



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 10:38 AM UTC

PDB ID : 5A3G / pdb_00005a3g
BMRB ID : 26580
Title : Structure of herpesvirus nuclear egress complex subunit M50
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Deposited on : 2015-06-01

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

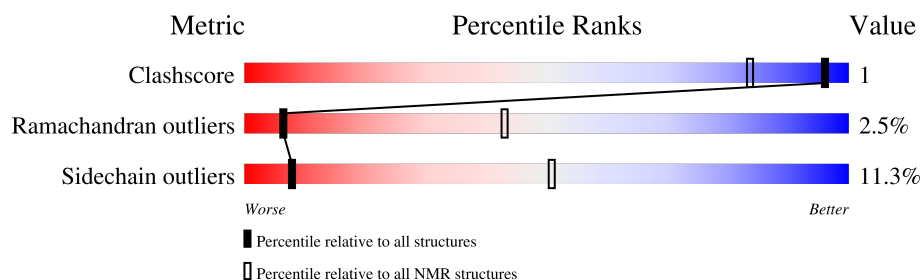
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 13%.

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	171	

2 Ensemble composition and analysis

This entry contains 15 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:7-A:171 (165)	1.61	12

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2711 atoms, of which 1356 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called M50.

Mol	Chain	Residues	Atoms						Trace
1	A	171	Total	C	H	N	O	S	0
			2711	851	1356	234	258	12	

There are 3 discrepancies between the modelled and reference sequences:

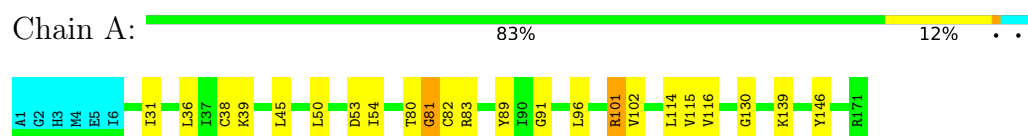
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP H2A365
A	2	GLY	-	expression tag	UNP H2A365
A	3	HIS	-	expression tag	UNP H2A365

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: M50

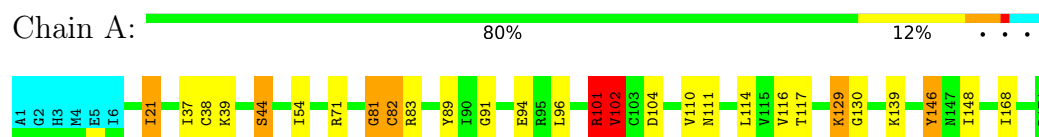


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

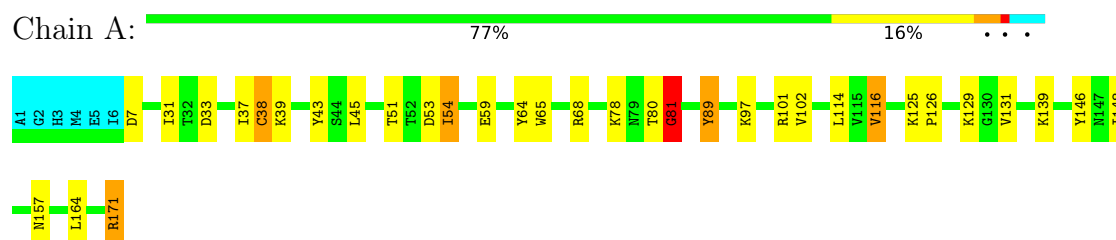
4.2.1 Score per residue for model 1

- Molecule 1: M50



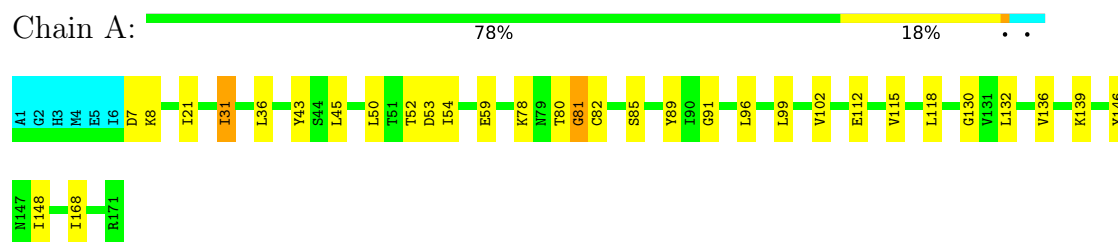
4.2.2 Score per residue for model 2

- Molecule 1: M50



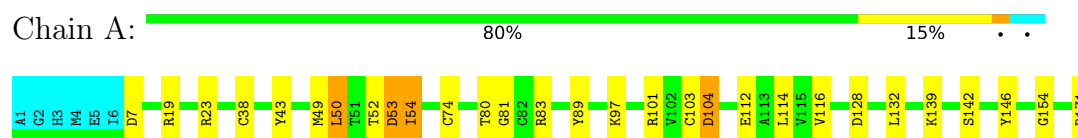
4.2.3 Score per residue for model 3

- Molecule 1: M50



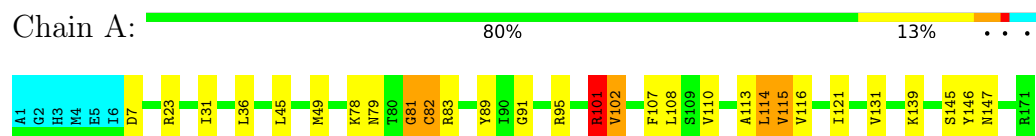
4.2.4 Score per residue for model 4

- Molecule 1: M50



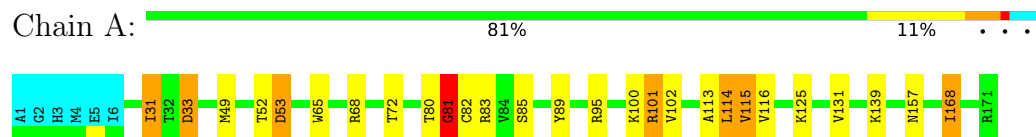
4.2.5 Score per residue for model 5

- Molecule 1: M50



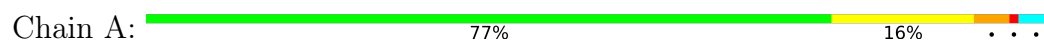
4.2.6 Score per residue for model 6

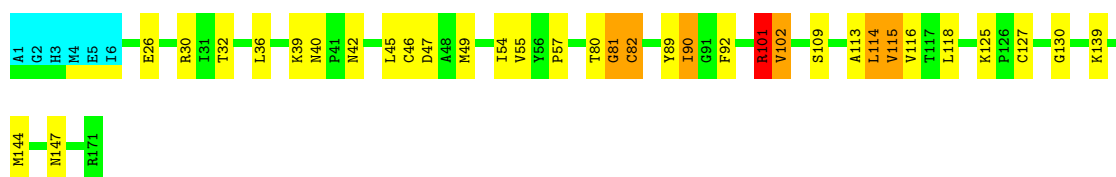
- Molecule 1: M50



4.2.7 Score per residue for model 7

- Molecule 1: M50

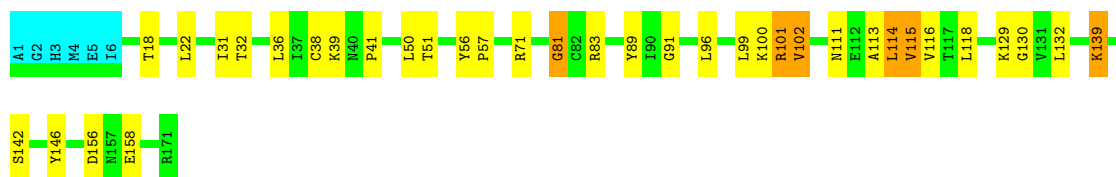




4.2.8 Score per residue for model 8

- Molecule 1: M50

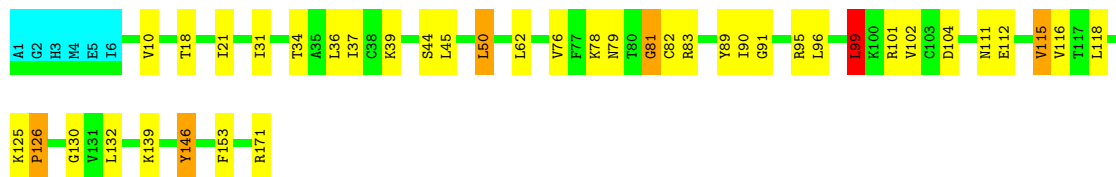
Chain A: 75% 18% . .



4.2.9 Score per residue for model 9

- Molecule 1: M50

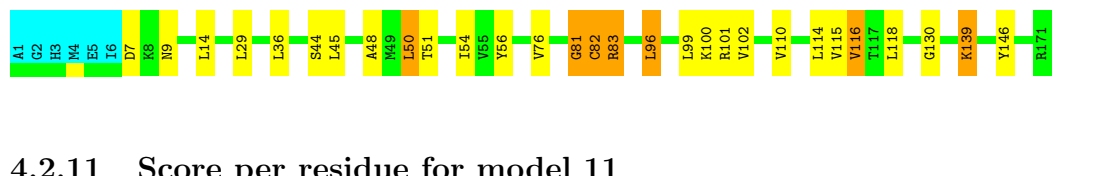
Chain A: 73% 20% . . .



4.2.10 Score per residue for model 10

- Molecule 1: M50

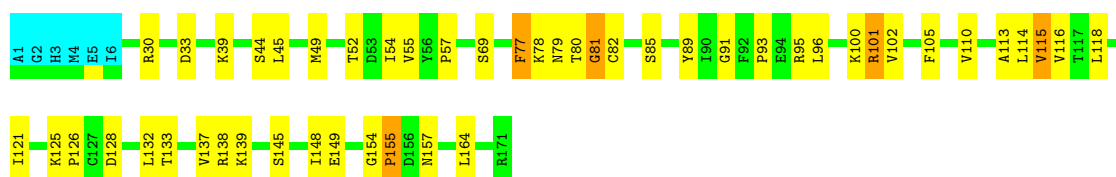
Chain A: 80% 13% . .



4.2.11 Score per residue for model 11

- Molecule 1: M50

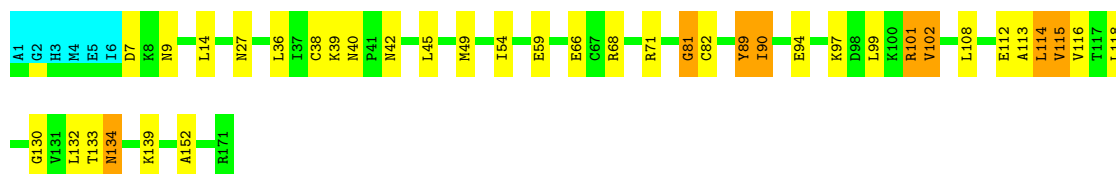
Chain A: 68% 26% . .



4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: M50

Chain A: 74% 18% 5% .



4.2.13 Score per residue for model 13

- Molecule 1: M50

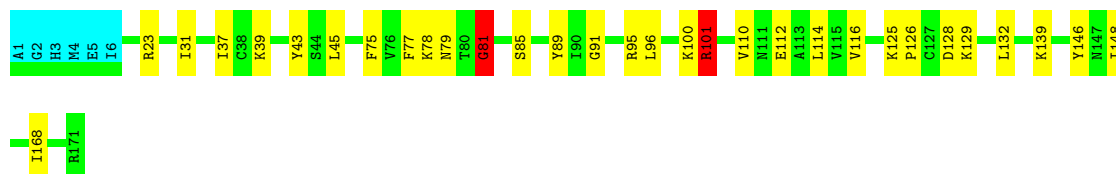
Chain A: 78% 16% . . .



4.2.14 Score per residue for model 14

- Molecule 1: M50

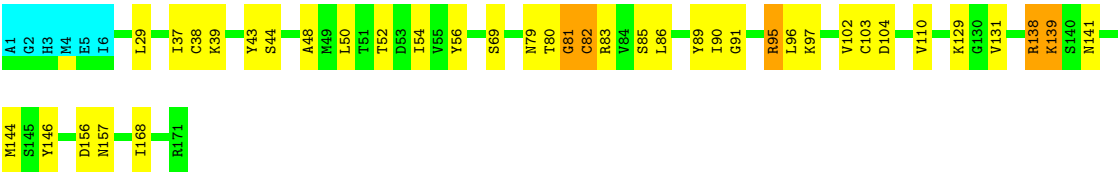
Chain A: 78% 17% . .



4.2.15 Score per residue for model 15

- Molecule 1: M50

Chain A: 74% 20% . .



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING WITH TORSION ANGLE DYNAMICS SIMULATION FOLLOWED BY RDC AND WATERBOX REFINEMENT*.

Of the 50 calculated structures, 15 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
Amber	refinement	
CYANA	structure solution	3.0
NMRDraw	structure solution	11
TALOS+	structure solution	1.2009.0605.17
CcpNmr Analysis	structure solution	2.4
NMRPipe	structure solution	11
hmsIST	structure solution	2.11
CARA	structure solution	1.8.4

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	300
Number of shifts mapped to atoms	300
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	13%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.88±0.01	0±0/1331 (0.0± 0.0%)	1.54±0.03	10±4/1801 (0.5± 0.2%)
All	All	0.88	0/19965 (0.0%)	1.54	145/27015 (0.5%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	9.3±2.0
All	All	0	140

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	91	GLY	N-CA-C	8.05	122.41	110.42	3	8
1	A	81	GLY	CA-C-N	-7.97	111.77	122.85	14	12
1	A	81	GLY	C-N-CA	-7.97	111.77	122.85	14	12
1	A	168	ILE	N-CA-C	7.08	117.90	111.81	6	1
1	A	77	PHE	CA-CB-CG	7.00	120.80	113.80	11	2
1	A	82	CYS	CA-C-N	6.72	134.38	121.54	5	7
1	A	82	CYS	C-N-CA	6.72	134.38	121.54	5	7
1	A	134	ASN	CA-CB-CG	6.53	119.13	112.60	12	1
1	A	53	ASP	N-CA-C	6.44	115.90	108.49	4	2
1	A	115	VAL	CA-CB-CG1	6.39	121.26	110.40	5	6
1	A	112	GLU	N-CA-C	6.35	124.32	110.80	9	1
1	A	37	ILE	CA-C-N	6.33	133.64	121.54	2	1
1	A	37	ILE	C-N-CA	6.33	133.64	121.54	2	1
1	A	101	ARG	CD-NE-CZ	6.33	133.27	124.40	1	4
1	A	100	LYS	N-CA-C	6.28	118.42	107.49	8	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	33	ASP	CA-CB-CG	6.25	118.85	112.60	6	2
1	A	103	CYS	CA-C-N	6.16	133.30	121.54	4	1
1	A	103	CYS	C-N-CA	6.16	133.30	121.54	4	1
1	A	89	TYR	N-CA-C	6.14	118.63	108.99	12	2
1	A	95	ARG	CA-C-N	6.13	128.77	120.38	14	5
1	A	95	ARG	C-N-CA	6.13	128.77	120.38	14	5
1	A	46	CYS	N-CA-C	5.95	115.71	107.73	13	1
1	A	116	VAL	CB-CA-C	5.92	118.17	110.12	1	4
1	A	99	LEU	N-CA-C	5.78	117.99	110.53	9	1
1	A	53	ASP	CA-C-N	5.77	132.36	121.97	3	2
1	A	53	ASP	C-N-CA	5.77	132.36	121.97	3	2
1	A	50	LEU	CA-C-N	5.74	132.88	122.02	3	2
1	A	50	LEU	C-N-CA	5.74	132.88	122.02	3	2
1	A	157	ASN	CA-C-N	5.64	128.62	120.38	6	2
1	A	157	ASN	C-N-CA	5.64	128.62	120.38	6	2
1	A	139	LYS	CB-CA-C	5.61	119.98	109.71	12	1
1	A	128	ASP	N-CA-C	5.57	119.82	113.19	14	1
1	A	50	LEU	N-CA-C	5.56	118.49	108.48	10	1
1	A	146	TYR	CA-CB-CG	5.55	123.88	113.90	9	1
1	A	79	ASN	CA-C-N	5.50	130.89	121.87	14	4
1	A	79	ASN	C-N-CA	5.50	130.89	121.87	14	4
1	A	101	ARG	CA-CB-CG	5.48	125.06	114.10	6	1
1	A	27	ASN	CA-CB-CG	5.47	118.07	112.60	12	1
1	A	108	LEU	N-CA-CB	-5.44	101.28	111.13	5	2
1	A	105	PHE	CA-CB-CG	5.41	119.21	113.80	11	1
1	A	56	TYR	CA-C-N	5.34	126.52	119.84	8	1
1	A	56	TYR	C-N-CA	5.34	126.52	119.84	8	1
1	A	101	ARG	CB-CG-CD	5.27	123.42	111.30	6	1
1	A	47	ASP	CA-CB-CG	5.26	117.86	112.60	7	1
1	A	115	VAL	CG1-CB-CG2	-5.25	99.25	110.80	8	3
1	A	154	GLY	CA-C-N	5.24	124.91	119.56	4	1
1	A	154	GLY	C-N-CA	5.24	124.91	119.56	4	1
1	A	141	ASN	CA-CB-CG	5.19	117.79	112.60	15	1
1	A	57	PRO	CA-C-N	5.14	127.78	120.53	7	1
1	A	57	PRO	C-N-CA	5.14	127.78	120.53	7	1
1	A	125	LYS	CA-C-N	5.14	126.26	119.84	2	1
1	A	125	LYS	C-N-CA	5.14	126.26	119.84	2	1
1	A	93	PRO	CA-C-N	5.11	127.84	120.38	11	1
1	A	93	PRO	C-N-CA	5.11	127.84	120.38	11	1
1	A	109	SER	CA-C-N	5.09	129.49	121.09	7	1
1	A	109	SER	C-N-CA	5.09	129.49	121.09	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	8	LYS	N-CA-C	5.05	116.79	111.28	3	1
1	A	128	ASP	CA-CB-CG	5.05	117.65	112.60	11	1
1	A	21	ILE	CA-CB-CG1	5.04	118.98	110.40	1	1
1	A	109	SER	N-CA-C	5.03	118.16	110.36	7	1
1	A	80	THR	CA-C-N	5.02	131.24	121.41	15	1
1	A	80	THR	C-N-CA	5.02	131.24	121.41	15	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	89	TYR	Sidechain,Peptide	12
1	A	102	VAL	Peptide	12
1	A	101	ARG	Peptide	9
1	A	82	CYS	Peptide	7
1	A	83	ARG	Peptide	7
1	A	146	TYR	Sidechain,Peptide	7
1	A	43	TYR	Peptide	6
1	A	80	THR	Peptide	6
1	A	49	MET	Peptide	6
1	A	39	LYS	Peptide	5
1	A	7	ASP	Peptide	5
1	A	44	SER	Peptide	4
1	A	81	GLY	Peptide	4
1	A	52	THR	Peptide	4
1	A	71	ARG	Sidechain	3
1	A	50	LEU	Peptide	3
1	A	115	VAL	Peptide	2
1	A	104	ASP	Peptide	2
1	A	112	GLU	Peptide	2
1	A	145	SER	Peptide	2
1	A	31	ILE	Peptide	2
1	A	42	ASN	Peptide	2
1	A	90	ILE	Peptide	2
1	A	138	ARG	Peptide	2
1	A	33	ASP	Peptide	1
1	A	51	THR	Peptide	1
1	A	171	ARG	Sidechain	1
1	A	23	ARG	Sidechain	1
1	A	74	CYS	Peptide	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	107	PHE	Peptide	1
1	A	147	ASN	Peptide	1
1	A	40	ASN	Peptide	1
1	A	127	CYS	Peptide	1
1	A	111	ASN	Peptide	1
1	A	34	THR	Peptide	1
1	A	79	ASN	Peptide	1
1	A	126	PRO	Peptide	1
1	A	153	PHE	Peptide	1
1	A	57	PRO	Peptide	1
1	A	149	GLU	Peptide	1
1	A	53	ASP	Peptide	1
1	A	54	ILE	Peptide	1
1	A	68	ARG	Sidechain	1
1	A	131	VAL	Peptide	1
1	A	56	TYR	Sidechain	1
1	A	129	LYS	Peptide	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1311	1313	1313	2±2
All	All	19665	19695	19695	34

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:VAL:HG22	1:A:115:VAL:HG22	0.86	1.48	10	3
1:A:113:ALA:C	1:A:114:LEU:HD23	0.67	2.15	13	6
1:A:29:LEU:HD11	1:A:48:ALA:HB1	0.58	1.76	15	2
1:A:139:LYS:HE2	1:A:146:TYR:CD1	0.55	2.36	15	3
1:A:53:ASP:C	1:A:54:ILE:HD13	0.55	2.27	4	3
1:A:101:ARG:CD	1:A:102:VAL:H	0.53	2.17	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:LYS:HE2	1:A:146:TYR:CG	0.52	2.40	8	2
1:A:99:LEU:HD11	1:A:115:VAL:HG23	0.51	1.82	10	1
1:A:52:THR:HG22	1:A:137:VAL:HG23	0.49	1.84	11	1
1:A:99:LEU:C	1:A:99:LEU:HD12	0.47	2.34	12	3
1:A:31:ILE:HD12	1:A:31:ILE:H	0.46	1.70	3	1
1:A:154:GLY:H	1:A:155:PRO:CD	0.44	2.25	11	1
1:A:101:ARG:CZ	1:A:102:VAL:H	0.44	2.24	1	1
1:A:99:LEU:CD1	1:A:115:VAL:HG23	0.44	2.43	10	1
1:A:133:THR:HG22	1:A:152:ALA:HA	0.43	1.89	12	1
1:A:78:LYS:HE3	1:A:113:ALA:HB2	0.43	1.91	11	1
1:A:139:LYS:HD2	1:A:146:TYR:CE1	0.42	2.50	1	1
1:A:96:LEU:HD11	1:A:115:VAL:HG21	0.42	1.92	10	1
1:A:90:ILE:HD13	1:A:90:ILE:H	0.42	1.74	12	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	164/171 (96%)	145±2 (88±2%)	15±2 (9±1%)	4±2 (3±1%)	6	43
All	All	2460/2565 (96%)	2176 (88%)	222 (9%)	62 (3%)	6	43

All 21 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	81	GLY	15
1	A	130	GLY	8
1	A	38	CYS	7
1	A	126	PRO	4
1	A	125	LYS	4
1	A	104	ASP	3
1	A	44	SER	2
1	A	157	ASN	2
1	A	142	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	144	MET	2
1	A	102	VAL	2
1	A	69	SER	2
1	A	129	LYS	1
1	A	33	ASP	1
1	A	41	PRO	1
1	A	57	PRO	1
1	A	111	ASN	1
1	A	155	PRO	1
1	A	82	CYS	1
1	A	94	GLU	1
1	A	156	ASP	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	148/152 (97%)	131±3 (89±2%)	17±3 (11±2%)	8	51
All	All	2220/2280 (97%)	1970 (89%)	250 (11%)	8	51

All 79 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	139	LYS	13
1	A	114	LEU	12
1	A	116	VAL	11
1	A	54	ILE	10
1	A	101	ARG	10
1	A	45	LEU	10
1	A	96	LEU	9
1	A	36	LEU	8
1	A	110	VAL	7
1	A	118	LEU	7
1	A	132	LEU	7
1	A	31	ILE	6
1	A	85	SER	6

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Mol	Chain	Res	Type	Models (Total)
1	A	115	VAL	6
1	A	37	ILE	5
1	A	148	ILE	5
1	A	168	ILE	5
1	A	78	LYS	5
1	A	39	LYS	5
1	A	102	VAL	4
1	A	129	LYS	4
1	A	97	LYS	4
1	A	131	VAL	4
1	A	50	LEU	4
1	A	21	ILE	3
1	A	59	GLU	3
1	A	68	ARG	3
1	A	171	ARG	3
1	A	30	ARG	3
1	A	90	ILE	3
1	A	65	TRP	2
1	A	164	LEU	2
1	A	99	LEU	2
1	A	112	GLU	2
1	A	23	ARG	2
1	A	121	ILE	2
1	A	83	ARG	2
1	A	125	LYS	2
1	A	32	THR	2
1	A	55	VAL	2
1	A	18	THR	2
1	A	51	THR	2
1	A	95	ARG	2
1	A	9	ASN	2
1	A	14	LEU	2
1	A	103	CYS	2
1	A	94	GLU	1
1	A	111	ASN	1
1	A	117	THR	1
1	A	38	CYS	1
1	A	64	TYR	1
1	A	89	TYR	1
1	A	136	VAL	1
1	A	7	ASP	1
1	A	19	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	128	ASP	1
1	A	53	ASP	1
1	A	72	THR	1
1	A	26	GLU	1
1	A	46	CYS	1
1	A	92	PHE	1
1	A	147	ASN	1
1	A	22	LEU	1
1	A	156	ASP	1
1	A	158	GLU	1
1	A	10	VAL	1
1	A	62	LEU	1
1	A	146	TYR	1
1	A	56	TYR	1
1	A	77	PHE	1
1	A	80	THR	1
1	A	133	THR	1
1	A	40	ASN	1
1	A	66	GLU	1
1	A	134	ASN	1
1	A	157	ASN	1
1	A	75	PHE	1
1	A	86	LEU	1
1	A	138	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 13% for the well-defined parts and 13% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

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	300
Number of shifts mapped to atoms	300
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 13%, i.e. 296 atoms were assigned a chemical shift out of a possible 2281. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/822 (0%)	0/332 (0%)	0/330 (0%)	0/160 (0%)
Sidechain	296/1315 (23%)	222/853 (26%)	74/402 (18%)	0/60 (0%)
Aromatic	0/144 (0%)	0/68 (0%)	0/75 (0%)	0/1 (0%)
Overall	296/2281 (13%)	222/1253 (18%)	74/807 (9%)	0/221 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 13%, i.e. 300 atoms were assigned a chemical shift out of a possible 2356. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/853 (0%)	0/345 (0%)	0/342 (0%)	0/166 (0%)
Sidechain	300/1352 (22%)	225/878 (26%)	75/414 (18%)	0/60 (0%)
Aromatic	0/151 (0%)	0/72 (0%)	0/77 (0%)	0/2 (0%)
Overall	300/2356 (13%)	225/1295 (17%)	75/833 (9%)	0/228 (0%)

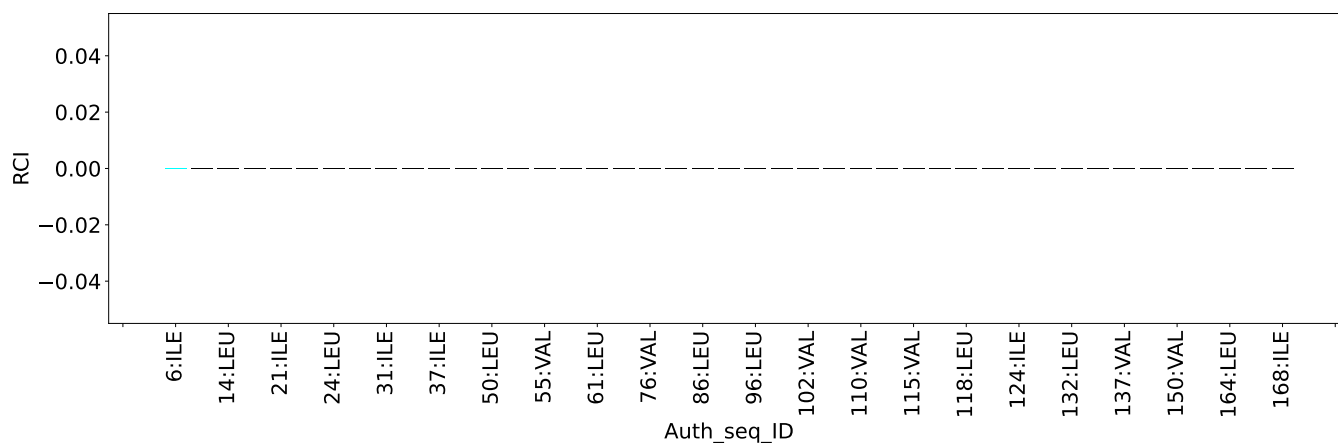
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1458
Intra-residue ($ i-j =0$)	300
Sequential ($ i-j =1$)	499
Medium range ($ i-j >1$ and $ i-j <5$)	221
Long range ($ i-j \geq 5$)	350
Inter-chain	0
Hydrogen bond restraints	88
Disulfide bond restraints	0
Total dihedral-angle restraints	282
Number of unmapped restraints	0
Number of restraints per residue	10.2
Number of long range restraints per residue ¹	2.3

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	23.4	0.2
0.2-0.5 (Medium)	23.1	0.5
>0.5 (Large)	28.9	2.36

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	46.5	10.0
10.0-20.0 (Medium)	5.1	19.92
>20.0 (Large)	2.5	44.78

9 Distance violation analysis ⓘ

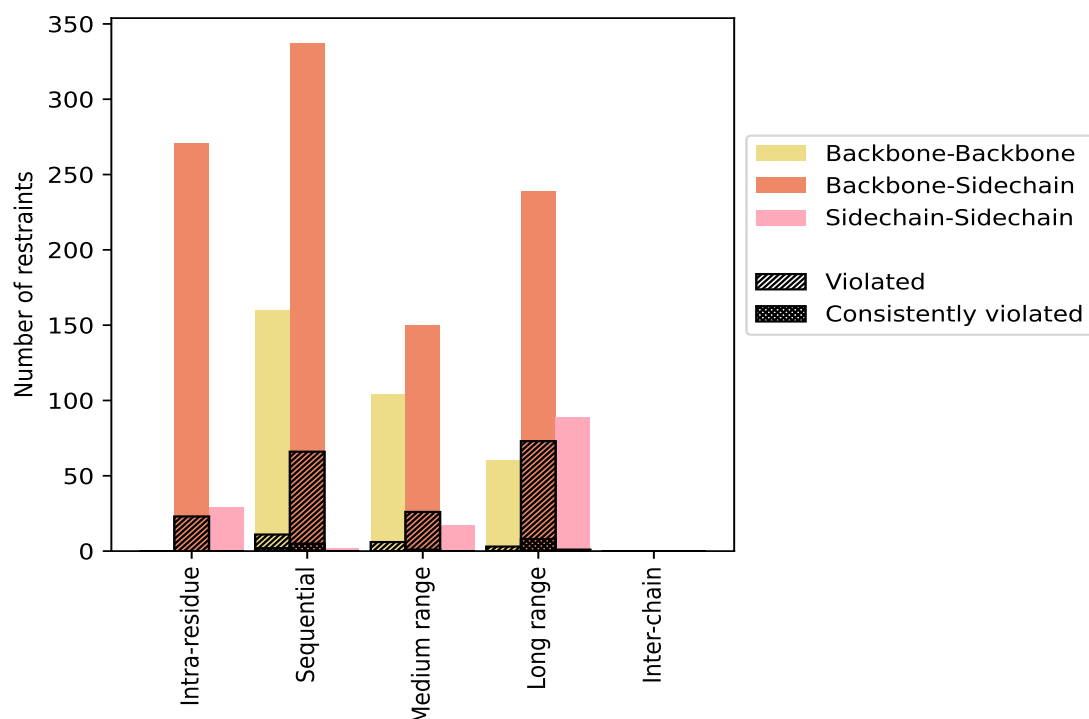
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	300	20.6	23	7.7	1.6	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	271	18.6	23	8.5	1.6	0	0.0	0.0
Sidechain-Sidechain	29	2.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	499	34.2	77	15.4	5.3	7	1.4	0.5
Backbone-Backbone	160	11.0	11	6.9	0.8	2	1.2	0.1
Backbone-Sidechain	337	23.1	66	19.6	4.5	5	1.5	0.3
Sidechain-Sidechain	2	0.1	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	221	15.2	29	13.1	2.0	1	0.5	0.1
Backbone-Backbone	104	7.1	6	5.8	0.4	0	0.0	0.0
Backbone-Sidechain	100	6.9	23	23.0	1.6	1	1.0	0.1
Sidechain-Sidechain	17	1.2	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	350	24.0	70	20.0	4.8	8	2.3	0.5
Backbone-Backbone	60	4.1	3	5.0	0.2	0	0.0	0.0
Backbone-Sidechain	201	13.8	66	32.8	4.5	8	4.0	0.5
Sidechain-Sidechain	89	6.1	1	1.1	0.1	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	88	6.0	10	11.4	0.7	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1458	100.0	209	14.3	14.3	16	1.1	1.1
Backbone-Backbone	324	22.2	20	6.2	1.4	2	0.6	0.1
Backbone-Sidechain	997	68.4	188	18.9	12.9	14	1.4	1.0
Sidechain-Sidechain	137	9.4	1	0.7	0.1	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	13	28	6	29	0	76	0.46	1.8	0.36	0.3
2	6	34	10	37	0	87	0.52	2.06	0.46	0.33
3	9	30	5	34	0	78	0.47	1.83	0.4	0.33
4	5	37	5	34	0	81	0.52	2.07	0.45	0.37
5	9	32	6	31	0	78	0.48	1.87	0.4	0.34
6	8	33	7	34	0	82	0.5	1.84	0.43	0.36
7	11	31	5	35	0	82	0.49	1.73	0.43	0.28
8	6	32	8	32	0	78	0.51	1.86	0.46	0.31
9	4	32	8	29	0	73	0.5	1.94	0.46	0.35
10	10	25	5	35	0	75	0.55	1.92	0.5	0.32

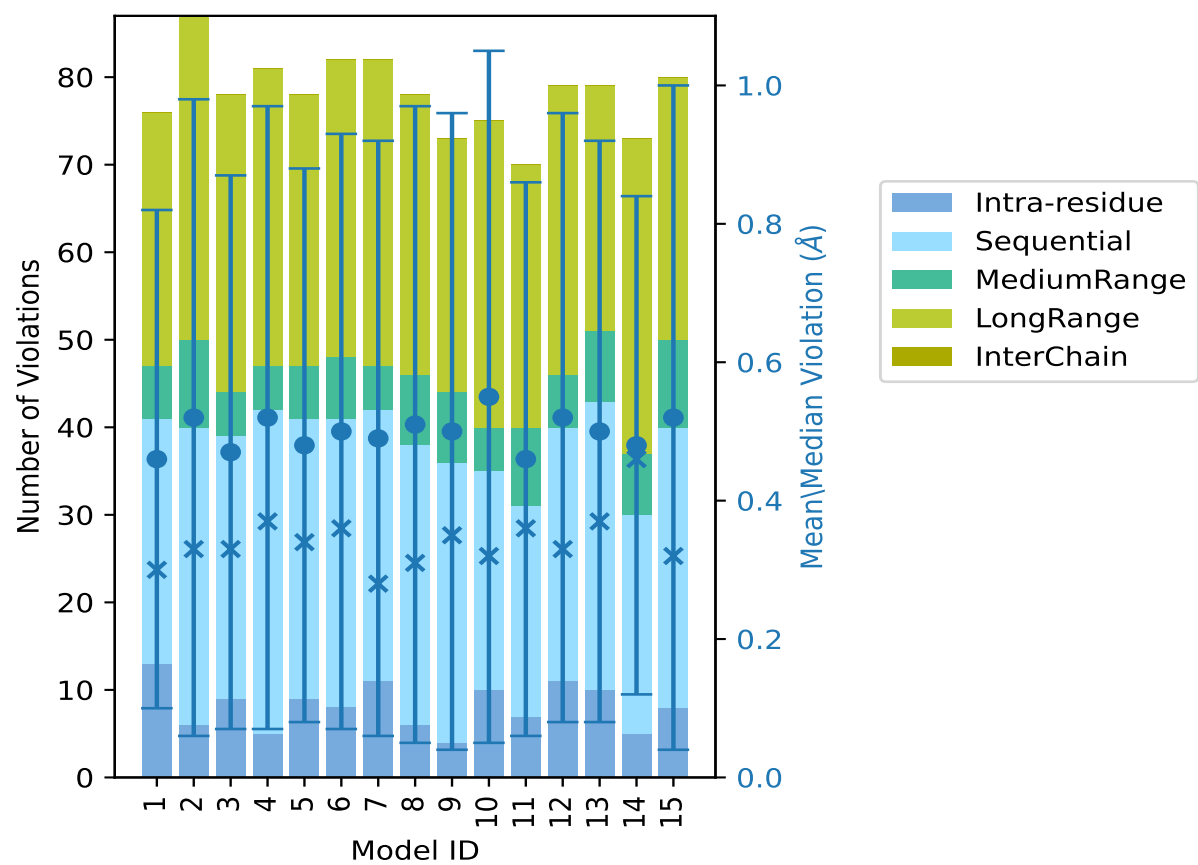
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	7	24	9	30	0	70	0.46	1.85	0.4	0.36
12	11	29	6	33	0	79	0.52	1.78	0.44	0.33
13	10	33	8	28	0	79	0.5	1.81	0.42	0.37
14	5	25	7	36	0	73	0.48	1.83	0.36	0.46
15	8	32	10	30	0	80	0.52	2.36	0.48	0.32

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

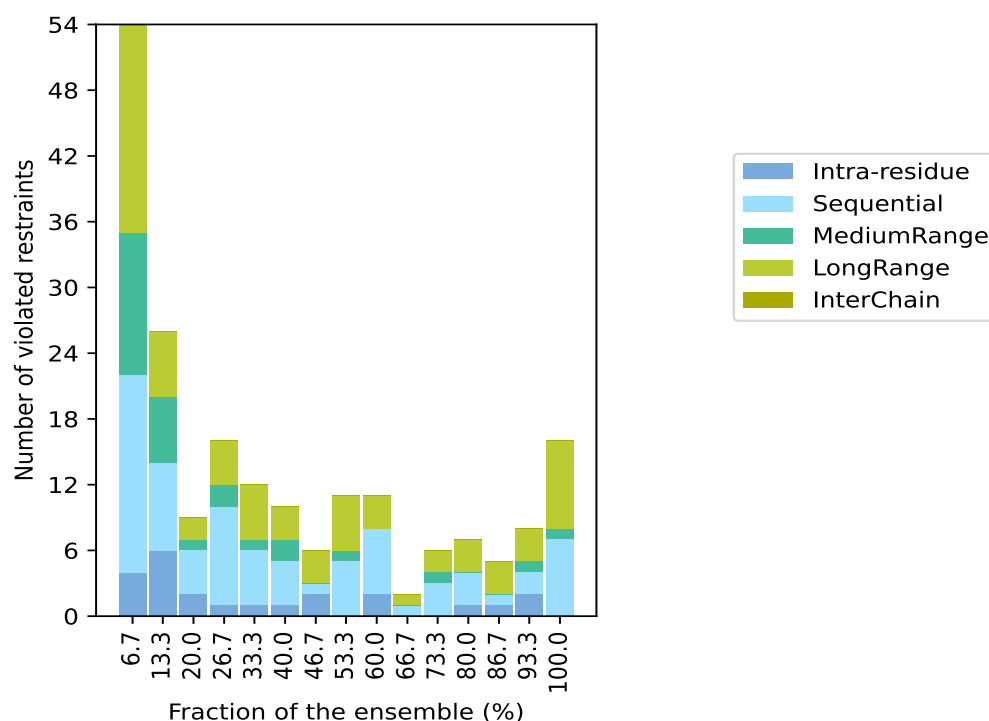
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1171(IR:277, SQ:422, MR:192, LR:280, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
4	18	13	19	0	54	1	6.7
6	8	6	6	0	26	2	13.3
2	4	1	2	0	9	3	20.0
1	9	2	4	0	16	4	26.7
1	5	1	5	0	12	5	33.3
1	4	2	3	0	10	6	40.0
2	1	0	3	0	6	7	46.7
0	5	1	5	0	11	8	53.3
2	6	0	3	0	11	9	60.0
0	1	0	1	0	2	10	66.7
0	3	1	2	0	6	11	73.3
1	3	0	3	0	7	12	80.0
1	1	0	3	0	5	13	86.7
2	2	1	3	0	8	14	93.3
0	7	1	8	0	16	15	100.0

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

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

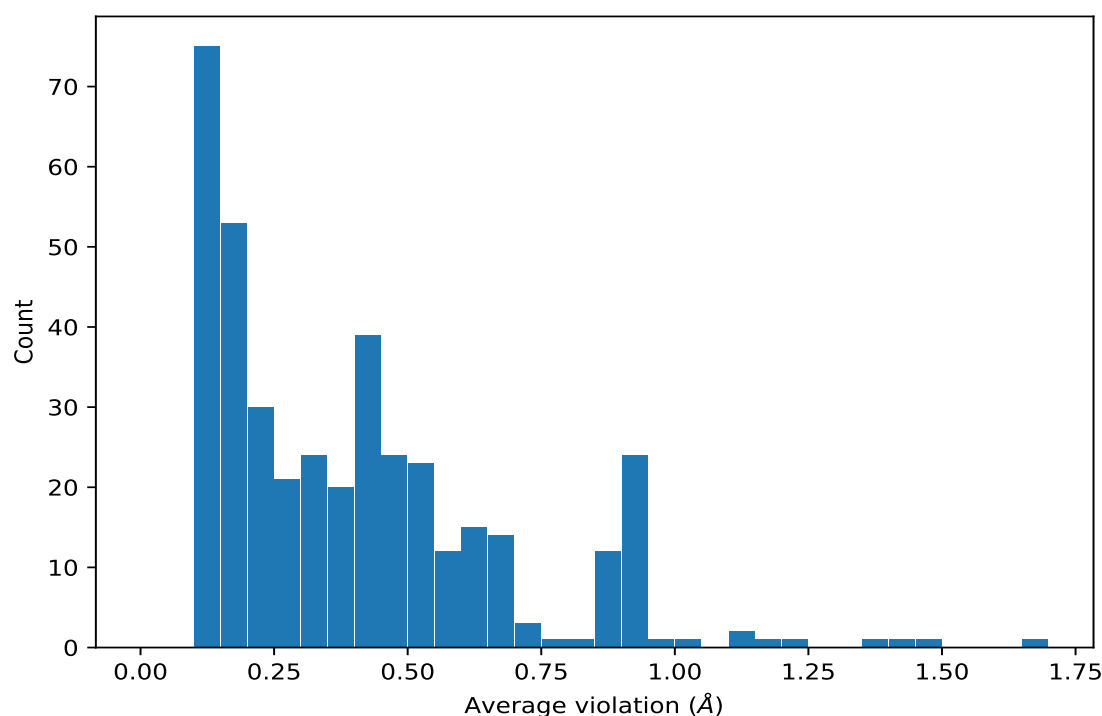
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	15	1.44	0.5	1.69
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	15	1.39	0.08	1.41
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	15	1.14	0.31	1.09
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	15	0.9	0.41	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	15	0.9	0.41	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	15	0.9	0.41	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	15	0.9	0.41	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	15	0.9	0.41	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	15	0.9	0.41	0.94
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	15	0.9	0.31	0.69
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	15	0.9	0.31	0.69
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	15	0.9	0.31	0.69
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	15	0.9	0.31	0.69
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	15	0.9	0.31	0.69
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	15	0.9	0.31	0.69
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	15	0.89	0.17	0.89

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	15	0.89	0.17	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	15	0.89	0.17	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	15	0.89	0.17	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	15	0.89	0.17	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	15	0.89	0.17	0.89
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	15	0.85	0.82	0.19
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	15	0.69	0.22	0.75
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	15	0.69	0.22	0.75
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	15	0.69	0.22	0.75
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	15	0.69	0.22	0.75
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	15	0.69	0.22	0.75
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	15	0.69	0.22	0.75
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	15	0.64	0.19	0.61
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	15	0.64	0.19	0.61
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	15	0.64	0.19	0.61
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	15	0.64	0.19	0.61
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	15	0.64	0.19	0.61
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	15	0.64	0.19	0.61
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	15	0.49	0.2	0.5
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	15	0.49	0.2	0.5
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	15	0.49	0.2	0.5
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	15	0.49	0.2	0.5
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	15	0.49	0.2	0.5
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	15	0.49	0.2	0.5
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	15	0.47	0.1	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	15	0.47	0.1	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	15	0.47	0.1	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	15	0.47	0.1	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	15	0.47	0.1	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	15	0.47	0.1	0.51
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	15	0.44	0.15	0.4
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	15	0.44	0.15	0.4
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	15	0.44	0.15	0.4
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	15	0.44	0.15	0.4
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	15	0.44	0.15	0.4
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	15	0.44	0.15	0.4
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	15	0.34	0.07	0.33
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	15	0.19	0.02	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	15	0.18	0.01	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	15	0.18	0.01	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	15	0.18	0.01	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	15	0.18	0.01	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	15	0.18	0.01	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	15	0.18	0.01	0.18
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	15	0.16	0.02	0.15
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	14	1.22	0.8	1.78
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	14	0.61	0.22	0.62
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	14	0.61	0.22	0.62
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	14	0.61	0.22	0.62
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	14	0.61	0.22	0.62
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	14	0.61	0.22	0.62
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	14	0.61	0.22	0.62
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	14	0.57	0.15	0.56
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	14	0.52	0.12	0.56
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	14	0.52	0.12	0.56
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	14	0.52	0.12	0.56
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	14	0.52	0.12	0.56
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	14	0.52	0.12	0.56
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	14	0.52	0.12	0.56
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	14	0.52	0.18	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	14	0.52	0.18	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	14	0.52	0.18	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	14	0.52	0.18	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	14	0.52	0.18	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	14	0.52	0.18	0.54
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	14	0.46	0.06	0.46
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	14	0.4	0.39	0.24
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	14	0.39	0.12	0.36
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	14	0.15	0.02	0.15
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	13	1.48	0.31	1.57
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	13	1.11	0.23	1.08
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	13	1.04	0.12	1.07
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	13	0.91	0.77	0.66
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	13	0.91	0.77	0.66
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	13	0.91	0.77	0.66
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	13	0.91	0.77	0.66
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	13	0.91	0.77	0.66
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	13	0.91	0.77	0.66
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	13	0.33	0.19	0.27
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	13	0.33	0.19	0.27
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	13	0.33	0.19	0.27
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	13	0.33	0.19	0.27
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	13	0.33	0.19	0.27
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	13	0.33	0.19	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,973)	1:72:A:THR:H	1:71:A:ARG:HG3	12	0.88	0.36	1.06
(1,987)	1:112:A:GLU:HG2	1:112:A:GLU:H	12	0.73	0.09	0.68
(1,974)	1:71:A:ARG:HD2	1:72:A:THR:H	12	0.7	0.23	0.8
(1,972)	1:71:A:ARG:HG2	1:72:A:THR:H	12	0.52	0.4	0.22
(1,1454)	1:95:A:ARG:H	1:78:A:LYS:HD3	12	0.49	0.53	0.27
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD11	12	0.41	0.13	0.38
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD12	12	0.41	0.13	0.38
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD13	12	0.41	0.13	0.38
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD21	12	0.41	0.13	0.38
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD22	12	0.41	0.13	0.38
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD23	12	0.41	0.13	0.38
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD3	12	0.15	0.03	0.15
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD2	12	0.15	0.03	0.15
(1,557)	1:54:A:ILE:HG12	1:55:A:VAL:H	11	0.75	0.31	0.63
(1,639)	1:166:A:ARG:HD2	1:167:A:ASP:H	11	0.57	0.38	0.41
(1,1039)	1:9:A:ASN:H	1:8:A:LYS:HE3	11	0.45	0.33	0.3
(1,884)	1:139:A:LYS:HE2	1:145:A:SER:H	11	0.32	0.1	0.3
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG11	11	0.24	0.07	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG12	11	0.24	0.07	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG13	11	0.24	0.07	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG21	11	0.24	0.07	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG22	11	0.24	0.07	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG23	11	0.24	0.07	0.27
(1,1411)	1:30:A:ARG:H	1:49:A:MET:O	11	0.14	0.02	0.14
(1,312)	1:78:A:LYS:H	1:87:A:SER:HA	11	0.13	0.03	0.13
(1,968)	1:69:A:SER:H	1:68:A:ARG:HD3	10	0.57	0.34	0.46
(1,397)	1:37:A:ILE:HD11	1:32:A:THR:H	10	0.15	0.03	0.15
(1,397)	1:37:A:ILE:HD12	1:32:A:THR:H	10	0.15	0.03	0.15
(1,397)	1:37:A:ILE:HD13	1:32:A:THR:H	10	0.15	0.03	0.15
(1,1040)	1:8:A:LYS:HE2	1:9:A:ASN:H	9	0.88	0.47	0.97
(1,731)	1:73:A:ALA:H	1:66:A:GLU:HB3	9	0.85	0.39	0.85
(1,670)	1:40:A:ASN:H	1:39:A:LYS:HE3	9	0.68	0.31	0.61
(1,1089)	1:85:A:SER:HB2	1:50:A:LEU:H	9	0.56	0.14	0.53
(1,890)	1:145:A:SER:H	1:139:A:LYS:HG3	9	0.44	0.36	0.34
(1,558)	1:55:A:VAL:H	1:54:A:ILE:HG13	9	0.44	0.18	0.54
(1,621)	1:27:A:ASN:H	1:26:A:GLU:HB3	9	0.43	0.12	0.47
(1,660)	1:79:A:ASN:H	1:78:A:LYS:HE3	9	0.38	0.26	0.34
(1,38)	1:145:A:SER:HB2	1:146:A:TYR:H	9	0.3	0.1	0.31
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD11	9	0.14	0.05	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD12	9	0.14	0.05	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD13	9	0.14	0.05	0.11
(1,924)	1:164:A:LEU:H	1:164:A:LEU:HG	9	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,671)	1:39:A:LYS:HE2	1:40:A:ASN:H	8	0.86	0.45	1.01
(1,1035)	1:9:A:ASN:H	1:8:A:LYS:HG3	8	0.64	0.23	0.68
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG21	8	0.5	0.15	0.52
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG22	8	0.5	0.15	0.52
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG23	8	0.5	0.15	0.52
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG11	8	0.5	0.15	0.52
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG12	8	0.5	0.15	0.52
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG13	8	0.5	0.15	0.52
(1,975)	1:72:A:THR:H	1:71:A:ARG:HD3	8	0.43	0.24	0.38
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG11	8	0.39	0.17	0.42
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG12	8	0.39	0.17	0.42
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG13	8	0.39	0.17	0.42
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG21	8	0.39	0.17	0.42
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG22	8	0.39	0.17	0.42
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG23	8	0.39	0.17	0.42
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD11	8	0.26	0.06	0.26
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD12	8	0.26	0.06	0.26
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD13	8	0.26	0.06	0.26
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD21	8	0.26	0.06	0.26
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD22	8	0.26	0.06	0.26
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD23	8	0.26	0.06	0.26
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG21	8	0.23	0.05	0.22
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG22	8	0.23	0.05	0.22
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG23	8	0.23	0.05	0.22
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG11	8	0.23	0.05	0.22
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG12	8	0.23	0.05	0.22
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG13	8	0.23	0.05	0.22
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD21	8	0.18	0.05	0.17
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD22	8	0.18	0.05	0.17
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD23	8	0.18	0.05	0.17
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD11	8	0.18	0.05	0.17
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD12	8	0.18	0.05	0.17
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD13	8	0.18	0.05	0.17
(1,328)	1:71:A:ARG:H	1:72:A:THR:H	8	0.16	0.03	0.15
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD2	8	0.14	0.03	0.13
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD3	8	0.14	0.03	0.13
(1,158)	1:96:A:LEU:H	1:99:A:LEU:HG	8	0.13	0.01	0.14
(1,1088)	1:50:A:LEU:H	1:85:A:SER:HB3	7	0.54	0.29	0.59
(1,612)	1:5:A:GLU:HG2	1:5:A:GLU:H	7	0.49	0.17	0.48
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG11	7	0.46	0.51	0.2
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG12	7	0.46	0.51	0.2
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG13	7	0.46	0.51	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG21	7	0.46	0.51	0.2
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG22	7	0.46	0.51	0.2
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG23	7	0.46	0.51	0.2
(1,618)	1:28:A:GLU:HG2	1:27:A:ASN:H	7	0.44	0.14	0.41
(1,613)	1:5:A:GLU:H	1:5:A:GLU:HG3	7	0.29	0.12	0.22
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG11	7	0.22	0.04	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG12	7	0.22	0.04	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG13	7	0.22	0.04	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG21	7	0.22	0.04	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG22	7	0.22	0.04	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG23	7	0.22	0.04	0.24
(1,889)	1:139:A:LYS:HG2	1:145:A:SER:H	6	1.65	0.24	1.66
(1,967)	1:68:A:ARG:HD2	1:69:A:SER:H	6	0.65	0.38	0.66
(1,638)	1:167:A:ASP:H	1:166:A:ARG:HD3	6	0.53	0.35	0.46
(1,1036)	1:8:A:LYS:HG2	1:9:A:ASN:H	6	0.47	0.4	0.28
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD11	6	0.4	0.08	0.43
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD12	6	0.4	0.08	0.43
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD13	6	0.4	0.08	0.43
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD21	6	0.4	0.08	0.43
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD22	6	0.4	0.08	0.43
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD23	6	0.4	0.08	0.43
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD21	6	0.36	0.13	0.36
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD22	6	0.36	0.13	0.36
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD23	6	0.36	0.13	0.36
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD11	6	0.36	0.13	0.36
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD12	6	0.36	0.13	0.36
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD13	6	0.36	0.13	0.36
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG21	6	0.33	0.06	0.32
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG22	6	0.33	0.06	0.32
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG23	6	0.33	0.06	0.32
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG11	6	0.33	0.06	0.32
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG12	6	0.33	0.06	0.32
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG13	6	0.33	0.06	0.32
(1,804)	1:16:A:SER:HB2	1:17:A:ASN:H	6	0.23	0.05	0.24
(1,251)	1:165:A:LEU:H	1:165:A:LEU:HG	6	0.16	0.03	0.15
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB3	6	0.14	0.03	0.13
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB2	6	0.14	0.03	0.13
(1,659)	1:78:A:LYS:HE2	1:79:A:ASN:H	5	1.15	0.36	1.27
(1,936)	1:140:A:SER:H	1:139:A:LYS:HE3	5	0.64	0.38	0.47
(1,834)	1:43:A:TYR:HB2	1:42:A:ASN:H	5	0.56	0.23	0.58
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG11	5	0.55	0.25	0.61
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG12	5	0.55	0.25	0.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG13	5	0.55	0.25	0.61
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG21	5	0.55	0.25	0.61
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG22	5	0.55	0.25	0.61
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG23	5	0.55	0.25	0.61
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG11	5	0.37	0.12	0.37
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG12	5	0.37	0.12	0.37
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG13	5	0.37	0.12	0.37
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG21	5	0.37	0.12	0.37
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG22	5	0.37	0.12	0.37
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG23	5	0.37	0.12	0.37
(1,37)	1:146:A:TYR:H	1:145:A:SER:HB3	5	0.28	0.05	0.28
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG11	5	0.18	0.06	0.15
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG12	5	0.18	0.06	0.15
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG13	5	0.18	0.06	0.15
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG21	5	0.18	0.06	0.15
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG22	5	0.18	0.06	0.15
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG23	5	0.18	0.06	0.15
(1,297)	1:37:A:ILE:HD11	1:43:A:TYR:H	5	0.15	0.02	0.15
(1,297)	1:37:A:ILE:HD12	1:43:A:TYR:H	5	0.15	0.02	0.15
(1,297)	1:37:A:ILE:HD13	1:43:A:TYR:H	5	0.15	0.02	0.15
(1,543)	1:129:A:LYS:H	1:128:A:ASP:H	5	0.15	0.02	0.14
(1,997)	1:108:A:LEU:HG	1:108:A:LEU:H	5	0.14	0.04	0.11
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG11	5	0.12	0.01	0.12
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG12	5	0.12	0.01	0.12
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG13	5	0.12	0.01	0.12
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD11	5	0.11	0.0	0.11
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD12	5	0.11	0.0	0.11
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD13	5	0.11	0.0	0.11
(1,945)	1:140:A:SER:H	1:139:A:LYS:HD3	4	0.86	0.24	0.82
(1,706)	1:168:A:ILE:HG12	1:169:A:TYR:H	4	0.84	0.12	0.86
(1,856)	1:101:A:ARG:HG2	1:115:A:VAL:H	4	0.55	0.37	0.47
(1,855)	1:115:A:VAL:H	1:101:A:ARG:HG3	4	0.53	0.29	0.5
(1,944)	1:139:A:LYS:HD2	1:140:A:SER:H	4	0.48	0.4	0.34
(1,705)	1:169:A:TYR:H	1:168:A:ILE:HG13	4	0.44	0.18	0.45
(1,887)	1:145:A:SER:HB2	1:145:A:SER:H	4	0.44	0.03	0.45
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD21	4	0.4	0.22	0.34
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD22	4	0.4	0.22	0.34
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD23	4	0.4	0.22	0.34
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD11	4	0.4	0.22	0.34
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD12	4	0.4	0.22	0.34
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD13	4	0.4	0.22	0.34
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD11	4	0.34	0.1	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD12	4	0.34	0.1	0.35
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD13	4	0.34	0.1	0.35
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD21	4	0.34	0.1	0.35
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD22	4	0.34	0.1	0.35
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD23	4	0.34	0.1	0.35
(1,805)	1:17:A:ASN:H	1:16:A:SER:HB3	4	0.32	0.14	0.34
(1,416)	1:6:A:ILE:H	1:7:A:ASP:H	4	0.15	0.03	0.16
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG11	4	0.15	0.03	0.15
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG12	4	0.15	0.03	0.15
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG13	4	0.15	0.03	0.15
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG21	4	0.15	0.03	0.15
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG22	4	0.15	0.03	0.15
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG23	4	0.15	0.03	0.15
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD11	4	0.12	0.01	0.12
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD12	4	0.12	0.01	0.12
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD13	4	0.12	0.01	0.12
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG21	4	0.12	0.02	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG22	4	0.12	0.02	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG23	4	0.12	0.02	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG11	4	0.12	0.02	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG12	4	0.12	0.02	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG13	4	0.12	0.02	0.11
(1,688)	1:84:A:VAL:H	1:80:A:THR:H	4	0.11	0.01	0.11
(1,748)	1:6:A:ILE:HB	1:7:A:ASP:H	4	0.11	0.01	0.11
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD11	3	0.93	0.18	0.84
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD12	3	0.93	0.18	0.84
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD13	3	0.93	0.18	0.84
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD21	3	0.93	0.18	0.84
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD22	3	0.93	0.18	0.84
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD23	3	0.93	0.18	0.84
(1,833)	1:42:A:ASN:H	1:43:A:TYR:HB3	3	0.7	0.16	0.6
(1,619)	1:27:A:ASN:H	1:28:A:GLU:HG3	3	0.41	0.25	0.35
(1,886)	1:145:A:SER:H	1:145:A:SER:HB3	3	0.28	0.08	0.29
(1,574)	1:139:A:LYS:H	1:139:A:LYS:HD3	3	0.2	0.06	0.22
(1,574)	1:139:A:LYS:H	1:139:A:LYS:HD2	3	0.2	0.06	0.22
(1,832)	1:42:A:ASN:H	1:43:A:TYR:HA	3	0.15	0.02	0.15
(1,1445)	1:104:A:ASP:H	1:150:A:VAL:O	3	0.15	0.06	0.12
(1,721)	1:99:A:LEU:HG	1:100:A:LYS:H	3	0.12	0.0	0.12
(1,1432)	1:112:A:GLU:H	1:79:A:ASN:O	3	0.12	0.01	0.12
(1,112)	1:47:A:ASP:H	1:45:A:LEU:HD21	3	0.11	0.01	0.11
(1,112)	1:47:A:ASP:H	1:45:A:LEU:HD22	3	0.11	0.01	0.11
(1,112)	1:47:A:ASP:H	1:45:A:LEU:HD23	3	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,283)	1:113:A:ALA:H	1:99:A:LEU:HD11	3	0.11	0.01	0.11
(1,283)	1:113:A:ALA:H	1:99:A:LEU:HD12	3	0.11	0.01	0.11
(1,283)	1:113:A:ALA:H	1:99:A:LEU:HD13	3	0.11	0.01	0.11
(1,653)	1:78:A:LYS:HD2	1:79:A:ASN:H	2	0.96	0.13	0.96
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD11	2	0.66	0.03	0.66
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD12	2	0.66	0.03	0.66
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD13	2	0.66	0.03	0.66
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD21	2	0.66	0.03	0.66
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD22	2	0.66	0.03	0.66
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD23	2	0.66	0.03	0.66
(1,519)	1:23:A:ARG:HD2	1:23:A:ARG:H	2	0.64	0.02	0.64
(1,941)	1:139:A:LYS:HG2	1:140:A:SER:H	2	0.54	0.41	0.54
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD21	2	0.4	0.06	0.4
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD22	2	0.4	0.06	0.4
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD23	2	0.4	0.06	0.4
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD11	2	0.4	0.06	0.4
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD12	2	0.4	0.06	0.4
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD13	2	0.4	0.06	0.4
(1,673)	1:39:A:LYS:HG2	1:40:A:ASN:H	2	0.34	0.02	0.34
(1,730)	1:66:A:GLU:HB2	1:73:A:ALA:H	2	0.34	0.14	0.34
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD21	2	0.28	0.09	0.28
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD22	2	0.28	0.09	0.28
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD23	2	0.28	0.09	0.28
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD11	2	0.28	0.09	0.28
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD12	2	0.28	0.09	0.28
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD13	2	0.28	0.09	0.28
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD11	2	0.28	0.02	0.28
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD12	2	0.28	0.02	0.28
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD13	2	0.28	0.02	0.28
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD21	2	0.28	0.02	0.28
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD22	2	0.28	0.02	0.28
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD23	2	0.28	0.02	0.28
(1,518)	1:23:A:ARG:H	1:23:A:ARG:HD3	2	0.24	0.01	0.24
(1,938)	1:139:A:LYS:HB2	1:140:A:SER:H	2	0.23	0.05	0.23
(1,488)	1:28:A:GLU:HG2	1:25:A:ASP:H	2	0.22	0.04	0.22
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD11	2	0.22	0.01	0.22
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD12	2	0.22	0.01	0.22
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD13	2	0.22	0.01	0.22
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD21	2	0.22	0.01	0.22
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD22	2	0.22	0.01	0.22
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD23	2	0.22	0.01	0.22
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD21	2	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD22	2	0.18	0.03	0.18
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD23	2	0.18	0.03	0.18
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD11	2	0.18	0.03	0.18
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD12	2	0.18	0.03	0.18
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD13	2	0.18	0.03	0.18
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG11	2	0.16	0.04	0.16
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG12	2	0.16	0.04	0.16
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG13	2	0.16	0.04	0.16
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG21	2	0.16	0.04	0.16
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG22	2	0.16	0.04	0.16
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG23	2	0.16	0.04	0.16
(1,45)	1:129:A:LYS:H	1:128:A:ASP:HA	2	0.14	0.04	0.14
(1,566)	1:54:A:ILE:HG21	1:55:A:VAL:H	2	0.14	0.04	0.14
(1,566)	1:54:A:ILE:HG22	1:55:A:VAL:H	2	0.14	0.04	0.14
(1,566)	1:54:A:ILE:HG23	1:55:A:VAL:H	2	0.14	0.04	0.14
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD21	2	0.13	0.03	0.13
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD22	2	0.13	0.03	0.13
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD23	2	0.13	0.03	0.13
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD11	2	0.13	0.03	0.13
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD12	2	0.13	0.03	0.13
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD13	2	0.13	0.03	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD21	2	0.13	0.0	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD22	2	0.13	0.0	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD23	2	0.13	0.0	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD11	2	0.13	0.0	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD12	2	0.13	0.0	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD13	2	0.13	0.0	0.13
(1,324)	1:71:A:ARG:H	1:71:A:ARG:HG2	2	0.12	0.02	0.12
(1,324)	1:71:A:ARG:H	1:71:A:ARG:HG3	2	0.12	0.02	0.12
(1,1456)	1:47:A:ASP:H	1:30:A:ARG:HB3	2	0.12	0.0	0.12
(1,1456)	1:47:A:ASP:H	1:30:A:ARG:HB2	2	0.12	0.0	0.12
(1,1427)	1:80:A:THR:H	1:83:A:ARG:O	2	0.12	0.02	0.12
(1,302)	1:31:A:ILE:HB	1:31:A:ILE:H	2	0.11	0.0	0.11
(1,410)	1:6:A:ILE:H	1:6:A:ILE:HG13	2	0.11	0.01	0.11
(1,410)	1:6:A:ILE:H	1:6:A:ILE:HG12	2	0.11	0.01	0.11
(1,816)	1:54:A:ILE:HD11	1:52:A:THR:H	2	0.11	0.0	0.11
(1,816)	1:54:A:ILE:HD12	1:52:A:THR:H	2	0.11	0.0	0.11
(1,816)	1:54:A:ILE:HD13	1:52:A:THR:H	2	0.11	0.0	0.11
(1,1323)	1:58:A:VAL:HG11	1:131:A:VAL:HG11	2	0.11	0.0	0.11
(1,1323)	1:58:A:VAL:HG11	1:131:A:VAL:HG12	2	0.11	0.0	0.11
(1,1323)	1:58:A:VAL:HG11	1:131:A:VAL:HG13	2	0.11	0.0	0.11
(1,1323)	1:58:A:VAL:HG12	1:131:A:VAL:HG11	2	0.11	0.0	0.11

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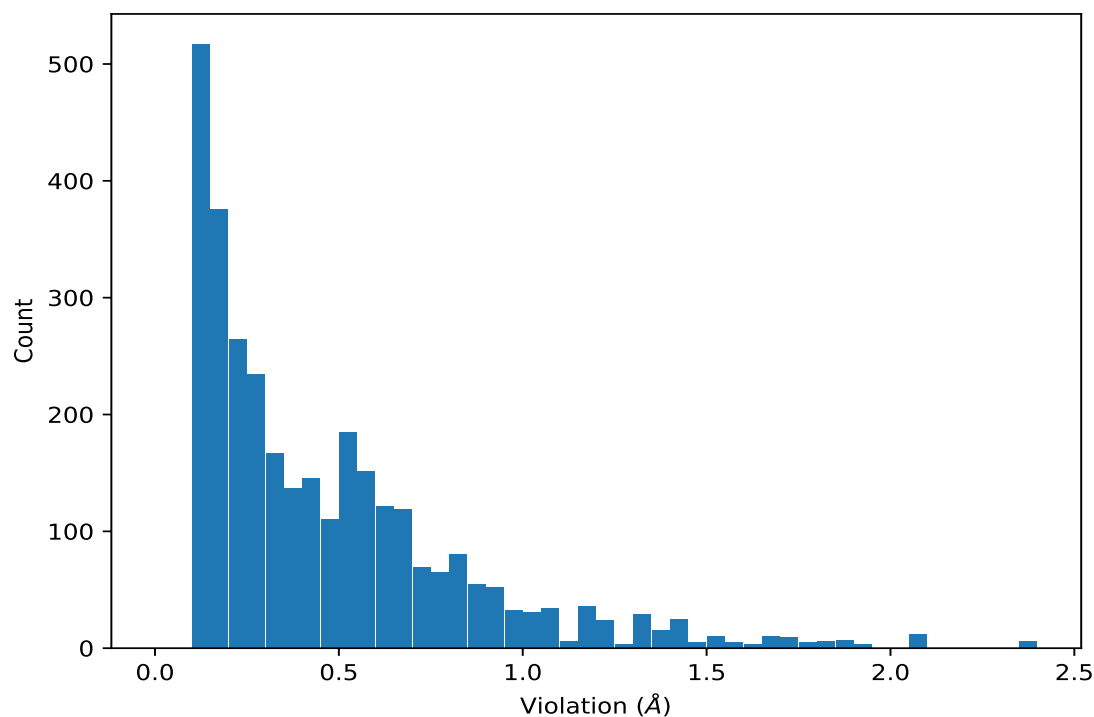
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1323)	1:58:A:VAL:HG12	1:131:A:VAL:HG12	2	0.11	0.0	0.11
(1,1323)	1:58:A:VAL:HG12	1:131:A:VAL:HG13	2	0.11	0.0	0.11
(1,1323)	1:58:A:VAL:HG13	1:131:A:VAL:HG11	2	0.11	0.0	0.11
(1,1323)	1:58:A:VAL:HG13	1:131:A:VAL:HG12	2	0.11	0.0	0.11
(1,1323)	1:58:A:VAL:HG13	1:131:A:VAL:HG13	2	0.11	0.0	0.11
(1,1452)	1:104:A:ASP:H	1:101:A:ARG:HD2	2	0.11	0.0	0.11
(1,1452)	1:104:A:ASP:H	1:101:A:ARG:HD3	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)
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	15	2.36
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	15	2.36
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	15	2.36
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	15	2.36
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	15	2.36
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	15	2.36
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	4	2.07
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	4	2.07
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	4	2.07
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	4	2.07
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	4	2.07
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	4	2.07
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	2	2.06
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	2	2.06
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	2	2.06
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	2	2.06
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	2	2.06
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	2	2.06
(1,889)	1:139:A:LYS:HG2	1:145:A:SER:H	9	1.94
(1,889)	1:139:A:LYS:HG2	1:145:A:SER:H	10	1.92
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	15	1.92
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	10	1.89
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	4	1.88
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	9	1.88
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	5	1.87
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	8	1.86
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	11	1.85
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	2	1.85
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	6	1.84
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	10	1.83
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	14	1.83
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	3	1.83
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	13	1.81
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	1	1.8
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	8	1.78
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	12	1.78
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	15	1.78
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	4	1.77
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	12	1.75
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	11	1.74
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	9	1.74
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	7	1.73
(1,889)	1:139:A:LYS:HG2	1:145:A:SER:H	8	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	7	1.73
(1,1454)	1:95:A:ARG:H	1:78:A:LYS:HD3	3	1.72
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	6	1.72
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	13	1.72
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	15	1.7
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	9	1.69
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	14	1.69
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	13	1.68
(1,1040)	1:8:A:LYS:HE2	1:9:A:ASN:H	6	1.67
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG11	2	1.66
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG12	2	1.66
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG13	2	1.66
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG21	2	1.66
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG22	2	1.66
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG23	2	1.66
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	8	1.64
(1,1454)	1:95:A:ARG:H	1:78:A:LYS:HD3	5	1.63
(1,731)	1:73:A:ALA:H	1:66:A:GLU:HB3	10	1.6
(1,889)	1:139:A:LYS:HG2	1:145:A:SER:H	15	1.58
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	3	1.57
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	7	1.57
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	12	1.56
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	10	1.55
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	13	1.54
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	13	1.54
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	13	1.54
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	13	1.54
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	13	1.54
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	13	1.54
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	8	1.53
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	10	1.53
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	2	1.51
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	2	1.5
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	12	1.49
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	7	1.48
(1,659)	1:78:A:LYS:HE2	1:79:A:ASN:H	5	1.46
(1,557)	1:54:A:ILE:HG12	1:55:A:VAL:H	6	1.46
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	10	1.46
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	7	1.44
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	11	1.43
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	13	1.43
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	15	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:139:A:LYS:HG2	1:145:A:SER:H	11	1.42
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	12	1.42
(1,659)	1:78:A:LYS:HE2	1:79:A:ASN:H	3	1.41
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	2	1.41
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	6	1.41
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	11	1.41
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	5	1.41
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	6	1.4
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	6	1.4
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	6	1.4
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	6	1.4
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	6	1.4
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	6	1.4
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	10	1.4
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	10	1.4
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	10	1.4
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	10	1.4
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	10	1.4
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	10	1.4
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	2	1.4
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	4	1.4
(1,671)	1:39:A:LYS:HE2	1:40:A:ASN:H	12	1.39
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	8	1.39
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	1	1.38
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	4	1.38
(1,890)	1:145:A:SER:H	1:139:A:LYS:HG3	12	1.37
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	4	1.37
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	9	1.36
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	9	1.36
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	9	1.36
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	9	1.36
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	9	1.36
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	9	1.36
(1,639)	1:166:A:ARG:HD2	1:167:A:ASP:H	1	1.36
(1,671)	1:39:A:LYS:HE2	1:40:A:ASN:H	10	1.35
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	13	1.35
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	14	1.34
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	8	1.33
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	8	1.33
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	8	1.33
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	8	1.33
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	8	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	8	1.33
(1,936)	1:140:A:SER:H	1:139:A:LYS:HE3	7	1.33
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	2	1.32
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	2	1.32
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	2	1.32
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	2	1.32
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	2	1.32
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	2	1.32
(1,731)	1:73:A:ALA:H	1:66:A:GLU:HB3	7	1.31
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	9	1.31
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	15	1.3
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	15	1.3
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	15	1.3
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	15	1.3
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	15	1.3
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	15	1.3
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	7	1.3
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	7	1.3
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	7	1.3
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	7	1.3
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	7	1.3
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	7	1.3
(1,889)	1:139:A:LYS:HG2	1:145:A:SER:H	1	1.3
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	3	1.29
(1,659)	1:78:A:LYS:HE2	1:79:A:ASN:H	2	1.27
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	3	1.25
(1,1040)	1:8:A:LYS:HE2	1:9:A:ASN:H	3	1.24
(1,1040)	1:8:A:LYS:HE2	1:9:A:ASN:H	4	1.24
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	4	1.23
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	4	1.23
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	4	1.23
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	4	1.23
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	4	1.23
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	4	1.23
(1,968)	1:69:A:SER:H	1:68:A:ARG:HD3	12	1.23
(1,670)	1:40:A:ASN:H	1:39:A:LYS:HE3	4	1.23
(1,508)	1:29:A:LEU:H	1:30:A:ARG:HB3	5	1.22
(1,945)	1:140:A:SER:H	1:139:A:LYS:HD3	10	1.21
(1,638)	1:167:A:ASP:H	1:166:A:ARG:HD3	13	1.21
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	6	1.21
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	13	1.21
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	11	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	11	1.2
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	11	1.2
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	11	1.2
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	11	1.2
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	11	1.2
(1,1036)	1:8:A:LYS:HG2	1:9:A:ASN:H	7	1.2
(1,973)	1:72:A:THR:H	1:71:A:ARG:HG3	5	1.2
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	6	1.2
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	2	1.19
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	2	1.19
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	2	1.19
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	2	1.19
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	2	1.19
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	2	1.19
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	10	1.19
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD11	15	1.18
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD12	15	1.18
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD13	15	1.18
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD21	15	1.18
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD22	15	1.18
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD23	15	1.18
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	12	1.18
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	12	1.18
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	12	1.18
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	12	1.18
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	12	1.18
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	12	1.18
(1,671)	1:39:A:LYS:HE2	1:40:A:ASN:H	1	1.18
(1,1040)	1:8:A:LYS:HE2	1:9:A:ASN:H	2	1.17
(1,659)	1:78:A:LYS:HE2	1:79:A:ASN:H	9	1.17
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	9	1.17
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	8	1.17
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	6	1.17
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	13	1.16
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	15	1.16
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	9	1.15
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	9	1.15
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	9	1.15
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	9	1.15
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	9	1.15
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	9	1.15
(1,967)	1:68:A:ARG:HD2	1:69:A:SER:H	9	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,944)	1:139:A:LYS:HD2	1:140:A:SER:H	7	1.15
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	12	1.15
(1,856)	1:101:A:ARG:HG2	1:115:A:VAL:H	4	1.14
(1,973)	1:72:A:THR:H	1:71:A:ARG:HG3	4	1.12
(1,671)	1:39:A:LYS:HE2	1:40:A:ASN:H	5	1.12
(1,973)	1:72:A:THR:H	1:71:A:ARG:HG3	9	1.11
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	2	1.1
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	5	1.1
(1,1039)	1:9:A:ASN:H	1:8:A:LYS:HE3	8	1.09
(1,972)	1:71:A:ARG:HG2	1:72:A:THR:H	10	1.09
(1,639)	1:166:A:ARG:HD2	1:167:A:ASP:H	8	1.09
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	7	1.09
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	14	1.09
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	10	1.08
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	10	1.08
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	10	1.08
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	10	1.08
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	10	1.08
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	10	1.08
(1,973)	1:72:A:THR:H	1:71:A:ARG:HG3	6	1.08
(1,973)	1:72:A:THR:H	1:71:A:ARG:HG3	7	1.08
(1,653)	1:78:A:LYS:HD2	1:79:A:ASN:H	3	1.08
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	6	1.08
(1,1039)	1:9:A:ASN:H	1:8:A:LYS:HE3	7	1.07
(1,973)	1:72:A:THR:H	1:71:A:ARG:HG3	14	1.07
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	4	1.07
(1,973)	1:72:A:THR:H	1:71:A:ARG:HG3	2	1.06
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	6	1.05
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	6	1.05
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	6	1.05
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	6	1.05
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	6	1.05
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	6	1.05
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	5	1.05
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	5	1.05
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	5	1.05
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	5	1.05
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	5	1.05
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	5	1.05
(1,973)	1:72:A:THR:H	1:71:A:ARG:HG3	3	1.05
(1,968)	1:69:A:SER:H	1:68:A:ARG:HD3	6	1.05
(1,660)	1:79:A:ASN:H	1:78:A:LYS:HE3	14	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:40:A:ASN:H	1:39:A:LYS:HE3	14	1.04
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	1	1.04
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	12	1.04
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	1	1.04
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	10	1.03
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	10	1.03
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	10	1.03
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	10	1.03
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	10	1.03
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	10	1.03
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	4	1.03
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	4	1.03
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	4	1.03
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	4	1.03
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	4	1.03
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	4	1.03
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	8	1.03
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	8	1.03
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	8	1.03
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	8	1.03
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	8	1.03
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	8	1.03
(1,557)	1:54:A:ILE:HG12	1:55:A:VAL:H	8	1.03
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	3	1.02
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	3	1.02
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	3	1.02
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	3	1.02
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	3	1.02
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	3	1.02
(1,967)	1:68:A:ARG:HD2	1:69:A:SER:H	11	1.01
(1,972)	1:71:A:ARG:HG2	1:72:A:THR:H	12	1.0
(1,706)	1:168:A:ILE:HG12	1:169:A:TYR:H	2	0.99
(1,557)	1:54:A:ILE:HG12	1:55:A:VAL:H	9	0.99
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	12	0.98
(1,1040)	1:8:A:LYS:HE2	1:9:A:ASN:H	5	0.97
(1,973)	1:72:A:THR:H	1:71:A:ARG:HG3	8	0.97
(1,972)	1:71:A:ARG:HG2	1:72:A:THR:H	15	0.97
(1,942)	1:140:A:SER:H	1:139:A:LYS:HG3	7	0.97
(1,731)	1:73:A:ALA:H	1:66:A:GLU:HB3	12	0.97
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	8	0.96
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	8	0.96
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	8	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	8	0.96
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	8	0.96
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	8	0.96
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	12	0.96
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	12	0.96
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	12	0.96
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	12	0.96
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	12	0.96
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	12	0.96
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	1	0.96
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	1	0.96
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	1	0.96
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	1	0.96
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	1	0.96
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	1	0.96
(1,557)	1:54:A:ILE:HG12	1:55:A:VAL:H	12	0.96
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	9	0.96
(1,972)	1:71:A:ARG:HG2	1:72:A:THR:H	1	0.95
(1,941)	1:139:A:LYS:HG2	1:140:A:SER:H	10	0.95
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	15	0.95
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	9	0.95
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	1	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	1	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	1	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	1	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	1	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	1	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	12	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	12	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	12	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	12	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	12	0.94
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	12	0.94
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	6	0.94
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	6	0.94
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	6	0.94
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	6	0.94
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	6	0.94
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	6	0.94
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	8	0.94
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	8	0.94
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	8	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	8	0.94
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	8	0.94
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	8	0.94
(1,987)	1:112:A:GLU:HG2	1:112:A:GLU:H	5	0.94
(1,855)	1:115:A:VAL:H	1:101:A:ARG:HG3	1	0.94
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	3	0.94
(1,1035)	1:9:A:ASN:H	1:8:A:LYS:HG3	2	0.93
(1,974)	1:71:A:ARG:HD2	1:72:A:THR:H	6	0.93
(1,974)	1:71:A:ARG:HD2	1:72:A:THR:H	7	0.93
(1,972)	1:71:A:ARG:HG2	1:72:A:THR:H	13	0.93
(1,945)	1:140:A:SER:H	1:139:A:LYS:HD3	8	0.93
(1,883)	1:145:A:SER:H	1:139:A:LYS:HE3	14	0.92
(1,833)	1:42:A:ASN:H	1:43:A:TYR:HB3	15	0.92
(1,975)	1:72:A:THR:H	1:71:A:ARG:HD3	12	0.91
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	10	0.91
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	11	0.91
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	15	0.9
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	15	0.9
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	15	0.9
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	15	0.9
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	15	0.9
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	15	0.9
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	10	0.9
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	10	0.9
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	10	0.9
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	10	0.9
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	10	0.9
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	10	0.9
(1,974)	1:71:A:ARG:HD2	1:72:A:THR:H	4	0.9
(1,974)	1:71:A:ARG:HD2	1:72:A:THR:H	14	0.9
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	5	0.9
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	11	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	11	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	11	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	11	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	11	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	11	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	12	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	12	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	12	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	12	0.89
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	12	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	12	0.89
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	13	0.89
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	13	0.89
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	13	0.89
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	13	0.89
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	13	0.89
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	13	0.89
(1,1088)	1:50:A:LEU:H	1:85:A:SER:HB3	3	0.89
(1,834)	1:43:A:TYR:HB2	1:42:A:ASN:H	5	0.89
(1,671)	1:39:A:LYS:HE2	1:40:A:ASN:H	13	0.89
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	7	0.89
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	14	0.88
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	14	0.88
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	14	0.88
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	14	0.88
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	14	0.88
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	14	0.88
(1,967)	1:68:A:ARG:HD2	1:69:A:SER:H	2	0.88
(1,731)	1:73:A:ALA:H	1:66:A:GLU:HB3	5	0.88
(1,706)	1:168:A:ILE:HG12	1:169:A:TYR:H	8	0.88
(1,670)	1:40:A:ASN:H	1:39:A:LYS:HE3	15	0.88
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	13	0.86
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	13	0.86
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	13	0.86
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	13	0.86
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	13	0.86
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	13	0.86
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	12	0.86
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	12	0.86
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	12	0.86
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	12	0.86
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	12	0.86
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	12	0.86
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	13	0.86
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	13	0.86
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	13	0.86
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	13	0.86
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	13	0.86
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	13	0.86
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	2	0.86
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	1	0.85
(1,974)	1:71:A:ARG:HD2	1:72:A:THR:H	9	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,731)	1:73:A:ALA:H	1:66:A:GLU:HB3	14	0.85
(1,706)	1:168:A:ILE:HG12	1:169:A:TYR:H	4	0.85
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	12	0.84
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	12	0.84
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	12	0.84
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	12	0.84
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	12	0.84
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	12	0.84
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	10	0.84
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	10	0.84
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	10	0.84
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	10	0.84
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	10	0.84
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	10	0.84
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD11	2	0.84
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD12	2	0.84
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD13	2	0.84
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD21	2	0.84
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD22	2	0.84
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD23	2	0.84
(1,1088)	1:50:A:LEU:H	1:85:A:SER:HB3	8	0.84
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	15	0.84
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	15	0.84
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	15	0.84
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	15	0.84
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	15	0.84
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	15	0.84
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	2	0.84
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	2	0.84
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	2	0.84
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	2	0.84
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	2	0.84
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	2	0.84
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	2	0.84
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	2	0.84
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	2	0.84
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	2	0.84
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	2	0.84
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	2	0.84
(1,1035)	1:9:A:ASN:H	1:8:A:LYS:HG3	8	0.84
(1,313)	1:78:A:LYS:H	1:78:A:LYS:HD3	14	0.84
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	11	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	8	0.83
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	8	0.83
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	8	0.83
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	8	0.83
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	8	0.83
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	8	0.83
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	13	0.83
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	13	0.83
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	13	0.83
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	13	0.83
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	13	0.83
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	13	0.83
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	4	0.83
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	4	0.83
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	4	0.83
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	4	0.83
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	4	0.83
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	4	0.83
(1,987)	1:112:A:GLU:HG2	1:112:A:GLU:H	7	0.83
(1,987)	1:112:A:GLU:HG2	1:112:A:GLU:H	15	0.83
(1,796)	1:135:A:CYS:HB2	1:151:A:VAL:H	10	0.83
(1,653)	1:78:A:LYS:HD2	1:79:A:ASN:H	5	0.83
(1,974)	1:71:A:ARG:HD2	1:72:A:THR:H	5	0.81
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	3	0.8
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	3	0.8
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	3	0.8
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	3	0.8
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	3	0.8
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	3	0.8
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	2	0.8
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	2	0.8
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	2	0.8
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	2	0.8
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	2	0.8
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	2	0.8
(1,1036)	1:8:A:LYS:HG2	1:9:A:ASN:H	6	0.8
(1,987)	1:112:A:GLU:HG2	1:112:A:GLU:H	4	0.8
(1,968)	1:69:A:SER:H	1:68:A:ARG:HD3	10	0.8
(1,639)	1:166:A:ARG:HD2	1:167:A:ASP:H	4	0.8
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	1	0.8
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	4	0.79
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	4	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	4	0.79
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	4	0.79
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	4	0.79
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	4	0.79
(1,974)	1:71:A:ARG:HD2	1:72:A:THR:H	13	0.79
(1,1088)	1:50:A:LEU:H	1:85:A:SER:HB3	15	0.78
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG11	5	0.78
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG12	5	0.78
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG13	5	0.78
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG21	5	0.78
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG22	5	0.78
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG23	5	0.78
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG11	14	0.78
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG12	14	0.78
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG13	14	0.78
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG21	14	0.78
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG22	14	0.78
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG23	14	0.78
(1,1035)	1:9:A:ASN:H	1:8:A:LYS:HG3	3	0.78
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	7	0.77
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	7	0.77
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	7	0.77
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	7	0.77
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	7	0.77
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	7	0.77
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD11	4	0.77
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD12	4	0.77
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD13	4	0.77
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD21	4	0.77
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD22	4	0.77
(1,1113)	1:63:A:SER:H	1:118:A:LEU:HD23	4	0.77
(1,1089)	1:85:A:SER:HB2	1:50:A:LEU:H	11	0.77
(1,987)	1:112:A:GLU:HG2	1:112:A:GLU:H	2	0.77
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	7	0.76
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	7	0.76
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	7	0.76
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	7	0.76
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	7	0.76
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	7	0.76
(1,1057)	1:68:A:ARG:H	1:14:A:LEU:HD11	15	0.76
(1,1057)	1:68:A:ARG:H	1:14:A:LEU:HD12	15	0.76
(1,1057)	1:68:A:ARG:H	1:14:A:LEU:HD13	15	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1057)	1:68:A:ARG:H	1:14:A:LEU:HD21	15	0.76
(1,1057)	1:68:A:ARG:H	1:14:A:LEU:HD22	15	0.76
(1,1057)	1:68:A:ARG:H	1:14:A:LEU:HD23	15	0.76
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	8	0.76
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	8	0.76
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	15	0.75
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	15	0.75
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	15	0.75
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	15	0.75
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	15	0.75
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	15	0.75
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	5	0.75
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	5	0.75
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	5	0.75
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	5	0.75
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	5	0.75
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	5	0.75
(1,652)	1:79:A:ASN:H	1:78:A:LYS:HD3	14	0.75
(1,639)	1:166:A:ARG:HD2	1:167:A:ASP:H	10	0.75
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	4	0.75
(1,7)	1:45:A:LEU:HB2	1:88:A:CYS:H	15	0.75
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD21	3	0.74
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD22	3	0.74
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD23	3	0.74
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD11	3	0.74
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD12	3	0.74
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD13	3	0.74
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	5	0.74
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	5	0.74
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	5	0.74
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	5	0.74
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	5	0.74
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	5	0.74
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	13	0.74
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	13	0.74
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	13	0.74
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	13	0.74
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	13	0.74
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	13	0.74
(1,1035)	1:9:A:ASN:H	1:8:A:LYS:HG3	15	0.74
(1,619)	1:27:A:ASN:H	1:28:A:GLU:HG3	1	0.74
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	13	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	13	0.73
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	13	0.73
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	13	0.73
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	13	0.73
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	13	0.73
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	7	0.73
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	7	0.73
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	7	0.73
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	7	0.73
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	7	0.73
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	7	0.73
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG21	4	0.73
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG22	4	0.73
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG23	4	0.73
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG11	4	0.73
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG12	4	0.73
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG13	4	0.73
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	10	0.73
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	10	0.73
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	10	0.73
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	10	0.73
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	10	0.73
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	10	0.73
(1,936)	1:140:A:SER:H	1:139:A:LYS:HE3	10	0.73
(1,670)	1:40:A:ASN:H	1:39:A:LYS:HE3	11	0.73
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	2	0.72
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	2	0.72
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	2	0.72
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	2	0.72
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	2	0.72
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	2	0.72
(1,1089)	1:85:A:SER:HB2	1:50:A:LEU:H	10	0.72
(1,612)	1:5:A:GLU:HG2	1:5:A:GLU:H	1	0.72
(1,618)	1:28:A:GLU:HG2	1:27:A:ASN:H	1	0.71
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	6	0.7
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	6	0.7
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	6	0.7
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	6	0.7
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	6	0.7
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	6	0.7
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	1	0.7
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	1	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	1	0.7
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	1	0.7
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	1	0.7
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	1	0.7
(1,945)	1:140:A:SER:H	1:139:A:LYS:HD3	15	0.7
(1,612)	1:5:A:GLU:HG2	1:5:A:GLU:H	12	0.7
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	8	0.69
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	8	0.69
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	8	0.69
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	8	0.69
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	8	0.69
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	8	0.69
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	8	0.69
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	8	0.69
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	8	0.69
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	8	0.69
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	8	0.69
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	8	0.69
(1,1089)	1:85:A:SER:HB2	1:50:A:LEU:H	9	0.69
(1,557)	1:54:A:ILE:HG12	1:55:A:VAL:H	2	0.69
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	11	0.68
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	11	0.68
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	11	0.68
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	11	0.68
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	11	0.68
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	11	0.68
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD11	13	0.68
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD12	13	0.68
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD13	13	0.68
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD21	13	0.68
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD22	13	0.68
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD23	13	0.68
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	9	0.68
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	9	0.68
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	9	0.68
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	9	0.68
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	9	0.68
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	9	0.68
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	15	0.68
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	15	0.68
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	15	0.68
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	15	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	15	0.68
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	15	0.68
(1,987)	1:112:A:GLU:HG2	1:112:A:GLU:H	3	0.68
(1,974)	1:71:A:ARG:HD2	1:72:A:THR:H	2	0.68
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	2	0.67
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	2	0.67
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	2	0.67
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	2	0.67
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	2	0.67
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	2	0.67
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	9	0.67
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	9	0.67
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	9	0.67
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	9	0.67
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	9	0.67
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	9	0.67
(1,987)	1:112:A:GLU:HG2	1:112:A:GLU:H	6	0.67
(1,987)	1:112:A:GLU:HG2	1:112:A:GLU:H	11	0.67
(1,987)	1:112:A:GLU:HG2	1:112:A:GLU:H	13	0.67
(1,731)	1:73:A:ALA:H	1:66:A:GLU:HB3	2	0.67
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	2	0.66
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	2	0.66
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	2	0.66
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	2	0.66
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	2	0.66
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	2	0.66
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	1	0.66
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	1	0.66
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	1	0.66
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	1	0.66
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	1	0.66
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	1	0.66
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	11	0.66
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	11	0.66
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	11	0.66
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	11	0.66
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	11	0.66
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	11	0.66
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG11	4	0.66
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG12	4	0.66
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG13	4	0.66
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG21	4	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG22	4	0.66
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG23	4	0.66
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	3	0.66
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	3	0.66
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	3	0.66
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	3	0.66
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	3	0.66
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	3	0.66
(1,1089)	1:85:A:SER:HB2	1:50:A:LEU:H	6	0.66
(1,1039)	1:9:A:ASN:H	1:8:A:LYS:HE3	12	0.66
(1,834)	1:43:A:TYR:HB2	1:42:A:ASN:H	3	0.66
(1,706)	1:168:A:ILE:HG12	1:169:A:TYR:H	5	0.66
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	1	0.66
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	4	0.65
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	4	0.65
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	4	0.65
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	4	0.65
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	4	0.65
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	4	0.65
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	3	0.65
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	3	0.65
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	3	0.65
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	3	0.65
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	3	0.65
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	3	0.65
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	1	0.65
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	1	0.65
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	1	0.65
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	1	0.65
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	1	0.65
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	1	0.65
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	10	0.65
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	10	0.65
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	10	0.65
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	10	0.65
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	10	0.65
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	10	0.65
(1,987)	1:112:A:GLU:HG2	1:112:A:GLU:H	1	0.65
(1,731)	1:73:A:ALA:H	1:66:A:GLU:HB3	6	0.65
(1,638)	1:167:A:ASP:H	1:166:A:ARG:HD3	15	0.65
(1,519)	1:23:A:ARG:HD2	1:23:A:ARG:H	1	0.65
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG21	15	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG22	15	0.64
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG23	15	0.64
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG11	15	0.64
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG12	15	0.64
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG13	15	0.64
(1,987)	1:112:A:GLU:HG2	1:112:A:GLU:H	8	0.64
(1,987)	1:112:A:GLU:HG2	1:112:A:GLU:H	10	0.64
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	13	0.63
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	13	0.63
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	13	0.63
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	13	0.63
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	13	0.63
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	13	0.63
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	4	0.63
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	4	0.63
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	4	0.63
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	4	0.63
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	4	0.63
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	4	0.63
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD11	6	0.63
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD12	6	0.63
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD13	6	0.63
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD21	6	0.63
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD22	6	0.63
(1,1170)	1:111:A:ASN:H	1:108:A:LEU:HD23	6	0.63
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	2	0.63
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	2	0.63
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	2	0.63
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	2	0.63
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	2	0.63
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	2	0.63
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD11	13	0.63
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD12	13	0.63
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD13	13	0.63
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD21	13	0.63
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD22	13	0.63
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD23	13	0.63
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	3	0.63
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	3	0.63
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	3	0.63
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	3	0.63
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	3	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	3	0.63
(1,855)	1:115:A:VAL:H	1:101:A:ARG:HG3	9	0.63
(1,705)	1:169:A:TYR:H	1:168:A:ILE:HG13	3	0.63
(1,557)	1:54:A:ILE:HG12	1:55:A:VAL:H	13	0.63
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	6	0.62
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	6	0.62
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	6	0.62
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	6	0.62
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	6	0.62
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	6	0.62
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	12	0.62
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	12	0.62
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	12	0.62
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	12	0.62
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	12	0.62
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	12	0.62
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	13	0.62
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	13	0.62
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	13	0.62
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	13	0.62
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	13	0.62
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	13	0.62
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD11	15	0.62
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD12	15	0.62
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD13	15	0.62
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD21	15	0.62
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD22	15	0.62
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD23	15	0.62
(1,1035)	1:9:A:ASN:H	1:8:A:LYS:HG3	14	0.62
(1,890)	1:145:A:SER:H	1:139:A:LYS:HG3	14	0.62
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	13	0.62
(1,639)	1:166:A:ARG:HD2	1:167:A:ASP:H	12	0.62
(1,557)	1:54:A:ILE:HG12	1:55:A:VAL:H	15	0.62
(1,519)	1:23:A:ARG:HD2	1:23:A:ARG:H	3	0.62
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	15	0.61
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	15	0.61
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	15	0.61
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	15	0.61
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	15	0.61
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	15	0.61
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG11	15	0.61
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG12	15	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG13	15	0.61
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG21	15	0.61
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG22	15	0.61
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG23	15	0.61
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	6	0.61
(1,705)	1:169:A:TYR:H	1:168:A:ILE:HG13	5	0.61
(1,670)	1:40:A:ASN:H	1:39:A:LYS:HE3	13	0.61
(1,558)	1:55:A:VAL:H	1:54:A:ILE:HG13	10	0.61
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	9	0.6
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	9	0.6
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	9	0.6
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	9	0.6
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	9	0.6
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	9	0.6
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	14	0.6
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	14	0.6
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	14	0.6
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	14	0.6
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	14	0.6
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	14	0.6
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	9	0.6
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	9	0.6
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	9	0.6
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	9	0.6
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	9	0.6
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	9	0.6
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	14	0.6
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	14	0.6
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	14	0.6
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	14	0.6
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	14	0.6
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	14	0.6
(1,1035)	1:9:A:ASN:H	1:8:A:LYS:HG3	5	0.6
(1,833)	1:42:A:ASN:H	1:43:A:TYR:HB3	11	0.6
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	10	0.6
(1,558)	1:55:A:VAL:H	1:54:A:ILE:HG13	7	0.6
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	3	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	3	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	3	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	3	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	3	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	3	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	7	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	7	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	7	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	7	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	7	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	7	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	11	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	11	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	11	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	11	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	11	0.59
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	11	0.59
(1,1088)	1:50:A:LEU:H	1:85:A:SER:HB3	14	0.59
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	7	0.59
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	7	0.59
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	7	0.59
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	7	0.59
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	7	0.59
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	7	0.59
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	14	0.59
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	14	0.59
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	14	0.59
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	14	0.59
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	14	0.59
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	14	0.59
(1,975)	1:72:A:THR:H	1:71:A:ARG:HD3	11	0.59
(1,945)	1:140:A:SER:H	1:139:A:LYS:HD3	9	0.59
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	5	0.58
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	5	0.58
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	5	0.58
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	5	0.58
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	5	0.58
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	5	0.58
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	14	0.58
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	14	0.58
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	14	0.58
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	14	0.58
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	14	0.58
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	14	0.58
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	6	0.58
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	6	0.58
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	6	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	6	0.58
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	6	0.58
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	6	0.58
(1,975)	1:72:A:THR:H	1:71:A:ARG:HD3	5	0.58
(1,834)	1:43:A:TYR:HB2	1:42:A:ASN:H	2	0.58
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	5	0.58
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	8	0.57
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	8	0.57
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	8	0.57
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	8	0.57
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	8	0.57
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	8	0.57
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	6	0.57
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	6	0.57
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	6	0.57
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	6	0.57
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	6	0.57
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	6	0.57
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	11	0.57
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	11	0.57
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	11	0.57
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	11	0.57
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	11	0.57
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	11	0.57
(1,833)	1:42:A:ASN:H	1:43:A:TYR:HB3	9	0.57
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	5	0.57
(1,612)	1:5:A:GLU:HG2	1:5:A:GLU:H	15	0.57
(1,558)	1:55:A:VAL:H	1:54:A:ILE:HG13	2	0.57
(1,558)	1:55:A:VAL:H	1:54:A:ILE:HG13	15	0.57
(1,557)	1:54:A:ILE:HG12	1:55:A:VAL:H	4	0.57
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	4	0.56
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	4	0.56
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	4	0.56
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	4	0.56
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	4	0.56
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	4	0.56
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	7	0.56
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	7	0.56
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	7	0.56
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	7	0.56
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	7	0.56
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	7	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG11	6	0.56
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG12	6	0.56
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG13	6	0.56
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG21	6	0.56
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG22	6	0.56
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG23	6	0.56
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	9	0.56
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	9	0.56
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	9	0.56
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	9	0.56
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	9	0.56
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	9	0.56
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	12	0.56
(1,968)	1:69:A:SER:H	1:68:A:ARG:HD3	4	0.56
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	7	0.56
(1,621)	1:27:A:ASN:H	1:26:A:GLU:HB3	6	0.56
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	5	0.56
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	14	0.55
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	14	0.55
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	14	0.55
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	14	0.55
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	14	0.55
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	14	0.55
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG11	7	0.55
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG12	7	0.55
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG13	7	0.55
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG21	7	0.55
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG22	7	0.55
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG23	7	0.55
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	6	0.55
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	6	0.55
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	6	0.55
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	6	0.55
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	6	0.55
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	6	0.55
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG21	3	0.55
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG22	3	0.55
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG23	3	0.55
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG11	3	0.55
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG12	3	0.55
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG13	3	0.55
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD21	1	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD22	1	0.55
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD23	1	0.55
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD11	1	0.55
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD12	1	0.55
(1,1090)	1:50:A:LEU:H	1:86:A:LEU:HD13	1	0.55
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD11	1	0.55
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD12	1	0.55
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD13	1	0.55
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD21	1	0.55
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD22	1	0.55
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD23	1	0.55
(1,890)	1:145:A:SER:H	1:139:A:LYS:HG3	13	0.55
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	14	0.55
(1,670)	1:40:A:ASN:H	1:39:A:LYS:HE3	3	0.55
(1,670)	1:40:A:ASN:H	1:39:A:LYS:HE3	6	0.55
(1,621)	1:27:A:ASN:H	1:26:A:GLU:HB3	3	0.55
(1,621)	1:27:A:ASN:H	1:26:A:GLU:HB3	9	0.55
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	8	0.55
(1,618)	1:28:A:GLU:HG2	1:27:A:ASN:H	13	0.55
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	11	0.54
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	11	0.54
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	11	0.54
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	11	0.54
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	11	0.54
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	11	0.54
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	5	0.54
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	5	0.54
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	5	0.54
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	5	0.54
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	5	0.54
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	5	0.54
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	1	0.54
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	1	0.54
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	1	0.54
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	1	0.54
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	1	0.54
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	1	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	11	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	11	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	11	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	11	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	11	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	11	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	12	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	12	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	12	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	12	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	12	0.54
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	12	0.54
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	14	0.54
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	15	0.54
(1,558)	1:55:A:VAL:H	1:54:A:ILE:HG13	13	0.54
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD21	13	0.53
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD22	13	0.53
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD23	13	0.53
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD11	13	0.53
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD12	13	0.53
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD13	13	0.53
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG21	13	0.53
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG22	13	0.53
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG23	13	0.53
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG11	13	0.53
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG12	13	0.53
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG13	13	0.53
(1,1089)	1:85:A:SER:HB2	1:50:A:LEU:H	7	0.53
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD11	14	0.53
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD12	14	0.53
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD13	14	0.53
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD21	14	0.53
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD22	14	0.53
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD23	14	0.53
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	14	0.53
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	14	0.53
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	14	0.53
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	14	0.53
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	14	0.53
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	14	0.53
(1,1040)	1:8:A:LYS:HE2	1:9:A:ASN:H	9	0.53
(1,1040)	1:8:A:LYS:HE2	1:9:A:ASN:H	11	0.53
(1,557)	1:54:A:ILE:HG12	1:55:A:VAL:H	1	0.53
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	3	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	3	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	3	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	3	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	3	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	3	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	11	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	11	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	11	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	11	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	11	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	11	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	13	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	13	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	13	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	13	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	13	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	13	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	14	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	14	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	14	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	14	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	14	0.52
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	14	0.52
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	14	0.52
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	14	0.52
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	14	0.52
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	14	0.52
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	14	0.52
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	14	0.52
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	5	0.52
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	5	0.52
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	5	0.52
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	5	0.52
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	5	0.52
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	5	0.52
(1,968)	1:69:A:SER:H	1:68:A:ARG:HD3	15	0.52
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	12	0.51
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	12	0.51
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	12	0.51
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	12	0.51
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	12	0.51
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	12	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	6	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	6	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	6	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	6	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	6	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	7	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	7	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	7	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	7	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	7	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	7	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	8	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	8	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	8	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	8	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	8	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	8	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	12	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	12	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	12	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	12	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	12	0.51
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	12	0.51
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG11	14	0.51
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG12	14	0.51
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG13	14	0.51
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG21	14	0.51
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG22	14	0.51
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG23	14	0.51
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	5	0.51
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	5	0.51
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	5	0.51
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	5	0.51
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	5	0.51
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	5	0.51
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG21	2	0.51
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG22	2	0.51
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG23	2	0.51
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG11	2	0.51
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG12	2	0.51
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG13	2	0.51
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	11	0.51
(1,884)	1:139:A:LYS:HE2	1:145:A:SER:H	14	0.51
(1,621)	1:27:A:ASN:H	1:26:A:GLU:HB3	14	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,613)	1:5:A:GLU:H	1:5:A:GLU:HG3	14	0.51
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	14	0.5
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	14	0.5
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	14	0.5
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	14	0.5
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	14	0.5
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	14	0.5
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD21	6	0.5
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD22	6	0.5
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD23	6	0.5
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD11	6	0.5
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD12	6	0.5
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD13	6	0.5
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	1	0.5
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	1	0.5
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	1	0.5
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	1	0.5
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	1	0.5
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	1	0.5
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	3	0.5
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	3	0.5
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	3	0.5
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	3	0.5
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	3	0.5
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	3	0.5
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	11	0.5
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	11	0.5
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	11	0.5
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	11	0.5
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	11	0.5
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	11	0.5
(1,1039)	1:9:A:ASN:H	1:8:A:LYS:HE3	9	0.5
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	8	0.5
(1,638)	1:167:A:ASP:H	1:166:A:ARG:HD3	7	0.5
(1,558)	1:55:A:VAL:H	1:54:A:ILE:HG13	4	0.5
(1,557)	1:54:A:ILE:HG12	1:55:A:VAL:H	14	0.5
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	6	0.49
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	6	0.49
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	6	0.49
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	6	0.49
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	6	0.49
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	4	0.49
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	4	0.49
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	4	0.49
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	4	0.49
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	4	0.49
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	4	0.49
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	9	0.49
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	9	0.49
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	9	0.49
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	9	0.49
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	9	0.49
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	9	0.49
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	12	0.49
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	12	0.49
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	12	0.49
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	12	0.49
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	12	0.49
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	12	0.49
(1,975)	1:72:A:THR:H	1:71:A:ARG:HD3	14	0.49
(1,974)	1:71:A:ARG:HD2	1:72:A:THR:H	12	0.49
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	1	0.48
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	9	0.48
(1,730)	1:66:A:GLU:HB2	1:73:A:ALA:H	12	0.48
(1,612)	1:5:A:GLU:HG2	1:5:A:GLU:H	11	0.48
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG11	14	0.47
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG12	14	0.47
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG13	14	0.47
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG21	14	0.47
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG22	14	0.47
(1,1141)	1:79:A:ASN:H	1:110:A:VAL:HG23	14	0.47
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG11	3	0.47
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG12	3	0.47
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG13	3	0.47
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG21	3	0.47
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG22	3	0.47
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG23	3	0.47
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG11	11	0.47
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG12	11	0.47
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG13	11	0.47
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG21	11	0.47
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG22	11	0.47
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG23	11	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	7	0.47
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	7	0.47
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	7	0.47
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	7	0.47
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	7	0.47
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	7	0.47
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG11	11	0.47
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG12	11	0.47
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG13	11	0.47
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG21	11	0.47
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG22	11	0.47
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG23	11	0.47
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	3	0.47
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	4	0.47
(1,936)	1:140:A:SER:H	1:139:A:LYS:HE3	15	0.47
(1,856)	1:101:A:ARG:HG2	1:115:A:VAL:H	1	0.47
(1,856)	1:101:A:ARG:HG2	1:115:A:VAL:H	2	0.47
(1,621)	1:27:A:ASN:H	1:26:A:GLU:HB3	13	0.47
(1,38)	1:145:A:SER:HB2	1:146:A:TYR:H	6	0.47
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD11	3	0.46
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD12	3	0.46
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD13	3	0.46
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD21	3	0.46
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD22	3	0.46
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD23	3	0.46
(1,1089)	1:85:A:SER:HB2	1:50:A:LEU:H	14	0.46
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	13	0.46
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	13	0.46
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	13	0.46
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	13	0.46
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	13	0.46
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	13	0.46
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD21	13	0.46
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD22	13	0.46
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD23	13	0.46
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD11	13	0.46
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD12	13	0.46
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD13	13	0.46
(1,834)	1:43:A:TYR:HB2	1:42:A:ASN:H	4	0.46
(1,805)	1:17:A:ASN:H	1:16:A:SER:HB3	5	0.46
(1,805)	1:17:A:ASN:H	1:16:A:SER:HB3	10	0.46
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:78:A:LYS:HE2	1:79:A:ASN:H	14	0.46
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	11	0.45
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	11	0.45
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	11	0.45
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	11	0.45
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	11	0.45
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	11	0.45
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	10	0.45
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	10	0.45
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	10	0.45
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	10	0.45
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	10	0.45
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	10	0.45
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	7	0.45
(1,887)	1:145:A:SER:HB2	1:145:A:SER:H	7	0.45
(1,887)	1:145:A:SER:HB2	1:145:A:SER:H	11	0.45
(1,887)	1:145:A:SER:HB2	1:145:A:SER:H	15	0.45
(1,884)	1:139:A:LYS:HE2	1:145:A:SER:H	5	0.45
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	11	0.45
(1,672)	1:40:A:ASN:H	1:39:A:LYS:HG3	5	0.45
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG21	9	0.44
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG22	9	0.44
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG23	9	0.44
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG11	9	0.44
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG12	9	0.44
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG13	9	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD11	4	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD12	4	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD13	4	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD21	4	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD22	4	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD23	4	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD11	6	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD12	6	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD13	6	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD21	6	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD22	6	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD23	6	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD11	8	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD12	8	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD13	8	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD21	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD22	8	0.44
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD23	8	0.44
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	8	0.44
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	8	0.44
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	8	0.44
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	8	0.44
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	8	0.44
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	8	0.44
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	1	0.44
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	1	0.44
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	1	0.44
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	1	0.44
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	1	0.44
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	1	0.44
(1,1040)	1:8:A:LYS:HE2	1:9:A:ASN:H	12	0.44
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	6	0.44
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	13	0.44
(1,618)	1:28:A:GLU:HG2	1:27:A:ASN:H	12	0.44
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD21	8	0.43
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD22	8	0.43
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD23	8	0.43
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD11	8	0.43
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD12	8	0.43
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD13	8	0.43
(1,1089)	1:85:A:SER:HB2	1:50:A:LEU:H	2	0.43
(1,974)	1:71:A:ARG:HD2	1:72:A:THR:H	11	0.43
(1,967)	1:68:A:ARG:HD2	1:69:A:SER:H	6	0.43
(1,944)	1:139:A:LYS:HD2	1:140:A:SER:H	4	0.43
(1,660)	1:79:A:ASN:H	1:78:A:LYS:HE3	4	0.43
(1,613)	1:5:A:GLU:H	1:5:A:GLU:HG3	6	0.43
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	7	0.42
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	7	0.42
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	7	0.42
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	7	0.42
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	7	0.42
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	7	0.42
(1,1089)	1:85:A:SER:HB2	1:50:A:LEU:H	15	0.42
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD11	1	0.42
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD12	1	0.42
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD13	1	0.42
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD21	1	0.42
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD22	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD23	1	0.42
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	5	0.42
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	5	0.42
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	5	0.42
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	5	0.42
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	5	0.42
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	5	0.42
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	10	0.42
(1,884)	1:139:A:LYS:HE2	1:145:A:SER:H	2	0.42
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	1	0.42
(1,638)	1:167:A:ASP:H	1:166:A:ARG:HD3	4	0.42
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	1	0.41
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	1	0.41
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	1	0.41
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	1	0.41
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	1	0.41
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	1	0.41
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG21	10	0.41
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG22	10	0.41
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG23	10	0.41
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG11	10	0.41
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG12	10	0.41
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG13	10	0.41
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG11	10	0.41
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG12	10	0.41
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG13	10	0.41
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG21	10	0.41
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG22	10	0.41
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG23	10	0.41
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG21	7	0.41
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG22	7	0.41
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG23	7	0.41
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG11	7	0.41
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG12	7	0.41
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG13	7	0.41
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD11	15	0.41
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD12	15	0.41
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD13	15	0.41
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD21	15	0.41
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD22	15	0.41
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD23	15	0.41
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD11	12	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD12	12	0.41
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD13	12	0.41
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD21	12	0.41
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD22	12	0.41
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD23	12	0.41
(1,884)	1:139:A:LYS:HE2	1:145:A:SER:H	6	0.41
(1,731)	1:73:A:ALA:H	1:66:A:GLU:HB3	4	0.41
(1,639)	1:166:A:ARG:HD2	1:167:A:ASP:H	11	0.41
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	10	0.41
(1,618)	1:28:A:GLU:HG2	1:27:A:ASN:H	4	0.41
(1,38)	1:145:A:SER:HB2	1:146:A:TYR:H	3	0.41
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	10	0.4
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	10	0.4
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	10	0.4
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	10	0.4
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	10	0.4
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	10	0.4
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD11	14	0.4
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD12	14	0.4
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD13	14	0.4
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD21	14	0.4
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD22	14	0.4
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD23	14	0.4
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD11	4	0.4
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD12	4	0.4
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD13	4	0.4
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD21	4	0.4
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD22	4	0.4
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD23	4	0.4
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	13	0.4
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	13	0.4
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	13	0.4
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	13	0.4
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	13	0.4
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	13	0.4
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	2	0.4
(1,968)	1:69:A:SER:H	1:68:A:ARG:HD3	8	0.4
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	6	0.4
(1,615)	1:5:A:GLU:H	1:4:A:MET:HG3	15	0.4
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	10	0.39
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	10	0.39
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	10	0.39
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	10	0.39
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	10	0.39
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	1	0.39
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	1	0.39
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	1	0.39
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	1	0.39
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	1	0.39
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	1	0.39
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG21	11	0.39
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG22	11	0.39
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG23	11	0.39
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG11	11	0.39
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG12	11	0.39
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG13	11	0.39
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	5	0.39
(1,887)	1:145:A:SER:HB2	1:145:A:SER:H	12	0.39
(1,621)	1:27:A:ASN:H	1:26:A:GLU:HB3	5	0.39
(1,38)	1:145:A:SER:HB2	1:146:A:TYR:H	5	0.39
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG11	12	0.38
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG12	12	0.38
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG13	12	0.38
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG21	12	0.38
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG22	12	0.38
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG23	12	0.38
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	10	0.38
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	10	0.38
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	10	0.38
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	10	0.38
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	10	0.38
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	10	0.38
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	6	0.38
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	6	0.38
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	6	0.38
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	6	0.38
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	6	0.38
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	6	0.38
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	9	0.38
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	9	0.38
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	9	0.38
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	9	0.38
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	9	0.38
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD11	13	0.38
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD12	13	0.38
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD13	13	0.38
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD21	13	0.38
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD22	13	0.38
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD23	13	0.38
(1,855)	1:115:A:VAL:H	1:101:A:ARG:HG3	4	0.38
(1,660)	1:79:A:ASN:H	1:78:A:LYS:HE3	5	0.38
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	6	0.38
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	9	0.38
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	2	0.37
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	2	0.37
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	2	0.37
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	2	0.37
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	2	0.37
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	2	0.37
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD21	12	0.37
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD22	12	0.37
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD23	12	0.37
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD11	12	0.37
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD12	12	0.37
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD13	12	0.37
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG11	1	0.37
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG12	1	0.37
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG13	1	0.37
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG21	1	0.37
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG22	1	0.37
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG23	1	0.37
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD21	2	0.37
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD22	2	0.37
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD23	2	0.37
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD11	2	0.37
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD12	2	0.37
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD13	2	0.37
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG11	4	0.37
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG12	4	0.37
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG13	4	0.37
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG21	4	0.37
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG22	4	0.37
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG23	4	0.37
(1,968)	1:69:A:SER:H	1:68:A:ARG:HD3	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,886)	1:145:A:SER:H	1:145:A:SER:HB3	13	0.37
(1,673)	1:39:A:LYS:HG2	1:40:A:ASN:H	11	0.37
(1,639)	1:166:A:ARG:HD2	1:167:A:ASP:H	13	0.37
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	9	0.37
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	14	0.37
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	14	0.37
(1,1089)	1:85:A:SER:HB2	1:50:A:LEU:H	12	0.36
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	9	0.36
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	9	0.36
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	9	0.36
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	9	0.36
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	9	0.36
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	9	0.36
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	7	0.36
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG11	7	0.35
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG12	7	0.35
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG13	7	0.35
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG21	7	0.35
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG22	7	0.35
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG23	7	0.35
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	2	0.35
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	2	0.35
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	2	0.35
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	2	0.35
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	2	0.35
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	2	0.35
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD11	2	0.35
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD12	2	0.35
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD13	2	0.35
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD21	2	0.35
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD22	2	0.35
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD23	2	0.35
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	3	0.35
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	3	0.35
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	3	0.35
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	3	0.35
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	3	0.35
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	3	0.35
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	7	0.35
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	7	0.35
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	7	0.35
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	7	0.35
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	7	0.35
(1,671)	1:39:A:LYS:HE2	1:40:A:ASN:H	4	0.35
(1,660)	1:79:A:ASN:H	1:78:A:LYS:HE3	9	0.35
(1,619)	1:27:A:ASN:H	1:28:A:GLU:HG3	14	0.35
(1,612)	1:5:A:GLU:HG2	1:5:A:GLU:H	6	0.35
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	11	0.35
(1,37)	1:146:A:TYR:H	1:145:A:SER:HB3	9	0.35
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	15	0.34
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	15	0.34
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	15	0.34
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	15	0.34
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	15	0.34
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	15	0.34
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD21	7	0.34
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD22	7	0.34
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD23	7	0.34
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD11	7	0.34
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD12	7	0.34
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD13	7	0.34
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	3	0.34
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	3	0.34
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	3	0.34
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	3	0.34
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	3	0.34
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	3	0.34
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	5	0.34
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	5	0.34
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	5	0.34
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	5	0.34
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	5	0.34
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	5	0.34
(1,1039)	1:9:A:ASN:H	1:8:A:LYS:HE3	4	0.34
(1,1035)	1:9:A:ASN:H	1:8:A:LYS:HG3	6	0.34
(1,974)	1:71:A:ARG:HD2	1:72:A:THR:H	3	0.34
(1,890)	1:145:A:SER:H	1:139:A:LYS:HG3	2	0.34
(1,890)	1:145:A:SER:H	1:139:A:LYS:HG3	3	0.34
(1,671)	1:39:A:LYS:HE2	1:40:A:ASN:H	14	0.34
(1,660)	1:79:A:ASN:H	1:78:A:LYS:HE3	2	0.34
(1,660)	1:79:A:ASN:H	1:78:A:LYS:HE3	3	0.34
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	8	0.34
(1,38)	1:145:A:SER:HB2	1:146:A:TYR:H	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	5	0.33
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD11	6	0.33
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD12	6	0.33
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD13	6	0.33
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD21	6	0.33
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD22	6	0.33
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD23	6	0.33
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD21	6	0.33
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD22	6	0.33
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD23	6	0.33
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD11	6	0.33
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD12	6	0.33
(1,1062)	1:19:A:ARG:H	1:61:A:LEU:HD13	6	0.33
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG11	3	0.33
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG12	3	0.33
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG13	3	0.33
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG21	3	0.33
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG22	3	0.33
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG23	3	0.33
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG11	5	0.33
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG12	5	0.33
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG13	5	0.33
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG21	5	0.33
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG22	5	0.33
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG23	5	0.33
(1,1036)	1:8:A:LYS:HG2	1:9:A:ASN:H	8	0.33
(1,974)	1:71:A:ARG:HD2	1:72:A:THR:H	8	0.33
(1,968)	1:69:A:SER:H	1:68:A:ARG:HD3	1	0.33
(1,936)	1:140:A:SER:H	1:139:A:LYS:HE3	4	0.33
(1,670)	1:40:A:ASN:H	1:39:A:LYS:HE3	12	0.33
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	3	0.33
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	13	0.33
(1,618)	1:28:A:GLU:HG2	1:27:A:ASN:H	8	0.33
(1,618)	1:28:A:GLU:HG2	1:27:A:ASN:H	11	0.33
(1,612)	1:5:A:GLU:HG2	1:5:A:GLU:H	13	0.33
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	2	0.33
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	3	0.33
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	4	0.33
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	2	0.33
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	14	0.33
(1,1205)	1:138:A:ARG:H	1:136:A:VAL:HG21	10	0.32
(1,1205)	1:138:A:ARG:H	1:136:A:VAL:HG22	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1205)	1:138:A:ARG:H	1:136:A:VAL:HG23	10	0.32
(1,1205)	1:138:A:ARG:H	1:136:A:VAL:HG11	10	0.32
(1,1205)	1:138:A:ARG:H	1:136:A:VAL:HG12	10	0.32
(1,1205)	1:138:A:ARG:H	1:136:A:VAL:HG13	10	0.32
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG21	10	0.32
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG22	10	0.32
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG23	10	0.32
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG11	10	0.32
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG12	10	0.32
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG13	10	0.32
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD11	7	0.32
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD12	7	0.32
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD13	7	0.32
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD21	7	0.32
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD22	7	0.32
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD23	7	0.32
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	15	0.32
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	15	0.32
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	15	0.32
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	15	0.32
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	15	0.32
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	15	0.32
(1,988)	1:112:A:GLU:H	1:112:A:GLU:HG3	15	0.32
(1,936)	1:140:A:SER:H	1:139:A:LYS:HE3	8	0.32
(1,884)	1:139:A:LYS:HE2	1:145:A:SER:H	7	0.32
(1,673)	1:39:A:LYS:HG2	1:40:A:ASN:H	12	0.32
(1,621)	1:27:A:ASN:H	1:26:A:GLU:HB3	4	0.32
(1,557)	1:54:A:ILE:HG12	1:55:A:VAL:H	5	0.32
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	1	0.32
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	15	0.32
(1,37)	1:146:A:TYR:H	1:145:A:SER:HB3	6	0.32
(1,1454)	1:95:A:ARG:H	1:78:A:LYS:HD3	4	0.31
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	10	0.31
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	10	0.31
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	10	0.31
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	10	0.31
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	10	0.31
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	10	0.31
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG21	5	0.31
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG22	5	0.31
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG23	5	0.31
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG11	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG12	5	0.31
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG13	5	0.31
(1,795)	1:151:A:VAL:H	1:135:A:CYS:HB3	3	0.31
(1,731)	1:73:A:ALA:H	1:66:A:GLU:HB3	3	0.31
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	4	0.31
(1,38)	1:145:A:SER:HB2	1:146:A:TYR:H	13	0.31
(1,1454)	1:95:A:ARG:H	1:78:A:LYS:HD3	13	0.3
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG11	13	0.3
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG12	13	0.3
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG13	13	0.3
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG21	13	0.3
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG22	13	0.3
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG23	13	0.3
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD11	15	0.3
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD12	15	0.3
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD13	15	0.3
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD21	15	0.3
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD22	15	0.3
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD23	15	0.3
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG21	9	0.3
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG22	9	0.3
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG23	9	0.3
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG11	9	0.3
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG12	9	0.3
(1,1129)	1:113:A:ALA:H	1:76:A:VAL:HG13	9	0.3
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	13	0.3
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	13	0.3
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	13	0.3
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	13	0.3
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	13	0.3
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	13	0.3
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD11	2	0.3
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD12	2	0.3
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD13	2	0.3
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD21	2	0.3
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD22	2	0.3
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD23	2	0.3
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD11	8	0.3
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD12	8	0.3
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD13	8	0.3
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD21	8	0.3
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD22	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD23	8	0.3
(1,1039)	1:9:A:ASN:H	1:8:A:LYS:HE3	2	0.3
(1,884)	1:139:A:LYS:HE2	1:145:A:SER:H	4	0.3
(1,640)	1:167:A:ASP:H	1:167:A:ASP:HB3	3	0.3
(1,638)	1:167:A:ASP:H	1:166:A:ARG:HD3	1	0.3
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	11	0.3
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	13	0.3
(1,1454)	1:95:A:ARG:H	1:78:A:LYS:HD3	2	0.29
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD21	8	0.29
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD22	8	0.29
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD23	8	0.29
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD11	8	0.29
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD12	8	0.29
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD13	8	0.29
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG21	2	0.29
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG22	2	0.29
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG23	2	0.29
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG11	2	0.29
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG12	2	0.29
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG13	2	0.29
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG21	12	0.29
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG22	12	0.29
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG23	12	0.29
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG11	12	0.29
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG12	12	0.29
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG13	12	0.29
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD11	11	0.29
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD12	11	0.29
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD13	11	0.29
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD21	11	0.29
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD22	11	0.29
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD23	11	0.29
(1,967)	1:68:A:ARG:HD2	1:69:A:SER:H	12	0.29
(1,886)	1:145:A:SER:H	1:145:A:SER:HB3	1	0.29
(1,705)	1:169:A:TYR:H	1:168:A:ILE:HG13	2	0.29
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	12	0.29
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	9	0.29
(1,1454)	1:95:A:ARG:H	1:78:A:LYS:HD3	9	0.28
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG21	1	0.28
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG22	1	0.28
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG23	1	0.28
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG11	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG12	1	0.28
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG13	1	0.28
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	12	0.28
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	12	0.28
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	12	0.28
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	12	0.28
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	12	0.28
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	12	0.28
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG11	2	0.28
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG12	2	0.28
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG13	2	0.28
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG21	2	0.28
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG22	2	0.28
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG23	2	0.28
(1,938)	1:139:A:LYS:HB2	1:140:A:SER:H	10	0.28
(1,804)	1:16:A:SER:HB2	1:17:A:ASN:H	7	0.28
(1,639)	1:166:A:ARG:HD2	1:167:A:ASP:H	5	0.28
(1,618)	1:28:A:GLU:HG2	1:27:A:ASN:H	10	0.28
(1,612)	1:5:A:GLU:HG2	1:5:A:GLU:H	7	0.28
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	7	0.28
(1,509)	1:30:A:ARG:HB2	1:29:A:LEU:H	10	0.28
(1,37)	1:146:A:TYR:H	1:145:A:SER:HB3	12	0.28
(1,1453)	1:78:A:LYS:HD2	1:95:A:ARG:H	3	0.27
(1,1191)	1:120:A:ASP:H	1:118:A:LEU:HD11	1	0.27
(1,1191)	1:120:A:ASP:H	1:118:A:LEU:HD12	1	0.27
(1,1191)	1:120:A:ASP:H	1:118:A:LEU:HD13	1	0.27
(1,1191)	1:120:A:ASP:H	1:118:A:LEU:HD21	1	0.27
(1,1191)	1:120:A:ASP:H	1:118:A:LEU:HD22	1	0.27
(1,1191)	1:120:A:ASP:H	1:118:A:LEU:HD23	1	0.27
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG21	3	0.27
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG22	3	0.27
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG23	3	0.27
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG11	3	0.27
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG12	3	0.27
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG13	3	0.27
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	5	0.27
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	5	0.27
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	5	0.27
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	5	0.27
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	5	0.27
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	5	0.27
(1,1088)	1:50:A:LEU:H	1:85:A:SER:HB3	13	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD11	5	0.27
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD12	5	0.27
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD13	5	0.27
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD21	5	0.27
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD22	5	0.27
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD23	5	0.27
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD11	2	0.27
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD12	2	0.27
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD13	2	0.27
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD21	2	0.27
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD22	2	0.27
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD23	2	0.27
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD11	7	0.27
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD12	7	0.27
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD13	7	0.27
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD21	7	0.27
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD22	7	0.27
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD23	7	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG11	9	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG12	9	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG13	9	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG21	9	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG22	9	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG23	9	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG11	11	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG12	11	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG13	11	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG21	11	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG22	11	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG23	11	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG11	12	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG12	12	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG13	12	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG21	12	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG22	12	0.27
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG23	12	0.27
(1,978)	1:105:A:PHE:HA	1:104:A:ASP:H	4	0.27
(1,975)	1:72:A:THR:H	1:71:A:ARG:HD3	1	0.27
(1,973)	1:72:A:THR:H	1:71:A:ARG:HG3	13	0.27
(1,968)	1:69:A:SER:H	1:68:A:ARG:HD3	7	0.27
(1,621)	1:27:A:ASN:H	1:26:A:GLU:HB3	7	0.27
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,613)	1:5:A:GLU:H	1:5:A:GLU:HG3	12	0.27
(1,574)	1:139:A:LYS:H	1:139:A:LYS:HD3	1	0.27
(1,574)	1:139:A:LYS:H	1:139:A:LYS:HD2	1	0.27
(1,398)	1:160:A:GLU:HG2	1:161:A:TYR:H	3	0.27
(1,38)	1:145:A:SER:HB2	1:146:A:TYR:H	10	0.27
(1,1454)	1:95:A:ARG:H	1:78:A:LYS:HD3	6	0.26
(1,1454)	1:95:A:ARG:H	1:78:A:LYS:HD3	7	0.26
(1,1454)	1:95:A:ARG:H	1:78:A:LYS:HD3	12	0.26
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD21	5	0.26
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD22	5	0.26
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD23	5	0.26
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD11	5	0.26
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD12	5	0.26
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD13	5	0.26
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD21	4	0.26
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD22	4	0.26
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD23	4	0.26
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD11	4	0.26
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD12	4	0.26
(1,1151)	1:85:A:SER:H	1:86:A:LEU:HD13	4	0.26
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD11	2	0.26
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD12	2	0.26
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD13	2	0.26
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD21	2	0.26
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD22	2	0.26
(1,1142)	1:79:A:ASN:H	1:114:A:LEU:HD23	2	0.26
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG11	7	0.26
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG12	7	0.26
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG13	7	0.26
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG21	7	0.26
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG22	7	0.26
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG23	7	0.26
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	3	0.26
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	3	0.26
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	3	0.26
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	3	0.26
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	3	0.26
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	3	0.26
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	4	0.26
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	4	0.26
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	4	0.26
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	4	0.26
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	4	0.26
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	15	0.26
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	15	0.26
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	15	0.26
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	15	0.26
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	15	0.26
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	15	0.26
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD11	3	0.26
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD12	3	0.26
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD13	3	0.26
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD21	3	0.26
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD22	3	0.26
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD23	3	0.26
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG11	14	0.26
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG12	14	0.26
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG13	14	0.26
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG21	14	0.26
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG22	14	0.26
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG23	14	0.26
(1,973)	1:72:A:THR:H	1:71:A:ARG:HG3	1	0.26
(1,944)	1:139:A:LYS:HD2	1:140:A:SER:H	5	0.26
(1,884)	1:139:A:LYS:HE2	1:145:A:SER:H	3	0.26
(1,884)	1:139:A:LYS:HE2	1:145:A:SER:H	13	0.26
(1,804)	1:16:A:SER:HB2	1:17:A:ASN:H	8	0.26
(1,804)	1:16:A:SER:HB2	1:17:A:ASN:H	12	0.26
(1,621)	1:27:A:ASN:H	1:26:A:GLU:HB3	8	0.26
(1,488)	1:28:A:GLU:HG2	1:25:A:ASP:H	9	0.26
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD11	14	0.26
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD12	14	0.26
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD13	14	0.26
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	1	0.26
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	4	0.26
(1,1454)	1:95:A:ARG:H	1:78:A:LYS:HD3	14	0.25
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD21	7	0.25
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD22	7	0.25
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD23	7	0.25
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD11	7	0.25
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD12	7	0.25
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD13	7	0.25
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG11	2	0.25
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG12	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG13	2	0.25
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG21	2	0.25
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG22	2	0.25
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG23	2	0.25
(1,1197)	1:129:A:LYS:H	1:131:A:VAL:HG11	2	0.25
(1,1197)	1:129:A:LYS:H	1:131:A:VAL:HG12	2	0.25
(1,1197)	1:129:A:LYS:H	1:131:A:VAL:HG13	2	0.25
(1,1197)	1:129:A:LYS:H	1:131:A:VAL:HG21	2	0.25
(1,1197)	1:129:A:LYS:H	1:131:A:VAL:HG22	2	0.25
(1,1197)	1:129:A:LYS:H	1:131:A:VAL:HG23	2	0.25
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG21	8	0.25
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG22	8	0.25
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG23	8	0.25
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG11	8	0.25
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG12	8	0.25
(1,1091)	1:50:A:LEU:H	1:137:A:VAL:HG13	8	0.25
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD21	1	0.25
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD22	1	0.25
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD23	1	0.25
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD11	1	0.25
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD12	1	0.25
(1,1067)	1:21:A:ILE:H	1:24:A:LEU:HD13	1	0.25
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	7	0.25
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	7	0.25
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	7	0.25
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	7	0.25
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	7	0.25
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	7	0.25
(1,1039)	1:9:A:ASN:H	1:8:A:LYS:HE3	6	0.25
(1,743)	1:102:A:VAL:H	1:116:A:VAL:HB	1	0.25
(1,518)	1:23:A:ARG:H	1:23:A:ARG:HD3	1	0.25
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG11	14	0.24
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG12	14	0.24
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG13	14	0.24
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG21	14	0.24
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG22	14	0.24
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG23	14	0.24
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG11	10	0.24
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG12	10	0.24
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG13	10	0.24
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG21	10	0.24
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG22	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:151:A:VAL:H	1:136:A:VAL:HG23	10	0.24
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	15	0.24
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	15	0.24
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	15	0.24
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	15	0.24
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	15	0.24
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	15	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG11	8	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG12	8	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG13	8	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG21	8	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG22	8	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG23	8	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG11	12	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG12	12	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG13	12	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG21	12	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG22	12	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG23	12	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG11	14	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG12	14	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG13	14	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG21	14	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG22	14	0.24
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG23	14	0.24
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	5	0.24
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	5	0.24
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	5	0.24
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	5	0.24
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	5	0.24
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	5	0.24
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	9	0.24
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	9	0.24
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	9	0.24
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	9	0.24
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	9	0.24
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	9	0.24
(1,671)	1:39:A:LYS:HE2	1:40:A:ASN:H	7	0.24
(1,639)	1:166:A:ARG:HD2	1:167:A:ASP:H	6	0.24
(1,1445)	1:104:A:ASP:H	1:150:A:VAL:O	4	0.23
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG11	1	0.23
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG12	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG13	1	0.23
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG21	1	0.23
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG22	1	0.23
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG23	1	0.23
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG11	6	0.23
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG12	6	0.23
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG13	6	0.23
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG21	6	0.23
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG22	6	0.23
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG23	6	0.23
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG21	15	0.23
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG22	15	0.23
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG23	15	0.23
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG11	15	0.23
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG12	15	0.23
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG13	15	0.23
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD11	10	0.23
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD12	10	0.23
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD13	10	0.23
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD21	10	0.23
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD22	10	0.23
(1,1084)	1:47:A:ASP:H	1:45:A:LEU:HD23	10	0.23
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD11	1	0.23
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD12	1	0.23
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD13	1	0.23
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD21	1	0.23
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD22	1	0.23
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD23	1	0.23
(1,1035)	1:9:A:ASN:H	1:8:A:LYS:HG3	7	0.23
(1,975)	1:72:A:THR:H	1:71:A:ARG:HD3	6	0.23
(1,973)	1:72:A:THR:H	1:71:A:ARG:HG3	12	0.23
(1,972)	1:71:A:ARG:HG2	1:72:A:THR:H	6	0.23
(1,884)	1:139:A:LYS:HE2	1:145:A:SER:H	10	0.23
(1,804)	1:16:A:SER:HB2	1:17:A:ASN:H	6	0.23
(1,660)	1:79:A:ASN:H	1:78:A:LYS:HE3	1	0.23
(1,518)	1:23:A:ARG:H	1:23:A:ARG:HD3	3	0.23
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	7	0.23
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	8	0.23
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	13	0.23
(1,37)	1:146:A:TYR:H	1:145:A:SER:HB3	3	0.23
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG21	9	0.22
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG22	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG23	9	0.22
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG11	9	0.22
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG12	9	0.22
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG13	9	0.22
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	1	0.22
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	1	0.22
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	1	0.22
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	1	0.22
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	1	0.22
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	1	0.22
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD11	7	0.22
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD12	7	0.22
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD13	7	0.22
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD21	7	0.22
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD22	7	0.22
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD23	7	0.22
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG11	4	0.22
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG12	4	0.22
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG13	4	0.22
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG21	4	0.22
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG22	4	0.22
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG23	4	0.22
(1,1039)	1:9:A:ASN:H	1:8:A:LYS:HE3	14	0.22
(1,1039)	1:9:A:ASN:H	1:8:A:LYS:HE3	15	0.22
(1,1036)	1:8:A:LYS:HG2	1:9:A:ASN:H	3	0.22
(1,997)	1:108:A:LEU:HG	1:108:A:LEU:H	5	0.22
(1,705)	1:169:A:TYR:H	1:168:A:ILE:HG13	8	0.22
(1,670)	1:40:A:ASN:H	1:39:A:LYS:HE3	2	0.22
(1,613)	1:5:A:GLU:H	1:5:A:GLU:HG3	7	0.22
(1,574)	1:139:A:LYS:H	1:139:A:LYS:HD3	11	0.22
(1,574)	1:139:A:LYS:H	1:139:A:LYS:HD2	11	0.22
(1,558)	1:55:A:VAL:H	1:54:A:ILE:HG13	11	0.22
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	4	0.22
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	6	0.22
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	7	0.22
(1,251)	1:165:A:LEU:H	1:165:A:LEU:HG	5	0.22
(1,38)	1:145:A:SER:HB2	1:146:A:TYR:H	2	0.22
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD21	12	0.21
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD22	12	0.21
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD23	12	0.21
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD11	12	0.21
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD12	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD13	12	0.21
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD11	2	0.21
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD12	2	0.21
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD13	2	0.21
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD21	2	0.21
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD22	2	0.21
(1,1138)	1:78:A:LYS:H	1:114:A:LEU:HD23	2	0.21
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG21	1	0.21
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG22	1	0.21
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG23	1	0.21
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG11	1	0.21
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG12	1	0.21
(1,1125)	1:76:A:VAL:H	1:115:A:VAL:HG13	1	0.21
(1,1088)	1:50:A:LEU:H	1:85:A:SER:HB3	5	0.21
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD21	14	0.21
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD22	14	0.21
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD23	14	0.21
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD11	14	0.21
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD12	14	0.21
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD13	14	0.21
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD11	11	0.21
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD12	11	0.21
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD13	11	0.21
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD21	11	0.21
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD22	11	0.21
(1,1079)	1:47:A:ASP:H	1:29:A:LEU:HD23	11	0.21
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD11	3	0.21
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD12	3	0.21
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD13	3	0.21
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD21	3	0.21
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD22	3	0.21
(1,1054)	1:13:A:ASP:H	1:14:A:LEU:HD23	3	0.21
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG11	10	0.21
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG12	10	0.21
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG13	10	0.21
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG21	10	0.21
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG22	10	0.21
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG23	10	0.21
(1,972)	1:71:A:ARG:HG2	1:72:A:THR:H	9	0.21
(1,890)	1:145:A:SER:H	1:139:A:LYS:HG3	7	0.21
(1,884)	1:139:A:LYS:HE2	1:145:A:SER:H	15	0.21
(1,805)	1:17:A:ASN:H	1:16:A:SER:HB3	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,804)	1:16:A:SER:HB2	1:17:A:ASN:H	1	0.21
(1,620)	1:26:A:GLU:HB2	1:27:A:ASN:H	2	0.21
(1,613)	1:5:A:GLU:H	1:5:A:GLU:HG3	13	0.21
(1,558)	1:55:A:VAL:H	1:54:A:ILE:HG13	3	0.21
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	8	0.21
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	12	0.21
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	7	0.21
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	12	0.21
(1,37)	1:146:A:TYR:H	1:145:A:SER:HB3	2	0.21
(1,1454)	1:95:A:ARG:H	1:78:A:LYS:HD3	11	0.2
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD3	1	0.2
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD2	1	0.2
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD11	15	0.2
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD12	15	0.2
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD13	15	0.2
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD21	15	0.2
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD22	15	0.2
(1,1223)	1:168:A:ILE:H	1:165:A:LEU:HD23	15	0.2
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD21	8	0.2
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD22	8	0.2
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD23	8	0.2
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD11	8	0.2
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD12	8	0.2
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD13	8	0.2
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG11	3	0.2
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG12	3	0.2
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG13	3	0.2
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG21	3	0.2
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG22	3	0.2
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG23	3	0.2
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG21	10	0.2
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG22	10	0.2
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG23	10	0.2
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG11	10	0.2
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG12	10	0.2
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG13	10	0.2
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG21	13	0.2
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG22	13	0.2
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG23	13	0.2
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG11	13	0.2
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG12	13	0.2
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG13	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	6	0.2
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	6	0.2
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	6	0.2
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	6	0.2
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	6	0.2
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	6	0.2
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG11	8	0.2
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG12	8	0.2
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG13	8	0.2
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG21	8	0.2
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG22	8	0.2
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG23	8	0.2
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD11	11	0.2
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD12	11	0.2
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD13	11	0.2
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD21	11	0.2
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD22	11	0.2
(1,1093)	1:78:A:LYS:H	1:50:A:LEU:HD23	11	0.2
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	14	0.2
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	14	0.2
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	14	0.2
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	14	0.2
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	14	0.2
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	14	0.2
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD21	4	0.2
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD22	4	0.2
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD23	4	0.2
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD11	4	0.2
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD12	4	0.2
(1,1058)	1:15:A:ILE:H	1:45:A:LEU:HD13	4	0.2
(1,1039)	1:9:A:ASN:H	1:8:A:LYS:HE3	11	0.2
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	3	0.2
(1,975)	1:72:A:THR:H	1:71:A:ARG:HD3	7	0.2
(1,972)	1:71:A:ARG:HG2	1:72:A:THR:H	7	0.2
(1,890)	1:145:A:SER:H	1:139:A:LYS:HG3	6	0.2
(1,834)	1:43:A:TYR:HB2	1:42:A:ASN:H	1	0.2
(1,730)	1:66:A:GLU:HB2	1:73:A:ALA:H	11	0.2
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	1	0.2
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD11	2	0.2
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD12	2	0.2
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD13	2	0.2
(1,328)	1:71:A:ARG:H	1:72:A:THR:H	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	15	0.2
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD3	7	0.19
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD2	7	0.19
(1,1200)	1:135:A:CYS:H	1:136:A:VAL:HG11	4	0.19
(1,1200)	1:135:A:CYS:H	1:136:A:VAL:HG12	4	0.19
(1,1200)	1:135:A:CYS:H	1:136:A:VAL:HG13	4	0.19
(1,1200)	1:135:A:CYS:H	1:136:A:VAL:HG21	4	0.19
(1,1200)	1:135:A:CYS:H	1:136:A:VAL:HG22	4	0.19
(1,1200)	1:135:A:CYS:H	1:136:A:VAL:HG23	4	0.19
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	6	0.19
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	6	0.19
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	6	0.19
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	6	0.19
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	6	0.19
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	6	0.19
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG11	3	0.19
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG12	3	0.19
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG13	3	0.19
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG21	3	0.19
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG22	3	0.19
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG23	3	0.19
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD21	13	0.19
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD22	13	0.19
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD23	13	0.19
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD11	13	0.19
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD12	13	0.19
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD13	13	0.19
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD21	15	0.19
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD22	15	0.19
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD23	15	0.19
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD11	15	0.19
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD12	15	0.19
(1,1110)	1:65:A:TRP:H	1:61:A:LEU:HD13	15	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	3	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	3	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	3	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	3	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	3	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	3	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	6	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	6	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	6	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	6	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	6	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	8	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	8	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	8	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	8	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	8	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	8	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	13	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	13	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	13	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	13	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	13	0.19
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	13	0.19
(1,1070)	1:22:A:LEU:H	1:24:A:LEU:HD11	2	0.19
(1,1070)	1:22:A:LEU:H	1:24:A:LEU:HD12	2	0.19
(1,1070)	1:22:A:LEU:H	1:24:A:LEU:HD13	2	0.19
(1,1070)	1:22:A:LEU:H	1:24:A:LEU:HD21	2	0.19
(1,1070)	1:22:A:LEU:H	1:24:A:LEU:HD22	2	0.19
(1,1070)	1:22:A:LEU:H	1:24:A:LEU:HD23	2	0.19
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD11	6	0.19
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD12	6	0.19
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD13	6	0.19
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD21	6	0.19
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD22	6	0.19
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD23	6	0.19
(1,972)	1:71:A:ARG:HG2	1:72:A:THR:H	4	0.19
(1,890)	1:145:A:SER:H	1:139:A:LYS:HG3	9	0.19
(1,884)	1:139:A:LYS:HE2	1:145:A:SER:H	8	0.19
(1,613)	1:5:A:GLU:H	1:5:A:GLU:HG3	1	0.19
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	3	0.19
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	9	0.19
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	10	0.19
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	14	0.19
(1,397)	1:37:A:ILE:HD11	1:32:A:THR:H	10	0.19
(1,397)	1:37:A:ILE:HD12	1:32:A:THR:H	10	0.19
(1,397)	1:37:A:ILE:HD13	1:32:A:THR:H	10	0.19
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	4	0.19
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	11	0.19
(1,328)	1:71:A:ARG:H	1:72:A:THR:H	8	0.19
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:37:A:ILE:HD11	1:43:A:TYR:H	5	0.19
(1,297)	1:37:A:ILE:HD12	1:43:A:TYR:H	5	0.19
(1,297)	1:37:A:ILE:HD13	1:43:A:TYR:H	5	0.19
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD3	14	0.18
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD2	14	0.18
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	6	0.18
(1,1411)	1:30:A:ARG:H	1:49:A:MET:O	1	0.18
(1,1411)	1:30:A:ARG:H	1:49:A:MET:O	8	0.18
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	11	0.18
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	11	0.18
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	11	0.18
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	11	0.18
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	11	0.18
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	11	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	1	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	1	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	1	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	1	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	1	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	1	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	2	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	2	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	2	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	2	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	2	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	2	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	5	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	5	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	5	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	5	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	5	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	5	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	7	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	7	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	7	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	7	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	7	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	7	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	10	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	10	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	10	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	10	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	10	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	15	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	15	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	15	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	15	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	15	0.18
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	15	0.18
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD2	2	0.18
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD3	2	0.18
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	2	0.18
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	10	0.18
(1,938)	1:139:A:LYS:HB2	1:140:A:SER:H	8	0.18
(1,832)	1:42:A:ASN:H	1:43:A:TYR:HA	13	0.18
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB3	5	0.18
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB2	5	0.18
(1,660)	1:79:A:ASN:H	1:78:A:LYS:HE3	11	0.18
(1,639)	1:166:A:ARG:HD2	1:167:A:ASP:H	9	0.18
(1,543)	1:129:A:LYS:H	1:128:A:ASP:H	5	0.18
(1,488)	1:28:A:GLU:HG2	1:25:A:ASP:H	11	0.18
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	5	0.18
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	10	0.18
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	13	0.18
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	14	0.18
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	15	0.18
(1,312)	1:78:A:LYS:H	1:87:A:SER:HA	7	0.18
(1,66)	1:130:A:GLY:H	1:131:A:VAL:H	1	0.18
(1,1454)	1:95:A:ARG:H	1:78:A:LYS:HD3	15	0.17
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD3	8	0.17
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD2	8	0.17
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	1	0.17
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD21	9	0.17
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD22	9	0.17
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD23	9	0.17
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD11	9	0.17
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD12	9	0.17
(1,1224)	1:169:A:TYR:H	1:165:A:LEU:HD13	9	0.17
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG11	6	0.17
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG12	6	0.17
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG13	6	0.17
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG21	6	0.17
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG22	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG23	6	0.17
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG11	10	0.17
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG12	10	0.17
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG13	10	0.17
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG21	10	0.17
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG22	10	0.17
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG23	10	0.17
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG11	11	0.17
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG12	11	0.17
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG13	11	0.17
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG21	11	0.17
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG22	11	0.17
(1,1100)	1:135:A:CYS:H	1:55:A:VAL:HG23	11	0.17
(1,1088)	1:50:A:LEU:H	1:85:A:SER:HB3	9	0.17
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	4	0.17
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	4	0.17
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	4	0.17
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	4	0.17
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	4	0.17
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	4	0.17
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	9	0.17
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	9	0.17
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	9	0.17
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	9	0.17
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	9	0.17
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	9	0.17
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD2	3	0.17
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD3	3	0.17
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD2	14	0.17
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD3	14	0.17
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	1	0.17
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	5	0.17
(1,972)	1:71:A:ARG:HG2	1:72:A:THR:H	3	0.17
(1,886)	1:145:A:SER:H	1:145:A:SER:HB3	15	0.17
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB3	2	0.17
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB2	2	0.17
(1,613)	1:5:A:GLU:H	1:5:A:GLU:HG3	10	0.17
(1,566)	1:54:A:ILE:HG21	1:55:A:VAL:H	2	0.17
(1,566)	1:54:A:ILE:HG22	1:55:A:VAL:H	2	0.17
(1,566)	1:54:A:ILE:HG23	1:55:A:VAL:H	2	0.17
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	15	0.17
(1,416)	1:6:A:ILE:H	1:7:A:ASP:H	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,416)	1:6:A:ILE:H	1:7:A:ASP:H	15	0.17
(1,397)	1:37:A:ILE:HD11	1:32:A:THR:H	3	0.17
(1,397)	1:37:A:ILE:HD12	1:32:A:THR:H	3	0.17
(1,397)	1:37:A:ILE:HD13	1:32:A:THR:H	3	0.17
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	1	0.17
(1,384)	1:31:A:ILE:HG12	1:30:A:ARG:H	12	0.17
(1,328)	1:71:A:ARG:H	1:72:A:THR:H	13	0.17
(1,312)	1:78:A:LYS:H	1:87:A:SER:HA	5	0.17
(1,45)	1:129:A:LYS:H	1:128:A:ASP:HA	13	0.17
(1,38)	1:145:A:SER:HB2	1:146:A:TYR:H	4	0.17
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD3	13	0.16
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD2	13	0.16
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	2	0.16
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	8	0.16
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	14	0.16
(1,1411)	1:30:A:ARG:H	1:49:A:MET:O	12	0.16
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG11	15	0.16
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG12	15	0.16
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG13	15	0.16
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG21	15	0.16
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG22	15	0.16
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG23	15	0.16
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG11	5	0.16
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG12	5	0.16
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG13	5	0.16
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG21	5	0.16
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG22	5	0.16
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG23	5	0.16
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	4	0.16
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	4	0.16
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	4	0.16
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	4	0.16
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	4	0.16
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	4	0.16
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	11	0.16
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	11	0.16
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	11	0.16
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	11	0.16
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	11	0.16
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	11	0.16
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD21	12	0.16
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD22	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD23	12	0.16
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD11	12	0.16
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD12	12	0.16
(1,1075)	1:49:A:MET:H	1:24:A:LEU:HD13	12	0.16
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	7	0.16
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	11	0.16
(1,975)	1:72:A:THR:H	1:71:A:ARG:HD3	9	0.16
(1,967)	1:68:A:ARG:HD2	1:69:A:SER:H	10	0.16
(1,890)	1:145:A:SER:H	1:139:A:LYS:HG3	10	0.16
(1,855)	1:115:A:VAL:H	1:101:A:ARG:HG3	2	0.16
(1,805)	1:17:A:ASN:H	1:16:A:SER:HB3	13	0.16
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD21	10	0.16
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD22	10	0.16
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD23	10	0.16
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD11	10	0.16
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD12	10	0.16
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD13	10	0.16
(1,558)	1:55:A:VAL:H	1:54:A:ILE:HG13	6	0.16
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	2	0.16
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	11	0.16
(1,420)	1:80:A:THR:H	1:81:A:GLY:H	13	0.16
(1,397)	1:37:A:ILE:HD11	1:32:A:THR:H	5	0.16
(1,397)	1:37:A:ILE:HD12	1:32:A:THR:H	5	0.16
(1,397)	1:37:A:ILE:HD13	1:32:A:THR:H	5	0.16
(1,397)	1:37:A:ILE:HD11	1:32:A:THR:H	8	0.16
(1,397)	1:37:A:ILE:HD12	1:32:A:THR:H	8	0.16
(1,397)	1:37:A:ILE:HD13	1:32:A:THR:H	8	0.16
(1,397)	1:37:A:ILE:HD11	1:32:A:THR:H	12	0.16
(1,397)	1:37:A:ILE:HD12	1:32:A:THR:H	12	0.16
(1,397)	1:37:A:ILE:HD13	1:32:A:THR:H	12	0.16
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	2	0.16
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	9	0.16
(1,360)	1:110:A:VAL:H	1:110:A:VAL:HB	13	0.16
(1,297)	1:37:A:ILE:HD11	1:43:A:TYR:H	12	0.16
(1,297)	1:37:A:ILE:HD12	1:43:A:TYR:H	12	0.16
(1,297)	1:37:A:ILE:HD13	1:43:A:TYR:H	12	0.16
(1,38)	1:145:A:SER:HB2	1:146:A:TYR:H	9	0.16
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD3	11	0.15
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD2	11	0.15
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	7	0.15
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	11	0.15
(1,1411)	1:30:A:ARG:H	1:49:A:MET:O	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1411)	1:30:A:ARG:H	1:49:A:MET:O	6	0.15
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG11	4	0.15
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG12	4	0.15
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG13	4	0.15
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG21	4	0.15
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG22	4	0.15
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG23	4	0.15
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG21	12	0.15
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG22	12	0.15
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG23	12	0.15
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG11	12	0.15
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG12	12	0.15
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG13	12	0.15
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD21	7	0.15
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD22	7	0.15
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD23	7	0.15
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD11	7	0.15
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD12	7	0.15
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD13	7	0.15
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD21	11	0.15
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD22	11	0.15
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD23	11	0.15
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD11	11	0.15
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD12	11	0.15
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD13	11	0.15
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG11	14	0.15
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG12	14	0.15
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG13	14	0.15
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG21	14	0.15
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG22	14	0.15
(1,1150)	1:139:A:LYS:H	1:84:A:VAL:HG23	14	0.15
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	12	0.15
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	12	0.15
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	12	0.15
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	12	0.15
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	12	0.15
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	12	0.15
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	14	0.15
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	14	0.15
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	14	0.15
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	14	0.15
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	14	0.15
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD21	11	0.15
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD22	11	0.15
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD23	11	0.15
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD11	11	0.15
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD12	11	0.15
(1,1081)	1:33:A:ASP:H	1:36:A:LEU:HD13	11	0.15
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD11	4	0.15
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD12	4	0.15
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD13	4	0.15
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD21	4	0.15
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD22	4	0.15
(1,1056)	1:14:A:LEU:H	1:45:A:LEU:HD23	4	0.15
(1,1039)	1:9:A:ASN:H	1:8:A:LYS:HE3	5	0.15
(1,1036)	1:8:A:LYS:HG2	1:9:A:ASN:H	15	0.15
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	6	0.15
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	8	0.15
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	12	0.15
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	13	0.15
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	15	0.15
(1,972)	1:71:A:ARG:HG2	1:72:A:THR:H	14	0.15
(1,966)	1:69:A:SER:H	1:70:A:GLY:H	11	0.15
(1,832)	1:42:A:ASN:H	1:43:A:TYR:HA	15	0.15
(1,543)	1:129:A:LYS:H	1:128:A:ASP:H	2	0.15
(1,416)	1:6:A:ILE:H	1:7:A:ASP:H	13	0.15
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	5	0.15
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	8	0.15
(1,328)	1:71:A:ARG:H	1:72:A:THR:H	1	0.15
(1,328)	1:71:A:ARG:H	1:72:A:THR:H	3	0.15
(1,297)	1:37:A:ILE:HD11	1:43:A:TYR:H	3	0.15
(1,297)	1:37:A:ILE:HD12	1:43:A:TYR:H	3	0.15
(1,297)	1:37:A:ILE:HD13	1:43:A:TYR:H	3	0.15
(1,297)	1:37:A:ILE:HD11	1:43:A:TYR:H	8	0.15
(1,297)	1:37:A:ILE:HD12	1:43:A:TYR:H	8	0.15
(1,297)	1:37:A:ILE:HD13	1:43:A:TYR:H	8	0.15
(1,251)	1:165:A:LEU:H	1:165:A:LEU:HG	6	0.15
(1,251)	1:165:A:LEU:H	1:165:A:LEU:HG	7	0.15
(1,251)	1:165:A:LEU:H	1:165:A:LEU:HG	8	0.15
(1,251)	1:165:A:LEU:H	1:165:A:LEU:HG	12	0.15
(1,158)	1:96:A:LEU:H	1:99:A:LEU:HG	11	0.15
(1,158)	1:96:A:LEU:H	1:99:A:LEU:HG	14	0.15
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD3	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD2	4	0.14
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	4	0.14
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	9	0.14
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	10	0.14
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	13	0.14
(1,1411)	1:30:A:ARG:H	1:49:A:MET:O	7	0.14
(1,1411)	1:30:A:ARG:H	1:49:A:MET:O	9	0.14
(1,1411)	1:30:A:ARG:H	1:49:A:MET:O	14	0.14
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG21	4	0.14
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG22	4	0.14
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG23	4	0.14
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG11	4	0.14
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG12	4	0.14
(1,1120)	1:74:A:CYS:H	1:115:A:VAL:HG13	4	0.14
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD11	14	0.14
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD12	14	0.14
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD13	14	0.14
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD21	14	0.14
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD22	14	0.14
(1,1114)	1:64:A:TYR:H	1:118:A:LEU:HD23	14	0.14
(1,1040)	1:8:A:LYS:HE2	1:9:A:ASN:H	15	0.14
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD2	6	0.14
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD3	6	0.14
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	14	0.14
(1,968)	1:69:A:SER:H	1:68:A:ARG:HD3	13	0.14
(1,956)	1:33:A:ASP:HB2	1:33:A:ASP:H	7	0.14
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB3	1	0.14
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB2	1	0.14
(1,619)	1:27:A:ASN:H	1:28:A:GLU:HG3	2	0.14
(1,543)	1:129:A:LYS:H	1:128:A:ASP:H	1	0.14
(1,543)	1:129:A:LYS:H	1:128:A:ASP:H	6	0.14
(1,472)	1:90:A:ILE:H	1:90:A:ILE:HD11	12	0.14
(1,472)	1:90:A:ILE:H	1:90:A:ILE:HD12	12	0.14
(1,472)	1:90:A:ILE:H	1:90:A:ILE:HD13	12	0.14
(1,324)	1:71:A:ARG:H	1:71:A:ARG:HG2	11	0.14
(1,324)	1:71:A:ARG:H	1:71:A:ARG:HG3	11	0.14
(1,312)	1:78:A:LYS:H	1:87:A:SER:HA	10	0.14
(1,158)	1:96:A:LEU:H	1:99:A:LEU:HG	13	0.14
(1,158)	1:96:A:LEU:H	1:99:A:LEU:HG	15	0.14
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD3	6	0.13
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD2	6	0.13
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD3	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD2	12	0.13
(1,1432)	1:112:A:GLU:H	1:79:A:ASN:O	9	0.13
(1,1427)	1:80:A:THR:H	1:83:A:ARG:O	15	0.13
(1,1426)	1:83:A:ARG:H	1:80:A:THR:O	12	0.13
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	3	0.13
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	12	0.13
(1,1411)	1:30:A:ARG:H	1:49:A:MET:O	4	0.13
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG11	15	0.13
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG12	15	0.13
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG13	15	0.13
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG21	15	0.13
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG22	15	0.13
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG23	15	0.13
(1,1198)	1:130:A:GLY:H	1:131:A:VAL:HG21	2	0.13
(1,1198)	1:130:A:GLY:H	1:131:A:VAL:HG22	2	0.13
(1,1198)	1:130:A:GLY:H	1:131:A:VAL:HG23	2	0.13
(1,1198)	1:130:A:GLY:H	1:131:A:VAL:HG11	2	0.13
(1,1198)	1:130:A:GLY:H	1:131:A:VAL:HG12	2	0.13
(1,1198)	1:130:A:GLY:H	1:131:A:VAL:HG13	2	0.13
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD11	5	0.13
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD12	5	0.13
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD13	5	0.13
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD21	5	0.13
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD22	5	0.13
(1,1188)	1:117:A:THR:H	1:118:A:LEU:HD23	5	0.13
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG11	4	0.13
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG12	4	0.13
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG13	4	0.13
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG21	4	0.13
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG22	4	0.13
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG23	4	0.13
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD21	5	0.13
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD22	5	0.13
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD23	5	0.13
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD11	5	0.13
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD12	5	0.13
(1,1181)	1:116:A:VAL:H	1:114:A:LEU:HD13	5	0.13
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD21	10	0.13
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD22	10	0.13
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD23	10	0.13
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD11	10	0.13
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD12	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD13	10	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD21	1	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD22	1	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD23	1	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD11	1	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD12	1	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD13	1	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD21	14	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD22	14	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD23	14	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD11	14	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD12	14	0.13
(1,1137)	1:78:A:LYS:H	1:86:A:LEU:HD13	14	0.13
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	3	0.13
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	3	0.13
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	3	0.13
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	3	0.13
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	3	0.13
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	3	0.13
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD11	8	0.13
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD12	8	0.13
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD13	8	0.13
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD21	8	0.13
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD22	8	0.13
(1,1080)	1:32:A:THR:H	1:45:A:LEU:HD23	8	0.13
(1,1036)	1:8:A:LYS:HG2	1:9:A:ASN:H	2	0.13
(1,997)	1:108:A:LEU:HG	1:108:A:LEU:H	2	0.13
(1,941)	1:139:A:LYS:HG2	1:140:A:SER:H	8	0.13
(1,924)	1:164:A:LEU:H	1:164:A:LEU:HG	4	0.13
(1,924)	1:164:A:LEU:H	1:164:A:LEU:HG	13	0.13
(1,832)	1:42:A:ASN:H	1:43:A:TYR:HA	6	0.13
(1,721)	1:99:A:LEU:HG	1:100:A:LYS:H	13	0.13
(1,674)	1:125:A:LYS:H	1:127:A:CYS:H	14	0.13
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD11	5	0.13
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD12	5	0.13
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD13	5	0.13
(1,397)	1:37:A:ILE:HD11	1:32:A:THR:H	1	0.13
(1,397)	1:37:A:ILE:HD12	1:32:A:THR:H	1	0.13
(1,397)	1:37:A:ILE:HD13	1:32:A:THR:H	1	0.13
(1,397)	1:37:A:ILE:HD11	1:32:A:THR:H	6	0.13
(1,397)	1:37:A:ILE:HD12	1:32:A:THR:H	6	0.13
(1,397)	1:37:A:ILE:HD13	1:32:A:THR:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:37:A:ILE:HD11	1:32:A:THR:H	15	0.13
(1,397)	1:37:A:ILE:HD12	1:32:A:THR:H	15	0.13
(1,397)	1:37:A:ILE:HD13	1:32:A:THR:H	15	0.13
(1,395)	1:31:A:ILE:HD11	1:32:A:THR:H	3	0.13
(1,395)	1:31:A:ILE:HD12	1:32:A:THR:H	3	0.13
(1,395)	1:31:A:ILE:HD13	1:32:A:THR:H	3	0.13
(1,385)	1:30:A:ARG:H	1:31:A:ILE:HG13	6	0.13
(1,328)	1:71:A:ARG:H	1:72:A:THR:H	12	0.13
(1,328)	1:71:A:ARG:H	1:72:A:THR:H	15	0.13
(1,312)	1:78:A:LYS:H	1:87:A:SER:HA	2	0.13
(1,312)	1:78:A:LYS:H	1:87:A:SER:HA	11	0.13
(1,312)	1:78:A:LYS:H	1:87:A:SER:HA	14	0.13
(1,274)	1:37:A:ILE:HD11	1:39:A:LYS:H	15	0.13
(1,274)	1:37:A:ILE:HD12	1:39:A:LYS:H	15	0.13
(1,274)	1:37:A:ILE:HD13	1:39:A:LYS:H	15	0.13
(1,251)	1:165:A:LEU:H	1:165:A:LEU:HG	3	0.13
(1,158)	1:96:A:LEU:H	1:99:A:LEU:HG	5	0.13
(1,158)	1:96:A:LEU:H	1:99:A:LEU:HG	9	0.13
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD11	9	0.13
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD12	9	0.13
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD13	9	0.13
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD11	12	0.13
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD12	12	0.13
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD13	12	0.13
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG11	5	0.13
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG12	5	0.13
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG13	5	0.13
(1,1456)	1:47:A:ASP:H	1:30:A:ARG:HB3	2	0.12
(1,1456)	1:47:A:ASP:H	1:30:A:ARG:HB2	2	0.12
(1,1456)	1:47:A:ASP:H	1:30:A:ARG:HB3	7	0.12
(1,1456)	1:47:A:ASP:H	1:30:A:ARG:HB2	7	0.12
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD3	9	0.12
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD2	9	0.12
(1,1445)	1:104:A:ASP:H	1:150:A:VAL:O	9	0.12
(1,1443)	1:140:A:SER:H	1:145:A:SER:O	8	0.12
(1,1432)	1:112:A:GLU:H	1:79:A:ASN:O	7	0.12
(1,1414)	1:84:A:VAL:H	1:50:A:LEU:O	5	0.12
(1,1255)	1:157:A:ASN:O	1:161:A:TYR:N	13	0.12
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG11	4	0.12
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG12	4	0.12
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG13	4	0.12
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG21	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG22	4	0.12
(1,1131)	1:115:A:VAL:H	1:76:A:VAL:HG23	4	0.12
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG11	15	0.12
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG12	15	0.12
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG13	15	0.12
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG21	15	0.12
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG22	15	0.12
(1,1096)	1:54:A:ILE:H	1:55:A:VAL:HG23	15	0.12
(1,1059)	1:18:A:THR:H	1:29:A:LEU:HD21	3	0.12
(1,1059)	1:18:A:THR:H	1:29:A:LEU:HD22	3	0.12
(1,1059)	1:18:A:THR:H	1:29:A:LEU:HD23	3	0.12
(1,1059)	1:18:A:THR:H	1:29:A:LEU:HD11	3	0.12
(1,1059)	1:18:A:THR:H	1:29:A:LEU:HD12	3	0.12
(1,1059)	1:18:A:THR:H	1:29:A:LEU:HD13	3	0.12
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG11	8	0.12
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG12	8	0.12
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG13	8	0.12
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG21	8	0.12
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG22	8	0.12
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG23	8	0.12
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG11	15	0.12
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG12	15	0.12
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG13	15	0.12
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG21	15	0.12
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG22	15	0.12
(1,1050)	1:13:A:ASP:H	1:10:A:VAL:HG23	15	0.12
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD2	7	0.12
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD3	7	0.12
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD2	13	0.12
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD3	13	0.12
(1,972)	1:71:A:ARG:HG2	1:72:A:THR:H	2	0.12
(1,856)	1:101:A:ARG:HG2	1:115:A:VAL:H	10	0.12
(1,804)	1:16:A:SER:HB2	1:17:A:ASN:H	2	0.12
(1,773)	1:76:A:VAL:H	1:115:A:VAL:HG11	6	0.12
(1,773)	1:76:A:VAL:H	1:115:A:VAL:HG12	6	0.12
(1,773)	1:76:A:VAL:H	1:115:A:VAL:HG13	6	0.12
(1,748)	1:6:A:ILE:HB	1:7:A:ASP:H	14	0.12
(1,721)	1:99:A:LEU:HG	1:100:A:LYS:H	6	0.12
(1,721)	1:99:A:LEU:HG	1:100:A:LYS:H	8	0.12
(1,693)	1:39:A:LYS:H	1:92:A:PHE:H	12	0.12
(1,688)	1:84:A:VAL:H	1:80:A:THR:H	4	0.12
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB3	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB2	6	0.12
(1,639)	1:166:A:ARG:HD2	1:167:A:ASP:H	2	0.12
(1,574)	1:139:A:LYS:H	1:139:A:LYS:HD3	10	0.12
(1,574)	1:139:A:LYS:H	1:139:A:LYS:HD2	10	0.12
(1,543)	1:129:A:LYS:H	1:128:A:ASP:H	4	0.12
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD11	8	0.12
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD12	8	0.12
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD13	8	0.12
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD11	9	0.12
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD12	9	0.12
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD13	9	0.12
(1,475)	1:90:A:ILE:H	1:45:A:LEU:HD21	2	0.12
(1,475)	1:90:A:ILE:H	1:45:A:LEU:HD22	2	0.12
(1,475)	1:90:A:ILE:H	1:45:A:LEU:HD23	2	0.12
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD11	13	0.12
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD12	13	0.12
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD13	13	0.12
(1,410)	1:6:A:ILE:H	1:6:A:ILE:HG13	1	0.12
(1,410)	1:6:A:ILE:H	1:6:A:ILE:HG12	1	0.12
(1,397)	1:37:A:ILE:HD11	1:32:A:THR:H	9	0.12
(1,397)	1:37:A:ILE:HD12	1:32:A:THR:H	9	0.12
(1,397)	1:37:A:ILE:HD13	1:32:A:THR:H	9	0.12
(1,328)	1:71:A:ARG:H	1:72:A:THR:H	4	0.12
(1,314)	1:78:A:LYS:HD2	1:78:A:LYS:H	10	0.12
(1,312)	1:78:A:LYS:H	1:87:A:SER:HA	4	0.12
(1,297)	1:37:A:ILE:HD11	1:43:A:TYR:H	10	0.12
(1,297)	1:37:A:ILE:HD12	1:43:A:TYR:H	10	0.12
(1,297)	1:37:A:ILE:HD13	1:43:A:TYR:H	10	0.12
(1,296)	1:43:A:TYR:H	1:40:A:ASN:HA	5	0.12
(1,283)	1:113:A:ALA:H	1:99:A:LEU:HD11	9	0.12
(1,283)	1:113:A:ALA:H	1:99:A:LEU:HD12	9	0.12
(1,283)	1:113:A:ALA:H	1:99:A:LEU:HD13	9	0.12
(1,221)	1:124:A:ILE:HG12	1:125:A:LYS:H	9	0.12
(1,158)	1:96:A:LEU:H	1:99:A:LEU:HG	8	0.12
(1,112)	1:47:A:ASP:H	1:45:A:LEU:HD21	5	0.12
(1,112)	1:47:A:ASP:H	1:45:A:LEU:HD22	5	0.12
(1,112)	1:47:A:ASP:H	1:45:A:LEU:HD23	5	0.12
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD11	10	0.12
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD12	10	0.12
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD13	10	0.12
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG11	7	0.12
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG12	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG13	7	0.12
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG11	8	0.12
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG12	8	0.12
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG13	8	0.12
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG11	12	0.12
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG12	12	0.12
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG13	12	0.12
(1,1452)	1:104:A:ASP:H	1:101:A:ARG:HD2	1	0.11
(1,1452)	1:104:A:ASP:H	1:101:A:ARG:HD3	1	0.11
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD3	10	0.11
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD2	10	0.11
(1,1444)	1:150:A:VAL:H	1:104:A:ASP:O	4	0.11
(1,1432)	1:112:A:GLU:H	1:79:A:ASN:O	2	0.11
(1,1411)	1:30:A:ARG:H	1:49:A:MET:O	11	0.11
(1,1323)	1:58:A:VAL:HG11	1:131:A:VAL:HG11	15	0.11
(1,1323)	1:58:A:VAL:HG11	1:131:A:VAL:HG12	15	0.11
(1,1323)	1:58:A:VAL:HG11	1:131:A:VAL:HG13	15	0.11
(1,1323)	1:58:A:VAL:HG12	1:131:A:VAL:HG11	15	0.11
(1,1323)	1:58:A:VAL:HG12	1:131:A:VAL:HG12	15	0.11
(1,1323)	1:58:A:VAL:HG12	1:131:A:VAL:HG13	15	0.11
(1,1323)	1:58:A:VAL:HG13	1:131:A:VAL:HG11	15	0.11
(1,1323)	1:58:A:VAL:HG13	1:131:A:VAL:HG12	15	0.11
(1,1323)	1:58:A:VAL:HG13	1:131:A:VAL:HG13	15	0.11
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG11	8	0.11
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG12	8	0.11
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG13	8	0.11
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG21	8	0.11
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG22	8	0.11
(1,1209)	1:148:A:ILE:H	1:137:A:VAL:HG23	8	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG21	8	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG22	8	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG23	8	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG11	8	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG12	8	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG13	8	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG21	10	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG22	10	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG23	10	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG11	10	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG12	10	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG13	10	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG21	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG22	15	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG23	15	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG11	15	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG12	15	0.11
(1,1203)	1:136:A:VAL:H	1:151:A:VAL:HG13	15	0.11
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG11	9	0.11
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG12	9	0.11
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG13	9	0.11
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG21	9	0.11
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG22	9	0.11
(1,1183)	1:115:A:VAL:H	1:116:A:VAL:HG23	9	0.11
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD21	6	0.11
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD22	6	0.11
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD23	6	0.11
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD11	6	0.11
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD12	6	0.11
(1,1180)	1:115:A:VAL:H	1:114:A:LEU:HD13	6	0.11
(1,1163)	1:100:A:LYS:H	1:115:A:VAL:HG21	8	0.11
(1,1163)	1:100:A:LYS:H	1:115:A:VAL:HG22	8	0.11
(1,1163)	1:100:A:LYS:H	1:115:A:VAL:HG23	8	0.11
(1,1163)	1:100:A:LYS:H	1:115:A:VAL:HG11	8	0.11
(1,1163)	1:100:A:LYS:H	1:115:A:VAL:HG12	8	0.11
(1,1163)	1:100:A:LYS:H	1:115:A:VAL:HG13	8	0.11
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG11	13	0.11
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG12	13	0.11
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG13	13	0.11
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG21	13	0.11
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG22	13	0.11
(1,1136)	1:78:A:LYS:H	1:84:A:VAL:HG23	13	0.11
(1,1132)	1:77:A:PHE:H	1:86:A:LEU:HD21	14	0.11
(1,1132)	1:77:A:PHE:H	1:86:A:LEU:HD22	14	0.11
(1,1132)	1:77:A:PHE:H	1:86:A:LEU:HD23	14	0.11
(1,1132)	1:77:A:PHE:H	1:86:A:LEU:HD11	14	0.11
(1,1132)	1:77:A:PHE:H	1:86:A:LEU:HD12	14	0.11
(1,1132)	1:77:A:PHE:H	1:86:A:LEU:HD13	14	0.11
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG11	4	0.11
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG12	4	0.11
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG13	4	0.11
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG21	4	0.11
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG22	4	0.11
(1,1052)	1:69:A:SER:H	1:10:A:VAL:HG23	4	0.11
(1,1042)	1:9:A:ASN:H	1:10:A:VAL:HG11	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:9:A:ASN:H	1:10:A:VAL:HG12	15	0.11
(1,1042)	1:9:A:ASN:H	1:10:A:VAL:HG13	15	0.11
(1,1027)	1:48:A:ALA:H	1:29:A:LEU:HD21	7	0.11
(1,1027)	1:48:A:ALA:H	1:29:A:LEU:HD22	7	0.11
(1,1027)	1:48:A:ALA:H	1:29:A:LEU:HD23	7	0.11
(1,997)	1:108:A:LEU:HG	1:108:A:LEU:H	1	0.11
(1,997)	1:108:A:LEU:HG	1:108:A:LEU:H	12	0.11
(1,997)	1:108:A:LEU:HG	1:108:A:LEU:H	15	0.11
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	4	0.11
(1,979)	1:105:A:PHE:H	1:104:A:ASP:H	9	0.11
(1,924)	1:164:A:LEU:H	1:164:A:LEU:HG	5	0.11
(1,924)	1:164:A:LEU:H	1:164:A:LEU:HG	7	0.11
(1,924)	1:164:A:LEU:H	1:164:A:LEU:HG	8	0.11
(1,924)	1:164:A:LEU:H	1:164:A:LEU:HG	9	0.11
(1,924)	1:164:A:LEU:H	1:164:A:LEU:HG	10	0.11
(1,843)	1:171:A:ARG:H	1:168:A:ILE:HA	15	0.11
(1,816)	1:54:A:ILE:HD11	1:52:A:THR:H	2	0.11
(1,816)	1:54:A:ILE:HD12	1:52:A:THR:H	2	0.11
(1,816)	1:54:A:ILE:HD13	1:52:A:THR:H	2	0.11
(1,816)	1:54:A:ILE:HD11	1:52:A:THR:H	13	0.11
(1,816)	1:54:A:ILE:HD12	1:52:A:THR:H	13	0.11
(1,816)	1:54:A:ILE:HD13	1:52:A:THR:H	13	0.11
(1,748)	1:6:A:ILE:HB	1:7:A:ASP:H	7	0.11
(1,748)	1:6:A:ILE:HB	1:7:A:ASP:H	9	0.11
(1,735)	1:154:A:GLY:H	1:131:A:VAL:HG11	6	0.11
(1,735)	1:154:A:GLY:H	1:131:A:VAL:HG12	6	0.11
(1,735)	1:154:A:GLY:H	1:131:A:VAL:HG13	6	0.11
(1,688)	1:84:A:VAL:H	1:80:A:THR:H	3	0.11
(1,688)	1:84:A:VAL:H	1:80:A:THR:H	6	0.11
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB3	7	0.11
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB2	7	0.11
(1,660)	1:79:A:ASN:H	1:78:A:LYS:HE3	13	0.11
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD11	2	0.11
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD12	2	0.11
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD13	2	0.11
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD11	11	0.11
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD12	11	0.11
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD13	11	0.11
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD11	14	0.11
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD12	14	0.11
(1,482)	1:170:A:ALA:H	1:168:A:ILE:HD13	14	0.11
(1,439)	1:49:A:MET:H	1:24:A:LEU:HD11	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:49:A:MET:H	1:24:A:LEU:HD12	3	0.11
(1,439)	1:49:A:MET:H	1:24:A:LEU:HD13	3	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD11	3	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD12	3	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD13	3	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD11	9	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD12	9	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD13	9	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD11	10	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD12	10	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD13	10	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD11	12	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD12	12	0.11
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD13	12	0.11
(1,336)	1:24:A:LEU:H	1:23:A:ARG:HD2	15	0.11
(1,336)	1:24:A:LEU:H	1:23:A:ARG:HD3	15	0.11
(1,327)	1:71:A:ARG:H	1:69:A:SER:H	12	0.11
(1,324)	1:71:A:ARG:H	1:71:A:ARG:HG2	10	0.11
(1,324)	1:71:A:ARG:H	1:71:A:ARG:HG3	10	0.11
(1,312)	1:78:A:LYS:H	1:87:A:SER:HA	8	0.11
(1,312)	1:78:A:LYS:H	1:87:A:SER:HA	9	0.11
(1,302)	1:31:A:ILE:HB	1:31:A:ILE:H	5	0.11
(1,302)	1:31:A:ILE:HB	1:31:A:ILE:H	6	0.11
(1,283)	1:113:A:ALA:H	1:99:A:LEU:HD11	11	0.11
(1,283)	1:113:A:ALA:H	1:99:A:LEU:HD12	11	0.11
(1,283)	1:113:A:ALA:H	1:99:A:LEU:HD13	11	0.11
(1,214)	1:166:A:ARG:H	1:164:A:LEU:HD11	15	0.11
(1,214)	1:166:A:ARG:H	1:164:A:LEU:HD12	15	0.11
(1,214)	1:166:A:ARG:H	1:164:A:LEU:HD13	15	0.11
(1,158)	1:96:A:LEU:H	1:99:A:LEU:HG	6	0.11
(1,112)	1:47:A:ASP:H	1:45:A:LEU:HD21	11	0.11
(1,112)	1:47:A:ASP:H	1:45:A:LEU:HD22	11	0.11
(1,112)	1:47:A:ASP:H	1:45:A:LEU:HD23	11	0.11
(1,74)	1:35:A:ALA:H	1:33:A:ASP:HB2	11	0.11
(1,74)	1:35:A:ALA:H	1:33:A:ASP:HB3	11	0.11
(1,57)	1:89:A:TYR:H	1:76:A:VAL:HG11	8	0.11
(1,57)	1:89:A:TYR:H	1:76:A:VAL:HG12	8	0.11
(1,57)	1:89:A:TYR:H	1:76:A:VAL:HG13	8	0.11
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD11	4	0.11
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD12	4	0.11
(1,23)	1:38:A:CYS:H	1:37:A:ILE:HD13	4	0.11
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG11	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG12	6	0.11
(1,12)	1:74:A:CYS:H	1:115:A:VAL:HG13	6	0.11
(1,11)	1:84:A:VAL:H	1:137:A:VAL:HB	8	0.11
(1,1457)	1:160:A:GLU:H	1:55:A:VAL:HG21	3	0.1
(1,1457)	1:160:A:GLU:H	1:55:A:VAL:HG22	3	0.1
(1,1457)	1:160:A:GLU:H	1:55:A:VAL:HG23	3	0.1
(1,1452)	1:104:A:ASP:H	1:101:A:ARG:HD2	9	0.1
(1,1452)	1:104:A:ASP:H	1:101:A:ARG:HD3	9	0.1
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD3	5	0.1
(1,1450)	1:99:A:LEU:H	1:78:A:LYS:HD2	5	0.1
(1,1445)	1:104:A:ASP:H	1:150:A:VAL:O	3	0.1
(1,1427)	1:80:A:THR:H	1:83:A:ARG:O	7	0.1
(1,1413)	1:32:A:THR:H	1:47:A:ASP:O	10	0.1
(1,1411)	1:30:A:ARG:H	1:49:A:MET:O	10	0.1
(1,1323)	1:58:A:VAL:HG11	1:131:A:VAL:HG11	5	0.1
(1,1323)	1:58:A:VAL:HG11	1:131:A:VAL:HG12	5	0.1
(1,1323)	1:58:A:VAL:HG11	1:131:A:VAL:HG13	5	0.1
(1,1323)	1:58:A:VAL:HG12	1:131:A:VAL:HG11	5	0.1
(1,1323)	1:58:A:VAL:HG12	1:131:A:VAL:HG12	5	0.1
(1,1323)	1:58:A:VAL:HG12	1:131:A:VAL:HG13	5	0.1
(1,1323)	1:58:A:VAL:HG13	1:131:A:VAL:HG11	5	0.1
(1,1323)	1:58:A:VAL:HG13	1:131:A:VAL:HG12	5	0.1
(1,1323)	1:58:A:VAL:HG13	1:131:A:VAL:HG13	5	0.1
(1,1173)	1:111:A:ASN:H	1:110:A:VAL:HG21	9	0.1
(1,1173)	1:111:A:ASN:H	1:110:A:VAL:HG22	9	0.1
(1,1173)	1:111:A:ASN:H	1:110:A:VAL:HG23	9	0.1
(1,1173)	1:111:A:ASN:H	1:110:A:VAL:HG11	9	0.1
(1,1173)	1:111:A:ASN:H	1:110:A:VAL:HG12	9	0.1
(1,1173)	1:111:A:ASN:H	1:110:A:VAL:HG13	9	0.1
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG11	8	0.1
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG12	8	0.1
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG13	8	0.1
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG21	8	0.1
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG22	8	0.1
(1,1105)	1:63:A:SER:H	1:58:A:VAL:HG23	8	0.1
(1,1104)	1:62:A:LEU:H	1:58:A:VAL:HG11	2	0.1
(1,1104)	1:62:A:LEU:H	1:58:A:VAL:HG12	2	0.1
(1,1104)	1:62:A:LEU:H	1:58:A:VAL:HG13	2	0.1
(1,1104)	1:62:A:LEU:H	1:58:A:VAL:HG21	2	0.1
(1,1104)	1:62:A:LEU:H	1:58:A:VAL:HG22	2	0.1
(1,1104)	1:62:A:LEU:H	1:58:A:VAL:HG23	2	0.1
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD2	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD3	5	0.1
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD2	12	0.1
(1,1016)	1:147:A:ASN:H	1:139:A:LYS:HD3	12	0.1
(1,1015)	1:147:A:ASN:H	1:148:A:ILE:HG13	3	0.1
(1,1015)	1:147:A:ASN:H	1:148:A:ILE:HG12	3	0.1
(1,1011)	1:147:A:ASN:H	1:137:A:VAL:HG21	11	0.1
(1,1011)	1:147:A:ASN:H	1:137:A:VAL:HG22	11	0.1
(1,1011)	1:147:A:ASN:H	1:137:A:VAL:HG23	11	0.1
(1,944)	1:139:A:LYS:HD2	1:140:A:SER:H	6	0.1
(1,939)	1:140:A:SER:H	1:139:A:LYS:HB3	7	0.1
(1,924)	1:164:A:LEU:H	1:164:A:LEU:HG	3	0.1
(1,924)	1:164:A:LEU:H	1:164:A:LEU:HG	12	0.1
(1,863)	1:102:A:VAL:H	1:115:A:VAL:H	7	0.1
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD21	5	0.1
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD22	5	0.1
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD23	5	0.1
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD11	5	0.1
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD12	5	0.1
(1,788)	1:36:A:LEU:H	1:36:A:LEU:HD13	5	0.1
(1,748)	1:6:A:ILE:HB	1:7:A:ASP:H	13	0.1
(1,688)	1:84:A:VAL:H	1:80:A:THR:H	1	0.1
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB3	11	0.1
(1,686)	1:84:A:VAL:H	1:139:A:LYS:HB2	11	0.1
(1,638)	1:167:A:ASP:H	1:166:A:ARG:HD3	5	0.1
(1,566)	1:54:A:ILE:HG21	1:55:A:VAL:H	13	0.1
(1,566)	1:54:A:ILE:HG22	1:55:A:VAL:H	13	0.1
(1,566)	1:54:A:ILE:HG23	1:55:A:VAL:H	13	0.1
(1,510)	1:29:A:LEU:H	1:28:A:GLU:H	1	0.1
(1,416)	1:6:A:ILE:H	1:7:A:ASP:H	7	0.1
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD11	1	0.1
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD12	1	0.1
(1,412)	1:6:A:ILE:H	1:6:A:ILE:HD13	1	0.1
(1,410)	1:6:A:ILE:H	1:6:A:ILE:HG13	7	0.1
(1,410)	1:6:A:ILE:H	1:6:A:ILE:HG12	7	0.1
(1,397)	1:37:A:ILE:HD11	1:32:A:THR:H	14	0.1
(1,397)	1:37:A:ILE:HD12	1:32:A:THR:H	14	0.1
(1,397)	1:37:A:ILE:HD13	1:32:A:THR:H	14	0.1
(1,320)	1:78:A:LYS:H	1:114:A:LEU:HD21	15	0.1
(1,320)	1:78:A:LYS:H	1:114:A:LEU:HD22	15	0.1
(1,320)	1:78:A:LYS:H	1:114:A:LEU:HD23	15	0.1
(1,317)	1:78:A:LYS:H	1:114:A:LEU:HD11	10	0.1
(1,317)	1:78:A:LYS:H	1:114:A:LEU:HD12	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,317)	1:78:A:LYS:H	1:114:A:LEU:HD13	10	0.1
(1,312)	1:78:A:LYS:H	1:87:A:SER:HA	3	0.1
(1,312)	1:78:A:LYS:H	1:87:A:SER:HA	12	0.1
(1,283)	1:113:A:ALA:H	1:99:A:LEU:HD11	14	0.1
(1,283)	1:113:A:ALA:H	1:99:A:LEU:HD12	14	0.1
(1,283)	1:113:A:ALA:H	1:99:A:LEU:HD13	14	0.1
(1,236)	1:168:A:ILE:H	1:170:A:ALA:H	13	0.1
(1,112)	1:47:A:ASP:H	1:45:A:LEU:HD21	2	0.1
(1,112)	1:47:A:ASP:H	1:45:A:LEU:HD22	2	0.1
(1,112)	1:47:A:ASP:H	1:45:A:LEU:HD23	2	0.1
(1,45)	1:129:A:LYS:H	1:128:A:ASP:HA	12	0.1
(1,18)	1:67:A:CYS:HB2	1:68:A:ARG:H	15	0.1

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

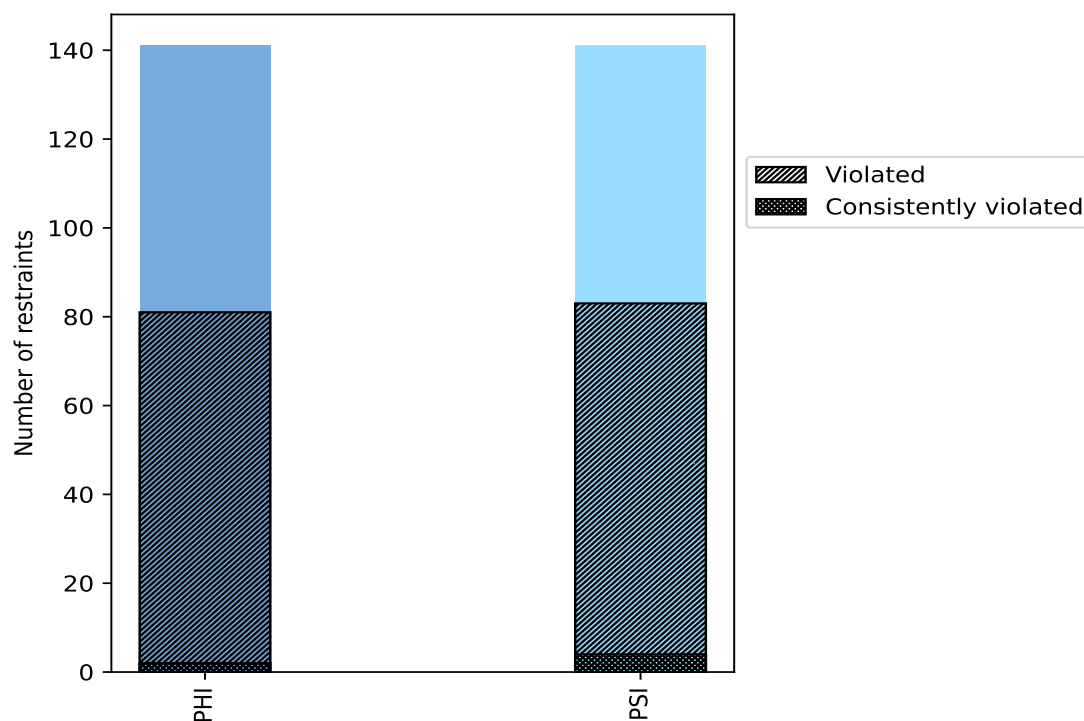
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	141	50.0	81	57.4	28.7	2	1.4	0.7
PSI	141	50.0	83	58.9	29.4	4	2.8	1.4
Total	282	100.0	164	58.2	58.2	6	2.1	2.1

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

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



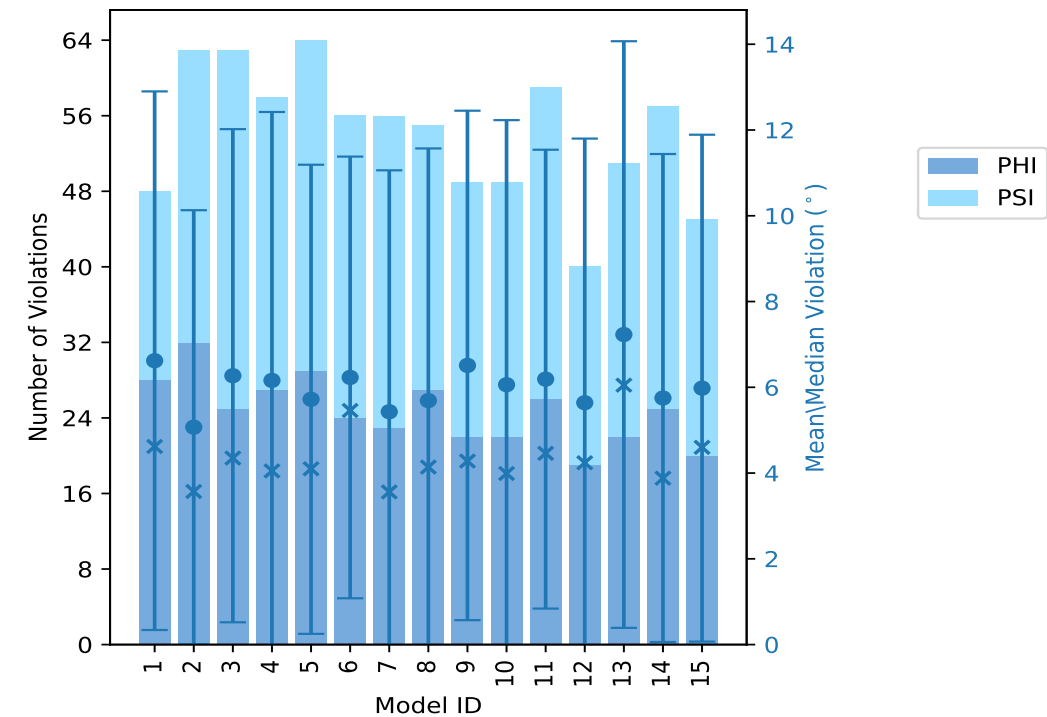
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	28	20	48	6.62	29.56	6.28	4.62
2	32	31	63	5.07	26.93	5.06	3.57
3	25	38	63	6.27	31.99	5.75	4.35
4	27	31	58	6.16	34.92	6.26	4.05
5	29	35	64	5.72	28.19	5.47	4.1
6	24	32	56	6.23	27.25	5.15	5.46
7	23	33	56	5.43	31.14	5.63	3.56
8	27	28	55	5.69	33.22	5.88	4.14
9	22	27	49	6.51	28.05	5.94	4.28
10	22	27	49	6.06	31.04	6.17	3.99
11	26	33	59	6.19	26.39	5.35	4.46
12	19	21	40	5.64	38.85	6.16	4.24
13	22	29	51	7.23	44.78	6.84	6.05
14	25	32	57	5.75	28.61	5.69	3.88
15	20	25	45	5.98	31.97	5.91	4.6

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

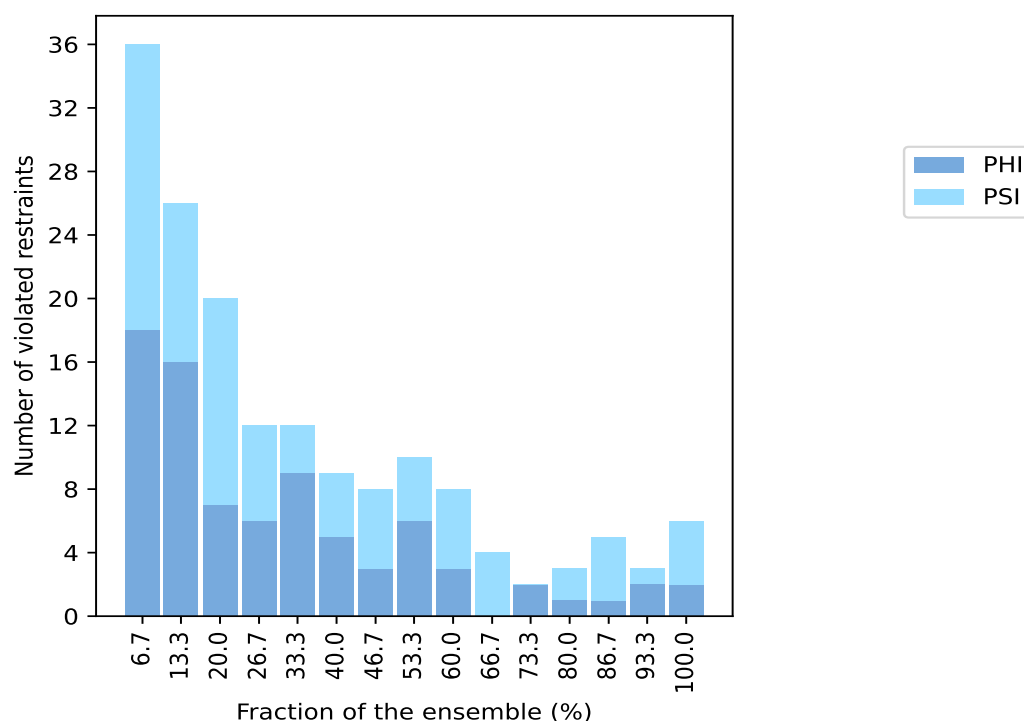
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
18	18	36	1	6.7
16	10	26	2	13.3
7	13	20	3	20.0
6	6	12	4	26.7
9	3	12	5	33.3
5	4	9	6	40.0
3	5	8	7	46.7
6	4	10	8	53.3
3	5	8	9	60.0
0	4	4	10	66.7
2	0	2	11	73.3
1	2	3	12	80.0
1	4	5	13	86.7
2	1	3	14	93.3
2	4	6	15	100.0

¹ Number of models with violations

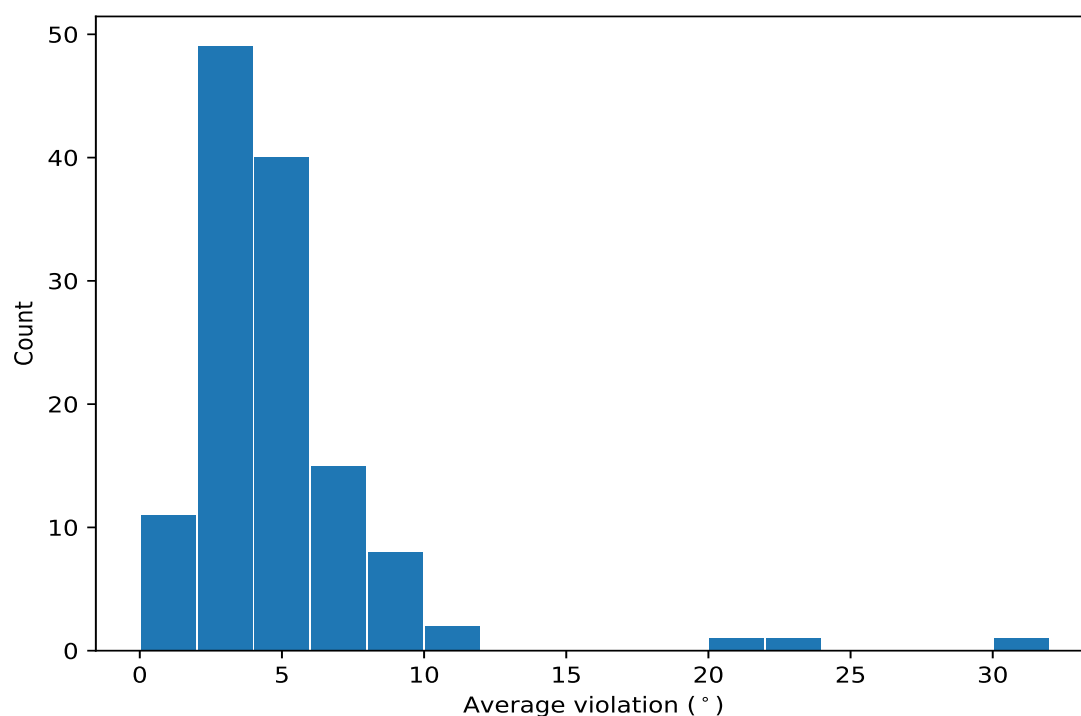
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	15	30.9	5.47	31.04
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	15	21.69	6.44	23.92
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	15	9.22	3.27	10.17
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	15	8.41	4.13	7.53
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	15	6.55	2.24	6.55
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	15	4.51	3.19	3.18
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	14	22.25	3.25	22.54
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	14	9.21	3.31	8.2
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	14	6.76	2.81	6.46
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	13	7.64	3.82	9.09
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	13	7.32	4.27	7.13
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	13	6.71	4.23	4.79
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	13	6.5	1.78	6.32
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	13	4.13	1.52	4.04
(1,222)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:SER:N	12	5.64	3.22	5.38
(1,111)	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	1:7:A:ASP:N	12	4.34	2.63	3.69
(1,194)	1:85:A:SER:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	12	3.94	1.37	3.32
(1,141)	1:33:A:ASP:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	11	11.24	4.1	11.43
(1,206)	1:95:A:ARG:C	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	11	4.81	1.48	4.6
(1,164)	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	1:52:A:THR:N	10	7.58	7.14	3.97
(1,82)	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1:125:A:LYS:N	10	4.52	2.47	4.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,242)	1:134:A:ASN:N	1:134:A:ASN:CA	1:134:A:ASN:C	1:135:A:CYS:N	10	4.2	2.51	3.4
(1,225)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:ASN:N	10	4.03	2.98	3.22
(1,142)	1:33:A:ASP:N	1:33:A:ASP:CA	1:33:A:ASP:C	1:34:A:THR:N	9	9.32	3.17	9.61
(1,172)	1:69:A:SER:C	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	9	6.68	1.54	6.07
(1,238)	1:130:A:GLY:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	9	6.16	2.28	7.33
(1,215)	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	1:102:A:VAL:N	9	4.62	3.44	3.22
(1,25)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:LYS:N	9	4.57	2.48	4.34
(1,143)	1:34:A:THR:C	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	9	4.48	2.89	4.02
(1,202)	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1:92:A:PHE:N	9	3.43	1.77	3.17
(1,138)	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	1:32:A:THR:N	9	3.21	1.96	2.44
(1,252)	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	1:140:A:SER:N	8	6.62	2.65	7.26
(1,54)	1:75:A:PHE:C	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	8	6.33	1.73	6.28
(1,109)	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1:6:A:ILE:N	8	6.24	3.85	6.7
(1,27)	1:44:A:SER:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	8	5.53	2.62	5.7
(1,227)	1:113:A:ALA:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	8	5.34	1.22	5.0
(1,56)	1:76:A:VAL:C	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	8	4.92	3.19	4.64
(1,241)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:THR:N	8	4.59	2.84	3.88
(1,161)	1:50:A:LEU:C	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	8	4.53	3.3	3.57
(1,106)	1:4:A:MET:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	8	4.26	1.94	3.95
(1,270)	1:153:A:PHE:N	1:153:A:PHE:CA	1:153:A:PHE:C	1:154:A:GLY:N	8	3.24	1.61	2.8
(1,147)	1:41:A:PRO:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	7	9.28	3.56	8.57
(1,152)	1:43:A:TYR:N	1:43:A:TYR:CA	1:43:A:TYR:C	1:44:A:SER:N	7	8.55	3.37	6.47
(1,181)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:VAL:N	7	6.28	2.92	6.37
(1,249)	1:138:A:ARG:C	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	7	4.83	2.62	5.03
(1,31)	1:55:A:VAL:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	7	4.23	1.85	4.79
(1,144)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:ALA:N	7	4.04	1.6	3.48
(1,280)	1:159:A:ALA:N	1:159:A:ALA:CA	1:159:A:ALA:C	1:160:A:GLU:N	7	2.36	0.69	2.47
(1,211)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:LEU:N	7	1.89	0.64	1.5
(1,166)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:VAL:N	6	10.17	3.65	9.68
(1,167)	1:54:A:ILE:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	6	8.64	3.18	8.42
(1,84)	1:132:A:LEU:C	1:133:A:THR:N	1:133:A:THR:CA	1:133:A:THR:C	6	4.77	1.88	4.62
(1,55)	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	1:77:A:PHE:N	6	3.81	2.33	2.89
(1,168)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:TYR:N	6	2.74	0.91	2.3
(1,33)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	6	2.71	0.97	2.76
(1,132)	1:28:A:GLU:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	6	2.37	1.75	1.72
(1,43)	1:64:A:TYR:N	1:64:A:TYR:CA	1:64:A:TYR:C	1:65:A:TRP:N	6	2.24	1.51	1.58
(1,61)	1:87:A:SER:C	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	6	1.84	0.78	1.64
(1,209)	1:97:A:LYS:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	5	6.97	3.86	8.09
(1,272)	1:154:A:GLY:N	1:154:A:GLY:CA	1:154:A:GLY:C	1:155:A:PRO:N	5	5.3	3.29	3.7
(1,203)	1:93:A:PRO:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	5	5.17	2.63	4.52
(1,108)	1:5:A:GLU:C	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	5	4.95	0.98	4.46
(1,204)	1:94:A:GLU:C	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	5	4.21	2.34	4.48
(1,110)	1:6:A:ILE:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	5	3.7	0.73	3.92
(1,73)	1:119:A:ALA:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	5	3.07	1.25	3.18
(1,174)	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	1:72:A:THR:N	5	3.0	0.92	3.03
(1,48)	1:66:A:GLU:C	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	5	2.96	1.15	3.36
(1,20)	1:35:A:ALA:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	5	2.63	0.92	2.72
(1,45)	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	1:66:A:GLU:N	5	2.39	0.47	2.15
(1,133)	1:29:A:LEU:C	1:30:A:ARG:N	1:30:A:ARG:CA	1:30:A:ARG:C	5	1.42	0.38	1.17
(1,273)	1:155:A:PRO:C	1:156:A:ASP:N	1:156:A:ASP:CA	1:156:A:ASP:C	4	4.81	3.27	3.67
(1,237)	1:127:A:CYS:N	1:127:A:CYS:CA	1:127:A:CYS:C	1:128:A:ASP:N	4	3.9	1.18	3.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,64)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ILE:N	4	3.75	1.82	3.82
(1,274)	1:156:A:ASP:N	1:156:A:ASP:CA	1:156:A:ASP:C	1:157:A:ASN:N	4	3.44	1.61	3.43
(1,47)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:CYS:N	4	3.43	1.57	3.78
(1,162)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:THR:N	4	3.4	0.95	3.24
(1,52)	1:70:A:GLY:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	4	2.66	0.89	2.67
(1,233)	1:115:A:VAL:N	1:115:A:VAL:CA	1:115:A:VAL:C	1:116:A:VAL:N	4	2.54	0.58	2.41
(1,116)	1:9:A:ASN:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	4	2.38	0.69	2.46
(1,214)	1:100:A:LYS:C	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	4	2.27	1.24	1.88
(1,261)	1:148:A:ILE:C	1:149:A:GLU:N	1:149:A:GLU:CA	1:149:A:GLU:C	4	1.87	0.6	1.88
(1,276)	1:158:A:GLU:C	1:159:A:ALA:N	1:159:A:ALA:CA	1:159:A:ALA:C	4	1.62	0.39	1.56
(1,103)	1:167:A:ASP:C	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	3	8.04	0.89	7.47
(1,197)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:CYS:N	3	5.78	3.26	6.36
(1,148)	1:42:A:ASN:C	1:43:A:TYR:N	1:43:A:TYR:CA	1:43:A:TYR:C	3	5.38	2.1	4.31
(1,262)	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	1:149:A:GLU:N	3	5.27	2.32	6.57
(1,22)	1:36:A:LEU:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	3	5.02	1.13	4.3
(1,246)	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	1:137:A:VAL:N	3	4.39	1.84	4.25
(1,151)	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	1:45:A:LEU:N	3	4.16	1.61	3.73
(1,23)	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	1:38:A:CYS:N	3	4.01	1.89	4.42
(1,165)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:ASP:N	3	3.81	1.97	4.99
(1,145)	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	1:36:A:LEU:N	3	3.33	1.5	2.29
(1,114)	1:8:A:LYS:C	1:9:A:ASN:N	1:9:A:ASN:CA	1:9:A:ASN:C	3	3.18	1.13	3.8
(1,171)	1:59:A:GLU:N	1:59:A:GLU:CA	1:59:A:GLU:C	1:60:A:TYR:N	3	3.13	1.33	3.43
(1,30)	1:53:A:ASP:C	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	3	2.92	1.08	2.65
(1,175)	1:71:A:ARG:C	1:72:A:THR:N	1:72:A:THR:CA	1:72:A:THR:C	3	2.74	1.21	3.47
(1,74)	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1:121:A:ILE:N	3	2.72	1.19	3.49
(1,131)	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	1:28:A:GLU:N	3	2.71	0.86	3.14
(1,44)	1:64:A:TYR:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	3	2.53	0.57	2.6
(1,153)	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	1:47:A:ASP:N	3	2.06	0.85	1.61
(1,21)	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	1:37:A:ILE:N	3	1.88	0.88	1.51
(1,236)	1:119:A:ALA:N	1:119:A:ALA:CA	1:119:A:ALA:C	1:120:A:ASP:N	3	1.86	0.58	2.26
(1,107)	1:4:A:MET:N	1:4:A:MET:CA	1:4:A:MET:C	1:5:A:GLU:N	2	6.86	2.41	6.86
(1,183)	1:77:A:PHE:C	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	2	5.02	1.22	5.02
(1,247)	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	1:138:A:ARG:N	2	4.81	1.9	4.81
(1,79)	1:122:A:GLU:C	1:123:A:ARG:N	1:123:A:ARG:CA	1:123:A:ARG:C	2	4.76	1.66	4.76
(1,186)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ASN:N	2	4.43	0.15	4.43
(1,136)	1:30:A:ARG:N	1:30:A:ARG:CA	1:30:A:ARG:C	1:31:A:ILE:N	2	4.07	1.34	4.07
(1,129)	1:26:A:GLU:C	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	2	4.0	2.96	4.0
(1,51)	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1:69:A:SER:N	2	4.0	2.64	4.0
(1,26)	1:38:A:CYS:C	1:39:A:LYS:N	1:39:A:LYS:CA	1:39:A:LYS:C	2	3.52	1.98	3.52
(1,88)	1:152:A:ALA:C	1:153:A:PHE:N	1:153:A:PHE:CA	1:153:A:PHE:C	2	3.45	1.87	3.45
(1,226)	1:112:A:GLU:C	1:113:A:ALA:N	1:113:A:ALA:CA	1:113:A:ALA:C	2	3.37	1.76	3.37
(1,179)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:PHE:N	2	3.36	0.52	3.36
(1,24)	1:37:A:ILE:C	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	2	3.3	0.27	3.3
(1,170)	1:58:A:VAL:C	1:59:A:GLU:N	1:59:A:GLU:CA	1:59:A:GLU:C	2	2.85	0.91	2.85
(1,15)	1:18:A:THR:C	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	2	2.82	1.78	2.82
(1,46)	1:65:A:TRP:C	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	2	2.79	0.34	2.79
(1,245)	1:135:A:CYS:N	1:135:A:CYS:CA	1:135:A:CYS:C	1:136:A:VAL:N	2	2.44	1.26	2.44
(1,19)	1:20:A:ARG:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	2	2.37	0.88	2.37
(1,67)	1:102:A:VAL:C	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	2	2.33	0.45	2.33
(1,83)	1:126:A:PRO:C	1:127:A:CYS:N	1:127:A:CYS:CA	1:127:A:CYS:C	2	2.33	1.31	2.33
(1,256)	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	1:146:A:TYR:N	2	2.25	1.01	2.25

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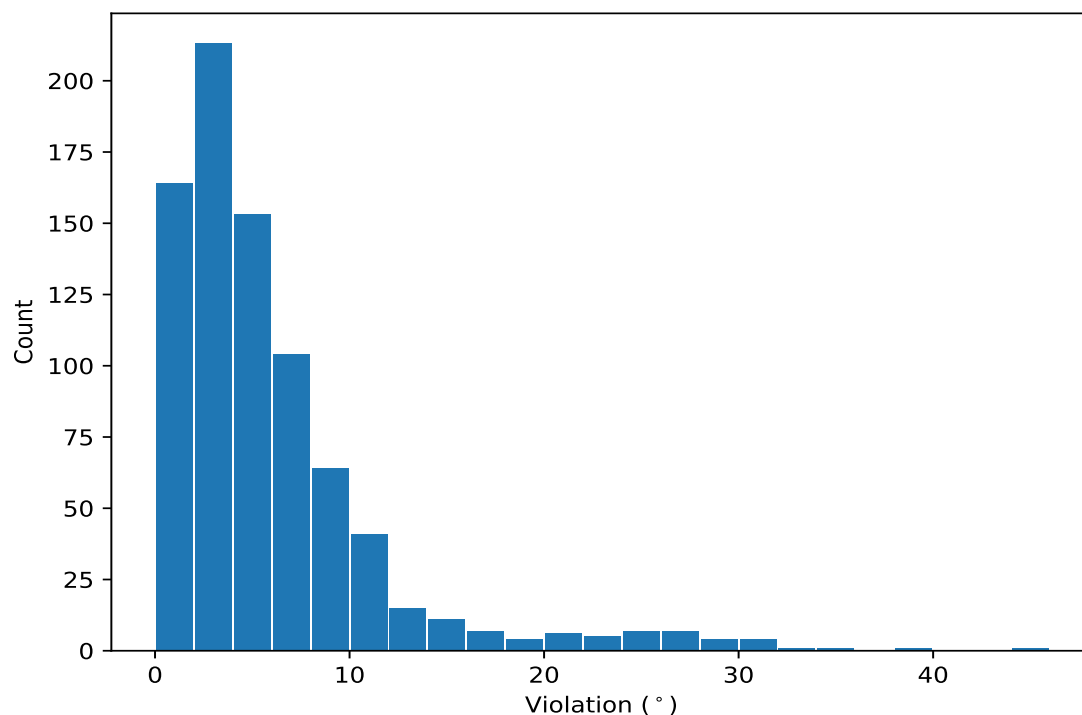
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,159)	1:49:A:MET:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	2	2.19	0.6	2.19
(1,118)	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	1:11:A:GLY:N	2	1.83	0.63	1.83
(1,104)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:TYR:N	2	1.6	0.16	1.6
(1,180)	1:74:A:CYS:C	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	2	1.54	0.24	1.54
(1,53)	1:73:A:ALA:C	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	2	1.36	0.05	1.36

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	13	44.78
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	12	38.85

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	4	34.92
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	8	33.22
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	3	31.99
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	15	31.97
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	7	31.14
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	10	31.04
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	1	29.56
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	14	28.61
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	5	28.19
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	9	28.05
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	5	27.46
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	6	27.25
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	1	27.16
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	2	26.93
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	11	26.39
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	15	26.19
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	7	26.08
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	11	25.99
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	9	25.8
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	10	25.68
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	2	25.5
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	11	24.32
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	14	24.19
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	14	24.01
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	8	23.92
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	4	22.91
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	6	22.8
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	3	22.58
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	13	22.5
(1,59)	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1:83:A:ARG:N	6	21.68
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1	21.25
(1,164)	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	1:52:A:THR:N	3	20.81
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	4	20.61
(1,164)	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	1:52:A:THR:N	4	20.51
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	8	20.34
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	9	19.92
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	5	19.65
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	2	19.15
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	7	18.44
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	3	17.91
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	10	17.58
(1,141)	1:33:A:ASP:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	9	17.55
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	3	16.73
(1,147)	1:41:A:PRO:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	8	16.69
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	1	16.24
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	6	16.03
(1,188)	1:80:A:THR:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	15	15.98
(1,141)	1:33:A:ASP:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	5	15.78
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	1	15.75
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	5	15.54
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	13	15.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,141)	1:33:A:ASP:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	10	15.45
(1,166)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:VAL:N	4	14.97
(1,167)	1:54:A:ILE:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	13	14.94
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	2	14.9
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	1	14.34
(1,166)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:VAL:N	13	14.2
(1,152)	1:43:A:TYR:N	1:43:A:TYR:CA	1:43:A:TYR:C	1:44:A:SER:N	9	13.94
(1,141)	1:33:A:ASP:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	3	13.89
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	10	13.67
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	12	13.51
(1,142)	1:33:A:ASP:N	1:33:A:ASP:CA	1:33:A:ASP:C	1:34:A:THR:N	7	13.21
(1,142)	1:33:A:ASP:N	1:33:A:ASP:CA	1:33:A:ASP:C	1:34:A:THR:N	10	13.07
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	9	12.98
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	15	12.93
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	1	12.71
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	3	12.61
(1,109)	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1:6:A:ILE:N	4	12.45
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	14	12.42
(1,209)	1:97:A:LYS:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	3	12.35
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	8	12.21
(1,217)	1:104:A:ASP:N	1:104:A:ASP:CA	1:104:A:ASP:C	1:105:A:PHE:N	4	12.12
(1,225)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:ASN:N	9	11.92
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	10	11.87
(1,147)	1:41:A:PRO:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	12	11.82
(1,142)	1:33:A:ASP:N	1:33:A:ASP:CA	1:33:A:ASP:C	1:34:A:THR:N	6	11.77
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	10	11.77
(1,161)	1:50:A:LEU:C	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	10	11.75
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	14	11.65
(1,152)	1:43:A:TYR:N	1:43:A:TYR:CA	1:43:A:TYR:C	1:44:A:SER:N	14	11.56
(1,141)	1:33:A:ASP:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	6	11.55
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	2	11.48
(1,152)	1:43:A:TYR:N	1:43:A:TYR:CA	1:43:A:TYR:C	1:44:A:SER:N	11	11.46
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	14	11.44
(1,141)	1:33:A:ASP:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	7	11.43
(1,272)	1:154:A:GLY:N	1:154:A:GLY:CA	1:154:A:GLY:C	1:155:A:PRO:N	11	11.37
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	11	11.31
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	14	11.22
(1,215)	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	1:102:A:VAL:N	13	11.2
(1,111)	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	1:7:A:ASP:N	5	11.18
(1,222)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:SER:N	13	11.05
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	4	10.96
(1,141)	1:33:A:ASP:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	11	10.93
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	5	10.91
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	7	10.84
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	11	10.83
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	15	10.76
(1,142)	1:33:A:ASP:N	1:33:A:ASP:CA	1:33:A:ASP:C	1:34:A:THR:N	11	10.69
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	4	10.68
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	9	10.65
(1,56)	1:76:A:VAL:C	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	4	10.57
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1	10.53

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	11	10.51
(1,141)	1:33:A:ASP:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	12	10.5
(1,222)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:SER:N	14	10.37
(1,109)	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1:6:A:ILE:N	13	10.34
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	13	10.31
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	13	10.17
(1,164)	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	1:52:A:THR:N	7	10.13
(1,273)	1:155:A:PRO:C	1:156:A:ASP:N	1:156:A:ASP:CA	1:156:A:ASP:C	13	10.12
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	12	10.05
(1,252)	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	1:140:A:SER:N	14	10.01
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	5	10.0
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	3	9.96
(1,215)	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	1:102:A:VAL:N	10	9.91
(1,181)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:VAL:N	8	9.85
(1,166)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:VAL:N	3	9.85
(1,249)	1:138:A:ARG:C	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	13	9.84
(1,54)	1:75:A:PHE:C	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	14	9.68
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	3	9.67
(1,203)	1:93:A:PRO:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	6	9.66
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	9	9.61
(1,181)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:VAL:N	5	9.61
(1,142)	1:33:A:ASP:N	1:33:A:ASP:CA	1:33:A:ASP:C	1:34:A:THR:N	3	9.61
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	13	9.6
(1,166)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:VAL:N	15	9.5
(1,197)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:CYS:N	8	9.46
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	9	9.34
(1,222)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:SER:N	4	9.32
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	5	9.31
(1,103)	1:167:A:ASP:C	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	15	9.3
(1,107)	1:4:A:MET:N	1:4:A:MET:CA	1:4:A:MET:C	1:5:A:GLU:N	11	9.27
(1,241)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:THR:N	7	9.25
(1,209)	1:97:A:LYS:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	2	9.16
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	8	9.09
(1,167)	1:54:A:ILE:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	4	9.06
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	11	9.05
(1,252)	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	1:140:A:SER:N	6	8.99
(1,164)	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	1:52:A:THR:N	13	8.96
(1,242)	1:134:A:ASN:N	1:134:A:ASN:CA	1:134:A:ASN:C	1:135:A:CYS:N	12	8.93
(1,27)	1:44:A:SER:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	14	8.92
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	3	8.9
(1,147)	1:41:A:PRO:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	1	8.9
(1,167)	1:54:A:ILE:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	3	8.88
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	2	8.88
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	11	8.85
(1,82)	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1:125:A:LYS:N	7	8.85
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	9	8.77
(1,142)	1:33:A:ASP:N	1:33:A:ASP:CA	1:33:A:ASP:C	1:34:A:THR:N	9	8.74
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	5	8.68
(1,172)	1:69:A:SER:C	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	12	8.68
(1,172)	1:69:A:SER:C	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	3	8.66
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	6	8.64

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	15	8.64
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	13	8.62
(1,238)	1:130:A:GLY:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	4	8.57
(1,147)	1:41:A:PRO:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	3	8.57
(1,238)	1:130:A:GLY:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	2	8.47
(1,166)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:VAL:N	2	8.44
(1,143)	1:34:A:THR:C	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	5	8.44
(1,252)	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	1:140:A:SER:N	10	8.36
(1,143)	1:34:A:THR:C	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	11	8.36
(1,82)	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1:125:A:LYS:N	14	8.34
(1,148)	1:42:A:ASN:C	1:43:A:TYR:N	1:43:A:TYR:CA	1:43:A:TYR:C	5	8.31
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	6	8.27
(1,25)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:LYS:N	13	8.26
(1,172)	1:69:A:SER:C	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1	8.16
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	4	8.15
(1,56)	1:76:A:VAL:C	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	3	8.14
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	8	8.11
(1,209)	1:97:A:LYS:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	9	8.09
(1,109)	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1:6:A:ILE:N	7	8.09
(1,27)	1:44:A:SER:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	9	8.08
(1,84)	1:132:A:LEU:C	1:133:A:THR:N	1:133:A:THR:CA	1:133:A:THR:C	1	8.05
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	4	8.05
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	4	8.01
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	13	8.0
(1,55)	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	1:77:A:PHE:N	1	7.98
(1,167)	1:54:A:ILE:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	2	7.95
(1,54)	1:75:A:PHE:C	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	12	7.93
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	8	7.75
(1,241)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:THR:N	6	7.72
(1,222)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:SER:N	15	7.7
(1,238)	1:130:A:GLY:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	15	7.68
(1,204)	1:94:A:GLU:C	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	13	7.65
(1,138)	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	1:32:A:THR:N	8	7.63
(1,181)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:VAL:N	6	7.62
(1,27)	1:44:A:SER:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	11	7.61
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	9	7.6
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	8	7.53
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	5	7.49
(1,172)	1:69:A:SER:C	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	13	7.48
(1,103)	1:167:A:ASP:C	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	4	7.47
(1,238)	1:130:A:GLY:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	5	7.43
(1,25)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:LYS:N	4	7.37
(1,27)	1:44:A:SER:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	13	7.36
(1,252)	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	1:140:A:SER:N	2	7.34
(1,111)	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	1:7:A:ASP:N	12	7.34
(1,103)	1:167:A:ASP:C	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	6	7.34
(1,238)	1:130:A:GLY:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	6	7.33
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	9	7.33
(1,109)	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1:6:A:ILE:N	3	7.33
(1,142)	1:33:A:ASP:N	1:33:A:ASP:CA	1:33:A:ASP:C	1:34:A:THR:N	5	7.28
(1,106)	1:4:A:MET:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	14	7.24

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,262)	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	1:149:A:GLU:N	6	7.22
(1,25)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:LYS:N	8	7.19
(1,252)	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	1:140:A:SER:N	3	7.18
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	1	7.16
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	14	7.13
(1,206)	1:95:A:ARG:C	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	1	7.12
(1,143)	1:34:A:THR:C	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	10	7.12
(1,227)	1:113:A:ALA:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	3	7.08
(1,129)	1:26:A:GLU:C	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	1	6.97
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	3	6.97
(1,54)	1:75:A:PHE:C	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	11	6.94
(1,144)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:ALA:N	11	6.9
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	7	6.88
(1,31)	1:55:A:VAL:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1	6.85
(1,227)	1:113:A:ALA:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	15	6.84
(1,241)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:THR:N	5	6.82
(1,147)	1:41:A:PRO:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	7	6.82
(1,242)	1:134:A:ASN:N	1:134:A:ASN:CA	1:134:A:ASN:C	1:135:A:CYS:N	13	6.77
(1,247)	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	1:138:A:ARG:N	11	6.71
(1,246)	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	1:137:A:VAL:N	6	6.71
(1,202)	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1:92:A:PHE:N	10	6.69
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	11	6.68
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	2	6.66
(1,56)	1:76:A:VAL:C	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	5	6.65
(1,51)	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1:69:A:SER:N	14	6.64
(1,108)	1:5:A:GLU:C	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	10	6.63
(1,238)	1:130:A:GLY:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	8	6.62
(1,142)	1:33:A:ASP:N	1:33:A:ASP:CA	1:33:A:ASP:C	1:34:A:THR:N	1	6.62
(1,22)	1:36:A:LEU:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	1	6.62
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	13	6.61
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	6	6.58
(1,262)	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	1:149:A:GLU:N	13	6.57
(1,106)	1:4:A:MET:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	6	6.55
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	6	6.55
(1,222)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:SER:N	3	6.54
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	8	6.54
(1,152)	1:43:A:TYR:N	1:43:A:TYR:CA	1:43:A:TYR:C	1:44:A:SER:N	6	6.47
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	7	6.46
(1,227)	1:113:A:ALA:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	1	6.44
(1,147)	1:41:A:PRO:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	5	6.44
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	12	6.42
(1,79)	1:122:A:GLU:C	1:123:A:ARG:N	1:123:A:ARG:CA	1:123:A:ARG:C	2	6.42
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	15	6.41
(1,181)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:VAL:N	7	6.37
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	6	6.37
(1,197)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:CYS:N	7	6.36
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	3	6.33
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	12	6.32
(1,151)	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	1:45:A:LEU:N	5	6.31
(1,54)	1:75:A:PHE:C	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	7	6.3
(1,249)	1:138:A:ARG:C	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	2	6.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,206)	1:95:A:ARG:C	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	5	6.26
(1,203)	1:93:A:PRO:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	8	6.26
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	5	6.25
(1,54)	1:75:A:PHE:C	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	8	6.25
(1,183)	1:77:A:PHE:C	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	9	6.24
(1,161)	1:50:A:LEU:C	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	4	6.24
(1,242)	1:134:A:ASN:N	1:134:A:ASN:CA	1:134:A:ASN:C	1:135:A:CYS:N	2	6.23
(1,252)	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	1:140:A:SER:N	13	6.22
(1,31)	1:55:A:VAL:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	2	6.22
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	2	6.21
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	5	6.2
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	12	6.2
(1,194)	1:85:A:SER:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	8	6.18
(1,181)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:VAL:N	12	6.17
(1,132)	1:28:A:GLU:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1	6.17
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	9	6.1
(1,23)	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	1:38:A:CYS:N	15	6.09
(1,206)	1:95:A:ARG:C	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	12	6.07
(1,172)	1:69:A:SER:C	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	14	6.07
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	13	6.07
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	7	6.06
(1,167)	1:54:A:ILE:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	6	6.06
(1,109)	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1:6:A:ILE:N	9	6.06
(1,194)	1:85:A:SER:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	13	6.05
(1,14)	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:C	1:19:A:ARG:N	15	6.05
(1,272)	1:154:A:GLY:N	1:154:A:GLY:CA	1:154:A:GLY:C	1:155:A:PRO:N	13	6.03
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	14	5.97
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	10	5.96
(1,141)	1:33:A:ASP:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	2	5.96
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	11	5.96
(1,161)	1:50:A:LEU:C	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	2	5.95
(1,242)	1:134:A:ASN:N	1:134:A:ASN:CA	1:134:A:ASN:C	1:135:A:CYS:N	3	5.91
(1,206)	1:95:A:ARG:C	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	14	5.91
(1,143)	1:34:A:THR:C	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	7	5.84
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	7	5.84
(1,237)	1:127:A:CYS:N	1:127:A:CYS:CA	1:127:A:CYS:C	1:128:A:ASP:N	9	5.82
(1,106)	1:4:A:MET:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	11	5.82
(1,141)	1:33:A:ASP:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	8	5.81
(1,222)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:SER:N	6	5.8
(1,152)	1:43:A:TYR:N	1:43:A:TYR:CA	1:43:A:TYR:C	1:44:A:SER:N	15	5.8
(1,64)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ILE:N	6	5.8
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	6	5.79
(1,172)	1:69:A:SER:C	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	8	5.78
(1,202)	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1:92:A:PHE:N	13	5.76
(1,152)	1:43:A:TYR:N	1:43:A:TYR:CA	1:43:A:TYR:C	1:44:A:SER:N	12	5.76
(1,55)	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	1:77:A:PHE:N	10	5.74
(1,270)	1:153:A:PHE:N	1:153:A:PHE:CA	1:153:A:PHE:C	1:154:A:GLY:N	9	5.73
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	12	5.72
(1,147)	1:41:A:PRO:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	4	5.71
(1,84)	1:132:A:LEU:C	1:133:A:THR:N	1:133:A:THR:CA	1:133:A:THR:C	15	5.71
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	2	5.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,172)	1:69:A:SER:C	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	5	5.69
(1,138)	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	1:32:A:THR:N	2	5.69
(1,60)	1:82:A:CYS:C	1:83:A:ARG:N	1:83:A:ARG:CA	1:83:A:ARG:C	10	5.68
(1,204)	1:94:A:GLU:C	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	8	5.67
(1,274)	1:156:A:ASP:N	1:156:A:ASP:CA	1:156:A:ASP:C	1:157:A:ASN:N	11	5.66
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	15	5.65
(1,56)	1:76:A:VAL:C	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	1	5.64
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	10	5.63
(1,82)	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1:125:A:LYS:N	4	5.63
(1,84)	1:132:A:LEU:C	1:133:A:THR:N	1:133:A:THR:CA	1:133:A:THR:C	6	5.56
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	1	5.55
(1,172)	1:69:A:SER:C	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	6	5.53
(1,25)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:LYS:N	1	5.53
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	11	5.52
(1,26)	1:38:A:CYS:C	1:39:A:LYS:N	1:39:A:LYS:CA	1:39:A:LYS:C	13	5.5
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	6	5.49
(1,215)	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	1:102:A:VAL:N	11	5.47
(1,111)	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	1:7:A:ASP:N	4	5.47
(1,145)	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	1:36:A:LEU:N	5	5.45
(1,108)	1:5:A:GLU:C	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	12	5.45
(1,43)	1:64:A:TYR:N	1:64:A:TYR:CA	1:64:A:TYR:C	1:65:A:TRP:N	15	5.44
(1,206)	1:95:A:ARG:C	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	6	5.43
(1,82)	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1:125:A:LYS:N	11	5.43
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	4	5.43
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	3	5.41
(1,165)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:ASP:N	11	5.4
(1,136)	1:30:A:ARG:N	1:30:A:ARG:CA	1:30:A:ARG:C	1:31:A:ILE:N	7	5.4
(1,88)	1:152:A:ALA:C	1:153:A:PHE:N	1:153:A:PHE:CA	1:153:A:PHE:C	2	5.32
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	7	5.3
(1,64)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ILE:N	4	5.29
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	14	5.28
(1,270)	1:153:A:PHE:N	1:153:A:PHE:CA	1:153:A:PHE:C	1:154:A:GLY:N	8	5.27
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	8	5.25
(1,227)	1:113:A:ALA:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	10	5.22
(1,194)	1:85:A:SER:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	12	5.19
(1,73)	1:119:A:ALA:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	8	5.18
(1,194)	1:85:A:SER:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	6	5.16
(1,69)	1:103:A:CYS:C	1:104:A:ASP:N	1:104:A:ASP:CA	1:104:A:ASP:C	4	5.16
(1,47)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:CYS:N	13	5.14
(1,226)	1:112:A:GLU:C	1:113:A:ALA:N	1:113:A:ALA:CA	1:113:A:ALA:C	9	5.13
(1,225)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:ASN:N	13	5.12
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	14	5.12
(1,161)	1:50:A:LEU:C	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	3	5.07
(1,144)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:ALA:N	5	5.05
(1,249)	1:138:A:ARG:C	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	14	5.04
(1,249)	1:138:A:ARG:C	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	3	5.03
(1,111)	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	1:7:A:ASP:N	11	5.02
(1,144)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:ALA:N	3	5.0
(1,165)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:ASP:N	3	4.99
(1,31)	1:55:A:VAL:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	14	4.98
(1,222)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:SER:N	10	4.96

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,167)	1:54:A:ILE:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	15	4.95
(1,87)	1:136:A:VAL:C	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	10	4.95
(1,152)	1:43:A:TYR:N	1:43:A:TYR:CA	1:43:A:TYR:C	1:44:A:SER:N	13	4.88
(1,225)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:ASN:N	6	4.87
(1,162)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:THR:N	4	4.86
(1,273)	1:155:A:PRO:C	1:156:A:ASP:N	1:156:A:ASP:CA	1:156:A:ASP:C	11	4.84
(1,225)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:ASN:N	14	4.83
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	5	4.79
(1,31)	1:55:A:VAL:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	6	4.79
(1,227)	1:113:A:ALA:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	9	4.78
(1,141)	1:33:A:ASP:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	15	4.77
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	15	4.77
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	1	4.73
(1,82)	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1:125:A:LYS:N	5	4.73
(1,227)	1:113:A:ALA:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	11	4.7
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	10	4.7
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	6	4.66
(1,110)	1:6:A:ILE:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	10	4.65
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	6	4.63
(1,242)	1:134:A:ASN:N	1:134:A:ASN:CA	1:134:A:ASN:C	1:135:A:CYS:N	4	4.6
(1,206)	1:95:A:ARG:C	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	15	4.6
(1,15)	1:18:A:THR:C	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	15	4.6
(1,171)	1:59:A:GLU:N	1:59:A:GLU:CA	1:59:A:GLU:C	1:60:A:TYR:N	12	4.59
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	7	4.59
(1,186)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ASN:N	3	4.58
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	7	4.58
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	14	4.55
(1,54)	1:75:A:PHE:C	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	6	4.55
(1,203)	1:93:A:PRO:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	5	4.52
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	13	4.52
(1,54)	1:75:A:PHE:C	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	1	4.52
(1,270)	1:153:A:PHE:N	1:153:A:PHE:CA	1:153:A:PHE:C	1:154:A:GLY:N	14	4.5
(1,204)	1:94:A:GLU:C	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	14	4.48
(1,54)	1:75:A:PHE:C	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	5	4.47
(1,108)	1:5:A:GLU:C	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	11	4.46
(1,206)	1:95:A:ARG:C	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	9	4.45
(1,206)	1:95:A:ARG:C	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	13	4.45
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	11	4.45
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	3	4.45
(1,107)	1:4:A:MET:N	1:4:A:MET:CA	1:4:A:MET:C	1:5:A:GLU:N	12	4.44
(1,47)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:CYS:N	10	4.44
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	2	4.43
(1,23)	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	1:38:A:CYS:N	13	4.42
(1,28)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:CYS:N	8	4.41
(1,194)	1:85:A:SER:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	7	4.38
(1,48)	1:66:A:GLU:C	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	8	4.38
(1,215)	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	1:102:A:VAL:N	5	4.36
(1,30)	1:53:A:ASP:C	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	3	4.35
(1,25)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:LYS:N	2	4.34
(1,111)	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	1:7:A:ASP:N	3	4.33
(1,148)	1:42:A:ASN:C	1:43:A:TYR:N	1:43:A:TYR:CA	1:43:A:TYR:C	3	4.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,22)	1:36:A:LEU:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	4	4.3
(1,214)	1:100:A:LYS:C	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	8	4.29
(1,186)	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	1:79:A:ASN:N	9	4.28
(1,108)	1:5:A:GLU:C	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	3	4.28
(1,241)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:THR:N	9	4.26
(1,174)	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	1:72:A:THR:N	5	4.26
(1,246)	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	1:137:A:VAL:N	11	4.25
(1,164)	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	1:52:A:THR:N	6	4.24
(1,238)	1:130:A:GLY:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	9	4.23
(1,105)	1:3:A:HIS:C	1:4:A:MET:N	1:4:A:MET:CA	1:4:A:MET:C	11	4.23
(1,168)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:TYR:N	2	4.22
(1,249)	1:138:A:ARG:C	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	6	4.21
(1,202)	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1:92:A:PHE:N	1	4.19
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	4	4.19
(1,110)	1:6:A:ILE:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	2	4.18
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	7	4.16
(1,111)	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	1:7:A:ASP:N	9	4.16
(1,114)	1:8:A:LYS:C	1:9:A:ASN:N	1:9:A:ASN:CA	1:9:A:ASN:C	8	4.14
(1,22)	1:36:A:LEU:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	8	4.14
(1,33)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	13	4.12
(1,166)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:VAL:N	11	4.08
(1,82)	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1:125:A:LYS:N	12	4.05
(1,27)	1:44:A:SER:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	15	4.05
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	14	4.04
(1,172)	1:69:A:SER:C	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	2	4.03
(1,143)	1:34:A:THR:C	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	9	4.02
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	10	3.99
(1,274)	1:156:A:ASP:N	1:156:A:ASP:CA	1:156:A:ASP:C	1:157:A:ASN:N	13	3.99
(1,106)	1:4:A:MET:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	10	3.96
(1,108)	1:5:A:GLU:C	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	5	3.94
(1,106)	1:4:A:MET:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1	3.94
(1,202)	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1:92:A:PHE:N	15	3.92
(1,110)	1:6:A:ILE:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	11	3.92
(1,227)	1:113:A:ALA:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	4	3.91
(1,80)	1:123:A:ARG:N	1:123:A:ARG:CA	1:123:A:ARG:C	1:124:A:ILE:N	8	3.91
(1,237)	1:127:A:CYS:N	1:127:A:CYS:CA	1:127:A:CYS:C	1:128:A:ASP:N	6	3.9
(1,52)	1:70:A:GLY:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	1	3.9
(1,179)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:PHE:N	14	3.88
(1,206)	1:95:A:ARG:C	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	11	3.86
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	15	3.8
(1,255)	1:145:A:SER:C	1:146:A:TYR:N	1:146:A:TYR:CA	1:146:A:TYR:C	11	3.8
(1,183)	1:77:A:PHE:C	1:78:A:LYS:N	1:78:A:LYS:CA	1:78:A:LYS:C	2	3.8
(1,114)	1:8:A:LYS:C	1:9:A:ASN:N	1:9:A:ASN:CA	1:9:A:ASN:C	2	3.8
(1,27)	1:44:A:SER:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	7	3.78
(1,48)	1:66:A:GLU:C	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	2	3.77
(1,170)	1:58:A:VAL:C	1:59:A:GLU:N	1:59:A:GLU:CA	1:59:A:GLU:C	6	3.76
(1,174)	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	1:72:A:THR:N	7	3.75
(1,227)	1:113:A:ALA:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	14	3.74
(1,168)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:TYR:N	11	3.74
(1,151)	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	1:45:A:LEU:N	4	3.73
(1,175)	1:71:A:ARG:C	1:72:A:THR:N	1:72:A:THR:CA	1:72:A:THR:C	9	3.72

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,272)	1:154:A:GLY:N	1:154:A:GLY:CA	1:154:A:GLY:C	1:155:A:PRO:N	3	3.7
(1,245)	1:135:A:CYS:N	1:135:A:CYS:CA	1:135:A:CYS:C	1:136:A:VAL:N	12	3.7
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	6	3.7
(1,164)	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	1:52:A:THR:N	2	3.7
(1,84)	1:132:A:LEU:C	1:133:A:THR:N	1:133:A:THR:CA	1:133:A:THR:C	5	3.69
(1,20)	1:35:A:ALA:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	1	3.69
(1,83)	1:126:A:PRO:C	1:127:A:CYS:N	1:127:A:CYS:CA	1:127:A:CYS:C	7	3.64
(1,74)	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1:121:A:ILE:N	6	3.64
(1,56)	1:76:A:VAL:C	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	11	3.63
(1,24)	1:37:A:ILE:C	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	2	3.57
(1,20)	1:35:A:ALA:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	8	3.53
(1,148)	1:42:A:ASN:C	1:43:A:TYR:N	1:43:A:TYR:CA	1:43:A:TYR:C	2	3.51
(1,241)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:THR:N	14	3.49
(1,74)	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1:121:A:ILE:N	11	3.49
(1,144)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:ALA:N	7	3.48
(1,131)	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	1:28:A:GLU:N	4	3.48
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	4	3.48
(1,175)	1:71:A:ARG:C	1:72:A:THR:N	1:72:A:THR:CA	1:72:A:THR:C	10	3.47
(1,233)	1:115:A:VAL:N	1:115:A:VAL:CA	1:115:A:VAL:C	1:116:A:VAL:N	3	3.46
(1,209)	1:97:A:LYS:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	4	3.45
(1,33)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	8	3.45
(1,171)	1:59:A:GLU:N	1:59:A:GLU:CA	1:59:A:GLU:C	1:60:A:TYR:N	7	3.43
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	2	3.42
(1,162)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:THR:N	9	3.39
(1,194)	1:85:A:SER:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	11	3.36
(1,48)	1:66:A:GLU:C	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	5	3.36
(1,27)	1:44:A:SER:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	6	3.35
(1,203)	1:93:A:PRO:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	3	3.33
(1,144)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:ALA:N	9	3.32
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	1	3.32
(1,225)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:ASN:N	5	3.31
(1,280)	1:159:A:ALA:N	1:159:A:ALA:CA	1:159:A:ALA:C	1:160:A:GLU:N	3	3.29
(1,194)	1:85:A:SER:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	2	3.27
(1,256)	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	1:146:A:TYR:N	13	3.26
(1,153)	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	1:47:A:ASP:N	1	3.26
(1,116)	1:9:A:ASN:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	4	3.25
(1,138)	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	1:32:A:THR:N	5	3.24
(1,19)	1:20:A:ARG:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	1	3.24
(1,272)	1:154:A:GLY:N	1:154:A:GLY:CA	1:154:A:GLY:C	1:155:A:PRO:N	7	3.22
(1,215)	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	1:102:A:VAL:N	14	3.22
(1,111)	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	1:7:A:ASP:N	7	3.22
(1,122)	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	1:23:A:ARG:N	14	3.21
(1,73)	1:119:A:ALA:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	10	3.2
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	15	3.19
(1,44)	1:64:A:TYR:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	15	3.19
(1,194)	1:85:A:SER:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	9	3.18
(1,73)	1:119:A:ALA:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	15	3.18
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1	3.18
(1,33)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	11	3.18
(1,202)	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1:92:A:PHE:N	3	3.17
(1,143)	1:34:A:THR:C	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	3	3.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,55)	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	1:77:A:PHE:N	3	3.15
(1,131)	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	1:28:A:GLU:N	1	3.14
(1,225)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:ASN:N	7	3.13
(1,46)	1:65:A:TRP:C	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	15	3.13
(1,47)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:CYS:N	1	3.12
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	11	3.11
(1,110)	1:6:A:ILE:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	3	3.11
(1,45)	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	1:66:A:GLU:N	4	3.11
(1,111)	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	1:7:A:ASP:N	2	3.1
(1,79)	1:122:A:GLU:C	1:123:A:ARG:N	1:123:A:ARG:CA	1:123:A:ARG:C	12	3.1
(1,61)	1:87:A:SER:C	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	7	3.1
(1,280)	1:159:A:ALA:N	1:159:A:ALA:CA	1:159:A:ALA:C	1:160:A:GLU:N	5	3.09
(1,162)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:THR:N	8	3.09
(1,21)	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	1:37:A:ILE:N	15	3.09
(1,225)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:ASN:N	12	3.08
(1,194)	1:85:A:SER:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	15	3.06
(1,237)	1:127:A:CYS:N	1:127:A:CYS:CA	1:127:A:CYS:C	1:128:A:ASP:N	3	3.04
(1,222)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:SER:N	5	3.04
(1,111)	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	1:7:A:ASP:N	10	3.04
(1,174)	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	1:72:A:THR:N	11	3.03
(1,194)	1:85:A:SER:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	5	3.02
(1,24)	1:37:A:ILE:C	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	4	3.02
(1,58)	1:81:A:GLY:C	1:82:A:CYS:N	1:82:A:CYS:CA	1:82:A:CYS:C	10	3.01
(1,215)	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	1:102:A:VAL:N	6	3.0
(1,270)	1:153:A:PHE:N	1:153:A:PHE:CA	1:153:A:PHE:C	1:154:A:GLY:N	15	2.97
(1,84)	1:132:A:LEU:C	1:133:A:THR:N	1:133:A:THR:CA	1:133:A:THR:C	9	2.93
(1,25)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:LYS:N	12	2.93
(1,247)	1:137:A:VAL:N	1:137:A:VAL:CA	1:137:A:VAL:C	1:138:A:ARG:N	10	2.91
(1,206)	1:95:A:ARG:C	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	8	2.9
(1,274)	1:156:A:ASP:N	1:156:A:ASP:CA	1:156:A:ASP:C	1:157:A:ASN:N	5	2.87
(1,142)	1:33:A:ASP:N	1:33:A:ASP:CA	1:33:A:ASP:C	1:34:A:THR:N	15	2.87
(1,144)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:ALA:N	10	2.85
(1,194)	1:85:A:SER:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	14	2.84
(1,179)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:PHE:N	8	2.84
(1,237)	1:127:A:CYS:N	1:127:A:CYS:CA	1:127:A:CYS:C	1:128:A:ASP:N	15	2.83
(1,211)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:LEU:N	9	2.82
(1,241)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:THR:N	4	2.81
(1,52)	1:70:A:GLY:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	12	2.8
(1,222)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:SER:N	9	2.79
(1,159)	1:49:A:MET:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	10	2.79
(1,238)	1:130:A:GLY:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1	2.78
(1,67)	1:102:A:VAL:C	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	14	2.78
(1,31)	1:55:A:VAL:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	12	2.78
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	9	2.76
(1,45)	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	1:66:A:GLU:N	5	2.75
(1,138)	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	1:32:A:THR:N	6	2.74
(1,109)	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1:6:A:ILE:N	14	2.74
(1,136)	1:30:A:ARG:N	1:30:A:ARG:CA	1:30:A:ARG:C	1:31:A:ILE:N	2	2.73
(1,20)	1:35:A:ALA:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	2	2.72
(1,211)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:LEU:N	3	2.7
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	5	2.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,252)	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	1:140:A:SER:N	4	2.69
(1,84)	1:132:A:LEU:C	1:133:A:THR:N	1:133:A:THR:CA	1:133:A:THR:C	4	2.68
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	15	2.68
(1,106)	1:4:A:MET:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	5	2.65
(1,30)	1:53:A:ASP:C	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	11	2.65
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	8	2.64
(1,280)	1:159:A:ALA:N	1:159:A:ALA:CA	1:159:A:ALA:C	1:160:A:GLU:N	8	2.63
(1,270)	1:153:A:PHE:N	1:153:A:PHE:CA	1:153:A:PHE:C	1:154:A:GLY:N	13	2.63
(1,116)	1:9:A:ASN:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	7	2.63
(1,55)	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	1:77:A:PHE:N	4	2.63
(1,25)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:LYS:N	14	2.63
(1,164)	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	1:52:A:THR:N	14	2.62
(1,110)	1:6:A:ILE:C	1:7:A:ASP:N	1:7:A:ASP:CA	1:7:A:ASP:C	12	2.62
(1,44)	1:64:A:TYR:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	5	2.6
(1,164)	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	1:52:A:THR:N	11	2.58
(1,111)	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	1:7:A:ASP:N	14	2.58
(1,261)	1:148:A:ILE:C	1:149:A:GLU:N	1:149:A:GLU:CA	1:149:A:GLU:C	3	2.56
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	5	2.56
(1,43)	1:64:A:TYR:N	1:64:A:TYR:CA	1:64:A:TYR:C	1:65:A:TRP:N	11	2.56
(1,158)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:MET:N	2	2.54
(1,82)	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1:125:A:LYS:N	2	2.54
(1,52)	1:70:A:GLY:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	13	2.54
(1,198)	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1:87:A:SER:N	14	2.52
(1,181)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:VAL:N	2	2.52
(1,135)	1:30:A:ARG:C	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	2	2.51
(1,61)	1:87:A:SER:C	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	12	2.51
(1,273)	1:155:A:PRO:C	1:156:A:ASP:N	1:156:A:ASP:CA	1:156:A:ASP:C	8	2.5
(1,280)	1:159:A:ALA:N	1:159:A:ALA:CA	1:159:A:ALA:C	1:160:A:GLU:N	11	2.47
(1,118)	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	1:11:A:GLY:N	10	2.46
(1,233)	1:115:A:VAL:N	1:115:A:VAL:CA	1:115:A:VAL:C	1:116:A:VAL:N	2	2.45
(1,151)	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	1:45:A:LEU:N	1	2.45
(1,46)	1:65:A:TRP:C	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	4	2.45
(1,138)	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	1:32:A:THR:N	11	2.44
(1,73)	1:119:A:ALA:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	11	2.4
(1,189)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:CYS:N	12	2.39
(1,233)	1:115:A:VAL:N	1:115:A:VAL:CA	1:115:A:VAL:C	1:116:A:VAL:N	15	2.37
(1,261)	1:148:A:ILE:C	1:149:A:GLU:N	1:149:A:GLU:CA	1:149:A:GLU:C	2	2.36
(1,64)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ILE:N	3	2.35
(1,33)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	2	2.34
(1,106)	1:4:A:MET:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	2	2.33
(1,168)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:TYR:N	14	2.32
(1,132)	1:28:A:GLU:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	7	2.32
(1,238)	1:130:A:GLY:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	10	2.31
(1,82)	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1:125:A:LYS:N	3	2.31
(1,211)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:LEU:N	7	2.3
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	8	2.3
(1,145)	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	1:36:A:LEU:N	7	2.29
(1,236)	1:119:A:ALA:N	1:119:A:ALA:CA	1:119:A:ALA:C	1:120:A:ASP:N	3	2.28
(1,116)	1:9:A:ASN:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	13	2.28
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	10	2.28
(1,249)	1:138:A:ARG:C	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	7	2.27

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	3	2.27
(1,168)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:TYR:N	10	2.27
(1,236)	1:119:A:ALA:N	1:119:A:ALA:CA	1:119:A:ALA:C	1:120:A:ASP:N	7	2.26
(1,81)	1:123:A:ARG:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	11	2.26
(1,145)	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	1:36:A:LEU:N	3	2.25
(1,162)	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	1:51:A:THR:N	3	2.24
(1,31)	1:55:A:VAL:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	5	2.22
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	2	2.21
(1,246)	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	1:137:A:VAL:N	5	2.2
(1,242)	1:134:A:ASN:N	1:134:A:ASN:CA	1:134:A:ASN:C	1:135:A:CYS:N	9	2.2
(1,214)	1:100:A:LYS:C	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	7	2.19
(1,202)	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1:92:A:PHE:N	11	2.19
(1,272)	1:154:A:GLY:N	1:154:A:GLY:CA	1:154:A:GLY:C	1:155:A:PRO:N	9	2.18
(1,68)	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	1:104:A:ASP:N	12	2.18
(1,252)	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	1:140:A:SER:N	5	2.17
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	7	2.17
(1,276)	1:158:A:GLU:C	1:159:A:ALA:N	1:159:A:ALA:CA	1:159:A:ALA:C	6	2.15
(1,45)	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	1:66:A:GLU:N	14	2.15
(1,242)	1:134:A:ASN:N	1:134:A:ASN:CA	1:134:A:ASN:C	1:135:A:CYS:N	6	2.14
(1,55)	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	1:77:A:PHE:N	5	2.14
(1,168)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:TYR:N	1	2.12
(1,203)	1:93:A:PRO:C	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	14	2.1
(1,222)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:SER:N	2	2.09
(1,61)	1:87:A:SER:C	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	11	2.08
(1,161)	1:50:A:LEU:C	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	1	2.07
(1,242)	1:134:A:ASN:N	1:134:A:ASN:CA	1:134:A:ASN:C	1:135:A:CYS:N	7	2.06
(1,138)	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	1:32:A:THR:N	13	2.06
(1,41)	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	1:64:A:TYR:N	14	2.06
(1,270)	1:153:A:PHE:N	1:153:A:PHE:CA	1:153:A:PHE:C	1:154:A:GLY:N	3	2.04
(1,222)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:SER:N	8	2.04
(1,161)	1:50:A:LEU:C	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	5	2.04
(1,48)	1:66:A:GLU:C	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	12	2.03
(1,45)	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	1:66:A:GLU:N	15	2.03
(1,40)	1:62:A:LEU:C	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	9	2.02
(1,262)	1:148:A:ILE:N	1:148:A:ILE:CA	1:148:A:ILE:C	1:149:A:GLU:N	4	2.01
(1,174)	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	1:72:A:THR:N	2	1.99
(1,174)	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	1:72:A:THR:N	6	1.99
(1,280)	1:159:A:ALA:N	1:159:A:ALA:CA	1:159:A:ALA:C	1:160:A:GLU:N	4	1.98
(1,280)	1:159:A:ALA:N	1:159:A:ALA:CA	1:159:A:ALA:C	1:160:A:GLU:N	1	1.97
(1,222)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:SER:N	7	1.97
(1,138)	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	1:32:A:THR:N	3	1.95
(1,170)	1:58:A:VAL:C	1:59:A:GLU:N	1:59:A:GLU:CA	1:59:A:GLU:C	8	1.94
(1,161)	1:50:A:LEU:C	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	14	1.93
(1,56)	1:76:A:VAL:C	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	10	1.93
(1,242)	1:134:A:ASN:N	1:134:A:ASN:CA	1:134:A:ASN:C	1:135:A:CYS:N	8	1.92
(1,173)	1:70:A:GLY:N	1:70:A:GLY:CA	1:70:A:GLY:C	1:71:A:ARG:N	15	1.92
(1,20)	1:35:A:ALA:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	13	1.92
(1,133)	1:29:A:LEU:C	1:30:A:ARG:N	1:30:A:ARG:CA	1:30:A:ARG:C	2	1.91
(1,202)	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1:92:A:PHE:N	4	1.9
(1,206)	1:95:A:ARG:C	1:96:A:LEU:N	1:96:A:LEU:CA	1:96:A:LEU:C	3	1.89
(1,45)	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	1:66:A:GLU:N	6	1.89

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,67)	1:102:A:VAL:C	1:103:A:CYS:N	1:103:A:CYS:CA	1:103:A:CYS:C	10	1.88
(1,132)	1:28:A:GLU:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	8	1.87
(1,233)	1:115:A:VAL:N	1:115:A:VAL:CA	1:115:A:VAL:C	1:116:A:VAL:N	9	1.86
(1,133)	1:29:A:LEU:C	1:30:A:ARG:N	1:30:A:ARG:CA	1:30:A:ARG:C	8	1.85
(1,96)	1:164:A:LEU:N	1:164:A:LEU:CA	1:164:A:LEU:C	1:165:A:LEU:N	6	1.85
(1,33)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	14	1.85
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	4	1.84
(1,276)	1:158:A:GLU:C	1:159:A:ALA:N	1:159:A:ALA:CA	1:159:A:ALA:C	3	1.84
(1,220)	1:107:A:PHE:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	5	1.82
(1,70)	1:116:A:VAL:C	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	5	1.82
(1,181)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:VAL:N	11	1.8
(1,44)	1:64:A:TYR:C	1:65:A:TRP:N	1:65:A:TRP:CA	1:65:A:TRP:C	2	1.8
(1,25)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:LYS:N	15	1.8
(1,273)	1:155:A:PRO:C	1:156:A:ASP:N	1:156:A:ASP:CA	1:156:A:ASP:C	7	1.79
(1,204)	1:94:A:GLU:C	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	11	1.79
(1,209)	1:97:A:LYS:C	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	7	1.78
(1,180)	1:74:A:CYS:C	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	14	1.78
(1,31)	1:55:A:VAL:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	7	1.78
(1,115)	1:8:A:LYS:N	1:8:A:LYS:CA	1:8:A:LYS:C	1:9:A:ASN:N	7	1.77
(1,168)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:TYR:N	5	1.76
(1,138)	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	1:32:A:THR:N	14	1.75
(1,104)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:TYR:N	8	1.75
(1,30)	1:53:A:ASP:C	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	5	1.75
(1,215)	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	1:102:A:VAL:N	7	1.72
(1,109)	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1:6:A:ILE:N	2	1.71
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	12	1.71
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	2	1.69
(1,144)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:ALA:N	6	1.67
(1,82)	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1:125:A:LYS:N	6	1.67
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	15	1.66
(1,62)	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	1:89:A:TYR:N	10	1.66
(1,270)	1:153:A:PHE:N	1:153:A:PHE:CA	1:153:A:PHE:C	1:154:A:GLY:N	5	1.65
(1,215)	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	1:102:A:VAL:N	12	1.65
(1,43)	1:64:A:TYR:N	1:64:A:TYR:CA	1:64:A:TYR:C	1:65:A:TRP:N	5	1.65
(1,232)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:THR:N	4	1.63
(1,106)	1:4:A:MET:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	7	1.63
(1,82)	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1:125:A:LYS:N	9	1.62
(1,226)	1:112:A:GLU:C	1:113:A:ALA:N	1:113:A:ALA:CA	1:113:A:ALA:C	2	1.61
(1,153)	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	1:47:A:ASP:N	4	1.61
(1,56)	1:76:A:VAL:C	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	9	1.61
(1,202)	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1:92:A:PHE:N	9	1.6
(1,114)	1:8:A:LYS:C	1:9:A:ASN:N	1:9:A:ASN:CA	1:9:A:ASN:C	12	1.6
(1,66)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:CYS:N	3	1.6
(1,159)	1:49:A:MET:C	1:50:A:LEU:N	1:50:A:LEU:CA	1:50:A:LEU:C	9	1.59
(1,88)	1:152:A:ALA:C	1:153:A:PHE:N	1:153:A:PHE:CA	1:153:A:PHE:C	13	1.58
(1,214)	1:100:A:LYS:C	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	14	1.57
(1,64)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:ILE:N	13	1.57
(1,194)	1:85:A:SER:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	1	1.56
(1,132)	1:28:A:GLU:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	4	1.56
(1,111)	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	1:7:A:ASP:N	13	1.55
(1,225)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:ASN:N	8	1.54

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,197)	1:87:A:SER:N	1:87:A:SER:CA	1:87:A:SER:C	1:88:A:CYS:N	2	1.53
(1,26)	1:38:A:CYS:C	1:39:A:LYS:N	1:39:A:LYS:CA	1:39:A:LYS:C	14	1.53
(1,199)	1:90:A:ILE:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	12	1.52
(1,43)	1:64:A:TYR:N	1:64:A:TYR:CA	1:64:A:TYR:C	1:65:A:TRP:N	9	1.52
(1,23)	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	1:38:A:CYS:N	14	1.52
(1,21)	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	1:37:A:ILE:N	7	1.51
(1,211)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:LEU:N	10	1.5
(1,131)	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	1:28:A:GLU:N	5	1.5
(1,19)	1:20:A:ARG:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	8	1.49
(1,204)	1:94:A:GLU:C	1:95:A:ARG:N	1:95:A:ARG:CA	1:95:A:ARG:C	7	1.48
(1,3)	1:12:A:ALA:C	1:13:A:ASP:N	1:13:A:ASP:CA	1:13:A:ASP:C	9	1.48
(1,282)	1:170:A:ALA:N	1:170:A:ALA:CA	1:170:A:ALA:C	1:171:A:ARG:N	9	1.46
(1,257)	1:146:A:TYR:C	1:147:A:ASN:N	1:147:A:ASN:CA	1:147:A:ASN:C	13	1.46
(1,104)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:TYR:N	5	1.44
(1,202)	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1:92:A:PHE:N	8	1.43
(1,156)	1:47:A:ASP:N	1:47:A:ASP:CA	1:47:A:ASP:C	1:48:A:ALA:N	2	1.42
(1,138)	1:31:A:ILE:N	1:31:A:ILE:CA	1:31:A:ILE:C	1:32:A:THR:N	1	1.42
(1,53)	1:73:A:ALA:C	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	12	1.41
(1,52)	1:70:A:GLY:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	3	1.4
(1,261)	1:148:A:ILE:C	1:149:A:GLU:N	1:149:A:GLU:CA	1:149:A:GLU:C	15	1.39
(1,211)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:LEU:N	6	1.39
(1,150)	1:43:A:TYR:C	1:44:A:SER:N	1:44:A:SER:CA	1:44:A:SER:C	1	1.39
(1,73)	1:119:A:ALA:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1	1.39
(1,225)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:ASN:N	11	1.38
(1,171)	1:59:A:GLU:N	1:59:A:GLU:CA	1:59:A:GLU:C	1:60:A:TYR:N	2	1.38
(1,5)	1:13:A:ASP:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	3	1.38
(1,235)	1:118:A:LEU:C	1:119:A:ALA:N	1:119:A:ALA:CA	1:119:A:ALA:C	5	1.37
(1,143)	1:34:A:THR:C	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	6	1.37
(1,51)	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1:69:A:SER:N	2	1.36
(1,211)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:LEU:N	11	1.34
(1,116)	1:9:A:ASN:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	1	1.34
(1,153)	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	1:47:A:ASP:N	15	1.32
(1,49)	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	1:68:A:ARG:N	11	1.32
(1,53)	1:73:A:ALA:C	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	8	1.3
(1,38)	1:61:A:LEU:C	1:62:A:LEU:N	1:62:A:LEU:CA	1:62:A:LEU:C	13	1.3
(1,33)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	10	1.3
(1,180)	1:74:A:CYS:C	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	4	1.29
(1,20)	1:35:A:ALA:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	4	1.29
(1,276)	1:158:A:GLU:C	1:159:A:ALA:N	1:159:A:ALA:CA	1:159:A:ALA:C	1	1.28
(1,250)	1:138:A:ARG:N	1:138:A:ARG:CA	1:138:A:ARG:C	1:139:A:LYS:N	12	1.27
(1,242)	1:134:A:ASN:N	1:134:A:ASN:CA	1:134:A:ASN:C	1:135:A:CYS:N	5	1.26
(1,241)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:THR:N	12	1.26
(1,132)	1:28:A:GLU:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	14	1.26
(1,48)	1:66:A:GLU:C	1:67:A:CYS:N	1:67:A:CYS:CA	1:67:A:CYS:C	10	1.26
(1,57)	1:79:A:ASN:C	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	8	1.25
(1,43)	1:64:A:TYR:N	1:64:A:TYR:CA	1:64:A:TYR:C	1:65:A:TRP:N	8	1.25
(1,274)	1:156:A:ASP:N	1:156:A:ASP:CA	1:156:A:ASP:C	1:157:A:ASN:N	8	1.24
(1,256)	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	1:146:A:TYR:N	3	1.24
(1,223)	1:109:A:SER:C	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	15	1.24
(1,276)	1:158:A:GLU:C	1:159:A:ALA:N	1:159:A:ALA:CA	1:159:A:ALA:C	4	1.23
(1,164)	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	1:52:A:THR:N	10	1.22

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,161)	1:50:A:LEU:C	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	7	1.22
(1,17)	1:19:A:ARG:C	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	13	1.22
(1,119)	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	1:22:A:LEU:N	13	1.21
(1,55)	1:76:A:VAL:N	1:76:A:VAL:CA	1:76:A:VAL:C	1:77:A:PHE:N	7	1.21
(1,211)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:LEU:N	2	1.2
(1,118)	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	1:11:A:GLY:N	4	1.2
(1,56)	1:76:A:VAL:C	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	7	1.2
(1,61)	1:87:A:SER:C	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	2	1.19
(1,245)	1:135:A:CYS:N	1:135:A:CYS:CA	1:135:A:CYS:C	1:136:A:VAL:N	14	1.18
(1,133)	1:29:A:LEU:C	1:30:A:ARG:N	1:30:A:ARG:CA	1:30:A:ARG:C	5	1.17
(1,261)	1:148:A:ILE:C	1:149:A:GLU:N	1:149:A:GLU:CA	1:149:A:GLU:C	1	1.16
(1,109)	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1:6:A:ILE:N	8	1.16
(1,270)	1:153:A:PHE:N	1:153:A:PHE:CA	1:153:A:PHE:C	1:154:A:GLY:N	10	1.12
(1,111)	1:6:A:ILE:N	1:6:A:ILE:CA	1:6:A:ILE:C	1:7:A:ASP:N	1	1.12
(1,61)	1:87:A:SER:C	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	5	1.12
(1,27)	1:44:A:SER:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	10	1.12
(1,280)	1:159:A:ALA:N	1:159:A:ALA:CA	1:159:A:ALA:C	1:160:A:GLU:N	14	1.11
(1,249)	1:138:A:ARG:C	1:139:A:LYS:N	1:139:A:LYS:CA	1:139:A:LYS:C	4	1.11
(1,187)	1:80:A:THR:N	1:80:A:THR:CA	1:80:A:THR:C	1:81:A:GLY:N	2	1.11
(1,169)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:GLU:N	3	1.11
(1,133)	1:29:A:LEU:C	1:30:A:ARG:N	1:30:A:ARG:CA	1:30:A:ARG:C	9	1.11
(1,225)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:ASN:N	15	1.1
(1,241)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:THR:N	3	1.09
(1,25)	1:38:A:CYS:N	1:38:A:CYS:CA	1:38:A:CYS:C	1:39:A:LYS:N	3	1.09
(1,98)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:ARG:N	7	1.08
(1,63)	1:88:A:CYS:C	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	11	1.08
(1,61)	1:87:A:SER:C	1:88:A:CYS:N	1:88:A:CYS:CA	1:88:A:CYS:C	6	1.07
(1,236)	1:119:A:ALA:N	1:119:A:ALA:CA	1:119:A:ALA:C	1:120:A:ASP:N	10	1.05
(1,165)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:ASP:N	4	1.04
(1,133)	1:29:A:LEU:C	1:30:A:ARG:N	1:30:A:ARG:CA	1:30:A:ARG:C	4	1.04
(1,132)	1:28:A:GLU:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	2	1.04
(1,129)	1:26:A:GLU:C	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	13	1.04
(1,74)	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1:121:A:ILE:N	10	1.04
(1,43)	1:64:A:TYR:N	1:64:A:TYR:CA	1:64:A:TYR:C	1:65:A:TRP:N	10	1.04
(1,21)	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	1:37:A:ILE:N	6	1.04
(1,15)	1:18:A:THR:C	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	14	1.04
(1,215)	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	1:102:A:VAL:N	8	1.03
(1,175)	1:71:A:ARG:C	1:72:A:THR:N	1:72:A:THR:CA	1:72:A:THR:C	12	1.03
(1,143)	1:34:A:THR:C	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	14	1.03
(1,214)	1:100:A:LYS:C	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	6	1.02
(1,83)	1:126:A:PRO:C	1:127:A:CYS:N	1:127:A:CYS:CA	1:127:A:CYS:C	4	1.02
(1,32)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:PRO:N	2	1.02
(1,47)	1:66:A:GLU:N	1:66:A:GLU:CA	1:66:A:GLU:C	1:67:A:CYS:N	8	1.01
(1,35)	1:60:A:TYR:N	1:60:A:TYR:CA	1:60:A:TYR:C	1:61:A:LEU:N	14	1.01
(1,164)	1:51:A:THR:N	1:51:A:THR:CA	1:51:A:THR:C	1:52:A:THR:N	5	1.0
(1,143)	1:34:A:THR:C	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	4	1.0