



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:34 PM UTC

PDB ID : 2M8T / pdb_00002m8t
BMRB ID : 19268
Title : Solution NMR structure of the V209M variant of the human prion protein (residues 90-231)
Authors : Mills, J.L.; Surewicz, K.; Surewicz, W.; Soennichsen, F.D.
Deposited on : 2013-05-28

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

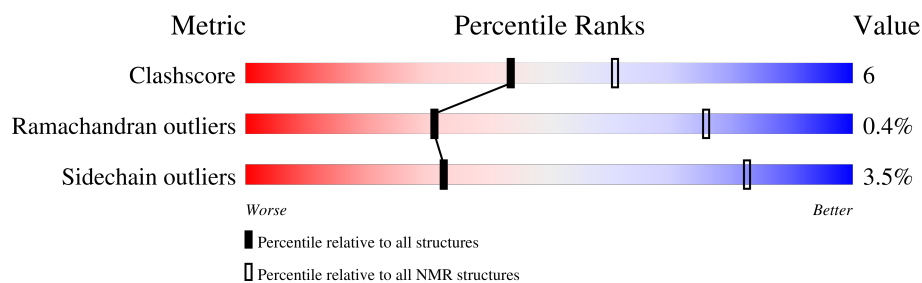
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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	146	

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:128-A:164, A:172-A:225 (91)	0.97	17

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 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1777 atoms, of which 856 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	112	Total	C	H	N	O	S	0
			1777	569	856	161	181	10	

There are 5 discrepancies between the modelled and reference sequences:

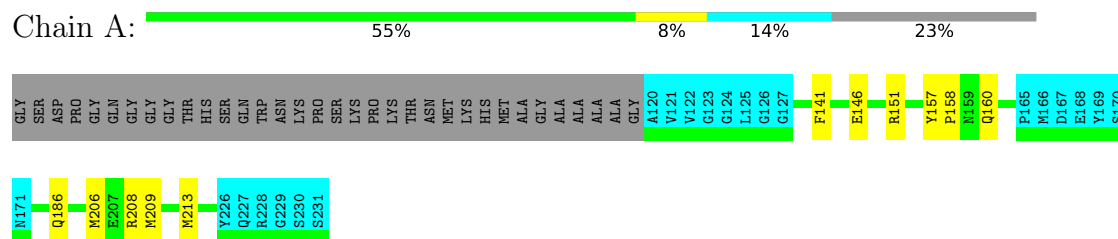
Chain	Residue	Modelled	Actual	Comment	Reference
A	86	GLY	-	expression tag	UNP P04156
A	87	SER	-	expression tag	UNP P04156
A	88	ASP	-	expression tag	UNP P04156
A	89	PRO	-	expression tag	UNP P04156
A	209	MET	VAL	engineered mutation	UNP P04156

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: Major prion protein

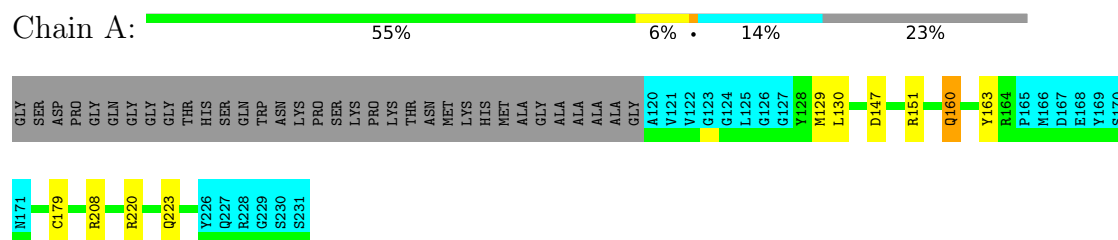


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

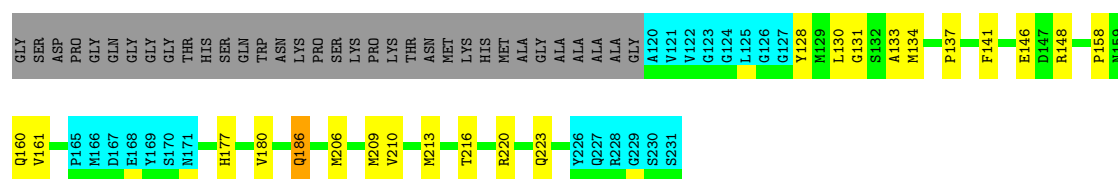
- Molecule 1: Major prion protein



4.2.2 Score per residue for model 2

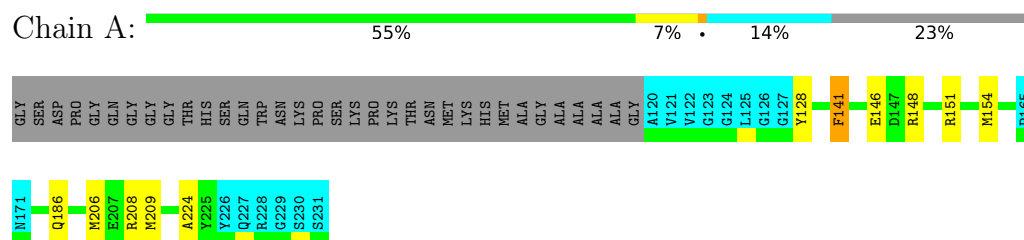
- Molecule 1: Major prion protein





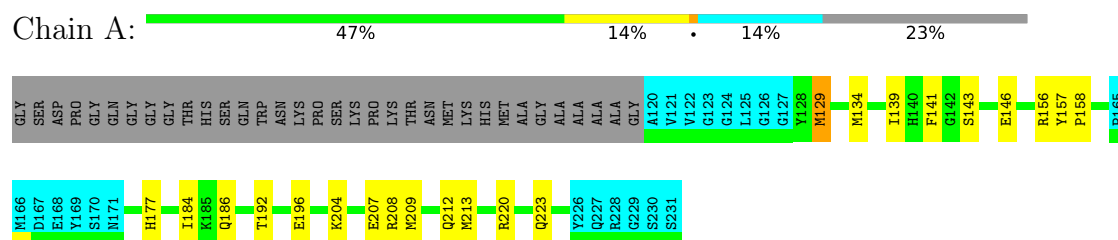
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



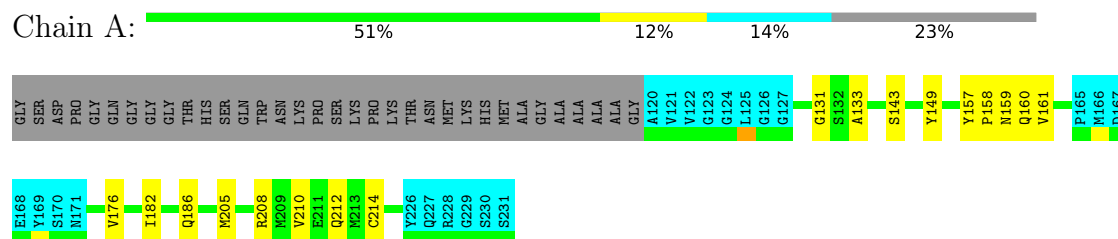
4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



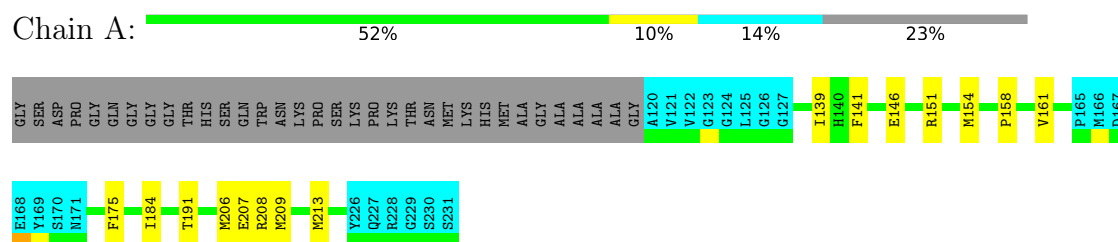
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



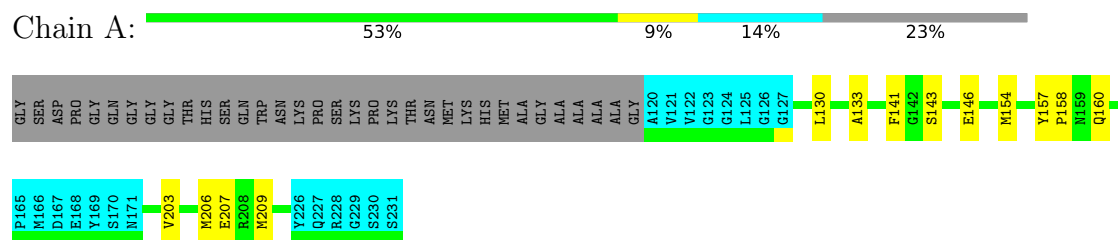
4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



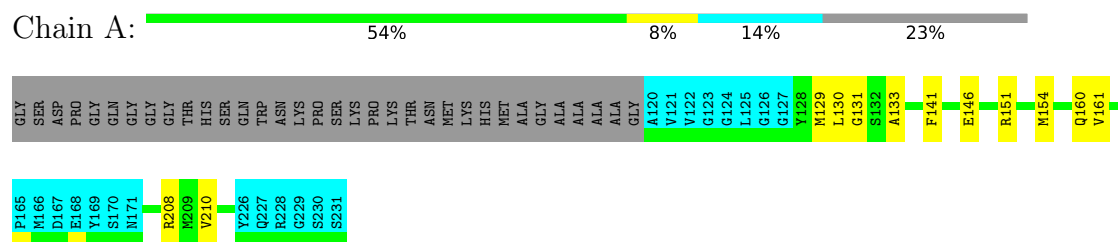
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



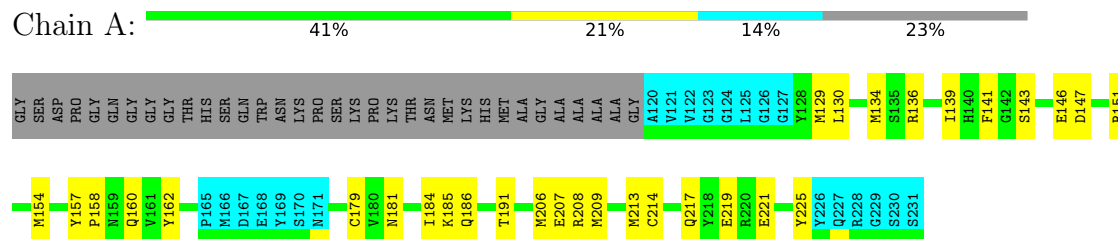
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



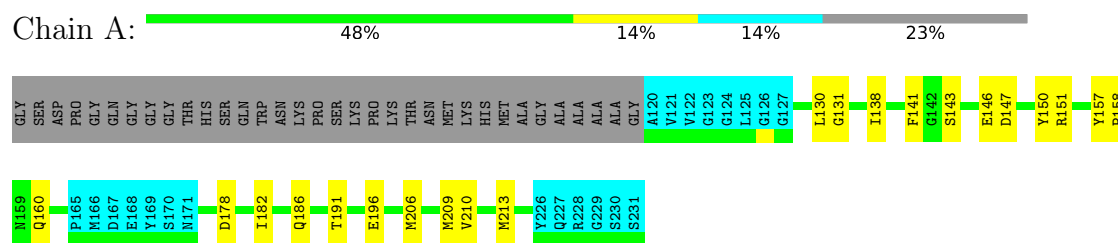
4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



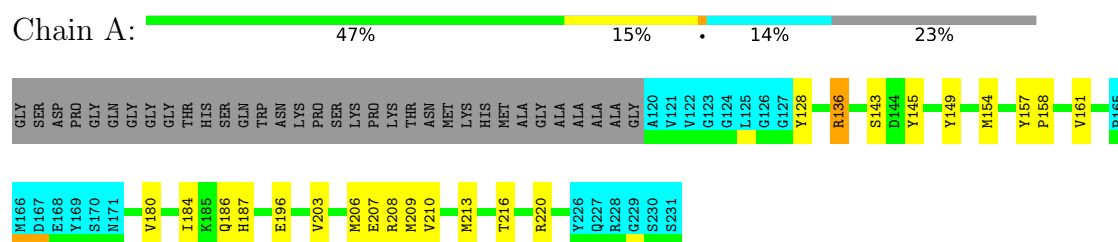
4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



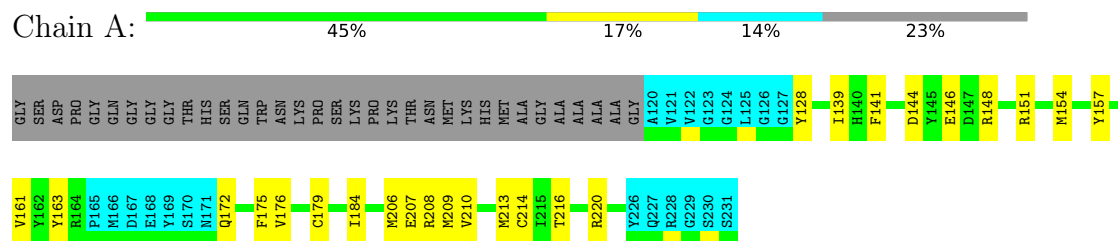
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



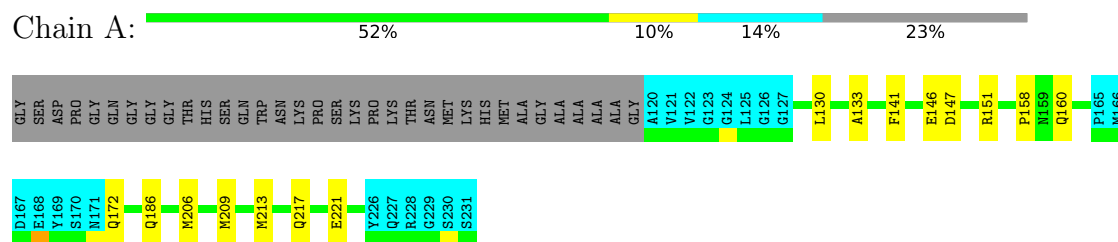
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



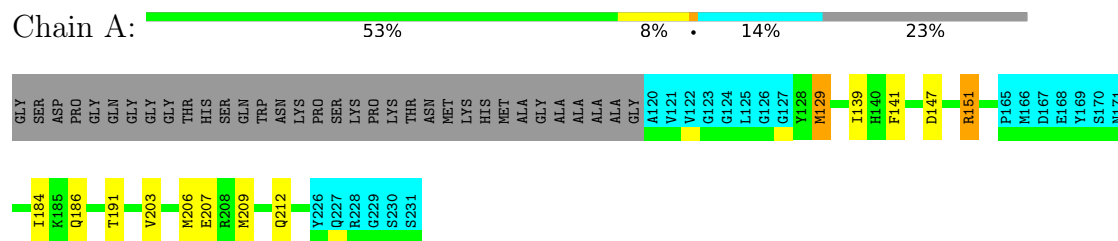
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



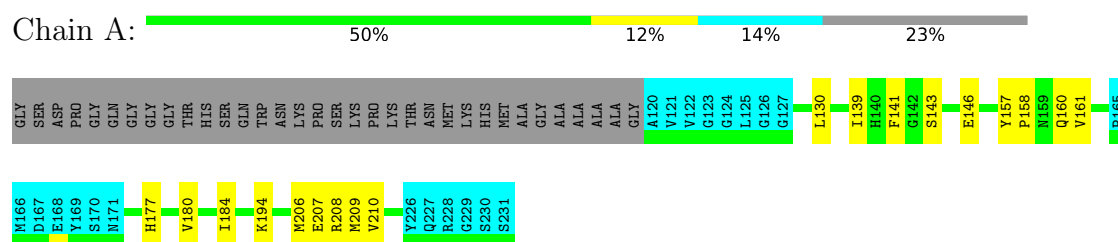
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



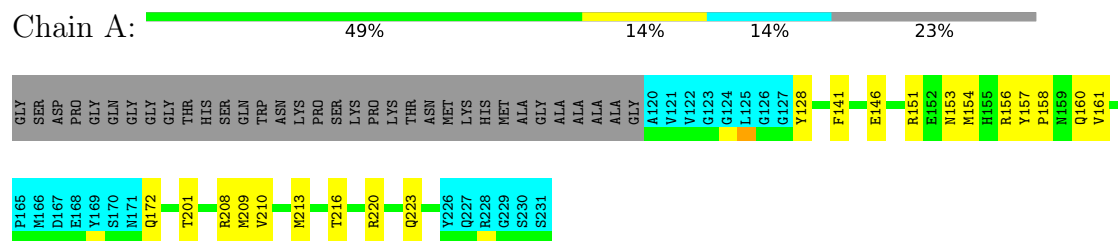
4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



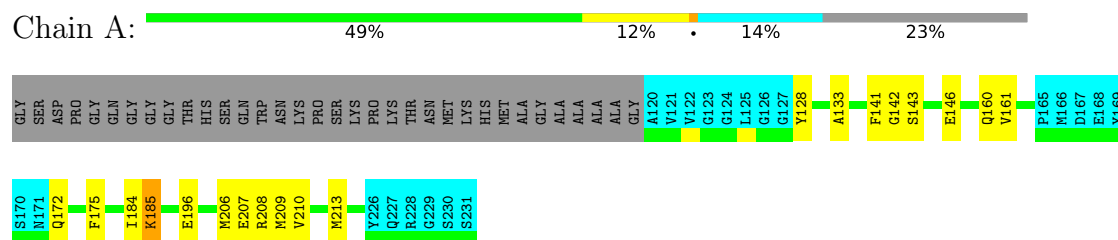
4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein



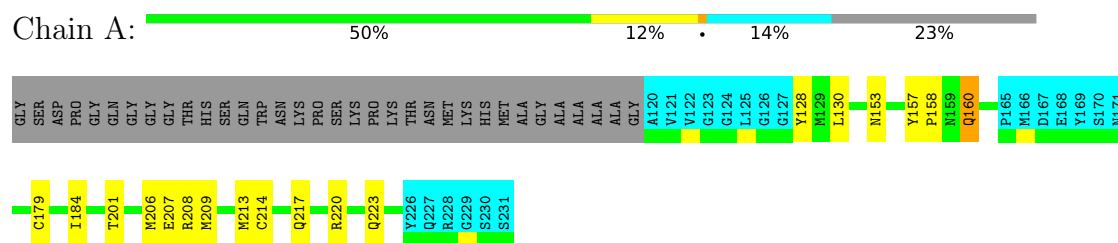
4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Major prion protein



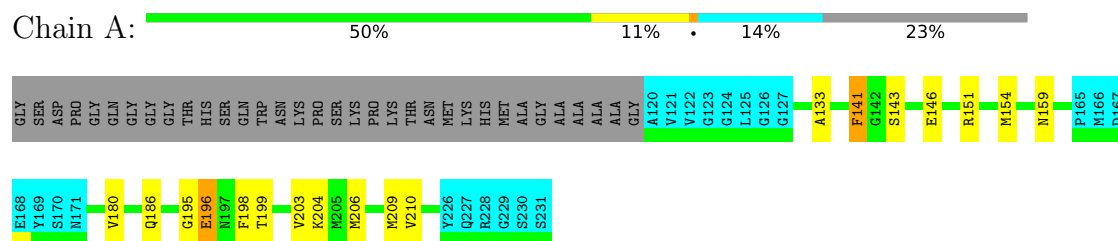
4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



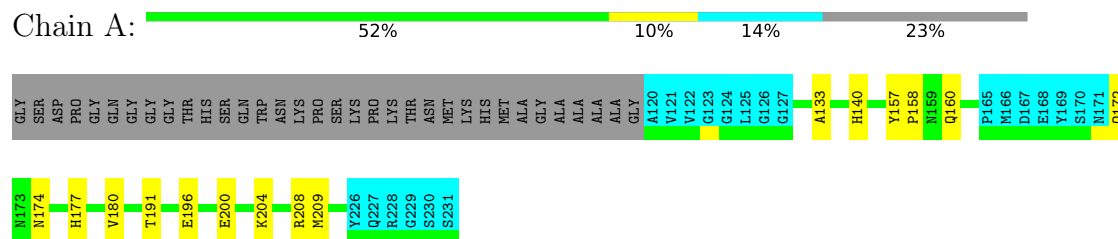
4.2.19 Score per residue for model 19

- Molecule 1: Major prion protein



4.2.20 Score per residue for model 20

- Molecule 1: Major prion protein



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
TALOS	geometry optimization	
CYANA	structure solution	
CNS	geometry optimization	
CYANA	refinement	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1503
Number of shifts mapped to atoms	1174
Number of unparsed shifts	0
Number of shifts with mapping errors	329
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	772	721	723	10±4
All	All	15440	14420	14460	194

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:THR:HB	1:A:196:GLU:HB3	0.78	1.53	20	1
1:A:204:LYS:HE2	1:A:204:LYS:HA	0.76	1.57	4	1
1:A:130:LEU:HD11	1:A:160:GLN:HG3	0.67	1.65	13	9
1:A:153:ASN:O	1:A:156:ARG:HG2	0.63	1.93	16	1
1:A:163:TYR:HB3	1:A:179:CYS:HB3	0.62	1.71	12	1
1:A:161:VAL:HG13	1:A:213:MET:SD	0.60	2.37	16	4
1:A:220:ARG:HA	1:A:223:GLN:HG2	0.59	1.74	2	4
1:A:154:MET:HA	1:A:157:TYR:CD2	0.58	2.34	11	2
1:A:180:VAL:HA	1:A:210:VAL:HG11	0.58	1.74	11	4
1:A:147:ASP:O	1:A:151:ARG:HG2	0.57	1.98	13	2
1:A:139:ILE:HD12	1:A:208:ARG:HG3	0.56	1.77	15	5
1:A:156:ARG:HA	1:A:156:ARG:HE	0.56	1.60	4	1
1:A:133:ALA:HB2	1:A:160:GLN:HB3	0.56	1.77	5	5
1:A:206:MET:O	1:A:210:VAL:HG23	0.55	2.02	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:195:GLY:O	1:A:196:GLU:HG2	0.54	2.03	19	1
1:A:129:MET:HE3	1:A:129:MET:HA	0.54	1.79	14	1
1:A:143:SER:HB2	1:A:146:GLU:OE2	0.53	2.03	7	2
1:A:129:MET:HA	1:A:129:MET:HE2	0.53	1.79	1	2
1:A:206:MET:HA	1:A:209:MET:HG2	0.53	1.81	15	13
1:A:157:TYR:HB3	1:A:158:PRO:HD2	0.53	1.79	9	8
1:A:192:THR:HA	1:A:196:GLU:O	0.52	2.05	4	1
1:A:203:VAL:O	1:A:206:MET:HG2	0.52	2.05	11	1
1:A:163:TYR:HB3	1:A:179:CYS:SG	0.51	2.45	1	1
1:A:187:HIS:CD2	1:A:206:MET:HE1	0.51	2.40	11	1
1:A:161:VAL:HG11	1:A:210:VAL:HG13	0.51	1.82	17	6
1:A:145:TYR:O	1:A:149:TYR:HB2	0.51	2.05	11	1
1:A:134:MET:SD	1:A:137:PRO:HA	0.51	2.46	2	1
1:A:141:PHE:HB2	1:A:146:GLU:OE1	0.50	2.06	8	13
1:A:213:MET:O	1:A:217:GLN:HG2	0.50	2.07	13	1
1:A:151:ARG:O	1:A:154:MET:HG2	0.49	2.07	12	7
1:A:141:PHE:CD1	1:A:146:GLU:HG2	0.48	2.42	7	2
1:A:133:ALA:HB1	1:A:159:ASN:OD1	0.48	2.08	19	1
1:A:184:ILE:HD11	1:A:207:GLU:CA	0.48	2.39	6	3
1:A:147:ASP:O	1:A:151:ARG:HB2	0.48	2.09	9	2
1:A:147:ASP:HB3	1:A:151:ARG:NH2	0.47	2.23	10	1
1:A:200:GLU:HB3	1:A:204:LYS:NZ	0.47	2.24	20	1
1:A:184:ILE:CD1	1:A:206:MET:HG3	0.47	2.39	14	5
1:A:158:PRO:O	1:A:209:MET:HE1	0.47	2.09	18	9
1:A:216:THR:O	1:A:220:ARG:HG3	0.47	2.09	2	4
1:A:172:GLN:HG3	1:A:175:PHE:H	0.47	1.69	17	2
1:A:209:MET:O	1:A:213:MET:HG3	0.47	2.09	4	3
1:A:178:ASP:O	1:A:182:ILE:HG12	0.47	2.09	10	1
1:A:149:TYR:CD2	1:A:205:MET:HG3	0.47	2.45	5	1
1:A:177:HIS:O	1:A:180:VAL:HB	0.47	2.10	20	1
1:A:153:ASN:HB3	1:A:157:TYR:CZ	0.46	2.44	18	1
1:A:134:MET:HB2	1:A:213:MET:SD	0.46	2.50	2	1
1:A:141:PHE:CD2	1:A:146:GLU:HG2	0.46	2.44	2	2
1:A:156:ARG:HA	1:A:156:ARG:NE	0.46	2.26	4	1
1:A:139:ILE:HD11	1:A:209:MET:HA	0.46	1.88	12	1
1:A:133:ALA:CB	1:A:160:GLN:HB3	0.46	2.40	7	1
1:A:146:GLU:CD	1:A:146:GLU:H	0.45	2.19	15	4
1:A:181:ASN:O	1:A:185:LYS:HG2	0.45	2.12	9	1
1:A:151:ARG:HA	1:A:154:MET:HE3	0.45	1.88	8	2
1:A:184:ILE:HD11	1:A:207:GLU:HA	0.45	1.88	6	7
1:A:176:VAL:HA	1:A:214:CYS:SG	0.45	2.52	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:PHE:CZ	1:A:208:ARG:HG3	0.45	2.47	3	1
1:A:136:ARG:HG2	1:A:136:ARG:O	0.44	2.12	11	1
1:A:149:TYR:HD2	1:A:205:MET:HG3	0.44	1.71	5	1
1:A:134:MET:HE3	1:A:213:MET:HG2	0.44	1.89	4	1
1:A:179:CYS:SG	1:A:214:CYS:SG	0.44	3.15	9	1
1:A:144:ASP:OD2	1:A:148:ARG:HD3	0.44	2.12	12	1
1:A:139:ILE:HG21	1:A:141:PHE:CE2	0.44	2.48	14	1
1:A:157:TYR:CE1	1:A:206:MET:HE2	0.43	2.48	11	1
1:A:217:GLN:O	1:A:221:GLU:HG2	0.43	2.13	9	1
1:A:204:LYS:HA	1:A:204:LYS:CE	0.43	2.38	4	1
1:A:203:VAL:HA	1:A:206:MET:HE3	0.43	1.91	11	1
1:A:182:ILE:O	1:A:186:GLN:HG2	0.43	2.14	5	1
1:A:210:VAL:HA	1:A:213:MET:HE2	0.43	1.90	10	1
1:A:186:GLN:C	1:A:186:GLN:HE21	0.42	2.22	2	1
1:A:185:LYS:NZ	1:A:185:LYS:HB2	0.42	2.29	17	1
1:A:157:TYR:CE2	1:A:206:MET:HB3	0.42	2.50	12	1
1:A:134:MET:HE3	1:A:213:MET:SD	0.41	2.55	9	1
1:A:151:ARG:HG3	1:A:154:MET:HE3	0.41	1.92	12	1
1:A:199:THR:O	1:A:203:VAL:HG23	0.41	2.16	19	1
1:A:138:ILE:HA	1:A:150:TYR:CE2	0.41	2.51	10	1
1:A:209:MET:SD	1:A:210:VAL:HG13	0.41	2.56	16	1
1:A:203:VAL:O	1:A:207:GLU:HB2	0.41	2.16	7	1
1:A:179:CYS:HB2	1:A:214:CYS:SG	0.41	2.56	18	1
1:A:162:TYR:CD1	1:A:162:TYR:N	0.40	2.89	9	1
1:A:203:VAL:O	1:A:207:GLU:HG3	0.40	2.16	14	1
1:A:133:ALA:HA	1:A:160:GLN:HB3	0.40	1.94	20	1
1:A:146:GLU:H	1:A:146:GLU:CD	0.40	2.24	8	1
1:A:184:ILE:HG13	1:A:207:GLU:HG2	0.40	1.93	15	1
1:A:157:TYR:HD2	1:A:209:MET:SD	0.40	2.40	12	1
1:A:209:MET:HG3	1:A:210:VAL:N	0.40	2.31	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	91/146 (62%)	87±1 (95±2%)	4±1 (4±1%)	0±1 (0±1%)	31	76
All	All	1820/2920 (62%)	1736 (95%)	76 (4%)	8 (0%)	31	76

All 4 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	131	GLY	4
1	A	141	PHE	2
1	A	142	GLY	1
1	A	196	GLU	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	86/123 (70%)	83±2 (96±2%)	3±2 (4±2%)	32	82
All	All	1720/2460 (70%)	1659 (96%)	61 (4%)	32	82

All 23 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	186	GLN	9
1	A	208	ARG	8
1	A	143	SER	7
1	A	191	THR	4
1	A	160	GLN	3
1	A	177	HIS	3
1	A	129	MET	3
1	A	212	GLN	3
1	A	196	GLU	3
1	A	148	ARG	2
1	A	136	ARG	2
1	A	172	GLN	2
1	A	201	THR	2
1	A	159	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	219	GLU	1
1	A	221	GLU	1
1	A	151	ARG	1
1	A	194	LYS	1
1	A	185	LYS	1
1	A	217	GLN	1
1	A	198	PHE	1
1	A	204	LYS	1
1	A	140	HIS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1503
Number of shifts mapped to atoms	1174
Number of unparsed shifts	0
Number of shifts with mapping errors	329
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 329 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	86	GLY	HA2	3.875	0.020	1
1	A	86	GLY	HA3	3.875	0.020	1
1	A	86	GLY	CA	43.411	0.300	1
1	A	87	SER	H	8.6	0.020	1
1	A	87	SER	HA	4.473	0.020	1
1	A	87	SER	HB2	3.811	0.020	1
1	A	87	SER	HB3	3.811	0.020	1
1	A	87	SER	CA	58.148	0.300	1
1	A	87	SER	CB	63.953	0.300	1
1	A	87	SER	N	115.741	0.300	1
1	A	88	ASP	H	8.438	0.020	1
1	A	88	ASP	HA	4.881	0.020	1
1	A	88	ASP	HB2	2.722	0.020	2
1	A	88	ASP	HB3	2.55	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	88	ASP	CA	54.716	0.300	1
1	A	88	ASP	CB	41.367	0.300	1
1	A	88	ASP	N	123.605	0.300	1
1	A	89	PRO	HA	4.4	0.020	1
1	A	89	PRO	HB2	2.26	0.020	2
1	A	89	PRO	HB3	1.909	0.020	2
1	A	89	PRO	HD2	3.776	0.020	2
1	A	89	PRO	HD3	3.605	0.020	2
1	A	89	PRO	HG2	1.987	0.020	1
1	A	89	PRO	HG3	1.987	0.020	1
1	A	89	PRO	CA	63.587	0.300	1
1	A	89	PRO	CB	32.113	0.300	1
1	A	89	PRO	CD	50.847	0.300	1
1	A	89	PRO	CG	27.136	0.300	1
1	A	90	GLY	H	8.482	0.020	1
1	A	90	GLY	HA2	3.902	0.020	1
1	A	90	GLY	HA3	3.902	0.020	1
1	A	90	GLY	CA	45.409	0.300	1
1	A	90	GLY	N	108.429	0.300	1
1	A	91	GLN	H	8.084	0.020	1
1	A	91	GLN	HA	4.324	0.020	1
1	A	91	GLN	HB2	2.142	0.020	2
1	A	91	GLN	HB3	1.962	0.020	2
1	A	91	GLN	HE21	7.362	0.020	2
1	A	91	GLN	HE22	6.793	0.020	2
1	A	91	GLN	HG2	2.325	0.020	1
1	A	91	GLN	HG3	2.325	0.020	1
1	A	91	GLN	CA	55.912	0.300	1
1	A	91	GLN	CB	29.28	0.300	1
1	A	91	GLN	CG	33.851	0.300	1
1	A	91	GLN	N	119.598	0.300	1
1	A	91	GLN	NE2	112.348	0.300	1
1	A	92	GLY	H	8.445	0.020	1
1	A	92	GLY	HA2	3.964	0.020	1
1	A	92	GLY	HA3	3.964	0.020	1
1	A	92	GLY	CA	45.43	0.300	1
1	A	92	GLY	N	109.845	0.300	1
1	A	93	GLY	H	8.291	0.020	1
1	A	93	GLY	HA2	3.913	0.020	1
1	A	93	GLY	HA3	3.913	0.020	1
1	A	93	GLY	CA	45.274	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	GLY	N	108.591	0.300	1
1	A	94	GLY	H	8.286	0.020	1
1	A	94	GLY	HA2	3.98	0.020	1
1	A	94	GLY	HA3	3.98	0.020	1
1	A	94	GLY	CA	45.229	0.300	1
1	A	94	GLY	N	108.815	0.300	1
1	A	95	THR	H	8.075	0.020	1
1	A	95	THR	HA	4.255	0.020	1
1	A	95	THR	HB	4.145	0.020	1
1	A	95	THR	HG21	1.135	0.020	1
1	A	95	THR	HG22	1.135	0.020	1
1	A	95	THR	HG23	1.135	0.020	1
1	A	95	THR	CA	62.262	0.300	1
1	A	95	THR	CB	69.627	0.300	1
1	A	95	THR	CG2	21.605	0.300	1
1	A	95	THR	N	113.428	0.300	1
1	A	96	HIS	H	8.522	0.020	1
1	A	96	HIS	HA	4.636	0.020	1
1	A	96	HIS	HB2	3.201	0.020	2
1	A	96	HIS	HB3	3.113	0.020	2
1	A	96	HIS	HD2	7.365	0.020	1
1	A	96	HIS	CA	55.268	0.300	1
1	A	96	HIS	CB	29.219	0.300	1
1	A	96	HIS	CD2	119.831	0.300	1
1	A	96	HIS	N	120.374	0.300	1
1	A	97	SER	H	8.258	0.020	1
1	A	97	SER	HA	4.361	0.020	1
1	A	97	SER	HB2	3.759	0.020	1
1	A	97	SER	HB3	3.759	0.020	1
1	A	97	SER	CA	58.543	0.300	1
1	A	97	SER	CB	63.874	0.300	1
1	A	97	SER	N	116.904	0.300	1
1	A	98	GLN	H	8.429	0.020	1
1	A	98	GLN	HA	4.256	0.020	1
1	A	98	GLN	HB2	1.93	0.020	2
1	A	98	GLN	HB3	1.838	0.020	2
1	A	98	GLN	HE21	7.425	0.020	2
1	A	98	GLN	HE22	6.791	0.020	2
1	A	98	GLN	HG2	2.14	0.020	1
1	A	98	GLN	HG3	2.14	0.020	1
1	A	98	GLN	CA	56.115	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	98	GLN	CB	29.287	0.300	1
1	A	98	GLN	CG	33.535	0.300	1
1	A	98	GLN	N	121.911	0.300	1
1	A	98	GLN	NE2	112.561	0.300	1
1	A	99	TRP	H	8.065	0.020	1
1	A	99	TRP	HA	4.652	0.020	1
1	A	99	TRP	HB2	3.269	0.020	2
1	A	99	TRP	HB3	3.171	0.020	2
1	A	99	TRP	HD1	7.212	0.020	1
1	A	99	TRP	HE1	10.071	0.020	1
1	A	99	TRP	HE3	7.575	0.020	1
1	A	99	TRP	HH2	7.184	0.020	1
1	A	99	TRP	HZ2	7.413	0.020	1
1	A	99	TRP	HZ3	7.09	0.020	1
1	A	99	TRP	CA	57.131	0.300	1
1	A	99	TRP	CB	29.585	0.300	1
1	A	99	TRP	CD1	126.676	0.300	1
1	A	99	TRP	CE3	120.455	0.300	1
1	A	99	TRP	CH2	124.243	0.300	1
1	A	99	TRP	CZ2	114.19	0.300	1
1	A	99	TRP	CZ3	121.629	0.300	1
1	A	99	TRP	N	121.53	0.300	1
1	A	99	TRP	NE1	129.392	0.300	1
1	A	100	ASN	H	8.065	0.020	1
1	A	100	ASN	HA	4.584	0.020	1
1	A	100	ASN	HB2	2.555	0.020	2
1	A	100	ASN	HB3	2.516	0.020	2
1	A	100	ASN	HD21	7.431	0.020	2
1	A	100	ASN	HD22	6.783	0.020	2
1	A	100	ASN	CA	52.795	0.300	1
1	A	100	ASN	CB	38.908	0.300	1
1	A	100	ASN	N	120.377	0.300	1
1	A	100	ASN	ND2	112.046	0.300	1
1	A	101	LYS	H	7.948	0.020	1
1	A	101	LYS	HA	4.43	0.020	1
1	A	101	LYS	HB2	1.747	0.020	2
1	A	101	LYS	HB3	1.616	0.020	2
1	A	101	LYS	HD2	1.624	0.020	1
1	A	101	LYS	HD3	1.624	0.020	1
1	A	101	LYS	HE2	2.941	0.020	1
1	A	101	LYS	HE3	2.941	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	LYS	HG2	1.365	0.020	1
1	A	101	LYS	HG3	1.365	0.020	1
1	A	101	LYS	CA	54.18	0.300	1
1	A	101	LYS	CB	32.388	0.300	1
1	A	101	LYS	CD	28.935	0.300	1
1	A	101	LYS	CE	42.056	0.300	1
1	A	101	LYS	CG	24.909	0.300	1
1	A	101	LYS	N	122.677	0.300	1
1	A	102	PRO	HA	4.406	0.020	1
1	A	102	PRO	HB2	2.267	0.020	2
1	A	102	PRO	HB3	1.884	0.020	2
1	A	102	PRO	HD2	3.774	0.020	2
1	A	102	PRO	HD3	3.605	0.020	2
1	A	102	PRO	HG2	1.992	0.020	1
1	A	102	PRO	HG3	1.992	0.020	1
1	A	102	PRO	CA	63.094	0.300	1
1	A	102	PRO	CB	32.192	0.300	1
1	A	102	PRO	CD	50.759	0.300	1
1	A	102	PRO	CG	27.373	0.300	1
1	A	103	SER	H	8.382	0.020	1
1	A	103	SER	HA	4.407	0.020	1
1	A	103	SER	HB2	3.82	0.020	1
1	A	103	SER	HB3	3.82	0.020	1
1	A	103	SER	CA	58.08	0.300	1
1	A	103	SER	CB	64.111	0.300	1
1	A	103	SER	N	116.909	0.300	1
1	A	104	LYS	H	8.279	0.020	1
1	A	104	LYS	HA	4.6	0.020	1
1	A	104	LYS	HB2	1.799	0.020	2
1	A	104	LYS	HB3	1.69	0.020	2
1	A	104	LYS	HD2	1.68	0.020	1
1	A	104	LYS	HD3	1.68	0.020	1
1	A	104	LYS	HE2	2.975	0.020	1
1	A	104	LYS	HE3	2.975	0.020	1
1	A	104	LYS	HG2	1.439	0.020	1
1	A	104	LYS	HG3	1.439	0.020	1
1	A	104	LYS	CA	54.184	0.300	1
1	A	104	LYS	CB	32.388	0.300	1
1	A	104	LYS	CD	28.935	0.300	1
1	A	104	LYS	CE	42.056	0.300	1
1	A	104	LYS	CG	24.4	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	104	LYS	N	124.225	0.300	1
1	A	105	PRO	HA	4.396	0.020	1
1	A	105	PRO	HB2	2.266	0.020	2
1	A	105	PRO	HB3	1.859	0.020	2
1	A	105	PRO	HD2	3.767	0.020	2
1	A	105	PRO	HD3	3.594	0.020	2
1	A	105	PRO	HG2	1.981	0.020	1
1	A	105	PRO	HG3	1.981	0.020	1
1	A	105	PRO	CA	63.018	0.300	1
1	A	105	PRO	CB	32.271	0.300	1
1	A	105	PRO	CD	50.759	0.300	1
1	A	105	PRO	CG	27.373	0.300	1
1	A	106	LYS	H	8.481	0.020	1
1	A	106	LYS	HA	4.321	0.020	1
1	A	106	LYS	HB2	1.84	0.020	2
1	A	106	LYS	HB3	1.747	0.020	2
1	A	106	LYS	HD2	1.679	0.020	1
1	A	106	LYS	HD3	1.679	0.020	1
1	A	106	LYS	HE2	2.995	0.020	1
1	A	106	LYS	HE3	2.995	0.020	1
1	A	106	LYS	HG2	1.464	0.020	2
1	A	106	LYS	HG3	1.428	0.020	2
1	A	106	LYS	CA	56.42	0.300	1
1	A	106	LYS	CB	33.061	0.300	1
1	A	106	LYS	CD	29.111	0.300	1
1	A	106	LYS	CE	42.305	0.300	1
1	A	106	LYS	CG	25.081	0.300	1
1	A	106	LYS	N	121.921	0.300	1
1	A	107	THR	H	8.102	0.020	1
1	A	107	THR	HA	4.304	0.020	1
1	A	107	THR	HB	4.158	0.020	1
1	A	107	THR	HG21	1.159	0.020	1
1	A	107	THR	HG22	1.159	0.020	1
1	A	107	THR	HG23	1.159	0.020	1
1	A	107	THR	CA	61.637	0.300	1
1	A	107	THR	CB	69.799	0.300	1
1	A	107	THR	CG2	21.605	0.300	1
1	A	107	THR	N	115.362	0.300	1
1	A	108	ASN	H	8.495	0.020	1
1	A	108	ASN	HA	4.694	0.020	1
1	A	108	ASN	HB2	2.816	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	108	ASN	HB3	2.723	0.020	2
1	A	108	ASN	HD21	7.557	0.020	2
1	A	108	ASN	HD22	6.86	0.020	2
1	A	108	ASN	CA	53.168	0.300	1
1	A	108	ASN	CB	38.75	0.300	1
1	A	108	ASN	N	121.166	0.300	1
1	A	108	ASN	ND2	112.704	0.300	1
1	A	109	MET	H	8.302	0.020	1
1	A	109	MET	HA	4.416	0.020	1
1	A	109	MET	HB2	2.037	0.020	2
1	A	109	MET	HB3	1.93	0.020	2
1	A	109	MET	HE1	1.363	0.020	1
1	A	109	MET	HE2	1.363	0.020	1
1	A	109	MET	HE3	1.363	0.020	1
1	A	109	MET	HG2	2.536	0.020	2
1	A	109	MET	HG3	2.48	0.020	2
1	A	109	MET	CA	55.573	0.300	1
1	A	109	MET	CB	31.007	0.300	1
1	A	109	MET	CE	19.096	0.300	1
1	A	109	MET	CG	32.388	0.300	1
1	A	109	MET	N	121.154	0.300	1
1	A	110	LYS	H	8.259	0.020	1
1	A	110	LYS	HA	4.21	0.020	1
1	A	110	LYS	HB2	1.698	0.020	1
1	A	110	LYS	HB3	1.698	0.020	1
1	A	110	LYS	HD2	1.643	0.020	1
1	A	110	LYS	HD3	1.643	0.020	1
1	A	110	LYS	HE2	2.961	0.020	1
1	A	110	LYS	HE3	2.961	0.020	1
1	A	110	LYS	HG2	1.388	0.020	2
1	A	110	LYS	HG3	1.322	0.020	2
1	A	110	LYS	CA	56.488	0.300	1
1	A	110	LYS	CB	33.14	0.300	1
1	A	110	LYS	CD	28.935	0.300	1
1	A	110	LYS	CE	42.147	0.300	1
1	A	110	LYS	CG	27.017	0.300	1
1	A	110	LYS	N	122.304	0.300	1
1	A	111	HIS	H	8.468	0.020	1
1	A	111	HIS	HA	4.619	0.020	1
1	A	111	HIS	HB2	3.216	0.020	2
1	A	111	HIS	HB3	3.107	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	111	HIS	HD2	7.198	0.020	1
1	A	111	HIS	CA	55.198	0.300	1
1	A	111	HIS	CB	29.111	0.300	1
1	A	111	HIS	CD2	119.62	0.300	1
1	A	111	HIS	N	119.597	0.300	1
1	A	112	MET	H	8.385	0.020	1
1	A	112	MET	HA	4.434	0.020	1
1	A	112	MET	HB2	2.042	0.020	2
1	A	112	MET	HB3	1.936	0.020	2
1	A	112	MET	HE1	2.061	0.020	1
1	A	112	MET	HE2	2.061	0.020	1
1	A	112	MET	HE3	2.061	0.020	1
1	A	112	MET	HG2	2.543	0.020	2
1	A	112	MET	HG3	2.478	0.020	2
1	A	112	MET	CA	55.302	0.300	1
1	A	112	MET	CB	33.078	0.300	1
1	A	112	MET	CE	16.934	0.300	1
1	A	112	MET	CG	32.042	0.300	1
1	A	112	MET	N	122.696	0.300	1
1	A	113	ALA	H	8.39	0.020	1
1	A	113	ALA	HA	4.295	0.020	1
1	A	113	ALA	HB1	1.357	0.020	1
1	A	113	ALA	HB2	1.357	0.020	1
1	A	113	ALA	HB3	1.357	0.020	1
1	A	113	ALA	CA	52.5	0.300	1
1	A	113	ALA	CB	19.0	0.300	1
1	A	113	ALA	N	125.77	0.300	1
1	A	114	GLY	H	8.356	0.020	1
1	A	114	GLY	HA2	3.914	0.020	1
1	A	114	GLY	HA3	3.914	0.020	1
1	A	114	GLY	CA	45.24	0.300	1
1	A	114	GLY	N	108.458	0.300	1
1	A	115	ALA	H	8.107	0.020	1
1	A	115	ALA	HA	4.277	0.020	1
1	A	115	ALA	HB1	1.349	0.020	1
1	A	115	ALA	HB2	1.349	0.020	1
1	A	115	ALA	HB3	1.349	0.020	1
1	A	115	ALA	CA	52.524	0.300	1
1	A	115	ALA	CB	19.393	0.300	1
1	A	115	ALA	N	123.843	0.300	1
1	A	116	ALA	H	8.241	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	ALA	HA	4.264	0.020	1
1	A	116	ALA	HB1	1.355	0.020	1
1	A	116	ALA	HB2	1.355	0.020	1
1	A	116	ALA	HB3	1.355	0.020	1
1	A	116	ALA	CA	52.472	0.300	1
1	A	116	ALA	CB	19.235	0.300	1
1	A	116	ALA	N	123.101	0.300	1
1	A	117	ALA	H	8.155	0.020	1
1	A	117	ALA	HA	4.246	0.020	1
1	A	117	ALA	HB1	1.355	0.020	1
1	A	117	ALA	HB2	1.355	0.020	1
1	A	117	ALA	HB3	1.355	0.020	1
1	A	117	ALA	CA	52.433	0.300	1
1	A	117	ALA	CB	19.235	0.300	1
1	A	117	ALA	N	123.228	0.300	1
1	A	118	ALA	H	8.188	0.020	1
1	A	118	ALA	HA	3.919	0.020	1
1	A	118	ALA	HB1	1.363	0.020	1
1	A	118	ALA	HB2	1.363	0.020	1
1	A	118	ALA	HB3	1.363	0.020	1
1	A	118	ALA	CA	52.539	0.300	1
1	A	118	ALA	CB	19.156	0.300	1
1	A	118	ALA	N	123.218	0.300	1
1	A	119	GLY	H	8.233	0.020	1
1	A	119	GLY	HA2	3.901	0.020	1
1	A	119	GLY	HA3	3.901	0.020	1
1	A	119	GLY	CA	45.24	0.300	1
1	A	119	GLY	N	108.025	0.300	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	142	-0.25 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	125	0.09 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	133	0.05 ± 0.16	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 1011 atoms were assigned a chemical shift out of a possible 1286. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	355/454 (78%)	176/183 (96%)	91/182 (50%)	88/89 (99%)
Sidechain	584/693 (84%)	390/444 (88%)	175/213 (82%)	19/36 (53%)
Aromatic	72/139 (52%)	51/67 (76%)	21/68 (31%)	0/4 (0%)
Overall	1011/1286 (79%)	617/694 (89%)	287/463 (62%)	107/129 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1174 atoms were assigned a chemical shift out of a possible 1529. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	424/562 (75%)	213/229 (93%)	108/224 (48%)	103/109 (94%)
Sidechain	666/810 (82%)	446/520 (86%)	198/249 (80%)	22/41 (54%)
Aromatic	84/157 (54%)	59/75 (79%)	25/78 (32%)	0/4 (0%)
Overall	1174/1529 (77%)	718/824 (87%)	331/551 (60%)	125/154 (81%)

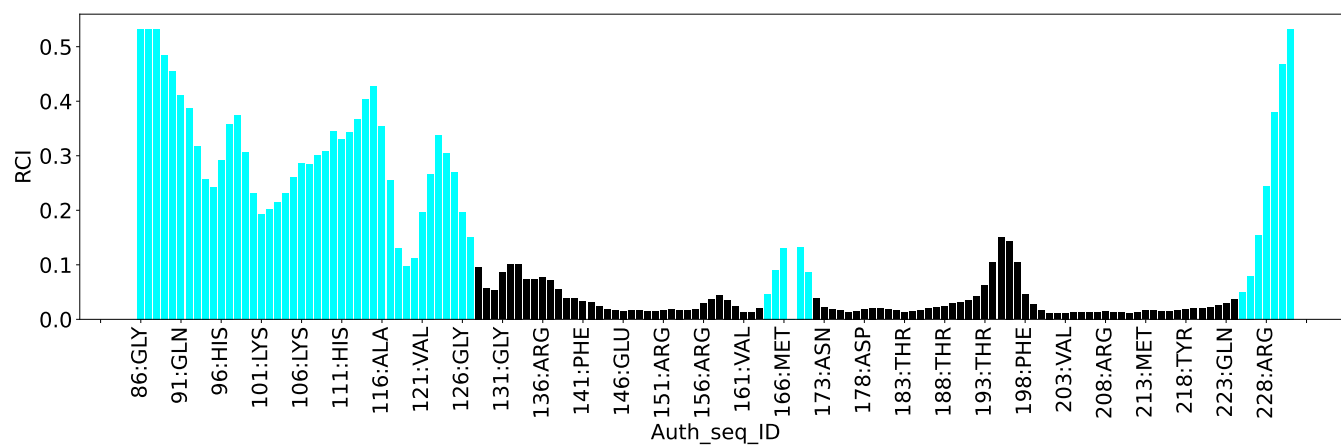
7.1.4 Statistically unusual chemical shifts [i](#)

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	1318
Intra-residue ($ i-j =0$)	462
Sequential ($ i-j =1$)	363
Medium range ($ i-j >1$ and $ i-j <5$)	216
Long range ($ i-j \geq 5$)	277
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	124
Number of unmapped restraints	0
Number of restraints per residue	9.9
Number of long range restraints per residue ¹	1.9

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)	23.0	0.2
0.2-0.5 (Medium)	34.2	0.5
>0.5 (Large)	45.1	18.31

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)	6.2	5.29
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

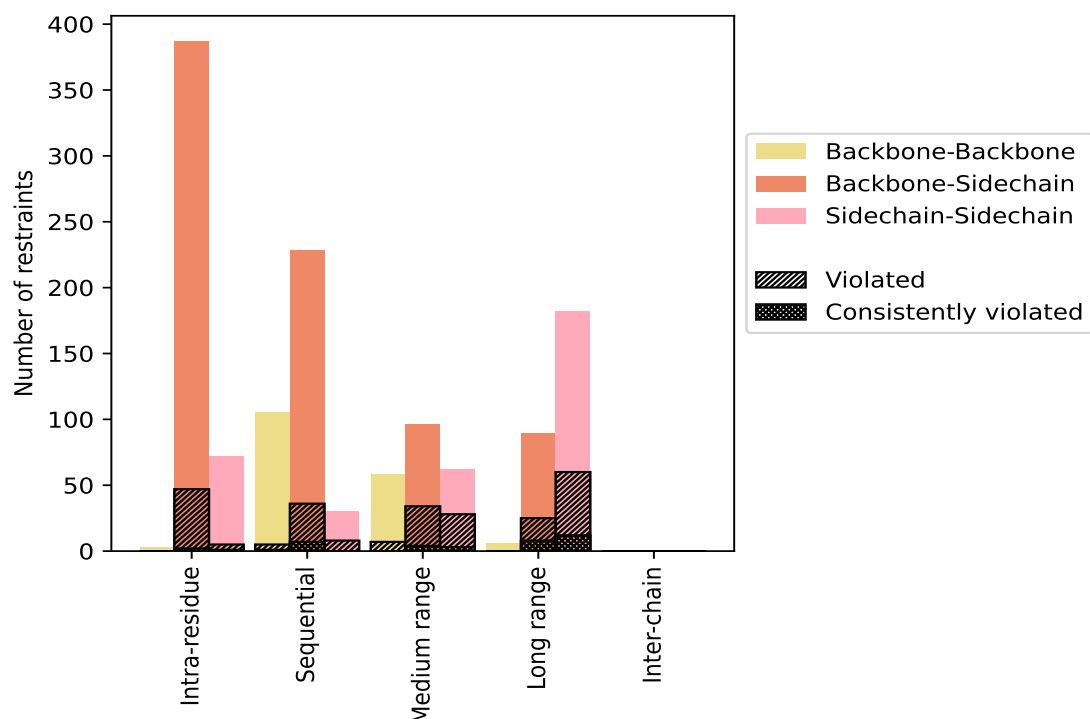
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	462	35.1	52	11.3	3.9	3	0.6	0.2
Backbone-Backbone	3	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	387	29.4	47	12.1	3.6	2	0.5	0.2
Sidechain-Sidechain	72	5.5	5	6.9	0.4	1	1.4	0.1
Sequential (i-j =1)	363	27.5	49	13.5	3.7	8	2.2	0.6
Backbone-Backbone	105	8.0	5	4.8	0.4	1	1.0	0.1
Backbone-Sidechain	228	17.3	36	15.8	2.7	7	3.1	0.5
Sidechain-Sidechain	30	2.3	8	26.7	0.6	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	216	16.4	69	31.9	5.2	7	3.2	0.5
Backbone-Backbone	58	4.4	7	12.1	0.5	0	0.0	0.0
Backbone-Sidechain	96	7.3	34	35.4	2.6	4	4.2	0.3
Sidechain-Sidechain	62	4.7	28	45.2	2.1	3	4.8	0.2
Long range (i-j ≥5)	277	21.0	85	30.7	6.4	20	7.2	1.5
Backbone-Backbone	6	0.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	89	6.8	25	28.1	1.9	8	9.0	0.6
Sidechain-Sidechain	182	13.8	60	33.0	4.6	12	6.6	0.9
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1318	100.0	255	19.3	19.3	38	2.9	2.9
Backbone-Backbone	172	13.1	12	7.0	0.9	1	0.6	0.1
Backbone-Sidechain	800	60.7	142	17.8	10.8	21	2.6	1.6
Sidechain-Sidechain	346	26.3	101	29.2	7.7	16	4.6	1.2

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	16	21	26	38	0	101	1.23	13.68	2.49	0.45
2	13	20	37	38	0	108	1.02	10.01	1.79	0.4
3	17	21	28	48	0	114	0.97	11.91	2.03	0.4
4	14	22	34	36	0	106	1.1	11.83	2.03	0.43
5	13	20	25	36	0	94	1.28	14.92	2.68	0.44
6	16	19	32	31	0	98	1.21	14.54	2.62	0.42
7	13	17	30	34	0	94	1.25	11.38	2.22	0.5
8	15	22	33	38	0	108	1.23	17.74	3.16	0.38
9	15	22	28	39	0	104	1.33	18.31	3.18	0.38
10	17	24	26	46	0	113	1.15	15.31	2.58	0.4

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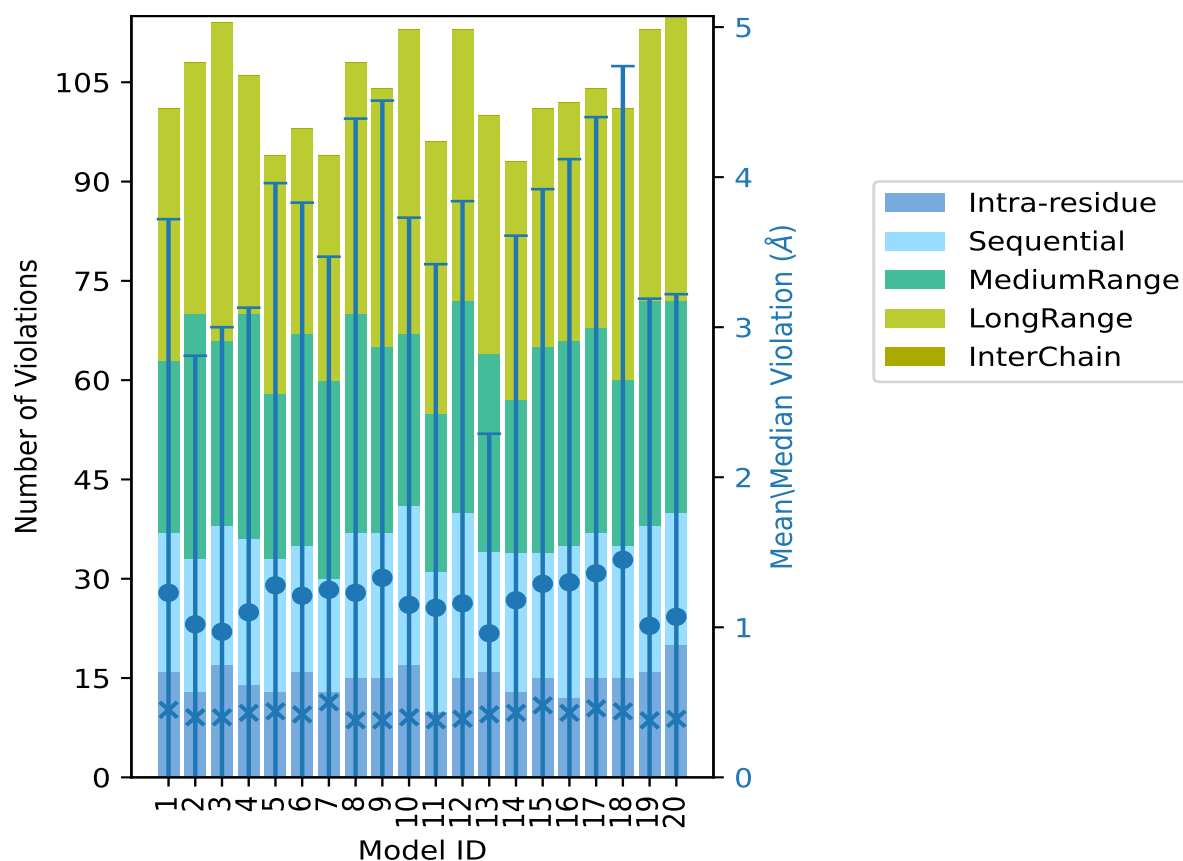
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	10	21	24	41	0	96	1.13	12.96	2.29	0.38
12	15	25	32	41	0	113	1.16	15.86	2.68	0.39
13	16	18	30	36	0	100	0.96	7.2	1.33	0.42
14	13	21	23	36	0	93	1.18	12.56	2.43	0.43
15	15	19	31	36	0	101	1.29	14.74	2.63	0.48
16	12	23	31	36	0	102	1.3	15.81	2.82	0.43
17	15	22	31	36	0	104	1.36	17.24	3.04	0.46
18	15	20	25	41	0	101	1.45	17.75	3.29	0.44
19	16	22	34	41	0	113	1.01	13.26	2.18	0.38
20	20	20	32	43	0	115	1.07	12.95	2.15	0.39

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

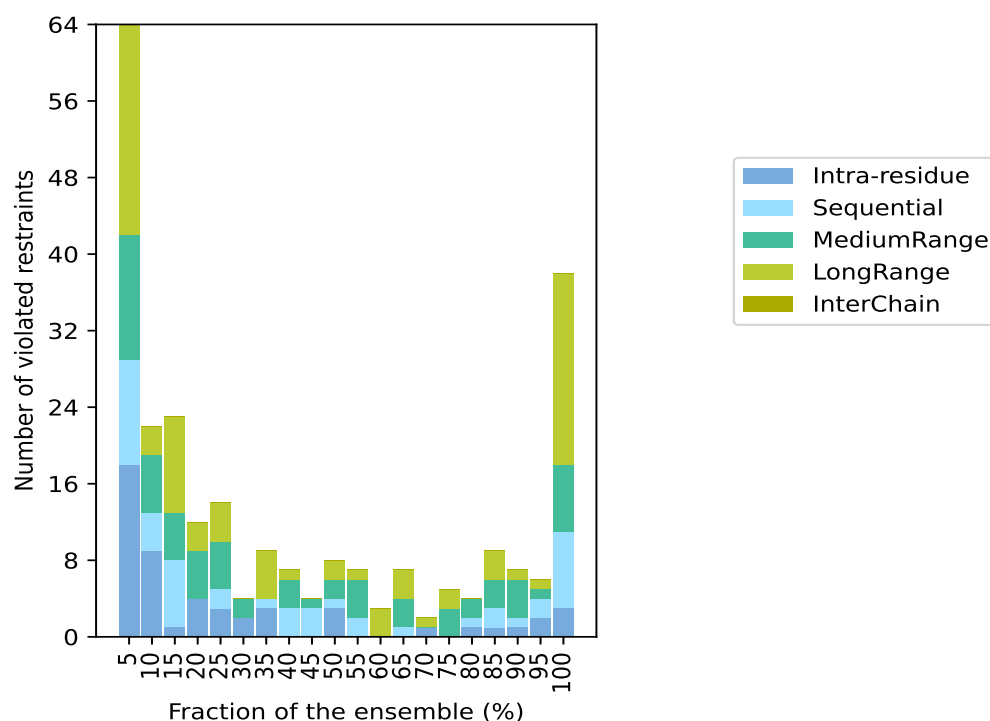
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1063(IR:410, SQ:314, MR:147, LR:192, IC:0) restraints are 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	%
18	11	13	22	0	64	1	5.0
9	4	6	3	0	22	2	10.0
1	7	5	10	0	23	3	15.0
4	0	5	3	0	12	4	20.0
3	2	5	4	0	14	5	25.0
2	0	2	0	0	4	6	30.0
3	1	0	5	0	9	7	35.0
0	3	3	1	0	7	8	40.0
0	3	1	0	0	4	9	45.0
3	1	2	2	0	8	10	50.0
0	2	4	1	0	7	11	55.0
0	0	0	3	0	3	12	60.0
0	1	3	3	0	7	13	65.0
1	0	0	1	0	2	14	70.0
0	0	3	2	0	5	15	75.0
1	1	2	0	0	4	16	80.0
1	2	3	3	0	9	17	85.0
1	1	4	1	0	7	18	90.0
2	2	1	1	0	6	19	95.0
3	8	7	20	0	38	20	100.0

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

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

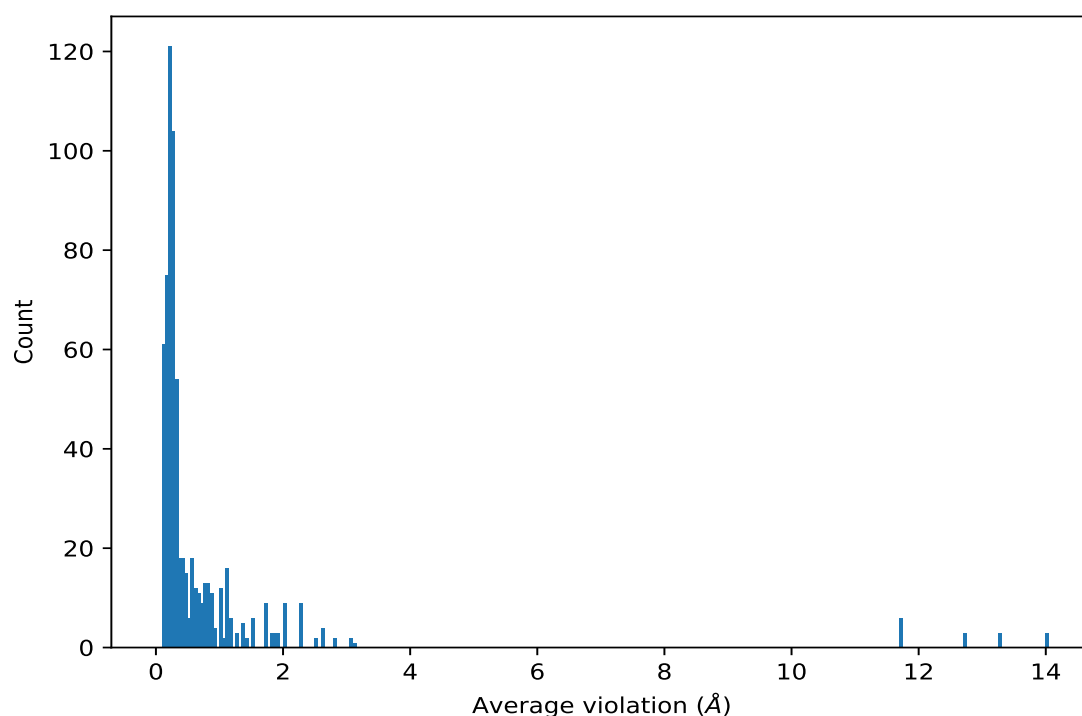
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	20	14.0	2.74	14.11
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	20	14.0	2.74	14.11
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	20	14.0	2.74	14.11
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	20	13.26	2.74	13.06
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	20	13.26	2.74	13.06
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	20	13.26	2.74	13.06
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	20	12.71	2.83	12.98
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	20	12.71	2.83	12.98
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	20	12.71	2.83	12.98
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	20	11.73	2.48	11.97
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	20	11.73	2.48	11.97
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	20	11.73	2.48	11.97
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	20	11.73	2.48	11.97
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	20	11.73	2.48	11.97
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	20	11.73	2.48	11.97
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	20	3.14	0.96	3.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	20	3.06	0.56	3.13
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	20	3.06	0.56	3.13
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	20	2.61	0.95	2.99
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	20	2.61	0.95	2.99
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	20	2.61	0.95	2.99
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	20	2.61	0.95	2.99
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	20	2.28	0.35	2.38
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	20	2.28	0.35	2.38
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	20	2.01	0.34	2.03
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	20	2.01	0.34	2.03
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	20	1.94	0.28	1.96
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	20	1.94	0.28	1.96
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	20	1.94	0.28	1.96
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	20	1.85	0.34	1.84
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	20	1.85	0.34	1.84
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	20	1.85	0.34	1.84
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	20	1.8	0.45	1.75
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	20	1.8	0.45	1.75
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	20	1.8	0.45	1.75
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	20	1.72	0.3	1.7
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	20	1.72	0.3	1.7
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	20	1.72	0.3	1.7
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	20	1.72	0.3	1.7
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	20	1.72	0.3	1.7
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	20	1.72	0.3	1.7
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	20	1.38	0.35	1.34
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	20	1.38	0.35	1.34
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	20	1.19	0.3	1.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	20	1.19	0.3	1.24
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	20	1.19	0.3	1.24
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	20	1.16	0.23	1.12
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	20	1.16	0.23	1.12
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	20	1.16	0.23	1.12
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	20	1.15	0.3	1.12
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	20	1.15	0.3	1.12
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	20	1.15	0.3	1.12
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	20	1.14	0.4	1.1
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	20	1.14	0.4	1.1
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	20	1.14	0.4	1.1
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	20	1.14	0.4	1.1
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	20	1.14	0.4	1.1
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	20	1.14	0.4	1.1
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	20	1.13	0.13	1.13
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	20	1.13	0.13	1.13
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	20	1.13	0.13	1.13
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	20	1.13	0.13	1.13
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	20	1.03	0.27	1.12
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	20	1.03	0.27	1.12
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	20	1.03	0.27	1.12
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	20	1.03	0.05	1.02
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	20	1.03	0.05	1.02
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	20	1.03	0.05	1.02
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	20	1.02	0.29	1.01
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	20	1.02	0.29	1.01
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	20	1.02	0.29	1.01
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	20	1.01	0.05	1.02
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	20	1.01	0.05	1.02
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	20	1.01	0.05	1.02
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	20	0.75	0.19	0.8
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	20	0.75	0.19	0.8
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	20	0.75	0.19	0.8
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	20	0.75	0.19	0.8
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	20	0.67	0.18	0.67
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	20	0.67	0.18	0.67
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	20	0.67	0.18	0.67
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	20	0.67	0.18	0.67
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	20	0.67	0.18	0.67
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	20	0.67	0.18	0.67
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	20	0.61	0.07	0.63
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	20	0.61	0.07	0.63

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	20	0.61	0.28	0.55
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	20	0.61	0.28	0.55
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	20	0.61	0.28	0.55
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	20	0.6	0.03	0.61
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	20	0.56	0.19	0.56
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	20	0.45	0.01	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	20	0.45	0.01	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	20	0.45	0.01	0.45
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	20	0.44	0.13	0.4
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	20	0.44	0.1	0.43
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	20	0.42	0.1	0.46
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	20	0.42	0.1	0.46
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	20	0.42	0.1	0.46
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	20	0.37	0.06	0.38
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	20	0.37	0.06	0.38
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	20	0.32	0.02	0.32
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	20	0.32	0.02	0.32
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	20	0.18	0.03	0.18
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	20	0.18	0.03	0.18
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	20	0.15	0.0	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	20	0.15	0.0	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	20	0.15	0.01	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	20	0.15	0.01	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	20	0.15	0.01	0.15
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	19	1.71	0.05	1.72
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	19	1.71	0.05	1.72
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	19	1.71	0.05	1.72
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	19	1.54	0.82	1.95
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	19	1.54	0.82	1.95
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	19	1.54	0.82	1.95
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	19	1.54	0.82	1.95
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	19	1.54	0.82	1.95
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	19	1.54	0.82	1.95
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	19	0.85	0.51	0.7
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	19	0.85	0.51	0.7
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	19	0.85	0.51	0.7
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	19	0.85	0.51	0.7
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	19	0.47	0.12	0.46
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	19	0.47	0.12	0.46
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	19	0.44	0.12	0.44
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	19	0.44	0.12	0.44
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	19	0.44	0.12	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	19	0.25	0.05	0.26
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	18	2.83	1.7	3.39
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	18	2.83	1.7	3.39
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	18	1.42	0.83	1.21
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	18	1.15	0.18	1.17
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	18	1.15	0.18	1.17
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	18	1.15	0.18	1.17
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	18	0.88	0.18	0.94
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	18	0.88	0.18	0.94
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	18	0.88	0.18	0.94
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	18	0.88	0.18	0.94
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	18	0.88	0.18	0.94
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	18	0.88	0.18	0.94
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	18	0.88	0.18	0.94
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	18	0.88	0.18	0.94
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	18	0.88	0.18	0.94
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	18	0.33	0.1	0.33
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	18	0.33	0.1	0.33
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	18	0.28	0.06	0.29
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	18	0.27	0.06	0.27
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	18	0.27	0.06	0.27
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	17	1.29	0.45	1.33
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	17	1.29	0.45	1.33
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	17	1.29	0.45	1.33
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	17	1.06	0.26	1.15
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	17	1.06	0.26	1.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	17	0.54	0.15	0.53
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	17	0.54	0.15	0.53
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	17	0.54	0.15	0.53
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	17	0.54	0.15	0.53
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	17	0.54	0.15	0.53
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	17	0.54	0.15	0.53
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	17	0.47	0.07	0.49
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	17	0.47	0.07	0.49
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	17	0.47	0.07	0.49
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	17	0.37	0.19	0.38
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	17	0.37	0.19	0.38
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	17	0.37	0.19	0.38
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	17	0.35	0.09	0.34
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	17	0.35	0.09	0.34
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	17	0.27	0.09	0.27
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	17	0.27	0.09	0.27
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	17	0.27	0.09	0.27
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	17	0.24	0.1	0.22
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	17	0.14	0.03	0.14
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	16	2.53	1.0	2.71
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	16	2.53	1.0	2.71
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	16	0.6	0.35	0.51
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	16	0.29	0.07	0.28
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	16	0.23	0.03	0.23
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	15	1.42	0.57	1.68
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	15	0.94	0.45	0.94
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	15	0.94	0.45	0.94
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	15	0.94	0.45	0.94
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	15	0.94	0.45	0.94
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	15	0.48	0.24	0.41
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	15	0.48	0.24	0.41
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	15	0.48	0.24	0.41
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	15	0.35	0.15	0.33
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	15	0.35	0.15	0.33
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	15	0.35	0.15	0.33
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	15	0.26	0.12	0.22
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	15	0.26	0.12	0.22
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	14	0.62	0.47	0.39
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	14	0.62	0.47	0.39
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	14	0.62	0.47	0.39
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	14	0.62	0.47	0.39
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	14	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	14	0.14	0.01	0.14
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	13	0.62	0.03	0.61
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	13	0.62	0.03	0.61
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	13	0.62	0.03	0.61
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	13	0.55	0.18	0.58
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	13	0.55	0.18	0.58
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	13	0.55	0.18	0.58
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	13	0.55	0.18	0.58
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	13	0.55	0.18	0.58
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	13	0.55	0.18	0.58
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	13	0.55	0.18	0.58
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	13	0.55	0.18	0.58
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	13	0.55	0.18	0.58
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	13	0.42	0.16	0.44
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	13	0.42	0.16	0.44
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	13	0.42	0.16	0.44
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	13	0.42	0.16	0.44
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	13	0.42	0.16	0.44
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	13	0.42	0.16	0.44
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	13	0.35	0.16	0.3
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	13	0.35	0.16	0.3
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	13	0.35	0.16	0.3
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	13	0.28	0.06	0.28
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	13	0.28	0.06	0.28
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	13	0.28	0.06	0.28
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	13	0.28	0.06	0.28
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	13	0.28	0.06	0.28
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	13	0.28	0.06	0.28
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	13	0.21	0.06	0.21
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	13	0.13	0.04	0.13
(1,217)	1:191:A:THR:HG21	1:197:A:ASN:HA	12	1.36	0.63	1.3
(1,217)	1:191:A:THR:HG22	1:197:A:ASN:HA	12	1.36	0.63	1.3
(1,217)	1:191:A:THR:HG23	1:197:A:ASN:HA	12	1.36	0.63	1.3
(1,763)	1:161:A:VAL:HG11	1:214:A:CYS:H	12	0.44	0.29	0.3
(1,763)	1:161:A:VAL:HG12	1:214:A:CYS:H	12	0.44	0.29	0.3
(1,763)	1:161:A:VAL:HG13	1:214:A:CYS:H	12	0.44	0.29	0.3
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG21	12	0.34	0.18	0.32
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG22	12	0.34	0.18	0.32
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG23	12	0.34	0.18	0.32
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG21	12	0.34	0.18	0.32
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG22	12	0.34	0.18	0.32
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG23	12	0.34	0.18	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,162)	1:217:A:GLN:HA	1:220:A:ARG:HG2	11	0.46	0.16	0.49
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG21	11	0.33	0.12	0.32
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG22	11	0.33	0.12	0.32
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG23	11	0.33	0.12	0.32
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB2	11	0.27	0.11	0.21
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB3	11	0.27	0.11	0.21
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB2	11	0.27	0.11	0.21
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB3	11	0.27	0.11	0.21
(1,365)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	11	0.26	0.12	0.22
(1,365)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	11	0.26	0.12	0.22
(1,365)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	11	0.26	0.12	0.22
(1,1121)	1:165:A:PRO:HB2	1:166:A:MET:H	11	0.26	0.07	0.3
(1,1121)	1:165:A:PRO:HB3	1:166:A:MET:H	11	0.26	0.07	0.3
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB2	11	0.21	0.08	0.22
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB3	11	0.21	0.08	0.22
(1,498)	1:141:A:PHE:HB3	1:143:A:SER:H	11	0.17	0.04	0.16
(1,11)	1:186:A:GLN:HA	1:189:A:VAL:HB	10	0.44	0.14	0.46
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG21	10	0.37	0.09	0.39
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG22	10	0.37	0.09	0.39
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG23	10	0.37	0.09	0.39
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE1	10	0.26	0.03	0.25
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE2	10	0.26	0.03	0.25
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE3	10	0.26	0.03	0.25
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE1	10	0.26	0.03	0.25
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE2	10	0.26	0.03	0.25
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE3	10	0.26	0.03	0.25
(1,819)	1:176:A:VAL:H	1:214:A:CYS:HB3	10	0.25	0.11	0.21
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB2	10	0.25	0.12	0.22
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB3	10	0.25	0.12	0.22
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG2	10	0.17	0.02	0.18
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG3	10	0.17	0.02	0.18
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE1	10	0.16	0.03	0.16
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE2	10	0.16	0.03	0.16
(1,27)	1:219:A:GLU:HA	1:219:A:GLU:HG3	10	0.16	0.02	0.16
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG11	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG12	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG13	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG21	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG22	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG23	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG11	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG12	9	0.27	0.03	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG13	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG21	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG22	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG23	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG11	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG12	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG13	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG21	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG22	9	0.27	0.03	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG23	9	0.27	0.03	0.28
(1,432)	1:228:A:ARG:H	1:229:A:GLY:H	9	0.21	0.05	0.2
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE1	9	0.18	0.07	0.17
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE2	9	0.18	0.07	0.17
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE3	9	0.18	0.07	0.17
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE1	9	0.18	0.07	0.17
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE2	9	0.18	0.07	0.17
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE3	9	0.18	0.07	0.17
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG12	9	0.12	0.01	0.11
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG13	9	0.12	0.01	0.11
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD2	8	0.86	0.21	0.8
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD3	8	0.86	0.21	0.8
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG2	8	0.37	0.3	0.25
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG3	8	0.37	0.3	0.25
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG2	8	0.37	0.3	0.25
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG3	8	0.37	0.3	0.25
(1,425)	1:165:A:PRO:HB3	1:166:A:MET:H	8	0.31	0.09	0.35
(1,180)	1:208:A:ARG:HB2	1:209:A:MET:HA	8	0.21	0.05	0.2
(1,180)	1:208:A:ARG:HB3	1:209:A:MET:HA	8	0.21	0.05	0.2
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD2	8	0.21	0.04	0.23
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD3	8	0.21	0.04	0.23
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD2	8	0.21	0.04	0.23
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD3	8	0.21	0.04	0.23
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD2	8	0.21	0.04	0.23
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD3	8	0.21	0.04	0.23
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB1	8	0.18	0.04	0.18
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB2	8	0.18	0.04	0.18
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB3	8	0.18	0.04	0.18
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB1	8	0.18	0.04	0.18
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB2	8	0.18	0.04	0.18
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB3	8	0.18	0.04	0.18
(1,865)	1:144:A:ASP:H	1:147:A:ASP:H	8	0.13	0.02	0.13
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG11	7	0.81	0.07	0.81

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG12	7	0.81	0.07	0.81
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG13	7	0.81	0.07	0.81
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG11	7	0.81	0.07	0.81
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG12	7	0.81	0.07	0.81
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG13	7	0.81	0.07	0.81
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG11	7	0.81	0.07	0.81
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG12	7	0.81	0.07	0.81
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG13	7	0.81	0.07	0.81
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG11	7	0.73	0.22	0.72
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG12	7	0.73	0.22	0.72
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG13	7	0.73	0.22	0.72
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG11	7	0.73	0.22	0.72
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG12	7	0.73	0.22	0.72
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG13	7	0.73	0.22	0.72
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG11	7	0.73	0.22	0.72
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG12	7	0.73	0.22	0.72
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG13	7	0.73	0.22	0.72
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB1	7	0.33	0.0	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB2	7	0.33	0.0	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB3	7	0.33	0.0	0.33
(1,674)	1:122:A:VAL:H	1:122:A:VAL:HB	7	0.32	0.09	0.32
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE1	7	0.3	0.17	0.22
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE2	7	0.3	0.17	0.22
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE3	7	0.3	0.17	0.22
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE1	7	0.28	0.09	0.32
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE2	7	0.28	0.09	0.32
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE3	7	0.28	0.09	0.32
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE1	7	0.26	0.06	0.24
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE2	7	0.26	0.06	0.24
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE3	7	0.26	0.06	0.24
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE1	7	0.26	0.06	0.24
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE2	7	0.26	0.06	0.24
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE3	7	0.26	0.06	0.24
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB1	7	0.23	0.02	0.22
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB2	7	0.23	0.02	0.22
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB3	7	0.23	0.02	0.22
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD2	7	0.21	0.05	0.22
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD3	7	0.21	0.05	0.22
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD2	7	0.21	0.05	0.22
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD3	7	0.21	0.05	0.22
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD2	7	0.21	0.05	0.22
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD3	7	0.21	0.05	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,605)	1:213:A:MET:H	1:213:A:MET:HG2	6	0.67	0.03	0.68
(1,605)	1:213:A:MET:H	1:213:A:MET:HG3	6	0.67	0.03	0.68
(1,463)	1:125:A:LEU:H	1:125:A:LEU:HB3	6	0.33	0.14	0.42
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE1	6	0.16	0.05	0.15
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE2	6	0.16	0.05	0.15
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE3	6	0.16	0.05	0.15
(1,944)	1:139:A:ILE:HD11	1:141:A:PHE:HZ	6	0.12	0.02	0.12
(1,944)	1:139:A:ILE:HD12	1:141:A:PHE:HZ	6	0.12	0.02	0.12
(1,944)	1:139:A:ILE:HD13	1:141:A:PHE:HZ	6	0.12	0.02	0.12
(1,663)	1:191:A:THR:H	1:191:A:THR:HG21	5	0.29	0.09	0.32
(1,663)	1:191:A:THR:H	1:191:A:THR:HG22	5	0.29	0.09	0.32
(1,663)	1:191:A:THR:H	1:191:A:THR:HG23	5	0.29	0.09	0.32
(1,150)	1:133:A:ALA:HB1	1:159:A:ASN:HB2	5	0.28	0.13	0.37
(1,150)	1:133:A:ALA:HB2	1:159:A:ASN:HB2	5	0.28	0.13	0.37
(1,150)	1:133:A:ALA:HB3	1:159:A:ASN:HB2	5	0.28	0.13	0.37
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE1	5	0.27	0.07	0.25
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE2	5	0.27	0.07	0.25
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE3	5	0.27	0.07	0.25
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE1	5	0.27	0.07	0.25
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE2	5	0.27	0.07	0.25
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE3	5	0.27	0.07	0.25
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE1	5	0.27	0.07	0.25
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE2	5	0.27	0.07	0.25
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE3	5	0.27	0.07	0.25
(1,1105)	1:156:A:ARG:HD2	1:157:A:TYR:H	5	0.25	0.12	0.28
(1,1105)	1:156:A:ARG:HD3	1:157:A:TYR:H	5	0.25	0.12	0.28
(1,938)	1:128:A:TYR:HE1	1:182:A:ILE:HB	5	0.25	0.14	0.22
(1,938)	1:128:A:TYR:HE2	1:182:A:ILE:HB	5	0.25	0.14	0.22
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE1	5	0.24	0.08	0.3
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE2	5	0.24	0.08	0.3
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE3	5	0.24	0.08	0.3
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE1	5	0.23	0.04	0.23
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE2	5	0.23	0.04	0.23
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE3	5	0.23	0.04	0.23
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG21	5	0.22	0.04	0.21
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG22	5	0.22	0.04	0.21
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG23	5	0.22	0.04	0.21
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE1	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE2	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE3	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE1	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE2	5	0.21	0.04	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE3	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE1	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE2	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE3	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE1	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE2	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE3	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE1	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE2	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE3	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE1	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE2	5	0.21	0.04	0.22
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE3	5	0.21	0.04	0.22
(1,185)	1:208:A:ARG:HA	1:211:A:GLU:HB2	5	0.2	0.09	0.24
(1,185)	1:208:A:ARG:HA	1:211:A:GLU:HB3	5	0.2	0.09	0.24
(1,394)	1:152:A:GLU:H	1:152:A:GLU:HG3	5	0.16	0.05	0.15
(1,893)	1:210:A:VAL:HA	1:214:A:CYS:H	5	0.15	0.02	0.16
(1,649)	1:196:A:GLU:HG3	1:197:A:ASN:H	5	0.14	0.02	0.14
(1,132)	1:208:A:ARG:HA	1:208:A:ARG:HG2	5	0.12	0.02	0.13
(1,981)	1:125:A:LEU:H	1:125:A:LEU:HB2	4	0.34	0.07	0.34
(1,981)	1:125:A:LEU:H	1:125:A:LEU:HB3	4	0.34	0.07	0.34
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE1	4	0.27	0.03	0.28
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE2	4	0.27	0.03	0.28
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE3	4	0.27	0.03	0.28
(1,358)	1:139:A:ILE:HG21	1:212:A:GLN:HG2	4	0.23	0.09	0.23
(1,358)	1:139:A:ILE:HG21	1:212:A:GLN:HG3	4	0.23	0.09	0.23
(1,358)	1:139:A:ILE:HG22	1:212:A:GLN:HG2	4	0.23	0.09	0.23
(1,358)	1:139:A:ILE:HG22	1:212:A:GLN:HG3	4	0.23	0.09	0.23
(1,358)	1:139:A:ILE:HG23	1:212:A:GLN:HG2	4	0.23	0.09	0.23
(1,358)	1:139:A:ILE:HG23	1:212:A:GLN:HG3	4	0.23	0.09	0.23
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD11	4	0.22	0.11	0.2
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD12	4	0.22	0.11	0.2
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD13	4	0.22	0.11	0.2
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE1	4	0.22	0.02	0.21
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE2	4	0.22	0.02	0.21
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE3	4	0.22	0.02	0.21
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE1	4	0.22	0.02	0.21
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE2	4	0.22	0.02	0.21
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE3	4	0.22	0.02	0.21
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE1	4	0.22	0.02	0.21
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE2	4	0.22	0.02	0.21
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE3	4	0.22	0.02	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1283)	1:222:A:SER:HA	1:225:A:TYR:HB2	4	0.21	0.08	0.23
(1,1283)	1:222:A:SER:HA	1:225:A:TYR:HB3	4	0.21	0.08	0.23
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG11	4	0.21	0.11	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG12	4	0.21	0.11	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG13	4	0.21	0.11	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG21	4	0.21	0.11	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG22	4	0.21	0.11	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG23	4	0.21	0.11	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG11	4	0.21	0.11	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG12	4	0.21	0.11	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG13	4	0.21	0.11	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG21	4	0.21	0.11	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG22	4	0.21	0.11	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG23	4	0.21	0.11	0.15
(1,152)	1:133:A:ALA:HB1	1:160:A:GLN:HB2	4	0.17	0.06	0.16
(1,152)	1:133:A:ALA:HB2	1:160:A:GLN:HB2	4	0.17	0.06	0.16
(1,152)	1:133:A:ALA:HB3	1:160:A:GLN:HB2	4	0.17	0.06	0.16
(1,109)	1:204:A:LYS:HA	1:204:A:LYS:HG3	4	0.16	0.04	0.16
(1,1181)	1:196:A:GLU:HA	1:196:A:GLU:HG2	4	0.16	0.01	0.16
(1,1181)	1:196:A:GLU:HA	1:196:A:GLU:HG3	4	0.16	0.01	0.16
(1,168)	1:216:A:THR:HA	1:219:A:GLU:HB3	4	0.14	0.02	0.13
(1,615)	1:207:A:GLU:H	1:207:A:GLU:HG2	4	0.11	0.0	0.11
(1,368)	1:176:A:VAL:HG11	1:215:A:ILE:HD11	3	0.78	0.19	0.77
(1,368)	1:176:A:VAL:HG11	1:215:A:ILE:HD12	3	0.78	0.19	0.77
(1,368)	1:176:A:VAL:HG11	1:215:A:ILE:HD13	3	0.78	0.19	0.77
(1,368)	1:176:A:VAL:HG12	1:215:A:ILE:HD11	3	0.78	0.19	0.77
(1,368)	1:176:A:VAL:HG12	1:215:A:ILE:HD12	3	0.78	0.19	0.77
(1,368)	1:176:A:VAL:HG12	1:215:A:ILE:HD13	3	0.78	0.19	0.77
(1,368)	1:176:A:VAL:HG13	1:215:A:ILE:HD11	3	0.78	0.19	0.77
(1,368)	1:176:A:VAL:HG13	1:215:A:ILE:HD12	3	0.78	0.19	0.77
(1,368)	1:176:A:VAL:HG13	1:215:A:ILE:HD13	3	0.78	0.19	0.77
(1,762)	1:176:A:VAL:HG11	1:214:A:CYS:H	3	0.66	0.26	0.8
(1,762)	1:176:A:VAL:HG12	1:214:A:CYS:H	3	0.66	0.26	0.8
(1,762)	1:176:A:VAL:HG13	1:214:A:CYS:H	3	0.66	0.26	0.8
(1,972)	1:175:A:PHE:HD1	1:176:A:VAL:HG21	3	0.59	0.24	0.69
(1,972)	1:175:A:PHE:HD1	1:176:A:VAL:HG22	3	0.59	0.24	0.69
(1,972)	1:175:A:PHE:HD1	1:176:A:VAL:HG23	3	0.59	0.24	0.69
(1,972)	1:175:A:PHE:HD2	1:176:A:VAL:HG21	3	0.59	0.24	0.69
(1,972)	1:175:A:PHE:HD2	1:176:A:VAL:HG22	3	0.59	0.24	0.69
(1,972)	1:175:A:PHE:HD2	1:176:A:VAL:HG23	3	0.59	0.24	0.69
(1,699)	1:120:A:ALA:HB1	1:122:A:VAL:H	3	0.46	0.19	0.42
(1,699)	1:120:A:ALA:HB2	1:122:A:VAL:H	3	0.46	0.19	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,699)	1:120:A:ALA:HB3	1:122:A:VAL:H	3	0.46	0.19	0.42
(1,341)	1:134:A:MET:HE1	1:217:A:GLN:HA	3	0.36	0.01	0.36
(1,341)	1:134:A:MET:HE2	1:217:A:GLN:HA	3	0.36	0.01	0.36
(1,341)	1:134:A:MET:HE3	1:217:A:GLN:HA	3	0.36	0.01	0.36
(1,475)	1:132:A:SER:HB2	1:133:A:ALA:H	3	0.32	0.07	0.28
(1,475)	1:132:A:SER:HB3	1:133:A:ALA:H	3	0.32	0.07	0.28
(1,1260)	1:215:A:ILE:HG21	1:219:A:GLU:HG2	3	0.25	0.08	0.2
(1,1260)	1:215:A:ILE:HG21	1:219:A:GLU:HG3	3	0.25	0.08	0.2
(1,1260)	1:215:A:ILE:HG22	1:219:A:GLU:HG2	3	0.25	0.08	0.2
(1,1260)	1:215:A:ILE:HG22	1:219:A:GLU:HG3	3	0.25	0.08	0.2
(1,1260)	1:215:A:ILE:HG23	1:219:A:GLU:HG2	3	0.25	0.08	0.2
(1,1260)	1:215:A:ILE:HG23	1:219:A:GLU:HG3	3	0.25	0.08	0.2
(1,813)	1:176:A:VAL:HB	1:177:A:HIS:H	3	0.24	0.08	0.21
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG11	3	0.22	0.05	0.24
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG12	3	0.22	0.05	0.24
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG13	3	0.22	0.05	0.24
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG21	3	0.22	0.05	0.24
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG22	3	0.22	0.05	0.24
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG23	3	0.22	0.05	0.24
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG11	3	0.22	0.05	0.24
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG12	3	0.22	0.05	0.24
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG13	3	0.22	0.05	0.24
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG21	3	0.22	0.05	0.24
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG22	3	0.22	0.05	0.24
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG23	3	0.22	0.05	0.24
(1,212)	1:200:A:GLU:HA	1:203:A:VAL:HG21	3	0.21	0.13	0.13
(1,212)	1:200:A:GLU:HA	1:203:A:VAL:HG22	3	0.21	0.13	0.13
(1,212)	1:200:A:GLU:HA	1:203:A:VAL:HG23	3	0.21	0.13	0.13
(1,234)	1:158:A:PRO:HB2	1:183:A:THR:HG21	3	0.2	0.14	0.11
(1,234)	1:158:A:PRO:HB2	1:183:A:THR:HG22	3	0.2	0.14	0.11
(1,234)	1:158:A:PRO:HB2	1:183:A:THR:HG23	3	0.2	0.14	0.11
(1,1174)	1:188:A:THR:HG21	1:198:A:PHE:HB2	3	0.2	0.01	0.19
(1,1174)	1:188:A:THR:HG21	1:198:A:PHE:HB3	3	0.2	0.01	0.19
(1,1174)	1:188:A:THR:HG22	1:198:A:PHE:HB2	3	0.2	0.01	0.19
(1,1174)	1:188:A:THR:HG22	1:198:A:PHE:HB3	3	0.2	0.01	0.19
(1,1174)	1:188:A:THR:HG23	1:198:A:PHE:HB2	3	0.2	0.01	0.19
(1,1174)	1:188:A:THR:HG23	1:198:A:PHE:HB3	3	0.2	0.01	0.19
(1,1183)	1:196:A:GLU:HG2	1:197:A:ASN:H	3	0.2	0.02	0.19
(1,1183)	1:196:A:GLU:HG3	1:197:A:ASN:H	3	0.2	0.02	0.19
(1,1016)	1:134:A:MET:HG2	1:216:A:THR:HG21	3	0.19	0.06	0.23
(1,1016)	1:134:A:MET:HG2	1:216:A:THR:HG22	3	0.19	0.06	0.23
(1,1016)	1:134:A:MET:HG2	1:216:A:THR:HG23	3	0.19	0.06	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1016)	1:134:A:MET:HG3	1:216:A:THR:HG21	3	0.19	0.06	0.23
(1,1016)	1:134:A:MET:HG3	1:216:A:THR:HG22	3	0.19	0.06	0.23
(1,1016)	1:134:A:MET:HG3	1:216:A:THR:HG23	3	0.19	0.06	0.23
(1,842)	1:196:A:GLU:HG2	1:197:A:ASN:H	3	0.18	0.04	0.19
(1,942)	1:139:A:ILE:HG21	1:141:A:PHE:HZ	3	0.18	0.09	0.12
(1,942)	1:139:A:ILE:HG22	1:141:A:PHE:HZ	3	0.18	0.09	0.12
(1,942)	1:139:A:ILE:HG23	1:141:A:PHE:HZ	3	0.18	0.09	0.12
(1,238)	1:183:A:THR:HG21	1:184:A:ILE:HA	3	0.16	0.02	0.15
(1,238)	1:183:A:THR:HG22	1:184:A:ILE:HA	3	0.16	0.02	0.15
(1,238)	1:183:A:THR:HG23	1:184:A:ILE:HA	3	0.16	0.02	0.15
(1,262)	1:161:A:VAL:HB	1:183:A:THR:HG21	3	0.16	0.02	0.16
(1,262)	1:161:A:VAL:HB	1:183:A:THR:HG22	3	0.16	0.02	0.16
(1,262)	1:161:A:VAL:HB	1:183:A:THR:HG23	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG11	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG12	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG13	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG21	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG22	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG23	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG11	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG12	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG13	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG21	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG22	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG23	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG11	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG12	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG13	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG21	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG22	3	0.16	0.02	0.16
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG23	3	0.16	0.02	0.16
(1,406)	1:176:A:VAL:H	1:176:A:VAL:HB	3	0.14	0.0	0.14
(1,157)	1:132:A:SER:HA	1:133:A:ALA:HB1	3	0.14	0.03	0.16
(1,157)	1:132:A:SER:HA	1:133:A:ALA:HB2	3	0.14	0.03	0.16
(1,157)	1:132:A:SER:HA	1:133:A:ALA:HB3	3	0.14	0.03	0.16
(1,178)	1:183:A:THR:HG21	1:210:A:VAL:HG21	3	0.13	0.01	0.12
(1,178)	1:183:A:THR:HG21	1:210:A:VAL:HG22	3	0.13	0.01	0.12
(1,178)	1:183:A:THR:HG21	1:210:A:VAL:HG23	3	0.13	0.01	0.12
(1,178)	1:183:A:THR:HG22	1:210:A:VAL:HG21	3	0.13	0.01	0.12
(1,178)	1:183:A:THR:HG22	1:210:A:VAL:HG22	3	0.13	0.01	0.12
(1,178)	1:183:A:THR:HG22	1:210:A:VAL:HG23	3	0.13	0.01	0.12
(1,178)	1:183:A:THR:HG23	1:210:A:VAL:HG21	3	0.13	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,178)	1:183:A:THR:HG23	1:210:A:VAL:HG22	3	0.13	0.01	0.12
(1,178)	1:183:A:THR:HG23	1:210:A:VAL:HG23	3	0.13	0.01	0.12
(1,249)	1:179:A:CYS:HA	1:182:A:ILE:HG21	3	0.12	0.01	0.12
(1,249)	1:179:A:CYS:HA	1:182:A:ILE:HG22	3	0.12	0.01	0.12
(1,249)	1:179:A:CYS:HA	1:182:A:ILE:HG23	3	0.12	0.01	0.12
(1,299)	1:129:A:MET:HB2	1:129:A:MET:HE1	2	0.38	0.01	0.38
(1,299)	1:129:A:MET:HB2	1:129:A:MET:HE2	2	0.38	0.01	0.38
(1,299)	1:129:A:MET:HB2	1:129:A:MET:HE3	2	0.38	0.01	0.38
(1,1242)	1:208:A:ARG:HG2	1:212:A:GLN:HG2	2	0.34	0.0	0.34
(1,1242)	1:208:A:ARG:HG2	1:212:A:GLN:HG3	2	0.34	0.0	0.34
(1,1242)	1:208:A:ARG:HG3	1:212:A:GLN:HG2	2	0.34	0.0	0.34
(1,1242)	1:208:A:ARG:HG3	1:212:A:GLN:HG3	2	0.34	0.0	0.34
(1,298)	1:129:A:MET:HA	1:129:A:MET:HE1	2	0.34	0.08	0.34
(1,298)	1:129:A:MET:HA	1:129:A:MET:HE2	2	0.34	0.08	0.34
(1,298)	1:129:A:MET:HA	1:129:A:MET:HE3	2	0.34	0.08	0.34
(1,1244)	1:209:A:MET:HB2	1:213:A:MET:HE1	2	0.3	0.01	0.3
(1,1244)	1:209:A:MET:HB2	1:213:A:MET:HE2	2	0.3	0.01	0.3
(1,1244)	1:209:A:MET:HB2	1:213:A:MET:HE3	2	0.3	0.01	0.3
(1,1244)	1:209:A:MET:HB3	1:213:A:MET:HE1	2	0.3	0.01	0.3
(1,1244)	1:209:A:MET:HB3	1:213:A:MET:HE2	2	0.3	0.01	0.3
(1,1244)	1:209:A:MET:HB3	1:213:A:MET:HE3	2	0.3	0.01	0.3
(1,1126)	1:176:A:VAL:HG11	1:179:A:CYS:HB2	2	0.29	0.14	0.29
(1,1126)	1:176:A:VAL:HG11	1:179:A:CYS:HB3	2	0.29	0.14	0.29
(1,1126)	1:176:A:VAL:HG12	1:179:A:CYS:HB2	2	0.29	0.14	0.29
(1,1126)	1:176:A:VAL:HG12	1:179:A:CYS:HB3	2	0.29	0.14	0.29
(1,1126)	1:176:A:VAL:HG13	1:179:A:CYS:HB2	2	0.29	0.14	0.29
(1,1126)	1:176:A:VAL:HG13	1:179:A:CYS:HB3	2	0.29	0.14	0.29
(1,1026)	1:138:A:ILE:HD11	1:151:A:ARG:HG2	2	0.23	0.03	0.23
(1,1026)	1:138:A:ILE:HD11	1:151:A:ARG:HG3	2	0.23	0.03	0.23
(1,1026)	1:138:A:ILE:HD12	1:151:A:ARG:HG2	2	0.23	0.03	0.23
(1,1026)	1:138:A:ILE:HD12	1:151:A:ARG:HG3	2	0.23	0.03	0.23
(1,1026)	1:138:A:ILE:HD13	1:151:A:ARG:HG2	2	0.23	0.03	0.23
(1,1026)	1:138:A:ILE:HD13	1:151:A:ARG:HG3	2	0.23	0.03	0.23
(1,1296)	1:228:A:ARG:H	1:228:A:ARG:HG2	2	0.21	0.04	0.21
(1,1296)	1:228:A:ARG:H	1:228:A:ARG:HG3	2	0.21	0.04	0.21
(1,718)	1:158:A:PRO:HB2	1:159:A:ASN:H	2	0.2	0.06	0.2
(1,476)	1:132:A:SER:HA	1:133:A:ALA:H	2	0.2	0.01	0.2
(1,45)	1:125:A:LEU:HA	1:125:A:LEU:HD11	2	0.18	0.08	0.18
(1,45)	1:125:A:LEU:HA	1:125:A:LEU:HD12	2	0.18	0.08	0.18
(1,45)	1:125:A:LEU:HA	1:125:A:LEU:HD13	2	0.18	0.08	0.18
(1,569)	1:228:A:ARG:H	1:228:A:ARG:HG2	2	0.18	0.02	0.18
(1,276)	1:138:A:ILE:HD11	1:151:A:ARG:HG3	2	0.18	0.04	0.18

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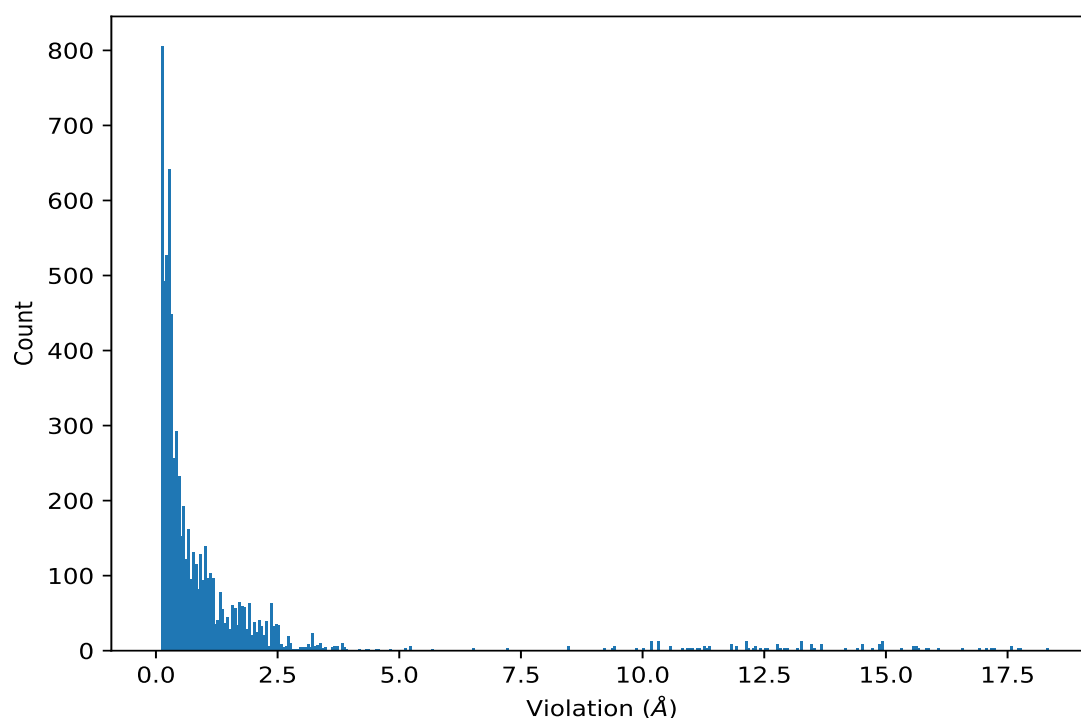
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,276)	1:138:A:ILE:HD12	1:151:A:ARG:HG3	2	0.18	0.04	0.18
(1,276)	1:138:A:ILE:HD13	1:151:A:ARG:HG3	2	0.18	0.04	0.18
(1,462)	1:122:A:VAL:HB	1:123:A:GLY:H	2	0.16	0.06	0.16
(1,370)	1:212:A:GLN:HA	1:215:A:ILE:HD11	2	0.16	0.04	0.16
(1,370)	1:212:A:GLN:HA	1:215:A:ILE:HD12	2	0.16	0.04	0.16
(1,370)	1:212:A:GLN:HA	1:215:A:ILE:HD13	2	0.16	0.04	0.16
(1,309)	1:202:A:ASP:HB2	1:206:A:MET:HE1	2	0.15	0.02	0.15
(1,309)	1:202:A:ASP:HB2	1:206:A:MET:HE2	2	0.15	0.02	0.15
(1,309)	1:202:A:ASP:HB2	1:206:A:MET:HE3	2	0.15	0.02	0.15
(1,705)	1:143:A:SER:H	1:147:A:ASP:H	2	0.15	0.02	0.15
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG11	2	0.15	0.04	0.15
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG12	2	0.15	0.04	0.15
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG13	2	0.15	0.04	0.15
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG21	2	0.15	0.04	0.15
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG22	2	0.15	0.04	0.15
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG23	2	0.15	0.04	0.15
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG11	2	0.15	0.04	0.15
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG12	2	0.15	0.04	0.15
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG13	2	0.15	0.04	0.15
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG21	2	0.15	0.04	0.15
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG22	2	0.15	0.04	0.15
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG23	2	0.15	0.04	0.15
(1,297)	1:129:A:MET:HB3	1:129:A:MET:HE1	2	0.14	0.01	0.14
(1,297)	1:129:A:MET:HB3	1:129:A:MET:HE2	2	0.14	0.01	0.14
(1,297)	1:129:A:MET:HB3	1:129:A:MET:HE3	2	0.14	0.01	0.14
(1,21)	1:200:A:GLU:HA	1:200:A:GLU:HB3	2	0.12	0.02	0.12
(1,34)	1:223:A:GLN:HA	1:223:A:GLN:HG2	2	0.11	0.01	0.11
(1,35)	1:223:A:GLN:HA	1:223:A:GLN:HG3	2	0.11	0.0	0.11
(1,855)	1:125:A:LEU:HD11	1:126:A:GLY:H	2	0.11	0.0	0.11
(1,855)	1:125:A:LEU:HD12	1:126:A:GLY:H	2	0.11	0.0	0.11
(1,855)	1:125:A:LEU:HD13	1:126:A:GLY:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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)
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	9	18.31
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	9	18.31
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	9	18.31
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	18	17.75
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	18	17.75
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	18	17.75
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	8	17.74
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	8	17.74
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	8	17.74
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	18	17.57
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	18	17.57
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	18	17.57
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	8	17.55
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	8	17.55
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	8	17.55
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	17	17.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	17	17.24
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	17	17.24
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	9	17.18
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	9	17.18
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	9	17.18
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	8	17.08
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	8	17.08
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	8	17.08
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	18	16.93
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	18	16.93
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	18	16.93
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	17	16.57
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	17	16.57
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	17	16.57
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	9	16.05
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	9	16.05
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	9	16.05
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	12	15.86
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	12	15.86
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	12	15.86
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	16	15.81
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	16	15.81
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	16	15.81
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	17	15.7
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	17	15.7
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	17	15.7
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	8	15.61
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	8	15.61
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	8	15.61
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	8	15.61
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	8	15.61
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	8	15.61
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	18	15.55
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	18	15.55
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	18	15.55
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	18	15.55
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	18	15.55
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	18	15.55
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	10	15.31
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	10	15.31
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	10	15.31
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	9	14.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	9	14.95
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	9	14.95
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	9	14.95
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	9	14.95
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	9	14.95
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	16	14.94
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	16	14.94
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	16	14.94
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	5	14.92
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	5	14.92
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	5	14.92
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	16	14.88
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	16	14.88
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	16	14.88
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	10	14.87
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	10	14.87
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	10	14.87
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	12	14.87
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	12	14.87
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	12	14.87
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	15	14.74
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	15	14.74
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	15	14.74
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	17	14.54
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	17	14.54
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	17	14.54
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	17	14.54
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	17	14.54
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	17	14.54
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	6	14.54
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	6	14.54
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	6	14.54
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	12	14.45
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	12	14.45
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	12	14.45
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	5	14.16
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	5	14.16
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	5	14.16
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	15	13.7
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	15	13.7
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	15	13.7
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	6	13.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	6	13.69
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	6	13.69
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	1	13.68
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	1	13.68
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	1	13.68
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	10	13.52
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	10	13.52
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	10	13.52
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	16	13.48
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	16	13.48
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	16	13.48
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	16	13.48
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	16	13.48
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	16	13.48
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	15	13.47
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	15	13.47
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	15	13.47
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	1	13.29
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	1	13.29
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	1	13.29
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	19	13.26
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	19	13.26
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	19	13.26
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	12	13.25
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	12	13.25
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	12	13.25
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	12	13.25
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	12	13.25
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	12	13.25
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	6	13.17
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	6	13.17
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	6	13.17
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	11	12.96
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	11	12.96
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	11	12.96
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	20	12.95
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	20	12.95
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	20	12.95
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	5	12.84
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	5	12.84
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	5	12.84
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	1	12.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	1	12.78
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	1	12.78
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	10	12.76
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	10	12.76
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	10	12.76
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	10	12.76
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	10	12.76
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	10	12.76
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	14	12.56
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	14	12.56
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	14	12.56
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	14	12.52
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	14	12.52
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	14	12.52
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	19	12.41
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	19	12.41
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	19	12.41
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	15	12.3
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	15	12.3
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	15	12.3
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	15	12.3
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	15	12.3
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	15	12.3
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	14	12.28
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	14	12.28
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	14	12.28
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	20	12.15
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	20	12.15
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	20	12.15
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	5	12.14
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	5	12.14
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	5	12.14
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	5	12.14
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	5	12.14
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	5	12.14
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	6	12.14
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	6	12.14
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	6	12.14
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	6	12.14
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	6	12.14
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	6	12.14
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	11	11.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	11	11.93
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	11	11.93
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	3	11.91
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	3	11.91
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	3	11.91
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	4	11.83
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	4	11.83
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	4	11.83
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	1	11.8
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	1	11.8
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	1	11.8
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	1	11.8
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	1	11.8
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	1	11.8
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	7	11.38
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	7	11.38
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	7	11.38
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	3	11.37
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	3	11.37
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	3	11.37
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	7	11.32
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	7	11.32
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	7	11.32
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	14	11.26
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	14	11.26
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	14	11.26
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	14	11.26
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	14	11.26
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	14	11.26
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	7	11.16
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	7	11.16
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	7	11.16
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	19	11.11
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	19	11.11
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	19	11.11
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	3	11.03
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	3	11.03
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	3	11.03
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	4	10.99
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	4	10.99
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	4	10.99
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	11	10.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	11	10.91
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	11	10.91
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	20	10.85
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	20	10.85
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	20	10.85
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	19	10.59
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	19	10.59
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	19	10.59
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	19	10.59
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	19	10.59
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	19	10.59
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	20	10.35
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	20	10.35
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	20	10.35
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	20	10.35
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	20	10.35
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	20	10.35
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	11	10.31
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	11	10.31
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	11	10.31
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	11	10.31
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	11	10.31
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	11	10.31
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	7	10.2
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	7	10.2
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	7	10.2
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	7	10.2
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	7	10.2
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	7	10.2
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	3	10.16
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	3	10.16
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	3	10.16
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	3	10.16
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	3	10.16
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	3	10.16
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	2	10.01
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	2	10.01
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	2	10.01
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	4	9.88
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	4	9.88
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	4	9.88
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	4	9.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	4	9.43
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	4	9.43
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	4	9.43
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	4	9.43
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	4	9.43
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	2	9.36
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	2	9.36
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	2	9.36
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	2	9.24
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	2	9.24
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	2	9.24
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	2	8.48
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	2	8.48
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	2	8.48
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	2	8.48
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	2	8.48
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	2	8.48
(1,1309)	1:166:A:MET:HE1	1:222:A:SER:HA	13	7.2
(1,1309)	1:166:A:MET:HE2	1:222:A:SER:HA	13	7.2
(1,1309)	1:166:A:MET:HE3	1:222:A:SER:HA	13	7.2
(1,1311)	1:166:A:MET:HE1	1:222:A:SER:HB3	13	6.52
(1,1311)	1:166:A:MET:HE2	1:222:A:SER:HB3	13	6.52
(1,1311)	1:166:A:MET:HE3	1:222:A:SER:HB3	13	6.52
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	18	5.69
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	18	5.69
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB2	13	5.24
(1,1312)	1:166:A:MET:HE1	1:222:A:SER:HB3	13	5.24
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB2	13	5.24
(1,1312)	1:166:A:MET:HE2	1:222:A:SER:HB3	13	5.24
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB2	13	5.24
(1,1312)	1:166:A:MET:HE3	1:222:A:SER:HB3	13	5.24
(1,1310)	1:166:A:MET:HE1	1:222:A:SER:HB2	13	5.13
(1,1310)	1:166:A:MET:HE2	1:222:A:SER:HB2	13	5.13
(1,1310)	1:166:A:MET:HE3	1:222:A:SER:HB2	13	5.13
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	13	4.84
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	13	4.84
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	20	4.6
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	20	4.6
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	7	4.53
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	7	4.53
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	18	4.36
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	18	4.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	9	4.34
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	9	4.34
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	17	4.15
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	17	4.15
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	9	3.94
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	9	3.94
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	17	3.88
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	18	3.85
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	9	3.85
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	9	3.85
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	12	3.84
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	12	3.84
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	1	3.83
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	1	3.83
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	8	3.82
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	8	3.82
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	8	3.82
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	8	3.82
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	11	3.81
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	11	3.81
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	14	3.73
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	4	3.73
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	4	3.73
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	15	3.73
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	15	3.73
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	15	3.73
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	4	3.69
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	12	3.69
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	12	3.69
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	12	3.69
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	12	3.69
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	12	3.68
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	10	3.61
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	10	3.61
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	7	3.6
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	16	3.6
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	19	3.58
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	15	3.47
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	7	3.47
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	7	3.47
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	5	3.45
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	15	3.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	15	3.44
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	8	3.43
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	13	3.4
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	20	3.38
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	20	3.38
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	6	3.37
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	2	3.36
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	1	3.35
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	9	3.35
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	9	3.35
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	9	3.35
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	9	3.35
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	11	3.34
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	2	3.33
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	5	3.33
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	5	3.33
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	5	3.33
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	5	3.33
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	9	3.32
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	3	3.25
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	3	3.25
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	3	3.25
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	3	3.25
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	19	3.25
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	19	3.25
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	6	3.24
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	6	3.24
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	1	3.21
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	1	3.21
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	1	3.21
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	1	3.21
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	4	3.21
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	4	3.21
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	4	3.21
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	4	3.21
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	4	3.21
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	4	3.21
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	4	3.21
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	4	3.21
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	4	3.21
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	11	3.2
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	11	3.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	11	3.2
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	11	3.2
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	20	3.2
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	20	3.2
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	13	3.2
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	13	3.2
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	6	3.17
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	6	3.17
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	10	3.17
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	10	3.17
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	8	3.14
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	8	3.14
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	2	3.12
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	2	3.12
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	2	3.12
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	2	3.12
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	4	3.12
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	4	3.12
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	18	3.09
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	18	3.09
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	18	3.09
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	18	3.09
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	17	3.0
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	17	3.0
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	17	3.0
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	17	3.0
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	15	2.97
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	15	2.97
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	15	2.97
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	15	2.97
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	5	2.93
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	5	2.93
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	2	2.9
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	2	2.9
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	13	2.81
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	13	2.81
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	16	2.8
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	16	2.8
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	16	2.8
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	16	2.8
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	15	2.79
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	15	2.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	10	2.76
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	10	2.76
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	10	2.76
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	10	2.76
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	13	2.72
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	13	2.72
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	13	2.72
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	4	2.72
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	4	2.72
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	4	2.72
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	4	2.72
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	4	2.72
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	4	2.72
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	4	2.72
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	4	2.72
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	4	2.72
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	1	2.72
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	1	2.72
(1,217)	1:191:A:THR:HG21	1:197:A:ASN:HA	18	2.7
(1,217)	1:191:A:THR:HG22	1:197:A:ASN:HA	18	2.7
(1,217)	1:191:A:THR:HG23	1:197:A:ASN:HA	18	2.7
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	10	2.7
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	10	2.7
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	2	2.67
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	2	2.67
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	6	2.66
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	6	2.66
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	6	2.66
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	6	2.66
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	14	2.63
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	14	2.63
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	18	2.62
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	18	2.62
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	20	2.58
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	20	2.58
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	20	2.58
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	20	2.58
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	20	2.58
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	20	2.58
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	20	2.58
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	20	2.58
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	20	2.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	4	2.55
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	4	2.55
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	4	2.55
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	17	2.54
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	17	2.54
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	10	2.54
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	10	2.54
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	10	2.54
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	10	2.54
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	10	2.54
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	10	2.54
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	10	2.54
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	10	2.54
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	10	2.54
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	3	2.53
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	3	2.53
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	7	2.53
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	7	2.53
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	7	2.53
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	7	2.53
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	7	2.53
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	7	2.53
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	7	2.53
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	7	2.53
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	7	2.53
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	18	2.5
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	18	2.5
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	18	2.5
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	18	2.5
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	18	2.5
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	18	2.5
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	18	2.5
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	18	2.5
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	18	2.5
(1,217)	1:191:A:THR:HG21	1:197:A:ASN:HA	20	2.47
(1,217)	1:191:A:THR:HG22	1:197:A:ASN:HA	20	2.47
(1,217)	1:191:A:THR:HG23	1:197:A:ASN:HA	20	2.47
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	10	2.46
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	10	2.46
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	10	2.46
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	10	2.46
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	10	2.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	10	2.46
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	10	2.46
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	10	2.46
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	10	2.46
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	16	2.46
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	16	2.46
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	16	2.46
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	16	2.46
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	16	2.46
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	16	2.46
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	16	2.46
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	16	2.46
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	16	2.46
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	1	2.45
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	1	2.45
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	18	2.45
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	18	2.45
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	18	2.45
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	16	2.45
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	16	2.45
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	16	2.45
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	16	2.45
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	16	2.45
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	16	2.45
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	16	2.45
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	16	2.45
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	16	2.45
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	3	2.43
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	3	2.43
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	3	2.43
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	3	2.43
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	3	2.43
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	3	2.43
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	3	2.43
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	3	2.43
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	3	2.43
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	2	2.42
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	2	2.42
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	2	2.42
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	2	2.42
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	2	2.42
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	2	2.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	2	2.42
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	2	2.42
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	2	2.42
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	16	2.41
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	16	2.41
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	16	2.41
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	15	2.41
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	15	2.41
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	15	2.41
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	15	2.41
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	15	2.41
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	15	2.41
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	15	2.41
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	15	2.41
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	15	2.41
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	17	2.41
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	17	2.41
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	17	2.41
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	17	2.4
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	17	2.4
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	17	2.4
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	17	2.4
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	17	2.4
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	17	2.4
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	17	2.4
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	17	2.4
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	17	2.4
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	12	2.39
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	12	2.39
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	12	2.39
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	12	2.39
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	12	2.39
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	12	2.39
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	7	2.39
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	7	2.39
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	7	2.39
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	3	2.38
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	3	2.38
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	3	2.38
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	3	2.38
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	3	2.38
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	3	2.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	8	2.38
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	8	2.38
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	8	2.38
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	8	2.38
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	8	2.38
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	8	2.38
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	8	2.38
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	8	2.38
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	8	2.38
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	17	2.37
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	17	2.37
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	17	2.37
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	17	2.37
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	17	2.37
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	17	2.37
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	5	2.37
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	5	2.37
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	5	2.37
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	5	2.37
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	5	2.37
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	5	2.37
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	5	2.37
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	5	2.37
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	5	2.37
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	20	2.36
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	20	2.36
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	20	2.36
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	20	2.36
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	20	2.36
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	20	2.36
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	13	2.36
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	13	2.36
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	13	2.36
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	13	2.36
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	13	2.36
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	13	2.36
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	13	2.36
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	13	2.36
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	13	2.36
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	1	2.33
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	1	2.33
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	1	2.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	19	2.31
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	19	2.31
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	19	2.31
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	19	2.3
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	19	2.3
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	19	2.3
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	19	2.3
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	14	2.3
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	14	2.3
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	6	2.29
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	6	2.29
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	6	2.29
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	6	2.29
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	6	2.29
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	6	2.29
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	1	2.28
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	1	2.28
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	1	2.28
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	18	2.28
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	18	2.28
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	18	2.28
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	14	2.28
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	14	2.28
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	14	2.28
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	14	2.28
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	14	2.28
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	14	2.28
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	17	2.26
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	17	2.26
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	17	2.26
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	17	2.26
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	17	2.26
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	17	2.26
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	17	2.26
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	17	2.26
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	17	2.26
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	16	2.25
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	16	2.25
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	16	2.25
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	16	2.25
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	16	2.25
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	16	2.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	16	2.24
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	16	2.24
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	16	2.24
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	13	2.21
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	13	2.21
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	13	2.21
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	13	2.21
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	13	2.21
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	13	2.21
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	7	2.21
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	7	2.21
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	7	2.21
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	20	2.21
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	20	2.21
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	20	2.21
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	20	2.21
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	20	2.21
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	20	2.21
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	20	2.21
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	20	2.21
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	20	2.21
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	18	2.19
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	18	2.19
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	18	2.19
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	18	2.19
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	18	2.19
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	18	2.19
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	7	2.18
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	7	2.18
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	7	2.18
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	7	2.18
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	7	2.18
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	7	2.18
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	7	2.18
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	7	2.18
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	7	2.18
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	7	2.18
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	7	2.18
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	7	2.18
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	16	2.17
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	16	2.17
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	2	2.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	14	2.16
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	14	2.16
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	14	2.16
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	14	2.16
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	14	2.16
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	14	2.16
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	14	2.16
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	14	2.16
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	14	2.16
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	17	2.15
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	17	2.15
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	17	2.15
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	2	2.13
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	2	2.13
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG2	7	2.13
(1,989)	1:128:A:TYR:H	1:186:A:GLN:HG3	7	2.13
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	15	2.13
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	15	2.13
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	15	2.13
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	15	2.13
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	15	2.13
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	15	2.13
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	15	2.13
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	15	2.13
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	15	2.13
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	18	2.13
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	18	2.13
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	18	2.13
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	18	2.13
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	18	2.13
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	18	2.13
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	18	2.13
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	18	2.13
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	18	2.13
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	9	2.12
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	9	2.12
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	9	2.12
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	9	2.12
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	9	2.12
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	9	2.12
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	14	2.12
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	14	2.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	16	2.12
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	16	2.12
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	16	2.12
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	10	2.12
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	10	2.12
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	10	2.12
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	12	2.12
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	12	2.12
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	12	2.12
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	4	2.12
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	4	2.12
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	2	2.09
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	2	2.09
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	2	2.09
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	13	2.09
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	13	2.09
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	13	2.09
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	13	2.09
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	13	2.09
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	13	2.09
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	13	2.09
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	13	2.09
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	13	2.09
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	6	2.08
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	6	2.08
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	6	2.08
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	15	2.08
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	15	2.08
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	15	2.08
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	6	2.07
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	6	2.07
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	6	2.07
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	6	2.07
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	6	2.07
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	6	2.07
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	5	2.05
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	12	2.04
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	12	2.04
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	12	2.04
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	12	2.04
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	12	2.04
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	12	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	12	2.04
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	12	2.04
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	12	2.04
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	14	2.02
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	14	2.02
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	14	2.02
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	14	2.02
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	5	2.02
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	5	2.02
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	5	2.02
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	5	2.02
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	5	2.02
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	5	2.02
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	5	2.02
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	5	2.02
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	5	2.02
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	9	2.01
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	9	2.01
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	9	2.01
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	9	2.01
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	9	2.01
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	9	2.01
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	9	2.01
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	9	2.01
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	9	2.01
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	17	2.0
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	17	2.0
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	17	2.0
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	20	2.0
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	20	2.0
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	20	2.0
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	12	1.98
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	12	1.98
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	12	1.98
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	12	1.98
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	12	1.98
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	12	1.98
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	12	1.98
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	12	1.98
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	12	1.98
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	7	1.97
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	7	1.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	7	1.97
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	7	1.97
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	7	1.97
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	7	1.97
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	3	1.97
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	3	1.97
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	3	1.97
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	11	1.97
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	11	1.97
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	11	1.97
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	1	1.95
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	1	1.95
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	1	1.95
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	1	1.95
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	1	1.95
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	1	1.95
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	7	1.95
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	7	1.95
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	7	1.95
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	7	1.95
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	7	1.95
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	7	1.95
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	1	1.95
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	1	1.95
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	1	1.95
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	1	1.95
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	1	1.95
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	1	1.95
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	11	1.95
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	11	1.95
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	11	1.95
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	11	1.95
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	11	1.95
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	11	1.95
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	11	1.95
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	11	1.95
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	11	1.95
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	19	1.94
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	19	1.94
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	19	1.94
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	19	1.94
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	19	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	19	1.94
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	20	1.94
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	20	1.94
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	20	1.94
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	20	1.94
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	20	1.94
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	20	1.94
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	2	1.94
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	2	1.94
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	2	1.94
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	4	1.94
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	4	1.94
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	4	1.94
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	16	1.93
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	16	1.93
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	16	1.93
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	16	1.93
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	16	1.93
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	16	1.93
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	20	1.93
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	20	1.93
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	20	1.93
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	20	1.93
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	19	1.93
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	19	1.93
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	15	1.92
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	15	1.92
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	15	1.92
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	5	1.91
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	5	1.91
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	5	1.91
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	1	1.89
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	11	1.89
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	11	1.89
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	11	1.89
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	11	1.89
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	11	1.89
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	11	1.89
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	11	1.89
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	11	1.89
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	11	1.89
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	19	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	19	1.88
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	10	1.87
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	10	1.87
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	10	1.87
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	10	1.87
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	10	1.87
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	10	1.87
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	16	1.87
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	16	1.87
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	12	1.86
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	12	1.86
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	12	1.86
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	12	1.86
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	12	1.86
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	12	1.86
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	9	1.85
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	9	1.85
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	9	1.85
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	4	1.84
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	4	1.84
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	4	1.84
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	13	1.84
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	13	1.84
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	15	1.84
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	15	1.84
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	15	1.84
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	20	1.84
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	20	1.84
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	20	1.84
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	20	1.84
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	9	1.84
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	9	1.84
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	9	1.84
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	18	1.84
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	18	1.84
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	18	1.84
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	8	1.83
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	8	1.83
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	8	1.83
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	14	1.83
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	14	1.83
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	14	1.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	14	1.83
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	14	1.83
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	14	1.83
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	14	1.83
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	14	1.83
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	14	1.83
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	16	1.82
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	6	1.82
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	6	1.82
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	6	1.82
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	6	1.82
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	6	1.82
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	6	1.82
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	6	1.82
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	6	1.82
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	6	1.82
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	5	1.82
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	5	1.82
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	5	1.82
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	18	1.81
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	4	1.8
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	4	1.8
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	4	1.8
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	4	1.8
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	4	1.8
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	4	1.8
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	3	1.8
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	12	1.8
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	10	1.8
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	10	1.8
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	10	1.8
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	13	1.8
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	13	1.8
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	13	1.8
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	13	1.79
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	13	1.79
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	13	1.79
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	17	1.77
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	17	1.77
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	17	1.77
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	17	1.77
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	5	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	5	1.77
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	5	1.77
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	16	1.76
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	16	1.76
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	16	1.76
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	2	1.76
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	2	1.76
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	2	1.76
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	15	1.75
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	15	1.75
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	15	1.75
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	15	1.75
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	15	1.75
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	15	1.75
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	10	1.75
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	10	1.75
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	10	1.75
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	14	1.75
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	14	1.75
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	14	1.75
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	7	1.75
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	7	1.75
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	16	1.75
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	16	1.75
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	1	1.75
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	1	1.75
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	1	1.75
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	1	1.75
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	1	1.75
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	1	1.75
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	1	1.75
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	1	1.75
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	1	1.75
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	11	1.75
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	11	1.75
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	11	1.75
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	16	1.75
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	16	1.75
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	16	1.75
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	1	1.75
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	1	1.75
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	1	1.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	2	1.75
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	2	1.75
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	2	1.75
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	7	1.75
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	7	1.75
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	7	1.75
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	11	1.75
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	11	1.75
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	11	1.75
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	14	1.74
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	14	1.74
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	14	1.74
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	16	1.74
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	16	1.74
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	16	1.74
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	11	1.73
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	11	1.73
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	11	1.73
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	11	1.73
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	11	1.73
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	11	1.73
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	12	1.73
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	12	1.73
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	12	1.73
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	12	1.73
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	7	1.73
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	19	1.73
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	19	1.73
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	19	1.73
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	19	1.73
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	19	1.73
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	19	1.73
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	19	1.73
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	19	1.73
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	19	1.73
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	13	1.73
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	13	1.73
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	13	1.73
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	6	1.72
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	6	1.72
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	6	1.72
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	6	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	6	1.72
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	6	1.72
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	6	1.72
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	6	1.72
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	6	1.72
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	8	1.72
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	8	1.72
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	8	1.72
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	15	1.72
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	15	1.72
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	15	1.72
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	19	1.72
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	19	1.72
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	19	1.72
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	20	1.72
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	20	1.72
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	20	1.72
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG21	19	1.71
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG22	19	1.71
(1,258)	1:134:A:MET:HE1	1:161:A:VAL:HG23	19	1.71
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG21	19	1.71
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG22	19	1.71
(1,258)	1:134:A:MET:HE2	1:161:A:VAL:HG23	19	1.71
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG21	19	1.71
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG22	19	1.71
(1,258)	1:134:A:MET:HE3	1:161:A:VAL:HG23	19	1.71
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	12	1.71
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	12	1.71
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	12	1.71
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	17	1.71
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	17	1.71
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	17	1.71
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	8	1.7
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	8	1.7
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	8	1.7
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	8	1.7
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	8	1.7
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	8	1.7
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	8	1.7
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	8	1.7
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	8	1.7
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	4	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	4	1.68
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	4	1.68
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	4	1.68
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	4	1.68
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	4	1.68
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	3	1.68
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	2	1.67
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	2	1.67
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	2	1.67
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	14	1.67
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	14	1.67
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	14	1.67
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	20	1.67
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	20	1.67
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	20	1.67
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	14	1.66
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	14	1.66
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	14	1.66
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	14	1.66
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	14	1.66
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	14	1.66
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	10	1.66
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	10	1.66
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	10	1.66
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	3	1.65
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	3	1.65
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	3	1.65
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	2	1.64
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	2	1.64
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	2	1.64
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	2	1.64
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	2	1.64
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	2	1.64
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	2	1.64
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	2	1.64
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	2	1.64
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	9	1.64
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	9	1.64
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	9	1.64
(1,217)	1:191:A:THR:HG21	1:197:A:ASN:HA	3	1.64
(1,217)	1:191:A:THR:HG22	1:197:A:ASN:HA	3	1.64
(1,217)	1:191:A:THR:HG23	1:197:A:ASN:HA	3	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	10	1.63
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	10	1.63
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	10	1.63
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	10	1.63
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	10	1.63
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	10	1.63
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	20	1.63
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	20	1.63
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	20	1.63
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	15	1.63
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	15	1.63
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	18	1.63
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	18	1.63
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	18	1.63
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	3	1.62
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	3	1.62
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	3	1.62
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	3	1.62
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	3	1.62
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	3	1.62
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	3	1.62
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	3	1.62
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	3	1.62
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	6	1.62
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	6	1.62
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	6	1.62
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	18	1.61
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	18	1.61
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	18	1.61
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	18	1.61
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	18	1.61
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	18	1.61
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	7	1.61
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	7	1.61
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	7	1.61
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	9	1.6
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	9	1.6
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	9	1.6
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	13	1.58
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	13	1.58
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	13	1.58
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	13	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	13	1.58
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	13	1.58
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	6	1.58
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	6	1.58
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	6	1.58
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	12	1.58
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	12	1.58
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	17	1.58
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	17	1.58
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	17	1.58
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	17	1.58
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	5	1.58
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	5	1.58
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	5	1.58
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	5	1.57
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	5	1.57
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	5	1.57
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	4	1.57
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	4	1.57
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	4	1.57
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	4	1.57
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	7	1.57
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	7	1.57
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	7	1.57
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	11	1.56
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	11	1.56
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	11	1.56
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	11	1.56
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	12	1.56
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	12	1.56
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	12	1.56
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	6	1.56
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	6	1.56
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	2	1.55
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	2	1.55
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	2	1.55
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	2	1.55
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	2	1.55
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	2	1.55
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	9	1.55
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	9	1.55
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	9	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	9	1.55
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	9	1.55
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	9	1.55
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	9	1.55
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	9	1.55
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	9	1.55
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	9	1.55
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	9	1.55
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	9	1.55
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	9	1.55
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	9	1.55
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	9	1.55
(1,222)	1:188:A:THR:HG21	1:189:A:VAL:HA	4	1.55
(1,222)	1:188:A:THR:HG22	1:189:A:VAL:HA	4	1.55
(1,222)	1:188:A:THR:HG23	1:189:A:VAL:HA	4	1.55
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	18	1.54
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	18	1.54
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	18	1.54
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	5	1.54
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	5	1.54
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	5	1.54
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	17	1.54
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	17	1.54
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	17	1.54
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	4	1.53
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	6	1.52
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	1	1.52
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	1	1.52
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	1	1.52
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	12	1.52
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	12	1.52
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	12	1.52
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	1	1.52
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	1	1.52
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	1	1.52
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	3	1.5
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	3	1.5
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	3	1.5
(1,257)	1:161:A:VAL:HG21	1:217:A:GLN:HA	8	1.5
(1,257)	1:161:A:VAL:HG22	1:217:A:GLN:HA	8	1.5
(1,257)	1:161:A:VAL:HG23	1:217:A:GLN:HA	8	1.5
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	3	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	3	1.5
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	3	1.5
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	14	1.49
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	14	1.49
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	14	1.49
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	4	1.49
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	4	1.49
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	4	1.49
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	19	1.48
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	19	1.48
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	19	1.48
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	2	1.48
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	2	1.48
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	2	1.48
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	4	1.48
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	4	1.48
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	4	1.48
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	9	1.47
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	9	1.47
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	9	1.47
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	9	1.47
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG11	1	1.47
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG12	1	1.47
(1,290)	1:134:A:MET:HE1	1:161:A:VAL:HG13	1	1.47
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG11	1	1.47
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG12	1	1.47
(1,290)	1:134:A:MET:HE2	1:161:A:VAL:HG13	1	1.47
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG11	1	1.47
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG12	1	1.47
(1,290)	1:134:A:MET:HE3	1:161:A:VAL:HG13	1	1.47
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	10	1.46
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	10	1.46
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	10	1.46
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	10	1.46
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	10	1.46
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	10	1.46
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	12	1.46
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	12	1.46
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	12	1.46
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	12	1.46
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	17	1.46
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	17	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	17	1.46
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	17	1.46
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	16	1.46
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	16	1.46
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	16	1.46
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	5	1.45
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	5	1.45
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	5	1.45
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	5	1.45
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	5	1.45
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	5	1.45
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	1	1.44
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	1	1.44
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	1	1.44
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	11	1.43
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	11	1.43
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	11	1.43
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	15	1.43
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	15	1.43
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	15	1.43
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	16	1.43
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	16	1.43
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	16	1.43
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	14	1.41
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	14	1.41
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	14	1.41
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	14	1.41
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	11	1.41
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	11	1.41
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	11	1.41
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	11	1.41
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	7	1.41
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	7	1.41
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	7	1.41
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	17	1.41
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	17	1.41
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	17	1.41
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	17	1.41
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	6	1.41
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	6	1.41
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	6	1.41
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	15	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	15	1.4
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	15	1.4
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	15	1.4
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	8	1.4
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	8	1.4
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	8	1.4
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	12	1.39
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	12	1.39
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	12	1.39
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	18	1.39
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	18	1.39
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	18	1.39
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	18	1.39
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	18	1.39
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	18	1.39
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	6	1.39
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	6	1.39
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	6	1.39
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	1	1.39
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	1	1.39
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	1	1.39
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	9	1.39
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	9	1.39
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	9	1.39
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	11	1.38
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	11	1.38
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	11	1.38
(1,217)	1:191:A:THR:HG21	1:197:A:ASN:HA	17	1.38
(1,217)	1:191:A:THR:HG22	1:197:A:ASN:HA	17	1.38
(1,217)	1:191:A:THR:HG23	1:197:A:ASN:HA	17	1.38
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	3	1.38
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	3	1.38
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	3	1.38
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	10	1.37
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	6	1.37
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	6	1.37
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	6	1.37
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	11	1.36
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	11	1.36
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	11	1.36
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	11	1.36
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	20	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	20	1.36
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	17	1.36
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	17	1.36
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	17	1.36
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	12	1.36
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	12	1.36
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	12	1.36
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	2	1.36
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	2	1.36
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	2	1.36
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	4	1.35
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	4	1.35
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	2	1.34
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	2	1.34
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	6	1.34
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	6	1.34
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	12	1.34
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	8	1.33
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	8	1.33
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	8	1.33
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	8	1.33
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	8	1.33
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	8	1.33
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	12	1.33
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	12	1.33
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	12	1.33
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	13	1.33
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	13	1.33
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	13	1.33
(1,217)	1:191:A:THR:HG21	1:197:A:ASN:HA	5	1.33
(1,217)	1:191:A:THR:HG22	1:197:A:ASN:HA	5	1.33
(1,217)	1:191:A:THR:HG23	1:197:A:ASN:HA	5	1.33
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	1	1.33
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	1	1.33
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	1	1.33
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	20	1.33
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	20	1.33
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	20	1.33
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	20	1.32
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	20	1.32
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	20	1.32
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	20	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	20	1.32
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	20	1.32
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	13	1.32
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	13	1.32
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	13	1.32
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	13	1.32
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	8	1.32
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	7	1.32
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	7	1.32
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	7	1.32
(1,217)	1:191:A:THR:HG21	1:197:A:ASN:HA	2	1.32
(1,217)	1:191:A:THR:HG22	1:197:A:ASN:HA	2	1.32
(1,217)	1:191:A:THR:HG23	1:197:A:ASN:HA	2	1.32
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	5	1.31
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	5	1.31
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	5	1.31
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	5	1.31
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	14	1.31
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	14	1.31
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	14	1.31
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	14	1.31
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	14	1.31
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	14	1.31
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	7	1.31
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	7	1.31
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	7	1.31
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	7	1.31
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	7	1.31
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	7	1.31
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	4	1.31
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	4	1.31
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	4	1.31
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	11	1.31
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	11	1.31
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	11	1.31
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	8	1.3
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	8	1.3
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	1	1.3
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	1	1.3
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	1	1.3
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	1	1.3
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	1	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	9	1.3
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	9	1.3
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	9	1.3
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	13	1.3
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	13	1.3
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	13	1.3
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB2	3	1.29
(1,1308)	1:161:A:VAL:HG21	1:217:A:GLN:HB3	3	1.29
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB2	3	1.29
(1,1308)	1:161:A:VAL:HG22	1:217:A:GLN:HB3	3	1.29
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB2	3	1.29
(1,1308)	1:161:A:VAL:HG23	1:217:A:GLN:HB3	3	1.29
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	13	1.29
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	13	1.29
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	13	1.29
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	10	1.28
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	10	1.28
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	10	1.28
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	1	1.28
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	1	1.28
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	1	1.28
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	19	1.27
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	19	1.27
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	19	1.27
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	15	1.27
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	15	1.27
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	15	1.27
(1,217)	1:191:A:THR:HG21	1:197:A:ASN:HA	12	1.27
(1,217)	1:191:A:THR:HG22	1:197:A:ASN:HA	12	1.27
(1,217)	1:191:A:THR:HG23	1:197:A:ASN:HA	12	1.27
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	5	1.26
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	5	1.26
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	7	1.25
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	7	1.25
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	9	1.25
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	9	1.25
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	9	1.25
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	9	1.25
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	6	1.25
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	6	1.25
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	6	1.25
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	20	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	20	1.25
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	5	1.25
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	5	1.25
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	5	1.25
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	16	1.24
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	16	1.24
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	16	1.24
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	16	1.24
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	18	1.24
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	18	1.24
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	18	1.24
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	17	1.24
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	17	1.24
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	17	1.24
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	4	1.23
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	4	1.23
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	10	1.23
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	10	1.23
(1,690)	1:134:A:MET:HE1	1:161:A:VAL:H	19	1.23
(1,690)	1:134:A:MET:HE2	1:161:A:VAL:H	19	1.23
(1,690)	1:134:A:MET:HE3	1:161:A:VAL:H	19	1.23
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	15	1.23
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	15	1.23
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	15	1.23
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	16	1.21
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	16	1.21
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	17	1.21
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	17	1.21
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	18	1.21
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	18	1.21
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	19	1.21
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	19	1.21
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	19	1.21
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	10	1.21
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	10	1.21
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	10	1.21
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	18	1.21
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	18	1.21
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	18	1.21
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	2	1.2
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	2	1.2
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	2	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	2	1.2
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	3	1.2
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	3	1.2
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	3	1.2
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	3	1.2
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	4	1.2
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	4	1.2
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	4	1.2
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	4	1.2
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	4	1.2
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	4	1.2
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	10	1.2
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	10	1.2
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	10	1.2
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	5	1.2
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	5	1.2
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	5	1.2
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	12	1.2
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	12	1.2
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	12	1.2
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	19	1.19
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	19	1.19
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	15	1.19
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	15	1.19
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	15	1.19
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	14	1.19
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	14	1.19
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	14	1.19
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	2	1.19
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	2	1.19
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	2	1.19
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	7	1.18
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	7	1.18
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	7	1.18
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	7	1.18
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	2	1.18
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	2	1.18
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	2	1.18
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	4	1.18
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	4	1.18
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	4	1.18
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	14	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	14	1.17
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	14	1.17
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	14	1.17
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	5	1.17
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	5	1.17
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	5	1.17
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	5	1.17
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	5	1.17
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	5	1.17
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	5	1.17
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	5	1.17
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	13	1.17
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	13	1.17
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	13	1.17
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	13	1.17
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	13	1.17
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	13	1.17
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	16	1.17
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	20	1.17
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	20	1.17
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	20	1.17
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	16	1.17
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	16	1.17
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	16	1.17
(1,217)	1:191:A:THR:HG21	1:197:A:ASN:HA	16	1.17
(1,217)	1:191:A:THR:HG22	1:197:A:ASN:HA	16	1.17
(1,217)	1:191:A:THR:HG23	1:197:A:ASN:HA	16	1.17
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	6	1.17
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	6	1.17
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	6	1.17
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	19	1.17
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	19	1.17
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	19	1.17
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	10	1.16
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	10	1.16
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	10	1.16
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	10	1.16
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	10	1.16
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	10	1.16
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	17	1.16
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	17	1.16
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	17	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	17	1.16
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	17	1.16
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	17	1.16
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	5	1.16
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	5	1.16
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	5	1.16
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	5	1.16
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	8	1.16
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	8	1.16
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	8	1.16
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	11	1.15
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	11	1.15
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	8	1.15
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	8	1.15
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	8	1.15
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	8	1.15
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	8	1.15
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	8	1.15
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	12	1.15
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	12	1.15
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	12	1.15
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	12	1.15
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	12	1.15
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	12	1.15
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	12	1.15
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	12	1.15
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	12	1.15
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	13	1.15
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	13	1.15
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	13	1.15
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	1	1.14
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	1	1.14
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	1	1.14
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	1	1.14
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	15	1.14
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	15	1.14
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	15	1.14
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	19	1.14
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	19	1.14
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	19	1.14
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD2	15	1.14
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD3	15	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	3	1.14
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	3	1.14
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	3	1.14
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	17	1.14
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	17	1.14
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	17	1.14
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	12	1.13
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	12	1.13
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG2	14	1.13
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG3	14	1.13
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG2	14	1.13
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG3	14	1.13
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	8	1.13
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	8	1.13
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	8	1.13
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD2	16	1.13
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD3	16	1.13
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	9	1.12
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	9	1.12
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	9	1.12
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	9	1.12
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	6	1.12
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	6	1.12
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	6	1.12
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	8	1.12
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	8	1.12
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	8	1.12
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	5	1.12
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	5	1.12
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	5	1.12
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	8	1.12
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	8	1.12
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	8	1.12
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	18	1.11
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	18	1.11
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	18	1.11
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	18	1.11
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	11	1.11
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	11	1.11
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	2	1.11
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	2	1.11
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	2	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	13	1.11
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	9	1.11
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	9	1.11
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	9	1.11
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	14	1.11
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	14	1.11
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	14	1.11
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	18	1.11
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	18	1.11
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	18	1.11
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	13	1.11
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	13	1.11
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	13	1.11
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	20	1.1
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	7	1.1
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	7	1.1
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	7	1.1
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	7	1.1
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	15	1.1
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	15	1.1
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	15	1.1
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	15	1.1
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	15	1.1
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	3	1.1
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	3	1.1
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	3	1.1
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	10	1.1
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	10	1.1
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	10	1.1
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	6	1.09
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	6	1.09
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	9	1.09
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	9	1.09
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	11	1.09
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	11	1.09
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	11	1.09
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	11	1.09
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	12	1.09
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	12	1.09
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	12	1.09
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	16	1.09
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	16	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	16	1.09
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG11	19	1.09
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG12	19	1.09
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG13	19	1.09
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG11	19	1.09
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG12	19	1.09
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG13	19	1.09
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG11	19	1.09
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG12	19	1.09
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG13	19	1.09
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	10	1.08
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	10	1.08
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	10	1.08
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	13	1.08
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	13	1.08
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	13	1.08
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	13	1.08
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	13	1.08
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	13	1.08
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	6	1.07
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	6	1.07
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	6	1.07
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	17	1.07
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	17	1.07
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	17	1.07
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	20	1.07
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	20	1.07
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	20	1.07
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	19	1.07
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	19	1.07
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	19	1.07
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	19	1.07
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	19	1.07
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	19	1.07
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	19	1.07
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	19	1.07
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	19	1.07
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	3	1.06
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	3	1.06
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	3	1.06
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	3	1.06
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	3	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	3	1.06
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	3	1.06
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	3	1.06
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	16	1.06
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	16	1.06
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	16	1.06
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	16	1.06
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	16	1.06
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	16	1.06
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	10	1.06
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	18	1.06
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	6	1.06
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	6	1.06
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	6	1.06
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	11	1.06
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	11	1.06
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	11	1.06
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD2	7	1.06
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD3	7	1.06
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	13	1.05
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	13	1.05
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	13	1.05
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	13	1.05
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	5	1.05
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	5	1.05
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	5	1.05
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	11	1.05
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	11	1.05
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	11	1.05
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	4	1.05
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	4	1.05
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	4	1.05
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	5	1.05
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	5	1.05
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	5	1.05
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	17	1.05
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	17	1.05
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	17	1.05
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	17	1.05
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	17	1.05
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	17	1.05
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	3	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	3	1.04
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	15	1.04
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	15	1.04
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	15	1.04
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	19	1.04
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	19	1.04
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	19	1.04
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	14	1.04
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	14	1.04
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	14	1.04
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	17	1.04
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	17	1.04
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	17	1.04
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	17	1.04
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	17	1.04
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	17	1.04
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	17	1.04
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	17	1.04
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	17	1.04
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	4	1.03
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	4	1.03
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	4	1.03
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	4	1.03
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	18	1.03
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	18	1.03
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	18	1.03
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	1	1.03
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	1	1.03
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	1	1.03
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	8	1.03
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	8	1.03
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	8	1.03
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	7	1.03
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	7	1.03
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	7	1.03
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	14	1.03
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	14	1.03
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	14	1.03
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	16	1.03
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	16	1.03
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	16	1.03
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	9	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	9	1.02
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	9	1.02
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	13	1.02
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	7	1.02
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	7	1.02
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	7	1.02
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	17	1.02
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	17	1.02
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	17	1.02
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	20	1.02
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	20	1.02
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	20	1.02
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	18	1.02
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	18	1.02
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	18	1.02
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	5	1.02
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	8	1.01
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	8	1.01
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	8	1.01
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	8	1.01
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	20	1.01
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	20	1.01
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	20	1.01
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	20	1.01
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	15	1.01
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	15	1.01
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	15	1.01
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	15	1.01
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	15	1.01
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	15	1.01
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	2	1.01
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	2	1.01
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	2	1.01
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	18	1.01
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	18	1.01
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	18	1.01
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	2	1.01
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	2	1.01
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	2	1.01
(1,368)	1:176:A:VAL:HG11	1:215:A:ILE:HD11	10	1.01
(1,368)	1:176:A:VAL:HG11	1:215:A:ILE:HD12	10	1.01
(1,368)	1:176:A:VAL:HG11	1:215:A:ILE:HD13	10	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,368)	1:176:A:VAL:HG12	1:215:A:ILE:HD11	10	1.01
(1,368)	1:176:A:VAL:HG12	1:215:A:ILE:HD12	10	1.01
(1,368)	1:176:A:VAL:HG12	1:215:A:ILE:HD13	10	1.01
(1,368)	1:176:A:VAL:HG13	1:215:A:ILE:HD11	10	1.01
(1,368)	1:176:A:VAL:HG13	1:215:A:ILE:HD12	10	1.01
(1,368)	1:176:A:VAL:HG13	1:215:A:ILE:HD13	10	1.01
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	2	1.01
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	2	1.01
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	2	1.01
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	2	1.01
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	2	1.01
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	2	1.01
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	2	1.01
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	2	1.01
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	2	1.01
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	8	1.01
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	8	1.01
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	8	1.01
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	9	1.01
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	9	1.01
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	9	1.01
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	16	1.0
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	16	1.0
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	16	1.0
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	12	1.0
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	12	1.0
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	12	1.0
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	16	1.0
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	16	1.0
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	16	1.0
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	20	1.0
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	20	1.0
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	20	1.0
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	1	1.0
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	1	1.0
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	1	1.0
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	1	1.0
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	1	1.0
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	1	1.0
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	1	1.0
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	1	1.0
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	1	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	13	1.0
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	13	1.0
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	13	1.0
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	13	1.0
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	13	1.0
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	13	1.0
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	13	1.0
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	13	1.0
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	13	1.0
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	7	1.0
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	7	1.0
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	7	1.0
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	17	0.99
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	17	0.99
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	17	0.99
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	17	0.99
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	10	0.99
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	2	0.99
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	2	0.99
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	11	0.99
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	11	0.99
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	11	0.99
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	11	0.99
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	11	0.99
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	11	0.99
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	11	0.99
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	5	0.99
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	5	0.99
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	5	0.99
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	1	0.99
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	20	0.99
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	20	0.99
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	20	0.99
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	15	0.99
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	15	0.99
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	15	0.99
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	14	0.99
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	14	0.99
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	14	0.99
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	19	0.98
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	19	0.98
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	19	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	19	0.98
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	6	0.98
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	6	0.98
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	6	0.98
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	6	0.98
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	6	0.98
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	6	0.98
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	1	0.98
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	1	0.98
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	1	0.98
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	8	0.98
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	8	0.98
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	8	0.98
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	15	0.98
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	15	0.98
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	15	0.98
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	15	0.98
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	4	0.97
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	4	0.97
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	4	0.97
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	4	0.97
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	6	0.97
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	6	0.97
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	6	0.97
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	6	0.97
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	20	0.97
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	20	0.97
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	20	0.97
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	19	0.97
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	19	0.97
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	19	0.97
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	6	0.97
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	6	0.97
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	6	0.97
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	6	0.97
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	6	0.97
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	6	0.97
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	6	0.97
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	6	0.97
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	6	0.97
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	5	0.97
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	5	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	5	0.97
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	1	0.96
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	1	0.96
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	17	0.96
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	9	0.96
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	9	0.96
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	9	0.96
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	13	0.96
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	13	0.96
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	13	0.96
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	5	0.96
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	5	0.96
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	5	0.96
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	5	0.96
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	5	0.96
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	5	0.96
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	5	0.96
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	5	0.96
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	5	0.96
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	18	0.96
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	18	0.96
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	18	0.96
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB2	12	0.95
(1,1318)	1:205:A:MET:HB2	1:209:A:MET:HB3	12	0.95
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB2	12	0.95
(1,1318)	1:205:A:MET:HB3	1:209:A:MET:HB3	12	0.95
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	11	0.95
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	11	0.95
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	11	0.95
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	11	0.95
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	11	0.95
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	11	0.95
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	11	0.95
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	10	0.95
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	10	0.95
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	10	0.95
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	3	0.95
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	3	0.95
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	3	0.95
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	3	0.95
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	3	0.95
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	3	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	3	0.95
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	3	0.95
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	3	0.95
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	10	0.94
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	10	0.94
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	10	0.94
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	10	0.94
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	4	0.94
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	4	0.94
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	4	0.94
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	11	0.94
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	11	0.94
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	11	0.94
(1,217)	1:191:A:THR:HG21	1:197:A:ASN:HA	15	0.94
(1,217)	1:191:A:THR:HG22	1:197:A:ASN:HA	15	0.94
(1,217)	1:191:A:THR:HG23	1:197:A:ASN:HA	15	0.94
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	8	0.93
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	8	0.93
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	8	0.93
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	8	0.93
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	8	0.93
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	8	0.93
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	8	0.93
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	8	0.93
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	8	0.93
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	8	0.93
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	3	0.93
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	3	0.93
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	3	0.93
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	9	0.93
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	9	0.93
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	9	0.93
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	20	0.92
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	20	0.92
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	17	0.92
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	17	0.92
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	4	0.92
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	4	0.92
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	4	0.92
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	4	0.92
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	13	0.92
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	13	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	13	0.92
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	5	0.92
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	13	0.92
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	3	0.92
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	3	0.92
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	3	0.92
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	4	0.92
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	4	0.92
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	4	0.92
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	4	0.92
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	4	0.92
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	4	0.92
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	4	0.92
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	4	0.92
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	4	0.92
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG11	17	0.92
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG12	17	0.92
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG13	17	0.92
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG11	17	0.92
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG12	17	0.92
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG13	17	0.92
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG11	17	0.92
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG12	17	0.92
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG13	17	0.92
(1,662)	1:191:A:THR:H	1:192:A:THR:HG21	15	0.91
(1,662)	1:191:A:THR:H	1:192:A:THR:HG22	15	0.91
(1,662)	1:191:A:THR:H	1:192:A:THR:HG23	15	0.91
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG11	5	0.91
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG12	5	0.91
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG13	5	0.91
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG11	5	0.91
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG12	5	0.91
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG13	5	0.91
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG11	5	0.91
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG12	5	0.91
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG13	5	0.91
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	12	0.91
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	12	0.91
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	12	0.91
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	19	0.91
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	19	0.91
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	19	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:191:A:THR:HG21	1:197:A:ASN:HA	1	0.91
(1,217)	1:191:A:THR:HG22	1:197:A:ASN:HA	1	0.91
(1,217)	1:191:A:THR:HG23	1:197:A:ASN:HA	1	0.91
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	8	0.9
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	8	0.9
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	8	0.9
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	4	0.9
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG11	8	0.9
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG12	8	0.9
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG13	8	0.9
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG11	8	0.9
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG12	8	0.9
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG13	8	0.9
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG11	8	0.9
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG12	8	0.9
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG13	8	0.9
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	3	0.9
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	3	0.9
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	3	0.9
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	4	0.9
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	4	0.9
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	4	0.9
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	8	0.9
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	8	0.9
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	8	0.9
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	15	0.89
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	15	0.89
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	9	0.89
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	9	0.89
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	9	0.89
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	9	0.89
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	9	0.89
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	9	0.89
(1,762)	1:176:A:VAL:HG11	1:214:A:CYS:H	20	0.89
(1,762)	1:176:A:VAL:HG12	1:214:A:CYS:H	20	0.89
(1,762)	1:176:A:VAL:HG13	1:214:A:CYS:H	20	0.89
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	9	0.89
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	9	0.89
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	9	0.89
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	9	0.89
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	9	0.89
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	9	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	9	0.89
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	9	0.89
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	9	0.89
(1,217)	1:191:A:THR:HG21	1:197:A:ASN:HA	19	0.89
(1,217)	1:191:A:THR:HG22	1:197:A:ASN:HA	19	0.89
(1,217)	1:191:A:THR:HG23	1:197:A:ASN:HA	19	0.89
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG21	14	0.88
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG22	14	0.88
(1,834)	1:214:A:CYS:H	1:216:A:THR:HG23	14	0.88
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	10	0.87
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	10	0.87
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	10	0.87
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	10	0.87
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	16	0.87
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	16	0.87
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	16	0.87
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	16	0.87
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	5	0.87
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	5	0.87
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	5	0.87
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	5	0.87
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	5	0.87
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	5	0.87
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	12	0.87
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	12	0.87
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	12	0.87
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	10	0.87
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	10	0.87
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	10	0.87
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	10	0.87
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	10	0.87
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	10	0.87
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	10	0.87
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	10	0.87
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	10	0.87
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	6	0.87
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	6	0.87
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	6	0.87
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	10	0.87
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	10	0.87
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	10	0.87
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	19	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	19	0.86
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	5	0.86
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	5	0.86
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	5	0.86
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	5	0.86
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	3	0.86
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	3	0.86
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	3	0.86
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	7	0.86
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	7	0.86
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	7	0.86
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	7	0.86
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	7	0.86
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	7	0.86
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG11	2	0.86
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG12	2	0.86
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG13	2	0.86
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG11	2	0.86
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG12	2	0.86
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG13	2	0.86
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG11	2	0.86
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG12	2	0.86
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG13	2	0.86
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	7	0.85
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	7	0.85
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	7	0.85
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	7	0.85
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	19	0.84
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	19	0.84
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	19	0.84
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	19	0.84
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	20	0.84
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	20	0.84
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	20	0.84
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	20	0.84
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	20	0.84
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	20	0.84
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	20	0.84
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	20	0.84
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	20	0.84
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	20	0.84
(1,896)	1:161:A:VAL:HG21	1:217:A:GLN:H	14	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,896)	1:161:A:VAL:HG22	1:217:A:GLN:H	14	0.84
(1,896)	1:161:A:VAL:HG23	1:217:A:GLN:H	14	0.84
(1,763)	1:161:A:VAL:HG11	1:214:A:CYS:H	12	0.84
(1,763)	1:161:A:VAL:HG12	1:214:A:CYS:H	12	0.84
(1,763)	1:161:A:VAL:HG13	1:214:A:CYS:H	12	0.84
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG11	17	0.84
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG12	17	0.84
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG13	17	0.84
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG11	17	0.84
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG12	17	0.84
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG13	17	0.84
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG11	17	0.84
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG12	17	0.84
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG13	17	0.84
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	9	0.84
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	9	0.84
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	9	0.84
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	20	0.84
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	20	0.84
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	20	0.84
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	20	0.84
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	20	0.84
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	20	0.84
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	20	0.84
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	20	0.84
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	20	0.84
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	14	0.84
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	14	0.84
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	14	0.84
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	20	0.84
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	20	0.84
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	20	0.84
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD2	19	0.84
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD3	19	0.84
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	18	0.83
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	18	0.83
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	18	0.83
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	18	0.83
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	18	0.83
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	18	0.83
(1,972)	1:175:A:PHE:HD1	1:176:A:VAL:HG21	10	0.83
(1,972)	1:175:A:PHE:HD1	1:176:A:VAL:HG22	10	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,972)	1:175:A:PHE:HD1	1:176:A:VAL:HG23	10	0.83
(1,972)	1:175:A:PHE:HD2	1:176:A:VAL:HG21	10	0.83
(1,972)	1:175:A:PHE:HD2	1:176:A:VAL:HG22	10	0.83
(1,972)	1:175:A:PHE:HD2	1:176:A:VAL:HG23	10	0.83
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	20	0.83
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	20	0.83
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	20	0.83
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	13	0.82
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	13	0.82
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	13	0.82
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	13	0.82
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	3	0.82
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	3	0.82
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	3	0.82
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	3	0.82
(1,763)	1:161:A:VAL:HG11	1:214:A:CYS:H	17	0.82
(1,763)	1:161:A:VAL:HG12	1:214:A:CYS:H	17	0.82
(1,763)	1:161:A:VAL:HG13	1:214:A:CYS:H	17	0.82
(1,763)	1:161:A:VAL:HG11	1:214:A:CYS:H	19	0.81
(1,763)	1:161:A:VAL:HG12	1:214:A:CYS:H	19	0.81
(1,763)	1:161:A:VAL:HG13	1:214:A:CYS:H	19	0.81
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	16	0.81
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	16	0.81
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	16	0.81
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	16	0.81
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	16	0.81
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	16	0.81
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	16	0.81
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	16	0.81
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	16	0.81
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG11	11	0.81
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG12	11	0.81
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG13	11	0.81
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG11	11	0.81
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG12	11	0.81
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG13	11	0.81
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG11	11	0.81
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG12	11	0.81
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG13	11	0.81
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	1	0.81
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	1	0.81
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	1	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	11	0.81
(1,187)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	11	0.81
(1,187)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	11	0.81
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	5	0.8
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	5	0.8
(1,762)	1:176:A:VAL:HG11	1:214:A:CYS:H	10	0.8
(1,762)	1:176:A:VAL:HG12	1:214:A:CYS:H	10	0.8
(1,762)	1:176:A:VAL:HG13	1:214:A:CYS:H	10	0.8
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	9	0.8
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	9	0.8
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	9	0.8
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	9	0.8
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	12	0.79
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	12	0.79
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	4	0.79
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	4	0.79
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	4	0.79
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	4	0.79
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	4	0.79
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	4	0.79
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	10	0.79
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	10	0.79
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	10	0.79
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	10	0.79
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	7	0.79
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	7	0.79
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	7	0.79
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	7	0.79
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	7	0.79
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	7	0.79
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	7	0.79
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	7	0.79
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	7	0.79
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	1	0.78
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	1	0.78
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	1	0.78
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	1	0.78
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	1	0.78
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	1	0.78
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	17	0.78
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	17	0.78
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	17	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	17	0.78
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	3	0.78
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	3	0.78
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	3	0.78
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	3	0.78
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	3	0.78
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	3	0.78
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	19	0.78
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	19	0.78
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	19	0.78
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	19	0.78
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	19	0.78
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	19	0.78
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	6	0.78
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	6	0.78
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	6	0.78
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	6	0.78
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	6	0.78
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	6	0.78
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	6	0.78
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	6	0.78
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	6	0.78
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	13	0.78
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	1	0.77
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	1	0.77
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	1	0.77
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	1	0.77
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	1	0.77
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	1	0.77
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	19	0.77
(1,368)	1:176:A:VAL:HG11	1:215:A:ILE:HD11	20	0.77
(1,368)	1:176:A:VAL:HG11	1:215:A:ILE:HD12	20	0.77
(1,368)	1:176:A:VAL:HG11	1:215:A:ILE:HD13	20	0.77
(1,368)	1:176:A:VAL:HG12	1:215:A:ILE:HD11	20	0.77
(1,368)	1:176:A:VAL:HG12	1:215:A:ILE:HD12	20	0.77
(1,368)	1:176:A:VAL:HG12	1:215:A:ILE:HD13	20	0.77
(1,368)	1:176:A:VAL:HG13	1:215:A:ILE:HD11	20	0.77
(1,368)	1:176:A:VAL:HG13	1:215:A:ILE:HD12	20	0.77
(1,368)	1:176:A:VAL:HG13	1:215:A:ILE:HD13	20	0.77
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	8	0.77
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	8	0.77
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	4	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	4	0.76
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	4	0.76
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	4	0.76
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	20	0.76
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	20	0.76
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	20	0.76
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	20	0.76
(1,763)	1:161:A:VAL:HG11	1:214:A:CYS:H	11	0.76
(1,763)	1:161:A:VAL:HG12	1:214:A:CYS:H	11	0.76
(1,763)	1:161:A:VAL:HG13	1:214:A:CYS:H	11	0.76
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	3	0.76
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	3	0.76
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	3	0.76
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	3	0.76
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG11	15	0.76
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG12	15	0.76
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG13	15	0.76
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG11	15	0.76
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG12	15	0.76
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG13	15	0.76
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG11	15	0.76
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG12	15	0.76
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG13	15	0.76
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	17	0.76
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	17	0.76
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	17	0.76
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	12	0.76
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	12	0.76
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	12	0.76
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	2	0.75
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	2	0.75
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	2	0.75
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	1	0.75
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	1	0.75
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	1	0.75
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	1	0.75
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	9	0.75
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	9	0.75
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	9	0.75
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	9	0.75
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	8	0.75
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	8	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	8	0.75
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	18	0.75
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	18	0.75
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	18	0.75
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	18	0.75
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	18	0.75
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	18	0.75
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	18	0.75
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	18	0.75
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	18	0.75
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD2	4	0.75
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD3	4	0.75
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD2	8	0.75
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD3	8	0.75
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	11	0.75
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	11	0.75
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	11	0.75
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	2	0.74
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	2	0.74
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	2	0.74
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	2	0.74
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	7	0.74
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	7	0.74
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	7	0.74
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	7	0.74
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	7	0.74
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	7	0.74
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	10	0.74
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	10	0.74
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	10	0.74
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	10	0.74
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	10	0.74
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	10	0.74
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	17	0.74
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	17	0.74
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	6	0.73
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	6	0.73
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	6	0.73
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	6	0.73
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	6	0.73
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	6	0.73
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG11	2	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG12	2	0.73
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG13	2	0.73
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG11	2	0.73
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG12	2	0.73
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG13	2	0.73
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG11	2	0.73
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG12	2	0.73
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG13	2	0.73
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG11	19	0.73
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG12	19	0.73
(1,346)	1:209:A:MET:HE1	1:210:A:VAL:HG13	19	0.73
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG11	19	0.73
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG12	19	0.73
(1,346)	1:209:A:MET:HE2	1:210:A:VAL:HG13	19	0.73
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG11	19	0.73
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG12	19	0.73
(1,346)	1:209:A:MET:HE3	1:210:A:VAL:HG13	19	0.73
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	13	0.73
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	13	0.73
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	13	0.73
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	14	0.72
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	14	0.72
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	18	0.72
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	18	0.72
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	18	0.72
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	18	0.72
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	11	0.72
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	11	0.72
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	11	0.72
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	11	0.72
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	11	0.72
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	11	0.72
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	11	0.72
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	3	0.72
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	3	0.72
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	3	0.72
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	20	0.72
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	20	0.72
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	20	0.72
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG11	15	0.72
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG12	15	0.72
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG13	15	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG11	15	0.72
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG12	15	0.72
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG13	15	0.72
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG11	15	0.72
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG12	15	0.72
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG13	15	0.72
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG21	3	0.71
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG22	3	0.71
(1,1300)	1:134:A:MET:HA	1:216:A:THR:HG23	3	0.71
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	14	0.71
(1,699)	1:120:A:ALA:HB1	1:122:A:VAL:H	4	0.71
(1,699)	1:120:A:ALA:HB2	1:122:A:VAL:H	4	0.71
(1,699)	1:120:A:ALA:HB3	1:122:A:VAL:H	4	0.71
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	14	0.71
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	14	0.71
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	15	0.71
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	15	0.71
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	14	0.71
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	14	0.71
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	14	0.71
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	2	0.71
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	2	0.71
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	2	0.71
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD2	5	0.71
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD3	5	0.71
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE1	19	0.71
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE2	19	0.71
(1,156)	1:133:A:ALA:HA	1:134:A:MET:HE3	19	0.71
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	12	0.7
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	12	0.7
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	12	0.7
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	12	0.7
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	12	0.7
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	12	0.7
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	3	0.7
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	3	0.7
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	3	0.7
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	3	0.7
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	9	0.7
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	9	0.7
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	9	0.7
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	9	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	9	0.7
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	9	0.7
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	15	0.7
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	15	0.7
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	2	0.7
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	2	0.7
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	2	0.7
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	2	0.7
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	13	0.7
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	13	0.7
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	13	0.7
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	13	0.7
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	11	0.7
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	18	0.7
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	20	0.7
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	20	0.7
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	20	0.7
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG21	10	0.7
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG22	10	0.7
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG23	10	0.7
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG21	10	0.7
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG22	10	0.7
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG23	10	0.7
(1,972)	1:175:A:PHE:HD1	1:176:A:VAL:HG21	3	0.69
(1,972)	1:175:A:PHE:HD1	1:176:A:VAL:HG22	3	0.69
(1,972)	1:175:A:PHE:HD1	1:176:A:VAL:HG23	3	0.69
(1,972)	1:175:A:PHE:HD2	1:176:A:VAL:HG21	3	0.69
(1,972)	1:175:A:PHE:HD2	1:176:A:VAL:HG22	3	0.69
(1,972)	1:175:A:PHE:HD2	1:176:A:VAL:HG23	3	0.69
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	5	0.69
(1,605)	1:213:A:MET:H	1:213:A:MET:HG2	2	0.69
(1,605)	1:213:A:MET:H	1:213:A:MET:HG3	2	0.69
(1,605)	1:213:A:MET:H	1:213:A:MET:HG2	3	0.69
(1,605)	1:213:A:MET:H	1:213:A:MET:HG3	3	0.69
(1,605)	1:213:A:MET:H	1:213:A:MET:HG2	9	0.69
(1,605)	1:213:A:MET:H	1:213:A:MET:HG3	9	0.69
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	12	0.69
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	12	0.69
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	12	0.69
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	12	0.69
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	12	0.69
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	12	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	12	0.69
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	12	0.69
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	12	0.69
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	7	0.69
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	17	0.68
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	17	0.68
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	17	0.68
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	17	0.68
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	17	0.68
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	17	0.68
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	2	0.68
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	2	0.68
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	2	0.68
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	2	0.68
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	2	0.68
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	2	0.68
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	8	0.68
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	8	0.68
(1,605)	1:213:A:MET:H	1:213:A:MET:HG2	8	0.68
(1,605)	1:213:A:MET:H	1:213:A:MET:HG3	8	0.68
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	19	0.68
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	19	0.68
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	19	0.68
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	19	0.68
(1,342)	1:134:A:MET:HE1	1:160:A:GLN:HA	19	0.68
(1,342)	1:134:A:MET:HE2	1:160:A:GLN:HA	19	0.68
(1,342)	1:134:A:MET:HE3	1:160:A:GLN:HA	19	0.68
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	4	0.68
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	4	0.68
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	4	0.68
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	15	0.67
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	15	0.67
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	15	0.67
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	15	0.67
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	15	0.67
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	15	0.67
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	2	0.67
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	2	0.67
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	2	0.67
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	2	0.67
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	2	0.67
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	2	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	16	0.67
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	16	0.67
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	16	0.67
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	16	0.67
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	16	0.67
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	16	0.67
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	15	0.67
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	15	0.67
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	15	0.67
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	15	0.67
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	16	0.67
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	16	0.67
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	6	0.67
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	6	0.67
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	6	0.67
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	4	0.67
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	4	0.67
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	4	0.67
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	12	0.67
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	12	0.67
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	12	0.67
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	13	0.66
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	13	0.66
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	13	0.66
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	13	0.66
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	13	0.66
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	13	0.66
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	14	0.66
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	2	0.66
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	2	0.66
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	19	0.66
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	19	0.66
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	7	0.66
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	7	0.66
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	7	0.66
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	7	0.66
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	7	0.66
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	7	0.66
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	7	0.66
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	7	0.66
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	7	0.66
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	15	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	15	0.66
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	15	0.66
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	3	0.66
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	1	0.65
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	4	0.65
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	4	0.65
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	5	0.65
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	5	0.65
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	13	0.65
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	13	0.65
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	13	0.65
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	13	0.65
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	13	0.65
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	13	0.65
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	13	0.65
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	13	0.65
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	13	0.65
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	20	0.65
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	20	0.65
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	20	0.65
(1,162)	1:217:A:GLN:HA	1:220:A:ARG:HG2	4	0.65
(1,11)	1:186:A:GLN:HA	1:189:A:VAL:HB	4	0.65
(1,1298)	1:128:A:TYR:HE1	1:182:A:ILE:HB	8	0.64
(1,1298)	1:128:A:TYR:HE2	1:182:A:ILE:HB	8	0.64
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	6	0.64
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	6	0.64
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	6	0.64
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	6	0.64
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	17	0.64
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	17	0.64
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	17	0.64
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	17	0.64
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	17	0.64
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	17	0.64
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	15	0.64
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	15	0.64
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	15	0.64
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	15	0.64
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	15	0.64
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	15	0.64
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	2	0.64
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	2	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	2	0.64
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	2	0.64
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	14	0.64
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	7	0.64
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	7	0.64
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	13	0.64
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	13	0.64
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	18	0.64
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	18	0.64
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	18	0.64
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	16	0.64
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	16	0.64
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	16	0.64
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	16	0.64
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	16	0.64
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	16	0.64
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	16	0.64
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	16	0.64
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	16	0.64
(1,1313)	1:176:A:VAL:HB	1:214:A:CYS:H	3	0.63
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	10	0.63
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	10	0.63
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	10	0.63
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	10	0.63
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	10	0.63
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	10	0.63
(1,605)	1:213:A:MET:H	1:213:A:MET:HG2	15	0.63
(1,605)	1:213:A:MET:H	1:213:A:MET:HG3	15	0.63
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	7	0.63
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	7	0.63
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	7	0.63
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	3	0.63
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	7	0.63
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	9	0.63
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	16	0.63
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	18	0.63
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	19	0.63
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	3	0.63
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	3	0.63
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	3	0.63
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	3	0.63
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	3	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	3	0.63
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	3	0.63
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	3	0.63
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	3	0.63
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	9	0.63
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	9	0.63
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	9	0.63
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	10	0.62
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	10	0.62
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	10	0.62
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	10	0.62
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	18	0.62
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	18	0.62
(1,605)	1:213:A:MET:H	1:213:A:MET:HG2	13	0.62
(1,605)	1:213:A:MET:H	1:213:A:MET:HG3	13	0.62
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	6	0.62
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	10	0.62
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	17	0.62
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	16	0.62
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	16	0.62
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	16	0.62
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	16	0.62
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	15	0.62
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	15	0.62
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	15	0.62
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	8	0.62
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	13	0.62
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	13	0.62
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	13	0.62
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	14	0.62
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	14	0.62
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	14	0.62
(1,162)	1:217:A:GLN:HA	1:220:A:ARG:HG2	16	0.62
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG11	5	0.62
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG12	5	0.62
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG13	5	0.62
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG11	5	0.62
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG12	5	0.62
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG13	5	0.62
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG11	5	0.62
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG12	5	0.62
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG13	5	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	8	0.61
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	11	0.61
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	11	0.61
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	8	0.61
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	12	0.61
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	7	0.61
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	7	0.61
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	7	0.61
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	15	0.61
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	16	0.61
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	10	0.61
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	10	0.61
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	10	0.61
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	18	0.61
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	18	0.61
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	18	0.61
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG2	17	0.61
(1,161)	1:224:A:ALA:HA	1:227:A:GLN:HG3	17	0.61
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	1	0.6
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	5	0.6
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	14	0.6
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	7	0.6
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	7	0.6
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	7	0.6
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	1	0.6
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	1	0.6
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	1	0.6
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	7	0.6
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	7	0.6
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	7	0.6
(1,162)	1:217:A:GLN:HA	1:220:A:ARG:HG2	10	0.6
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	13	0.59
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	13	0.59
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	13	0.59
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	13	0.59
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	13	0.59
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	13	0.59
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	4	0.59
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	4	0.59
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	19	0.59
(1,763)	1:161:A:VAL:HG11	1:214:A:CYS:H	15	0.59
(1,763)	1:161:A:VAL:HG12	1:214:A:CYS:H	15	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:161:A:VAL:HG13	1:214:A:CYS:H	15	0.59
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	1	0.59
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	1	0.59
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	17	0.59
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	17	0.59
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	11	0.59
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	20	0.59
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	10	0.59
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	10	0.59
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	10	0.59
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	14	0.59
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	14	0.59
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	14	0.59
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	14	0.59
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	14	0.59
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	14	0.59
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	14	0.59
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	14	0.59
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	14	0.59
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	3	0.59
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	3	0.59
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	3	0.59
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	6	0.59
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	6	0.59
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	6	0.59
(1,228)	1:184:A:ILE:HD11	1:210:A:VAL:HB	16	0.59
(1,228)	1:184:A:ILE:HD12	1:210:A:VAL:HB	16	0.59
(1,228)	1:184:A:ILE:HD13	1:210:A:VAL:HB	16	0.59
(1,11)	1:186:A:GLN:HA	1:189:A:VAL:HB	3	0.59
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	3	0.58
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	3	0.58
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	3	0.58
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	3	0.58
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	3	0.58
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	3	0.58
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	1	0.58
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	1	0.58
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	1	0.58
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	1	0.58
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	1	0.58
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	1	0.58
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	1	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	1	0.58
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	1	0.58
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	1	0.58
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	1	0.58
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	1	0.58
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	1	0.58
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	1	0.58
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	1	0.58
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	1	0.58
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	1	0.58
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	1	0.58
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	20	0.58
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	20	0.58
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	17	0.58
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	17	0.58
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	17	0.58
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	4	0.58
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	13	0.58
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	7	0.58
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	7	0.58
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	7	0.58
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	9	0.58
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	9	0.58
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	9	0.58
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	9	0.58
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	9	0.58
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	9	0.58
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	9	0.58
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	9	0.58
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	9	0.58
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE1	3	0.58
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE2	3	0.58
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE3	3	0.58
(1,11)	1:186:A:GLN:HA	1:189:A:VAL:HB	10	0.58
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	19	0.57
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	19	0.57
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	19	0.57
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	19	0.57
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	19	0.57
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	19	0.57
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	18	0.57
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	5	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	17	0.57
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	16	0.57
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	16	0.57
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	16	0.57
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	10	0.57
(1,162)	1:217:A:GLN:HA	1:220:A:ARG:HG2	9	0.57
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE1	12	0.56
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE2	12	0.56
(1,1042)	1:139:A:ILE:HG12	1:213:A:MET:HE3	12	0.56
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE1	12	0.56
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE2	12	0.56
(1,1042)	1:139:A:ILE:HG13	1:213:A:MET:HE3	12	0.56
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	1	0.56
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	11	0.56
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	3	0.56
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	3	0.56
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	3	0.56
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG21	20	0.56
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG22	20	0.56
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG23	20	0.56
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG21	20	0.56
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG22	20	0.56
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG23	20	0.56
(1,162)	1:217:A:GLN:HA	1:220:A:ARG:HG2	14	0.56
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	19	0.55
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	19	0.55
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	19	0.55
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	19	0.55
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	19	0.55
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	19	0.55
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	7	0.55
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	7	0.55
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	7	0.55
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	7	0.55
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	7	0.55
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	7	0.55
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	12	0.55
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	12	0.55
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	12	0.55
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	12	0.55
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	12	0.55
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	12	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	4	0.55
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	4	0.55
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	4	0.55
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	4	0.55
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	4	0.55
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	4	0.55
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	8	0.55
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	8	0.55
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	9	0.55
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	9	0.55
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	9	0.55
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	9	0.55
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	12	0.55
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	12	0.55
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	9	0.55
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	9	0.55
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	9	0.55
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	18	0.55
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	18	0.55
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	18	0.55
(1,368)	1:176:A:VAL:HG11	1:215:A:ILE:HD11	3	0.55
(1,368)	1:176:A:VAL:HG11	1:215:A:ILE:HD12	3	0.55
(1,368)	1:176:A:VAL:HG11	1:215:A:ILE:HD13	3	0.55
(1,368)	1:176:A:VAL:HG12	1:215:A:ILE:HD11	3	0.55
(1,368)	1:176:A:VAL:HG12	1:215:A:ILE:HD12	3	0.55
(1,368)	1:176:A:VAL:HG12	1:215:A:ILE:HD13	3	0.55
(1,368)	1:176:A:VAL:HG13	1:215:A:ILE:HD11	3	0.55
(1,368)	1:176:A:VAL:HG13	1:215:A:ILE:HD12	3	0.55
(1,368)	1:176:A:VAL:HG13	1:215:A:ILE:HD13	3	0.55
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	18	0.55
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	18	0.55
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	18	0.55
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	18	0.55
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	18	0.55
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	18	0.55
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	18	0.55
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	18	0.55
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	18	0.55
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	17	0.55
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	19	0.55
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	6	0.55
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	6	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	6	0.55
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	19	0.54
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	19	0.54
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	19	0.54
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	19	0.54
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	19	0.54
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	19	0.54
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	4	0.54
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	4	0.54
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	4	0.54
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	4	0.54
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	8	0.54
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	8	0.54
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	8	0.54
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	16	0.54
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	16	0.54
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	16	0.54
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	6	0.54
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	6	0.54
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	6	0.54
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	6	0.54
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	2	0.54
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	17	0.54
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	17	0.54
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	17	0.54
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	8	0.53
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	8	0.53
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	8	0.53
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	2	0.53
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	2	0.53
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	2	0.53
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	2	0.53
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	2	0.53
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	2	0.53
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	10	0.53
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	10	0.53
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	10	0.53
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	10	0.53
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	10	0.53
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	10	0.53
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	14	0.53
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	14	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	14	0.53
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	14	0.53
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	14	0.53
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	2	0.53
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	1	0.53
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	1	0.53
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	1	0.53
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	1	0.53
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	1	0.53
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	1	0.53
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	1	0.53
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	1	0.53
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	1	0.53
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD2	9	0.53
(1,205)	1:201:A:THR:HA	1:204:A:LYS:HD3	9	0.53
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	12	0.53
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	12	0.53
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	12	0.53
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	6	0.52
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	6	0.52
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	10	0.52
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	10	0.52
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	10	0.52
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	9	0.52
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	9	0.52
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	9	0.52
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	4	0.52
(1,11)	1:186:A:GLN:HA	1:189:A:VAL:HB	6	0.52
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	7	0.51
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	7	0.51
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	20	0.51
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	20	0.51
(1,819)	1:176:A:VAL:H	1:214:A:CYS:HB3	9	0.51
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	15	0.51
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	10	0.51
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	10	0.51
(1,387)	1:135:A:SER:HA	1:136:A:ARG:H	15	0.51
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	20	0.51
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	20	0.51
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	20	0.51
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	10	0.51
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	10	0.51
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	18	0.51
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	18	0.51
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	18	0.51
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	12	0.51
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	12	0.51
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	12	0.51
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	5	0.51
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	5	0.51
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	5	0.51
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	9	0.51
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	9	0.51
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	9	0.51
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	10	0.51
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	10	0.51
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	10	0.51
(1,11)	1:186:A:GLN:HA	1:189:A:VAL:HB	16	0.51
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	9	0.5
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	9	0.5
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	9	0.5
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	11	0.5
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	11	0.5
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	14	0.5
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	14	0.5
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	14	0.5
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	14	0.5
(1,938)	1:128:A:TYR:HE1	1:182:A:ILE:HB	14	0.5
(1,938)	1:128:A:TYR:HE2	1:182:A:ILE:HB	14	0.5
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	10	0.5
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	10	0.5
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	19	0.5
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	19	0.5
(1,858)	1:135:A:SER:HA	1:136:A:ARG:HE	7	0.5
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	7	0.5
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	19	0.5
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	8	0.5
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	8	0.5
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	8	0.5
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	8	0.5
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	2	0.5
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	2	0.5
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	2	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	3	0.5
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	3	0.5
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	3	0.5
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	15	0.5
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	15	0.5
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	15	0.5
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG21	4	0.5
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG22	4	0.5
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG23	4	0.5
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG21	4	0.5
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG22	4	0.5
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG23	4	0.5
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	2	0.5
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	2	0.5
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	2	0.5
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	13	0.5
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	13	0.5
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	13	0.5
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG11	11	0.5
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG12	11	0.5
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG13	11	0.5
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG11	11	0.5
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG12	11	0.5
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG13	11	0.5
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG11	11	0.5
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG12	11	0.5
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG13	11	0.5
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	5	0.49
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	5	0.49
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	5	0.49
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	5	0.49
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	5	0.49
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	5	0.49
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	18	0.49
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	18	0.49
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	18	0.49
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	18	0.49
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	18	0.49
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	18	0.49
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	12	0.49
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	12	0.49
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	12	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	12	0.49
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	2	0.49
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	2	0.49
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	2	0.49
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	2	0.49
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	2	0.49
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	2	0.49
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	1	0.49
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	1	0.49
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	1	0.49
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	1	0.49
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	1	0.49
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	1	0.49
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	12	0.49
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	12	0.49
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	12	0.49
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	6	0.49
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	6	0.49
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	6	0.49
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	11	0.49
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	11	0.49
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	11	0.49
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	13	0.49
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	13	0.49
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	13	0.49
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	1	0.49
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	1	0.49
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	1	0.49
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	3	0.49
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	3	0.49
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	3	0.49
(1,162)	1:217:A:GLN:HA	1:220:A:ARG:HG2	15	0.49
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG21	18	0.49
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG22	18	0.49
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG23	18	0.49
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	6	0.48
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	6	0.48
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	6	0.48
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	6	0.48
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	6	0.48
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	6	0.48
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	6	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	6	0.48
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	6	0.48
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	6	0.48
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	6	0.48
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	6	0.48
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	6	0.48
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	6	0.48
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	6	0.48
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	6	0.48
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	6	0.48
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	6	0.48
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	7	0.48
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	7	0.48
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	15	0.48
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	1	0.48
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	1	0.48
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	1	0.48
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	9	0.48
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	9	0.48
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	9	0.48
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	2	0.48
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	2	0.48
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	2	0.48
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	17	0.48
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	17	0.48
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	17	0.48
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	19	0.48
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	19	0.48
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	19	0.48
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG21	13	0.48
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG22	13	0.48
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG23	13	0.48
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG21	13	0.48
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG22	13	0.48
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG23	13	0.48
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG21	3	0.48
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG22	3	0.48
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG23	3	0.48
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	18	0.48
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	18	0.48
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	18	0.48
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	17	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	17	0.47
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	17	0.47
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	17	0.47
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	17	0.47
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	17	0.47
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	18	0.47
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	18	0.47
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	13	0.47
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	7	0.47
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	3	0.47
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	3	0.47
(1,681)	1:134:A:MET:HB2	1:135:A:SER:H	3	0.47
(1,681)	1:134:A:MET:HB3	1:135:A:SER:H	3	0.47
(1,674)	1:122:A:VAL:H	1:122:A:VAL:HB	15	0.47
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	19	0.47
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	19	0.47
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	19	0.47
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	8	0.47
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	8	0.47
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	8	0.47
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	16	0.47
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	16	0.47
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	16	0.47
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG21	19	0.47
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG22	19	0.47
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG23	19	0.47
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	8	0.47
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	8	0.47
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	8	0.47
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB2	16	0.46
(1,1287)	1:224:A:ALA:HA	1:227:A:GLN:HB3	16	0.46
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	12	0.46
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	12	0.46
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	17	0.46
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	17	0.46
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	17	0.46
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	12	0.46
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	12	0.46
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	12	0.46
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	1	0.46
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	1	0.46
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	7	0.46
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	7	0.46
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	7	0.46
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	8	0.46
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	8	0.46
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	8	0.46
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	1	0.46
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	1	0.46
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	1	0.46
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	2	0.46
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	2	0.46
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	2	0.46
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	6	0.46
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	6	0.46
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	6	0.46
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG21	17	0.46
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG22	17	0.46
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG23	17	0.46
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	20	0.45
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	20	0.45
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	20	0.45
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	20	0.45
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	20	0.45
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	20	0.45
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB2	12	0.45
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB3	12	0.45
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	4	0.45
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	4	0.45
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	4	0.45
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	4	0.45
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	16	0.45
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	16	0.45
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	1	0.45
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	3	0.45
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	3	0.45
(1,463)	1:125:A:LEU:H	1:125:A:LEU:HB3	20	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	1	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	1	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	1	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	3	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	3	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	3	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	6	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	6	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	6	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	7	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	7	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	7	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	8	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	8	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	8	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	9	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	9	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	9	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	10	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	10	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	10	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	11	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	11	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	11	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	12	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	12	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	12	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	13	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	13	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	13	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	16	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	16	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	16	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	18	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	18	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	18	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	19	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	19	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	19	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	20	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	20	0.45
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	20	0.45
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE1	1	0.45
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE2	1	0.45
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE3	1	0.45
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG21	12	0.45
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG22	12	0.45
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG23	12	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	19	0.45
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	19	0.45
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	19	0.45
(1,162)	1:217:A:GLN:HA	1:220:A:ARG:HG2	18	0.45
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG21	7	0.45
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG22	7	0.45
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG23	7	0.45
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	14	0.44
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	14	0.44
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	14	0.44
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	14	0.44
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	14	0.44
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	14	0.44
(1,1105)	1:156:A:ARG:HD2	1:157:A:TYR:H	18	0.44
(1,1105)	1:156:A:ARG:HD3	1:157:A:TYR:H	18	0.44
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	2	0.44
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	2	0.44
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	3	0.44
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	3	0.44
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	5	0.44
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	5	0.44
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	10	0.44
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	10	0.44
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	4	0.44
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	18	0.44
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	12	0.44
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	12	0.44
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	12	0.44
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	2	0.44
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	2	0.44
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	2	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	2	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	2	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	2	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	4	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	4	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	4	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	5	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	5	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	5	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	14	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	14	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	14	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	17	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	17	0.44
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	17	0.44
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	18	0.44
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	18	0.44
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	18	0.44
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	3	0.44
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	3	0.44
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	3	0.44
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	10	0.44
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	10	0.44
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	10	0.44
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB2	14	0.43
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB3	14	0.43
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB2	14	0.43
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB3	14	0.43
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	4	0.43
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	4	0.43
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	4	0.43
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	4	0.43
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	4	0.43
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	4	0.43
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	4	0.43
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	4	0.43
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	4	0.43
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	4	0.43
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	4	0.43
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	4	0.43
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	4	0.43
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	4	0.43
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	4	0.43
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	4	0.43
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	4	0.43
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	4	0.43
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB2	4	0.43
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB3	4	0.43
(1,1126)	1:176:A:VAL:HG11	1:179:A:CYS:HB2	4	0.43
(1,1126)	1:176:A:VAL:HG11	1:179:A:CYS:HB3	4	0.43
(1,1126)	1:176:A:VAL:HG12	1:179:A:CYS:HB2	4	0.43
(1,1126)	1:176:A:VAL:HG12	1:179:A:CYS:HB3	4	0.43
(1,1126)	1:176:A:VAL:HG13	1:179:A:CYS:HB2	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1126)	1:176:A:VAL:HG13	1:179:A:CYS:HB3	4	0.43
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	14	0.43
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	14	0.43
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	14	0.43
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	14	0.43
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	14	0.43
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	14	0.43
(1,983)	1:125:A:LEU:HA	1:125:A:LEU:HD11	5	0.43
(1,983)	1:125:A:LEU:HA	1:125:A:LEU:HD12	5	0.43
(1,983)	1:125:A:LEU:HA	1:125:A:LEU:HD13	5	0.43
(1,983)	1:125:A:LEU:HA	1:125:A:LEU:HD21	5	0.43
(1,983)	1:125:A:LEU:HA	1:125:A:LEU:HD22	5	0.43
(1,983)	1:125:A:LEU:HA	1:125:A:LEU:HD23	5	0.43
(1,981)	1:125:A:LEU:H	1:125:A:LEU:HB2	1	0.43
(1,981)	1:125:A:LEU:H	1:125:A:LEU:HB3	1	0.43
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	6	0.43
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	6	0.43
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	5	0.43
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	5	0.43
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	5	0.43
(1,455)	1:192:A:THR:H	1:192:A:THR:HG21	15	0.43
(1,455)	1:192:A:THR:H	1:192:A:THR:HG22	15	0.43
(1,455)	1:192:A:THR:H	1:192:A:THR:HG23	15	0.43
(1,365)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	6	0.43
(1,365)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	6	0.43
(1,365)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	6	0.43
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	13	0.43
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	13	0.43
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	13	0.43
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	16	0.43
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	16	0.43
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	16	0.43
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	6	0.43
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG21	11	0.43
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG22	11	0.43
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG23	11	0.43
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG21	11	0.43
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG22	11	0.43
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG23	11	0.43
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG11	8	0.43
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG12	8	0.43
(1,73)	1:184:A:ILE:HD11	1:210:A:VAL:HG13	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG11	8	0.43
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG12	8	0.43
(1,73)	1:184:A:ILE:HD12	1:210:A:VAL:HG13	8	0.43
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG11	8	0.43
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG12	8	0.43
(1,73)	1:184:A:ILE:HD13	1:210:A:VAL:HG13	8	0.43
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG21	16	0.43
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG22	16	0.43
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG23	16	0.43
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB2	18	0.42
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB3	18	0.42
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB2	18	0.42
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB3	18	0.42
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	6	0.42
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	6	0.42
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	6	0.42
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	6	0.42
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	6	0.42
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	6	0.42
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	12	0.42
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	12	0.42
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	12	0.42
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	12	0.42
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	12	0.42
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	12	0.42
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG2	17	0.42
(1,1046)	1:139:A:ILE:HD11	1:209:A:MET:HG3	17	0.42
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG2	17	0.42
(1,1046)	1:139:A:ILE:HD12	1:209:A:MET:HG3	17	0.42
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG2	17	0.42
(1,1046)	1:139:A:ILE:HD13	1:209:A:MET:HG3	17	0.42
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG2	20	0.42
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG3	20	0.42
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG2	20	0.42
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG3	20	0.42
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	13	0.42
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	13	0.42
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	9	0.42
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	9	0.42
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	12	0.42
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	12	0.42
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	19	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	20	0.42
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	6	0.42
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	6	0.42
(1,699)	1:120:A:ALA:HB1	1:122:A:VAL:H	2	0.42
(1,699)	1:120:A:ALA:HB2	1:122:A:VAL:H	2	0.42
(1,699)	1:120:A:ALA:HB3	1:122:A:VAL:H	2	0.42
(1,463)	1:125:A:LEU:H	1:125:A:LEU:HB3	1	0.42
(1,463)	1:125:A:LEU:H	1:125:A:LEU:HB3	7	0.42
(1,463)	1:125:A:LEU:H	1:125:A:LEU:HB3	8	0.42
(1,425)	1:165:A:PRO:HB3	1:166:A:MET:H	14	0.42
(1,365)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	4	0.42
(1,365)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	4	0.42
(1,365)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	4	0.42
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE1	13	0.42
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE2	13	0.42
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE3	13	0.42
(1,298)	1:129:A:MET:HA	1:129:A:MET:HE1	15	0.42
(1,298)	1:129:A:MET:HA	1:129:A:MET:HE2	15	0.42
(1,298)	1:129:A:MET:HA	1:129:A:MET:HE3	15	0.42
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD11	4	0.42
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD12	4	0.42
(1,242)	1:179:A:CYS:HA	1:182:A:ILE:HD13	4	0.42
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	4	0.42
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	4	0.42
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	4	0.42
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG21	20	0.42
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG22	20	0.42
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG23	20	0.42
(1,11)	1:186:A:GLN:HA	1:189:A:VAL:HB	20	0.42
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB2	13	0.41
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB3	13	0.41
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB2	13	0.41
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB3	13	0.41
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	11	0.41
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	11	0.41
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	11	0.41
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	11	0.41
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	11	0.41
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	11	0.41
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	19	0.41
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	19	0.41
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	19	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	19	0.41
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	4	0.41
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	4	0.41
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	7	0.41
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	7	0.41
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	16	0.41
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	16	0.41
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	3	0.41
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	3	0.41
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	3	0.41
(1,475)	1:132:A:SER:HB2	1:133:A:ALA:H	9	0.41
(1,475)	1:132:A:SER:HB3	1:133:A:ALA:H	9	0.41
(1,365)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	1	0.41
(1,365)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	1	0.41
(1,365)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	1	0.41
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	5	0.41
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	5	0.41
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	5	0.41
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	20	0.41
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	20	0.41
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	20	0.41
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	20	0.41
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	20	0.41
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	20	0.41
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	20	0.41
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	20	0.41
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	20	0.41
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	1	0.41
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	1	0.41
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	1	0.41
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE1	11	0.41
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE2	11	0.41
(1,301)	1:184:A:ILE:HG21	1:206:A:MET:HE3	11	0.41
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE1	11	0.41
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE2	11	0.41
(1,301)	1:184:A:ILE:HG22	1:206:A:MET:HE3	11	0.41
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE1	11	0.41
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE2	11	0.41
(1,301)	1:184:A:ILE:HG23	1:206:A:MET:HE3	11	0.41
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	20	0.41
(1,162)	1:217:A:GLN:HA	1:220:A:ARG:HG2	7	0.41
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG21	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG22	5	0.41
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG23	5	0.41
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	3	0.4
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	3	0.4
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	3	0.4
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	3	0.4
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	3	0.4
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	3	0.4
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	3	0.4
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	3	0.4
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	3	0.4
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	3	0.4
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	3	0.4
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	3	0.4
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	3	0.4
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	3	0.4
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	3	0.4
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	3	0.4
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	3	0.4
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	3	0.4
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	8	0.4
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	8	0.4
(1,663)	1:191:A:THR:H	1:191:A:THR:HG21	4	0.4
(1,663)	1:191:A:THR:H	1:191:A:THR:HG22	4	0.4
(1,663)	1:191:A:THR:H	1:191:A:THR:HG23	4	0.4
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	11	0.4
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	11	0.4
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	11	0.4
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	13	0.4
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	13	0.4
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	13	0.4
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	7	0.4
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	7	0.4
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	7	0.4
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	1	0.4
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	1	0.4
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	1	0.4
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	1	0.4
(1,234)	1:158:A:PRO:HB2	1:183:A:THR:HG21	10	0.4
(1,234)	1:158:A:PRO:HB2	1:183:A:THR:HG22	10	0.4
(1,234)	1:158:A:PRO:HB2	1:183:A:THR:HG23	10	0.4
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG21	16	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG22	16	0.4
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG23	16	0.4
(1,150)	1:133:A:ALA:HB1	1:159:A:ASN:HB2	17	0.4
(1,150)	1:133:A:ALA:HB2	1:159:A:ASN:HB2	17	0.4
(1,150)	1:133:A:ALA:HB3	1:159:A:ASN:HB2	17	0.4
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	14	0.39
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	14	0.39
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	14	0.39
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG11	8	0.39
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG12	8	0.39
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG13	8	0.39
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG21	8	0.39
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG22	8	0.39
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG23	8	0.39
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG11	8	0.39
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG12	8	0.39
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG13	8	0.39
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG21	8	0.39
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG22	8	0.39
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG23	8	0.39
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	6	0.39
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	6	0.39
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	7	0.39
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	19	0.39
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	1	0.39
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	20	0.39
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	18	0.39
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	20	0.39
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	20	0.39
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	10	0.39
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	10	0.39
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	10	0.39
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD11	1	0.39
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD12	1	0.39
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD13	1	0.39
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	6	0.39
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	6	0.39
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	6	0.39
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	9	0.39
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	9	0.39
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	9	0.39
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	12	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:200:A:GLU:HA	1:203:A:VAL:HG21	8	0.39
(1,212)	1:200:A:GLU:HA	1:203:A:VAL:HG22	8	0.39
(1,212)	1:200:A:GLU:HA	1:203:A:VAL:HG23	8	0.39
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	7	0.39
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	7	0.39
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	7	0.39
(1,150)	1:133:A:ALA:HB1	1:159:A:ASN:HB2	12	0.39
(1,150)	1:133:A:ALA:HB2	1:159:A:ASN:HB2	12	0.39
(1,150)	1:133:A:ALA:HB3	1:159:A:ASN:HB2	12	0.39
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	5	0.38
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	5	0.38
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	5	0.38
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	2	0.38
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	2	0.38
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	2	0.38
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	2	0.38
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	2	0.38
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	2	0.38
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	8	0.38
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	8	0.38
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	8	0.38
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	8	0.38
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	8	0.38
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	8	0.38
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	18	0.38
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	18	0.38
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	1	0.38
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	1	0.38
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	8	0.38
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	7	0.38
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	16	0.38
(1,674)	1:122:A:VAL:H	1:122:A:VAL:HB	19	0.38
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	5	0.38
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	5	0.38
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	5	0.38
(1,341)	1:134:A:MET:HE1	1:217:A:GLN:HA	4	0.38
(1,341)	1:134:A:MET:HE2	1:217:A:GLN:HA	4	0.38
(1,341)	1:134:A:MET:HE3	1:217:A:GLN:HA	4	0.38
(1,299)	1:129:A:MET:HB2	1:129:A:MET:HE1	9	0.38
(1,299)	1:129:A:MET:HB2	1:129:A:MET:HE2	9	0.38
(1,299)	1:129:A:MET:HB2	1:129:A:MET:HE3	9	0.38
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG21	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG22	7	0.38
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG23	7	0.38
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG21	7	0.38
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG22	7	0.38
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG23	7	0.38
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE1	19	0.38
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE2	19	0.38
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE3	19	0.38
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE1	19	0.38
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE2	19	0.38
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE3	19	0.38
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE1	19	0.38
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE2	19	0.38
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE3	19	0.38
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	1	0.38
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	1	0.38
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	1	0.38
(1,11)	1:186:A:GLN:HA	1:189:A:VAL:HB	9	0.38
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG2	11	0.37
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG3	11	0.37
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG2	11	0.37
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG3	11	0.37
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	8	0.37
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	8	0.37
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	8	0.37
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	8	0.37
(1,981)	1:125:A:LEU:H	1:125:A:LEU:HB2	7	0.37
(1,981)	1:125:A:LEU:H	1:125:A:LEU:HB3	7	0.37
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	8	0.37
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	8	0.37
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	8	0.37
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	8	0.37
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	8	0.37
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	8	0.37
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	5	0.37
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	5	0.37
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	11	0.37
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	11	0.37
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	16	0.37
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	16	0.37
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	18	0.37
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	18	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	20	0.37
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	20	0.37
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	3	0.37
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	3	0.37
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	10	0.37
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	13	0.37
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	10	0.37
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	11	0.37
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	11	0.37
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	14	0.37
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	14	0.37
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	7	0.37
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	7	0.37
(1,425)	1:165:A:PRO:HB3	1:166:A:MET:H	3	0.37
(1,299)	1:129:A:MET:HB2	1:129:A:MET:HE1	20	0.37
(1,299)	1:129:A:MET:HB2	1:129:A:MET:HE2	20	0.37
(1,299)	1:129:A:MET:HB2	1:129:A:MET:HE3	20	0.37
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE1	18	0.37
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE2	18	0.37
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE3	18	0.37
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	2	0.37
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	2	0.37
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	2	0.37
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	3	0.37
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	3	0.37
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	3	0.37
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	9	0.37
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	9	0.37
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	9	0.37
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	19	0.37
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	19	0.37
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	19	0.37
(1,150)	1:133:A:ALA:HB1	1:159:A:ASN:HB2	10	0.37
(1,150)	1:133:A:ALA:HB2	1:159:A:ASN:HB2	10	0.37
(1,150)	1:133:A:ALA:HB3	1:159:A:ASN:HB2	10	0.37
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG21	12	0.37
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG22	12	0.37
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG23	12	0.37
(1,1303)	1:139:A:ILE:HG21	1:146:A:GLU:HB2	14	0.36
(1,1303)	1:139:A:ILE:HG21	1:146:A:GLU:HB3	14	0.36
(1,1303)	1:139:A:ILE:HG22	1:146:A:GLU:HB2	14	0.36
(1,1303)	1:139:A:ILE:HG22	1:146:A:GLU:HB3	14	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1303)	1:139:A:ILE:HG23	1:146:A:GLU:HB2	14	0.36
(1,1303)	1:139:A:ILE:HG23	1:146:A:GLU:HB3	14	0.36
(1,1260)	1:215:A:ILE:HG21	1:219:A:GLU:HG2	4	0.36
(1,1260)	1:215:A:ILE:HG21	1:219:A:GLU:HG3	4	0.36
(1,1260)	1:215:A:ILE:HG22	1:219:A:GLU:HG2	4	0.36
(1,1260)	1:215:A:ILE:HG22	1:219:A:GLU:HG3	4	0.36
(1,1260)	1:215:A:ILE:HG23	1:219:A:GLU:HG2	4	0.36
(1,1260)	1:215:A:ILE:HG23	1:219:A:GLU:HG3	4	0.36
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	8	0.36
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	8	0.36
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	8	0.36
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	8	0.36
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	8	0.36
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	8	0.36
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	8	0.36
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	8	0.36
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	8	0.36
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	8	0.36
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	8	0.36
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	8	0.36
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	8	0.36
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	8	0.36
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	8	0.36
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	8	0.36
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	8	0.36
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	8	0.36
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	9	0.36
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	9	0.36
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	9	0.36
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	9	0.36
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	9	0.36
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	9	0.36
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	9	0.36
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	9	0.36
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	9	0.36
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	9	0.36
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	9	0.36
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	9	0.36
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	9	0.36
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	9	0.36
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	9	0.36
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	9	0.36
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	9	0.36
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	19	0.36
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	19	0.36
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	19	0.36
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	19	0.36
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	19	0.36
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	19	0.36
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	19	0.36
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	19	0.36
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	19	0.36
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	19	0.36
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	19	0.36
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	19	0.36
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	19	0.36
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	19	0.36
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	19	0.36
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	19	0.36
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	19	0.36
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	19	0.36
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	7	0.36
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	2	0.36
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	2	0.36
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	17	0.36
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	17	0.36
(1,819)	1:176:A:VAL:H	1:214:A:CYS:HB3	14	0.36
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	17	0.36
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	8	0.36
(1,663)	1:191:A:THR:H	1:191:A:THR:HG21	10	0.36
(1,663)	1:191:A:THR:H	1:191:A:THR:HG22	10	0.36
(1,663)	1:191:A:THR:H	1:191:A:THR:HG23	10	0.36
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	15	0.36
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	15	0.36
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	15	0.36
(1,425)	1:165:A:PRO:HB3	1:166:A:MET:H	8	0.36
(1,425)	1:165:A:PRO:HB3	1:166:A:MET:H	10	0.36
(1,341)	1:134:A:MET:HE1	1:217:A:GLN:HA	8	0.36
(1,341)	1:134:A:MET:HE2	1:217:A:GLN:HA	8	0.36
(1,341)	1:134:A:MET:HE3	1:217:A:GLN:HA	8	0.36
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	18	0.36
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	18	0.36
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	18	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD11	10	0.36
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD12	10	0.36
(1,241)	1:178:A:ASP:HB3	1:182:A:ILE:HD13	10	0.36
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG21	3	0.36
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG22	3	0.36
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG23	3	0.36
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG21	17	0.36
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG22	17	0.36
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG23	17	0.36
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB2	7	0.35
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB3	7	0.35
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB2	7	0.35
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB3	7	0.35
(1,1242)	1:208:A:ARG:HG2	1:212:A:GLN:HG2	17	0.35
(1,1242)	1:208:A:ARG:HG2	1:212:A:GLN:HG3	17	0.35
(1,1242)	1:208:A:ARG:HG3	1:212:A:GLN:HG2	17	0.35
(1,1242)	1:208:A:ARG:HG3	1:212:A:GLN:HG3	17	0.35
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	16	0.35
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	16	0.35
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	16	0.35
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	16	0.35
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	16	0.35
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	16	0.35
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE1	18	0.35
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE2	18	0.35
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE3	18	0.35
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE1	18	0.35
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE2	18	0.35
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE3	18	0.35
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	18	0.35
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	18	0.35
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	18	0.35
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	18	0.35
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	18	0.35
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	18	0.35
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	18	0.35
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	18	0.35
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	18	0.35
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	18	0.35
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	18	0.35
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	18	0.35
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	18	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	18	0.35
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	18	0.35
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	18	0.35
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	18	0.35
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	18	0.35
(1,1121)	1:165:A:PRO:HB2	1:166:A:MET:H	10	0.35
(1,1121)	1:165:A:PRO:HB3	1:166:A:MET:H	10	0.35
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	12	0.35
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	14	0.35
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	14	0.35
(1,813)	1:176:A:VAL:HB	1:177:A:HIS:H	10	0.35
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	15	0.35
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	12	0.35
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	3	0.35
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	6	0.35
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	8	0.35
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	10	0.35
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	10	0.35
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	12	0.35
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	12	0.35
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	13	0.35
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	13	0.35
(1,358)	1:139:A:ILE:HG21	1:212:A:GLN:HG2	16	0.35
(1,358)	1:139:A:ILE:HG21	1:212:A:GLN:HG3	16	0.35
(1,358)	1:139:A:ILE:HG22	1:212:A:GLN:HG2	16	0.35
(1,358)	1:139:A:ILE:HG22	1:212:A:GLN:HG3	16	0.35
(1,358)	1:139:A:ILE:HG23	1:212:A:GLN:HG2	16	0.35
(1,358)	1:139:A:ILE:HG23	1:212:A:GLN:HG3	16	0.35
(1,341)	1:134:A:MET:HE1	1:217:A:GLN:HA	3	0.35
(1,341)	1:134:A:MET:HE2	1:217:A:GLN:HA	3	0.35
(1,341)	1:134:A:MET:HE3	1:217:A:GLN:HA	3	0.35
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	7	0.35
(1,1242)	1:208:A:ARG:HG2	1:212:A:GLN:HG2	5	0.34
(1,1242)	1:208:A:ARG:HG2	1:212:A:GLN:HG3	5	0.34
(1,1242)	1:208:A:ARG:HG3	1:212:A:GLN:HG2	5	0.34
(1,1242)	1:208:A:ARG:HG3	1:212:A:GLN:HG3	5	0.34
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	9	0.34
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	9	0.34
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	9	0.34
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	9	0.34
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	9	0.34
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	12	0.34
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	12	0.34
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	12	0.34
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	12	0.34
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	12	0.34
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	12	0.34
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	12	0.34
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	12	0.34
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	12	0.34
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	12	0.34
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	12	0.34
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	12	0.34
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	12	0.34
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	12	0.34
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	12	0.34
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	12	0.34
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	12	0.34
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	12	0.34
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	5	0.34
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	5	0.34
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	16	0.34
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	8	0.34
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	8	0.34
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	2	0.34
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	2	0.34
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	16	0.34
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	16	0.34
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	16	0.34
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	16	0.34
(1,425)	1:165:A:PRO:HB3	1:166:A:MET:H	12	0.34
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	15	0.34
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	15	0.34
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	15	0.34
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	17	0.34
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	17	0.34
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	17	0.34
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	5	0.34
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	5	0.34
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	5	0.34
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	13	0.34
(1,162)	1:217:A:GLN:HA	1:220:A:ARG:HG2	8	0.34
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE1	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE2	8	0.33
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE3	8	0.33
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE1	8	0.33
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE2	8	0.33
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE3	8	0.33
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE1	15	0.33
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE2	15	0.33
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE3	15	0.33
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE1	15	0.33
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE2	15	0.33
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE3	15	0.33
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	16	0.33
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	16	0.33
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	16	0.33
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	16	0.33
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	16	0.33
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	16	0.33
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB2	9	0.33
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB3	9	0.33
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	8	0.33
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	8	0.33
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	8	0.33
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	8	0.33
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	20	0.33
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	20	0.33
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	20	0.33
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	20	0.33
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	5	0.33
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	5	0.33
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	5	0.33
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	5	0.33
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	5	0.33
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	5	0.33
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	16	0.33
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	16	0.33
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	16	0.33
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	16	0.33
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	16	0.33
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	16	0.33
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	14	0.33
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	14	0.33
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	16	0.33
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	8	0.33
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	9	0.33
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	9	0.33
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	19	0.33
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	19	0.33
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	1	0.33
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	1	0.33
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	4	0.33
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	4	0.33
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	11	0.33
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	11	0.33
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	14	0.33
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	14	0.33
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	18	0.33
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	18	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB1	4	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB2	4	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB3	4	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB1	16	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB2	16	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB3	16	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB1	17	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB2	17	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB3	17	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB1	18	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB2	18	0.33
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB3	18	0.33
(1,432)	1:228:A:ARG:H	1:229:A:GLY:H	18	0.33
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB2	12	0.33
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB3	12	0.33
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	8	0.33
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	8	0.33
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	8	0.33
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	4	0.33
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	4	0.33
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	4	0.33
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	9	0.33
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	9	0.33
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	9	0.33
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	19	0.33
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	19	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	19	0.33
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	1	0.33
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	3	0.33
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE1	8	0.33
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE2	8	0.33
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE3	8	0.33
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE1	16	0.33
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE2	16	0.33
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE3	16	0.33
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	12	0.33
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	12	0.33
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	12	0.33
(1,11)	1:186:A:GLN:HA	1:189:A:VAL:HB	18	0.33
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	3	0.32
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	3	0.32
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	3	0.32
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	5	0.32
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	5	0.32
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	5	0.32
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	5	0.32
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	5	0.32
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	5	0.32
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	5	0.32
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	5	0.32
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	5	0.32
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	5	0.32
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	5	0.32
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	5	0.32
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	5	0.32
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	5	0.32
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	5	0.32
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	5	0.32
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	5	0.32
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	5	0.32
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	16	0.32
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	16	0.32
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	16	0.32
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	16	0.32
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	16	0.32
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	16	0.32
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	16	0.32
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	16	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	16	0.32
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	16	0.32
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	16	0.32
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	16	0.32
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	16	0.32
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	16	0.32
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	16	0.32
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	16	0.32
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	16	0.32
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	16	0.32
(1,1121)	1:165:A:PRO:HB2	1:166:A:MET:H	3	0.32
(1,1121)	1:165:A:PRO:HB3	1:166:A:MET:H	3	0.32
(1,1121)	1:165:A:PRO:HB2	1:166:A:MET:H	8	0.32
(1,1121)	1:165:A:PRO:HB3	1:166:A:MET:H	8	0.32
(1,1121)	1:165:A:PRO:HB2	1:166:A:MET:H	12	0.32
(1,1121)	1:165:A:PRO:HB3	1:166:A:MET:H	12	0.32
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	2	0.32
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	2	0.32
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	2	0.32
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	2	0.32
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	9	0.32
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	9	0.32
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	9	0.32
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	9	0.32
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	9	0.32
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	9	0.32
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	11	0.32
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	11	0.32
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	11	0.32
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	11	0.32
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	11	0.32
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	11	0.32
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	18	0.32
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	18	0.32
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	18	0.32
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	18	0.32
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	18	0.32
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	18	0.32
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	9	0.32
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	1	0.32
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	1	0.32
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	5	0.32
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	10	0.32
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	10	0.32
(1,674)	1:122:A:VAL:H	1:122:A:VAL:HB	12	0.32
(1,674)	1:122:A:VAL:H	1:122:A:VAL:HB	17	0.32
(1,674)	1:122:A:VAL:H	1:122:A:VAL:HB	18	0.32
(1,663)	1:191:A:THR:H	1:191:A:THR:HG21	9	0.32
(1,663)	1:191:A:THR:H	1:191:A:THR:HG22	9	0.32
(1,663)	1:191:A:THR:H	1:191:A:THR:HG23	9	0.32
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	5	0.32
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	5	0.32
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	6	0.32
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	6	0.32
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	7	0.32
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	7	0.32
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	15	0.32
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	15	0.32
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	17	0.32
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	17	0.32
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	20	0.32
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	20	0.32
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	1	0.32
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	1	0.32
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	17	0.32
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	17	0.32
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB1	1	0.32
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB2	1	0.32
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB3	1	0.32
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB1	6	0.32
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB2	6	0.32
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB3	6	0.32
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB1	11	0.32
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB2	11	0.32
(1,456)	1:120:A:ALA:H	1:120:A:ALA:HB3	11	0.32
(1,365)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	12	0.32
(1,365)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	12	0.32
(1,365)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	12	0.32
(1,365)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	17	0.32
(1,365)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	17	0.32
(1,365)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	17	0.32
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	1	0.32
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	1	0.32
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	4	0.32
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	4	0.32
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	4	0.32
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	4	0.32
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	4	0.32
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	4	0.32
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	4	0.32
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	4	0.32
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	4	0.32
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	9	0.32
(1,217)	1:191:A:THR:HG21	1:197:A:ASN:HA	11	0.32
(1,217)	1:191:A:THR:HG22	1:197:A:ASN:HA	11	0.32
(1,217)	1:191:A:THR:HG23	1:197:A:ASN:HA	11	0.32
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG21	18	0.32
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG22	18	0.32
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG23	18	0.32
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE1	15	0.32
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE2	15	0.32
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE3	15	0.32
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	13	0.32
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	13	0.32
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	13	0.32
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG11	16	0.31
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG12	16	0.31
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG13	16	0.31
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG21	16	0.31
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG22	16	0.31
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG23	16	0.31
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG11	16	0.31
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG12	16	0.31
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG13	16	0.31
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG21	16	0.31
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG22	16	0.31
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG23	16	0.31
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG11	16	0.31
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG12	16	0.31
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG13	16	0.31
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG21	16	0.31
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG22	16	0.31
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG23	16	0.31
(1,1244)	1:209:A:MET:HB2	1:213:A:MET:HE1	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1244)	1:209:A:MET:HB2	1:213:A:MET:HE2	14	0.31
(1,1244)	1:209:A:MET:HB2	1:213:A:MET:HE3	14	0.31
(1,1244)	1:209:A:MET:HB3	1:213:A:MET:HE1	14	0.31
(1,1244)	1:209:A:MET:HB3	1:213:A:MET:HE2	14	0.31
(1,1244)	1:209:A:MET:HB3	1:213:A:MET:HE3	14	0.31
(1,1226)	1:206:A:MET:HB2	1:206:A:MET:HE1	15	0.31
(1,1226)	1:206:A:MET:HB2	1:206:A:MET:HE2	15	0.31
(1,1226)	1:206:A:MET:HB2	1:206:A:MET:HE3	15	0.31
(1,1226)	1:206:A:MET:HB3	1:206:A:MET:HE1	15	0.31
(1,1226)	1:206:A:MET:HB3	1:206:A:MET:HE2	15	0.31
(1,1226)	1:206:A:MET:HB3	1:206:A:MET:HE3	15	0.31
(1,1160)	1:183:A:THR:HB	1:210:A:VAL:HG11	10	0.31
(1,1160)	1:183:A:THR:HB	1:210:A:VAL:HG12	10	0.31
(1,1160)	1:183:A:THR:HB	1:210:A:VAL:HG13	10	0.31
(1,1160)	1:183:A:THR:HB	1:210:A:VAL:HG21	10	0.31
(1,1160)	1:183:A:THR:HB	1:210:A:VAL:HG22	10	0.31
(1,1160)	1:183:A:THR:HB	1:210:A:VAL:HG23	10	0.31
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	15	0.31
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	15	0.31
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	15	0.31
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	15	0.31
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	15	0.31
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	15	0.31
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE1	14	0.31
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE2	14	0.31
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE3	14	0.31
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE1	14	0.31
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE2	14	0.31
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE3	14	0.31
(1,1087)	1:151:A:ARG:HG2	1:154:A:MET:HE1	13	0.31
(1,1087)	1:151:A:ARG:HG2	1:154:A:MET:HE2	13	0.31
(1,1087)	1:151:A:ARG:HG2	1:154:A:MET:HE3	13	0.31
(1,1087)	1:151:A:ARG:HG3	1:154:A:MET:HE1	13	0.31
(1,1087)	1:151:A:ARG:HG3	1:154:A:MET:HE2	13	0.31
(1,1087)	1:151:A:ARG:HG3	1:154:A:MET:HE3	13	0.31
(1,819)	1:176:A:VAL:H	1:214:A:CYS:HB3	12	0.31
(1,763)	1:161:A:VAL:HG11	1:214:A:CYS:H	6	0.31
(1,763)	1:161:A:VAL:HG12	1:214:A:CYS:H	6	0.31
(1,763)	1:161:A:VAL:HG13	1:214:A:CYS:H	6	0.31
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE1	1	0.31
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE2	1	0.31
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE3	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	6	0.31
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	13	0.31
(1,674)	1:122:A:VAL:H	1:122:A:VAL:HB	14	0.31
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	19	0.31
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	19	0.31
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	4	0.31
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	4	0.31
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	10	0.31
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	10	0.31
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	19	0.31
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	19	0.31
(1,425)	1:165:A:PRO:HB3	1:166:A:MET:H	1	0.31
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	14	0.31
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	14	0.31
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	14	0.31
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE1	13	0.31
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE2	13	0.31
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE3	13	0.31
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	11	0.31
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	11	0.31
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	11	0.31
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE1	19	0.31
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE2	19	0.31
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE3	19	0.31
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	14	0.31
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	4	0.31
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	4	0.31
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	4	0.31
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE1	9	0.31
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE2	9	0.31
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE3	9	0.31
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	11	0.31
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	11	0.31
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	11	0.31
(1,188)	1:184:A:ILE:HD11	1:207:A:GLU:HG2	16	0.31
(1,188)	1:184:A:ILE:HD12	1:207:A:GLU:HG2	16	0.31
(1,188)	1:184:A:ILE:HD13	1:207:A:GLU:HG2	16	0.31
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	19	0.3
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	19	0.3
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	19	0.3
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB2	8	0.3
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB3	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB2	8	0.3
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB3	8	0.3
(1,1121)	1:165:A:PRO:HB2	1:166:A:MET:H	1	0.3
(1,1121)	1:165:A:PRO:HB3	1:166:A:MET:H	1	0.3
(1,1121)	1:165:A:PRO:HB2	1:166:A:MET:H	9	0.3
(1,1121)	1:165:A:PRO:HB3	1:166:A:MET:H	9	0.3
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE1	8	0.3
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE2	8	0.3
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE3	8	0.3
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE1	8	0.3
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE2	8	0.3
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE3	8	0.3
(1,981)	1:125:A:LEU:H	1:125:A:LEU:HB2	8	0.3
(1,981)	1:125:A:LEU:H	1:125:A:LEU:HB3	8	0.3
(1,942)	1:139:A:ILE:HG21	1:141:A:PHE:HZ	17	0.3
(1,942)	1:139:A:ILE:HG22	1:141:A:PHE:HZ	17	0.3
(1,942)	1:139:A:ILE:HG23	1:141:A:PHE:HZ	17	0.3
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	13	0.3
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	13	0.3
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	1	0.3
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	16	0.3
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	13	0.3
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE1	10	0.3
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE2	10	0.3
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE3	10	0.3
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE1	13	0.3
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE2	13	0.3
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE3	13	0.3
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	9	0.3
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	13	0.3
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	20	0.3
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	14	0.3
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	14	0.3
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	4	0.3
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	4	0.3
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	4	0.3
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	10	0.3
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	15	0.3
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	17	0.3
(1,223)	1:188:A:THR:HG21	1:191:A:THR:HB	6	0.3
(1,223)	1:188:A:THR:HG22	1:191:A:THR:HB	6	0.3
(1,223)	1:188:A:THR:HG23	1:191:A:THR:HB	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:208:A:ARG:HB2	1:209:A:MET:HA	15	0.3
(1,180)	1:208:A:ARG:HB3	1:209:A:MET:HA	15	0.3
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	8	0.3
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	8	0.3
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	8	0.3
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	18	0.29
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	18	0.29
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	18	0.29
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD1	7	0.29
(1,1304)	1:157:A:TYR:HE1	1:198:A:PHE:HD2	7	0.29
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD1	7	0.29
(1,1304)	1:157:A:TYR:HE2	1:198:A:PHE:HD2	7	0.29
(1,1283)	1:222:A:SER:HA	1:225:A:TYR:HB2	4	0.29
(1,1283)	1:222:A:SER:HA	1:225:A:TYR:HB3	4	0.29
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG11	11	0.29
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG12	11	0.29
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG13	11	0.29
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG21	11	0.29
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG22	11	0.29
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG23	11	0.29
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG11	11	0.29
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG12	11	0.29
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG13	11	0.29
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG21	11	0.29
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG22	11	0.29
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG23	11	0.29
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG11	11	0.29
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG12	11	0.29
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG13	11	0.29
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG21	11	0.29
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG22	11	0.29
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG23	11	0.29
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG11	17	0.29
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG12	17	0.29
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG13	17	0.29
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG21	17	0.29
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG22	17	0.29
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG23	17	0.29
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG11	17	0.29
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG12	17	0.29
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG13	17	0.29
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG21	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG22	17	0.29
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG23	17	0.29
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG11	17	0.29
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG12	17	0.29
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG13	17	0.29
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG21	17	0.29
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG22	17	0.29
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG23	17	0.29
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG2	7	0.29
(1,1209)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	7	0.29
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG2	7	0.29
(1,1209)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	7	0.29
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG2	7	0.29
(1,1209)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	7	0.29
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	13	0.29
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	13	0.29
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	13	0.29
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	13	0.29
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	13	0.29
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	13	0.29
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	13	0.29
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	13	0.29
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	13	0.29
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	13	0.29
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	13	0.29
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	13	0.29
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	13	0.29
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	13	0.29
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	13	0.29
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	13	0.29
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	13	0.29
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	13	0.29
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	17	0.29
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	17	0.29
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	17	0.29
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	17	0.29
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	17	0.29
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	17	0.29
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	17	0.29
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	17	0.29
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	17	0.29
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	17	0.29
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	17	0.29
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	17	0.29
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	17	0.29
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	17	0.29
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	17	0.29
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	17	0.29
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	17	0.29
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE1	1	0.29
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE2	1	0.29
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE3	1	0.29
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE1	1	0.29
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE2	1	0.29
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE3	1	0.29
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	5	0.29
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	10	0.29
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	18	0.29
(1,763)	1:161:A:VAL:HG11	1:214:A:CYS:H	1	0.29
(1,763)	1:161:A:VAL:HG12	1:214:A:CYS:H	1	0.29
(1,763)	1:161:A:VAL:HG13	1:214:A:CYS:H	1	0.29
(1,762)	1:176:A:VAL:HG11	1:214:A:CYS:H	3	0.29
(1,762)	1:176:A:VAL:HG12	1:214:A:CYS:H	3	0.29
(1,762)	1:176:A:VAL:HG13	1:214:A:CYS:H	3	0.29
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	2	0.29
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	4	0.29
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	8	0.29
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB2	6	0.29
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB3	6	0.29
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB2	7	0.29
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB3	7	0.29
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	4	0.29
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	4	0.29
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	4	0.29
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	20	0.29
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	20	0.29
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	20	0.29
(1,310)	1:206:A:MET:HA	1:206:A:MET:HE1	15	0.29
(1,310)	1:206:A:MET:HA	1:206:A:MET:HE2	15	0.29
(1,310)	1:206:A:MET:HA	1:206:A:MET:HE3	15	0.29
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	5	0.29
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	8	0.29
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	16	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	20	0.29
(1,185)	1:208:A:ARG:HA	1:211:A:GLU:HB2	8	0.29
(1,185)	1:208:A:ARG:HA	1:211:A:GLU:HB3	8	0.29
(1,185)	1:208:A:ARG:HA	1:211:A:GLU:HB2	15	0.29
(1,185)	1:208:A:ARG:HA	1:211:A:GLU:HB3	15	0.29
(1,151)	1:133:A:ALA:HB1	1:159:A:ASN:HB3	2	0.29
(1,151)	1:133:A:ALA:HB2	1:159:A:ASN:HB3	2	0.29
(1,151)	1:133:A:ALA:HB3	1:159:A:ASN:HB3	2	0.29
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	15	0.28
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	15	0.28
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	15	0.28
(1,1283)	1:222:A:SER:HA	1:225:A:TYR:HB2	14	0.28
(1,1283)	1:222:A:SER:HA	1:225:A:TYR:HB3	14	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG11	5	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG12	5	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG13	5	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG21	5	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG22	5	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG23	5	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG11	5	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG12	5	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG13	5	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG21	5	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG22	5	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG23	5	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG11	5	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG12	5	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG13	5	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG21	5	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG22	5	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG23	5	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG11	15	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG12	15	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG13	15	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG21	15	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG22	15	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG23	15	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG11	15	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG12	15	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG13	15	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG21	15	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG22	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG23	15	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG11	15	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG12	15	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG13	15	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG21	15	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG22	15	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG23	15	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG11	19	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG12	19	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG13	19	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG21	19	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG22	19	0.28
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG23	19	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG11	19	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG12	19	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG13	19	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG21	19	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG22	19	0.28
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG23	19	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG11	19	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG12	19	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG13	19	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG21	19	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG22	19	0.28
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG23	19	0.28
(1,1244)	1:209:A:MET:HB2	1:213:A:MET:HE1	20	0.28
(1,1244)	1:209:A:MET:HB2	1:213:A:MET:HE2	20	0.28
(1,1244)	1:209:A:MET:HB2	1:213:A:MET:HE3	20	0.28
(1,1244)	1:209:A:MET:HB3	1:213:A:MET:HE1	20	0.28
(1,1244)	1:209:A:MET:HB3	1:213:A:MET:HE2	20	0.28
(1,1244)	1:209:A:MET:HB3	1:213:A:MET:HE3	20	0.28
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE1	19	0.28
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE2	19	0.28
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE3	19	0.28
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE1	19	0.28
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE2	19	0.28
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE3	19	0.28
(1,1105)	1:156:A:ARG:HD2	1:157:A:TYR:H	13	0.28
(1,1105)	1:156:A:ARG:HD3	1:157:A:TYR:H	13	0.28
(1,1105)	1:156:A:ARG:HD2	1:157:A:TYR:H	15	0.28
(1,1105)	1:156:A:ARG:HD3	1:157:A:TYR:H	15	0.28
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD2	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD3	4	0.28
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD2	4	0.28
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD3	4	0.28
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD2	4	0.28
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD3	4	0.28
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	1	0.28
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	1	0.28
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	1	0.28
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	1	0.28
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	1	0.28
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	1	0.28
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	2	0.28
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	2	0.28
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	2	0.28
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	2	0.28
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	2	0.28
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	2	0.28
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	3	0.28
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	3	0.28
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	3	0.28
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	3	0.28
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	3	0.28
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	3	0.28
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	15	0.28
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	15	0.28
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	19	0.28
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	19	0.28
(1,819)	1:176:A:VAL:H	1:214:A:CYS:HB3	5	0.28
(1,763)	1:161:A:VAL:HG11	1:214:A:CYS:H	2	0.28
(1,763)	1:161:A:VAL:HG12	1:214:A:CYS:H	2	0.28
(1,763)	1:161:A:VAL:HG13	1:214:A:CYS:H	2	0.28
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	9	0.28
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	7	0.28
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	7	0.28
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	19	0.28
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	3	0.28
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	3	0.28
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	8	0.28
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	8	0.28
(1,582)	1:223:A:GLN:HB2	1:224:A:ALA:H	9	0.28
(1,582)	1:223:A:GLN:HB3	1:224:A:ALA:H	9	0.28
(1,475)	1:132:A:SER:HB2	1:133:A:ALA:H	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:132:A:SER:HB3	1:133:A:ALA:H	10	0.28
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	18	0.28
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	18	0.28
(1,432)	1:228:A:ARG:H	1:229:A:GLY:H	2	0.28
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB2	10	0.28
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB3	10	0.28
(1,358)	1:139:A:ILE:HG21	1:212:A:GLN:HG2	3	0.28
(1,358)	1:139:A:ILE:HG21	1:212:A:GLN:HG3	3	0.28
(1,358)	1:139:A:ILE:HG22	1:212:A:GLN:HG2	3	0.28
(1,358)	1:139:A:ILE:HG22	1:212:A:GLN:HG3	3	0.28
(1,358)	1:139:A:ILE:HG23	1:212:A:GLN:HG2	3	0.28
(1,358)	1:139:A:ILE:HG23	1:212:A:GLN:HG3	3	0.28
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE1	6	0.28
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE2	6	0.28
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE3	6	0.28
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE1	20	0.28
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE2	20	0.28
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE3	20	0.28
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	18	0.28
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG21	10	0.28
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG22	10	0.28
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG23	10	0.28
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE1	3	0.28
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE2	3	0.28
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE3	3	0.28
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE1	3	0.28
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE2	3	0.28
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE3	3	0.28
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE1	3	0.28
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE2	3	0.28
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE3	3	0.28
(1,180)	1:208:A:ARG:HB2	1:209:A:MET:HA	14	0.28
(1,180)	1:208:A:ARG:HB3	1:209:A:MET:HA	14	0.28
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	11	0.27
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	11	0.27
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	11	0.27
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	11	0.27
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	11	0.27
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	11	0.27
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG11	8	0.27
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG12	8	0.27
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG13	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG21	8	0.27
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG22	8	0.27
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG23	8	0.27
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG11	8	0.27
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG12	8	0.27
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG13	8	0.27
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG21	8	0.27
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG22	8	0.27
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG23	8	0.27
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG11	8	0.27
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG12	8	0.27
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG13	8	0.27
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG21	8	0.27
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG22	8	0.27
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG23	8	0.27
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	20	0.27
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	20	0.27
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	20	0.27
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	20	0.27
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	20	0.27
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	20	0.27
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	20	0.27
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	20	0.27
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	20	0.27
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	20	0.27
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	20	0.27
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	20	0.27
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	20	0.27
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	20	0.27
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	20	0.27
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	20	0.27
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	20	0.27
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	20	0.27
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB2	19	0.27
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB3	19	0.27
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG11	11	0.27
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG12	11	0.27
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG13	11	0.27
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG21	11	0.27
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG22	11	0.27
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG23	11	0.27
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG11	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG12	11	0.27
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG13	11	0.27
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG21	11	0.27
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG22	11	0.27
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG23	11	0.27
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	5	0.27
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	11	0.27
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	6	0.27
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	14	0.27
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	5	0.27
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	12	0.27
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	17	0.27
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB1	13	0.27
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB2	13	0.27
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB3	13	0.27
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	15	0.27
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	15	0.27
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	15	0.27
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	14	0.27
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	14	0.27
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	14	0.27
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	14	0.27
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	14	0.27
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	14	0.27
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	14	0.27
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	14	0.27
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	14	0.27
(1,240)	1:164:A:ARG:HG2	1:182:A:ILE:HD11	4	0.27
(1,240)	1:164:A:ARG:HG2	1:182:A:ILE:HD12	4	0.27
(1,240)	1:164:A:ARG:HG2	1:182:A:ILE:HD13	4	0.27
(1,240)	1:164:A:ARG:HG3	1:182:A:ILE:HD11	4	0.27
(1,240)	1:164:A:ARG:HG3	1:182:A:ILE:HD12	4	0.27
(1,240)	1:164:A:ARG:HG3	1:182:A:ILE:HD13	4	0.27
(1,230)	1:162:A:TYR:HB2	1:183:A:THR:HA	10	0.27
(1,230)	1:162:A:TYR:HB3	1:183:A:THR:HA	10	0.27
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD2	8	0.27
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD3	8	0.27
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD2	8	0.27
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD3	8	0.27
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD2	8	0.27
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD3	8	0.27
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	10	0.27
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	10	0.27
(1,152)	1:133:A:ALA:HB1	1:160:A:GLN:HB2	1	0.27
(1,152)	1:133:A:ALA:HB2	1:160:A:GLN:HB2	1	0.27
(1,152)	1:133:A:ALA:HB3	1:160:A:GLN:HB2	1	0.27
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	7	0.27
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	17	0.27
(1,45)	1:125:A:LEU:HA	1:125:A:LEU:HD11	5	0.27
(1,45)	1:125:A:LEU:HA	1:125:A:LEU:HD12	5	0.27
(1,45)	1:125:A:LEU:HA	1:125:A:LEU:HD13	5	0.27
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	16	0.26
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	16	0.26
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	16	0.26
(1,1305)	1:157:A:TYR:HE1	1:206:A:MET:HB2	15	0.26
(1,1305)	1:157:A:TYR:HE1	1:206:A:MET:HB3	15	0.26
(1,1305)	1:157:A:TYR:HE2	1:206:A:MET:HB2	15	0.26
(1,1305)	1:157:A:TYR:HE2	1:206:A:MET:HB3	15	0.26
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE1	19	0.26
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE2	19	0.26
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE3	19	0.26
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE1	19	0.26
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE2	19	0.26
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE3	19	0.26
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE1	19	0.26
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE2	19	0.26
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE3	19	0.26
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE1	19	0.26
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE2	19	0.26
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE3	19	0.26
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE1	19	0.26
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE2	19	0.26
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE3	19	0.26
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE1	19	0.26
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE2	19	0.26
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE3	19	0.26
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE1	16	0.26
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE2	16	0.26
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE3	16	0.26
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE1	16	0.26
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE2	16	0.26
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE3	16	0.26
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB2	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB3	18	0.26
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG2	9	0.26
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG3	9	0.26
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG2	9	0.26
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG3	9	0.26
(1,1026)	1:138:A:ILE:HD11	1:151:A:ARG:HG2	3	0.26
(1,1026)	1:138:A:ILE:HD11	1:151:A:ARG:HG3	3	0.26
(1,1026)	1:138:A:ILE:HD12	1:151:A:ARG:HG2	3	0.26
(1,1026)	1:138:A:ILE:HD12	1:151:A:ARG:HG3	3	0.26
(1,1026)	1:138:A:ILE:HD13	1:151:A:ARG:HG2	3	0.26
(1,1026)	1:138:A:ILE:HD13	1:151:A:ARG:HG3	3	0.26
(1,972)	1:175:A:PHE:HD1	1:176:A:VAL:HG21	20	0.26
(1,972)	1:175:A:PHE:HD1	1:176:A:VAL:HG22	20	0.26
(1,972)	1:175:A:PHE:HD1	1:176:A:VAL:HG23	20	0.26
(1,972)	1:175:A:PHE:HD2	1:176:A:VAL:HG21	20	0.26
(1,972)	1:175:A:PHE:HD2	1:176:A:VAL:HG22	20	0.26
(1,972)	1:175:A:PHE:HD2	1:176:A:VAL:HG23	20	0.26
(1,938)	1:128:A:TYR:HE1	1:182:A:ILE:HB	19	0.26
(1,938)	1:128:A:TYR:HE2	1:182:A:ILE:HB	19	0.26
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	2	0.26
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	2	0.26
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	2	0.26
(1,718)	1:158:A:PRO:HB2	1:159:A:ASN:H	8	0.26
(1,707)	1:143:A:SER:H	1:146:A:GLU:HB3	2	0.26
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	11	0.26
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	15	0.26
(1,671)	1:188:A:THR:HB	1:189:A:VAL:H	11	0.26
(1,498)	1:141:A:PHE:HB3	1:143:A:SER:H	12	0.26
(1,475)	1:132:A:SER:HB2	1:133:A:ALA:H	1	0.26
(1,475)	1:132:A:SER:HB3	1:133:A:ALA:H	1	0.26
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	3	0.26
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	3	0.26
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	5	0.26
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	5	0.26
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD11	4	0.26
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD12	4	0.26
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD13	4	0.26
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	7	0.26
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	7	0.26
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	7	0.26
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	7	0.26
(1,298)	1:129:A:MET:HA	1:129:A:MET:HE1	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:129:A:MET:HA	1:129:A:MET:HE2	20	0.26
(1,298)	1:129:A:MET:HA	1:129:A:MET:HE3	20	0.26
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	6	0.26
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG21	18	0.26
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG22	18	0.26
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG23	18	0.26
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG21	18	0.26
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG22	18	0.26
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG23	18	0.26
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB1	10	0.26
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB2	10	0.26
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB3	10	0.26
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB1	10	0.26
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB2	10	0.26
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB3	10	0.26
(1,1296)	1:228:A:ARG:H	1:228:A:ARG:HG2	16	0.25
(1,1296)	1:228:A:ARG:H	1:228:A:ARG:HG3	16	0.25
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	2	0.25
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	2	0.25
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	2	0.25
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	2	0.25
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	2	0.25
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	2	0.25
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	2	0.25
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	2	0.25
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	2	0.25
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	2	0.25
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	2	0.25
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	2	0.25
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	2	0.25
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	2	0.25
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	2	0.25
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	2	0.25
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	2	0.25
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	2	0.25
(1,1121)	1:165:A:PRO:HB2	1:166:A:MET:H	14	0.25
(1,1121)	1:165:A:PRO:HB3	1:166:A:MET:H	14	0.25
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE1	3	0.25
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE2	3	0.25
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE3	3	0.25
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE1	3	0.25
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE2	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE3	3	0.25
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE1	12	0.25
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE2	12	0.25
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE3	12	0.25
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE1	12	0.25
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE2	12	0.25
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE3	12	0.25
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE1	18	0.25
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE2	18	0.25
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE3	18	0.25
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE1	18	0.25
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE2	18	0.25
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE3	18	0.25
(1,981)	1:125:A:LEU:H	1:125:A:LEU:HB2	20	0.25
(1,981)	1:125:A:LEU:H	1:125:A:LEU:HB3	20	0.25
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	15	0.25
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	15	0.25
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	15	0.25
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	15	0.25
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	15	0.25
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	15	0.25
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	17	0.25
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	10	0.25
(1,699)	1:120:A:ALA:HB1	1:122:A:VAL:H	19	0.25
(1,699)	1:120:A:ALA:HB2	1:122:A:VAL:H	19	0.25
(1,699)	1:120:A:ALA:HB3	1:122:A:VAL:H	19	0.25
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	20	0.25
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	20	0.25
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG21	10	0.25
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG22	10	0.25
(1,347)	1:209:A:MET:HE1	1:210:A:VAL:HG23	10	0.25
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG21	10	0.25
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG22	10	0.25
(1,347)	1:209:A:MET:HE2	1:210:A:VAL:HG23	10	0.25
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG21	10	0.25
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG22	10	0.25
(1,347)	1:209:A:MET:HE3	1:210:A:VAL:HG23	10	0.25
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	19	0.25
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	19	0.25
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	19	0.25
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE1	1	0.25
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE2	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE3	1	0.25
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE1	1	0.25
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE2	1	0.25
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE3	1	0.25
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE1	1	0.25
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE2	1	0.25
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE3	1	0.25
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	9	0.25
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	12	0.25
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG21	20	0.25
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG22	20	0.25
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG23	20	0.25
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG21	1	0.25
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG22	1	0.25
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG23	1	0.25
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG21	15	0.25
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG22	15	0.25
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG23	15	0.25
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD2	7	0.25
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD3	7	0.25
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD2	7	0.25
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD3	7	0.25
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD2	7	0.25
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD3	7	0.25
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE1	6	0.25
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE2	6	0.25
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE3	6	0.25
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE1	6	0.25
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE2	6	0.25
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE3	6	0.25
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE1	6	0.25
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE2	6	0.25
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE3	6	0.25
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE1	14	0.25
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE2	14	0.25
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE3	14	0.25
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE1	14	0.25
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE2	14	0.25
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE3	14	0.25
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE1	14	0.25
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE2	14	0.25
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE3	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	6	0.25
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	6	0.25
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	6	0.25
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	4	0.25
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	15	0.25
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	19	0.25
(1,11)	1:186:A:GLN:HA	1:189:A:VAL:HB	8	0.25
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	5	0.24
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	5	0.24
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	5	0.24
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	5	0.24
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	5	0.24
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	5	0.24
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE1	2	0.24
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE2	2	0.24
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE3	2	0.24
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE1	2	0.24
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE2	2	0.24
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE3	2	0.24
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE1	2	0.24
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE2	2	0.24
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE3	2	0.24
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE1	2	0.24
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE2	2	0.24
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE3	2	0.24
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE1	2	0.24
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE2	2	0.24
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE3	2	0.24
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE1	2	0.24
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE2	2	0.24
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE3	2	0.24
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG11	2	0.24
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG12	2	0.24
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG13	2	0.24
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG21	2	0.24
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG22	2	0.24
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG23	2	0.24
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG11	2	0.24
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG12	2	0.24
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG13	2	0.24
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG21	2	0.24
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG22	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG23	2	0.24
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG11	2	0.24
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG12	2	0.24
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG13	2	0.24
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG21	2	0.24
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG22	2	0.24
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG23	2	0.24
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE1	2	0.24
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE2	2	0.24
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE3	2	0.24
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE1	2	0.24
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE2	2	0.24
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE3	2	0.24
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE1	8	0.24
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE2	8	0.24
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE3	8	0.24
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE1	8	0.24
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE2	8	0.24
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE3	8	0.24
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE1	9	0.24
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE2	9	0.24
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE3	9	0.24
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE1	9	0.24
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE2	9	0.24
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE3	9	0.24
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG11	3	0.24
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG12	3	0.24
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG13	3	0.24
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG21	3	0.24
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG22	3	0.24
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG23	3	0.24
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG11	3	0.24
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG12	3	0.24
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG13	3	0.24
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG21	3	0.24
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG22	3	0.24
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG23	3	0.24
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE1	6	0.24
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE2	6	0.24
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE3	6	0.24
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE1	6	0.24
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE2	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE3	6	0.24
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE1	11	0.24
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE2	11	0.24
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE3	11	0.24
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE1	11	0.24
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE2	11	0.24
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE3	11	0.24
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG2	2	0.24
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG3	2	0.24
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG2	2	0.24
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG3	2	0.24
(1,1016)	1:134:A:MET:HG2	1:216:A:THR:HG21	20	0.24
(1,1016)	1:134:A:MET:HG2	1:216:A:THR:HG22	20	0.24
(1,1016)	1:134:A:MET:HG2	1:216:A:THR:HG23	20	0.24
(1,1016)	1:134:A:MET:HG3	1:216:A:THR:HG21	20	0.24
(1,1016)	1:134:A:MET:HG3	1:216:A:THR:HG22	20	0.24
(1,1016)	1:134:A:MET:HG3	1:216:A:THR:HG23	20	0.24
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	19	0.24
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	19	0.24
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	19	0.24
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	19	0.24
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	10	0.24
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	10	0.24
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	10	0.24
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	10	0.24
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	10	0.24
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	10	0.24
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	13	0.24
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	13	0.24
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	20	0.24
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	20	0.24
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	9	0.24
(1,706)	1:143:A:SER:H	1:146:A:GLU:HB2	2	0.24
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	7	0.24
(1,432)	1:228:A:ARG:H	1:229:A:GLY:H	11	0.24
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB1	9	0.24
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB2	9	0.24
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB3	9	0.24
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	18	0.24
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	18	0.24
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	18	0.24
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE1	3	0.24
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE2	3	0.24
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE3	3	0.24
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG21	5	0.24
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG22	5	0.24
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG23	5	0.24
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD2	16	0.24
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD3	16	0.24
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD2	16	0.24
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD3	16	0.24
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD2	16	0.24
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD3	16	0.24
(1,185)	1:208:A:ARG:HA	1:211:A:GLU:HB2	20	0.24
(1,185)	1:208:A:ARG:HA	1:211:A:GLU:HB3	20	0.24
(1,162)	1:217:A:GLN:HA	1:220:A:ARG:HG2	3	0.24
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	12	0.24
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	12	0.24
(1,134)	1:228:A:ARG:HA	1:228:A:ARG:HG3	4	0.24
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	8	0.24
(1,1183)	1:196:A:GLU:HG2	1:197:A:ASN:H	6	0.23
(1,1183)	1:196:A:GLU:HG3	1:197:A:ASN:H	6	0.23
(1,1121)	1:165:A:PRO:HB2	1:166:A:MET:H	17	0.23
(1,1121)	1:165:A:PRO:HB3	1:166:A:MET:H	17	0.23
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE1	2	0.23
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE2	2	0.23
(1,1109)	1:158:A:PRO:HG2	1:209:A:MET:HE3	2	0.23
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE1	2	0.23
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE2	2	0.23
(1,1109)	1:158:A:PRO:HG3	1:209:A:MET:HE3	2	0.23
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG2	18	0.23
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG3	18	0.23
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG2	18	0.23
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG3	18	0.23
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD2	6	0.23
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD3	6	0.23
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD2	6	0.23
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD3	6	0.23
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD2	6	0.23
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD3	6	0.23
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD2	10	0.23
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD3	10	0.23
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD2	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD3	10	0.23
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD2	10	0.23
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD3	10	0.23
(1,1016)	1:134:A:MET:HG2	1:216:A:THR:HG21	16	0.23
(1,1016)	1:134:A:MET:HG2	1:216:A:THR:HG22	16	0.23
(1,1016)	1:134:A:MET:HG2	1:216:A:THR:HG23	16	0.23
(1,1016)	1:134:A:MET:HG3	1:216:A:THR:HG21	16	0.23
(1,1016)	1:134:A:MET:HG3	1:216:A:THR:HG22	16	0.23
(1,1016)	1:134:A:MET:HG3	1:216:A:THR:HG23	16	0.23
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	14	0.23
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	14	0.23
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	14	0.23
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	14	0.23
(1,918)	1:145:A:TYR:HD1	1:146:A:GLU:HB2	16	0.23
(1,918)	1:145:A:TYR:HD2	1:146:A:GLU:HB2	16	0.23
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	5	0.23
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	5	0.23
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	9	0.23
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	6	0.23
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	6	0.23
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	6	0.23
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	2	0.23
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	2	0.23
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB1	6	0.23
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB2	6	0.23
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB3	6	0.23
(1,394)	1:152:A:GLU:H	1:152:A:GLU:HG3	3	0.23
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB2	15	0.23
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB3	15	0.23
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	18	0.23
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	18	0.23
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	18	0.23
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	13	0.23
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	13	0.23
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	13	0.23
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE1	2	0.23
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE2	2	0.23
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE3	2	0.23
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE1	11	0.23
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE2	11	0.23
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE3	11	0.23
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE1	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE2	14	0.23
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE3	14	0.23
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	4	0.23
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG21	5	0.23
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG22	5	0.23
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG23	5	0.23
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG21	5	0.23
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG22	5	0.23
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG23	5	0.23
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD2	5	0.23
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD3	5	0.23
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD2	5	0.23
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD3	5	0.23
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD2	5	0.23
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD3	5	0.23
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD2	9	0.23
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD3	9	0.23
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD2	9	0.23
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD3	9	0.23
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD2	9	0.23
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD3	9	0.23
(1,180)	1:208:A:ARG:HB2	1:209:A:MET:HA	2	0.23
(1,180)	1:208:A:ARG:HB3	1:209:A:MET:HA	2	0.23
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	16	0.23
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	16	0.23
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	16	0.23
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB1	16	0.23
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB2	16	0.23
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB3	16	0.23
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB1	16	0.23
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB2	16	0.23
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB3	16	0.23
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	3	0.23
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	13	0.23
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	16	0.23
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	18	0.23
(1,1279)	1:221:A:GLU:H	1:221:A:GLU:HG2	13	0.22
(1,1279)	1:221:A:GLU:H	1:221:A:GLU:HG3	13	0.22
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE1	8	0.22
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE2	8	0.22
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE3	8	0.22
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE1	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE2	8	0.22
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE3	8	0.22
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE1	8	0.22
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE2	8	0.22
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE3	8	0.22
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE1	8	0.22
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE2	8	0.22
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE3	8	0.22
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE1	8	0.22
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE2	8	0.22
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE3	8	0.22
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE1	8	0.22
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE2	8	0.22
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE3	8	0.22
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE1	5	0.22
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE2	5	0.22
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE3	5	0.22
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE1	5	0.22
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE2	5	0.22
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE3	5	0.22
(1,1174)	1:188:A:THR:HG21	1:198:A:PHE:HB2	1	0.22
(1,1174)	1:188:A:THR:HG21	1:198:A:PHE:HB3	1	0.22
(1,1174)	1:188:A:THR:HG22	1:198:A:PHE:HB2	1	0.22
(1,1174)	1:188:A:THR:HG22	1:198:A:PHE:HB3	1	0.22
(1,1174)	1:188:A:THR:HG23	1:198:A:PHE:HB2	1	0.22
(1,1174)	1:188:A:THR:HG23	1:198:A:PHE:HB3	1	0.22
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	9	0.22
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	9	0.22
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	9	0.22
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	9	0.22
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	9	0.22
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	9	0.22
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	15	0.22
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	15	0.22
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	15	0.22
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	15	0.22
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	15	0.22
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	15	0.22
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	15	0.22
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	15	0.22
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	15	0.22
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	15	0.22
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	15	0.22
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	15	0.22
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	15	0.22
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	15	0.22
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	15	0.22
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	15	0.22
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	15	0.22
(1,1108)	1:158:A:PRO:HB3	1:210:A:VAL:HG11	11	0.22
(1,1108)	1:158:A:PRO:HB3	1:210:A:VAL:HG12	11	0.22
(1,1108)	1:158:A:PRO:HB3	1:210:A:VAL:HG13	11	0.22
(1,1108)	1:158:A:PRO:HB3	1:210:A:VAL:HG21	11	0.22
(1,1108)	1:158:A:PRO:HB3	1:210:A:VAL:HG22	11	0.22
(1,1108)	1:158:A:PRO:HB3	1:210:A:VAL:HG23	11	0.22
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD2	2	0.22
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD3	2	0.22
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD2	2	0.22
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD3	2	0.22
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD2	2	0.22
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD3	2	0.22
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD2	12	0.22
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD3	12	0.22
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD2	12	0.22
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD3	12	0.22
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD2	12	0.22
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD3	12	0.22
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	12	0.22
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	12	0.22
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	12	0.22
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	12	0.22
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	12	0.22
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	12	0.22
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE1	14	0.22
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE2	14	0.22
(1,938)	1:128:A:TYR:HE1	1:182:A:ILE:HB	13	0.22
(1,938)	1:128:A:TYR:HE2	1:182:A:ILE:HB	13	0.22
(1,931)	1:128:A:TYR:HE1	1:182:A:ILE:HG21	14	0.22
(1,931)	1:128:A:TYR:HE1	1:182:A:ILE:HG22	14	0.22
(1,931)	1:128:A:TYR:HE1	1:182:A:ILE:HG23	14	0.22
(1,931)	1:128:A:TYR:HE2	1:182:A:ILE:HG21	14	0.22
(1,931)	1:128:A:TYR:HE2	1:182:A:ILE:HG22	14	0.22
(1,931)	1:128:A:TYR:HE2	1:182:A:ILE:HG23	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	11	0.22
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	11	0.22
(1,891)	1:191:A:THR:HA	1:195:A:GLY:H	15	0.22
(1,842)	1:196:A:GLU:HG2	1:197:A:ASN:H	15	0.22
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	2	0.22
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	11	0.22
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	15	0.22
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	19	0.22
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	18	0.22
(1,498)	1:141:A:PHE:HB3	1:143:A:SER:H	15	0.22
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	20	0.22
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	20	0.22
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	20	0.22
(1,462)	1:122:A:VAL:HB	1:123:A:GLY:H	12	0.22
(1,425)	1:165:A:PRO:HB3	1:166:A:MET:H	9	0.22
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB1	1	0.22
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB2	1	0.22
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB3	1	0.22
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB2	3	0.22
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB3	3	0.22
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB2	20	0.22
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB3	20	0.22
(1,365)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	3	0.22
(1,365)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	3	0.22
(1,365)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	3	0.22
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG2	12	0.22
(1,359)	1:208:A:ARG:HB2	1:212:A:GLN:HG3	12	0.22
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG2	12	0.22
(1,359)	1:208:A:ARG:HB3	1:212:A:GLN:HG3	12	0.22
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE1	19	0.22
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE2	19	0.22
(1,338)	1:151:A:ARG:HA	1:154:A:MET:HE3	19	0.22
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE1	10	0.22
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE2	10	0.22
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE3	10	0.22
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE1	8	0.22
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE2	8	0.22
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE3	8	0.22
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	11	0.22
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	11	0.22
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	11	0.22
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE1	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE2	12	0.22
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE3	12	0.22
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE1	12	0.22
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE2	12	0.22
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE3	12	0.22
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE1	12	0.22
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE2	12	0.22
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE3	12	0.22
(1,276)	1:138:A:ILE:HD11	1:151:A:ARG:HG3	13	0.22
(1,276)	1:138:A:ILE:HD12	1:151:A:ARG:HG3	13	0.22
(1,276)	1:138:A:ILE:HD13	1:151:A:ARG:HG3	13	0.22
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG21	9	0.22
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG22	9	0.22
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG23	9	0.22
(1,180)	1:208:A:ARG:HB2	1:209:A:MET:HA	10	0.22
(1,180)	1:208:A:ARG:HB3	1:209:A:MET:HA	10	0.22
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	20	0.22
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	10	0.22
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	20	0.22
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG21	2	0.22
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG22	2	0.22
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG23	2	0.22
(1,10)	1:183:A:THR:HA	1:183:A:THR:HG21	10	0.22
(1,10)	1:183:A:THR:HA	1:183:A:THR:HG22	10	0.22
(1,10)	1:183:A:THR:HA	1:183:A:THR:HG23	10	0.22
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB2	20	0.21
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB3	20	0.21
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB2	20	0.21
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB3	20	0.21
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE1	1	0.21
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE2	1	0.21
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE3	1	0.21
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE1	1	0.21
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE2	1	0.21
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE3	1	0.21
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE1	20	0.21
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE2	20	0.21
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE3	20	0.21
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE1	20	0.21
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE2	20	0.21
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE3	20	0.21
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	9	0.21
(1,819)	1:176:A:VAL:H	1:214:A:CYS:HB3	7	0.21
(1,819)	1:176:A:VAL:H	1:214:A:CYS:HB3	13	0.21
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	4	0.21
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	14	0.21
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	12	0.21
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	17	0.21
(1,813)	1:176:A:VAL:HB	1:177:A:HIS:H	20	0.21
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	18	0.21
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	18	0.21
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	3	0.21
(1,663)	1:191:A:THR:H	1:191:A:THR:HG21	14	0.21
(1,663)	1:191:A:THR:H	1:191:A:THR:HG22	14	0.21
(1,663)	1:191:A:THR:H	1:191:A:THR:HG23	14	0.21
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	13	0.21
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	13	0.21
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB1	11	0.21
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB2	11	0.21
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB3	11	0.21
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB1	12	0.21
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB2	12	0.21
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB3	12	0.21
(1,370)	1:212:A:GLN:HA	1:215:A:ILE:HD11	20	0.21
(1,370)	1:212:A:GLN:HA	1:215:A:ILE:HD12	20	0.21
(1,370)	1:212:A:GLN:HA	1:215:A:ILE:HD13	20	0.21
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	17	0.21
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	17	0.21
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	17	0.21
(1,308)	1:198:A:PHE:HB2	1:206:A:MET:HE1	20	0.21
(1,308)	1:198:A:PHE:HB2	1:206:A:MET:HE2	20	0.21
(1,308)	1:198:A:PHE:HB2	1:206:A:MET:HE3	20	0.21
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG21	12	0.21
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG22	12	0.21
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG23	12	0.21
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	5	0.21
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	5	0.21
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	5	0.21
(1,109)	1:204:A:LYS:HA	1:204:A:LYS:HG3	4	0.21
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	9	0.21
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	12	0.21
(1,11)	1:186:A:GLN:HA	1:189:A:VAL:HB	19	0.21
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	7	0.2
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	7	0.2
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB2	19	0.2
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB3	19	0.2
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB2	19	0.2
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB3	19	0.2
(1,1260)	1:215:A:ILE:HG21	1:219:A:GLU:HG2	14	0.2
(1,1260)	1:215:A:ILE:HG21	1:219:A:GLU:HG3	14	0.2
(1,1260)	1:215:A:ILE:HG22	1:219:A:GLU:HG2	14	0.2
(1,1260)	1:215:A:ILE:HG22	1:219:A:GLU:HG3	14	0.2
(1,1260)	1:215:A:ILE:HG23	1:219:A:GLU:HG2	14	0.2
(1,1260)	1:215:A:ILE:HG23	1:219:A:GLU:HG3	14	0.2
(1,1121)	1:165:A:PRO:HB2	1:166:A:MET:H	18	0.2
(1,1121)	1:165:A:PRO:HB3	1:166:A:MET:H	18	0.2
(1,1026)	1:138:A:ILE:HD11	1:151:A:ARG:HG2	13	0.2
(1,1026)	1:138:A:ILE:HD11	1:151:A:ARG:HG3	13	0.2
(1,1026)	1:138:A:ILE:HD12	1:151:A:ARG:HG2	13	0.2
(1,1026)	1:138:A:ILE:HD12	1:151:A:ARG:HG3	13	0.2
(1,1026)	1:138:A:ILE:HD13	1:151:A:ARG:HG2	13	0.2
(1,1026)	1:138:A:ILE:HD13	1:151:A:ARG:HG3	13	0.2
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	11	0.2
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	16	0.2
(1,569)	1:228:A:ARG:H	1:228:A:ARG:HG2	6	0.2
(1,498)	1:141:A:PHE:HB3	1:143:A:SER:H	4	0.2
(1,498)	1:141:A:PHE:HB3	1:143:A:SER:H	6	0.2
(1,479)	1:134:A:MET:H	1:134:A:MET:HE1	19	0.2
(1,479)	1:134:A:MET:H	1:134:A:MET:HE2	19	0.2
(1,479)	1:134:A:MET:H	1:134:A:MET:HE3	19	0.2
(1,476)	1:132:A:SER:HA	1:133:A:ALA:H	12	0.2
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	8	0.2
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	8	0.2
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	9	0.2
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	9	0.2
(1,432)	1:228:A:ARG:H	1:229:A:GLY:H	5	0.2
(1,432)	1:228:A:ARG:H	1:229:A:GLY:H	19	0.2
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB1	17	0.2
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB2	17	0.2
(1,408)	1:133:A:ALA:H	1:133:A:ALA:HB3	17	0.2
(1,394)	1:152:A:GLU:H	1:152:A:GLU:HG3	6	0.2
(1,365)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	13	0.2
(1,365)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	13	0.2
(1,365)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE1	12	0.2
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE2	12	0.2
(1,318)	1:209:A:MET:HB3	1:213:A:MET:HE3	12	0.2
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE1	3	0.2
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE2	3	0.2
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE3	3	0.2
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE1	3	0.2
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE2	3	0.2
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE3	3	0.2
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE1	3	0.2
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE2	3	0.2
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE3	3	0.2
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG21	19	0.2
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG22	19	0.2
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG23	19	0.2
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	18	0.2
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	18	0.2
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	19	0.2
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	19	0.2
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB1	5	0.2
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB2	5	0.2
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB3	5	0.2
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB1	5	0.2
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB2	5	0.2
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB3	5	0.2
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	6	0.2
(1,27)	1:219:A:GLU:HA	1:219:A:GLU:HG3	18	0.2
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG21	11	0.2
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG22	11	0.2
(1,14)	1:188:A:THR:HA	1:191:A:THR:HG23	11	0.2
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG21	19	0.19
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG22	19	0.19
(1,1306)	1:158:A:PRO:HD2	1:210:A:VAL:HG23	19	0.19
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG21	19	0.19
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG22	19	0.19
(1,1306)	1:158:A:PRO:HD3	1:210:A:VAL:HG23	19	0.19
(1,1260)	1:215:A:ILE:HG21	1:219:A:GLU:HG2	15	0.19
(1,1260)	1:215:A:ILE:HG21	1:219:A:GLU:HG3	15	0.19
(1,1260)	1:215:A:ILE:HG22	1:219:A:GLU:HG2	15	0.19
(1,1260)	1:215:A:ILE:HG22	1:219:A:GLU:HG3	15	0.19
(1,1260)	1:215:A:ILE:HG23	1:219:A:GLU:HG2	15	0.19
(1,1260)	1:215:A:ILE:HG23	1:219:A:GLU:HG3	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG11	6	0.19
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG12	6	0.19
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG13	6	0.19
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG21	6	0.19
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG22	6	0.19
(1,1247)	1:209:A:MET:HE1	1:210:A:VAL:HG23	6	0.19
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG11	6	0.19
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG12	6	0.19
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG13	6	0.19
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG21	6	0.19
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG22	6	0.19
(1,1247)	1:209:A:MET:HE2	1:210:A:VAL:HG23	6	0.19
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG11	6	0.19
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG12	6	0.19
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG13	6	0.19
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG21	6	0.19
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG22	6	0.19
(1,1247)	1:209:A:MET:HE3	1:210:A:VAL:HG23	6	0.19
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG2	12	0.19
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG3	12	0.19
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG2	13	0.19
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG3	13	0.19
(1,1183)	1:196:A:GLU:HG2	1:197:A:ASN:H	2	0.19
(1,1183)	1:196:A:GLU:HG3	1:197:A:ASN:H	2	0.19
(1,1174)	1:188:A:THR:HG21	1:198:A:PHE:HB2	19	0.19
(1,1174)	1:188:A:THR:HG21	1:198:A:PHE:HB3	19	0.19
(1,1174)	1:188:A:THR:HG22	1:198:A:PHE:HB2	19	0.19
(1,1174)	1:188:A:THR:HG22	1:198:A:PHE:HB3	19	0.19
(1,1174)	1:188:A:THR:HG23	1:198:A:PHE:HB2	19	0.19
(1,1174)	1:188:A:THR:HG23	1:198:A:PHE:HB3	19	0.19
(1,1174)	1:188:A:THR:HG21	1:198:A:PHE:HB2	20	0.19
(1,1174)	1:188:A:THR:HG21	1:198:A:PHE:HB3	20	0.19
(1,1174)	1:188:A:THR:HG22	1:198:A:PHE:HB2	20	0.19
(1,1174)	1:188:A:THR:HG22	1:198:A:PHE:HB3	20	0.19
(1,1174)	1:188:A:THR:HG23	1:198:A:PHE:HB2	20	0.19
(1,1174)	1:188:A:THR:HG23	1:198:A:PHE:HB3	20	0.19
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG11	5	0.19
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG12	5	0.19
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG13	5	0.19
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG21	5	0.19
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG22	5	0.19
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG23	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG11	5	0.19
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG12	5	0.19
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG13	5	0.19
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG21	5	0.19
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG22	5	0.19
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG23	5	0.19
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG11	5	0.19
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG12	5	0.19
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG13	5	0.19
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG21	5	0.19
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG22	5	0.19
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG23	5	0.19
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG11	19	0.19
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG12	19	0.19
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG13	19	0.19
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG21	19	0.19
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG22	19	0.19
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG23	19	0.19
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG11	19	0.19
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG12	19	0.19
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG13	19	0.19
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG21	19	0.19
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG22	19	0.19
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG23	19	0.19
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	4	0.19
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	4	0.19
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	4	0.19
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	4	0.19
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	4	0.19
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	4	0.19
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	7	0.19
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	7	0.19
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	7	0.19
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	7	0.19
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	7	0.19
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	7	0.19
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	7	0.19
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	7	0.19
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	7	0.19
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	7	0.19
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	7	0.19
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	7	0.19
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	7	0.19
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	7	0.19
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	7	0.19
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	7	0.19
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	7	0.19
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB2	1	0.19
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB3	1	0.19
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB2	17	0.19
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB3	17	0.19
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE1	6	0.19
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE2	6	0.19
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE1	18	0.19
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE2	18	0.19
(1,893)	1:210:A:VAL:HA	1:214:A:CYS:H	1	0.19
(1,842)	1:196:A:GLU:HG2	1:197:A:ASN:H	1	0.19
(1,824)	1:162:A:TYR:HD1	1:163:A:TYR:H	11	0.19
(1,824)	1:162:A:TYR:HD2	1:163:A:TYR:H	11	0.19
(1,819)	1:176:A:VAL:H	1:214:A:CYS:HB3	15	0.19
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	7	0.19
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	17	0.19
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	1	0.19
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	14	0.19
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	18	0.19
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	9	0.19
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE1	3	0.19
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE2	3	0.19
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE3	3	0.19
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	1	0.19
(1,652)	1:192:A:THR:HA	1:195:A:GLY:H	15	0.19
(1,476)	1:132:A:SER:HA	1:133:A:ALA:H	17	0.19
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	6	0.19
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	6	0.19
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	3	0.19
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	3	0.19
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	3	0.19
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE1	9	0.19
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE2	9	0.19
(1,313)	1:210:A:VAL:HG21	1:213:A:MET:HE3	9	0.19
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE1	9	0.19
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE2	9	0.19
(1,313)	1:210:A:VAL:HG22	1:213:A:MET:HE3	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE1	9	0.19
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE2	9	0.19
(1,313)	1:210:A:VAL:HG23	1:213:A:MET:HE3	9	0.19
(1,238)	1:183:A:THR:HG21	1:184:A:ILE:HA	9	0.19
(1,238)	1:183:A:THR:HG22	1:184:A:ILE:HA	9	0.19
(1,238)	1:183:A:THR:HG23	1:184:A:ILE:HA	9	0.19
(1,180)	1:208:A:ARG:HB2	1:209:A:MET:HA	4	0.19
(1,180)	1:208:A:ARG:HB3	1:209:A:MET:HA	4	0.19
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	15	0.19
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	15	0.19
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	15	0.19
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	13	0.19
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	13	0.19
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	17	0.19
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	17	0.19
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	20	0.19
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	20	0.19
(1,152)	1:133:A:ALA:HB1	1:160:A:GLN:HB2	18	0.19
(1,152)	1:133:A:ALA:HB2	1:160:A:GLN:HB2	18	0.19
(1,152)	1:133:A:ALA:HB3	1:160:A:GLN:HB2	18	0.19
(1,109)	1:204:A:LYS:HA	1:204:A:LYS:HG3	19	0.19
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB2	2	0.18
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB3	2	0.18
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB2	2	0.18
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB3	2	0.18
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB2	3	0.18
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB3	3	0.18
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB2	3	0.18
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB3	3	0.18
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB2	5	0.18
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB3	5	0.18
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB2	5	0.18
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB3	5	0.18
(1,1283)	1:222:A:SER:HA	1:225:A:TYR:HB2	2	0.18
(1,1283)	1:222:A:SER:HA	1:225:A:TYR:HB3	2	0.18
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG2	4	0.18
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG3	4	0.18
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG2	6	0.18
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG3	6	0.18
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG2	14	0.18
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG3	14	0.18
(1,1183)	1:196:A:GLU:HG2	1:197:A:ASN:H	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1183)	1:196:A:GLU:HG3	1:197:A:ASN:H	8	0.18
(1,1107)	1:158:A:PRO:HB2	1:210:A:VAL:HG11	11	0.18
(1,1107)	1:158:A:PRO:HB2	1:210:A:VAL:HG12	11	0.18
(1,1107)	1:158:A:PRO:HB2	1:210:A:VAL:HG13	11	0.18
(1,1107)	1:158:A:PRO:HB2	1:210:A:VAL:HG21	11	0.18
(1,1107)	1:158:A:PRO:HB2	1:210:A:VAL:HG22	11	0.18
(1,1107)	1:158:A:PRO:HB2	1:210:A:VAL:HG23	11	0.18
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD2	9	0.18
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD3	9	0.18
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD2	9	0.18
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD3	9	0.18
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD2	9	0.18
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD3	9	0.18
(1,960)	1:150:A:TYR:HE1	1:157:A:TYR:HE1	10	0.18
(1,960)	1:150:A:TYR:HE1	1:157:A:TYR:HE2	10	0.18
(1,960)	1:150:A:TYR:HE2	1:157:A:TYR:HE1	10	0.18
(1,960)	1:150:A:TYR:HE2	1:157:A:TYR:HE2	10	0.18
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE1	20	0.18
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE2	20	0.18
(1,845)	1:188:A:THR:H	1:191:A:THR:HG21	4	0.18
(1,845)	1:188:A:THR:H	1:191:A:THR:HG22	4	0.18
(1,845)	1:188:A:THR:H	1:191:A:THR:HG23	4	0.18
(1,774)	1:125:A:LEU:H	1:126:A:GLY:H	12	0.18
(1,700)	1:139:A:ILE:HB	1:140:A:HIS:H	12	0.18
(1,649)	1:196:A:GLU:HG3	1:197:A:ASN:H	9	0.18
(1,432)	1:228:A:ARG:H	1:229:A:GLY:H	10	0.18
(1,432)	1:228:A:ARG:H	1:229:A:GLY:H	15	0.18
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	2	0.18
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	2	0.18
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	2	0.18
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE1	1	0.18
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE2	1	0.18
(1,319)	1:210:A:VAL:HA	1:213:A:MET:HE3	1	0.18
(1,291)	1:198:A:PHE:HA	1:199:A:THR:HG21	13	0.18
(1,291)	1:198:A:PHE:HA	1:199:A:THR:HG22	13	0.18
(1,291)	1:198:A:PHE:HA	1:199:A:THR:HG23	13	0.18
(1,262)	1:161:A:VAL:HB	1:183:A:THR:HG21	18	0.18
(1,262)	1:161:A:VAL:HB	1:183:A:THR:HG22	18	0.18
(1,262)	1:161:A:VAL:HB	1:183:A:THR:HG23	18	0.18
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	20	0.18
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	20	0.18
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	5	0.18
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	5	0.18
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	6	0.18
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	6	0.18
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	7	0.18
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	7	0.18
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	11	0.18
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	11	0.18
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB1	2	0.18
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB2	2	0.18
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB3	2	0.18
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB1	2	0.18
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB2	2	0.18
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB3	2	0.18
(1,27)	1:219:A:GLU:HA	1:219:A:GLU:HG3	5	0.18
(1,1296)	1:228:A:ARG:H	1:228:A:ARG:HG2	10	0.17
(1,1296)	1:228:A:ARG:H	1:228:A:ARG:HG3	10	0.17
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE1	15	0.17
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE2	15	0.17
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE3	15	0.17
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE1	15	0.17
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE2	15	0.17
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE3	15	0.17
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE1	15	0.17
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE2	15	0.17
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE3	15	0.17
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE1	15	0.17
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE2	15	0.17
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE3	15	0.17
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE1	15	0.17
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE2	15	0.17
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE3	15	0.17
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE1	15	0.17
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE2	15	0.17
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE3	15	0.17
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG2	20	0.17
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG3	20	0.17
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE1	4	0.17
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE2	4	0.17
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE3	4	0.17
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE1	4	0.17
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE2	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE3	4	0.17
(1,1181)	1:196:A:GLU:HA	1:196:A:GLU:HG2	1	0.17
(1,1181)	1:196:A:GLU:HA	1:196:A:GLU:HG3	1	0.17
(1,1181)	1:196:A:GLU:HA	1:196:A:GLU:HG2	20	0.17
(1,1181)	1:196:A:GLU:HA	1:196:A:GLU:HG3	20	0.17
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG2	18	0.17
(1,991)	1:128:A:TYR:HE1	1:186:A:GLN:HG3	18	0.17
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG2	18	0.17
(1,991)	1:128:A:TYR:HE2	1:186:A:GLN:HG3	18	0.17
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE1	19	0.17
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE2	19	0.17
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	10	0.17
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	10	0.17
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	17	0.17
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	17	0.17
(1,865)	1:144:A:ASP:H	1:147:A:ASP:H	7	0.17
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	13	0.17
(1,705)	1:143:A:SER:H	1:147:A:ASP:H	2	0.17
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	14	0.17
(1,569)	1:228:A:ARG:H	1:228:A:ARG:HG2	12	0.17
(1,498)	1:141:A:PHE:HB3	1:143:A:SER:H	2	0.17
(1,365)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	19	0.17
(1,365)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	19	0.17
(1,365)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	19	0.17
(1,358)	1:139:A:ILE:HG21	1:212:A:GLN:HG2	19	0.17
(1,358)	1:139:A:ILE:HG21	1:212:A:GLN:HG3	19	0.17
(1,358)	1:139:A:ILE:HG22	1:212:A:GLN:HG2	19	0.17
(1,358)	1:139:A:ILE:HG22	1:212:A:GLN:HG3	19	0.17
(1,358)	1:139:A:ILE:HG23	1:212:A:GLN:HG2	19	0.17
(1,358)	1:139:A:ILE:HG23	1:212:A:GLN:HG3	19	0.17
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	11	0.17
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	11	0.17
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	11	0.17
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE1	4	0.17
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE2	4	0.17
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE3	4	0.17
(1,309)	1:202:A:ASP:HB2	1:206:A:MET:HE1	8	0.17
(1,309)	1:202:A:ASP:HB2	1:206:A:MET:HE2	8	0.17
(1,309)	1:202:A:ASP:HB2	1:206:A:MET:HE3	8	0.17
(1,268)	1:141:A:PHE:HB3	1:146:A:GLU:HB3	14	0.17
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG21	17	0.17
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG22	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	1:161:A:VAL:HA	1:183:A:THR:HG23	17	0.17
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE1	2	0.17
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE2	2	0.17
(1,204)	1:203:A:VAL:HG21	1:206:A:MET:HE3	2	0.17
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE1	2	0.17
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE2	2	0.17
(1,204)	1:203:A:VAL:HG22	1:206:A:MET:HE3	2	0.17
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE1	2	0.17
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE2	2	0.17
(1,204)	1:203:A:VAL:HG23	1:206:A:MET:HE3	2	0.17
(1,180)	1:208:A:ARG:HB2	1:209:A:MET:HA	6	0.17
(1,180)	1:208:A:ARG:HB3	1:209:A:MET:HA	6	0.17
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	11	0.17
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	11	0.17
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	11	0.17
(1,168)	1:216:A:THR:HA	1:219:A:GLU:HB3	1	0.17
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	1	0.17
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	1	0.17
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	2	0.17
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	2	0.17
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	8	0.17
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	8	0.17
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	14	0.17
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	14	0.17
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	15	0.17
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	15	0.17
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	16	0.17
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	16	0.17
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB1	4	0.17
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB2	4	0.17
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB3	4	0.17
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB1	4	0.17
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB2	4	0.17
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB3	4	0.17
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB1	8	0.17
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB2	8	0.17
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB3	8	0.17
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB1	8	0.17
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB2	8	0.17
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB3	8	0.17
(1,140)	1:209:A:MET:HA	1:209:A:MET:HG2	16	0.17
(1,138)	1:207:A:GLU:HA	1:207:A:GLU:HG3	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	10	0.17
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	19	0.17
(1,1314)	1:176:A:VAL:HG11	1:215:A:ILE:HG12	10	0.16
(1,1314)	1:176:A:VAL:HG11	1:215:A:ILE:HG13	10	0.16
(1,1314)	1:176:A:VAL:HG12	1:215:A:ILE:HG12	10	0.16
(1,1314)	1:176:A:VAL:HG12	1:215:A:ILE:HG13	10	0.16
(1,1314)	1:176:A:VAL:HG13	1:215:A:ILE:HG12	10	0.16
(1,1314)	1:176:A:VAL:HG13	1:215:A:ILE:HG13	10	0.16
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	13	0.16
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	13	0.16
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	13	0.16
(1,1267)	1:217:A:GLN:HA	1:220:A:ARG:HB2	13	0.16
(1,1267)	1:217:A:GLN:HA	1:220:A:ARG:HB3	13	0.16
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE1	11	0.16
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE2	11	0.16
(1,1252)	1:210:A:VAL:HG11	1:213:A:MET:HE3	11	0.16
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE1	11	0.16
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE2	11	0.16
(1,1252)	1:210:A:VAL:HG12	1:213:A:MET:HE3	11	0.16
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE1	11	0.16
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE2	11	0.16
(1,1252)	1:210:A:VAL:HG13	1:213:A:MET:HE3	11	0.16
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE1	11	0.16
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE2	11	0.16
(1,1252)	1:210:A:VAL:HG21	1:213:A:MET:HE3	11	0.16
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE1	11	0.16
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE2	11	0.16
(1,1252)	1:210:A:VAL:HG22	1:213:A:MET:HE3	11	0.16
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE1	11	0.16
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE2	11	0.16
(1,1252)	1:210:A:VAL:HG23	1:213:A:MET:HE3	11	0.16
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG2	9	0.16
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG3	9	0.16
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG2	10	0.16
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG3	10	0.16
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	1	0.16
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	1	0.16
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	6	0.16
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	6	0.16
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	20	0.16
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	20	0.16
(1,1196)	1:200:A:GLU:H	1:200:A:GLU:HG2	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1196)	1:200:A:GLU:H	1:200:A:GLU:HG3	14	0.16
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE1	5	0.16
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE2	5	0.16
(1,1193)	1:198:A:PHE:HB2	1:206:A:MET:HE3	5	0.16
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE1	5	0.16
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE2	5	0.16
(1,1193)	1:198:A:PHE:HB3	1:206:A:MET:HE3	5	0.16
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG11	19	0.16
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG12	19	0.16
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG13	19	0.16
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG21	19	0.16
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG22	19	0.16
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG23	19	0.16
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG11	19	0.16
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG12	19	0.16
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG13	19	0.16
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG21	19	0.16
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG22	19	0.16
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG23	19	0.16
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG11	19	0.16
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG12	19	0.16
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG13	19	0.16
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG21	19	0.16
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG22	19	0.16
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG23	19	0.16
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG2	5	0.16
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG3	5	0.16
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG2	5	0.16
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG3	5	0.16
(1,971)	1:154:A:MET:HA	1:157:A:TYR:HE1	1	0.16
(1,971)	1:154:A:MET:HA	1:157:A:TYR:HE2	1	0.16
(1,951)	1:129:A:MET:HB2	1:163:A:TYR:HE1	3	0.16
(1,951)	1:129:A:MET:HB2	1:163:A:TYR:HE2	3	0.16
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	4	0.16
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	4	0.16
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	8	0.16
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	8	0.16
(1,893)	1:210:A:VAL:HA	1:214:A:CYS:H	6	0.16
(1,893)	1:210:A:VAL:HA	1:214:A:CYS:H	12	0.16
(1,865)	1:144:A:ASP:H	1:147:A:ASP:H	8	0.16
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	6	0.16
(1,813)	1:176:A:VAL:HB	1:177:A:HIS:H	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:161:A:VAL:HG11	1:214:A:CYS:H	14	0.16
(1,763)	1:161:A:VAL:HG12	1:214:A:CYS:H	14	0.16
(1,763)	1:161:A:VAL:HG13	1:214:A:CYS:H	14	0.16
(1,663)	1:191:A:THR:H	1:191:A:THR:HG21	6	0.16
(1,663)	1:191:A:THR:H	1:191:A:THR:HG22	6	0.16
(1,663)	1:191:A:THR:H	1:191:A:THR:HG23	6	0.16
(1,498)	1:141:A:PHE:HB3	1:143:A:SER:H	10	0.16
(1,498)	1:141:A:PHE:HB3	1:143:A:SER:H	19	0.16
(1,498)	1:141:A:PHE:HB3	1:143:A:SER:H	20	0.16
(1,432)	1:228:A:ARG:H	1:229:A:GLY:H	4	0.16
(1,432)	1:228:A:ARG:H	1:229:A:GLY:H	16	0.16
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	14	0.16
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	14	0.16
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	14	0.16
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE1	12	0.16
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE2	12	0.16
(1,320)	1:209:A:MET:HA	1:213:A:MET:HE3	12	0.16
(1,262)	1:161:A:VAL:HB	1:183:A:THR:HG21	7	0.16
(1,262)	1:161:A:VAL:HB	1:183:A:THR:HG22	7	0.16
(1,262)	1:161:A:VAL:HB	1:183:A:THR:HG23	7	0.16
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG21	12	0.16
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG22	12	0.16
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG23	12	0.16
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG21	12	0.16
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG22	12	0.16
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG23	12	0.16
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE1	3	0.16
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE2	3	0.16
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE3	3	0.16
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD2	4	0.16
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD3	4	0.16
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD2	4	0.16
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD3	4	0.16
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD2	4	0.16
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD3	4	0.16
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD2	15	0.16
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD3	15	0.16
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD2	15	0.16
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD3	15	0.16
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD2	15	0.16
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD3	15	0.16
(1,209)	1:201:A:THR:HG21	1:205:A:MET:HG3	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:201:A:THR:HG22	1:205:A:MET:HG3	16	0.16
(1,209)	1:201:A:THR:HG23	1:205:A:MET:HG3	16	0.16
(1,180)	1:208:A:ARG:HB2	1:209:A:MET:HA	9	0.16
(1,180)	1:208:A:ARG:HB3	1:209:A:MET:HA	9	0.16
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	4	0.16
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	4	0.16
(1,157)	1:132:A:SER:HA	1:133:A:ALA:HB1	12	0.16
(1,157)	1:132:A:SER:HA	1:133:A:ALA:HB2	12	0.16
(1,157)	1:132:A:SER:HA	1:133:A:ALA:HB3	12	0.16
(1,157)	1:132:A:SER:HA	1:133:A:ALA:HB1	17	0.16
(1,157)	1:132:A:SER:HA	1:133:A:ALA:HB2	17	0.16
(1,157)	1:132:A:SER:HA	1:133:A:ALA:HB3	17	0.16
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	7	0.16
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	14	0.16
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	16	0.16
(1,27)	1:219:A:GLU:HA	1:219:A:GLU:HG3	1	0.16
(1,27)	1:219:A:GLU:HA	1:219:A:GLU:HG3	11	0.16
(1,27)	1:219:A:GLU:HA	1:219:A:GLU:HG3	12	0.16
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	1	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	1	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	5	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	5	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	6	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	6	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	8	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	8	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	12	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	12	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	13	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	13	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	15	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	15	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	16	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	16	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	17	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	17	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	18	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	18	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	19	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	19	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	20	0.15
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1269)	1:217:A:GLN:HA	1:220:A:ARG:HD2	7	0.15
(1,1269)	1:217:A:GLN:HA	1:220:A:ARG:HD3	7	0.15
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG2	2	0.15
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG3	2	0.15
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	4	0.15
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	4	0.15
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	12	0.15
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	12	0.15
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	17	0.15
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	17	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG11	17	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG12	17	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG13	17	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG21	17	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG22	17	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG23	17	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG11	17	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG12	17	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG13	17	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG21	17	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG22	17	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG23	17	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG11	19	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG12	19	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG13	19	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG21	19	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG22	19	0.15
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG23	19	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG11	19	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG12	19	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG13	19	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG21	19	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG22	19	0.15
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG23	19	0.15
(1,1181)	1:196:A:GLU:HA	1:196:A:GLU:HG2	15	0.15
(1,1181)	1:196:A:GLU:HA	1:196:A:GLU:HG3	15	0.15
(1,1126)	1:176:A:VAL:HG11	1:179:A:CYS:HB2	12	0.15
(1,1126)	1:176:A:VAL:HG11	1:179:A:CYS:HB3	12	0.15
(1,1126)	1:176:A:VAL:HG12	1:179:A:CYS:HB2	12	0.15
(1,1126)	1:176:A:VAL:HG12	1:179:A:CYS:HB3	12	0.15
(1,1126)	1:176:A:VAL:HG13	1:179:A:CYS:HB2	12	0.15
(1,1126)	1:176:A:VAL:HG13	1:179:A:CYS:HB3	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1121)	1:165:A:PRO:HB2	1:166:A:MET:H	16	0.15
(1,1121)	1:165:A:PRO:HB3	1:166:A:MET:H	16	0.15
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG11	12	0.15
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG12	12	0.15
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG13	12	0.15
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG21	12	0.15
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG22	12	0.15
(1,1110)	1:158:A:PRO:HG2	1:210:A:VAL:HG23	12	0.15
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG11	12	0.15
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG12	12	0.15
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG13	12	0.15
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG21	12	0.15
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG22	12	0.15
(1,1110)	1:158:A:PRO:HG3	1:210:A:VAL:HG23	12	0.15
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE1	17	0.15
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE2	17	0.15
(1,973)	1:198:A:PHE:HD1	1:206:A:MET:HE3	17	0.15
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE1	17	0.15
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE2	17	0.15
(1,973)	1:198:A:PHE:HD2	1:206:A:MET:HE3	17	0.15
(1,944)	1:139:A:ILE:HD11	1:141:A:PHE:HZ	15	0.15
(1,944)	1:139:A:ILE:HD12	1:141:A:PHE:HZ	15	0.15
(1,944)	1:139:A:ILE:HD13	1:141:A:PHE:HZ	15	0.15
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE1	1	0.15
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE2	1	0.15
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE1	8	0.15
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE2	8	0.15
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	6	0.15
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	6	0.15
(1,913)	1:223:A:GLN:HB2	1:225:A:TYR:H	12	0.15
(1,913)	1:223:A:GLN:HB3	1:225:A:TYR:H	12	0.15
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	4	0.15
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	12	0.15
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	17	0.15
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	15	0.15
(1,763)	1:161:A:VAL:HG11	1:214:A:CYS:H	10	0.15
(1,763)	1:161:A:VAL:HG12	1:214:A:CYS:H	10	0.15
(1,763)	1:161:A:VAL:HG13	1:214:A:CYS:H	10	0.15
(1,718)	1:158:A:PRO:HB2	1:159:A:ASN:H	19	0.15
(1,685)	1:138:A:ILE:H	1:138:A:ILE:HG13	6	0.15
(1,674)	1:122:A:VAL:H	1:122:A:VAL:HB	13	0.15
(1,651)	1:196:A:GLU:H	1:196:A:GLU:HB2	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,651)	1:196:A:GLU:H	1:196:A:GLU:HB3	19	0.15
(1,649)	1:196:A:GLU:HG3	1:197:A:ASN:H	12	0.15
(1,463)	1:125:A:LEU:H	1:125:A:LEU:HB3	19	0.15
(1,430)	1:228:A:ARG:HA	1:229:A:GLY:H	1	0.15
(1,406)	1:176:A:VAL:H	1:176:A:VAL:HB	3	0.15
(1,394)	1:152:A:GLU:H	1:152:A:GLU:HG3	1	0.15
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB2	16	0.15
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB3	16	0.15
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	11	0.15
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	11	0.15
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	11	0.15
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	1	0.15
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	1	0.15
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	1	0.15
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE1	6	0.15
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE2	6	0.15
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE3	6	0.15
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE1	19	0.15
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE2	19	0.15
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE3	19	0.15
(1,238)	1:183:A:THR:HG21	1:184:A:ILE:HA	11	0.15
(1,238)	1:183:A:THR:HG22	1:184:A:ILE:HA	11	0.15
(1,238)	1:183:A:THR:HG23	1:184:A:ILE:HA	11	0.15
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG21	8	0.15
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG22	8	0.15
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG23	8	0.15
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG21	8	0.15
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG22	8	0.15
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG23	8	0.15
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG21	19	0.15
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG22	19	0.15
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG23	19	0.15
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG21	19	0.15
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG22	19	0.15
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG23	19	0.15
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD2	19	0.15
(1,210)	1:201:A:THR:HG21	1:204:A:LYS:HD3	19	0.15
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD2	19	0.15
(1,210)	1:201:A:THR:HG22	1:204:A:LYS:HD3	19	0.15
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD2	19	0.15
(1,210)	1:201:A:THR:HG23	1:204:A:LYS:HD3	19	0.15
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	7	0.15
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	7	0.15
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	9	0.15
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	9	0.15
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	10	0.15
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	10	0.15
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	13	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	2	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	2	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	2	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	3	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	3	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	3	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	4	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	4	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	4	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	7	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	7	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	7	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	8	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	8	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	8	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	9	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	9	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	9	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	10	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	10	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	10	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	12	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	12	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	12	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	13	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	13	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	13	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	14	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	14	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	14	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	17	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	17	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	17	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	18	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	18	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	20	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	20	0.15
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	20	0.15
(1,27)	1:219:A:GLU:HA	1:219:A:GLU:HG3	2	0.15
(1,27)	1:219:A:GLU:HA	1:219:A:GLU:HG3	3	0.15
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE1	4	0.14
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE2	4	0.14
(1,1307)	1:159:A:ASN:H	1:213:A:MET:HE3	4	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	2	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	2	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	3	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	3	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	4	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	4	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	7	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	7	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	9	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	9	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	10	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	10	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	11	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	11	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG2	14	0.14
(1,1285)	1:223:A:GLN:HA	1:223:A:GLN:HG3	14	0.14
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG2	15	0.14
(1,1235)	1:208:A:ARG:H	1:208:A:ARG:HG3	15	0.14
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	5	0.14
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	5	0.14
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	13	0.14
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	13	0.14
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG11	4	0.14
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG12	4	0.14
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG13	4	0.14
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG21	4	0.14
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG22	4	0.14
(1,1228)	1:206:A:MET:HB2	1:210:A:VAL:HG23	4	0.14
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG11	4	0.14
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG12	4	0.14
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG13	4	0.14
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG21	4	0.14
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG22	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1228)	1:206:A:MET:HB3	1:210:A:VAL:HG23	4	0.14
(1,1181)	1:196:A:GLU:HA	1:196:A:GLU:HG2	19	0.14
(1,1181)	1:196:A:GLU:HA	1:196:A:GLU:HG3	19	0.14
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB2	15	0.14
(1,1166)	1:184:A:ILE:HG12	1:206:A:MET:HB3	15	0.14
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB2	15	0.14
(1,1166)	1:184:A:ILE:HG13	1:206:A:MET:HB3	15	0.14
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE21	3	0.14
(1,1159)	1:182:A:ILE:HG21	1:186:A:GLN:HE22	3	0.14
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE21	3	0.14
(1,1159)	1:182:A:ILE:HG22	1:186:A:GLN:HE22	3	0.14
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE21	3	0.14
(1,1159)	1:182:A:ILE:HG23	1:186:A:GLN:HE22	3	0.14
(1,1105)	1:156:A:ARG:HD2	1:157:A:TYR:H	4	0.14
(1,1105)	1:156:A:ARG:HD3	1:157:A:TYR:H	4	0.14
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG2	1	0.14
(1,1039)	1:139:A:ILE:HG12	1:209:A:MET:HG3	1	0.14
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG2	1	0.14
(1,1039)	1:139:A:ILE:HG13	1:209:A:MET:HG3	1	0.14
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	7	0.14
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	7	0.14
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	7	0.14
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	7	0.14
(1,865)	1:144:A:ASP:H	1:147:A:ASP:H	20	0.14
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	8	0.14
(1,819)	1:176:A:VAL:H	1:214:A:CYS:HB3	8	0.14
(1,819)	1:176:A:VAL:H	1:214:A:CYS:HB3	11	0.14
(1,819)	1:176:A:VAL:H	1:214:A:CYS:HB3	18	0.14
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	3	0.14
(1,649)	1:196:A:GLU:HG3	1:197:A:ASN:H	14	0.14
(1,607)	1:212:A:GLN:H	1:212:A:GLN:HG2	17	0.14
(1,607)	1:212:A:GLN:H	1:212:A:GLN:HG3	17	0.14
(1,567)	1:228:A:ARG:HG2	1:229:A:GLY:H	6	0.14
(1,498)	1:141:A:PHE:HB3	1:143:A:SER:H	16	0.14
(1,425)	1:165:A:PRO:HB3	1:166:A:MET:H	16	0.14
(1,406)	1:176:A:VAL:H	1:176:A:VAL:HB	10	0.14
(1,406)	1:176:A:VAL:H	1:176:A:VAL:HB	20	0.14
(1,365)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	2	0.14
(1,365)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	2	0.14
(1,365)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	2	0.14
(1,362)	1:176:A:VAL:HG21	1:215:A:ILE:HA	6	0.14
(1,362)	1:176:A:VAL:HG22	1:215:A:ILE:HA	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,362)	1:176:A:VAL:HG23	1:215:A:ILE:HA	6	0.14
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	20	0.14
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	20	0.14
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	20	0.14
(1,297)	1:129:A:MET:HB3	1:129:A:MET:HE1	9	0.14
(1,297)	1:129:A:MET:HB3	1:129:A:MET:HE2	9	0.14
(1,297)	1:129:A:MET:HB3	1:129:A:MET:HE3	9	0.14
(1,276)	1:138:A:ILE:HD11	1:151:A:ARG:HG3	3	0.14
(1,276)	1:138:A:ILE:HD12	1:151:A:ARG:HG3	3	0.14
(1,276)	1:138:A:ILE:HD13	1:151:A:ARG:HG3	3	0.14
(1,270)	1:139:A:ILE:HD11	1:208:A:ARG:HB2	10	0.14
(1,270)	1:139:A:ILE:HD11	1:208:A:ARG:HB3	10	0.14
(1,270)	1:139:A:ILE:HD12	1:208:A:ARG:HB2	10	0.14
(1,270)	1:139:A:ILE:HD12	1:208:A:ARG:HB3	10	0.14
(1,270)	1:139:A:ILE:HD13	1:208:A:ARG:HB2	10	0.14
(1,270)	1:139:A:ILE:HD13	1:208:A:ARG:HB3	10	0.14
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	19	0.14
(1,262)	1:161:A:VAL:HB	1:183:A:THR:HG21	4	0.14
(1,262)	1:161:A:VAL:HB	1:183:A:THR:HG22	4	0.14
(1,262)	1:161:A:VAL:HB	1:183:A:THR:HG23	4	0.14
(1,238)	1:183:A:THR:HG21	1:184:A:ILE:HA	18	0.14
(1,238)	1:183:A:THR:HG22	1:184:A:ILE:HA	18	0.14
(1,238)	1:183:A:THR:HG23	1:184:A:ILE:HA	18	0.14
(1,180)	1:208:A:ARG:HB2	1:209:A:MET:HA	12	0.14
(1,180)	1:208:A:ARG:HB3	1:209:A:MET:HA	12	0.14
(1,178)	1:183:A:THR:HG21	1:210:A:VAL:HG21	9	0.14
(1,178)	1:183:A:THR:HG21	1:210:A:VAL:HG22	9	0.14
(1,178)	1:183:A:THR:HG21	1:210:A:VAL:HG23	9	0.14
(1,178)	1:183:A:THR:HG22	1:210:A:VAL:HG21	9	0.14
(1,178)	1:183:A:THR:HG22	1:210:A:VAL:HG22	9	0.14
(1,178)	1:183:A:THR:HG22	1:210:A:VAL:HG23	9	0.14
(1,178)	1:183:A:THR:HG23	1:210:A:VAL:HG21	9	0.14
(1,178)	1:183:A:THR:HG23	1:210:A:VAL:HG22	9	0.14
(1,178)	1:183:A:THR:HG23	1:210:A:VAL:HG23	9	0.14
(1,175)	1:220:A:ARG:HA	1:220:A:ARG:HG2	13	0.14
(1,168)	1:216:A:THR:HA	1:219:A:GLU:HB3	6	0.14
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB1	7	0.14
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB2	7	0.14
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB3	7	0.14
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB1	7	0.14
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB2	7	0.14
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB3	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,132)	1:208:A:ARG:HA	1:208:A:ARG:HG2	2	0.14
(1,132)	1:208:A:ARG:HA	1:208:A:ARG:HG2	15	0.14
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	1	0.14
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	2	0.14
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	11	0.14
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	18	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	6	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	6	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	6	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	11	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	11	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	11	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	15	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	15	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	15	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	16	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	16	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	16	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	19	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	19	0.14
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	19	0.14
(1,27)	1:219:A:GLU:HA	1:219:A:GLU:HG3	8	0.14
(1,27)	1:219:A:GLU:HA	1:219:A:GLU:HG3	19	0.14
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB2	16	0.13
(1,1292)	1:226:A:TYR:HB2	1:227:A:GLN:HB3	16	0.13
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB2	16	0.13
(1,1292)	1:226:A:TYR:HB3	1:227:A:GLN:HB3	16	0.13
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	3	0.13
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	3	0.13
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	9	0.13
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	9	0.13
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	10	0.13
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	10	0.13
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	18	0.13
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	18	0.13
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE1	6	0.13
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE2	6	0.13
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE3	6	0.13
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE1	6	0.13
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE2	6	0.13
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE3	6	0.13
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE1	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE2	18	0.13
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE3	18	0.13
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE1	18	0.13
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE2	18	0.13
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE3	18	0.13
(1,1195)	1:199:A:THR:HG21	1:202:A:ASP:HB2	18	0.13
(1,1195)	1:199:A:THR:HG21	1:202:A:ASP:HB3	18	0.13
(1,1195)	1:199:A:THR:HG22	1:202:A:ASP:HB2	18	0.13
(1,1195)	1:199:A:THR:HG22	1:202:A:ASP:HB3	18	0.13
(1,1195)	1:199:A:THR:HG23	1:202:A:ASP:HB2	18	0.13
(1,1195)	1:199:A:THR:HG23	1:202:A:ASP:HB3	18	0.13
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG11	17	0.13
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG12	17	0.13
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG13	17	0.13
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG21	17	0.13
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG22	17	0.13
(1,1170)	1:184:A:ILE:HD11	1:210:A:VAL:HG23	17	0.13
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG11	17	0.13
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG12	17	0.13
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG13	17	0.13
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG21	17	0.13
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG22	17	0.13
(1,1170)	1:184:A:ILE:HD12	1:210:A:VAL:HG23	17	0.13
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG11	17	0.13
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG12	17	0.13
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG13	17	0.13
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG21	17	0.13
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG22	17	0.13
(1,1170)	1:184:A:ILE:HD13	1:210:A:VAL:HG23	17	0.13
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG12	1	0.13
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG13	1	0.13
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG12	11	0.13
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG13	11	0.13
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG12	19	0.13
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG13	19	0.13
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG2	3	0.13
(1,990)	1:128:A:TYR:HD1	1:186:A:GLN:HG3	3	0.13
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG2	3	0.13
(1,990)	1:128:A:TYR:HD2	1:186:A:GLN:HG3	3	0.13
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE1	5	0.13
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE2	5	0.13
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE1	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE2	17	0.13
(1,938)	1:128:A:TYR:HE1	1:182:A:ILE:HB	7	0.13
(1,938)	1:128:A:TYR:HE2	1:182:A:ILE:HB	7	0.13
(1,938)	1:128:A:TYR:HE1	1:182:A:ILE:HB	16	0.13
(1,938)	1:128:A:TYR:HE2	1:182:A:ILE:HB	16	0.13
(1,893)	1:210:A:VAL:HA	1:214:A:CYS:H	9	0.13
(1,865)	1:144:A:ASP:H	1:147:A:ASP:H	13	0.13
(1,865)	1:144:A:ASP:H	1:147:A:ASP:H	15	0.13
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	2	0.13
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	10	0.13
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	16	0.13
(1,789)	1:188:A:THR:H	1:191:A:THR:HB	19	0.13
(1,772)	1:228:A:ARG:HB2	1:230:A:SER:H	12	0.13
(1,763)	1:161:A:VAL:HG11	1:214:A:CYS:H	16	0.13
(1,763)	1:161:A:VAL:HG12	1:214:A:CYS:H	16	0.13
(1,763)	1:161:A:VAL:HG13	1:214:A:CYS:H	16	0.13
(1,705)	1:143:A:SER:H	1:147:A:ASP:H	19	0.13
(1,649)	1:196:A:GLU:HG3	1:197:A:ASN:H	5	0.13
(1,617)	1:207:A:GLU:H	1:207:A:GLU:HG3	20	0.13
(1,498)	1:141:A:PHE:HB3	1:143:A:SER:H	17	0.13
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE1	11	0.13
(1,469)	1:128:A:TYR:H	1:128:A:TYR:HE2	11	0.13
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD11	12	0.13
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD12	12	0.13
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD13	12	0.13
(1,366)	1:184:A:ILE:HD11	1:207:A:GLU:HG3	20	0.13
(1,366)	1:184:A:ILE:HD12	1:207:A:GLU:HG3	20	0.13
(1,366)	1:184:A:ILE:HD13	1:207:A:GLU:HG3	20	0.13
(1,365)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	10	0.13
(1,365)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	10	0.13
(1,365)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	10	0.13
(1,358)	1:139:A:ILE:HG21	1:212:A:GLN:HG2	18	0.13
(1,358)	1:139:A:ILE:HG21	1:212:A:GLN:HG3	18	0.13
(1,358)	1:139:A:ILE:HG22	1:212:A:GLN:HG2	18	0.13
(1,358)	1:139:A:ILE:HG22	1:212:A:GLN:HG3	18	0.13
(1,358)	1:139:A:ILE:HG23	1:212:A:GLN:HG2	18	0.13
(1,358)	1:139:A:ILE:HG23	1:212:A:GLN:HG3	18	0.13
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE1	9	0.13
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE2	9	0.13
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE3	9	0.13
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE1	20	0.13
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE2	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,331)	1:150:A:TYR:HA	1:205:A:MET:HE3	20	0.13
(1,329)	1:149:A:TYR:HA	1:205:A:MET:HE1	3	0.13
(1,329)	1:149:A:TYR:HA	1:205:A:MET:HE2	3	0.13
(1,329)	1:149:A:TYR:HA	1:205:A:MET:HE3	3	0.13
(1,309)	1:202:A:ASP:HB2	1:206:A:MET:HE1	11	0.13
(1,309)	1:202:A:ASP:HB2	1:206:A:MET:HE2	11	0.13
(1,309)	1:202:A:ASP:HB2	1:206:A:MET:HE3	11	0.13
(1,297)	1:129:A:MET:HB3	1:129:A:MET:HE1	20	0.13
(1,297)	1:129:A:MET:HB3	1:129:A:MET:HE2	20	0.13
(1,297)	1:129:A:MET:HB3	1:129:A:MET:HE3	20	0.13
(1,264)	1:149:A:TYR:HA	1:152:A:GLU:HB2	3	0.13
(1,264)	1:149:A:TYR:HA	1:152:A:GLU:HB3	3	0.13
(1,249)	1:179:A:CYS:HA	1:182:A:ILE:HG21	6	0.13
(1,249)	1:179:A:CYS:HA	1:182:A:ILE:HG22	6	0.13
(1,249)	1:179:A:CYS:HA	1:182:A:ILE:HG23	6	0.13
(1,212)	1:200:A:GLU:HA	1:203:A:VAL:HG21	13	0.13
(1,212)	1:200:A:GLU:HA	1:203:A:VAL:HG22	13	0.13
(1,212)	1:200:A:GLU:HA	1:203:A:VAL:HG23	13	0.13
(1,150)	1:133:A:ALA:HB1	1:159:A:ASN:HB2	8	0.13
(1,150)	1:133:A:ALA:HB2	1:159:A:ASN:HB2	8	0.13
(1,150)	1:133:A:ALA:HB3	1:159:A:ASN:HB2	8	0.13
(1,150)	1:133:A:ALA:HB1	1:159:A:ASN:HB2	11	0.13
(1,150)	1:133:A:ALA:HB2	1:159:A:ASN:HB2	11	0.13
(1,150)	1:133:A:ALA:HB3	1:159:A:ASN:HB2	11	0.13
(1,132)	1:208:A:ARG:HA	1:208:A:ARG:HG2	10	0.13
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	8	0.13
(1,103)	1:220:A:ARG:HA	1:220:A:ARG:HG3	13	0.13
(1,95)	1:146:A:GLU:HA	1:146:A:GLU:HG2	2	0.13
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	1	0.13
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	1	0.13
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	1	0.13
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD11	5	0.13
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD12	5	0.13
(1,68)	1:182:A:ILE:HB	1:182:A:ILE:HD13	5	0.13
(1,27)	1:219:A:GLU:HA	1:219:A:GLU:HG3	10	0.13
(1,21)	1:200:A:GLU:HA	1:200:A:GLU:HB3	14	0.13
(1,1315)	1:188:A:THR:HG21	1:203:A:VAL:HG11	11	0.12
(1,1315)	1:188:A:THR:HG21	1:203:A:VAL:HG12	11	0.12
(1,1315)	1:188:A:THR:HG21	1:203:A:VAL:HG13	11	0.12
(1,1315)	1:188:A:THR:HG22	1:203:A:VAL:HG11	11	0.12
(1,1315)	1:188:A:THR:HG22	1:203:A:VAL:HG12	11	0.12
(1,1315)	1:188:A:THR:HG22	1:203:A:VAL:HG13	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1315)	1:188:A:THR:HG23	1:203:A:VAL:HG11	11	0.12
(1,1315)	1:188:A:THR:HG23	1:203:A:VAL:HG12	11	0.12
(1,1315)	1:188:A:THR:HG23	1:203:A:VAL:HG13	11	0.12
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB2	18	0.12
(1,1299)	1:134:A:MET:H	1:159:A:ASN:HB3	18	0.12
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	2	0.12
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	2	0.12
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG2	19	0.12
(1,1229)	1:207:A:GLU:H	1:207:A:GLU:HG3	19	0.12
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE1	17	0.12
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE2	17	0.12
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE3	17	0.12
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE1	17	0.12
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE2	17	0.12
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE3	17	0.12
(1,1186)	1:197:A:ASN:HB2	1:198:A:PHE:H	20	0.12
(1,1186)	1:197:A:ASN:HB3	1:198:A:PHE:H	20	0.12
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB2	11	0.12
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB3	11	0.12
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB2	16	0.12
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB3	16	0.12
(1,1121)	1:165:A:PRO:HB2	1:166:A:MET:H	4	0.12
(1,1121)	1:165:A:PRO:HB3	1:166:A:MET:H	4	0.12
(1,1088)	1:151:A:ARG:HD2	1:154:A:MET:HE1	10	0.12
(1,1088)	1:151:A:ARG:HD2	1:154:A:MET:HE2	10	0.12
(1,1088)	1:151:A:ARG:HD2	1:154:A:MET:HE3	10	0.12
(1,1088)	1:151:A:ARG:HD3	1:154:A:MET:HE1	10	0.12
(1,1088)	1:151:A:ARG:HD3	1:154:A:MET:HE2	10	0.12
(1,1088)	1:151:A:ARG:HD3	1:154:A:MET:HE3	10	0.12
(1,1055)	1:143:A:SER:HB2	1:144:A:ASP:H	14	0.12
(1,1055)	1:143:A:SER:HB3	1:144:A:ASP:H	14	0.12
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG12	2	0.12
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG13	2	0.12
(1,1011)	1:133:A:ALA:H	1:160:A:GLN:HE21	10	0.12
(1,1011)	1:133:A:ALA:H	1:160:A:GLN:HE22	10	0.12
(1,944)	1:139:A:ILE:HD11	1:141:A:PHE:HZ	6	0.12
(1,944)	1:139:A:ILE:HD12	1:141:A:PHE:HZ	6	0.12
(1,944)	1:139:A:ILE:HD13	1:141:A:PHE:HZ	6	0.12
(1,944)	1:139:A:ILE:HD11	1:141:A:PHE:HZ	17	0.12
(1,944)	1:139:A:ILE:HD12	1:141:A:PHE:HZ	17	0.12
(1,944)	1:139:A:ILE:HD13	1:141:A:PHE:HZ	17	0.12
(1,942)	1:139:A:ILE:HG21	1:141:A:PHE:HZ	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,942)	1:139:A:ILE:HG22	1:141:A:PHE:HZ	16	0.12
(1,942)	1:139:A:ILE:HG23	1:141:A:PHE:HZ	16	0.12
(1,893)	1:210:A:VAL:HA	1:214:A:CYS:H	11	0.12
(1,865)	1:144:A:ASP:H	1:147:A:ASP:H	12	0.12
(1,856)	1:125:A:LEU:HD21	1:126:A:GLY:H	20	0.12
(1,856)	1:125:A:LEU:HD22	1:126:A:GLY:H	20	0.12
(1,856)	1:125:A:LEU:HD23	1:126:A:GLY:H	20	0.12
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	7	0.12
(1,842)	1:196:A:GLU:HG2	1:197:A:ASN:H	20	0.12
(1,763)	1:161:A:VAL:HG11	1:214:A:CYS:H	8	0.12
(1,763)	1:161:A:VAL:HG12	1:214:A:CYS:H	8	0.12
(1,763)	1:161:A:VAL:HG13	1:214:A:CYS:H	8	0.12
(1,737)	1:191:A:THR:HG21	1:192:A:THR:H	20	0.12
(1,737)	1:191:A:THR:HG22	1:192:A:THR:H	20	0.12
(1,737)	1:191:A:THR:HG23	1:192:A:THR:H	20	0.12
(1,667)	1:188:A:THR:HG21	1:189:A:VAL:H	19	0.12
(1,667)	1:188:A:THR:HG22	1:189:A:VAL:H	19	0.12
(1,667)	1:188:A:THR:HG23	1:189:A:VAL:H	19	0.12
(1,498)	1:141:A:PHE:HB3	1:143:A:SER:H	8	0.12
(1,394)	1:152:A:GLU:H	1:152:A:GLU:HG3	8	0.12
(1,370)	1:212:A:GLN:HA	1:215:A:ILE:HD11	16	0.12
(1,370)	1:212:A:GLN:HA	1:215:A:ILE:HD12	16	0.12
(1,370)	1:212:A:GLN:HA	1:215:A:ILE:HD13	16	0.12
(1,365)	1:203:A:VAL:HG11	1:207:A:GLU:HG3	20	0.12
(1,365)	1:203:A:VAL:HG12	1:207:A:GLU:HG3	20	0.12
(1,365)	1:203:A:VAL:HG13	1:207:A:GLU:HG3	20	0.12
(1,296)	1:176:A:VAL:HG11	1:214:A:CYS:HB2	3	0.12
(1,296)	1:176:A:VAL:HG12	1:214:A:CYS:HB2	3	0.12
(1,296)	1:176:A:VAL:HG13	1:214:A:CYS:HB2	3	0.12
(1,288)	1:133:A:ALA:HA	1:161:A:VAL:HG11	20	0.12
(1,288)	1:133:A:ALA:HA	1:161:A:VAL:HG12	20	0.12
(1,288)	1:133:A:ALA:HA	1:161:A:VAL:HG13	20	0.12
(1,249)	1:179:A:CYS:HA	1:182:A:ILE:HG21	17	0.12
(1,249)	1:179:A:CYS:HA	1:182:A:ILE:HG22	17	0.12
(1,249)	1:179:A:CYS:HA	1:182:A:ILE:HG23	17	0.12
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE1	5	0.12
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE2	5	0.12
(1,213)	1:198:A:PHE:HB3	1:206:A:MET:HE3	5	0.12
(1,178)	1:183:A:THR:HG21	1:210:A:VAL:HG21	6	0.12
(1,178)	1:183:A:THR:HG21	1:210:A:VAL:HG22	6	0.12
(1,178)	1:183:A:THR:HG21	1:210:A:VAL:HG23	6	0.12
(1,178)	1:183:A:THR:HG22	1:210:A:VAL:HG21	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:183:A:THR:HG22	1:210:A:VAL:HG22	6	0.12
(1,178)	1:183:A:THR:HG22	1:210:A:VAL:HG23	6	0.12
(1,178)	1:183:A:THR:HG23	1:210:A:VAL:HG21	6	0.12
(1,178)	1:183:A:THR:HG23	1:210:A:VAL:HG22	6	0.12
(1,178)	1:183:A:THR:HG23	1:210:A:VAL:HG23	6	0.12
(1,178)	1:183:A:THR:HG21	1:210:A:VAL:HG21	12	0.12
(1,178)	1:183:A:THR:HG21	1:210:A:VAL:HG22	12	0.12
(1,178)	1:183:A:THR:HG21	1:210:A:VAL:HG23	12	0.12
(1,178)	1:183:A:THR:HG22	1:210:A:VAL:HG21	12	0.12
(1,178)	1:183:A:THR:HG22	1:210:A:VAL:HG22	12	0.12
(1,178)	1:183:A:THR:HG22	1:210:A:VAL:HG23	12	0.12
(1,178)	1:183:A:THR:HG23	1:210:A:VAL:HG21	12	0.12
(1,178)	1:183:A:THR:HG23	1:210:A:VAL:HG22	12	0.12
(1,178)	1:183:A:THR:HG23	1:210:A:VAL:HG23	12	0.12
(1,168)	1:216:A:THR:HA	1:219:A:GLU:HB3	2	0.12
(1,162)	1:217:A:GLN:HA	1:220:A:ARG:HG2	20	0.12
(1,152)	1:133:A:ALA:HB1	1:160:A:GLN:HB2	14	0.12
(1,152)	1:133:A:ALA:HB2	1:160:A:GLN:HB2	14	0.12
(1,152)	1:133:A:ALA:HB3	1:160:A:GLN:HB2	14	0.12
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB1	3	0.12
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB2	3	0.12
(1,149)	1:132:A:SER:HB2	1:133:A:ALA:HB3	3	0.12
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB1	3	0.12
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB2	3	0.12
(1,149)	1:132:A:SER:HB3	1:133:A:ALA:HB3	3	0.12
(1,142)	1:186:A:GLN:HA	1:186:A:GLN:HG2	17	0.12
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	4	0.12
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	12	0.12
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	17	0.12
(1,109)	1:204:A:LYS:HA	1:204:A:LYS:HG3	16	0.12
(1,34)	1:223:A:GLN:HA	1:223:A:GLN:HG2	12	0.12
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE1	20	0.11
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE2	20	0.11
(1,1227)	1:206:A:MET:HB2	1:209:A:MET:HE3	20	0.11
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE1	20	0.11
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE2	20	0.11
(1,1227)	1:206:A:MET:HB3	1:209:A:MET:HE3	20	0.11
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG11	17	0.11
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG12	17	0.11
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG13	17	0.11
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG21	17	0.11
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG22	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1167)	1:184:A:ILE:HG12	1:210:A:VAL:HG23	17	0.11
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG11	17	0.11
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG12	17	0.11
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG13	17	0.11
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG21	17	0.11
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG22	17	0.11
(1,1167)	1:184:A:ILE:HG13	1:210:A:VAL:HG23	17	0.11
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD11	10	0.11
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD12	10	0.11
(1,1144)	1:180:A:VAL:HG11	1:184:A:ILE:HD13	10	0.11
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD11	10	0.11
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD12	10	0.11
(1,1144)	1:180:A:VAL:HG12	1:184:A:ILE:HD13	10	0.11
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD11	10	0.11
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD12	10	0.11
(1,1144)	1:180:A:VAL:HG13	1:184:A:ILE:HD13	10	0.11
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD11	10	0.11
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD12	10	0.11
(1,1144)	1:180:A:VAL:HG21	1:184:A:ILE:HD13	10	0.11
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD11	10	0.11
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD12	10	0.11
(1,1144)	1:180:A:VAL:HG22	1:184:A:ILE:HD13	10	0.11
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD11	10	0.11
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD12	10	0.11
(1,1144)	1:180:A:VAL:HG23	1:184:A:ILE:HD13	10	0.11
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB2	6	0.11
(1,1131)	1:178:A:ASP:H	1:179:A:CYS:HB3	6	0.11
(1,1124)	1:174:A:ASN:H	1:174:A:ASN:HD21	5	0.11
(1,1124)	1:174:A:ASN:H	1:174:A:ASN:HD22	5	0.11
(1,1105)	1:156:A:ARG:HD2	1:157:A:TYR:H	17	0.11
(1,1105)	1:156:A:ARG:HD3	1:157:A:TYR:H	17	0.11
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG12	4	0.11
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG13	4	0.11
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG12	8	0.11
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG13	8	0.11
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG12	9	0.11
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG13	9	0.11
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG12	13	0.11
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG13	13	0.11
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG12	16	0.11
(1,1022)	1:138:A:ILE:HB	1:139:A:ILE:HG13	16	0.11
(1,1016)	1:134:A:MET:HG2	1:216:A:THR:HG21	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1016)	1:134:A:MET:HG2	1:216:A:THR:HG22	13	0.11
(1,1016)	1:134:A:MET:HG2	1:216:A:THR:HG23	13	0.11
(1,1016)	1:134:A:MET:HG3	1:216:A:THR:HG21	13	0.11
(1,1016)	1:134:A:MET:HG3	1:216:A:THR:HG22	13	0.11
(1,1016)	1:134:A:MET:HG3	1:216:A:THR:HG23	13	0.11
(1,1009)	1:131:A:GLY:HA2	1:161:A:VAL:HG21	8	0.11
(1,1009)	1:131:A:GLY:HA2	1:161:A:VAL:HG22	8	0.11
(1,1009)	1:131:A:GLY:HA2	1:161:A:VAL:HG23	8	0.11
(1,1009)	1:131:A:GLY:HA3	1:161:A:VAL:HG21	8	0.11
(1,1009)	1:131:A:GLY:HA3	1:161:A:VAL:HG22	8	0.11
(1,1009)	1:131:A:GLY:HA3	1:161:A:VAL:HG23	8	0.11
(1,944)	1:139:A:ILE:HD11	1:141:A:PHE:HZ	2	0.11
(1,944)	1:139:A:ILE:HD12	1:141:A:PHE:HZ	2	0.11
(1,944)	1:139:A:ILE:HD13	1:141:A:PHE:HZ	2	0.11
(1,944)	1:139:A:ILE:HD11	1:141:A:PHE:HZ	12	0.11
(1,944)	1:139:A:ILE:HD12	1:141:A:PHE:HZ	12	0.11
(1,944)	1:139:A:ILE:HD13	1:141:A:PHE:HZ	12	0.11
(1,942)	1:139:A:ILE:HG21	1:141:A:PHE:HZ	20	0.11
(1,942)	1:139:A:ILE:HG22	1:141:A:PHE:HZ	20	0.11
(1,942)	1:139:A:ILE:HG23	1:141:A:PHE:HZ	20	0.11
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE1	3	0.11
(1,939)	1:225:A:TYR:HA	1:225:A:TYR:HE2	3	0.11
(1,865)	1:144:A:ASP:H	1:147:A:ASP:H	2	0.11
(1,855)	1:125:A:LEU:HD11	1:126:A:GLY:H	9	0.11
(1,855)	1:125:A:LEU:HD12	1:126:A:GLY:H	9	0.11
(1,855)	1:125:A:LEU:HD13	1:126:A:GLY:H	9	0.11
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	6	0.11
(1,817)	1:190:A:THR:HA	1:192:A:THR:H	9	0.11
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	3	0.11
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG2	4	0.11
(1,701)	1:136:A:ARG:H	1:137:A:PRO:HG3	4	0.11
(1,649)	1:196:A:GLU:HG3	1:197:A:ASN:H	16	0.11
(1,615)	1:207:A:GLU:H	1:207:A:GLU:HG2	3	0.11
(1,615)	1:207:A:GLU:H	1:207:A:GLU:HG2	6	0.11
(1,615)	1:207:A:GLU:H	1:207:A:GLU:HG2	12	0.11
(1,462)	1:122:A:VAL:HB	1:123:A:GLY:H	17	0.11
(1,454)	1:190:A:THR:H	1:191:A:THR:HG21	4	0.11
(1,454)	1:190:A:THR:H	1:191:A:THR:HG22	4	0.11
(1,454)	1:190:A:THR:H	1:191:A:THR:HG23	4	0.11
(1,394)	1:152:A:GLU:H	1:152:A:GLU:HG3	18	0.11
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB2	19	0.11
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB3	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD11	19	0.11
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD12	19	0.11
(1,372)	1:176:A:VAL:HB	1:215:A:ILE:HD13	19	0.11
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE1	8	0.11
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE2	8	0.11
(1,352)	1:157:A:TYR:HA	1:209:A:MET:HE3	8	0.11
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE1	2	0.11
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE2	2	0.11
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE3	2	0.11
(1,304)	1:206:A:MET:HB2	1:206:A:MET:HE1	15	0.11
(1,304)	1:206:A:MET:HB2	1:206:A:MET:HE2	15	0.11
(1,304)	1:206:A:MET:HB2	1:206:A:MET:HE3	15	0.11
(1,252)	1:178:A:ASP:HA	1:181:A:ASN:HB3	11	0.11
(1,249)	1:179:A:CYS:HA	1:182:A:ILE:HG21	2	0.11
(1,249)	1:179:A:CYS:HA	1:182:A:ILE:HG22	2	0.11
(1,249)	1:179:A:CYS:HA	1:182:A:ILE:HG23	2	0.11
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG21	14	0.11
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG22	14	0.11
(1,236)	1:162:A:TYR:HB2	1:183:A:THR:HG23	14	0.11
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG21	14	0.11
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG22	14	0.11
(1,236)	1:162:A:TYR:HB3	1:183:A:THR:HG23	14	0.11
(1,234)	1:158:A:PRO:HB2	1:183:A:THR:HG21	3	0.11
(1,234)	1:158:A:PRO:HB2	1:183:A:THR:HG22	3	0.11
(1,234)	1:158:A:PRO:HB2	1:183:A:THR:HG23	3	0.11
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG21	2	0.11
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG22	2	0.11
(1,214)	1:198:A:PHE:HB3	1:203:A:VAL:HG23	2	0.11
(1,212)	1:200:A:GLU:HA	1:203:A:VAL:HG21	14	0.11
(1,212)	1:200:A:GLU:HA	1:203:A:VAL:HG22	14	0.11
(1,212)	1:200:A:GLU:HA	1:203:A:VAL:HG23	14	0.11
(1,168)	1:216:A:THR:HA	1:219:A:GLU:HB3	13	0.11
(1,152)	1:133:A:ALA:HB1	1:160:A:GLN:HB2	9	0.11
(1,152)	1:133:A:ALA:HB2	1:160:A:GLN:HB2	9	0.11
(1,152)	1:133:A:ALA:HB3	1:160:A:GLN:HB2	9	0.11
(1,132)	1:208:A:ARG:HA	1:208:A:ARG:HG2	9	0.11
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	3	0.11
(1,113)	1:184:A:ILE:HA	1:184:A:ILE:HG13	5	0.11
(1,109)	1:204:A:LYS:HA	1:204:A:LYS:HG3	7	0.11
(1,35)	1:223:A:GLN:HA	1:223:A:GLN:HG3	7	0.11
(1,35)	1:223:A:GLN:HA	1:223:A:GLN:HG3	10	0.11
(1,1301)	1:134:A:MET:HE1	1:216:A:THR:HG21	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1301)	1:134:A:MET:HE1	1:216:A:THR:HG22	13	0.1
(1,1301)	1:134:A:MET:HE1	1:216:A:THR:HG23	13	0.1
(1,1301)	1:134:A:MET:HE2	1:216:A:THR:HG21	13	0.1
(1,1301)	1:134:A:MET:HE2	1:216:A:THR:HG22	13	0.1
(1,1301)	1:134:A:MET:HE2	1:216:A:THR:HG23	13	0.1
(1,1301)	1:134:A:MET:HE3	1:216:A:THR:HG21	13	0.1
(1,1301)	1:134:A:MET:HE3	1:216:A:THR:HG22	13	0.1
(1,1301)	1:134:A:MET:HE3	1:216:A:THR:HG23	13	0.1
(1,1283)	1:222:A:SER:HA	1:225:A:TYR:HB2	11	0.1
(1,1283)	1:222:A:SER:HA	1:225:A:TYR:HB3	11	0.1
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD2	13	0.1
(1,1032)	1:139:A:ILE:HG21	1:208:A:ARG:HD3	13	0.1
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD2	13	0.1
(1,1032)	1:139:A:ILE:HG22	1:208:A:ARG:HD3	13	0.1
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD2	13	0.1
(1,1032)	1:139:A:ILE:HG23	1:208:A:ARG:HD3	13	0.1
(1,944)	1:139:A:ILE:HD11	1:141:A:PHE:HZ	9	0.1
(1,944)	1:139:A:ILE:HD12	1:141:A:PHE:HZ	9	0.1
(1,944)	1:139:A:ILE:HD13	1:141:A:PHE:HZ	9	0.1
(1,865)	1:144:A:ASP:H	1:147:A:ASP:H	3	0.1
(1,855)	1:125:A:LEU:HD11	1:126:A:GLY:H	12	0.1
(1,855)	1:125:A:LEU:HD12	1:126:A:GLY:H	12	0.1
(1,855)	1:125:A:LEU:HD13	1:126:A:GLY:H	12	0.1
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	3	0.1
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	13	0.1
(1,851)	1:141:A:PHE:HA	1:143:A:SER:H	15	0.1
(1,816)	1:177:A:HIS:H	1:178:A:ASP:HB2	4	0.1
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE1	20	0.1
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE2	20	0.1
(1,712)	1:150:A:TYR:H	1:205:A:MET:HE3	20	0.1
(1,615)	1:207:A:GLU:H	1:207:A:GLU:HG2	7	0.1
(1,463)	1:125:A:LEU:H	1:125:A:LEU:HB3	10	0.1
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB2	11	0.1
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB3	11	0.1
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB2	14	0.1
(1,374)	1:220:A:ARG:HA	1:223:A:GLN:HB3	14	0.1
(1,349)	1:209:A:MET:HE1	1:210:A:VAL:HA	10	0.1
(1,349)	1:209:A:MET:HE2	1:210:A:VAL:HA	10	0.1
(1,349)	1:209:A:MET:HE3	1:210:A:VAL:HA	10	0.1
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE1	13	0.1
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE2	13	0.1
(1,306)	1:203:A:VAL:HB	1:206:A:MET:HE3	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:146:A:GLU:HA	1:149:A:TYR:HB2	2	0.1
(1,265)	1:145:A:TYR:HA	1:148:A:ARG:HB2	12	0.1
(1,265)	1:145:A:TYR:HA	1:148:A:ARG:HB3	12	0.1
(1,234)	1:158:A:PRO:HB2	1:183:A:THR:HG21	20	0.1
(1,234)	1:158:A:PRO:HB2	1:183:A:THR:HG22	20	0.1
(1,234)	1:158:A:PRO:HB2	1:183:A:THR:HG23	20	0.1
(1,185)	1:208:A:ARG:HA	1:211:A:GLU:HB2	5	0.1
(1,185)	1:208:A:ARG:HA	1:211:A:GLU:HB3	5	0.1
(1,185)	1:208:A:ARG:HA	1:211:A:GLU:HB2	9	0.1
(1,185)	1:208:A:ARG:HA	1:211:A:GLU:HB3	9	0.1
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG21	18	0.1
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG22	18	0.1
(1,173)	1:213:A:MET:HA	1:216:A:THR:HG23	18	0.1
(1,160)	1:223:A:GLN:HB2	1:224:A:ALA:HA	3	0.1
(1,160)	1:223:A:GLN:HB3	1:224:A:ALA:HA	3	0.1
(1,157)	1:132:A:SER:HA	1:133:A:ALA:HB1	10	0.1
(1,157)	1:132:A:SER:HA	1:133:A:ALA:HB2	10	0.1
(1,157)	1:132:A:SER:HA	1:133:A:ALA:HB3	10	0.1
(1,132)	1:208:A:ARG:HA	1:208:A:ARG:HG2	14	0.1
(1,108)	1:204:A:LYS:HA	1:204:A:LYS:HG2	8	0.1
(1,45)	1:125:A:LEU:HA	1:125:A:LEU:HD11	3	0.1
(1,45)	1:125:A:LEU:HA	1:125:A:LEU:HD12	3	0.1
(1,45)	1:125:A:LEU:HA	1:125:A:LEU:HD13	3	0.1
(1,34)	1:223:A:GLN:HA	1:223:A:GLN:HG2	18	0.1
(1,21)	1:200:A:GLU:HA	1:200:A:GLU:HB3	3	0.1

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

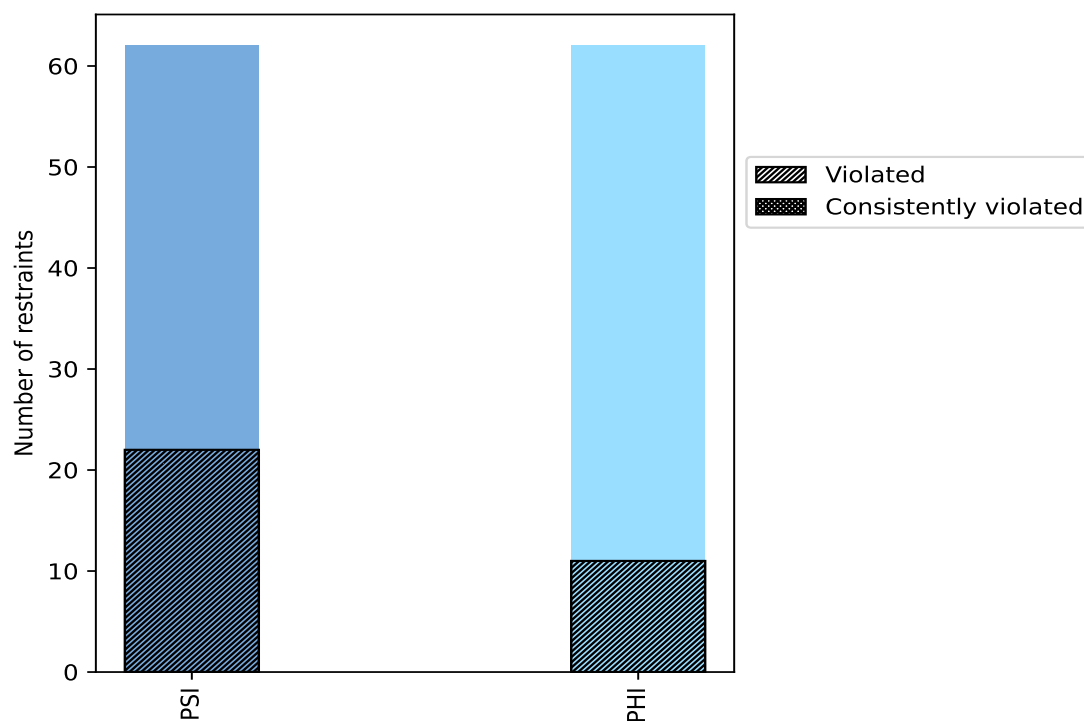
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	62	50.0	22	35.5	17.7	0	0.0	0.0
PHI	62	50.0	11	17.7	8.9	0	0.0	0.0
Total	124	100.0	33	26.6	26.6	0	0.0	0.0

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

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



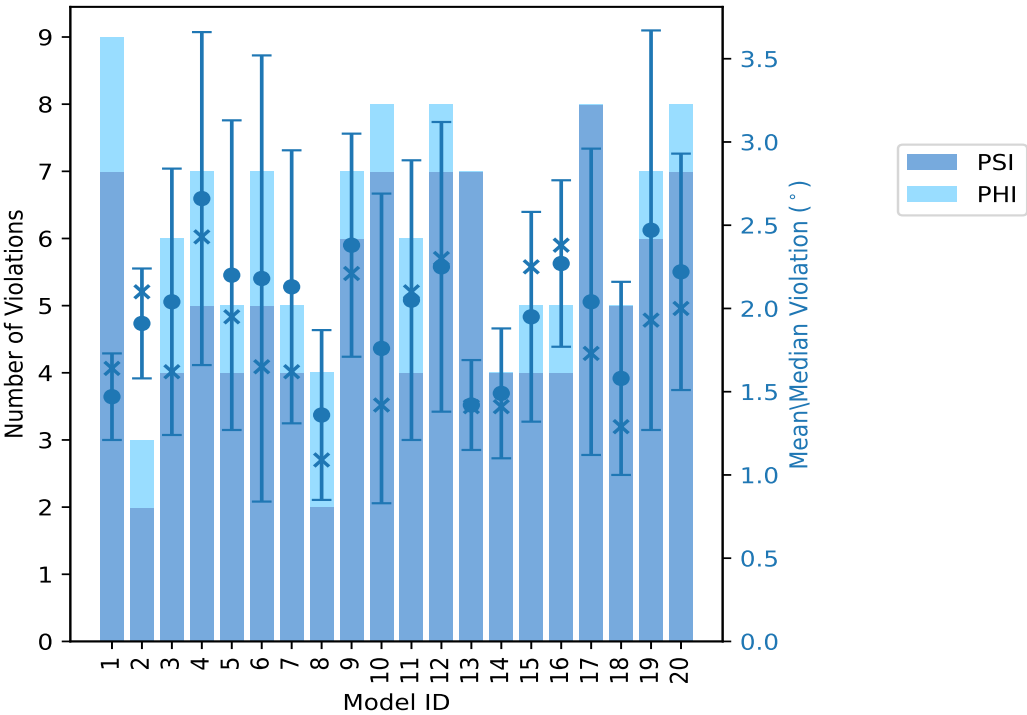
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	7	2	9	1.47	1.78	0.26	1.64
2	2	1	3	1.91	2.19	0.33	2.1
3	4	2	6	2.04	3.64	0.8	1.62
4	5	2	7	2.66	4.48	1.0	2.43
5	4	1	5	2.2	3.95	0.93	1.95
6	5	2	7	2.18	5.29	1.34	1.65
7	4	1	5	2.13	3.25	0.82	1.62
8	2	2	4	1.36	2.25	0.51	1.09
9	6	1	7	2.38	3.94	0.67	2.21
10	7	1	8	1.76	4.18	0.93	1.42
11	4	2	6	2.05	3.45	0.84	2.1
12	7	1	8	2.25	3.57	0.87	2.3
13	7	0	7	1.42	1.91	0.27	1.41
14	4	0	4	1.49	2.11	0.39	1.41
15	4	1	5	1.95	2.63	0.63	2.25
16	4	1	5	2.27	2.79	0.5	2.38
17	8	0	8	2.04	3.7	0.92	1.73
18	5	0	5	1.58	2.48	0.58	1.29
19	6	1	7	2.47	4.85	1.2	1.93
20	7	1	8	2.22	3.49	0.71	2.0

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
9	7	16	1	5.0
2	3	5	2	10.0
1	0	1	3	15.0
3	0	3	4	20.0
1	0	1	5	25.0
1	0	1	6	30.0
0	0	0	7	35.0
1	0	1	8	40.0
1	1	2	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

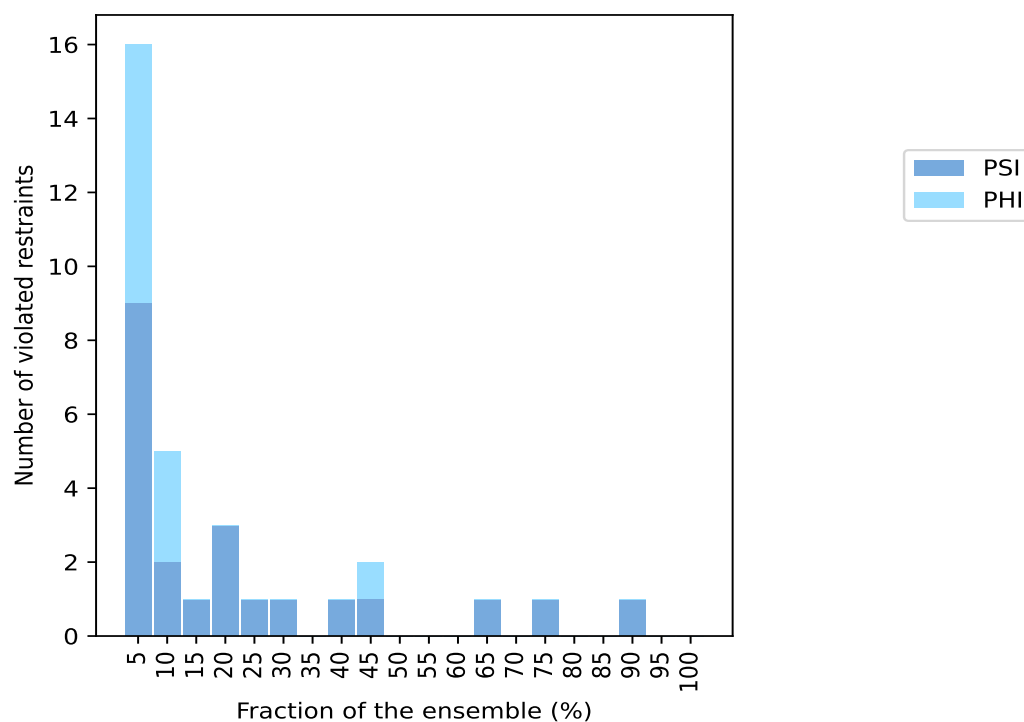
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	60.0
1	0	1	13	65.0
0	0	0	14	70.0
1	0	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
1	0	1	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

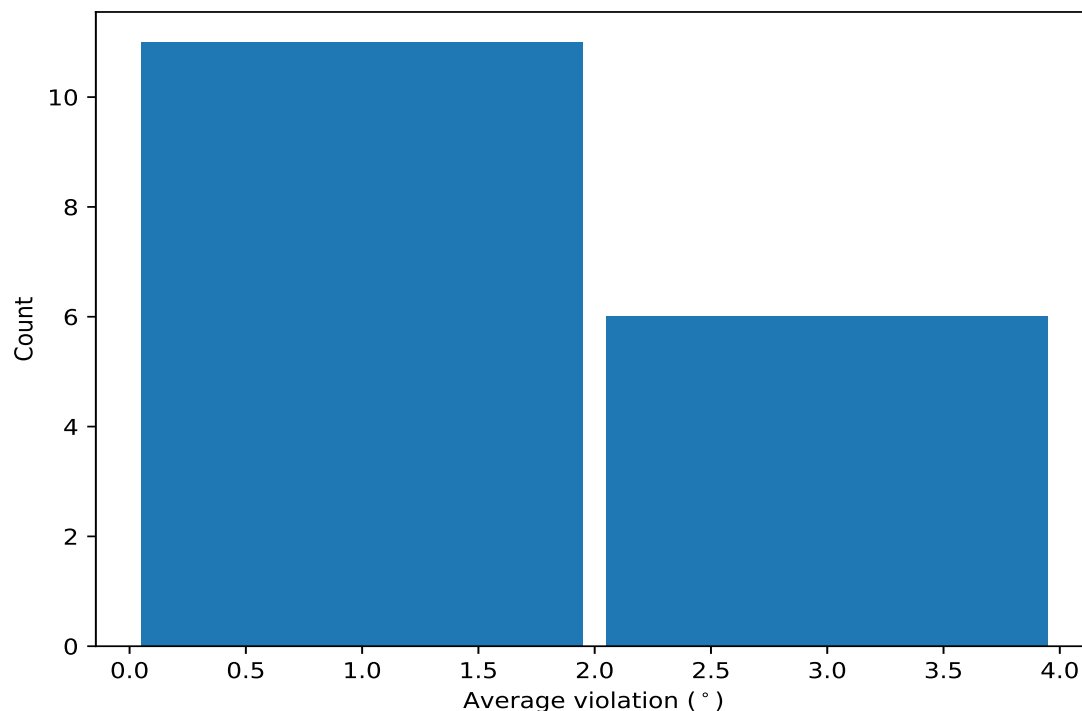


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [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.

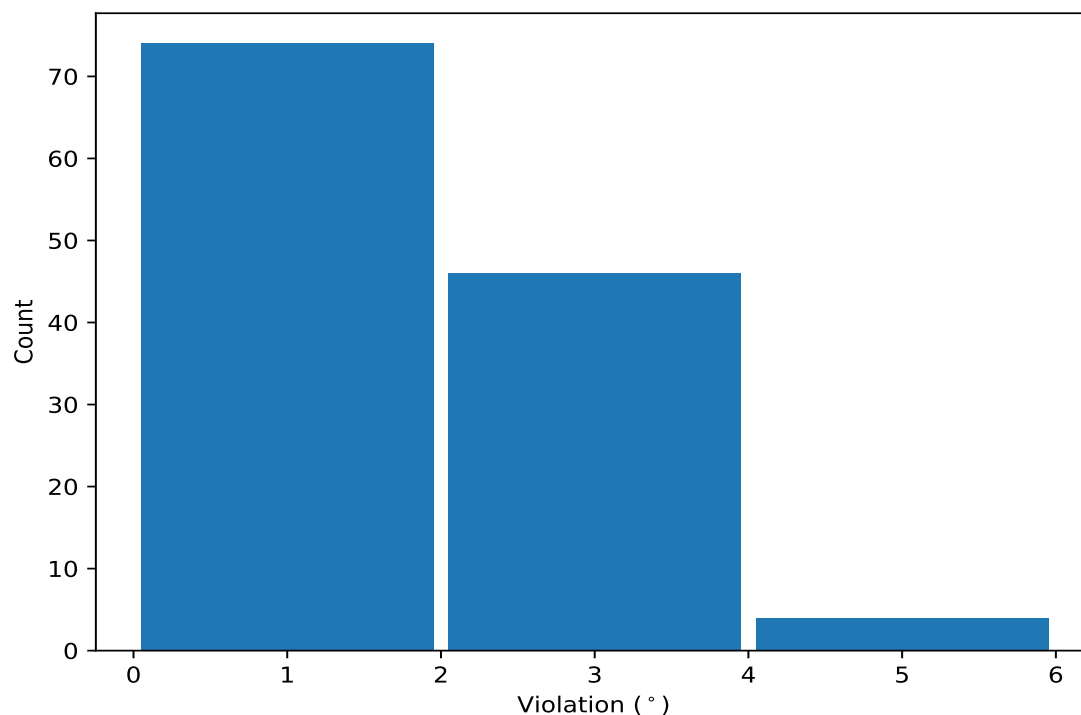
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	18	2.53	1.0	2.16
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	15	2.65	1.12	2.25
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	13	2.06	0.51	1.95
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	9	2.35	1.0	1.9
(1,41)	1:176:A:VAL:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	9	1.94	0.72	1.64
(1,6)	1:145:A:TYR:N	1:145:A:TYR:CA	1:145:A:TYR:C	1:146:A:GLU:N	8	1.67	0.41	1.6
(1,86)	1:206:A:MET:N	1:206:A:MET:CA	1:206:A:MET:C	1:207:A:GLU:N	6	1.44	0.27	1.38
(1,124)	1:225:A:TYR:N	1:225:A:TYR:CA	1:225:A:TYR:C	1:226:A:TYR:N	5	1.78	0.52	1.76
(1,106)	1:216:A:THR:N	1:216:A:THR:CA	1:216:A:THR:C	1:217:A:GLN:N	4	2.45	0.99	2.32
(1,10)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ARG:N	4	1.69	0.46	1.58
(1,100)	1:213:A:MET:N	1:213:A:MET:CA	1:213:A:MET:C	1:214:A:CYS:N	4	1.52	0.16	1.54
(1,120)	1:223:A:GLN:N	1:223:A:GLN:CA	1:223:A:GLN:C	1:224:A:ALA:N	3	1.13	0.07	1.12
(1,18)	1:151:A:ARG:N	1:151:A:ARG:CA	1:151:A:ARG:C	1:152:A:GLU:N	2	2.16	0.83	2.16
(1,99)	1:212:A:GLN:C	1:213:A:MET:N	1:213:A:MET:CA	1:213:A:MET:C	2	1.94	0.26	1.94
(1,21)	1:152:A:GLU:C	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	2	1.88	0.42	1.88
(1,98)	1:212:A:GLN:N	1:212:A:GLN:CA	1:212:A:GLN:C	1:213:A:MET:N	2	1.38	0.28	1.38
(1,31)	1:163:A:TYR:C	1:164:A:ARG:N	1:164:A:ARG:CA	1:164:A:ARG:C	2	1.23	0.11	1.23

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 (°)
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	6	5.29
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	19	4.85
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	4	4.48
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	10	4.18
(1,106)	1:216:A:THR:N	1:216:A:THR:CA	1:216:A:THR:C	1:217:A:GLN:N	5	3.95
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	9	3.94
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	17	3.7
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	3	3.64
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	12	3.57
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	19	3.53
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	20	3.49
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	11	3.45
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	17	3.37
(1,61)	1:187:A:HIS:C	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	4	3.28

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,41)	1:176:A:VAL:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	4	3.27
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	7	3.25
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	12	3.16
(1,60)	1:187:A:HIS:N	1:187:A:HIS:CA	1:187:A:HIS:C	1:188:A:THR:N	20	3.15
(1,18)	1:151:A:ARG:N	1:151:A:ARG:CA	1:151:A:ARG:C	1:152:A:GLU:N	7	2.99
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	12	2.89
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	16	2.79
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	15	2.63
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	6	2.62
(1,106)	1:216:A:THR:N	1:216:A:THR:CA	1:216:A:THR:C	1:217:A:GLN:N	16	2.55
(1,41)	1:176:A:VAL:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	19	2.5
(1,124)	1:225:A:TYR:N	1:225:A:TYR:CA	1:225:A:TYR:C	1:226:A:TYR:N	15	2.49
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	18	2.48
(1,41)	1:176:A:VAL:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	3	2.48
(1,6)	1:145:A:TYR:N	1:145:A:TYR:CA	1:145:A:TYR:C	1:146:A:GLU:N	11	2.48
(1,41)	1:176:A:VAL:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	12	2.47
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	4	2.43
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	11	2.43
(1,10)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ARG:N	20	2.43
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	9	2.38
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	16	2.38
(1,21)	1:152:A:GLU:C	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	16	2.3
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	8	2.25
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	15	2.25
(1,124)	1:225:A:TYR:N	1:225:A:TYR:CA	1:225:A:TYR:C	1:226:A:TYR:N	9	2.23
(1,99)	1:212:A:GLN:C	1:213:A:MET:N	1:213:A:MET:CA	1:213:A:MET:C	9	2.21
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	2	2.19
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	9	2.18
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	5	2.14
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	12	2.12
(1,6)	1:145:A:TYR:N	1:145:A:TYR:CA	1:145:A:TYR:C	1:146:A:GLU:N	14	2.11
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	20	2.1
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	2	2.1
(1,106)	1:216:A:THR:N	1:216:A:THR:CA	1:216:A:THR:C	1:217:A:GLN:N	17	2.09
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	9	2.06
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	18	2.05
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	17	1.97
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	5	1.95
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	19	1.93
(1,40)	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	1:177:A:HIS:N	4	1.92
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	13	1.91
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	20	1.9
(1,86)	1:206:A:MET:N	1:206:A:MET:CA	1:206:A:MET:C	1:207:A:GLU:N	4	1.84
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	1	1.78
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	10	1.78
(1,124)	1:225:A:TYR:N	1:225:A:TYR:CA	1:225:A:TYR:C	1:226:A:TYR:N	11	1.76
(1,6)	1:145:A:TYR:N	1:145:A:TYR:CA	1:145:A:TYR:C	1:146:A:GLU:N	5	1.76
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	3	1.73
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	13	1.72
(1,100)	1:213:A:MET:N	1:213:A:MET:CA	1:213:A:MET:C	1:214:A:CYS:N	1	1.7
(1,86)	1:206:A:MET:N	1:206:A:MET:CA	1:206:A:MET:C	1:207:A:GLU:N	6	1.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	20	1.69
(1,99)	1:212:A:GLN:C	1:213:A:MET:N	1:213:A:MET:CA	1:213:A:MET:C	1	1.68
(1,6)	1:145:A:TYR:N	1:145:A:TYR:CA	1:145:A:TYR:C	1:146:A:GLU:N	1	1.68
(1,98)	1:212:A:GLN:N	1:212:A:GLN:CA	1:212:A:GLN:C	1:213:A:MET:N	9	1.67
(1,100)	1:213:A:MET:N	1:213:A:MET:CA	1:213:A:MET:C	1:214:A:CYS:N	19	1.66
(1,10)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ARG:N	6	1.65
(1,41)	1:176:A:VAL:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1	1.64
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	7	1.62
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	10	1.59
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	19	1.58
(1,26)	1:161:A:VAL:N	1:161:A:VAL:CA	1:161:A:VAL:C	1:162:A:TYR:N	20	1.55
(1,10)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ARG:N	10	1.51
(1,6)	1:145:A:TYR:N	1:145:A:TYR:CA	1:145:A:TYR:C	1:146:A:GLU:N	3	1.51
(1,41)	1:176:A:VAL:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	6	1.5
(1,86)	1:206:A:MET:N	1:206:A:MET:CA	1:206:A:MET:C	1:207:A:GLU:N	17	1.49
(1,21)	1:152:A:GLU:C	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	2	1.45
(1,3)	1:143:A:SER:C	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	7	1.45
(1,116)	1:221:A:GLU:N	1:221:A:GLU:CA	1:221:A:GLU:C	1:222:A:SER:N	12	1.44
(1,41)	1:176:A:VAL:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	20	1.44
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	3	1.43
(1,59)	1:186:A:GLN:C	1:187:A:HIS:N	1:187:A:HIS:CA	1:187:A:HIS:C	3	1.42
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	14	1.42
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	13	1.42
(1,100)	1:213:A:MET:N	1:213:A:MET:CA	1:213:A:MET:C	1:214:A:CYS:N	13	1.41
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	14	1.4
(1,22)	1:153:A:ASN:N	1:153:A:ASN:CA	1:153:A:ASN:C	1:154:A:MET:N	4	1.37
(1,58)	1:186:A:GLN:N	1:186:A:GLN:CA	1:186:A:GLN:C	1:187:A:HIS:N	16	1.34
(1,31)	1:163:A:TYR:C	1:164:A:ARG:N	1:164:A:ARG:CA	1:164:A:ARG:C	6	1.34
(1,124)	1:225:A:TYR:N	1:225:A:TYR:CA	1:225:A:TYR:C	1:226:A:TYR:N	10	1.33
(1,100)	1:213:A:MET:N	1:213:A:MET:CA	1:213:A:MET:C	1:214:A:CYS:N	12	1.33
(1,18)	1:151:A:ARG:N	1:151:A:ARG:CA	1:151:A:ARG:C	1:152:A:GLU:N	17	1.33
(1,6)	1:145:A:TYR:N	1:145:A:TYR:CA	1:145:A:TYR:C	1:146:A:GLU:N	7	1.33
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	1	1.32
(1,6)	1:145:A:TYR:N	1:145:A:TYR:CA	1:145:A:TYR:C	1:146:A:GLU:N	18	1.29
(1,86)	1:206:A:MET:N	1:206:A:MET:CA	1:206:A:MET:C	1:207:A:GLU:N	1	1.28
(1,42)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:ASP:N	17	1.27
(1,5)	1:144:A:ASP:C	1:145:A:TYR:N	1:145:A:TYR:CA	1:145:A:TYR:C	10	1.26
(1,6)	1:145:A:TYR:N	1:145:A:TYR:CA	1:145:A:TYR:C	1:146:A:GLU:N	15	1.24
(1,86)	1:206:A:MET:N	1:206:A:MET:CA	1:206:A:MET:C	1:207:A:GLU:N	19	1.23
(1,120)	1:223:A:GLN:N	1:223:A:GLN:CA	1:223:A:GLN:C	1:224:A:ALA:N	10	1.22
(1,107)	1:216:A:THR:C	1:217:A:GLN:N	1:217:A:GLN:CA	1:217:A:GLN:C	5	1.22
(1,106)	1:216:A:THR:N	1:216:A:THR:CA	1:216:A:THR:C	1:217:A:GLN:N	10	1.22
(1,70)	1:192:A:THR:N	1:192:A:THR:CA	1:192:A:THR:C	1:193:A:THR:N	13	1.19
(1,10)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ARG:N	13	1.19
(1,41)	1:176:A:VAL:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	15	1.15
(1,62)	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	1:189:A:VAL:N	6	1.13
(1,120)	1:223:A:GLN:N	1:223:A:GLN:CA	1:223:A:GLN:C	1:224:A:ALA:N	13	1.12
(1,31)	1:163:A:TYR:C	1:164:A:ARG:N	1:164:A:ARG:CA	1:164:A:ARG:C	11	1.12
(1,124)	1:225:A:TYR:N	1:225:A:TYR:CA	1:225:A:TYR:C	1:226:A:TYR:N	1	1.1
(1,98)	1:212:A:GLN:N	1:212:A:GLN:CA	1:212:A:GLN:C	1:213:A:MET:N	17	1.1
(1,55)	1:184:A:ILE:C	1:185:A:LYS:N	1:185:A:LYS:CA	1:185:A:LYS:C	8	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,122)	1:224:A:ALA:N	1:224:A:ALA:CA	1:224:A:ALA:C	1:225:A:TYR:N	1	1.09
(1,86)	1:206:A:MET:N	1:206:A:MET:CA	1:206:A:MET:C	1:207:A:GLU:N	18	1.09
(1,24)	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1:155:A:HIS:N	8	1.08
(1,11)	1:147:A:ASP:C	1:148:A:ARG:N	1:148:A:ARG:CA	1:148:A:ARG:C	11	1.07
(1,120)	1:223:A:GLN:N	1:223:A:GLN:CA	1:223:A:GLN:C	1:224:A:ALA:N	14	1.04
(1,114)	1:220:A:ARG:N	1:220:A:ARG:CA	1:220:A:ARG:C	1:221:A:GLU:N	12	1.04
(1,41)	1:176:A:VAL:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	8	1.01
(1,4)	1:144:A:ASP:N	1:144:A:ASP:CA	1:144:A:ASP:C	1:145:A:TYR:N	18	1.01