18	0.14
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	18	0.14
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	18	0.14
(1,878)	2:149:B:THR:HG21	2:148:B:GLN:HA	9	0.14
(1,868)	2:152:B:M3L:H	2:151:B:ARG:HD2	10	0.14
(1,820)	1:121:A:LEU:HD21	1:121:A:LEU:H	9	0.14
(1,785)	1:128:A:GLU:HG3	1:128:A:GLU:H	3	0.14
(1,785)	1:128:A:GLU:HG3	1:128:A:GLU:H	8	0.14
(1,766)	1:109:A:PRO:HA	1:90:A:MET:H	15	0.14
(1,756)	1:112:A:TYR:HD1	1:95:A:VAL:H	14	0.14
(1,739)	1:130:A:LEU:HD13	1:129:A:TRP:H	17	0.14
(1,696)	1:90:A:MET:HE3	1:92:A:PHE:HD1	10	0.14
(1,677)	1:112:A:TYR:HB3	1:129:A:TRP:HZ3	20	0.14
(1,670)	1:117:A:LEU:HD13	1:129:A:TRP:HH2	5	0.14
(1,670)	1:117:A:LEU:HD13	1:129:A:TRP:HH2	6	0.14
(1,609)	1:132:A:PRO:HD3	1:129:A:TRP:HH2	10	0.14
(1,608)	1:98:A:ASP:HA	1:92:A:PHE:HD1	12	0.14
(1,600)	1:111:A:SER:HB2	1:102:A:LEU:HD13	11	0.14
(1,576)	1:136:A:CYS:HA	1:137:A:PRO:HD2	12	0.14
(1,464)	1:135:A:THR:H	1:133:A:ARG:HB3	10	0.14
(1,464)	1:135:A:THR:H	1:133:A:ARG:HB3	18	0.14
(1,396)	1:105:A:CYS:H	1:103:A:LEU:H	1	0.14
(1,396)	1:105:A:CYS:H	1:103:A:LEU:H	11	0.14
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	4	0.14
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	13	0.14
(1,365)	1:95:A:VAL:H	1:96:A:CYS:HA	18	0.14
(1,344)	1:102:A:LEU:HD13	1:103:A:LEU:H	11	0.14
(1,344)	1:102:A:LEU:HD12	1:103:A:LEU:H	17	0.14
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	11	0.14
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	6	0.14
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	8	0.14
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:117:A:LEU:HD11	1:118:A:ASN:H	8	0.14
(1,182)	1:118:A:ASN:H	1:117:A:LEU:H	11	0.14
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	1	0.14
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	2	0.14
(1,171)	1:135:A:THR:HG23	1:136:A:CYS:H	16	0.14
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	10	0.14
(1,108)	1:117:A:LEU:HA	1:129:A:TRP:HZ2	12	0.14
(1,108)	1:117:A:LEU:HA	1:129:A:TRP:HZ2	17	0.14
(1,108)	1:117:A:LEU:HA	1:129:A:TRP:HZ2	18	0.14
(1,88)	1:135:A:THR:HA	1:130:A:LEU:HD11	7	0.14
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD11	5	0.14
(1,77)	1:95:A:VAL:HB	1:116:A:CYS:HB2	7	0.14
(1,70)	1:130:A:LEU:HD13	1:128:A:GLU:HG2	3	0.14
(1,65)	1:121:A:LEU:HD21	1:114:A:ILE:HA	16	0.14
(1,19)	1:112:A:TYR:HE2	1:95:A:VAL:H	5	0.14
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD2	9	0.13
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD3	9	0.13
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	3	0.13
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	3	0.13
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	14	0.13
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	14	0.13
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	2	0.13
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	2	0.13
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	2	0.13
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	2	0.13
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	2	0.13
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	2	0.13
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	3	0.13
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	3	0.13
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	3	0.13
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	3	0.13
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	3	0.13
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	3	0.13
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	20	0.13
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	20	0.13
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	20	0.13
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	20	0.13
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	20	0.13
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	20	0.13
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	10	0.13
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	10	0.13
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	10	0.13
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	10	0.13
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	10	0.13
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG2	16	0.13
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG3	16	0.13
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG2	16	0.13
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG3	16	0.13
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG2	16	0.13
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG3	16	0.13
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG2	16	0.13
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG3	16	0.13
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG2	16	0.13
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG3	16	0.13
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG2	16	0.13
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG3	16	0.13
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD2	1	0.13
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD3	1	0.13
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD2	1	0.13
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD3	1	0.13
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD2	1	0.13
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD3	1	0.13
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD2	1	0.13
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD3	1	0.13
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD2	1	0.13
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD3	1	0.13
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD2	1	0.13
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD3	1	0.13
(1,980)	1:101:A:GLU:HG2	2:148:B:GLN:HA	2	0.13
(1,980)	1:101:A:GLU:HG3	2:148:B:GLN:HA	2	0.13
(1,980)	1:101:A:GLU:HG2	2:148:B:GLN:HA	7	0.13
(1,980)	1:101:A:GLU:HG3	2:148:B:GLN:HA	7	0.13
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB1	12	0.13
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB2	12	0.13
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB3	12	0.13
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG21	11	0.13
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG22	11	0.13
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG23	11	0.13
(1,951)	1:124:A:ILE:HA	2:144:B:ALA:HB1	7	0.13
(1,951)	1:124:A:ILE:HA	2:144:B:ALA:HB2	7	0.13
(1,951)	1:124:A:ILE:HA	2:144:B:ALA:HB3	7	0.13
(1,946)	1:98:A:ASP:HA	2:152:B:M3L:HA	11	0.13
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	1	0.13
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	1	0.13
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	3	0.13
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	3	0.13
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	3	0.13
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	14	0.13
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	14	0.13
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	14	0.13
(1,931)	1:98:A:ASP:H	2:152:B:M3L:HE2	3	0.13
(1,931)	1:98:A:ASP:H	2:152:B:M3L:HE2	6	0.13
(1,931)	1:98:A:ASP:H	2:152:B:M3L:HE2	8	0.13
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	13	0.13
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	13	0.13
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	13	0.13
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	1	0.13
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	6	0.13
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	9	0.13
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	13	0.13
(1,915)	1:101:A:GLU:H	2:151:B:ARG:HG2	13	0.13
(1,915)	1:101:A:GLU:H	2:151:B:ARG:HG3	13	0.13
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	19	0.13
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	19	0.13
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	19	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	2	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	2	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	2	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	7	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	7	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	7	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	8	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	8	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	8	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	17	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	17	0.13
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	17	0.13
(1,901)	1:102:A:LEU:HD11	2:147:B:LYS:HE2	9	0.13
(1,901)	1:102:A:LEU:HD12	2:147:B:LYS:HE2	9	0.13
(1,901)	1:102:A:LEU:HD13	2:147:B:LYS:HE2	9	0.13
(1,893)	1:103:A:LEU:HD21	2:144:B:ALA:HB1	17	0.13
(1,893)	1:103:A:LEU:HD21	2:144:B:ALA:HB2	17	0.13
(1,893)	1:103:A:LEU:HD21	2:144:B:ALA:HB3	17	0.13
(1,893)	1:103:A:LEU:HD22	2:144:B:ALA:HB1	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	1:103:A:LEU:HD22	2:144:B:ALA:HB2	17	0.13
(1,893)	1:103:A:LEU:HD22	2:144:B:ALA:HB3	17	0.13
(1,893)	1:103:A:LEU:HD23	2:144:B:ALA:HB1	17	0.13
(1,893)	1:103:A:LEU:HD23	2:144:B:ALA:HB2	17	0.13
(1,893)	1:103:A:LEU:HD23	2:144:B:ALA:HB3	17	0.13
(1,869)	2:147:B:LYS:H	2:146:B:THR:HG23	12	0.13
(1,855)	2:148:B:GLN:H	2:149:B:THR:HG23	1	0.13
(1,825)	1:110:A:SER:HB3	1:111:A:SER:H	15	0.13
(1,820)	1:121:A:LEU:HD23	1:121:A:LEU:H	15	0.13
(1,805)	1:135:A:THR:HA	1:136:A:CYS:H	20	0.13
(1,756)	1:112:A:TYR:HD1	1:95:A:VAL:H	6	0.13
(1,739)	1:130:A:LEU:HD11	1:129:A:TRP:H	16	0.13
(1,738)	1:130:A:LEU:HD22	1:129:A:TRP:H	15	0.13
(1,730)	1:111:A:SER:HB2	1:112:A:TYR:H	7	0.13
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	13	0.13
(1,642)	1:105:A:CYS:HA	1:89:A:HIS:HD2	20	0.13
(1,558)	1:125:A:PRO:HB3	1:129:A:TRP:HD1	8	0.13
(1,558)	1:125:A:PRO:HB3	1:129:A:TRP:HD1	16	0.13
(1,545)	1:102:A:LEU:HA	1:103:A:LEU:HD23	3	0.13
(1,529)	1:131:A:CYS:HA	1:129:A:TRP:HZ3	7	0.13
(1,529)	1:131:A:CYS:HA	1:129:A:TRP:HZ3	10	0.13
(1,529)	1:131:A:CYS:HA	1:129:A:TRP:HZ3	19	0.13
(1,520)	1:113:A:HIS:H	1:116:A:CYS:HA	7	0.13
(1,505)	1:92:A:PHE:H	1:92:A:PHE:HD1	17	0.13
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD21	1	0.13
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD22	4	0.13
(1,487)	1:116:A:CYS:H	1:117:A:LEU:HD12	6	0.13
(1,487)	1:116:A:CYS:H	1:117:A:LEU:HD11	19	0.13
(1,424)	1:102:A:LEU:HD13	1:93:A:CYS:H	16	0.13
(1,396)	1:105:A:CYS:H	1:103:A:LEU:H	3	0.13
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	2	0.13
(1,390)	1:98:A:ASP:H	1:98:A:ASP:HB3	18	0.13
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	4	0.13
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	7	0.13
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	9	0.13
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	20	0.13
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	5	0.13
(1,240)	1:93:A:CYS:HA	1:96:A:CYS:H	19	0.13
(1,234)	1:95:A:VAL:HG11	1:96:A:CYS:H	17	0.13
(1,234)	1:95:A:VAL:HG11	1:96:A:CYS:H	20	0.13
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	10	0.13
(1,177)	1:97:A:LYS:H	1:97:A:LYS:HB3	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	16	0.13
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD12	6	0.13
(1,25)	1:131:A:CYS:HA	1:105:A:CYS:H	2	0.13
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	20	0.12
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	20	0.12
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	4	0.12
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	4	0.12
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	4	0.12
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	4	0.12
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	4	0.12
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	4	0.12
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	6	0.12
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	6	0.12
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	6	0.12
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	6	0.12
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	6	0.12
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	6	0.12
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	7	0.12
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	7	0.12
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	7	0.12
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	7	0.12
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	7	0.12
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	7	0.12
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	12	0.12
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	12	0.12
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	12	0.12
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	12	0.12
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	12	0.12
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	12	0.12
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	8	0.12
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	8	0.12
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	8	0.12
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	8	0.12
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	8	0.12
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	8	0.12
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	20	0.12
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	20	0.12
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	20	0.12
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	20	0.12
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	20	0.12
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	20	0.12
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD2	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD3	5	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD2	5	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD3	5	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD2	5	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD3	5	0.12
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD2	5	0.12
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD3	5	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD2	5	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD3	5	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD2	5	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD3	5	0.12
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD2	7	0.12
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD3	7	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD2	7	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD3	7	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD2	7	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD3	7	0.12
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD2	7	0.12
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD3	7	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD2	7	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD3	7	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD2	7	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD3	7	0.12
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD2	8	0.12
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD3	8	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD2	8	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD3	8	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD2	8	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD3	8	0.12
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD2	8	0.12
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD3	8	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD2	8	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD3	8	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD2	8	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD3	8	0.12
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD2	17	0.12
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD3	17	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD2	17	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD3	17	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD2	17	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD3	17	0.12
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD2	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD3	17	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD2	17	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD3	17	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD2	17	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD3	17	0.12
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD2	18	0.12
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD3	18	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD2	18	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD3	18	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD2	18	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD3	18	0.12
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD2	18	0.12
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD3	18	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD2	18	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD3	18	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD2	18	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD3	18	0.12
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD2	20	0.12
(1,985)	1:102:A:LEU:HD11	2:147:B:LYS:HD3	20	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD2	20	0.12
(1,985)	1:102:A:LEU:HD12	2:147:B:LYS:HD3	20	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD2	20	0.12
(1,985)	1:102:A:LEU:HD13	2:147:B:LYS:HD3	20	0.12
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD2	20	0.12
(1,985)	1:102:A:LEU:HD21	2:147:B:LYS:HD3	20	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD2	20	0.12
(1,985)	1:102:A:LEU:HD22	2:147:B:LYS:HD3	20	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD2	20	0.12
(1,985)	1:102:A:LEU:HD23	2:147:B:LYS:HD3	20	0.12
(1,980)	1:101:A:GLU:HG2	2:148:B:GLN:HA	20	0.12
(1,980)	1:101:A:GLU:HG3	2:148:B:GLN:HA	20	0.12
(1,977)	1:101:A:GLU:HB2	2:148:B:GLN:HA	15	0.12
(1,977)	1:101:A:GLU:HB3	2:148:B:GLN:HA	15	0.12
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG21	17	0.12
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG22	17	0.12
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG23	17	0.12
(1,950)	1:103:A:LEU:HD21	2:146:B:THR:HG21	17	0.12
(1,950)	1:103:A:LEU:HD21	2:146:B:THR:HG22	17	0.12
(1,950)	1:103:A:LEU:HD21	2:146:B:THR:HG23	17	0.12
(1,950)	1:103:A:LEU:HD22	2:146:B:THR:HG21	17	0.12
(1,950)	1:103:A:LEU:HD22	2:146:B:THR:HG22	17	0.12
(1,950)	1:103:A:LEU:HD22	2:146:B:THR:HG23	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:103:A:LEU:HD23	2:146:B:THR:HG21	17	0.12
(1,950)	1:103:A:LEU:HD23	2:146:B:THR:HG22	17	0.12
(1,950)	1:103:A:LEU:HD23	2:146:B:THR:HG23	17	0.12
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	8	0.12
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	8	0.12
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	8	0.12
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	17	0.12
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	17	0.12
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	17	0.12
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	10	0.12
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	10	0.12
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	10	0.12
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	18	0.12
(1,915)	1:101:A:GLU:H	2:151:B:ARG:HG2	19	0.12
(1,915)	1:101:A:GLU:H	2:151:B:ARG:HG3	19	0.12
(1,914)	1:101:A:GLU:H	2:148:B:GLN:HG2	17	0.12
(1,914)	1:101:A:GLU:H	2:148:B:GLN:HG3	17	0.12
(1,908)	1:101:A:GLU:H	2:151:B:ARG:HD2	4	0.12
(1,908)	1:101:A:GLU:H	2:151:B:ARG:HD3	4	0.12
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	1	0.12
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	1	0.12
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	1	0.12
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG21	2	0.12
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG22	2	0.12
(1,905)	1:92:A:PHE:H	2:149:B:THR:HG23	2	0.12
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	5	0.12
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	5	0.12
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	5	0.12
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	11	0.12
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	11	0.12
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	11	0.12
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	12	0.12
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	12	0.12
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	12	0.12
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	20	0.12
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	20	0.12
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	20	0.12
(1,896)	1:102:A:LEU:HD21	2:147:B:LYS:HE2	15	0.12
(1,896)	1:102:A:LEU:HD22	2:147:B:LYS:HE2	15	0.12
(1,896)	1:102:A:LEU:HD23	2:147:B:LYS:HE2	15	0.12
(1,893)	1:103:A:LEU:HD21	2:144:B:ALA:HB1	18	0.12
(1,893)	1:103:A:LEU:HD21	2:144:B:ALA:HB2	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	1:103:A:LEU:HD21	2:144:B:ALA:HB3	18	0.12
(1,893)	1:103:A:LEU:HD22	2:144:B:ALA:HB1	18	0.12
(1,893)	1:103:A:LEU:HD22	2:144:B:ALA:HB2	18	0.12
(1,893)	1:103:A:LEU:HD22	2:144:B:ALA:HB3	18	0.12
(1,893)	1:103:A:LEU:HD23	2:144:B:ALA:HB1	18	0.12
(1,893)	1:103:A:LEU:HD23	2:144:B:ALA:HB2	18	0.12
(1,893)	1:103:A:LEU:HD23	2:144:B:ALA:HB3	18	0.12
(1,883)	2:148:B:GLN:HE21	2:146:B:THR:HG21	14	0.12
(1,871)	2:146:B:THR:H	2:145:B:ARG:HD3	10	0.12
(1,861)	2:146:B:THR:H	2:145:B:ARG:HG2	3	0.12
(1,858)	2:148:B:GLN:H	2:147:B:LYS:HB2	10	0.12
(1,845)	1:115:A:HIS:HB2	1:117:A:LEU:H	1	0.12
(1,820)	1:121:A:LEU:HD22	1:121:A:LEU:H	10	0.12
(1,820)	1:121:A:LEU:HD23	1:121:A:LEU:H	18	0.12
(1,793)	1:103:A:LEU:HB3	1:104:A:CYS:H	8	0.12
(1,785)	1:128:A:GLU:HG3	1:128:A:GLU:H	12	0.12
(1,756)	1:112:A:TYR:HD1	1:95:A:VAL:H	4	0.12
(1,754)	1:89:A:HIS:HD2	1:103:A:LEU:H	3	0.12
(1,709)	1:94:A:ARG:HD2	1:94:A:ARG:H	2	0.12
(1,696)	1:90:A:MET:HE3	1:92:A:PHE:HD1	6	0.12
(1,696)	1:90:A:MET:HE3	1:92:A:PHE:HD1	11	0.12
(1,677)	1:112:A:TYR:HB3	1:129:A:TRP:HZ3	2	0.12
(1,651)	1:114:A:ILE:HG21	1:125:A:PRO:HD2	17	0.12
(1,608)	1:98:A:ASP:HA	1:92:A:PHE:HD1	1	0.12
(1,608)	1:98:A:ASP:HA	1:92:A:PHE:HD1	14	0.12
(1,606)	1:89:A:HIS:HA	1:88:A:HIS:HE1	3	0.12
(1,581)	1:93:A:CYS:HB3	1:102:A:LEU:HD11	3	0.12
(1,578)	1:130:A:LEU:HD11	1:106:A:ASP:HB2	6	0.12
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	6	0.12
(1,554)	1:97:A:LYS:HA	1:92:A:PHE:HE1	11	0.12
(1,520)	1:113:A:HIS:H	1:116:A:CYS:HA	2	0.12
(1,517)	1:117:A:LEU:H	1:117:A:LEU:HD22	6	0.12
(1,501)	1:121:A:LEU:HB2	1:123:A:GLU:H	17	0.12
(1,466)	1:130:A:LEU:HD22	1:135:A:THR:H	14	0.12
(1,464)	1:135:A:THR:H	1:133:A:ARG:HB3	17	0.12
(1,421)	1:92:A:PHE:HB3	1:93:A:CYS:H	17	0.12
(1,396)	1:105:A:CYS:H	1:103:A:LEU:H	12	0.12
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	5	0.12
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	12	0.12
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	14	0.12
(1,286)	1:102:A:LEU:HB2	1:112:A:TYR:H	17	0.12
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	16	0.12
(1,214)	1:133:A:ARG:H	1:134:A:CYS:HB3	14	0.12
(1,182)	1:118:A:ASN:H	1:117:A:LEU:H	8	0.12
(1,161)	1:129:A:TRP:HB3	1:130:A:LEU:H	9	0.12
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD23	5	0.12
(1,103)	1:131:A:CYS:HA	1:133:A:ARG:HB3	6	0.12
(1,85)	1:109:A:PRO:HA	1:108:A:CYS:HB3	3	0.12
(1,85)	1:109:A:PRO:HA	1:108:A:CYS:HB3	14	0.12
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD13	4	0.12
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD13	8	0.12
(1,77)	1:95:A:VAL:HB	1:116:A:CYS:HB2	15	0.12
(1,77)	1:95:A:VAL:HB	1:116:A:CYS:HB2	17	0.12
(1,77)	1:95:A:VAL:HB	1:116:A:CYS:HB2	20	0.12
(1,51)	1:95:A:VAL:HG23	1:96:A:CYS:HB2	17	0.12
(1,51)	1:95:A:VAL:HG21	1:96:A:CYS:HB2	20	0.12
(1,42)	1:102:A:LEU:HD11	1:99:A:GLY:HA3	6	0.12
(1,26)	1:131:A:CYS:HB3	1:105:A:CYS:H	2	0.12
(1,16)	1:117:A:LEU:HD11	1:114:A:ILE:H	15	0.12
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD2	3	0.11
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD3	3	0.11
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD2	11	0.11
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD3	11	0.11
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD2	20	0.11
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD3	20	0.11
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	2	0.11
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	2	0.11
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	6	0.11
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	6	0.11
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	11	0.11
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	11	0.11
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	9	0.11
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	9	0.11
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	9	0.11
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	9	0.11
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	9	0.11
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	9	0.11
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	15	0.11
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	15	0.11
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	15	0.11
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	15	0.11
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	15	0.11
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	1	0.11
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	1	0.11
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	1	0.11
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	1	0.11
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	1	0.11
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	1	0.11
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	7	0.11
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	7	0.11
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	7	0.11
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	7	0.11
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	7	0.11
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	7	0.11
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG2	18	0.11
(1,988)	1:102:A:LEU:HD11	2:148:B:GLN:HG3	18	0.11
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG2	18	0.11
(1,988)	1:102:A:LEU:HD12	2:148:B:GLN:HG3	18	0.11
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG2	18	0.11
(1,988)	1:102:A:LEU:HD13	2:148:B:GLN:HG3	18	0.11
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG2	18	0.11
(1,988)	1:102:A:LEU:HD21	2:148:B:GLN:HG3	18	0.11
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG2	18	0.11
(1,988)	1:102:A:LEU:HD22	2:148:B:GLN:HG3	18	0.11
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG2	18	0.11
(1,988)	1:102:A:LEU:HD23	2:148:B:GLN:HG3	18	0.11
(1,980)	1:101:A:GLU:HG2	2:148:B:GLN:HA	8	0.11
(1,980)	1:101:A:GLU:HG3	2:148:B:GLN:HA	8	0.11
(1,980)	1:101:A:GLU:HG2	2:148:B:GLN:HA	18	0.11
(1,980)	1:101:A:GLU:HG3	2:148:B:GLN:HA	18	0.11
(1,979)	1:101:A:GLU:HG2	2:146:B:THR:HG21	9	0.11
(1,979)	1:101:A:GLU:HG2	2:146:B:THR:HG22	9	0.11
(1,979)	1:101:A:GLU:HG2	2:146:B:THR:HG23	9	0.11
(1,979)	1:101:A:GLU:HG3	2:146:B:THR:HG21	9	0.11
(1,979)	1:101:A:GLU:HG3	2:146:B:THR:HG22	9	0.11
(1,979)	1:101:A:GLU:HG3	2:146:B:THR:HG23	9	0.11
(1,977)	1:101:A:GLU:HB2	2:148:B:GLN:HA	11	0.11
(1,977)	1:101:A:GLU:HB3	2:148:B:GLN:HA	11	0.11
(1,977)	1:101:A:GLU:HB2	2:148:B:GLN:HA	20	0.11
(1,977)	1:101:A:GLU:HB3	2:148:B:GLN:HA	20	0.11
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB1	11	0.11
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB2	11	0.11
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB3	11	0.11
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG21	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG22	3	0.11
(1,952)	1:102:A:LEU:HA	2:146:B:THR:HG23	3	0.11
(1,950)	1:103:A:LEU:HD21	2:146:B:THR:HG21	4	0.11
(1,950)	1:103:A:LEU:HD21	2:146:B:THR:HG22	4	0.11
(1,950)	1:103:A:LEU:HD21	2:146:B:THR:HG23	4	0.11
(1,950)	1:103:A:LEU:HD22	2:146:B:THR:HG21	4	0.11
(1,950)	1:103:A:LEU:HD22	2:146:B:THR:HG22	4	0.11
(1,950)	1:103:A:LEU:HD22	2:146:B:THR:HG23	4	0.11
(1,950)	1:103:A:LEU:HD23	2:146:B:THR:HG21	4	0.11
(1,950)	1:103:A:LEU:HD23	2:146:B:THR:HG22	4	0.11
(1,950)	1:103:A:LEU:HD23	2:146:B:THR:HG23	4	0.11
(1,942)	1:124:A:ILE:HG21	2:146:B:THR:HB	11	0.11
(1,942)	1:124:A:ILE:HG22	2:146:B:THR:HB	11	0.11
(1,942)	1:124:A:ILE:HG23	2:146:B:THR:HB	11	0.11
(1,941)	1:98:A:ASP:HA	2:152:B:M3L:HD2	19	0.11
(1,941)	1:98:A:ASP:HA	2:152:B:M3L:HD3	19	0.11
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB1	19	0.11
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB2	19	0.11
(1,936)	1:129:A:TRP:HA	2:144:B:ALA:HB3	19	0.11
(1,931)	1:98:A:ASP:H	2:152:B:M3L:HE2	17	0.11
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	16	0.11
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	16	0.11
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	16	0.11
(1,925)	1:101:A:GLU:H	2:148:B:GLN:HE22	5	0.11
(1,925)	1:101:A:GLU:H	2:148:B:GLN:HE22	20	0.11
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD2	13	0.11
(1,921)	1:99:A:GLY:H	2:151:B:ARG:HD3	13	0.11
(1,920)	1:103:A:LEU:H	2:146:B:THR:HA	11	0.11
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB1	7	0.11
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB2	7	0.11
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB3	7	0.11
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB1	19	0.11
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB2	19	0.11
(1,919)	1:99:A:GLY:H	2:150:B:ALA:HB3	19	0.11
(1,914)	1:101:A:GLU:H	2:148:B:GLN:HG2	16	0.11
(1,914)	1:101:A:GLU:H	2:148:B:GLN:HG3	16	0.11
(1,912)	1:99:A:GLY:H	2:149:B:THR:HG21	19	0.11
(1,912)	1:99:A:GLY:H	2:149:B:THR:HG22	19	0.11
(1,912)	1:99:A:GLY:H	2:149:B:THR:HG23	19	0.11
(1,909)	1:98:A:ASP:H	2:152:B:M3L:HM12	11	0.11
(1,908)	1:101:A:GLU:H	2:151:B:ARG:HD2	5	0.11
(1,908)	1:101:A:GLU:H	2:151:B:ARG:HD3	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,908)	1:101:A:GLU:H	2:151:B:ARG:HD2	13	0.11
(1,908)	1:101:A:GLU:H	2:151:B:ARG:HD3	13	0.11
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG21	19	0.11
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG22	19	0.11
(1,903)	1:124:A:ILE:HB	2:146:B:THR:HG23	19	0.11
(1,896)	1:102:A:LEU:HD21	2:147:B:LYS:HE2	10	0.11
(1,896)	1:102:A:LEU:HD22	2:147:B:LYS:HE2	10	0.11
(1,896)	1:102:A:LEU:HD23	2:147:B:LYS:HE2	10	0.11
(1,894)	1:102:A:LEU:HD21	2:147:B:LYS:HG2	15	0.11
(1,894)	1:102:A:LEU:HD21	2:147:B:LYS:HG3	15	0.11
(1,894)	1:102:A:LEU:HD22	2:147:B:LYS:HG2	15	0.11
(1,894)	1:102:A:LEU:HD22	2:147:B:LYS:HG3	15	0.11
(1,894)	1:102:A:LEU:HD23	2:147:B:LYS:HG2	15	0.11
(1,894)	1:102:A:LEU:HD23	2:147:B:LYS:HG3	15	0.11
(1,890)	1:91:A:GLU:HA	2:147:B:LYS:HB2	5	0.11
(1,821)	1:130:A:LEU:HD11	1:135:A:THR:H	10	0.11
(1,815)	1:133:A:ARG:HG2	1:134:A:CYS:H	20	0.11
(1,797)	1:119:A:PRO:HA	1:118:A:ASN:H	7	0.11
(1,793)	1:103:A:LEU:HB3	1:104:A:CYS:H	3	0.11
(1,785)	1:128:A:GLU:HG3	1:128:A:GLU:H	2	0.11
(1,785)	1:128:A:GLU:HG3	1:128:A:GLU:H	9	0.11
(1,766)	1:109:A:PRO:HA	1:90:A:MET:H	3	0.11
(1,734)	1:117:A:LEU:HD11	1:114:A:ILE:H	16	0.11
(1,730)	1:111:A:SER:HB2	1:112:A:TYR:H	2	0.11
(1,729)	1:110:A:SER:HA	1:112:A:TYR:H	8	0.11
(1,723)	1:89:A:HIS:HB3	1:110:A:SER:H	13	0.11
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	4	0.11
(1,721)	1:109:A:PRO:HD3	1:110:A:SER:H	20	0.11
(1,701)	1:111:A:SER:HB2	1:89:A:HIS:HD2	6	0.11
(1,701)	1:111:A:SER:HB2	1:89:A:HIS:HD2	8	0.11
(1,696)	1:90:A:MET:HE2	1:92:A:PHE:HD1	7	0.11
(1,654)	1:132:A:PRO:HD2	1:117:A:LEU:HD22	15	0.11
(1,651)	1:114:A:ILE:HG22	1:125:A:PRO:HD2	19	0.11
(1,625)	1:129:A:TRP:HB3	1:103:A:LEU:HD22	20	0.11
(1,606)	1:89:A:HIS:HA	1:88:A:HIS:HE1	17	0.11
(1,602)	1:137:A:PRO:HD2	1:136:A:CYS:HB2	11	0.11
(1,598)	1:111:A:SER:HA	1:102:A:LEU:HD11	14	0.11
(1,597)	1:121:A:LEU:HD22	1:129:A:TRP:HD1	8	0.11
(1,578)	1:130:A:LEU:HD13	1:106:A:ASP:HB2	7	0.11
(1,578)	1:130:A:LEU:HD11	1:106:A:ASP:HB2	15	0.11
(1,562)	1:112:A:TYR:HE1	1:117:A:LEU:HD21	12	0.11
(1,539)	1:112:A:TYR:HA	1:102:A:LEU:HD11	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,529)	1:131:A:CYS:HA	1:129:A:TRP:HZ3	3	0.11
(1,529)	1:131:A:CYS:HA	1:129:A:TRP:HZ3	15	0.11
(1,520)	1:113:A:HIS:H	1:116:A:CYS:HA	16	0.11
(1,517)	1:117:A:LEU:H	1:117:A:LEU:HD22	5	0.11
(1,501)	1:121:A:LEU:HB2	1:123:A:GLU:H	19	0.11
(1,488)	1:116:A:CYS:H	1:117:A:LEU:HD21	8	0.11
(1,466)	1:130:A:LEU:HD22	1:135:A:THR:H	6	0.11
(1,391)	1:92:A:PHE:HB3	1:98:A:ASP:H	3	0.11
(1,365)	1:95:A:VAL:H	1:96:A:CYS:HA	1	0.11
(1,365)	1:95:A:VAL:H	1:96:A:CYS:HA	6	0.11
(1,365)	1:95:A:VAL:H	1:96:A:CYS:HA	13	0.11
(1,337)	1:100:A:GLY:H	1:92:A:PHE:HA	4	0.11
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	6	0.11
(1,259)	1:109:A:PRO:HD2	1:108:A:CYS:H	18	0.11
(1,240)	1:93:A:CYS:HA	1:96:A:CYS:H	11	0.11
(1,182)	1:118:A:ASN:H	1:117:A:LEU:H	18	0.11
(1,108)	1:117:A:LEU:HA	1:129:A:TRP:HZ2	1	0.11
(1,108)	1:117:A:LEU:HA	1:129:A:TRP:HZ2	9	0.11
(1,108)	1:117:A:LEU:HA	1:129:A:TRP:HZ2	19	0.11
(1,104)	1:131:A:CYS:HA	1:117:A:LEU:HD23	4	0.11
(1,85)	1:109:A:PRO:HA	1:108:A:CYS:HB3	9	0.11
(1,16)	1:117:A:LEU:HD13	1:114:A:ILE:H	17	0.11
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD2	12	0.1
(1,996)	1:104:A:CYS:H	2:145:B:ARG:HD3	12	0.1
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	15	0.1
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	15	0.1
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB2	16	0.1
(1,995)	1:104:A:CYS:H	2:145:B:ARG:HB3	16	0.1
(1,993)	1:103:A:LEU:HD11	2:146:B:THR:HB	14	0.1
(1,993)	1:103:A:LEU:HD12	2:146:B:THR:HB	14	0.1
(1,993)	1:103:A:LEU:HD13	2:146:B:THR:HB	14	0.1
(1,993)	1:103:A:LEU:HD21	2:146:B:THR:HB	14	0.1
(1,993)	1:103:A:LEU:HD22	2:146:B:THR:HB	14	0.1
(1,993)	1:103:A:LEU:HD23	2:146:B:THR:HB	14	0.1
(1,989)	1:102:A:LEU:HD11	2:149:B:THR:HB	19	0.1
(1,989)	1:102:A:LEU:HD12	2:149:B:THR:HB	19	0.1
(1,989)	1:102:A:LEU:HD13	2:149:B:THR:HB	19	0.1
(1,989)	1:102:A:LEU:HD21	2:149:B:THR:HB	19	0.1
(1,989)	1:102:A:LEU:HD22	2:149:B:THR:HB	19	0.1
(1,989)	1:102:A:LEU:HD23	2:149:B:THR:HB	19	0.1
(1,980)	1:101:A:GLU:HG2	2:148:B:GLN:HA	1	0.1
(1,980)	1:101:A:GLU:HG3	2:148:B:GLN:HA	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,980)	1:101:A:GLU:HG2	2:148:B:GLN:HA	4	0.1
(1,980)	1:101:A:GLU:HG3	2:148:B:GLN:HA	4	0.1
(1,963)	1:91:A:GLU:HA	2:147:B:LYS:HB2	6	0.1
(1,963)	1:91:A:GLU:HA	2:147:B:LYS:HB3	6	0.1
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB1	10	0.1
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB2	10	0.1
(1,962)	1:129:A:TRP:HE3	2:144:B:ALA:HB3	10	0.1
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB1	9	0.1
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB2	9	0.1
(1,927)	1:128:A:GLU:H	2:144:B:ALA:HB3	9	0.1
(1,925)	1:101:A:GLU:H	2:148:B:GLN:HE22	6	0.1
(1,915)	1:101:A:GLU:H	2:151:B:ARG:HG2	9	0.1
(1,915)	1:101:A:GLU:H	2:151:B:ARG:HG3	9	0.1
(1,912)	1:99:A:GLY:H	2:149:B:THR:HG21	1	0.1
(1,912)	1:99:A:GLY:H	2:149:B:THR:HG22	1	0.1
(1,912)	1:99:A:GLY:H	2:149:B:THR:HG23	1	0.1
(1,896)	1:102:A:LEU:HD21	2:147:B:LYS:HE2	6	0.1
(1,896)	1:102:A:LEU:HD22	2:147:B:LYS:HE2	6	0.1
(1,896)	1:102:A:LEU:HD23	2:147:B:LYS:HE2	6	0.1
(1,858)	2:148:B:GLN:H	2:147:B:LYS:HB2	2	0.1
(1,805)	1:135:A:THR:HA	1:136:A:CYS:H	7	0.1
(1,785)	1:128:A:GLU:HG3	1:128:A:GLU:H	1	0.1
(1,779)	1:90:A:MET:HG2	1:94:A:ARG:H	15	0.1
(1,756)	1:112:A:TYR:HD1	1:95:A:VAL:H	1	0.1
(1,756)	1:112:A:TYR:HD1	1:95:A:VAL:H	9	0.1
(1,756)	1:112:A:TYR:HD1	1:95:A:VAL:H	11	0.1
(1,729)	1:110:A:SER:HA	1:112:A:TYR:H	15	0.1
(1,709)	1:94:A:ARG:HD2	1:94:A:ARG:H	9	0.1
(1,663)	1:118:A:ASN:HA	1:120:A:PRO:HD2	1	0.1
(1,656)	1:92:A:PHE:HB3	1:102:A:LEU:HD23	12	0.1
(1,569)	1:91:A:GLU:HG3	1:92:A:PHE:HD1	16	0.1
(1,569)	1:91:A:GLU:HG3	1:92:A:PHE:HD1	17	0.1
(1,529)	1:131:A:CYS:HA	1:129:A:TRP:HZ3	16	0.1
(1,529)	1:131:A:CYS:HA	1:129:A:TRP:HZ3	18	0.1
(1,365)	1:95:A:VAL:H	1:96:A:CYS:HA	10	0.1
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	2	0.1
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	8	0.1
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	11	0.1
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	15	0.1
(1,330)	1:130:A:LEU:HG	1:131:A:CYS:H	16	0.1
(1,313)	1:90:A:MET:H	1:90:A:MET:HB3	15	0.1
(1,230)	1:114:A:ILE:H	1:103:A:LEU:HD12	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,189)	1:117:A:LEU:HD21	1:118:A:ASN:H	9	0.1
(1,182)	1:118:A:ASN:H	1:117:A:LEU:H	6	0.1
(1,118)	1:112:A:TYR:HA	1:117:A:LEU:HD23	15	0.1
(1,108)	1:117:A:LEU:HA	1:129:A:TRP:HZ2	2	0.1
(1,108)	1:117:A:LEU:HA	1:129:A:TRP:HZ2	8	0.1
(1,85)	1:109:A:PRO:HA	1:108:A:CYS:HB3	6	0.1
(1,85)	1:109:A:PRO:HA	1:108:A:CYS:HB3	11	0.1
(1,85)	1:109:A:PRO:HA	1:108:A:CYS:HB3	12	0.1
(1,79)	1:107:A:THR:HB	1:130:A:LEU:HD12	14	0.1
(1,74)	1:107:A:THR:HG21	1:130:A:LEU:HG	19	0.1
(1,69)	1:130:A:LEU:HD12	1:128:A:GLU:HB2	17	0.1
(1,21)	1:93:A:CYS:HB3	1:113:A:HIS:H	11	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found