



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 08:54 PM UTC

PDB ID : 2M8D / pdb_00002m8d
BMRB ID : 19248
Title : Structure of SRSF1 RRM2 in complex with the RNA 5'-UGAAGGAC-3'
Authors : Clery, A.; Sinha, R.; Anczukow, O.; Corrionero, A.; Moursy, A.; Daubner, G.;
Valcarcel, J.; Krainer, A.R.; Allain, F.H.T.
Deposited on : 2013-05-17

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

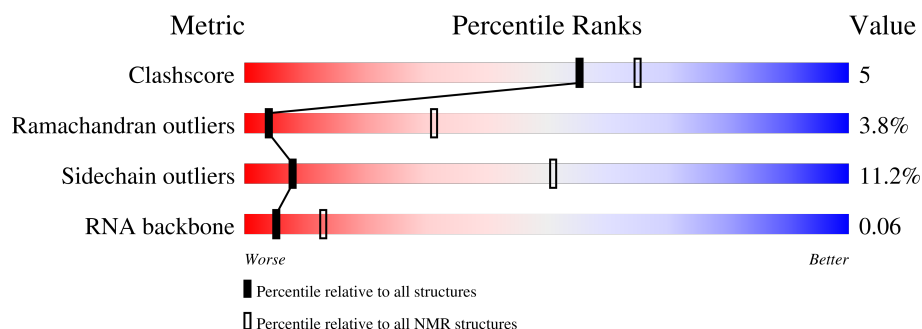
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 74%.

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
RNA backbone	8273	777

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	8	25% 62% 12%
2	B	91	67% 14% 19%

2 Ensemble composition and analysis

This entry contains 16 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	B:117-B:181, B:187-B:195 (74)	0.49	3

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

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

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

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1692 atoms, of which 795 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3').

Mol	Chain	Residues	Atoms						Trace
1	A	8	Total	C	H	N	O	P	0
			261	78	89	35	52	7	

- Molecule 2 is a protein called Serine/arginine-rich splicing factor 1.

Mol	Chain	Residues	Atoms						Trace
2	B	91	Total	C	H	N	O	S	0
			1431	446	706	137	138	4	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	106	MET	-	initiating methionine	UNP Q07955

4 Residue-property plots

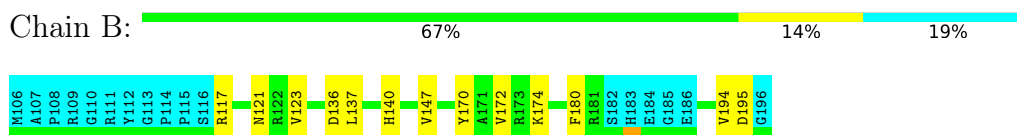
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')



- Molecule 2: Serine/arginine-rich splicing factor 1

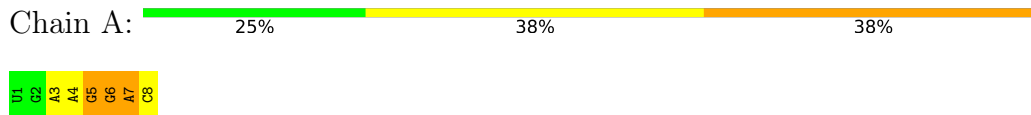


4.2 Scores per residue for each member of the ensemble

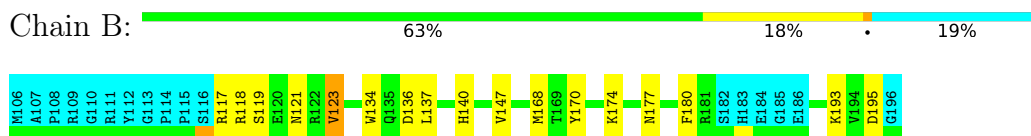
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

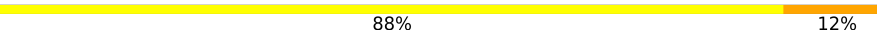


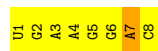
- Molecule 2: Serine/arginine-rich splicing factor 1



4.2.2 Score per residue for model 2

- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

Chain A:  88% 12%



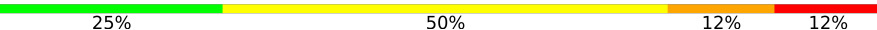
- Molecule 2: Serine/arginine-rich splicing factor 1

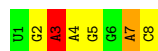
Chain B:  67% 13% 19%



4.2.3 Score per residue for model 3 (medoid)

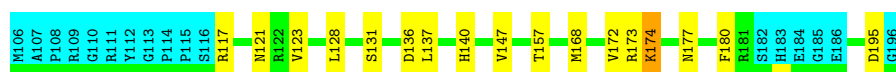
- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

Chain A:  25% 50% 12% 12%



- Molecule 2: Serine/arginine-rich splicing factor 1

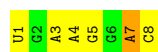
Chain B:  63% 18% 19%



4.2.4 Score per residue for model 4

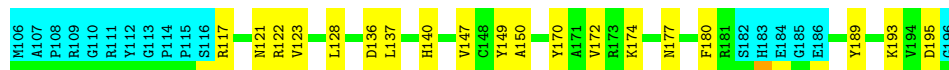
- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

Chain A:  25% 62% 12%



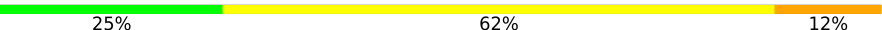
- Molecule 2: Serine/arginine-rich splicing factor 1

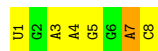
Chain B:  60% 21% 19%



4.2.5 Score per residue for model 5

- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

Chain A:  25% 62% 12%



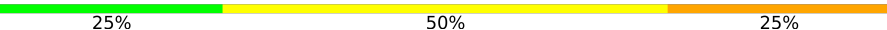
- Molecule 2: Serine/arginine-rich splicing factor 1

Chain B:  65% 14% 19%



4.2.6 Score per residue for model 6

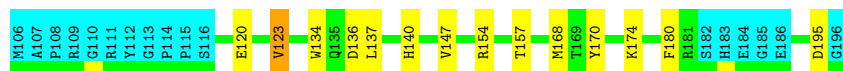
- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

Chain A:  25% 50% 25%



- Molecule 2: Serine/arginine-rich splicing factor 1

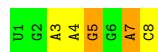
Chain B:  66% 14% 19%



4.2.7 Score per residue for model 7

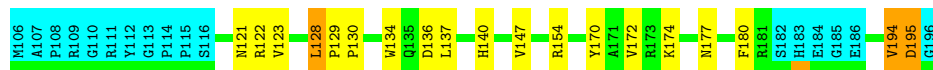
- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

Chain A:  38% 38% 25%



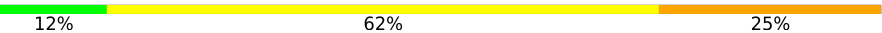
- Molecule 2: Serine/arginine-rich splicing factor 1

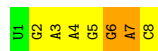
Chain B:  60% 18% 19%



4.2.8 Score per residue for model 8

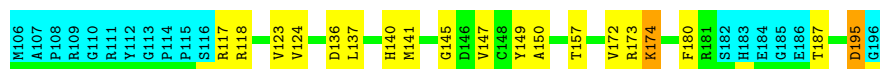
- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

Chain A:  12% 62% 25%



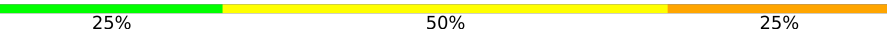
- Molecule 2: Serine/arginine-rich splicing factor 1

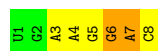
Chain B:  60% 19% 19%



4.2.9 Score per residue for model 9

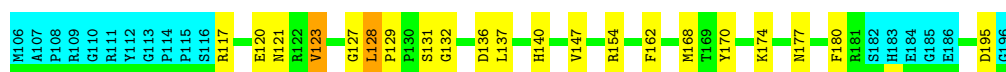
- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

Chain A:  25% 50% 25%



- Molecule 2: Serine/arginine-rich splicing factor 1

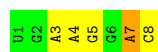
Chain B:  58% 21% 19%



4.2.10 Score per residue for model 10

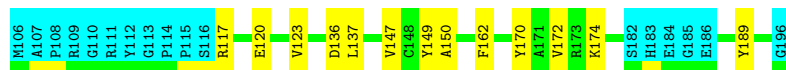
- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

Chain A:  38% 50% 12%



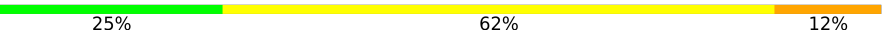
- Molecule 2: Serine/arginine-rich splicing factor 1

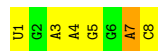
Chain B:  67% 14% 19%



4.2.11 Score per residue for model 11

- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

Chain A:  25% 62% 12%



- Molecule 2: Serine/arginine-rich splicing factor 1

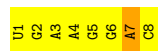
Chain B:  65% 16% 19%



4.2.12 Score per residue for model 12

- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

Chain A:  88% 12%



- Molecule 2: Serine/arginine-rich splicing factor 1

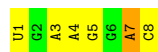
Chain B:  65% 14% 19%



4.2.13 Score per residue for model 13

- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

Chain A:  25% 62% 12%



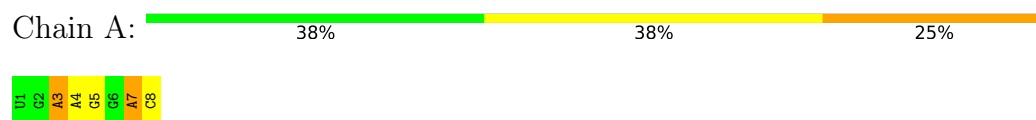
- Molecule 2: Serine/arginine-rich splicing factor 1

Chain B:  63% 16% 19%

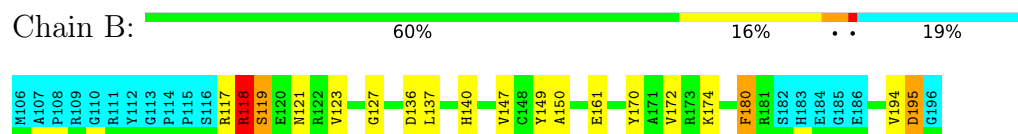


4.2.14 Score per residue for model 14

- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')

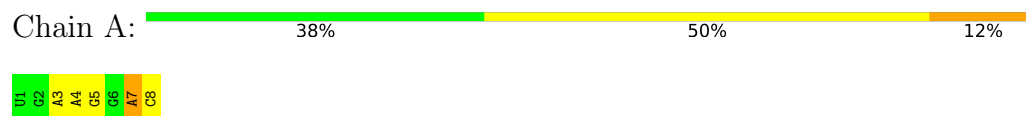


- Molecule 2: Serine/arginine-rich splicing factor 1



4.2.15 Score per residue for model 15

- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')



- Molecule 2: Serine/arginine-rich splicing factor 1

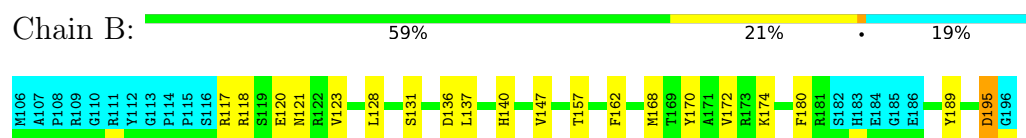


4.2.16 Score per residue for model 16

- Molecule 1: RNA (5'-R(*UP*GP*AP*AP*GP*GP*AP*C)-3')



- Molecule 2: Serine/arginine-rich splicing factor 1



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 16 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
Amber	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	998
Number of shifts mapped to atoms	998
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.70±0.02	0±0/193 (0.0± 0.0%)	1.13±0.06	0±1/300 (0.1± 0.2%)
2	B	0.54±0.01	0±0/611 (0.0± 0.0%)	1.11±0.02	1±1/824 (0.1± 0.1%)
All	All	0.58	0/12864 (0.0%)	1.12	19/17984 (0.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	120	GLU	N-CA-CB	-5.78	103.31	111.00	9	6
1	A	6	G	O4'-C1'-N9	5.54	116.51	108.20	9	3
1	A	6	G	N9-C1'-C2'	-5.54	105.70	114.00	8	1
2	B	127	GLY	CA-C-N	5.51	128.05	120.39	14	2
2	B	127	GLY	C-N-CA	5.51	128.05	120.39	14	2
2	B	194	VAL	N-CA-C	5.38	117.77	111.05	11	1
1	A	3	A	C5'-C4'-C3'	-5.17	108.24	116.00	3	1
2	B	194	VAL	CA-CB-CG1	-5.14	101.66	110.40	15	2
1	A	6	G	C5'-C4'-C3'	-5.11	107.54	115.20	16	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	3	A	Sidechain	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	172	89	89	2±0
2	B	600	592	592	7±2
All	All	12352	10896	10896	116

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:A:N6	2:B:136:ASP:OD1	0.62	2.33	8	16
2:B:180:PHE:C	2:B:180:PHE:CD1	0.60	2.79	12	1
2:B:170:TYR:CE2	2:B:174:LYS:HE3	0.57	2.34	4	9
2:B:123:VAL:HG13	2:B:168:MET:SD	0.56	2.41	2	1
2:B:173:ARG:C	2:B:174:LYS:HE2	0.54	2.27	15	4
2:B:140:HIS:CE1	2:B:180:PHE:HA	0.54	2.38	16	12
1:A:7:A:H61	2:B:136:ASP:CG	0.53	2.11	2	16
2:B:168:MET:SD	2:B:168:MET:C	0.51	2.94	2	1
2:B:170:TYR:CE2	2:B:174:LYS:CE	0.51	2.94	16	9
2:B:128:LEU:N	2:B:129:PRO:CD	0.50	2.74	9	2
2:B:123:VAL:CG1	2:B:168:MET:SD	0.50	3.00	2	1
1:A:3:A:H5''	1:A:3:A:C8	0.47	2.45	3	1
2:B:194:VAL:O	2:B:195:ASP:CB	0.47	2.63	7	3
2:B:128:LEU:N	2:B:129:PRO:HD3	0.46	2.26	9	2
2:B:172:VAL:O	2:B:172:VAL:HG22	0.46	2.11	13	1
2:B:149:TYR:CG	2:B:150:ALA:N	0.45	2.85	10	5
2:B:118:ARG:HA	2:B:118:ARG:CZ	0.44	2.41	12	1
2:B:121:ASN:C	2:B:168:MET:SD	0.44	3.01	16	6
1:A:5:G:C8	2:B:134:TRP:CZ2	0.43	3.06	1	1
1:A:5:G:C6	2:B:134:TRP:CE3	0.43	3.07	7	2
2:B:128:LEU:C	2:B:130:PRO:HD2	0.43	2.38	7	1
2:B:172:VAL:O	2:B:172:VAL:CG2	0.43	2.67	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:181:ARG:HB3	2:B:187:THR:HA	0.42	1.90	12	1
2:B:121:ASN:ND2	2:B:121:ASN:N	0.42	2.67	14	1
2:B:162:PHE:CD1	2:B:162:PHE:N	0.42	2.88	16	4
2:B:123:VAL:HG13	2:B:168:MET:CG	0.42	2.45	2	5
2:B:140:HIS:CD2	2:B:140:HIS:C	0.42	2.97	2	2
2:B:127:GLY:C	2:B:129:PRO:CD	0.41	2.93	9	1
2:B:181:ARG:CB	2:B:187:THR:HA	0.41	2.45	12	1
2:B:170:TYR:CD1	2:B:170:TYR:C	0.40	2.99	11	2
1:A:7:A:N1	2:B:133:SER:CB	0.40	2.84	13	1
2:B:118:ARG:HG3	2:B:119:SER:H	0.40	1.75	14	1
2:B:180:PHE:CG	2:B:181:ARG:N	0.40	2.90	5	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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	
2	B	74/91 (81%)	57±14 (77±19%)	10±3 (13±4%)	3±1 (4±2%)	4	33
All	All	1107/1456 (76%)	907 (82%)	158 (14%)	42 (4%)	4	31

All 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	195	ASP	13
2	B	117	ARG	6
2	B	122	ARG	5
2	B	154	ARG	5
2	B	118	ARG	4
2	B	128	LEU	2
2	B	194	VAL	2
2	B	145	GLY	1
2	B	131	SER	1
2	B	132	GLY	1
2	B	181	ARG	1

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Mol	Chain	Res	Type	Models (Total)
2	B	172	VAL	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	65/77 (84%)	58±2 (89±3%)	7±2 (11±3%)	8	51
All	All	1040/1232 (84%)	924 (89%)	116 (11%)	8	51

All 21 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)
2	B	123	VAL	16
2	B	147	VAL	16
2	B	137	LEU	14
2	B	172	VAL	12
2	B	177	ASN	8
2	B	157	THR	8
2	B	174	LYS	7
2	B	189	TYR	6
2	B	121	ASN	4
2	B	124	VAL	4
2	B	117	ARG	3
2	B	128	LEU	3
2	B	180	PHE	3
2	B	119	SER	2
2	B	193	LYS	2
2	B	131	SER	2
2	B	187	THR	2
2	B	194	VAL	1
2	B	141	MET	1
2	B	118	ARG	1
2	B	161	GLU	1

6.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	7/8 (88%)	5±0 (71±0%)	2±1 (30±16%)	0.12±0.00
All	All	119/128 (93%)	80 (67%)	34 (29%)	0.12

The overall RNA backbone suiteness is 0.06.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	3	A	16
1	A	4	A	16
1	A	5	G	16
1	A	7	A	16
1	A	8	C	16

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	3	A	13
1	A	1	U	7
1	A	6	G	5
1	A	2	G	4
1	A	7	A	4
1	A	4	A	1

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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 74% for the well-defined parts and 72% 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	998
Number of shifts mapped to atoms	998
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	83	-0.20 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	76	-0.24 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	83	1.31 ± 0.57	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 74%, i.e. 883 atoms were assigned a chemical shift out of a possible 1189. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	294/371 (79%)	150/151 (99%)	72/148 (49%)	72/72 (100%)
Sidechain	475/590 (81%)	325/378 (86%)	145/177 (82%)	5/35 (14%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	56/75 (75%)	34/36 (94%)	21/37 (57%)	1/2 (50%)
Sugar	46/88 (52%)	46/48 (96%)	0/40 (0%)	0/0 (—%)
Base	12/65 (18%)	12/41 (29%)	0/13 (0%)	0/11 (0%)
Overall	883/1189 (74%)	567/654 (87%)	238/415 (57%)	78/120 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 997 atoms were assigned a chemical shift out of a possible 1392. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	344/454 (76%)	178/186 (96%)	83/182 (46%)	83/86 (97%)
Sidechain	529/693 (76%)	361/444 (81%)	163/208 (78%)	5/41 (12%)
Aromatic	66/92 (72%)	40/44 (91%)	25/44 (57%)	1/4 (25%)
Sugar	46/88 (52%)	46/48 (96%)	0/40 (0%)	0/0 (—%)
Base	12/65 (18%)	12/41 (29%)	0/13 (0%)	0/11 (0%)
Overall	997/1392 (72%)	637/763 (83%)	271/487 (56%)	89/142 (63%)

7.1.4 Statistically unusual chemical shifts ⓘ

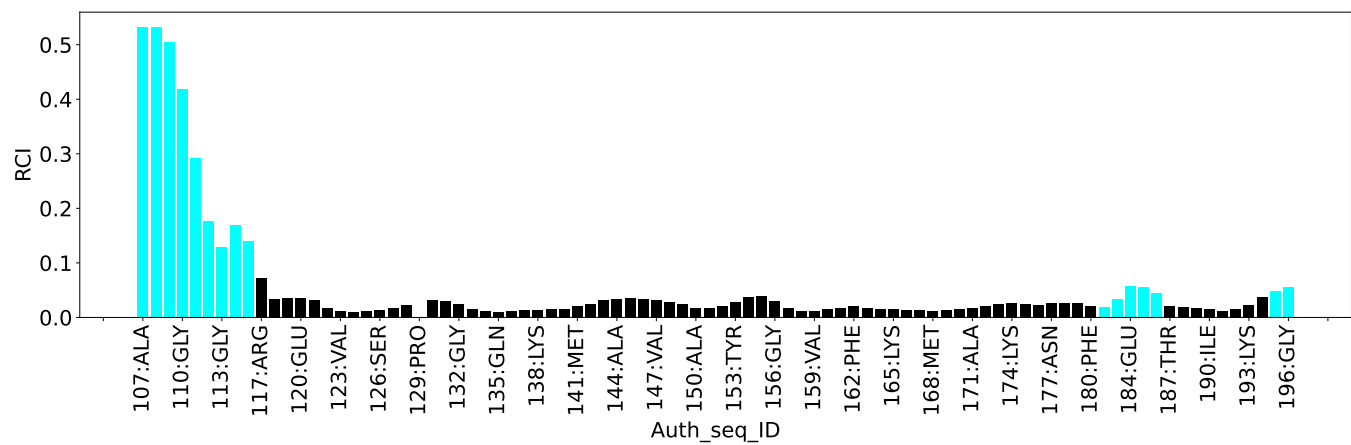
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	135	GLN	HG3	-1.40	0.91 – 3.68	-13.3
1	B	135	GLN	HG2	0.53	1.01 – 3.62	-6.8

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1508
Intra-residue ($ i-j =0$)	304
Sequential ($ i-j =1$)	367
Medium range ($ i-j >1$ and $ i-j <5$)	195
Long range ($ i-j \geq 5$)	558
Inter-chain	28
Hydrogen bond restraints	56
Disulfide bond restraints	0
Total dihedral-angle restraints	351
Number of unmapped restraints	0
Number of restraints per residue	18.8
Number of long range restraints per residue ¹	5.9

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)	32.8	0.2
0.2-0.5 (Medium)	10.8	0.5
>0.5 (Large)	81.9	19.13

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)	3.9	9.36
10.0-20.0 (Medium)	0.8	18.86
>20.0 (Large)	2.3	55.69

9 Distance violation analysis ⓘ

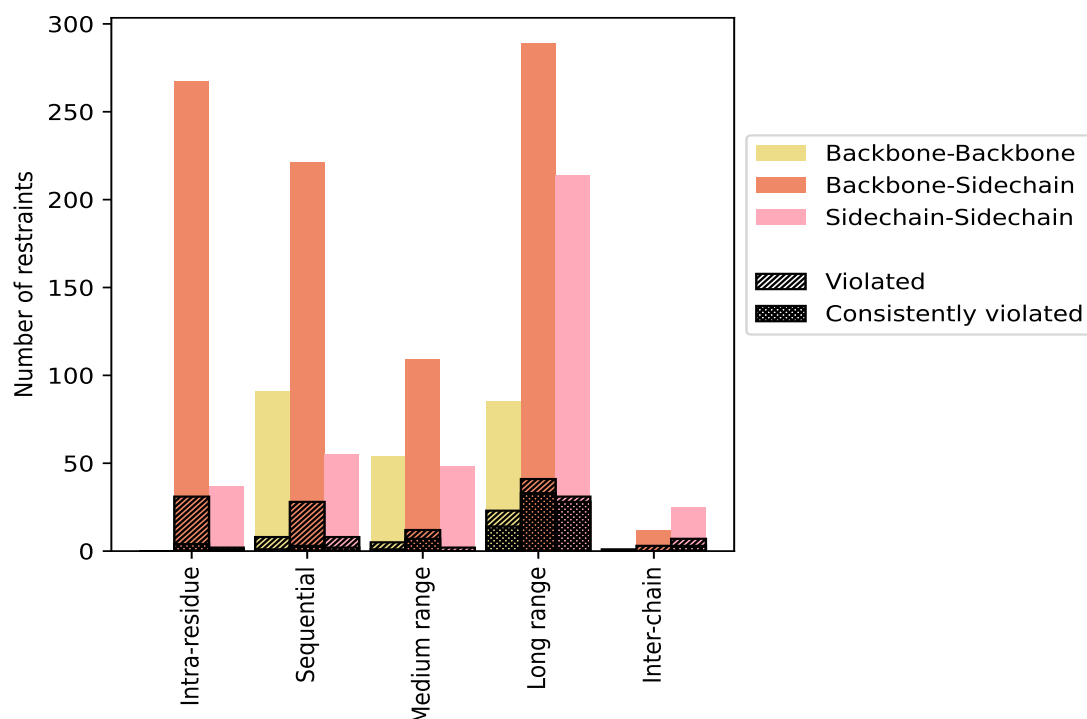
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	304	20.2	33	10.9	2.2	5	1.6	0.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	267	17.7	31	11.6	2.1	4	1.5	0.3
Sidechain-Sidechain	37	2.5	2	5.4	0.1	1	2.7	0.1
Sequential ($i-j =1$)	367	24.3	44	12.0	2.9	6	1.6	0.4
Backbone-Backbone	91	6.0	8	8.8	0.5	1	1.1	0.1
Backbone-Sidechain	221	14.7	28	12.7	1.9	3	1.4	0.2
Sidechain-Sidechain	55	3.6	8	14.5	0.5	2	3.6	0.1
Medium range ($i-j >1$ & $i-j <5$)	195	12.9	19	9.7	1.3	8	4.1	0.5
Backbone-Backbone	54	3.6	5	9.3	0.3	1	1.9	0.1
Backbone-Sidechain	93	6.2	12	12.9	0.8	7	7.5	0.5
Sidechain-Sidechain	48	3.2	2	4.2	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	558	37.0	95	17.0	6.3	75	13.4	5.0
Backbone-Backbone	85	5.6	23	27.1	1.5	14	16.5	0.9
Backbone-Sidechain	261	17.3	41	15.7	2.7	33	12.6	2.2
Sidechain-Sidechain	212	14.1	31	14.6	2.1	28	13.2	1.9
Inter-chain	28	1.9	6	21.4	0.4	1	3.6	0.1
Backbone-Backbone	1	0.1	1	100.0	0.1	0	0.0	0.0
Backbone-Sidechain	10	0.7	3	30.0	0.2	0	0.0	0.0
Sidechain-Sidechain	17	1.1	2	11.8	0.1	1	5.9	0.1
Hydrogen bond	56	3.7	5	8.9	0.3	2	3.6	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1508	100.0	202	13.4	13.4	97	6.4	6.4
Backbone-Backbone	231	15.3	37	16.0	2.5	16	6.9	1.1
Backbone-Sidechain	898	59.5	115	12.8	7.6	47	5.2	3.1
Sidechain-Sidechain	379	25.1	50	13.2	3.3	34	9.0	2.3

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	12	16	9	80	8	125	4.43	17.51	4.75	2.97
2	10	16	10	80	9	125	4.4	17.51	4.69	3.22
3	14	18	10	81	8	131	4.19	17.29	4.59	2.58
4	15	15	10	80	8	128	4.43	17.82	4.84	2.7
5	13	19	10	81	8	131	4.31	17.8	4.82	2.48
6	11	15	11	82	6	125	4.33	16.99	4.55	3.23
7	13	17	9	81	6	126	4.39	17.46	4.68	2.96
8	13	16	11	81	9	130	4.21	17.65	4.68	2.55
9	13	20	12	84	8	137	4.02	17.35	4.63	2.26
10	14	19	12	79	6	130	4.39	18.31	4.9	2.55

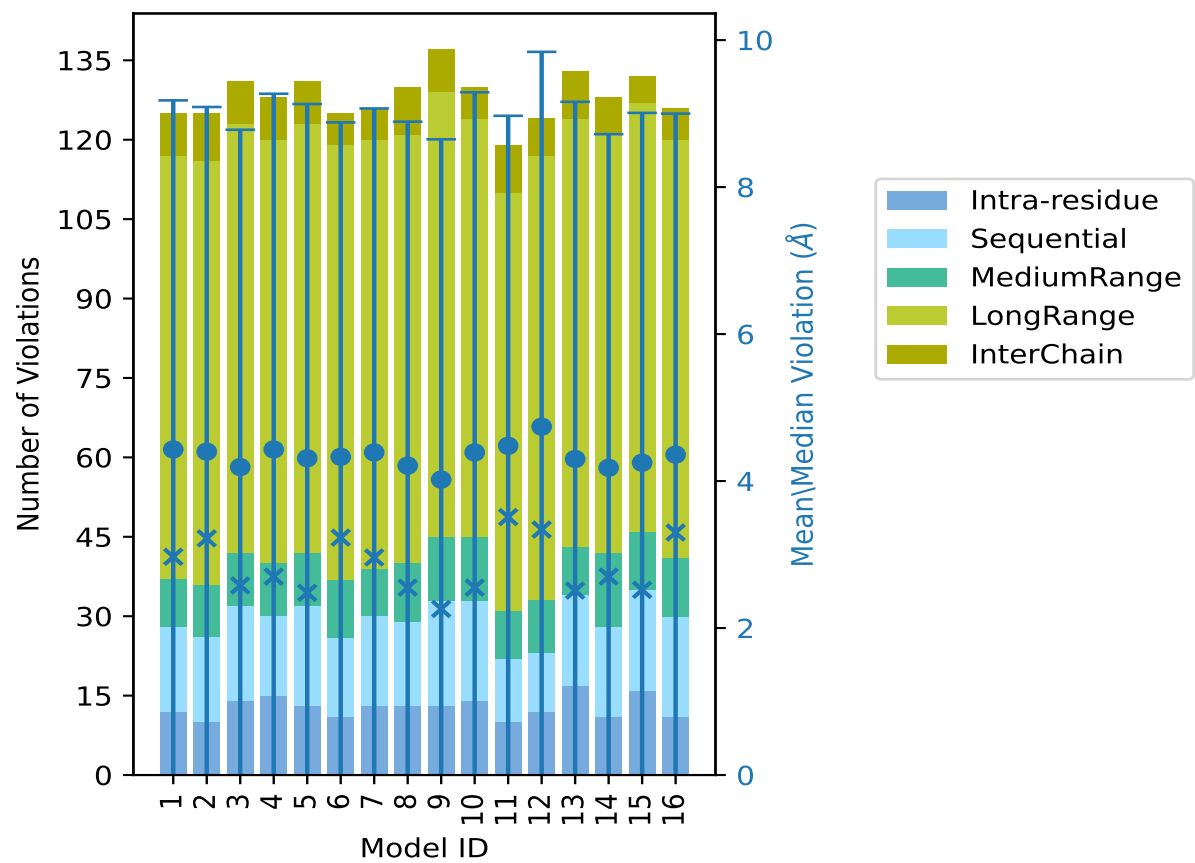
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	10	12	9	79	9	119	4.48	17.4	4.49	3.51
12	12	11	10	84	7	124	4.74	19.13	5.1	3.34
13	17	17	9	81	9	133	4.3	18.17	4.86	2.51
14	11	17	14	79	7	128	4.18	17.17	4.54	2.7
15	16	19	11	81	5	132	4.25	17.67	4.76	2.52
16	11	19	11	79	6	126	4.36	17.46	4.64	3.3

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

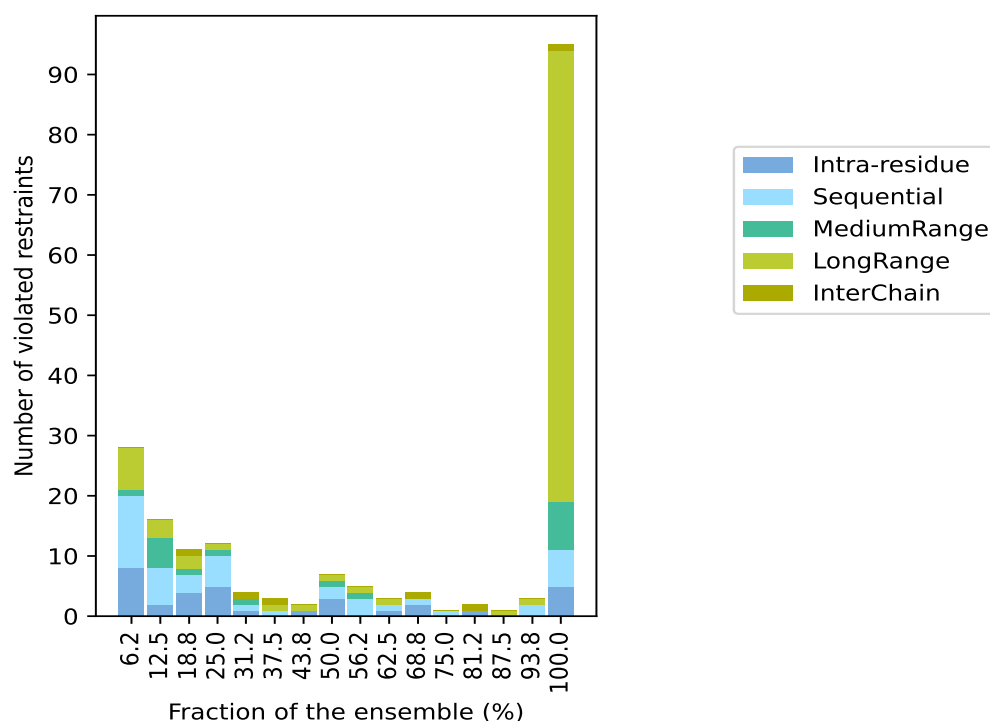
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1255(IR:271, SQ:323, MR:176, LR:463, IC:22) restraints are 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	%
8	12	1	7	0	28	1	6.2
2	6	5	3	0	16	2	12.5
4	3	1	2	1	11	3	18.8
5	5	1	1	0	12	4	25.0
1	1	1	0	1	4	5	31.2
0	1	0	1	1	3	6	37.5
1	0	0	1	0	2	7	43.8
3	2	1	1	0	7	8	50.0
0	3	1	1	0	5	9	56.2
1	1	0	1	0	3	10	62.5
2	1	0	0	1	4	11	68.8
0	1	0	0	0	1	12	75.0
1	0	0	0	1	2	13	81.2
0	0	0	1	0	1	14	87.5
0	2	0	1	0	3	15	93.8
5	6	8	75	1	95	16	100.0

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

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

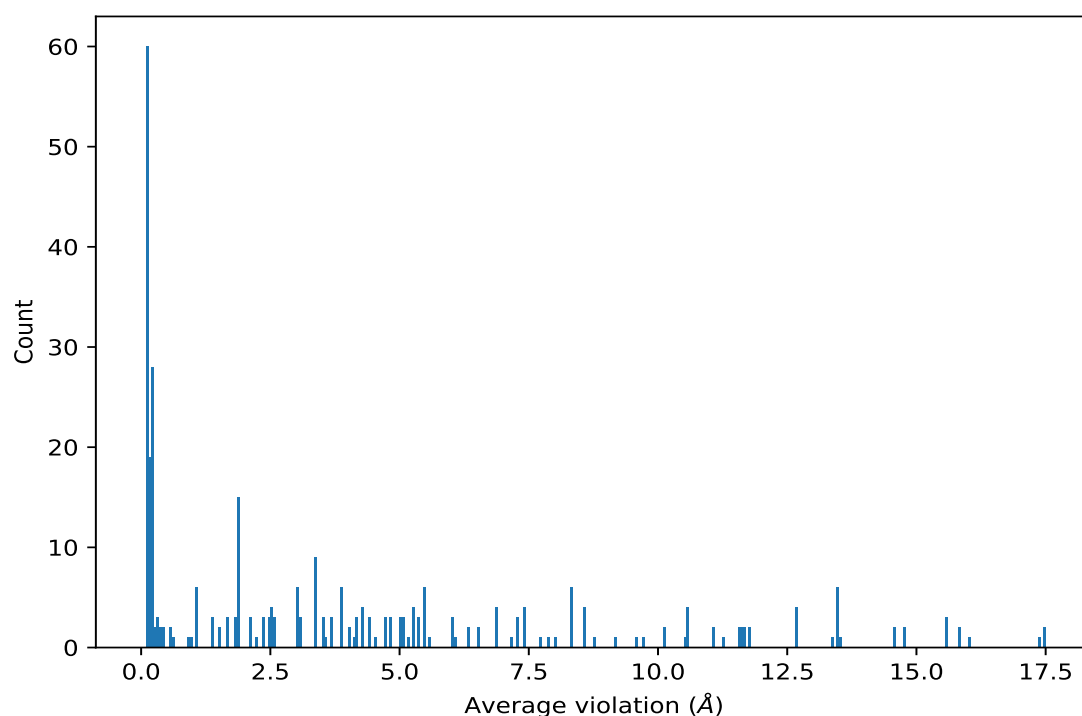
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	16	17.46	0.39	17.51
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	16	17.46	0.39	17.51
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	16	17.36	0.69	17.13
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	16	16.0	0.8	15.72
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	16	15.81	0.47	15.78
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	16	15.81	0.47	15.78
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	16	15.6	0.36	15.52
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	16	15.6	0.36	15.52
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	16	15.6	0.36	15.52
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	16	14.76	0.31	14.8
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	16	14.76	0.31	14.8
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	16	14.56	0.57	14.56
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	16	14.56	0.57	14.56
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	16	13.54	0.57	13.4
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	16	13.49	0.27	13.55
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	16	13.49	0.27	13.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	16	13.49	0.27	13.55
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	16	13.49	0.27	13.55
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	16	13.49	0.27	13.55
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	16	13.49	0.27	13.55
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	16	13.37	0.43	13.28
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	16	12.68	0.52	12.69
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	16	12.68	0.52	12.69
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	16	12.68	0.52	12.69
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	16	12.68	0.52	12.69
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	16	11.76	0.41	11.79
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	16	11.76	0.41	11.79
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	16	11.67	0.6	11.56
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	16	11.67	0.6	11.56
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	16	11.61	0.67	11.48
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	16	11.61	0.67	11.48
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	16	11.59	0.43	11.68
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	16	11.59	0.43	11.68
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	16	11.26	0.27	11.25
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	16	11.08	0.78	10.8
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	16	11.08	0.78	10.8
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	16	10.57	0.53	10.56
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	16	10.57	0.53	10.56
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	16	10.57	0.53	10.56
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	16	10.57	0.53	10.56
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	16	10.54	0.36	10.47
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	16	10.11	0.47	10.06
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	16	10.11	0.47	10.06
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	16	9.74	0.39	9.72
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	16	9.6	0.25	9.66
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	16	9.17	0.28	9.22
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	16	8.77	0.41	8.75
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	16	8.59	0.61	8.57
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	16	8.59	0.61	8.57
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	16	8.59	0.61	8.57
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	16	8.59	0.61	8.57
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	16	8.31	0.39	8.23
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	16	8.31	0.39	8.23
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	16	8.31	0.39	8.23
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	16	8.31	0.39	8.23
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	16	8.31	0.39	8.23
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	16	8.31	0.39	8.23
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	16	8.01	0.37	7.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	16	7.88	0.39	7.84
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	16	7.72	0.43	7.68
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	16	7.41	0.57	7.22
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	16	7.41	0.57	7.22
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	16	7.41	0.57	7.22
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	16	7.41	0.57	7.22
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	16	7.26	0.41	7.12
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	16	7.26	0.41	7.12
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	16	7.26	0.41	7.12
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	16	7.16	0.2	7.14
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	16	6.87	0.59	6.74
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	16	6.87	0.59	6.74
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	16	6.87	0.59	6.74
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	16	6.87	0.59	6.74
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	16	6.52	0.1	6.53
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	16	6.5	0.16	6.56
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	16	6.34	0.46	6.29
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	16	6.34	0.46	6.29
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	16	6.08	0.19	6.11
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	16	6.04	0.12	6.07
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	16	6.04	0.12	6.07
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	16	6.04	0.12	6.07
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	16	5.6	0.18	5.66
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	16	5.46	0.69	5.04
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	16	5.46	0.69	5.04
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	16	5.46	0.69	5.04
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	16	5.46	0.69	5.04
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	16	5.46	0.69	5.04
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	16	5.46	0.69	5.04
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	16	5.36	0.12	5.36
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	16	5.36	0.12	5.36
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	16	5.36	0.12	5.36
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	16	5.28	0.14	5.32
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	16	5.25	0.21	5.24
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	16	5.25	0.21	5.24
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	16	5.25	0.21	5.24
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	16	5.15	0.15	5.12
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	16	5.06	0.14	5.06
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	16	5.06	0.14	5.06
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	16	5.06	0.14	5.06
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	16	5.03	0.13	5.0
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	16	5.03	0.13	5.0

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	16	5.03	0.13	5.0
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	16	4.81	0.12	4.84
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	16	4.81	0.12	4.84
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	16	4.81	0.12	4.84
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	16	4.72	0.12	4.72
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	16	4.72	0.12	4.72
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	16	4.72	0.12	4.72
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	16	4.53	0.04	4.53
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	16	4.42	0.13	4.45
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	16	4.42	0.13	4.45
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	16	4.42	0.13	4.45
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	16	4.29	0.14	4.28
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	16	4.29	0.1	4.3
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	16	4.29	0.1	4.3
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	16	4.29	0.1	4.3
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	16	4.16	0.17	4.21
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	16	4.16	0.17	4.21
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	16	4.16	0.17	4.21
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	16	4.12	0.03	4.11
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	16	4.04	0.23	3.98
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	16	4.04	0.23	3.98
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	16	3.89	0.11	3.9
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	16	3.89	0.11	3.9
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	16	3.89	0.11	3.9
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	16	3.88	0.28	3.84
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	16	3.88	0.28	3.84
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	16	3.88	0.28	3.84
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	16	3.69	0.19	3.66
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	16	3.69	0.19	3.66
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	16	3.69	0.19	3.66
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	16	3.56	0.22	3.56
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	16	3.54	0.12	3.5
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	16	3.54	0.12	3.5
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	16	3.54	0.12	3.5
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	16	3.37	0.08	3.36
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	16	3.37	0.08	3.36
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	16	3.37	0.08	3.36
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	16	3.37	0.08	3.36
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	16	3.37	0.08	3.36
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	16	3.37	0.08	3.36
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	16	3.36	0.09	3.37
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	16	3.36	0.09	3.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	16	3.36	0.09	3.37
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	16	3.09	0.15	3.08
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	16	3.09	0.15	3.08
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	16	3.09	0.15	3.08
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	16	3.05	0.4	3.06
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	16	3.05	0.4	3.06
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	16	3.05	0.4	3.06
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	16	3.05	0.4	3.06
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	16	3.05	0.4	3.06
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	16	3.05	0.4	3.06
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	16	2.56	0.08	2.57
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	16	2.56	0.08	2.57
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	16	2.56	0.08	2.57
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	16	2.55	0.09	2.58
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	16	2.51	0.06	2.52
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	16	2.51	0.06	2.52
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	16	2.51	0.06	2.52
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	16	2.45	0.05	2.45
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	16	2.45	0.05	2.45
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	16	2.45	0.05	2.45
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	16	2.4	0.13	2.38
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	16	2.4	0.13	2.38
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	16	2.4	0.13	2.38
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	16	2.23	0.14	2.2
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	16	2.13	0.2	2.12
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	16	2.13	0.2	2.12
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	16	2.13	0.2	2.12
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	16	1.88	0.05	1.88
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	16	1.88	0.05	1.88
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	16	1.88	0.05	1.88
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	16	1.88	0.05	1.88
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	16	1.88	0.05	1.88
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	16	1.88	0.05	1.88
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	16	1.88	0.05	1.88
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	16	1.88	0.05	1.88
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	16	1.88	0.05	1.88
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	16	1.88	0.05	1.88
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	16	1.88	0.05	1.88
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	16	1.88	0.05	1.88
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	16	1.85	0.08	1.86
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	16	1.85	0.08	1.86
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	16	1.85	0.08	1.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	16	1.82	0.08	1.83
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	16	1.82	0.08	1.83
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	16	1.82	0.08	1.83
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	16	1.7	0.14	1.64
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	16	1.7	0.14	1.64
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	16	1.7	0.14	1.64
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	16	1.54	0.03	1.54
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	16	1.54	0.03	1.54
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	16	1.37	0.11	1.36
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	16	1.37	0.11	1.36
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	16	1.37	0.11	1.36
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	16	1.06	0.04	1.06
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	16	1.06	0.04	1.06
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	16	1.06	0.04	1.06
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	16	1.06	0.04	1.06
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	16	1.06	0.04	1.06
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	16	1.06	0.04	1.06
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	16	0.97	0.09	0.98
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	16	0.95	0.08	0.95
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	16	0.64	0.15	0.6
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	16	0.57	0.2	0.61
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	16	0.56	0.33	0.4
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	16	0.26	0.04	0.26
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	16	0.22	0.03	0.23
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	16	0.22	0.03	0.21
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	16	0.2	0.03	0.2
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	16	0.18	0.02	0.18
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	16	0.18	0.02	0.18
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	16	0.18	0.03	0.19
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	16	0.16	0.03	0.16
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	16	0.15	0.02	0.15
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	16	0.14	0.02	0.14
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	16	0.14	0.01	0.13
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	16	0.14	0.01	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	16	0.14	0.0	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	16	0.14	0.0	0.14
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	16	0.12	0.02	0.12
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	15	0.19	0.06	0.18
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	15	0.15	0.02	0.15
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	15	0.14	0.01	0.14
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	14	0.33	0.1	0.32
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	14	0.19	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	13	0.37	0.18	0.3
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	13	0.2	0.04	0.21
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	13	0.15	0.02	0.15
(1,717)	2:193:B:LYS:HB2	2:194:B:VAL:H	12	0.13	0.02	0.13
(1,1362)	1:2:A:G:H8	1:2:A:G:H1'	11	0.22	0.08	0.24
(1,826)	2:172:B:VAL:H	2:172:B:VAL:HB	11	0.19	0.01	0.19
(1,414)	2:119:B:SER:HB2	2:120:B:GLU:HG3	11	0.14	0.02	0.13
(1,1414)	1:5:A:G:H1	2:134:B:TRP:HB3	11	0.13	0.03	0.11
(1,292)	2:120:B:GLU:H	2:120:B:GLU:HG2	10	0.16	0.06	0.15
(1,744)	2:131:B:SER:H	2:184:B:GLU:HG2	10	0.16	0.05	0.14
(1,724)	2:159:B:VAL:HB	2:160:B:VAL:H	10	0.11	0.01	0.12
(1,247)	2:116:B:SER:H	2:117:B:ARG:HB2	9	0.33	0.21	0.37
(1,115)	2:121:B:ASN:H	2:122:B:ARG:HB2	9	0.18	0.05	0.21
(1,36)	2:119:B:SER:HB3	2:122:B:ARG:H	9	0.15	0.02	0.15
(1,76)	2:147:B:VAL:H	2:148:B:CYS:H	9	0.14	0.01	0.14
(1,110)	2:162:B:PHE:H	2:168:B:MET:HB3	9	0.12	0.01	0.13
(1,311)	2:186:B:GLU:HG3	2:187:B:THR:H	8	0.19	0.03	0.17
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG11	8	0.15	0.02	0.15
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG12	8	0.15	0.02	0.15
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG13	8	0.15	0.02	0.15
(1,344)	2:177:B:ASN:H	2:177:B:ASN:HD22	8	0.13	0.01	0.13
(1,162)	2:142:B:ARG:H	2:147:B:VAL:H	8	0.13	0.01	0.13
(1,634)	2:136:B:ASP:HB3	2:138:B:LYS:H	8	0.12	0.02	0.12
(1,723)	2:143:B:GLU:HA	2:143:B:GLU:HG2	8	0.11	0.01	0.11
(1,392)	2:145:B:GLY:H	2:146:B:ASP:H	8	0.1	0.0	0.1
(1,809)	2:194:B:VAL:H	2:194:B:VAL:HB	7	0.2	0.01	0.2
(1,56)	2:126:B:SER:H	2:193:B:LYS:H	7	0.17	0.04	0.16
(2,52)	1:6:A:G:N2	2:139:B:ASP:OD1	6	0.25	0.11	0.2
(1,863)	2:154:B:ARG:HB3	2:155:B:ASP:HB2	6	0.21	0.01	0.21
(1,1422)	1:6:A:G:H1'	2:135:B:GLN:HA	6	0.12	0.01	0.12
(1,740)	2:151:B:ASP:H	2:159:B:VAL:HB	6	0.1	0.0	0.11
(1,566)	2:131:B:SER:HB3	2:132:B:GLY:HA3	5	0.16	0.05	0.14
(1,1389)	1:8:A:C:H6	1:8:A:C:H3'	5	0.15	0.01	0.15
(1,1426)	1:6:A:G:H2'	2:134:B:TRP:HZ2	5	0.14	0.02	0.15
(1,212)	2:189:B:TYR:HB3	2:191:B:ARG:H	5	0.12	0.01	0.12
(1,892)	2:174:B:LYS:HB3	2:174:B:LYS:HD3	4	0.39	0.0	0.39
(1,890)	2:174:B:LYS:HA	2:174:B:LYS:HD3	4	0.2	0.01	0.2
(1,660)	2:191:B:ARG:HD2	2:192:B:VAL:H	4	0.16	0.02	0.16
(1,1404)	1:7:A:A:H1'	1:6:A:G:H1'	4	0.15	0.02	0.16
(1,1300)	2:183:B:HIS:HA	2:183:B:HIS:HD2	4	0.15	0.04	0.14
(1,1407)	1:8:A:C:H6	1:7:A:A:H4'	4	0.14	0.02	0.14
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG11	4	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG12	4	0.14	0.02	0.14
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG13	4	0.14	0.02	0.14
(1,1360)	1:1:A:U:H3'	1:1:A:U:H6	4	0.13	0.02	0.13
(1,87)	2:190:B:ILE:H	2:192:B:VAL:H	4	0.13	0.03	0.12
(1,388)	2:177:B:ASN:HB2	2:178:B:THR:H	4	0.12	0.01	0.12
(1,757)	2:176:B:ASP:H	2:192:B:VAL:HB	4	0.11	0.01	0.12
(1,956)	2:193:B:LYS:HG2	2:194:B:VAL:H	4	0.11	0.01	0.11
(1,956)	2:193:B:LYS:HG3	2:194:B:VAL:H	4	0.11	0.01	0.11
(1,806)	2:179:B:LYS:HB3	2:180:B:PHE:HA	3	0.42	0.03	0.43
(1,813)	2:178:B:THR:HA	2:179:B:LYS:HB2	3	0.42	0.18	0.44
(1,933)	2:191:B:ARG:HG3	2:192:B:VAL:H	3	0.33	0.05	0.36
(1,1047)	2:128:B:LEU:HD21	2:160:B:VAL:HG21	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD21	2:160:B:VAL:HG22	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD21	2:160:B:VAL:HG23	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD22	2:160:B:VAL:HG21	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD22	2:160:B:VAL:HG22	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD22	2:160:B:VAL:HG23	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD23	2:160:B:VAL:HG21	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD23	2:160:B:VAL:HG22	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD23	2:160:B:VAL:HG23	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD12	2:160:B:VAL:HG21	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD12	2:160:B:VAL:HG22	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD12	2:160:B:VAL:HG23	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD13	2:160:B:VAL:HG21	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD13	2:160:B:VAL:HG22	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD13	2:160:B:VAL:HG23	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD11	2:160:B:VAL:HG21	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD11	2:160:B:VAL:HG22	3	0.22	0.04	0.24
(1,1047)	2:128:B:LEU:HD11	2:160:B:VAL:HG23	3	0.22	0.04	0.24
(1,628)	2:122:B:ARG:HB2	2:195:B:ASP:HB3	3	0.16	0.05	0.14
(1,596)	2:164:B:ARG:H	2:164:B:ARG:HD2	3	0.14	0.0	0.14
(1,211)	2:191:B:ARG:H	2:191:B:ARG:HD2	3	0.13	0.03	0.12
(1,1370)	1:3:A:A:H8	1:3:A:A:H4'	3	0.12	0.02	0.11
(1,1417)	1:5:A:G:H3'	2:134:B:TRP:HZ2	3	0.12	0.01	0.12
(1,1034)	2:194:B:VAL:H	2:194:B:VAL:HG21	3	0.11	0.02	0.1
(1,1034)	2:194:B:VAL:H	2:194:B:VAL:HG22	3	0.11	0.02	0.1
(1,1034)	2:194:B:VAL:H	2:194:B:VAL:HG23	3	0.11	0.02	0.1
(1,136)	2:174:B:LYS:HB3	2:176:B:ASP:H	3	0.11	0.0	0.11
(1,934)	2:178:B:THR:HB	2:179:B:LYS:HG2	2	0.2	0.0	0.2
(1,316)	2:119:B:SER:HB2	2:121:B:ASN:HD22	2	0.2	0.04	0.2
(1,149)	2:142:B:ARG:H	2:142:B:ARG:HB2	2	0.19	0.03	0.19
(1,355)	2:127:B:GLY:H	2:128:B:LEU:HB3	2	0.19	0.06	0.19

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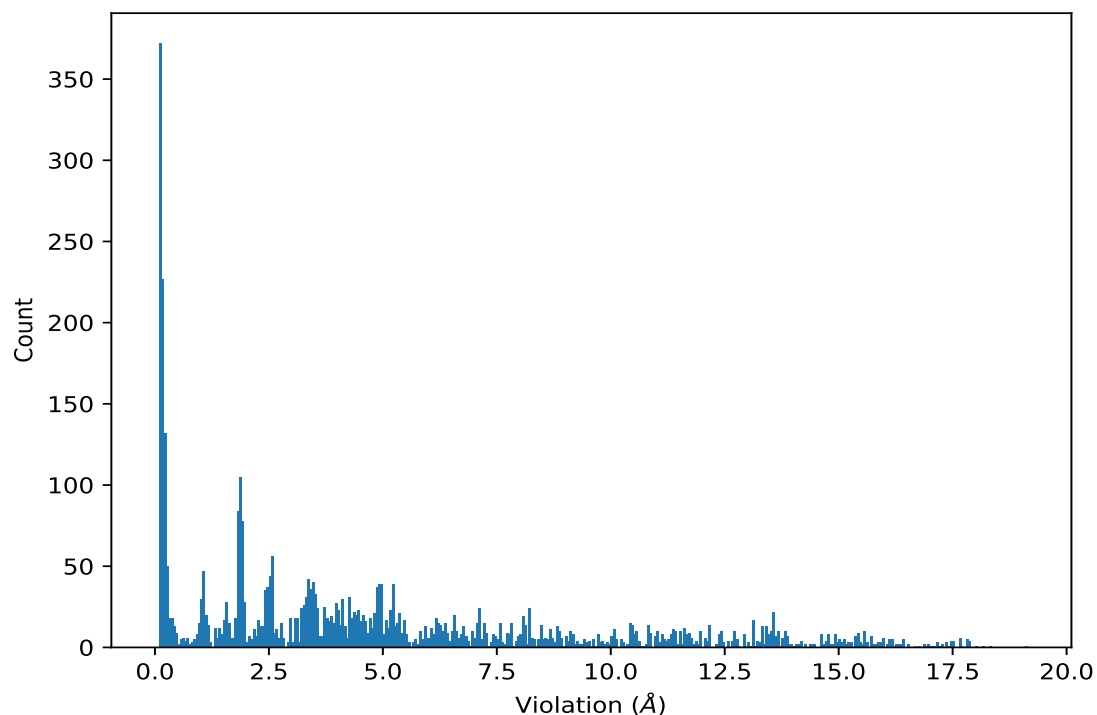
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,41)	2:120:B:GLU:HA	2:122:B:ARG:H	2	0.18	0.04	0.18
(1,556)	2:121:B:ASN:HA	2:165:B:LYS:HA	2	0.16	0.02	0.16
(1,731)	2:119:B:SER:HB3	2:120:B:GLU:HG2	2	0.15	0.03	0.15
(1,1310)	2:134:B:TRP:HE3	2:138:B:LYS:HB3	2	0.14	0.01	0.14
(1,373)	2:126:B:SER:HB2	2:158:B:GLY:H	2	0.12	0.01	0.12
(1,743)	2:184:B:GLU:HG2	2:185:B:GLY:H	2	0.12	0.01	0.12
(1,430)	2:126:B:SER:HB3	2:127:B:GLY:H	2	0.12	0.01	0.12
(1,1392)	1:3:A:A:H8	1:2:A:G:H1'	2	0.12	0.02	0.12
(1,199)	2:124:B:VAL:HB	2:126:B:SER:H	2	0.12	0.0	0.12
(1,238)	2:116:B:SER:HA	2:118:B:ARG:H	2	0.12	0.0	0.12
(1,437)	2:131:B:SER:HB2	2:184:B:GLU:HB2	2	0.11	0.0	0.11
(1,1380)	1:6:A:G:H3'	1:6:A:G:H8	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	12	19.13
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	10	18.31
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	13	18.17
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	12	18.01
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	12	17.87
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	12	17.87
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	13	17.85
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	13	17.85
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	10	17.83
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	10	17.83
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	4	17.82
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	5	17.8
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	5	17.8
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	5	17.74
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	15	17.67
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	15	17.67
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	4	17.65
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	4	17.65
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	8	17.65
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	8	17.65
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	1	17.51
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	1	17.51
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	2	17.51
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	2	17.51
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	7	17.46
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	7	17.46
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	16	17.46
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	16	17.46
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	11	17.4
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	15	17.39
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	9	17.35
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	9	17.35
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	3	17.29
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	3	17.29
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	10	17.21
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	14	17.17
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	14	17.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	7	17.15
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	1	17.11
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	13	17.05
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	8	17.04
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	6	16.99
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	6	16.99
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	9	16.92
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	2	16.89
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	16	16.88
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	3	16.78
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	14	16.68
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	12	16.54
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	12	16.54
(1,907)	2:170:B:TYR:HA	2:181:B:ARG:HG2	6	16.41
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	4	16.41
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	12	16.4
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	12	16.4
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	12	16.4
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	13	16.35
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	13	16.35
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	10	16.33
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	10	16.33
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD2	11	16.26
(1,408)	2:169:B:THR:HB	2:181:B:ARG:HD3	11	16.26
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	5	16.24
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	10	16.17
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	10	16.17
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	10	16.17
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	5	16.16
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	5	16.16
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	11	16.13
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	12	16.11
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	12	16.11
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	15	16.11
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	15	16.11
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	4	16.09
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	4	16.09
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	8	15.98
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	8	15.98
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	15	15.97
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	5	15.96
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	5	15.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	5	15.96
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	13	15.93
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	13	15.93
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	13	15.93
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	4	15.86
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	4	15.86
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	4	15.86
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	7	15.81
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	7	15.81
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	1	15.76
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	1	15.76
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	2	15.73
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	2	15.73
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	1	15.72
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	16	15.72
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	16	15.72
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	7	15.71
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	8	15.7
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	15	15.62
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	15	15.62
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	15	15.62
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	3	15.59
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	3	15.59
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	9	15.59
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	9	15.59
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	11	15.57
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	11	15.57
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	11	15.57
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	1	15.55
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	1	15.55
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	1	15.55
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	9	15.52
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	2	15.5
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	2	15.48
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	2	15.48
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	2	15.48
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	14	15.44
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	14	15.44
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	7	15.42
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	7	15.42
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	7	15.42
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	16	15.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	9	15.41
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	9	15.41
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	9	15.41
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	8	15.37
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	8	15.37
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	8	15.37
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	3	15.37
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	16	15.35
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	16	15.35
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	16	15.35
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	14	15.26
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	14	15.26
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	14	15.26
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	3	15.21
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	3	15.21
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	3	15.21
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	6	15.19
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	6	15.19
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	10	15.14
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	10	15.14
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	13	15.13
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	13	15.13
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	14	15.12
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	12	15.08
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	4	15.08
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	4	15.08
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	5	15.02
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	5	15.02
(1,1031)	2:169:B:THR:HG21	2:181:B:ARG:HG2	6	15.01
(1,1031)	2:169:B:THR:HG22	2:181:B:ARG:HG2	6	15.01
(1,1031)	2:169:B:THR:HG23	2:181:B:ARG:HG2	6	15.01
(1,692)	2:170:B:TYR:HB2	2:181:B:ARG:HG2	6	14.98
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	15	14.95
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	15	14.95
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	15	14.94
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	15	14.94
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	13	14.93
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	13	14.93
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	8	14.92
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	8	14.92
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	2	14.91
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	2	14.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	1	14.85
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	1	14.85
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	12	14.81
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	12	14.81
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	16	14.79
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	16	14.79
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	5	14.78
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	5	14.78
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	4	14.77
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	4	14.77
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	10	14.75
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	10	14.75
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	7	14.71
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	7	14.71
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	9	14.71
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	9	14.71
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	1	14.67
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	1	14.67
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	14	14.63
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	14	14.63
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	8	14.62
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	8	14.62
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	3	14.62
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	3	14.62
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD2	11	14.6
(1,601)	2:170:B:TYR:HA	2:181:B:ARG:HD3	11	14.6
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	3	14.49
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	3	14.49
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	9	14.42
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	9	14.42
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	6	14.37
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	6	14.37
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	7	14.29
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	7	14.29
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	13	14.19
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	12	14.18
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	2	14.16
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	2	14.16
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	16	14.13
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	16	14.13
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	6	14.07
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	6	14.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	5	14.0
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	4	13.98
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	10	13.97
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	14	13.93
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	14	13.93
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	10	13.89
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	10	13.89
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	10	13.89
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	10	13.89
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	10	13.89
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	10	13.89
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	4	13.86
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	13	13.84
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	13	13.84
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	13	13.84
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	13	13.84
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	13	13.84
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	13	13.84
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	5	13.82
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	13	13.81
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD2	11	13.8
(1,602)	2:169:B:THR:HA	2:181:B:ARG:HD3	11	13.8
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	5	13.75
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	5	13.75
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	5	13.75
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	5	13.75
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	5	13.75
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	5	13.75
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	10	13.74
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	12	13.66
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	12	13.66
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	12	13.66
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	12	13.66
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	15	13.65
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	15	13.65
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	15	13.65
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	15	13.65
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	15	13.65
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	15	13.65
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	2	13.6
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	2	13.6
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	2	13.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	2	13.6
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	2	13.6
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	2	13.6
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	1	13.6
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	8	13.59
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	8	13.59
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	8	13.59
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	8	13.59
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	8	13.59
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	8	13.59
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	15	13.59
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	12	13.57
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	12	13.57
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	12	13.57
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	12	13.57
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	12	13.57
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	12	13.57
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE2	11	13.57
(1,635)	2:181:B:ARG:HG3	2:174:B:LYS:HE3	11	13.57
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	1	13.56
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	1	13.56
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	1	13.56
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	1	13.56
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	1	13.56
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	1	13.56
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	1	13.56
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	4	13.54
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	4	13.54
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	4	13.54
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	4	13.54
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	4	13.54
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	4	13.54
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	13	13.5
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	13	13.5
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	13	13.5
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	13	13.5
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	16	13.49
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	16	13.49
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	16	13.49
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	16	13.49
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	16	13.49
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	16	13.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	12	13.48
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	12	13.48
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	7	13.43
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	7	13.43
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	7	13.43
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	7	13.43
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	7	13.43
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	7	13.43
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	9	13.43
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	9	13.42
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	9	13.42
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	9	13.42
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	9	13.42
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	9	13.42
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	9	13.42
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	15	13.39
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	2	13.36
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	14	13.34
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	14	13.34
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	14	13.34
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	14	13.34
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	14	13.34
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	14	13.34
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	9	13.32
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	3	13.31
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	3	13.31
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	3	13.31
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	3	13.31
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	3	13.31
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	3	13.31
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	12	13.27
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	12	13.27
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	7	13.25
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	2	13.23
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	7	13.23
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	8	13.21
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	11	13.2
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	8	13.19
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	6	13.14
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	6	13.14
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	6	13.14
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	6	13.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	6	13.14
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	6	13.14
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	16	13.13
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	15	13.11
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	15	13.11
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	15	13.11
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	15	13.11
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	12	13.1
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	12	13.1
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	10	13.1
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	10	13.1
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	10	13.1
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	10	13.1
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	3	13.08
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	6	13.03
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	16	13.03
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	6	13.0
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	3	12.99
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	4	12.93
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	4	12.93
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	4	12.93
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	4	12.93
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	5	12.9
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	5	12.9
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	5	12.9
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	5	12.9
(1,909)	2:181:B:ARG:HG2	2:174:B:LYS:H	14	12.8
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	14	12.78
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	8	12.77
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	8	12.77
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	8	12.77
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	8	12.77
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD2	11	12.72
(1,1030)	2:169:B:THR:HG21	2:181:B:ARG:HD3	11	12.72
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD2	11	12.72
(1,1030)	2:169:B:THR:HG22	2:181:B:ARG:HD3	11	12.72
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD2	11	12.72
(1,1030)	2:169:B:THR:HG23	2:181:B:ARG:HD3	11	12.72
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	1	12.72
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	1	12.72
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	1	12.72
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	1	12.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	2	12.66
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	2	12.66
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	2	12.66
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	2	12.66
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	9	12.57
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	9	12.57
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	9	12.57
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	9	12.57
(1,913)	2:181:B:ARG:HG3	2:174:B:LYS:H	11	12.48
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	10	12.46
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	10	12.46
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	7	12.43
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	7	12.43
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	7	12.43
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	7	12.43
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	4	12.41
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	4	12.41
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	3	12.4
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	3	12.4
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	3	12.4
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	3	12.4
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	13	12.36
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	13	12.36
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	16	12.36
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	16	12.36
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	16	12.36
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	16	12.36
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	13	12.36
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	13	12.36
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	12	12.32
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	12	12.32
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	10	12.19
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	10	12.19
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	6	12.17
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	6	12.17
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	6	12.17
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	6	12.17
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	5	12.16
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	5	12.16
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	13	12.16
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	13	12.16
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	14	12.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	14	12.15
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	14	12.15
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	14	12.15
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	4	12.14
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	4	12.14
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	13	12.12
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	13	12.12
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	10	12.08
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	10	12.08
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	10	12.08
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	10	12.08
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	5	12.06
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	5	12.06
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	4	11.99
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	4	11.99
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	8	11.99
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	8	11.99
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	12	11.97
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	12	11.97
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	15	11.96
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	15	11.96
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	1	11.95
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	1	11.95
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	5	11.92
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	5	11.92
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	5	11.88
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	5	11.88
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	15	11.87
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	15	11.87
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	1	11.81
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	1	11.81
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	2	11.77
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	2	11.77
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	7	11.77
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	7	11.77
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	10	11.75
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	10	11.75
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	16	11.74
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	16	11.74
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	4	11.74
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	4	11.74
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	2	11.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	2	11.73
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	5	11.71
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	9	11.7
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	9	11.7
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	1	11.69
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	1	11.69
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	8	11.67
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	8	11.67
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	12	11.65
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	12	11.65
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	12	11.65
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	12	11.65
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	8	11.64
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	8	11.64
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	3	11.64
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	3	11.64
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	9	11.64
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	9	11.64
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	10	11.61
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	15	11.6
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	15	11.6
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	7	11.6
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	7	11.6
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	16	11.6
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	1	11.59
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	1	11.59
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	7	11.54
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	7	11.54
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	9	11.54
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	9	11.54
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	15	11.51
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	15	11.51
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE2	11	11.5
(1,639)	2:181:B:ARG:HD2	2:174:B:LYS:HE3	11	11.5
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE2	11	11.5
(1,639)	2:181:B:ARG:HD3	2:174:B:LYS:HE3	11	11.5
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	15	11.47
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	4	11.45
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	2	11.44
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	2	11.44
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	4	11.44
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	4	11.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	6	11.43
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	6	11.43
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	14	11.42
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	14	11.42
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	7	11.41
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	7	11.41
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	13	11.37
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	13	11.37
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	16	11.37
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	16	11.37
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	12	11.37
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	12	11.37
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	16	11.36
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	16	11.36
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	12	11.36
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	7	11.35
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	13	11.35
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	3	11.34
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	3	11.34
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	9	11.32
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	9	11.32
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	16	11.31
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	16	11.31
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	3	11.3
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	3	11.3
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	6	11.28
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	6	11.28
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	5	11.27
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	5	11.27
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	14	11.26
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	3	11.24
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	6	11.21
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	6	11.21
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	1	11.2
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	2	11.17
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	2	11.17
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	2	11.17
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	11	11.15
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	11	11.15
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	14	11.13
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	14	11.13
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	11	11.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	11	11.12
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	11	11.12
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	8	11.11
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	8	11.1
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	8	11.1
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	15	11.06
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	15	11.06
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	9	11.05
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	3	11.04
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	3	11.04
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	14	11.04
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	14	11.04
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	14	11.01
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	14	11.01
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	13	11.01
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	13	11.01
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	13	11.01
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	13	11.01
(1,1204)	2:170:B:TYR:HD1	2:181:B:ARG:HG3	6	10.98
(1,1204)	2:170:B:TYR:HD2	2:181:B:ARG:HG3	6	10.98
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	10	10.97
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	10	10.97
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	10	10.97
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	10	10.97
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	10	10.97
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	4	10.89
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	4	10.89
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	4	10.89
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	4	10.89
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	15	10.89
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	15	10.89
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	15	10.89
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	15	10.89
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	5	10.88
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	5	10.83
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	5	10.83
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	5	10.83
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	5	10.83
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	6	10.83
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	8	10.82
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	8	10.82
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	8	10.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	8	10.82
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	4	10.82
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	1	10.8
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	1	10.8
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	8	10.8
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	8	10.8
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	7	10.76
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	7	10.76
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	13	10.71
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	1	10.69
(1,489)	2:172:B:VAL:HA	2:181:B:ARG:HA	12	10.64
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	15	10.62
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	9	10.61
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	9	10.61
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	2	10.57
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	2	10.57
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	1	10.57
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	1	10.57
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	1	10.57
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	1	10.57
(1,599)	2:181:B:ARG:HD2	2:174:B:LYS:H	11	10.55
(1,599)	2:181:B:ARG:HD3	2:174:B:LYS:H	11	10.55
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	10	10.55
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	10	10.55
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	7	10.54
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	7	10.54
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	7	10.54
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	7	10.54
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD2	11	10.51
(1,604)	2:171:B:ALA:H	2:181:B:ARG:HD3	11	10.51
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	3	10.5
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	3	10.5
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	2	10.49
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	2	10.49
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	2	10.49
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	2	10.49
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	5	10.48
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	5	10.48
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	2	10.48
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	16	10.47
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	16	10.47
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	13	10.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	13	10.47
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	12	10.46
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	9	10.46
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	16	10.46
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	3	10.43
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	3	10.43
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	3	10.43
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	3	10.43
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	4	10.42
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	4	10.42
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	7	10.42
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	16	10.41
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	16	10.41
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	16	10.41
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	16	10.41
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	9	10.4
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	9	10.4
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	9	10.4
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	9	10.4
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG2	11	10.38
(1,915)	2:181:B:ARG:HG3	2:174:B:LYS:HG3	11	10.38
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	3	10.32
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	15	10.28
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	15	10.28
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	6	10.27
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	14	10.24
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	14	10.24
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	8	10.24
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	1	10.2
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	1	10.2
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	4	10.14
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	5	10.14
(1,910)	2:170:B:TYR:HD1	2:181:B:ARG:HG2	6	10.12
(1,910)	2:170:B:TYR:HD2	2:181:B:ARG:HG2	6	10.12
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	10	10.12
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	14	10.09
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	14	10.09
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	14	10.09
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	14	10.09
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	5	10.08
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	2	10.08
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	2	10.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	12	10.07
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	12	10.07
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	12	10.07
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	12	10.07
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	9	10.04
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	9	10.04
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	6	10.01
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	6	10.01
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	6	10.01
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	6	10.01
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	1	10.0
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	15	9.98
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	14	9.97
(1,269)	2:181:B:ARG:H	2:174:B:LYS:H	11	9.94
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	7	9.92
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	7	9.92
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	13	9.88
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	15	9.85
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	8	9.83
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	8	9.83
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	2	9.81
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	4	9.81
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	1	9.79
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	16	9.78
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	16	9.78
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	9	9.73
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	10	9.73
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	3	9.72
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	3	9.72
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	2	9.71
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	13	9.71
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	6	9.71
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	6	9.71
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	16	9.69
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	9	9.64
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	6	9.62
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	5	9.62
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	7	9.6
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	16	9.6
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	12	9.56
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	14	9.52
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	14	9.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	3	9.51
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	7	9.51
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	12	9.48
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	4	9.47
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	10	9.45
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	15	9.44
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	3	9.42
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	6	9.4
(1,272)	2:181:B:ARG:HB2	2:174:B:LYS:H	11	9.4
(1,272)	2:181:B:ARG:HB3	2:174:B:LYS:H	11	9.4
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	1	9.39
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	8	9.36
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	8	9.31
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	2	9.31
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	10	9.27
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	14	9.27
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	13	9.26
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	4	9.25
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	16	9.22
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	9	9.21
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD2	11	9.17
(1,614)	2:170:B:TYR:HD1	2:181:B:ARG:HD3	11	9.17
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD2	11	9.17
(1,614)	2:170:B:TYR:HD2	2:181:B:ARG:HD3	11	9.17
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	12	9.16
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	12	9.16
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	12	9.16
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	12	9.16
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	5	9.14
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	12	9.14
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	13	9.13
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	13	9.13
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	13	9.13
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	13	9.13
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	13	9.13
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	13	9.13
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	7	9.11
(1,488)	2:181:B:ARG:HA	2:176:B:ASP:H	11	9.1
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	10	9.08
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	10	9.08
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	10	9.08
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	10	9.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	1	9.04
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	14	9.04
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	13	9.01
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	13	9.01
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	13	9.01
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	13	9.01
(1,513)	2:181:B:ARG:H	2:174:B:LYS:HA	11	9.01
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	15	8.95
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	4	8.93
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	4	8.93
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	4	8.93
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	4	8.93
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	6	8.93
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	3	8.92
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	5	8.89
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	5	8.89
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	5	8.89
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	5	8.89
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	15	8.89
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	15	8.89
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	15	8.89
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	15	8.89
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	12	8.89
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	12	8.87
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	2	8.84
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	2	8.84
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	2	8.84
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	2	8.84
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	2	8.84
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	2	8.84
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	1	8.82
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	1	8.82
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	1	8.82
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	1	8.82
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	1	8.82
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	1	8.82
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	13	8.8
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	8	8.79
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	9	8.77
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	14	8.77
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	16	8.74
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	8	8.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	8	8.73
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	8	8.73
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	8	8.73
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	2	8.7
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	12	8.69
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	12	8.69
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	12	8.69
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	12	8.69
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	9	8.68
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	9	8.68
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	9	8.68
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	9	8.68
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	9	8.68
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	9	8.68
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	7	8.67
(1,306)	2:181:B:ARG:HA	2:175:B:LEU:H	11	8.64
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	1	8.6
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	1	8.6
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	1	8.6
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	1	8.6
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	12	8.58
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	6	8.55
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	2	8.55
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	2	8.55
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	2	8.55
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	2	8.55
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	7	8.51
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	7	8.51
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	7	8.51
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	7	8.51
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	3	8.5
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	10	8.48
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	6	8.46
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	6	8.46
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	6	8.46
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	6	8.46
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	6	8.46
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	6	8.46
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	10	8.46
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	10	8.46
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	10	8.46
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	10	8.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	10	8.46
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	10	8.46
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	10	8.45
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	9	8.43
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	9	8.43
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	9	8.43
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	9	8.43
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	5	8.4
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	8	8.35
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	4	8.31
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	16	8.3
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	16	8.3
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	16	8.3
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	16	8.3
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	4	8.29
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	3	8.28
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	3	8.28
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	3	8.28
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	3	8.28
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	10	8.28
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	15	8.23
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	15	8.23
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	15	8.23
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	15	8.23
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	15	8.23
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	15	8.23
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	16	8.23
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	16	8.23
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	16	8.23
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	16	8.23
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	16	8.23
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	16	8.23
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	8	8.22
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	8	8.22
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	8	8.22
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	8	8.22
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	8	8.22
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	8	8.22
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	5	8.2
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	5	8.2
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	5	8.2
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	5	8.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	5	8.2
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	5	8.2
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	5	8.19
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	4	8.17
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	1	8.14
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	5	8.13
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	7	8.12
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	7	8.12
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	7	8.12
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	7	8.12
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	7	8.12
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	7	8.12
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	14	8.1
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	14	8.1
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	14	8.1
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	14	8.1
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	14	8.1
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	14	8.1
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	12	8.08
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	12	8.08
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	12	8.08
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	13	8.08
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	4	8.07
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	4	8.07
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	4	8.07
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	4	8.07
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	4	8.07
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	4	8.07
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	15	8.06
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	6	8.05
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	6	8.05
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	6	8.05
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	6	8.05
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	14	8.05
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	14	8.05
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	14	8.05
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	14	8.05
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	3	8.04
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	3	8.04
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	3	8.04
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	3	8.04
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	3	8.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	3	8.04
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	11	8.04
(1,781)	2:181:B:ARG:H	2:174:B:LYS:HB2	14	8.03
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	16	7.99
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	15	7.98
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	1	7.98
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	10	7.97
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	10	7.97
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	10	7.97
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	13	7.95
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	2	7.94
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	16	7.93
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	7	7.93
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	9	7.93
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	7	7.88
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	13	7.84
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	13	7.84
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	13	7.84
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	12	7.83
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	12	7.83
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	12	7.83
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	12	7.83
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	12	7.83
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	12	7.83
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	1	7.81
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	15	7.81
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	13	7.8
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	13	7.8
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	13	7.8
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	13	7.8
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	10	7.79
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	10	7.79
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	10	7.79
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	10	7.79
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	15	7.76
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	15	7.76
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	15	7.76
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	15	7.76
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	4	7.73
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	4	7.73
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	4	7.73
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	4	7.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	3	7.71
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	6	7.71
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	3	7.7
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	9	7.7
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	16	7.7
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	8	7.69
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	7	7.67
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	8	7.62
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	2	7.61
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	2	7.61
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	9	7.59
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	13	7.59
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD2	11	7.58
(1,1011)	2:172:B:VAL:HG11	2:181:B:ARG:HD3	11	7.58
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD2	11	7.58
(1,1011)	2:172:B:VAL:HG12	2:181:B:ARG:HD3	11	7.58
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD2	11	7.58
(1,1011)	2:172:B:VAL:HG13	2:181:B:ARG:HD3	11	7.58
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	5	7.58
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	5	7.58
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	5	7.58
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	5	7.58
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	12	7.58
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	12	7.58
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	16	7.55
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	5	7.52
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	5	7.52
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	5	7.52
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	6	7.51
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	14	7.5
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	4	7.49
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	4	7.49
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	4	7.49
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	14	7.47
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	11	7.46
(1,252)	2:181:B:ARG:H	2:175:B:LEU:H	11	7.46
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	7	7.45
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	1	7.43
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	1	7.43
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	1	7.43
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	1	7.43
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	10	7.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	10	7.43
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	10	7.43
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	10	7.43
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	6	7.37
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	3	7.37
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	13	7.35
(1,253)	2:171:B:ALA:HA	2:181:B:ARG:H	6	7.32
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	11	7.28
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	11	7.28
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	11	7.28
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	5	7.27
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	3	7.26
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	9	7.25
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	9	7.25
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	9	7.25
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	9	7.25
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	13	7.22
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	13	7.22
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	13	7.22
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	13	7.22
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	15	7.2
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	15	7.2
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	15	7.2
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	2	7.2
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	2	7.2
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	2	7.2
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	2	7.2
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	8	7.2
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	8	7.2
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	8	7.2
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	8	7.2
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	11	7.18
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	4	7.16
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	4	7.16
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	4	7.16
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	4	7.16
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	9	7.14
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	1	7.13
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	1	7.13
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	1	7.13
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	1	7.13
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	7	7.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	7	7.13
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	7	7.13
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	7	7.13
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	8	7.13
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	3	7.12
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	3	7.12
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	3	7.12
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	3	7.12
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD2	11	7.12
(1,600)	2:170:B:TYR:HE1	2:181:B:ARG:HD3	11	7.12
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD2	11	7.12
(1,600)	2:170:B:TYR:HE2	2:181:B:ARG:HD3	11	7.12
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	2	7.11
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	2	7.11
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	2	7.11
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	8	7.11
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	8	7.11
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	8	7.11
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	15	7.09
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	15	7.09
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	15	7.09
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	15	7.09
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	15	7.08
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	11	7.08
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	8	7.06
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	7	7.06
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	7	7.06
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	7	7.06
(1,251)	2:181:B:ARG:H	2:174:B:LYS:HB3	14	7.06
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	5	7.05
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	5	7.05
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	5	7.05
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	5	7.05
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	16	7.03
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	16	7.03
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	16	7.03
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	9	7.02
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	9	7.02
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	9	7.02
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	2	6.99
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	14	6.98
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	16	6.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	16	6.97
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	16	6.97
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	16	6.97
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	4	6.96
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	3	6.96
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	3	6.96
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	3	6.96
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	12	6.92
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	6	6.89
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	6	6.89
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	6	6.89
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	6	6.89
(1,1285)	2:134:B:TRP:HD1	2:160:B:VAL:H	10	6.81
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	14	6.81
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	14	6.81
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	14	6.81
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	14	6.81
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	10	6.81
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	10	6.81
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	14	6.76
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	14	6.76
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	14	6.76
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	1	6.76
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	1	6.76
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	1	6.76
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	1	6.76
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	5	6.76
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	5	6.76
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	8	6.75
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	8	6.75
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	8	6.75
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	8	6.75
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	7	6.74
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	7	6.74
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	7	6.74
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	7	6.74
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE2	11	6.72
(1,843)	2:181:B:ARG:HB2	2:174:B:LYS:HE3	11	6.72
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE2	11	6.72
(1,843)	2:181:B:ARG:HB3	2:174:B:LYS:HE3	11	6.72
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	1	6.68
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	11	6.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	4	6.66
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	4	6.66
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	12	6.66
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	9	6.65
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	2	6.63
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	2	6.63
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	2	6.63
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	2	6.63
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	14	6.62
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	6	6.61
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	3	6.61
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	4	6.61
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	13	6.6
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	15	6.6
(1,908)	2:171:B:ALA:HB1	2:181:B:ARG:HG2	6	6.59
(1,908)	2:171:B:ALA:HB2	2:181:B:ARG:HG2	6	6.59
(1,908)	2:171:B:ALA:HB3	2:181:B:ARG:HG2	6	6.59
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	13	6.59
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	13	6.59
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	9	6.58
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	9	6.58
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	9	6.58
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	9	6.58
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	1	6.57
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	10	6.57
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	9	6.57
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	10	6.57
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	3	6.56
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	3	6.56
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	3	6.56
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	3	6.56
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	3	6.56
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	8	6.56
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	16	6.55
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	16	6.53
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	16	6.53
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	16	6.53
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	16	6.53
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	8	6.53
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	12	6.53
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	2	6.52
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	11	6.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	14	6.51
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	2	6.5
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	7	6.48
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	15	6.48
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	15	6.47
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	15	6.47
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	4	6.44
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	1	6.41
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	1	6.41
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	7	6.4
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	7	6.4
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	7	6.4
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	7	6.4
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	7	6.4
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	7	6.4
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	6	6.39
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	13	6.38
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	13	6.38
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	13	6.38
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	13	6.38
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	13	6.38
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	13	6.38
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	13	6.36
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	6	6.35
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	6	6.35
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	6	6.35
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	6	6.35
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	6	6.35
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	6	6.35
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	7	6.35
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	16	6.34
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	15	6.33
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	15	6.33
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	15	6.33
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	15	6.33
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	15	6.33
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	15	6.33
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	5	6.31
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	2	6.31
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	2	6.31
(1,522)	2:160:B:VAL:HA	2:153:B:TYR:HA	16	6.29
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	7	6.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	9	6.27
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	9	6.27
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	9	6.26
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	9	6.26
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	9	6.26
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	9	6.26
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	9	6.26
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	9	6.26
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	14	6.26
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	14	6.26
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	14	6.26
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	14	6.26
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	11	6.23
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	11	6.23
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	11	6.23
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	11	6.23
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	6	6.23
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	5	6.22
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	5	6.22
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	5	6.22
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	5	6.22
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	5	6.22
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	5	6.22
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	12	6.2
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	12	6.2
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	12	6.2
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	9	6.2
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB2	6	6.19
(1,842)	2:170:B:TYR:HD1	2:181:B:ARG:HB3	6	6.19
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB2	6	6.19
(1,842)	2:170:B:TYR:HD2	2:181:B:ARG:HB3	6	6.19
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	2	6.19
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	2	6.19
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	2	6.19
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	7	6.19
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	7	6.19
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	15	6.19
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	4	6.18
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	4	6.18
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	4	6.18
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	11	6.18
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	10	6.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	10	6.16
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	10	6.16
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	5	6.15
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	1	6.12
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	1	6.12
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	1	6.12
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	14	6.12
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	14	6.12
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	14	6.12
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	3	6.12
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	13	6.1
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	9	6.08
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	9	6.08
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	9	6.08
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	16	6.08
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	16	6.08
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	3	6.07
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	3	6.07
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	3	6.07
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	11	6.07
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	11	6.07
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	11	6.07
(1,230)	2:160:B:VAL:HA	2:154:B:ARG:H	5	6.07
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	8	6.04
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	8	6.04
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	8	6.04
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	15	6.01
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	15	6.01
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	15	6.01
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	8	5.99
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	8	5.99
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	6	5.97
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	6	5.97
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	6	5.97
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	1	5.95
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	13	5.94
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	13	5.94
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	13	5.94
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	4	5.93
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	10	5.93
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	14	5.93
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	4	5.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	6	5.91
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	6	5.91
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	12	5.91
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	16	5.9
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	16	5.9
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	16	5.9
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	3	5.89
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	3	5.89
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	7	5.87
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	7	5.87
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	7	5.87
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	8	5.83
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	8	5.83
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	8	5.83
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	2	5.83
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	14	5.82
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	14	5.82
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	12	5.81
(1,691)	2:160:B:VAL:HG21	2:153:B:TYR:HB2	5	5.8
(1,691)	2:160:B:VAL:HG22	2:153:B:TYR:HB2	5	5.8
(1,691)	2:160:B:VAL:HG23	2:153:B:TYR:HB2	5	5.8
(1,283)	2:134:B:TRP:H	2:160:B:VAL:H	8	5.78
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	8	5.78
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	3	5.73
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	11	5.72
(1,303)	2:181:B:ARG:HB2	2:175:B:LEU:H	11	5.71
(1,303)	2:181:B:ARG:HB3	2:175:B:LEU:H	11	5.71
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	1	5.7
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	10	5.69
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	2	5.66
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	14	5.66
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	11	5.58
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	11	5.58
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	11	5.58
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	9	5.54
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	15	5.52
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	3	5.51
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	3	5.51
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	3	5.51
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	7	5.51
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	7	5.51
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	7	5.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	8	5.48
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	8	5.48
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	8	5.48
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	8	5.48
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	8	5.48
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	8	5.48
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	12	5.47
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	6	5.47
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	7	5.47
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	16	5.46
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	16	5.46
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	16	5.46
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	4	5.46
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	12	5.46
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	12	5.46
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	12	5.46
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	13	5.46
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	6	5.44
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	6	5.44
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	6	5.44
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	15	5.42
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	15	5.42
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	15	5.42
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	14	5.41
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	14	5.41
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	14	5.41
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	7	5.39
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	10	5.39
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	10	5.39
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	10	5.39
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	13	5.38
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	10	5.38
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	3	5.37
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	4	5.37
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	4	5.37
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	4	5.37
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	3	5.37
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	2	5.36
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	1	5.36
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	1	5.36
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	1	5.36
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	12	5.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	12	5.35
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	12	5.35
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	13	5.35
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	13	5.35
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	13	5.35
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	1	5.33
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	16	5.33
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	5	5.32
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	5	5.32
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	5	5.32
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	8	5.32
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	11	5.32
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	4	5.32
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	4	5.32
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	4	5.32
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	6	5.31
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	14	5.31
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	4	5.3
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	4	5.3
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	4	5.3
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	9	5.29
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	9	5.29
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	9	5.29
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	9	5.28
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	9	5.28
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	9	5.28
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	9	5.26
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	15	5.26
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	15	5.26
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	15	5.26
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	10	5.25
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	10	5.25
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	10	5.25
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	11	5.24
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	7	5.24
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	7	5.24
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	7	5.24
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	15	5.24
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	13	5.23
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	13	5.23
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	13	5.23
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	2	5.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	2	5.23
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	2	5.23
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	3	5.22
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	3	5.22
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	3	5.22
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	6	5.22
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	3	5.22
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	3	5.22
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	3	5.22
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	3	5.22
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	3	5.22
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	3	5.22
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	16	5.21
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	8	5.21
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	8	5.21
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	8	5.21
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	6	5.21
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	6	5.21
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	6	5.21
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	11	5.21
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	11	5.21
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	11	5.21
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	2	5.21
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	2	5.21
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	2	5.21
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	11	5.21
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	11	5.21
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	11	5.21
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	13	5.2
(1,233)	2:160:B:VAL:HB	2:154:B:ARG:H	5	5.2
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	14	5.19
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	14	5.19
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	14	5.19
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	7	5.19
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	8	5.19
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	8	5.19
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	8	5.19
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	5	5.18
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG13	1	5.18
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG11	1	5.18
(1,1110)	2:133:B:SER:HA	2:160:B:VAL:HG12	1	5.18
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	12	5.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	12	5.18
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	12	5.18
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	6	5.17
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	6	5.17
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	6	5.17
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	7	5.17
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	7	5.17
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	7	5.17
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	2	5.16
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	2	5.16
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	2	5.16
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	4	5.14
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	4	5.14
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	4	5.14
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	4	5.14
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	4	5.14
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	4	5.14
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	4	5.12
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	11	5.12
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	11	5.12
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	11	5.12
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	2	5.11
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	8	5.11
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	16	5.09
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	16	5.09
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	16	5.09
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	13	5.09
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	13	5.09
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	13	5.09
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	10	5.09
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	10	5.09
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	10	5.09
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	14	5.08
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	14	5.08
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	14	5.08
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	5	5.07
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	5	5.07
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	5	5.07
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	12	5.06
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	15	5.06
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	1	5.04
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	7	5.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	7	5.04
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	7	5.04
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	8	5.0
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	8	5.0
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	8	5.0
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	5	5.0
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	9	4.99
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	10	4.99
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	2	4.99
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	2	4.99
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	2	4.99
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	4	4.99
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	4	4.99
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	4	4.99
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	12	4.99
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	12	4.99
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	12	4.99
(1,741)	2:160:B:VAL:HB	2:153:B:TYR:H	16	4.97
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	13	4.97
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	13	4.97
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	13	4.97
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	15	4.96
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	15	4.96
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	15	4.96
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	5	4.96
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	5	4.96
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	5	4.96
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	6	4.96
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	6	4.96
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	6	4.96
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	16	4.96
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	16	4.96
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	16	4.96
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	12	4.95
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	12	4.95
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	12	4.95
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	12	4.95
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	12	4.95
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	12	4.95
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	12	4.95
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	12	4.95
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	12	4.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	9	4.95
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	9	4.95
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	9	4.95
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	1	4.94
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	1	4.94
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	1	4.94
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	1	4.94
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	1	4.94
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	1	4.94
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	1	4.94
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	1	4.94
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	1	4.94
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	4	4.94
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	4	4.94
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	4	4.94
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	3	4.92
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	3	4.92
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	3	4.92
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	3	4.92
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	3	4.92
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	3	4.92
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	15	4.92
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	15	4.92
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	15	4.92
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	11	4.91
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	11	4.91
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	11	4.91
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	11	4.91
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	11	4.91
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	11	4.91
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	9	4.9
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	9	4.9
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	9	4.9
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	1	4.9
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	1	4.9
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	1	4.9
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	10	4.9
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	10	4.9
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	10	4.9
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	1	4.9
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	1	4.9
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	1	4.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	10	4.89
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	10	4.89
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	10	4.89
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	14	4.89
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	14	4.89
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	14	4.89
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	7	4.88
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	7	4.88
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	7	4.88
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	3	4.87
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	3	4.87
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	3	4.87
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	11	4.87
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	11	4.87
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	11	4.87
(1,1282)	2:134:B:TRP:HD1	2:160:B:VAL:HB	14	4.86
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	10	4.86
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	10	4.86
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	10	4.86
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	10	4.86
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	10	4.86
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	10	4.86
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	2	4.85
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	2	4.85
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	2	4.85
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	2	4.85
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	2	4.85
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	2	4.85
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	2	4.85
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	2	4.85
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	2	4.85
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	3	4.85
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	3	4.85
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	3	4.85
(1,347)	2:160:B:VAL:HG21	2:156:B:GLY:H	16	4.85
(1,347)	2:160:B:VAL:HG22	2:156:B:GLY:H	16	4.85
(1,347)	2:160:B:VAL:HG23	2:156:B:GLY:H	16	4.85
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	6	4.84
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	6	4.84
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	6	4.84
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	9	4.84
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	9	4.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	9	4.84
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	16	4.83
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	16	4.83
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	16	4.83
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	11	4.83
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	11	4.83
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	11	4.83
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	15	4.83
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	15	4.83
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	15	4.83
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	8	4.82
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	8	4.82
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	8	4.82
(1,210)	2:160:B:VAL:HG13	2:155:B:ASP:H	5	4.81
(1,210)	2:160:B:VAL:HG11	2:155:B:ASP:H	5	4.81
(1,210)	2:160:B:VAL:HG12	2:155:B:ASP:H	5	4.81
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	13	4.79
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	13	4.79
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	13	4.79
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	14	4.78
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	14	4.78
(1,1122)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	14	4.78
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	6	4.76
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	6	4.76
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	6	4.76
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	5	4.75
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	5	4.75
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	5	4.75
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	14	4.73
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	14	4.73
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	14	4.73
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	14	4.73
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	14	4.73
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	14	4.73
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	4	4.72
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	4	4.72
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	4	4.72
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	15	4.72
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	15	4.72
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	15	4.72
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	13	4.72
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	13	4.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	13	4.72
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	12	4.7
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	12	4.7
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	12	4.7
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	7	4.67
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	7	4.67
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	7	4.67
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	12	4.67
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	12	4.67
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	12	4.67
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	10	4.66
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	10	4.66
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	10	4.66
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG2	16	4.64
(1,1113)	2:160:B:VAL:HG13	2:154:B:ARG:HG3	16	4.64
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG2	16	4.64
(1,1113)	2:160:B:VAL:HG11	2:154:B:ARG:HG3	16	4.64
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG2	16	4.64
(1,1113)	2:160:B:VAL:HG12	2:154:B:ARG:HG3	16	4.64
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	9	4.64
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	9	4.64
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	9	4.64
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	2	4.62
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	2	4.62
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	2	4.62
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	12	4.6
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	12	4.6
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	12	4.6
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	1	4.6
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	9	4.59
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	11	4.58
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	16	4.57
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	16	4.57
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	16	4.57
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	16	4.57
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	16	4.57
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	4	4.57
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	1	4.56
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	1	4.56
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	1	4.56
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	8	4.55
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	8	4.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	8	4.55
(1,1042)	2:160:B:VAL:HG21	2:153:B:TYR:H	5	4.55
(1,1042)	2:160:B:VAL:HG22	2:153:B:TYR:H	5	4.55
(1,1042)	2:160:B:VAL:HG23	2:153:B:TYR:H	5	4.55
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	2	4.55
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	3	4.55
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	15	4.55
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	9	4.54
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	9	4.54
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	9	4.54
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	8	4.53
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	10	4.53
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	13	4.53
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	14	4.53
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	14	4.52
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	14	4.52
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	14	4.52
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	15	4.51
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	15	4.51
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	15	4.51
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	6	4.51
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	7	4.5
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	12	4.5
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG13	14	4.49
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG11	14	4.49
(1,1106)	2:134:B:TRP:H	2:160:B:VAL:HG12	14	4.49
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	6	4.48
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	6	4.48
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	6	4.48
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	11	4.48
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	11	4.48
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	11	4.48
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	16	4.48
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	7	4.47
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	8	4.47
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	8	4.47
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	8	4.47
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	3	4.46
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	11	4.45
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	16	4.45
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	2	4.45
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	2	4.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	2	4.45
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	7	4.45
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	7	4.45
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	7	4.45
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	10	4.44
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	10	4.44
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	10	4.44
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	11	4.43
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	11	4.43
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	11	4.43
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	6	4.43
(1,284)	2:160:B:VAL:H	2:153:B:TYR:H	5	4.42
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	4	4.41
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	4	4.41
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	4	4.41
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	4	4.41
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	4	4.41
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	4	4.41
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	15	4.4
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	15	4.4
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	15	4.4
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	1	4.4
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	1	4.4
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	1	4.4
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	12	4.39
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	12	4.39
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	12	4.39
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	12	4.38
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	12	4.38
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	12	4.38
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	3	4.38
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	3	4.38
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	3	4.38
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	16	4.37
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	16	4.37
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	16	4.37
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	3	4.35
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	3	4.35
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	3	4.35
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	6	4.35
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	6	4.35
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	6	4.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	13	4.35
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	13	4.35
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	13	4.35
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	13	4.35
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	9	4.34
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	9	4.34
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	9	4.34
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	5	4.32
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	5	4.32
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	7	4.32
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	7	4.32
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	1	4.31
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	1	4.31
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	1	4.31
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	14	4.3
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	14	4.3
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	14	4.3
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	5	4.3
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	15	4.3
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	5	4.3
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	5	4.3
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	5	4.3
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	1	4.29
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	1	4.29
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	1	4.29
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	4	4.29
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	4	4.29
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	4	4.29
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	7	4.29
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	7	4.29
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	7	4.29
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	14	4.29
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	14	4.29
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	14	4.29
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	10	4.28
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	10	4.28
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	10	4.28
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	4	4.27
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	12	4.26
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	6	4.26
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	6	4.26
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	10	4.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	10	4.26
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	10	4.26
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	3	4.25
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	3	4.25
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	3	4.25
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	10	4.25
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	10	4.25
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	10	4.25
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	11	4.25
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	11	4.25
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	11	4.25
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	8	4.24
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	8	4.24
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	8	4.24
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	9	4.23
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	10	4.2
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	16	4.2
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	13	4.19
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	13	4.19
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	13	4.19
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	13	4.18
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	13	4.18
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	2	4.18
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	2	4.18
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	2	4.18
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	2	4.15
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	6	4.15
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	9	4.15
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	9	4.15
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	9	4.15
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	7	4.14
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	13	4.14
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	15	4.14
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	15	4.14
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	15	4.14
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	5	4.13
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	5	4.13
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	5	4.13
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	4	4.13
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	1	4.12
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	3	4.12
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	3	4.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	2	4.12
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	3	4.12
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	12	4.11
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	12	4.11
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	12	4.11
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	12	4.11
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	12	4.11
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	12	4.11
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	16	4.11
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	1	4.11
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	5	4.11
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	9	4.11
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	11	4.11
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	15	4.11
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	2	4.1
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	2	4.1
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	2	4.1
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	14	4.1
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG21	8	4.08
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG22	8	4.08
(1,1043)	2:133:B:SER:HA	2:160:B:VAL:HG23	8	4.08
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	8	4.08
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	10	4.08
(1,285)	2:151:B:ASP:HA	2:160:B:VAL:H	12	4.08
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	8	4.07
(1,749)	2:134:B:TRP:H	2:160:B:VAL:HB	14	4.06
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	4	4.05
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	4	4.05
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	4	4.05
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	4	4.05
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	4	4.05
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	4	4.05
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	16	4.04
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	16	4.04
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	16	4.04
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	5	4.04
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	5	4.04
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	5	4.04
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	6	4.04
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	6	4.04
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	6	4.04
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	12	4.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	12	4.02
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	12	4.02
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	3	4.01
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	3	4.01
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	3	4.01
(1,342)	2:160:B:VAL:HG21	2:157:B:THR:H	16	4.01
(1,342)	2:160:B:VAL:HG22	2:157:B:THR:H	16	4.01
(1,342)	2:160:B:VAL:HG23	2:157:B:THR:H	16	4.01
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	13	4.01
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	13	4.01
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	13	4.01
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	11	4.0
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	11	4.0
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	2	3.99
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	2	3.99
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	2	3.99
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	9	3.99
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	9	3.99
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	4	3.99
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	4	3.99
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	4	3.99
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	8	3.98
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	8	3.98
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	8	3.98
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	7	3.98
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	7	3.98
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	7	3.98
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	10	3.97
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	10	3.97
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	10	3.97
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	1	3.97
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	1	3.97
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	13	3.97
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	13	3.97
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	13	3.97
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	11	3.96
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	11	3.96
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	11	3.96
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	15	3.96
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	15	3.96
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	12	3.94
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	12	3.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	12	3.94
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	16	3.92
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	16	3.92
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	16	3.92
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	7	3.91
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	7	3.91
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	7	3.91
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	1	3.91
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	1	3.91
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	1	3.91
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	16	3.9
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	16	3.9
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	16	3.9
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	6	3.88
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	6	3.88
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	6	3.88
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	15	3.88
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	15	3.88
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	15	3.88
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	13	3.86
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	13	3.86
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	13	3.86
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	3	3.86
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	3	3.86
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	3	3.86
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	4	3.86
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	4	3.86
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	8	3.86
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	8	3.86
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	1	3.85
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	1	3.85
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	1	3.85
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	14	3.83
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	14	3.83
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	14	3.83
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	2	3.83
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	2	3.83
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	14	3.83
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	14	3.83
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	12	3.82
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	12	3.82
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	7	3.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	9	3.8
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	9	3.8
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	9	3.8
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	2	3.8
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	2	3.8
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	2	3.8
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	15	3.79
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	15	3.79
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	15	3.79
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	7	3.78
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	7	3.78
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	7	3.78
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	9	3.78
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	9	3.78
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	9	3.78
(1,231)	2:160:B:VAL:HG21	2:154:B:ARG:H	5	3.78
(1,231)	2:160:B:VAL:HG22	2:154:B:ARG:H	5	3.78
(1,231)	2:160:B:VAL:HG23	2:154:B:ARG:H	5	3.78
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	8	3.77
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	8	3.77
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	8	3.77
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	3	3.76
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	3	3.76
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	3	3.76
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	14	3.74
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	14	3.74
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	14	3.74
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	7	3.73
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	7	3.73
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	7	3.73
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	13	3.73
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	13	3.73
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	13	3.73
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	5	3.73
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	5	3.73
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	5	3.73
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	11	3.73
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	11	3.73
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	11	3.73
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	5	3.73
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	6	3.72
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	3	3.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	3	3.71
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	3	3.71
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	15	3.7
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	15	3.7
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	15	3.7
(1,287)	2:134:B:TRP:HB2	2:160:B:VAL:H	10	3.7
(1,287)	2:134:B:TRP:HB3	2:160:B:VAL:H	10	3.7
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	10	3.69
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	10	3.69
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	10	3.69
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	11	3.69
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	6	3.66
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	6	3.66
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	6	3.66
(1,1107)	2:160:B:VAL:HG13	2:153:B:TYR:H	16	3.63
(1,1107)	2:160:B:VAL:HG11	2:153:B:TYR:H	16	3.63
(1,1107)	2:160:B:VAL:HG12	2:153:B:TYR:H	16	3.63
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	1	3.63
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	1	3.63
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	1	3.63
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	3	3.6
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	11	3.59
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	11	3.59
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	11	3.59
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	5	3.59
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	5	3.59
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	5	3.59
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	13	3.59
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	2	3.58
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	2	3.58
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	2	3.58
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	5	3.57
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	5	3.57
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	5	3.57
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	9	3.57
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	9	3.57
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	9	3.57
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	16	3.56
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	16	3.56
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	16	3.56
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	9	3.56
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	7	3.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	7	3.55
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	7	3.55
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	15	3.55
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	6	3.52
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	6	3.52
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	6	3.52
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	8	3.51
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	8	3.51
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	8	3.51
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	11	3.51
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	11	3.51
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	11	3.51
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	14	3.51
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	14	3.51
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	14	3.51
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	3	3.5
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	3	3.5
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	3	3.5
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	3	3.5
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	3	3.5
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	3	3.5
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	13	3.5
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	13	3.5
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	13	3.5
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	13	3.5
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	13	3.5
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	13	3.5
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	2	3.5
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	2	3.5
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	2	3.5
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	4	3.5
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	4	3.5
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	4	3.5
(1,250)	2:171:B:ALA:HB1	2:181:B:ARG:H	6	3.5
(1,250)	2:171:B:ALA:HB2	2:181:B:ARG:H	6	3.5
(1,250)	2:171:B:ALA:HB3	2:181:B:ARG:H	6	3.5
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	15	3.49
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	15	3.49
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	15	3.49
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	6	3.47
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	6	3.47
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	6	3.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	6	3.47
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	6	3.47
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	6	3.47
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	7	3.46
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	7	3.46
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	7	3.46
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	7	3.46
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	7	3.46
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	7	3.46
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	12	3.46
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	12	3.46
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	12	3.46
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	13	3.46
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	13	3.46
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	13	3.46
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	6	3.46
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	6	3.46
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	6	3.46
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	11	3.46
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	11	3.46
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	11	3.46
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	1	3.46
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	2	3.45
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	2	3.45
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	2	3.45
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	2	3.45
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	2	3.45
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	2	3.45
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	3	3.45
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	3	3.45
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	3	3.45
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	16	3.45
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	16	3.45
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	16	3.45
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	1	3.44
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	1	3.44
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	1	3.44
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	10	3.43
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	10	3.43
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	10	3.43
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	12	3.43
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	12	3.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	12	3.43
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	15	3.43
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	15	3.43
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	15	3.43
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	4	3.43
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	14	3.42
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	14	3.42
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	14	3.42
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	14	3.42
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	14	3.42
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	14	3.42
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	11	3.41
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	11	3.41
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	11	3.41
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	11	3.41
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	11	3.41
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	11	3.41
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	9	3.41
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	9	3.41
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	9	3.41
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	2	3.41
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	16	3.4
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	16	3.4
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	16	3.4
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	16	3.4
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	16	3.4
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	16	3.4
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	14	3.4
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG21	8	3.39
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG22	8	3.39
(1,1046)	2:132:B:GLY:HA3	2:160:B:VAL:HG23	8	3.39
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	7	3.39
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	7	3.39
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	7	3.39
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	9	3.38
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	9	3.38
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	9	3.38
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	12	3.37
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	12	3.37
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	12	3.37
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	12	3.37
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	12	3.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	12	3.37
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	15	3.36
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	15	3.36
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	15	3.36
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	15	3.36
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	15	3.36
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	15	3.36
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	1	3.36
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	1	3.36
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	1	3.36
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	4	3.36
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	4	3.36
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	4	3.36
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	13	3.36
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	13	3.36
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	13	3.36
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	1	3.35
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	1	3.35
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	1	3.35
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	1	3.35
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	1	3.35
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	1	3.35
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	4	3.35
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	4	3.35
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	4	3.35
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	4	3.35
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	4	3.35
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	4	3.35
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	5	3.31
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	5	3.31
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	5	3.31
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	5	3.31
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	5	3.31
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	5	3.31
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	9	3.31
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	9	3.31
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	9	3.31
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	9	3.31
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	9	3.31
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	9	3.31
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG13	14	3.31
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG11	14	3.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1112)	2:134:B:TRP:HB3	2:160:B:VAL:HG12	14	3.31
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	12	3.31
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	16	3.3
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	16	3.3
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	16	3.3
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	16	3.3
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	16	3.3
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	16	3.3
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	2	3.3
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	2	3.3
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	2	3.3
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	2	3.3
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	2	3.3
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	2	3.3
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	14	3.3
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	14	3.3
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	14	3.3
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	8	3.29
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	8	3.29
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	8	3.29
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	8	3.29
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	8	3.29
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	8	3.29
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	7	3.29
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	7	3.29
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	7	3.29
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	16	3.29
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	16	3.29
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	16	3.29
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	10	3.29
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	10	3.29
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	10	3.29
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	8	3.29
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	10	3.27
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	10	3.27
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	10	3.27
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	10	3.27
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	10	3.27
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	10	3.27
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	5	3.25
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	5	3.25
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	5	3.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,286)	2:134:B:TRP:HA	2:160:B:VAL:H	10	3.25
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	5	3.24
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	5	3.24
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	5	3.24
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	6	3.23
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	6	3.23
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	6	3.23
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	11	3.23
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	11	3.23
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	11	3.23
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG11	14	3.22
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG12	14	3.22
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG13	14	3.22
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	14	3.22
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	14	3.22
(1,1288)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	14	3.22
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	13	3.22
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	13	3.22
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	13	3.22
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	2	3.22
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	2	3.22
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	2	3.22
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	3	3.21
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	3	3.21
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	3	3.21
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG21	8	3.16
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG22	8	3.16
(1,1041)	2:134:B:TRP:H	2:160:B:VAL:HG23	8	3.16
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	8	3.14
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	8	3.14
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	8	3.14
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	8	3.14
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	8	3.14
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	8	3.14
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	11	3.14
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	11	3.14
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	11	3.14
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	11	3.14
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	11	3.14
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	11	3.14
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	10	3.11
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	10	3.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	10	3.11
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	10	3.11
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	10	3.11
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	10	3.11
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	2	3.09
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	2	3.09
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	2	3.09
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	4	3.08
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	4	3.08
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	4	3.08
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	13	3.07
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	13	3.07
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	13	3.07
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	13	3.07
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	13	3.07
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	13	3.07
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	3	3.05
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	3	3.05
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	3	3.05
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	3	3.05
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	3	3.05
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	3	3.05
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	15	3.0
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	15	3.0
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	15	3.0
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	8	2.98
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	8	2.98
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	8	2.98
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	9	2.97
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	9	2.97
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	9	2.97
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	9	2.97
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	9	2.97
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	9	2.97
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	1	2.97
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	1	2.97
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	1	2.97
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	12	2.96
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	12	2.96
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	12	2.96
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	9	2.95
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	9	2.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	9	2.95
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	10	2.9
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	10	2.9
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	10	2.9
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	4	2.84
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	4	2.84
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	4	2.84
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	4	2.84
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	4	2.84
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	4	2.84
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	1	2.77
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	1	2.77
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	1	2.77
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	1	2.77
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	1	2.77
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	1	2.77
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG13	14	2.77
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG11	14	2.77
(1,1109)	2:135:B:GLN:H	2:160:B:VAL:HG12	14	2.77
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	5	2.76
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	5	2.76
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	5	2.76
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	5	2.76
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	5	2.76
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	5	2.76
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	15	2.72
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	15	2.72
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	15	2.72
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	15	2.72
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	15	2.72
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	15	2.72
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	3	2.68
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	3	2.68
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	3	2.68
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	13	2.68
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	13	2.68
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	13	2.68
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	12	2.68
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	6	2.66
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	6	2.66
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	6	2.66
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	9	2.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	14	2.63
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	15	2.63
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	7	2.62
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	7	2.62
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	7	2.62
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	11	2.61
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	12	2.6
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	12	2.6
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	12	2.6
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	11	2.59
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	11	2.59
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	11	2.59
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	7	2.59
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	7	2.59
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	7	2.59
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	7	2.59
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	7	2.59
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	7	2.59
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	6	2.59
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	8	2.59
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	16	2.58
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	16	2.58
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	16	2.58
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	3	2.58
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	3	2.58
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	3	2.58
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	1	2.58
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	10	2.58
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	7	2.57
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	7	2.57
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	7	2.57
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	7	2.57
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	7	2.57
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	7	2.57
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	1	2.57
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	1	2.57
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	1	2.57
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	15	2.57
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	15	2.57
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	15	2.57
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	5	2.57
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	5	2.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	5	2.57
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	4	2.56
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	4	2.56
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	4	2.56
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	6	2.56
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	6	2.56
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	6	2.56
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	13	2.56
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	13	2.56
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	13	2.56
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	3	2.56
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	3	2.56
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	3	2.56
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	16	2.56
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	16	2.56
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	16	2.56
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	2	2.55
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	2	2.55
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	2	2.55
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	11	2.55
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	11	2.55
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	11	2.55
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	2	2.55
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	4	2.54
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	4	2.54
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	4	2.54
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	12	2.54
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	12	2.54
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	12	2.54
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	16	2.54
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	16	2.54
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	16	2.54
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	3	2.54
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	7	2.54
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	6	2.53
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	6	2.53
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	6	2.53
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	10	2.52
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	10	2.52
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	10	2.52
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	10	2.52
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	10	2.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	10	2.52
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	12	2.52
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	12	2.52
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	12	2.52
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	16	2.52
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	16	2.52
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	16	2.52
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	9	2.51
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	9	2.51
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	9	2.51
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	8	2.51
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	8	2.51
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	8	2.51
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	13	2.51
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	13	2.51
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	13	2.51
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	4	2.5
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	4	2.5
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	4	2.5
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	9	2.5
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	9	2.5
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	9	2.5
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	14	2.5
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	14	2.5
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	14	2.5
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	2	2.49
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	2	2.49
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	2	2.49
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	11	2.48
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	11	2.48
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	11	2.48
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	5	2.48
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	5	2.48
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	5	2.48
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	13	2.48
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	2	2.47
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	2	2.47
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	2	2.47
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	15	2.47
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	15	2.47
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	15	2.47
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	5	2.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	5	2.46
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	5	2.46
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	8	2.46
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	8	2.46
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	8	2.46
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	10	2.46
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	10	2.46
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	10	2.46
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	13	2.46
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	5	2.46
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	7	2.45
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	3	2.45
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	3	2.45
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	3	2.45
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	6	2.45
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	6	2.45
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	6	2.45
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	4	2.45
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	4	2.45
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	4	2.45
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	3	2.44
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	7	2.44
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	7	2.44
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	7	2.44
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG21	14	2.43
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG22	14	2.43
(1,1060)	2:134:B:TRP:HD1	2:160:B:VAL:HG23	14	2.43
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	1	2.43
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	1	2.43
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	1	2.43
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	5	2.43
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	5	2.43
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	5	2.43
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	14	2.43
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	14	2.43
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	14	2.43
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	15	2.43
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	15	2.43
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	15	2.43
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	4	2.43
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	1	2.42
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	1	2.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	1	2.42
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	4	2.41
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	4	2.41
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	4	2.41
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	8	2.4
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	8	2.4
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	8	2.4
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	11	2.4
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	11	2.4
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	11	2.4
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	13	2.4
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	13	2.4
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	13	2.4
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG13	9	2.38
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG11	9	2.38
(1,550)	2:151:B:ASP:HA	2:160:B:VAL:HG12	9	2.38
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	3	2.38
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	3	2.38
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	3	2.38
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	6	2.37
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	2	2.36
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	2	2.36
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	2	2.36
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	15	2.35
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	15	2.35
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	15	2.35
(1,570)	2:160:B:VAL:HG21	2:158:B:GLY:HA2	16	2.34
(1,570)	2:160:B:VAL:HG22	2:158:B:GLY:HA2	16	2.34
(1,570)	2:160:B:VAL:HG23	2:158:B:GLY:HA2	16	2.34
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	12	2.34
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	12	2.34
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	12	2.34
(1,455)	2:160:B:VAL:HA	2:158:B:GLY:HA3	16	2.32
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG13	6	2.31
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG11	6	2.31
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG12	6	2.31
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG21	6	2.31
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG22	6	2.31
(1,1409)	1:4:A:A:H2	2:160:B:VAL:HG23	6	2.31
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	11	2.28
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	8	2.27
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	8	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	8	2.27
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	10	2.27
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	10	2.27
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	10	2.27
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	1	2.26
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	1	2.26
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	1	2.26
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	9	2.26
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	9	2.26
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	9	2.26
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	5	2.25
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	7	2.25
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	7	2.25
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	7	2.25
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	16	2.23
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	11	2.22
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	11	2.22
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	11	2.22
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	4	2.21
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	2	2.2
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	8	2.2
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	15	2.17
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	5	2.17
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	5	2.17
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	5	2.17
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG13	14	2.16
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG11	14	2.16
(1,461)	2:134:B:TRP:HA	2:160:B:VAL:HG12	14	2.16
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	14	2.16
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	14	2.16
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	14	2.16
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	12	2.15
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	12	2.14
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	12	2.14
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	12	2.14
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	1	2.12
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	10	2.11
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	6	2.09
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	6	2.09
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	6	2.09
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	9	2.08
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	1	2.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	1	2.06
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	1	2.06
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	2	2.03
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	2	2.03
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	2	2.03
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	2	1.99
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	2	1.99
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	2	1.99
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	2	1.99
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	2	1.99
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	2	1.99
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	2	1.99
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	2	1.99
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	2	1.99
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	2	1.99
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	2	1.99
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	2	1.99
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	13	1.98
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	13	1.98
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	13	1.98
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	3	1.97
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	3	1.97
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	3	1.97
(1,898)	2:134:B:TRP:HB3	2:160:B:VAL:HB	14	1.97
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	12	1.96
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	12	1.96
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	12	1.96
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	13	1.96
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	13	1.96
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	13	1.96
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	10	1.95
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	10	1.95
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	10	1.95
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	10	1.94
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	10	1.94
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	10	1.94
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	10	1.94
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	10	1.94
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	10	1.94
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	10	1.94
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	10	1.94
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	10	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	10	1.94
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	10	1.94
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	10	1.94
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	15	1.94
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	15	1.94
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	15	1.94
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	4	1.93
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	4	1.93
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	4	1.93
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	4	1.93
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	4	1.93
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	4	1.93
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	4	1.93
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	4	1.93
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	4	1.93
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	4	1.93
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	4	1.93
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	4	1.93
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	6	1.93
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	6	1.93
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	6	1.93
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	3	1.92
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	3	1.92
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	3	1.92
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	3	1.92
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	3	1.92
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	3	1.92
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	3	1.92
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	3	1.92
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	3	1.92
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	3	1.92
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	3	1.92
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	3	1.92
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	12	1.92
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	12	1.92
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	12	1.92
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	12	1.92
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	12	1.92
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	12	1.92
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	12	1.92
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	12	1.92
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	12	1.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	12	1.92
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	12	1.92
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	12	1.92
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	15	1.91
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	15	1.91
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	15	1.91
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	6	1.9
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	6	1.9
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	6	1.9
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	6	1.9
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	6	1.9
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	6	1.9
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	6	1.9
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	6	1.9
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	6	1.9
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	6	1.9
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	6	1.9
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	6	1.9
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	14	1.9
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	14	1.9
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	14	1.9
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	7	1.9
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	7	1.9
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	7	1.9
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	13	1.9
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	13	1.9
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	13	1.9
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	7	1.89
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	7	1.89
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	7	1.89
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	12	1.89
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	12	1.89
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	12	1.89
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	7	1.88
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	7	1.88
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	7	1.88
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	7	1.88
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	7	1.88
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	7	1.88
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	7	1.88
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	7	1.88
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	7	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	7	1.88
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	7	1.88
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	7	1.88
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	8	1.88
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	8	1.88
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	8	1.88
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	8	1.88
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	8	1.88
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	8	1.88
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	8	1.88
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	8	1.88
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	8	1.88
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	8	1.88
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	8	1.88
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	8	1.88
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	9	1.88
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	9	1.88
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	9	1.88
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	9	1.88
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	9	1.88
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	9	1.88
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	9	1.88
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	9	1.88
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	9	1.88
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	9	1.88
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	9	1.88
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	9	1.88
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	1	1.88
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	1	1.88
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	1	1.88
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	10	1.88
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	10	1.88
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	10	1.88
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	11	1.87
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	11	1.87
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	11	1.87
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	11	1.87
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	11	1.87
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	11	1.87
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	11	1.87
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	11	1.87
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	11	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	11	1.87
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	11	1.87
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	11	1.87
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	13	1.87
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	13	1.87
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	13	1.87
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	13	1.87
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	13	1.87
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	13	1.87
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	13	1.87
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	13	1.87
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	13	1.87
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	13	1.87
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	13	1.87
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	13	1.87
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	14	1.87
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	14	1.87
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	14	1.87
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	14	1.87
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	14	1.87
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	14	1.87
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	14	1.87
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	14	1.87
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	14	1.87
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	14	1.87
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	14	1.87
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	14	1.87
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	11	1.87
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	11	1.87
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	11	1.87
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	2	1.87
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	2	1.87
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	2	1.87
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	3	1.87
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	3	1.87
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	3	1.87
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	9	1.86
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	9	1.86
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	9	1.86
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	15	1.86
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	15	1.86
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	15	1.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	6	1.85
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	6	1.85
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	6	1.85
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	9	1.85
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	9	1.85
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	9	1.85
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	4	1.84
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	4	1.84
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	4	1.84
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	4	1.84
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	4	1.84
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	4	1.84
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	6	1.84
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	6	1.84
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	6	1.84
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	15	1.83
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	15	1.83
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	15	1.83
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	15	1.83
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	15	1.83
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	15	1.83
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	15	1.83
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	15	1.83
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	15	1.83
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	15	1.83
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	15	1.83
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	15	1.83
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	9	1.83
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	9	1.83
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	9	1.83
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	1	1.82
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	1	1.82
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	1	1.82
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	1	1.82
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	1	1.82
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	1	1.82
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	1	1.82
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	1	1.82
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	1	1.82
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	1	1.82
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	1	1.82
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	1	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	5	1.82
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	5	1.82
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	5	1.82
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	5	1.82
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	5	1.82
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	5	1.82
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	5	1.82
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	5	1.82
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	5	1.82
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	5	1.82
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	5	1.82
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	5	1.82
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	5	1.82
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	5	1.82
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	5	1.82
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	16	1.82
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	16	1.82
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	16	1.82
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG21	8	1.82
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG22	8	1.82
(1,62)	2:133:B:SER:H	2:160:B:VAL:HG23	8	1.82
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	1	1.81
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	1	1.81
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	1	1.81
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	3	1.81
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	3	1.81
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	3	1.81
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	7	1.81
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	7	1.81
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	7	1.81
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD1	16	1.8
(1,1224)	2:160:B:VAL:HG11	2:153:B:TYR:HD2	16	1.8
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD1	16	1.8
(1,1224)	2:160:B:VAL:HG12	2:153:B:TYR:HD2	16	1.8
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD1	16	1.8
(1,1224)	2:160:B:VAL:HG13	2:153:B:TYR:HD2	16	1.8
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD1	16	1.8
(1,1224)	2:160:B:VAL:HG21	2:153:B:TYR:HD2	16	1.8
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD1	16	1.8
(1,1224)	2:160:B:VAL:HG22	2:153:B:TYR:HD2	16	1.8
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD1	16	1.8
(1,1224)	2:160:B:VAL:HG23	2:153:B:TYR:HD2	16	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	10	1.8
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	10	1.8
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	10	1.8
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	8	1.8
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	8	1.8
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	8	1.8
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	2	1.79
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	2	1.79
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	2	1.79
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	8	1.79
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	8	1.79
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	8	1.79
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	16	1.79
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	16	1.79
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	16	1.79
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	5	1.78
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	5	1.78
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	5	1.78
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	11	1.78
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	11	1.78
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	11	1.78
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	14	1.77
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	14	1.77
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	14	1.77
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	13	1.74
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	13	1.74
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	13	1.74
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	11	1.71
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	11	1.71
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	11	1.71
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG21	5	1.69
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG22	5	1.69
(1,1063)	2:134:B:TRP:HB3	2:160:B:VAL:HG23	5	1.69
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	8	1.65
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	8	1.65
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	8	1.65
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	4	1.64
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	4	1.64
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	4	1.64
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	12	1.64
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	12	1.64
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	12	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	2	1.62
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	2	1.62
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	2	1.62
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	15	1.61
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	15	1.61
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	15	1.61
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	1	1.6
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	1	1.6
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	1	1.6
(1,1045)	2:160:B:VAL:HG21	2:158:B:GLY:HA3	16	1.59
(1,1045)	2:160:B:VAL:HG22	2:158:B:GLY:HA3	16	1.59
(1,1045)	2:160:B:VAL:HG23	2:158:B:GLY:HA3	16	1.59
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	6	1.59
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	6	1.59
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	16	1.59
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	16	1.59
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	16	1.59
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	13	1.58
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	13	1.58
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	10	1.56
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	10	1.56
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	10	1.56
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	2	1.56
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	2	1.56
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	4	1.56
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	4	1.56
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	7	1.56
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	7	1.56
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	9	1.55
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	9	1.55
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	9	1.55
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	3	1.55
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	3	1.55
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	12	1.55
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	12	1.55
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	16	1.55
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	16	1.55
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	8	1.53
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	8	1.53
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	10	1.53
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	10	1.53
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	11	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	11	1.52
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	14	1.52
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	14	1.52
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	9	1.51
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	9	1.51
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	15	1.51
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	15	1.51
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	1	1.5
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	1	1.5
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	6	1.5
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	6	1.5
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	6	1.5
(1,288)	2:151:B:ASP:HB2	2:160:B:VAL:H	5	1.48
(1,288)	2:151:B:ASP:HB3	2:160:B:VAL:H	5	1.48
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	7	1.46
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	7	1.46
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	7	1.46
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	11	1.45
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	11	1.45
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	11	1.45
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG13	14	1.44
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG11	14	1.44
(1,897)	2:134:B:TRP:HB2	2:160:B:VAL:HG12	14	1.44
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	3	1.44
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	3	1.44
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	3	1.44
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	5	1.41
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	5	1.41
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	5	1.41
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	13	1.4
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	13	1.4
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	13	1.4
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	1	1.38
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	1	1.38
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	1	1.38
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	15	1.35
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	15	1.35
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	15	1.35
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	4	1.34
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	4	1.34
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	4	1.34
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	9	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	9	1.34
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	9	1.34
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	12	1.32
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	12	1.32
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	12	1.32
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	2	1.31
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	2	1.31
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	2	1.31
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	8	1.21
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	8	1.21
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	8	1.21
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	14	1.19
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	14	1.19
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	14	1.19
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	11	1.18
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	10	1.17
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG21	10	1.16
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG22	10	1.16
(1,29)	2:135:B:GLN:H	2:160:B:VAL:HG23	10	1.16
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	2	1.15
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	2	1.15
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	2	1.15
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	2	1.15
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	2	1.15
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	2	1.15
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	12	1.13
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	5	1.11
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	5	1.11
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	5	1.11
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	5	1.11
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	5	1.11
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	5	1.11
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	4	1.11
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	9	1.1
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	9	1.1
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	9	1.1
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	9	1.1
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	9	1.1
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	9	1.1
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	13	1.1
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	13	1.1
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	13	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	13	1.1
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	13	1.1
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	13	1.1
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	10	1.09
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	10	1.09
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	10	1.09
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	10	1.09
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	10	1.09
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	10	1.09
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	6	1.08
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	6	1.08
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	6	1.08
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	6	1.08
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	6	1.08
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	6	1.08
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	12	1.08
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	5	1.08
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	15	1.07
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	15	1.07
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	15	1.07
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	15	1.07
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	15	1.07
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	15	1.07
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	16	1.07
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	16	1.07
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	16	1.07
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	16	1.07
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	16	1.07
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	16	1.07
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	13	1.07
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	4	1.06
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	4	1.06
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	4	1.06
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	4	1.06
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	4	1.06
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	4	1.06
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	14	1.06
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	14	1.06
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	14	1.06
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	14	1.06
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	14	1.06
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	14	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	10	1.06
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	3	1.05
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	3	1.05
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	3	1.05
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	3	1.05
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	3	1.05
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	3	1.05
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	2	1.05
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	1	1.04
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	1	1.04
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	1	1.04
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	1	1.04
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	1	1.04
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	1	1.04
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	16	1.04
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	4	1.04
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	12	1.03
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	12	1.03
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	12	1.03
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	12	1.03
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	12	1.03
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	12	1.03
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	14	1.03
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	7	1.02
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	7	1.02
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	7	1.02
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	7	1.02
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	7	1.02
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	7	1.02
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	8	1.02
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	8	1.02
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	8	1.02
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	8	1.02
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	8	1.02
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	8	1.02
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	3	1.0
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	3	1.0
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	7	1.0
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE1	11	0.99
(1,1061)	2:160:B:VAL:HG21	2:153:B:TYR:HE2	11	0.99
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE1	11	0.99
(1,1061)	2:160:B:VAL:HG22	2:153:B:TYR:HE2	11	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE1	11	0.99
(1,1061)	2:160:B:VAL:HG23	2:153:B:TYR:HE2	11	0.99
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	6	0.99
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	2	0.98
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	9	0.98
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	8	0.97
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	15	0.97
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	1	0.96
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	9	0.96
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	7	0.95
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	15	0.95
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	16	0.94
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	6	0.94
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	12	0.93
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	1	0.93
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	5	0.93
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	11	0.93
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	10	0.9
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	14	0.9
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	13	0.89
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	13	0.89
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	7	0.87
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	11	0.85
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	16	0.85
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	3	0.82
(1,906)	2:181:B:ARG:H	2:181:B:ARG:HG2	8	0.81
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	11	0.81
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	6	0.79
(1,247)	2:116:B:SER:H	2:117:B:ARG:HB2	4	0.76
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	15	0.74
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	13	0.74
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	5	0.73
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	6	0.72
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	5	0.72
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	9	0.7
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	10	0.69
(1,748)	2:160:B:VAL:HB	2:158:B:GLY:HA3	16	0.69
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	12	0.68
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	1	0.66
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	3	0.64
(1,813)	2:178:B:THR:HA	2:179:B:LYS:HB2	5	0.64
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	4	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	4	0.61
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	14	0.61
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	7	0.6
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	16	0.59
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	15	0.58
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	2	0.57
(1,247)	2:116:B:SER:H	2:117:B:ARG:HB2	15	0.57
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	12	0.56
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	11	0.5
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	9	0.5
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	13	0.49
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	1	0.48
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	4	0.47
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	10	0.47
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	8	0.46
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	16	0.46
(1,806)	2:179:B:LYS:HB3	2:180:B:PHE:HA	5	0.46
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	2	0.45
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	8	0.45
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	3	0.44
(1,813)	2:178:B:THR:HA	2:179:B:LYS:HB2	13	0.44
(2,52)	1:6:A:G:N2	2:139:B:ASP:OD1	5	0.43
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	2	0.43
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	5	0.43
(1,806)	2:179:B:LYS:HB3	2:180:B:PHE:HA	13	0.43
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	15	0.42
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	8	0.42
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	11	0.41
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	13	0.41
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	6	0.4
(1,892)	2:174:B:LYS:HB3	2:174:B:LYS:HD3	13	0.4
(1,754)	2:134:B:TRP:HA	2:160:B:VAL:HB	14	0.4
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	10	0.39
(1,892)	2:174:B:LYS:HB3	2:174:B:LYS:HD3	3	0.39
(1,892)	2:174:B:LYS:HB3	2:174:B:LYS:HD3	8	0.39
(1,892)	2:174:B:LYS:HB3	2:174:B:LYS:HD3	15	0.39
(1,247)	2:116:B:SER:H	2:117:B:ARG:HB2	16	0.39
(2,52)	1:6:A:G:N2	2:139:B:ASP:OD1	9	0.38
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	2	0.38
(1,806)	2:179:B:LYS:HB3	2:180:B:PHE:HA	14	0.38
(1,247)	2:116:B:SER:H	2:117:B:ARG:HB2	10	0.38
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	12	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	1:3:A:A:H8	1:3:A:A:H3'	7	0.37
(1,933)	2:191:B:ARG:HG3	2:192:B:VAL:H	6	0.37
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	1	0.37
(1,247)	2:116:B:SER:H	2:117:B:ARG:HB2	8	0.37
(1,933)	2:191:B:ARG:HG3	2:192:B:VAL:H	2	0.36
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	1	0.35
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	6	0.35
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	9	0.35
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	3	0.34
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	7	0.33
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	14	0.33
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	15	0.33
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	16	0.33
(1,1362)	1:2:A:G:H8	1:2:A:G:H1'	10	0.32
(1,1362)	1:2:A:G:H8	1:2:A:G:H1'	12	0.32
(1,1362)	1:2:A:G:H8	1:2:A:G:H1'	15	0.32
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	15	0.32
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	4	0.31
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	7	0.31
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	14	0.31
(1,914)	2:181:B:ARG:H	2:181:B:ARG:HG3	8	0.31
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	5	0.31
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	9	0.31
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	4	0.3
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	14	0.3
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	10	0.3
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	1	0.29
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	3	0.29
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	4	0.29
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	1	0.29
(1,1362)	1:2:A:G:H8	1:2:A:G:H1'	13	0.28
(1,1362)	1:2:A:G:H8	1:2:A:G:H1'	14	0.28
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	13	0.28
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	6	0.27
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	12	0.27
(1,115)	2:121:B:ASN:H	2:122:B:ARG:HB2	16	0.27
(1,56)	2:126:B:SER:H	2:193:B:LYS:H	2	0.27
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	3	0.26
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	13	0.26
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	3	0.26
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	7	0.26
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	13	0.26
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	10	0.26
(1,715)	2:166:B:GLU:HA	2:166:B:GLU:HG3	13	0.26
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	4	0.25
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	5	0.25
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	8	0.25
(1,1047)	2:128:B:LEU:HD21	2:160:B:VAL:HG21	9	0.25
(1,1047)	2:128:B:LEU:HD21	2:160:B:VAL:HG22	9	0.25
(1,1047)	2:128:B:LEU:HD21	2:160:B:VAL:HG23	9	0.25
(1,1047)	2:128:B:LEU:HD22	2:160:B:VAL:HG21	9	0.25
(1,1047)	2:128:B:LEU:HD22	2:160:B:VAL:HG22	9	0.25
(1,1047)	2:128:B:LEU:HD22	2:160:B:VAL:HG23	9	0.25
(1,1047)	2:128:B:LEU:HD23	2:160:B:VAL:HG21	9	0.25
(1,1047)	2:128:B:LEU:HD23	2:160:B:VAL:HG22	9	0.25
(1,1047)	2:128:B:LEU:HD23	2:160:B:VAL:HG23	9	0.25
(1,1047)	2:128:B:LEU:HD12	2:160:B:VAL:HG21	9	0.25
(1,1047)	2:128:B:LEU:HD12	2:160:B:VAL:HG22	9	0.25
(1,1047)	2:128:B:LEU:HD12	2:160:B:VAL:HG23	9	0.25
(1,1047)	2:128:B:LEU:HD13	2:160:B:VAL:HG21	9	0.25
(1,1047)	2:128:B:LEU:HD13	2:160:B:VAL:HG22	9	0.25
(1,1047)	2:128:B:LEU:HD13	2:160:B:VAL:HG23	9	0.25
(1,1047)	2:128:B:LEU:HD11	2:160:B:VAL:HG21	9	0.25
(1,1047)	2:128:B:LEU:HD11	2:160:B:VAL:HG22	9	0.25
(1,1047)	2:128:B:LEU:HD11	2:160:B:VAL:HG23	9	0.25
(1,933)	2:191:B:ARG:HG3	2:192:B:VAL:H	14	0.25
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	9	0.25
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	16	0.25
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	7	0.25
(1,744)	2:131:B:SER:H	2:184:B:GLU:HG2	5	0.25
(1,744)	2:131:B:SER:H	2:184:B:GLU:HG2	12	0.25
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	14	0.25
(1,355)	2:127:B:GLY:H	2:128:B:LEU:HB3	16	0.25
(1,311)	2:186:B:GLU:HG3	2:187:B:THR:H	10	0.25
(1,292)	2:120:B:GLU:H	2:120:B:GLU:HG2	7	0.25
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	11	0.24
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	2	0.24
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	5	0.24
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	9	0.24
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	2	0.24
(1,1362)	1:2:A:G:H8	1:2:A:G:H1'	1	0.24
(1,1047)	2:128:B:LEU:HD21	2:160:B:VAL:HG21	7	0.24
(1,1047)	2:128:B:LEU:HD21	2:160:B:VAL:HG22	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1047)	2:128:B:LEU:HD21	2:160:B:VAL:HG23	7	0.24
(1,1047)	2:128:B:LEU:HD22	2:160:B:VAL:HG21	7	0.24
(1,1047)	2:128:B:LEU:HD22	2:160:B:VAL:HG22	7	0.24
(1,1047)	2:128:B:LEU:HD22	2:160:B:VAL:HG23	7	0.24
(1,1047)	2:128:B:LEU:HD23	2:160:B:VAL:HG21	7	0.24
(1,1047)	2:128:B:LEU:HD23	2:160:B:VAL:HG22	7	0.24
(1,1047)	2:128:B:LEU:HD23	2:160:B:VAL:HG23	7	0.24
(1,1047)	2:128:B:LEU:HD12	2:160:B:VAL:HG21	7	0.24
(1,1047)	2:128:B:LEU:HD12	2:160:B:VAL:HG22	7	0.24
(1,1047)	2:128:B:LEU:HD12	2:160:B:VAL:HG23	7	0.24
(1,1047)	2:128:B:LEU:HD13	2:160:B:VAL:HG21	7	0.24
(1,1047)	2:128:B:LEU:HD13	2:160:B:VAL:HG22	7	0.24
(1,1047)	2:128:B:LEU:HD13	2:160:B:VAL:HG23	7	0.24
(1,1047)	2:128:B:LEU:HD11	2:160:B:VAL:HG21	7	0.24
(1,1047)	2:128:B:LEU:HD11	2:160:B:VAL:HG22	7	0.24
(1,1047)	2:128:B:LEU:HD11	2:160:B:VAL:HG23	7	0.24
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	15	0.24
(1,863)	2:154:B:ARG:HB3	2:155:B:ASP:HB2	9	0.24
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	5	0.24
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	5	0.24
(1,311)	2:186:B:GLU:HG3	2:187:B:THR:H	3	0.24
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	7	0.23
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	14	0.23
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	3	0.23
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	11	0.23
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	12	0.23
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	4	0.23
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	16	0.23
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	6	0.23
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	2	0.23
(1,628)	2:122:B:ARG:HB2	2:195:B:ASP:HB3	8	0.23
(1,566)	2:131:B:SER:HB3	2:132:B:GLY:HA3	10	0.23
(1,316)	2:119:B:SER:HB2	2:121:B:ASN:HD22	14	0.23
(1,292)	2:120:B:GLU:H	2:120:B:GLU:HG2	2	0.23
(1,292)	2:120:B:GLU:H	2:120:B:GLU:HG2	13	0.23
(1,170)	2:185:B:GLY:H	2:186:B:GLU:H	10	0.23
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	1	0.22
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	13	0.22
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	6	0.22
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	8	0.22
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	11	0.22
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	12	0.22
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	15	0.22
(1,1362)	1:2:A:G:H8	1:2:A:G:H1'	9	0.22
(1,890)	2:174:B:LYS:HA	2:174:B:LYS:HD3	3	0.22
(1,878)	2:193:B:LYS:HD2	2:194:B:VAL:H	11	0.22
(1,878)	2:193:B:LYS:HD3	2:194:B:VAL:H	11	0.22
(1,863)	2:154:B:ARG:HB3	2:155:B:ASP:HB2	5	0.22
(1,863)	2:154:B:ARG:HB3	2:155:B:ASP:HB2	7	0.22
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	3	0.22
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	11	0.22
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	15	0.22
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	12	0.22
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	14	0.22
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	8	0.22
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	15	0.22
(1,566)	2:131:B:SER:HB3	2:132:B:GLY:HA3	4	0.22
(1,149)	2:142:B:ARG:H	2:142:B:ARG:HB2	10	0.22
(1,115)	2:121:B:ASN:H	2:122:B:ARG:HB2	15	0.22
(1,41)	2:120:B:GLU:HA	2:122:B:ARG:H	2	0.22
(1,1414)	1:5:A:G:H1	2:134:B:TRP:HB3	1	0.21
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	16	0.21
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	4	0.21
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	6	0.21
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	1	0.21
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	16	0.21
(1,1300)	2:183:B:HIS:HA	2:183:B:HIS:HD2	5	0.21
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	2	0.21
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	13	0.21
(1,890)	2:174:B:LYS:HA	2:174:B:LYS:HD3	8	0.21
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	6	0.21
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	12	0.21
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	14	0.21
(1,826)	2:172:B:VAL:H	2:172:B:VAL:HB	5	0.21
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	8	0.21
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	11	0.21
(1,809)	2:194:B:VAL:H	2:194:B:VAL:HB	7	0.21
(1,809)	2:194:B:VAL:H	2:194:B:VAL:HB	14	0.21
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	5	0.21
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	10	0.21
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	15	0.21
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	16	0.21
(1,311)	2:186:B:GLU:HG3	2:187:B:THR:H	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	2:121:B:ASN:H	2:122:B:ARG:HB2	5	0.21
(1,115)	2:121:B:ASN:H	2:122:B:ARG:HB2	9	0.21
(1,115)	2:121:B:ASN:H	2:122:B:ARG:HB2	10	0.21
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	2	0.21
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	8	0.21
(2,52)	1:6:A:G:N2	2:139:B:ASP:OD1	2	0.2
(2,52)	1:6:A:G:N2	2:139:B:ASP:OD1	8	0.2
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	1	0.2
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	12	0.2
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	15	0.2
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	14	0.2
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	15	0.2
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	7	0.2
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	10	0.2
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	4	0.2
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	5	0.2
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	7	0.2
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	8	0.2
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	15	0.2
(1,934)	2:178:B:THR:HB	2:179:B:LYS:HG2	7	0.2
(1,934)	2:178:B:THR:HB	2:179:B:LYS:HG2	8	0.2
(1,890)	2:174:B:LYS:HA	2:174:B:LYS:HD3	15	0.2
(1,874)	2:120:B:GLU:HB3	2:121:B:ASN:HB3	7	0.2
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	12	0.2
(1,863)	2:154:B:ARG:HB3	2:155:B:ASP:HB2	6	0.2
(1,863)	2:154:B:ARG:HB3	2:155:B:ASP:HB2	13	0.2
(1,863)	2:154:B:ARG:HB3	2:155:B:ASP:HB2	15	0.2
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	2	0.2
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	8	0.2
(1,826)	2:172:B:VAL:H	2:172:B:VAL:HB	4	0.2
(1,826)	2:172:B:VAL:H	2:172:B:VAL:HB	8	0.2
(1,822)	2:162:B:PHE:HA	2:163:B:VAL:HB	2	0.2
(1,809)	2:194:B:VAL:H	2:194:B:VAL:HB	6	0.2
(1,809)	2:194:B:VAL:H	2:194:B:VAL:HB	10	0.2
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	14	0.2
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	3	0.2
(1,292)	2:120:B:GLU:H	2:120:B:GLU:HG2	4	0.2
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	10	0.2
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	14	0.2
(1,36)	2:119:B:SER:HB3	2:122:B:ARG:H	10	0.2
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	9	0.19
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	2	0.19
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	8	0.19
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	11	0.19
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	16	0.19
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	1	0.19
(1,890)	2:174:B:LYS:HA	2:174:B:LYS:HD3	13	0.19
(1,826)	2:172:B:VAL:H	2:172:B:VAL:HB	3	0.19
(1,826)	2:172:B:VAL:H	2:172:B:VAL:HB	7	0.19
(1,826)	2:172:B:VAL:H	2:172:B:VAL:HB	15	0.19
(1,826)	2:172:B:VAL:H	2:172:B:VAL:HB	16	0.19
(1,813)	2:178:B:THR:HA	2:179:B:LYS:HB2	14	0.19
(1,809)	2:194:B:VAL:H	2:194:B:VAL:HB	9	0.19
(1,809)	2:194:B:VAL:H	2:194:B:VAL:HB	12	0.19
(1,744)	2:131:B:SER:H	2:184:B:GLU:HG2	10	0.19
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	5	0.19
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	11	0.19
(1,717)	2:193:B:LYS:HB2	2:194:B:VAL:H	2	0.19
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	8	0.19
(1,431)	2:130:B:PRO:HA	2:132:B:GLY:H	9	0.19
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	3	0.19
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	6	0.19
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	9	0.19
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	15	0.19
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	16	0.19
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	1	0.19
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	2	0.18
(2,50)	1:6:A:G:N1	2:139:B:ASP:OD2	8	0.18
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	7	0.18
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	11	0.18
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	13	0.18
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	6	0.18
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	11	0.18
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	14	0.18
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG11	10	0.18
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG12	10	0.18
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG13	10	0.18
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	3	0.18
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	7	0.18
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	10	0.18
(1,826)	2:172:B:VAL:H	2:172:B:VAL:HB	10	0.18
(1,826)	2:172:B:VAL:H	2:172:B:VAL:HB	11	0.18
(1,826)	2:172:B:VAL:H	2:172:B:VAL:HB	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,809)	2:194:B:VAL:H	2:194:B:VAL:HB	15	0.18
(1,731)	2:119:B:SER:HB3	2:120:B:GLU:HG2	1	0.18
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	4	0.18
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	6	0.18
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	7	0.18
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	10	0.18
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	13	0.18
(1,556)	2:121:B:ASN:HA	2:165:B:LYS:HA	13	0.18
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	9	0.18
(1,115)	2:121:B:ASN:H	2:122:B:ARG:HB2	1	0.18
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	5	0.18
(1,56)	2:126:B:SER:H	2:193:B:LYS:H	6	0.18
(1,36)	2:119:B:SER:HB3	2:122:B:ARG:H	16	0.18
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	1	0.18
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	2	0.18
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	6	0.18
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	10	0.18
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	10	0.17
(1,1414)	1:5:A:G:H1	2:134:B:TRP:HB3	5	0.17
(1,1404)	1:7:A:A:H1'	1:6:A:G:H1'	1	0.17
(1,1404)	1:7:A:A:H1'	1:6:A:G:H1'	8	0.17
(1,1389)	1:8:A:C:H6	1:8:A:C:H3'	10	0.17
(1,1382)	1:7:A:A:H8	1:7:A:A:H1'	13	0.17
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	14	0.17
(1,1360)	1:1:A:U:H3'	1:1:A:U:H6	16	0.17
(1,1358)	1:1:A:U:H1'	1:1:A:U:H6	1	0.17
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	3	0.17
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	16	0.17
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	11	0.17
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	14	0.17
(1,826)	2:172:B:VAL:H	2:172:B:VAL:HB	14	0.17
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	10	0.17
(1,744)	2:131:B:SER:H	2:184:B:GLU:HG2	4	0.17
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	1	0.17
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	3	0.17
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	9	0.17
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	12	0.17
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	16	0.17
(1,660)	2:191:B:ARG:HD2	2:192:B:VAL:H	13	0.17
(1,660)	2:191:B:ARG:HD2	2:192:B:VAL:H	15	0.17
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	6	0.17
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,545)	2:181:B:ARG:HA	2:187:B:THR:HA	12	0.17
(1,525)	2:184:B:GLU:HA	2:184:B:GLU:HG2	4	0.17
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	6	0.17
(1,414)	2:119:B:SER:HB2	2:120:B:GLU:HG3	14	0.17
(1,311)	2:186:B:GLU:HG3	2:187:B:THR:H	5	0.17
(1,311)	2:186:B:GLU:HG3	2:187:B:THR:H	9	0.17
(1,311)	2:186:B:GLU:HG3	2:187:B:THR:H	13	0.17
(1,311)	2:186:B:GLU:HG3	2:187:B:THR:H	15	0.17
(1,292)	2:120:B:GLU:H	2:120:B:GLU:HG2	11	0.17
(1,211)	2:191:B:ARG:H	2:191:B:ARG:HD2	13	0.17
(1,87)	2:190:B:ILE:H	2:192:B:VAL:H	14	0.17
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	1	0.17
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	12	0.17
(1,56)	2:126:B:SER:H	2:193:B:LYS:H	1	0.17
(1,36)	2:119:B:SER:HB3	2:122:B:ARG:H	8	0.17
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	4	0.17
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	9	0.17
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	11	0.17
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	16	0.17
(2,52)	1:6:A:G:N2	2:139:B:ASP:OD1	11	0.16
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	14	0.16
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	16	0.16
(1,1426)	1:6:A:G:H2'	2:134:B:TRP:HZ2	8	0.16
(1,1407)	1:8:A:C:H6	1:7:A:A:H4'	7	0.16
(1,1389)	1:8:A:C:H6	1:8:A:C:H3'	9	0.16
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	9	0.16
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	9	0.16
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	10	0.16
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG11	9	0.16
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG12	9	0.16
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG13	9	0.16
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG11	16	0.16
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG12	16	0.16
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG13	16	0.16
(1,1047)	2:128:B:LEU:HD21	2:160:B:VAL:HG21	8	0.16
(1,1047)	2:128:B:LEU:HD21	2:160:B:VAL:HG22	8	0.16
(1,1047)	2:128:B:LEU:HD21	2:160:B:VAL:HG23	8	0.16
(1,1047)	2:128:B:LEU:HD22	2:160:B:VAL:HG21	8	0.16
(1,1047)	2:128:B:LEU:HD22	2:160:B:VAL:HG22	8	0.16
(1,1047)	2:128:B:LEU:HD22	2:160:B:VAL:HG23	8	0.16
(1,1047)	2:128:B:LEU:HD23	2:160:B:VAL:HG21	8	0.16
(1,1047)	2:128:B:LEU:HD23	2:160:B:VAL:HG22	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1047)	2:128:B:LEU:HD23	2:160:B:VAL:HG23	8	0.16
(1,1047)	2:128:B:LEU:HD12	2:160:B:VAL:HG21	8	0.16
(1,1047)	2:128:B:LEU:HD12	2:160:B:VAL:HG22	8	0.16
(1,1047)	2:128:B:LEU:HD12	2:160:B:VAL:HG23	8	0.16
(1,1047)	2:128:B:LEU:HD13	2:160:B:VAL:HG21	8	0.16
(1,1047)	2:128:B:LEU:HD13	2:160:B:VAL:HG22	8	0.16
(1,1047)	2:128:B:LEU:HD13	2:160:B:VAL:HG23	8	0.16
(1,1047)	2:128:B:LEU:HD11	2:160:B:VAL:HG21	8	0.16
(1,1047)	2:128:B:LEU:HD11	2:160:B:VAL:HG22	8	0.16
(1,1047)	2:128:B:LEU:HD11	2:160:B:VAL:HG23	8	0.16
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	1	0.16
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	1	0.16
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	1	0.16
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	4	0.16
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	9	0.16
(1,717)	2:193:B:LYS:HB2	2:194:B:VAL:H	1	0.16
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	2	0.16
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	8	0.16
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	8	0.16
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	9	0.16
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	10	0.16
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	14	0.16
(1,414)	2:119:B:SER:HB2	2:120:B:GLU:HG3	12	0.16
(1,344)	2:177:B:ASN:H	2:177:B:ASN:HD22	1	0.16
(1,316)	2:119:B:SER:HB2	2:121:B:ASN:HD22	1	0.16
(1,311)	2:186:B:GLU:HG3	2:187:B:THR:H	11	0.16
(1,149)	2:142:B:ARG:H	2:142:B:ARG:HB2	12	0.16
(1,56)	2:126:B:SER:H	2:193:B:LYS:H	13	0.16
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	2	0.16
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	3	0.16
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	10	0.16
(2,52)	1:6:A:G:N2	2:139:B:ASP:OD1	13	0.15
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	3	0.15
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	5	0.15
(1,1426)	1:6:A:G:H2'	2:134:B:TRP:HZ2	3	0.15
(1,1426)	1:6:A:G:H2'	2:134:B:TRP:HZ2	9	0.15
(1,1407)	1:8:A:C:H6	1:7:A:A:H4'	5	0.15
(1,1389)	1:8:A:C:H6	1:8:A:C:H3'	4	0.15
(1,1388)	1:8:A:C:H6	1:8:A:C:H2'	7	0.15
(1,1367)	1:3:A:A:H8	1:3:A:A:H1'	9	0.15
(1,1362)	1:2:A:G:H8	1:2:A:G:H1'	16	0.15
(1,1310)	2:134:B:TRP:HE3	2:138:B:LYS:HB3	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1300)	2:183:B:HIS:HA	2:183:B:HIS:HD2	13	0.15
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG11	4	0.15
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG12	4	0.15
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG13	4	0.15
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG11	13	0.15
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG12	13	0.15
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG13	13	0.15
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG11	1	0.15
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG12	1	0.15
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG13	1	0.15
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG11	15	0.15
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG12	15	0.15
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG13	15	0.15
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	2	0.15
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	10	0.15
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	11	0.15
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	14	0.15
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	15	0.15
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	16	0.15
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	8	0.15
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	13	0.15
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	7	0.15
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	16	0.15
(1,722)	2:143:B:GLU:HG2	2:144:B:ALA:H	15	0.15
(1,717)	2:193:B:LYS:HB2	2:194:B:VAL:H	13	0.15
(1,717)	2:193:B:LYS:HB2	2:194:B:VAL:H	16	0.15
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	4	0.15
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	5	0.15
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	1	0.15
(1,634)	2:136:B:ASP:HB3	2:138:B:LYS:H	15	0.15
(1,634)	2:136:B:ASP:HB3	2:138:B:LYS:H	16	0.15
(1,596)	2:164:B:ARG:H	2:164:B:ARG:HD2	15	0.15
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	5	0.15
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	6	0.15
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	10	0.15
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	5	0.15
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	7	0.15
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	13	0.15
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	16	0.15
(1,556)	2:121:B:ASN:HA	2:165:B:LYS:HA	7	0.15
(1,414)	2:119:B:SER:HB2	2:120:B:GLU:HG3	9	0.15
(1,414)	2:119:B:SER:HB2	2:120:B:GLU:HG3	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,247)	2:116:B:SER:H	2:117:B:ARG:HB2	9	0.15
(1,162)	2:142:B:ARG:H	2:147:B:VAL:H	12	0.15
(1,110)	2:162:B:PHE:H	2:168:B:MET:HB3	3	0.15
(1,76)	2:147:B:VAL:H	2:148:B:CYS:H	10	0.15
(1,76)	2:147:B:VAL:H	2:148:B:CYS:H	15	0.15
(1,76)	2:147:B:VAL:H	2:148:B:CYS:H	16	0.15
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	7	0.15
(1,56)	2:126:B:SER:H	2:193:B:LYS:H	5	0.15
(1,56)	2:126:B:SER:H	2:193:B:LYS:H	9	0.15
(1,36)	2:119:B:SER:HB3	2:122:B:ARG:H	6	0.15
(1,36)	2:119:B:SER:HB3	2:122:B:ARG:H	15	0.15
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	14	0.15
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	4	0.15
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	9	0.15
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	12	0.15
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	1	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	1	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	3	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	3	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	6	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	6	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	8	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	8	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	9	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	9	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	11	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	11	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	12	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	12	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	14	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	14	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	15	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	15	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	16	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	16	0.14
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	6	0.14
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	8	0.14
(1,1422)	1:6:A:G:H1'	2:135:B:GLN:HA	1	0.14
(1,1414)	1:5:A:G:H1	2:134:B:TRP:HB3	12	0.14
(1,1404)	1:7:A:A:H1'	1:6:A:G:H1'	9	0.14
(1,1389)	1:8:A:C:H6	1:8:A:C:H3'	1	0.14
(1,1389)	1:8:A:C:H6	1:8:A:C:H3'	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1370)	1:3:A:A:H8	1:3:A:A:H4'	9	0.14
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG11	4	0.14
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG12	4	0.14
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG13	4	0.14
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG11	13	0.14
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG12	13	0.14
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG13	13	0.14
(1,1034)	2:194:B:VAL:H	2:194:B:VAL:HG21	15	0.14
(1,1034)	2:194:B:VAL:H	2:194:B:VAL:HG22	15	0.14
(1,1034)	2:194:B:VAL:H	2:194:B:VAL:HG23	15	0.14
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	1	0.14
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	9	0.14
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	13	0.14
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	9	0.14
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	6	0.14
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	15	0.14
(1,744)	2:131:B:SER:H	2:184:B:GLU:HG2	15	0.14
(1,724)	2:159:B:VAL:HB	2:160:B:VAL:H	8	0.14
(1,717)	2:193:B:LYS:HB2	2:194:B:VAL:H	7	0.14
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	1	0.14
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	2	0.14
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	3	0.14
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	7	0.14
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	8	0.14
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	10	0.14
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	12	0.14
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	16	0.14
(1,660)	2:191:B:ARG:HD2	2:192:B:VAL:H	9	0.14
(1,660)	2:191:B:ARG:HD2	2:192:B:VAL:H	10	0.14
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	4	0.14
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	5	0.14
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	6	0.14
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	9	0.14
(1,634)	2:136:B:ASP:HB3	2:138:B:LYS:H	4	0.14
(1,628)	2:122:B:ARG:HB2	2:195:B:ASP:HB3	3	0.14
(1,596)	2:164:B:ARG:H	2:164:B:ARG:HD2	3	0.14
(1,596)	2:164:B:ARG:H	2:164:B:ARG:HD2	5	0.14
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	12	0.14
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	14	0.14
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	1	0.14
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	3	0.14
(1,566)	2:131:B:SER:HB3	2:132:B:GLY:HA3	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	2:119:B:SER:HB2	2:120:B:GLU:HG3	5	0.14
(1,360)	2:184:B:GLU:HG3	2:185:B:GLY:H	12	0.14
(1,344)	2:177:B:ASN:H	2:177:B:ASN:HD22	4	0.14
(1,344)	2:177:B:ASN:H	2:177:B:ASN:HD22	11	0.14
(1,266)	2:138:B:LYS:HB2	2:139:B:ASP:H	11	0.14
(1,212)	2:189:B:TYR:HB3	2:191:B:ARG:H	14	0.14
(1,162)	2:142:B:ARG:H	2:147:B:VAL:H	5	0.14
(1,162)	2:142:B:ARG:H	2:147:B:VAL:H	7	0.14
(1,115)	2:121:B:ASN:H	2:122:B:ARG:HB2	14	0.14
(1,76)	2:147:B:VAL:H	2:148:B:CYS:H	3	0.14
(1,76)	2:147:B:VAL:H	2:148:B:CYS:H	4	0.14
(1,76)	2:147:B:VAL:H	2:148:B:CYS:H	9	0.14
(1,56)	2:126:B:SER:H	2:193:B:LYS:H	12	0.14
(1,36)	2:119:B:SER:HB3	2:122:B:ARG:H	5	0.14
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	8	0.14
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	13	0.14
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	15	0.14
(1,19)	2:123:B:VAL:HA	2:195:B:ASP:H	5	0.14
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	3	0.14
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	11	0.14
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	14	0.14
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	15	0.14
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	2	0.13
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	2	0.13
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	4	0.13
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	4	0.13
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	5	0.13
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	5	0.13
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	7	0.13
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	7	0.13
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	10	0.13
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	10	0.13
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	13	0.13
(2,53)	1:7:A:A:H61	2:136:B:ASP:OD1	13	0.13
(2,49)	1:6:A:G:H1	2:139:B:ASP:OD2	5	0.13
(1,1426)	1:6:A:G:H2'	2:134:B:TRP:HZ2	13	0.13
(1,1422)	1:6:A:G:H1'	2:135:B:GLN:HA	11	0.13
(1,1422)	1:6:A:G:H1'	2:135:B:GLN:HA	13	0.13
(1,1417)	1:5:A:G:H3'	2:134:B:TRP:HZ2	3	0.13
(1,1414)	1:5:A:G:H1	2:134:B:TRP:HB3	6	0.13
(1,1407)	1:8:A:C:H6	1:7:A:A:H4'	3	0.13
(1,1404)	1:7:A:A:H1'	1:6:A:G:H1'	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1392)	1:3:A:A:H8	1:2:A:G:H1'	13	0.13
(1,1360)	1:1:A:U:H3'	1:1:A:U:H6	3	0.13
(1,1360)	1:1:A:U:H3'	1:1:A:U:H6	8	0.13
(1,1310)	2:134:B:TRP:HE3	2:138:B:LYS:HB3	14	0.13
(1,1300)	2:183:B:HIS:HA	2:183:B:HIS:HD2	2	0.13
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	4	0.13
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	5	0.13
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	12	0.13
(1,827)	2:169:B:THR:HA	2:172:B:VAL:HB	6	0.13
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	2	0.13
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	5	0.13
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	8	0.13
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	11	0.13
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	12	0.13
(1,744)	2:131:B:SER:H	2:184:B:GLU:HG2	2	0.13
(1,743)	2:184:B:GLU:HG2	2:185:B:GLY:H	16	0.13
(1,717)	2:193:B:LYS:HB2	2:194:B:VAL:H	3	0.13
(1,717)	2:193:B:LYS:HB2	2:194:B:VAL:H	5	0.13
(1,717)	2:193:B:LYS:HB2	2:194:B:VAL:H	8	0.13
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	9	0.13
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	15	0.13
(1,658)	2:141:B:MET:HA	2:175:B:LEU:HB3	13	0.13
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	2	0.13
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	13	0.13
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	1	0.13
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	4	0.13
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	7	0.13
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	9	0.13
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	11	0.13
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	13	0.13
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	15	0.13
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	16	0.13
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	2	0.13
(1,588)	2:195:B:ASP:HB2	2:196:B:GLY:HA2	4	0.13
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	4	0.13
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	7	0.13
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	12	0.13
(1,430)	2:126:B:SER:HB3	2:127:B:GLY:H	16	0.13
(1,414)	2:119:B:SER:HB2	2:120:B:GLU:HG3	1	0.13
(1,414)	2:119:B:SER:HB2	2:120:B:GLU:HG3	8	0.13
(1,414)	2:119:B:SER:HB2	2:120:B:GLU:HG3	10	0.13
(1,414)	2:119:B:SER:HB2	2:120:B:GLU:HG3	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	2:177:B:ASN:HB2	2:178:B:THR:H	2	0.13
(1,373)	2:126:B:SER:HB2	2:158:B:GLY:H	9	0.13
(1,355)	2:127:B:GLY:H	2:128:B:LEU:HB3	9	0.13
(1,344)	2:177:B:ASN:H	2:177:B:ASN:HD22	3	0.13
(1,344)	2:177:B:ASN:H	2:177:B:ASN:HD22	7	0.13
(1,344)	2:177:B:ASN:H	2:177:B:ASN:HD22	13	0.13
(1,292)	2:120:B:GLU:H	2:120:B:GLU:HG2	14	0.13
(1,247)	2:116:B:SER:H	2:117:B:ARG:HB2	2	0.13
(1,247)	2:116:B:SER:H	2:117:B:ARG:HB2	3	0.13
(1,162)	2:142:B:ARG:H	2:147:B:VAL:H	3	0.13
(1,162)	2:142:B:ARG:H	2:147:B:VAL:H	11	0.13
(1,162)	2:142:B:ARG:H	2:147:B:VAL:H	15	0.13
(1,110)	2:162:B:PHE:H	2:168:B:MET:HB3	6	0.13
(1,110)	2:162:B:PHE:H	2:168:B:MET:HB3	8	0.13
(1,110)	2:162:B:PHE:H	2:168:B:MET:HB3	9	0.13
(1,110)	2:162:B:PHE:H	2:168:B:MET:HB3	15	0.13
(1,87)	2:190:B:ILE:H	2:192:B:VAL:H	16	0.13
(1,76)	2:147:B:VAL:H	2:148:B:CYS:H	1	0.13
(1,76)	2:147:B:VAL:H	2:148:B:CYS:H	13	0.13
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	11	0.13
(1,41)	2:120:B:GLU:HA	2:122:B:ARG:H	4	0.13
(1,36)	2:119:B:SER:HB3	2:122:B:ARG:H	3	0.13
(1,36)	2:119:B:SER:HB3	2:122:B:ARG:H	9	0.13
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	6	0.13
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	7	0.13
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	16	0.13
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	7	0.13
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	1	0.12
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	2	0.12
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	4	0.12
(1,1432)	1:7:A:A:H2	2:133:B:SER:HA	12	0.12
(1,1422)	1:6:A:G:H1'	2:135:B:GLN:HA	9	0.12
(1,1417)	1:5:A:G:H3'	2:134:B:TRP:HZ2	10	0.12
(1,1414)	1:5:A:G:H1	2:134:B:TRP:HB3	9	0.12
(1,1395)	1:3:A:A:H2	1:2:A:G:H4'	7	0.12
(1,1377)	1:5:A:G:H3'	1:5:A:G:H8	12	0.12
(1,1362)	1:2:A:G:H8	1:2:A:G:H1'	8	0.12
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG11	1	0.12
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG12	1	0.12
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG13	1	0.12
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG11	8	0.12
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG12	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	2:194:B:VAL:H	2:194:B:VAL:HG13	8	0.12
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG11	3	0.12
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG12	3	0.12
(1,1071)	2:147:B:VAL:H	2:147:B:VAL:HG13	3	0.12
(1,956)	2:193:B:LYS:HG2	2:194:B:VAL:H	3	0.12
(1,956)	2:193:B:LYS:HG3	2:194:B:VAL:H	3	0.12
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	3	0.12
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	6	0.12
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	8	0.12
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	4	0.12
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	3	0.12
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	13	0.12
(1,757)	2:176:B:ASP:H	2:192:B:VAL:HB	2	0.12
(1,757)	2:176:B:ASP:H	2:192:B:VAL:HB	9	0.12
(1,744)	2:131:B:SER:H	2:184:B:GLU:HG2	8	0.12
(1,743)	2:184:B:GLU:HG2	2:185:B:GLY:H	3	0.12
(1,731)	2:119:B:SER:HB3	2:120:B:GLU:HG2	14	0.12
(1,724)	2:159:B:VAL:HB	2:160:B:VAL:H	1	0.12
(1,724)	2:159:B:VAL:HB	2:160:B:VAL:H	5	0.12
(1,724)	2:159:B:VAL:HB	2:160:B:VAL:H	6	0.12
(1,724)	2:159:B:VAL:HB	2:160:B:VAL:H	16	0.12
(1,723)	2:143:B:GLU:HA	2:143:B:GLU:HG2	2	0.12
(1,723)	2:143:B:GLU:HA	2:143:B:GLU:HG2	8	0.12
(1,717)	2:193:B:LYS:HB2	2:194:B:VAL:H	14	0.12
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	6	0.12
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	11	0.12
(1,710)	2:166:B:GLU:HG2	2:167:B:ASP:HA	14	0.12
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	14	0.12
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	15	0.12
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	16	0.12
(1,634)	2:136:B:ASP:HB3	2:138:B:LYS:H	6	0.12
(1,634)	2:136:B:ASP:HB3	2:138:B:LYS:H	9	0.12
(1,589)	2:144:B:ALA:H	2:145:B:GLY:HA3	3	0.12
(1,566)	2:131:B:SER:HB3	2:132:B:GLY:HA3	5	0.12
(1,388)	2:177:B:ASN:HB2	2:178:B:THR:H	16	0.12
(1,373)	2:126:B:SER:HB2	2:158:B:GLY:H	2	0.12
(1,344)	2:177:B:ASN:H	2:177:B:ASN:HD22	9	0.12
(1,344)	2:177:B:ASN:H	2:177:B:ASN:HD22	15	0.12
(1,247)	2:116:B:SER:H	2:117:B:ARG:HB2	14	0.12
(1,239)	2:117:B:ARG:H	2:118:B:ARG:H	14	0.12
(1,238)	2:116:B:SER:HA	2:118:B:ARG:H	14	0.12
(1,212)	2:189:B:TYR:HB3	2:191:B:ARG:H	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	2:189:B:TYR:HB3	2:191:B:ARG:H	8	0.12
(1,212)	2:189:B:TYR:HB3	2:191:B:ARG:H	11	0.12
(1,211)	2:191:B:ARG:H	2:191:B:ARG:HD2	9	0.12
(1,199)	2:124:B:VAL:HB	2:126:B:SER:H	7	0.12
(1,162)	2:142:B:ARG:H	2:147:B:VAL:H	6	0.12
(1,110)	2:162:B:PHE:H	2:168:B:MET:HB3	10	0.12
(1,110)	2:162:B:PHE:H	2:168:B:MET:HB3	16	0.12
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	4	0.12
(1,36)	2:119:B:SER:HB3	2:122:B:ARG:H	12	0.12
(1,34)	2:153:B:TYR:H	2:159:B:VAL:H	12	0.12
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	13	0.12
(2,51)	1:6:A:G:H21	2:139:B:ASP:OD1	12	0.11
(1,1426)	1:6:A:G:H2'	2:134:B:TRP:HZ2	5	0.11
(1,1422)	1:6:A:G:H1'	2:135:B:GLN:HA	8	0.11
(1,1414)	1:5:A:G:H1	2:134:B:TRP:HB3	2	0.11
(1,1414)	1:5:A:G:H1	2:134:B:TRP:HB3	11	0.11
(1,1414)	1:5:A:G:H1	2:134:B:TRP:HB3	14	0.11
(1,1414)	1:5:A:G:H1	2:134:B:TRP:HB3	15	0.11
(1,1407)	1:8:A:C:H6	1:7:A:A:H4'	10	0.11
(1,1398)	1:4:A:A:H8	1:3:A:A:H3'	15	0.11
(1,1383)	1:7:A:A:H8	1:7:A:A:H2'	5	0.11
(1,1380)	1:6:A:G:H3'	1:6:A:G:H8	6	0.11
(1,1374)	1:4:A:A:H8	1:4:A:A:H3'	5	0.11
(1,1370)	1:3:A:A:H8	1:3:A:A:H4'	2	0.11
(1,1362)	1:2:A:G:H8	1:2:A:G:H1'	4	0.11
(1,1300)	2:183:B:HIS:HA	2:183:B:HIS:HD2	4	0.11
(1,1195)	2:183:B:HIS:HB2	2:183:B:HIS:HE1	12	0.11
(1,956)	2:193:B:LYS:HG2	2:194:B:VAL:H	8	0.11
(1,956)	2:193:B:LYS:HG3	2:194:B:VAL:H	8	0.11
(1,956)	2:193:B:LYS:HG2	2:194:B:VAL:H	16	0.11
(1,956)	2:193:B:LYS:HG3	2:194:B:VAL:H	16	0.11
(1,873)	2:120:B:GLU:HB3	2:121:B:ASN:HD22	7	0.11
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	13	0.11
(1,824)	2:146:B:ASP:HB3	2:163:B:VAL:HB	14	0.11
(1,757)	2:176:B:ASP:H	2:192:B:VAL:HB	1	0.11
(1,746)	2:184:B:GLU:HA	2:184:B:GLU:HG3	5	0.11
(1,744)	2:131:B:SER:H	2:184:B:GLU:HG2	6	0.11
(1,744)	2:131:B:SER:H	2:184:B:GLU:HG2	13	0.11
(1,744)	2:131:B:SER:H	2:184:B:GLU:HG2	14	0.11
(1,740)	2:151:B:ASP:H	2:159:B:VAL:HB	1	0.11
(1,740)	2:151:B:ASP:H	2:159:B:VAL:HB	4	0.11
(1,740)	2:151:B:ASP:H	2:159:B:VAL:HB	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	2:159:B:VAL:HB	2:160:B:VAL:H	7	0.11
(1,724)	2:159:B:VAL:HB	2:160:B:VAL:H	12	0.11
(1,723)	2:143:B:GLU:HA	2:143:B:GLU:HG2	3	0.11
(1,723)	2:143:B:GLU:HA	2:143:B:GLU:HG2	7	0.11
(1,723)	2:143:B:GLU:HA	2:143:B:GLU:HG2	13	0.11
(1,723)	2:143:B:GLU:HA	2:143:B:GLU:HG2	15	0.11
(1,717)	2:193:B:LYS:HB2	2:194:B:VAL:H	6	0.11
(1,717)	2:193:B:LYS:HB2	2:194:B:VAL:H	9	0.11
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	3	0.11
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	7	0.11
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	8	0.11
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	12	0.11
(1,634)	2:136:B:ASP:HB3	2:138:B:LYS:H	5	0.11
(1,634)	2:136:B:ASP:HB3	2:138:B:LYS:H	10	0.11
(1,625)	2:122:B:ARG:H	2:195:B:ASP:HB2	7	0.11
(1,546)	2:128:B:LEU:HA	2:190:B:ILE:HA	9	0.11
(1,437)	2:131:B:SER:HB2	2:184:B:GLU:HB2	9	0.11
(1,437)	2:131:B:SER:HB2	2:184:B:GLU:HB2	16	0.11
(1,430)	2:126:B:SER:HB3	2:127:B:GLY:H	4	0.11
(1,414)	2:119:B:SER:HB2	2:120:B:GLU:HG3	3	0.11
(1,414)	2:119:B:SER:HB2	2:120:B:GLU:HG3	6	0.11
(1,402)	2:181:B:ARG:HA	2:187:B:THR:HB	12	0.11
(1,392)	2:145:B:GLY:H	2:146:B:ASP:H	5	0.11
(1,392)	2:145:B:GLY:H	2:146:B:ASP:H	7	0.11
(1,392)	2:145:B:GLY:H	2:146:B:ASP:H	9	0.11
(1,388)	2:177:B:ASN:HB2	2:178:B:THR:H	6	0.11
(1,388)	2:177:B:ASN:HB2	2:178:B:THR:H	10	0.11
(1,292)	2:120:B:GLU:H	2:120:B:GLU:HG2	3	0.11
(1,292)	2:120:B:GLU:H	2:120:B:GLU:HG2	5	0.11
(1,292)	2:120:B:GLU:H	2:120:B:GLU:HG2	6	0.11
(1,292)	2:120:B:GLU:H	2:120:B:GLU:HG2	10	0.11
(1,238)	2:116:B:SER:HA	2:118:B:ARG:H	15	0.11
(1,212)	2:189:B:TYR:HB3	2:191:B:ARG:H	3	0.11
(1,211)	2:191:B:ARG:H	2:191:B:ARG:HD2	10	0.11
(1,199)	2:124:B:VAL:HB	2:126:B:SER:H	10	0.11
(1,162)	2:142:B:ARG:H	2:147:B:VAL:H	4	0.11
(1,136)	2:174:B:LYS:HB3	2:176:B:ASP:H	10	0.11
(1,136)	2:174:B:LYS:HB3	2:176:B:ASP:H	12	0.11
(1,136)	2:174:B:LYS:HB3	2:176:B:ASP:H	14	0.11
(1,115)	2:121:B:ASN:H	2:122:B:ARG:HB2	6	0.11
(1,110)	2:162:B:PHE:H	2:168:B:MET:HB3	12	0.11
(1,87)	2:190:B:ILE:H	2:192:B:VAL:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	2:147:B:VAL:H	2:148:B:CYS:H	7	0.11
(1,64)	2:168:B:MET:HB2	2:170:B:TYR:H	13	0.11
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	5	0.11
(1,1)	2:180:B:PHE:H	2:190:B:ILE:H	8	0.11
(1,1422)	1:6:A:G:H1'	2:135:B:GLN:HA	2	0.1
(1,1417)	1:5:A:G:H3'	2:134:B:TRP:HZ2	4	0.1
(1,1414)	1:5:A:G:H1	2:134:B:TRP:HB3	4	0.1
(1,1414)	1:5:A:G:H1	2:134:B:TRP:HB3	16	0.1
(1,1392)	1:3:A:A:H8	1:2:A:G:H1'	9	0.1
(1,1380)	1:6:A:G:H3'	1:6:A:G:H8	16	0.1
(1,1370)	1:3:A:A:H8	1:3:A:A:H4'	14	0.1
(1,1362)	1:2:A:G:H8	1:2:A:G:H1'	6	0.1
(1,1360)	1:1:A:U:H3'	1:1:A:U:H6	7	0.1
(1,1305)	2:134:B:TRP:HE3	2:135:B:GLN:HG2	2	0.1
(1,1034)	2:194:B:VAL:H	2:194:B:VAL:HG21	5	0.1
(1,1034)	2:194:B:VAL:H	2:194:B:VAL:HG22	5	0.1
(1,1034)	2:194:B:VAL:H	2:194:B:VAL:HG23	5	0.1
(1,1034)	2:194:B:VAL:H	2:194:B:VAL:HG21	12	0.1
(1,1034)	2:194:B:VAL:H	2:194:B:VAL:HG22	12	0.1
(1,1034)	2:194:B:VAL:H	2:194:B:VAL:HG23	12	0.1
(1,956)	2:193:B:LYS:HG2	2:194:B:VAL:H	4	0.1
(1,956)	2:193:B:LYS:HG3	2:194:B:VAL:H	4	0.1
(1,883)	2:122:B:ARG:HG3	2:123:B:VAL:H	7	0.1
(1,872)	2:120:B:GLU:HB3	2:121:B:ASN:H	2	0.1
(1,757)	2:176:B:ASP:H	2:192:B:VAL:HB	6	0.1
(1,740)	2:151:B:ASP:H	2:159:B:VAL:HB	3	0.1
(1,740)	2:151:B:ASP:H	2:159:B:VAL:HB	14	0.1
(1,740)	2:151:B:ASP:H	2:159:B:VAL:HB	15	0.1
(1,724)	2:159:B:VAL:HB	2:160:B:VAL:H	2	0.1
(1,724)	2:159:B:VAL:HB	2:160:B:VAL:H	4	0.1
(1,724)	2:159:B:VAL:HB	2:160:B:VAL:H	11	0.1
(1,723)	2:143:B:GLU:HA	2:143:B:GLU:HG2	10	0.1
(1,723)	2:143:B:GLU:HA	2:143:B:GLU:HG2	11	0.1
(1,717)	2:193:B:LYS:HB2	2:194:B:VAL:H	4	0.1
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	10	0.1
(1,645)	2:174:B:LYS:HB2	2:175:B:LEU:HB2	11	0.1
(1,634)	2:136:B:ASP:HB3	2:138:B:LYS:H	8	0.1
(1,628)	2:122:B:ARG:HB2	2:195:B:ASP:HB3	11	0.1
(1,572)	2:127:B:GLY:H	2:156:B:GLY:HA2	12	0.1
(1,566)	2:131:B:SER:HB3	2:132:B:GLY:HA3	13	0.1
(1,470)	2:121:B:ASN:H	2:165:B:LYS:HA	11	0.1
(1,392)	2:145:B:GLY:H	2:146:B:ASP:H	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,392)	2:145:B:GLY:H	2:146:B:ASP:H	3	0.1
(1,392)	2:145:B:GLY:H	2:146:B:ASP:H	10	0.1
(1,392)	2:145:B:GLY:H	2:146:B:ASP:H	13	0.1
(1,392)	2:145:B:GLY:H	2:146:B:ASP:H	15	0.1
(1,336)	2:195:B:ASP:HA	2:196:B:GLY:H	15	0.1
(1,124)	2:188:B:ALA:H	2:189:B:TYR:H	8	0.1
(1,115)	2:121:B:ASN:H	2:122:B:ARG:HB2	3	0.1
(1,110)	2:162:B:PHE:H	2:168:B:MET:HB3	5	0.1
(1,87)	2:190:B:ILE:H	2:192:B:VAL:H	13	0.1

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

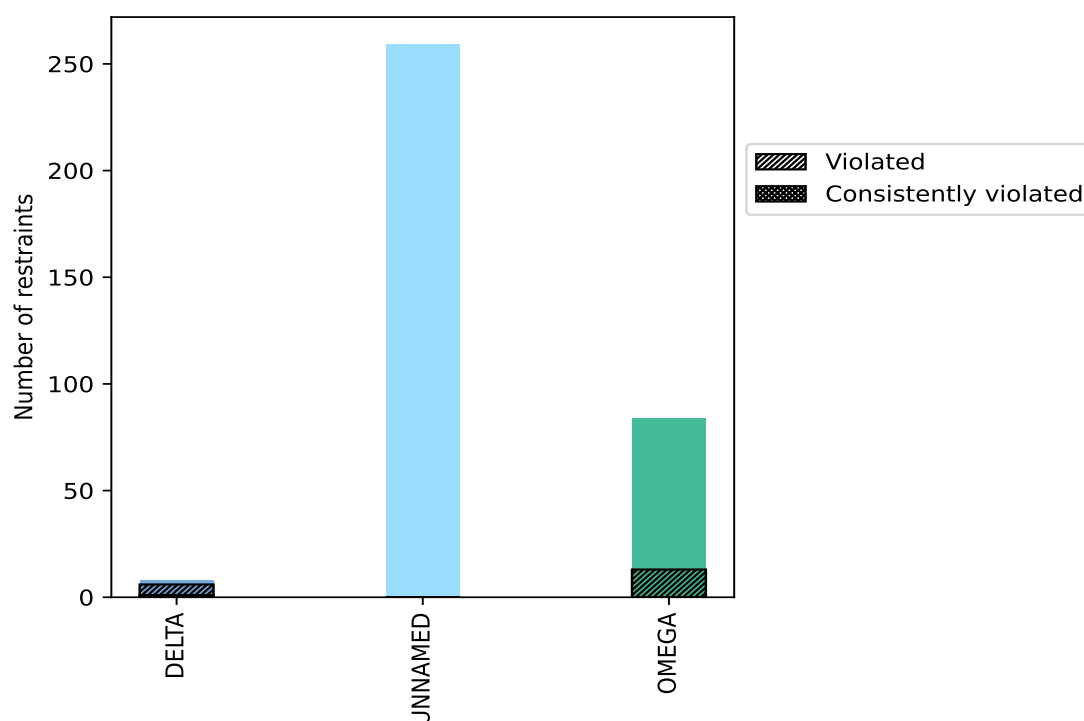
10.1 Summary of dihedral-angle violations [i](#)

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
DELTA	8	2.3	6	75.0	1.7	1	12.5	0.3
UNNAMED	259	73.8	0	0.0	0.0	0	0.0	0.0
OMEGA	84	23.9	13	15.5	3.7	0	0.0	0.0
Total	351	100.0	19	5.4	5.4	1	0.3	0.3

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](#)



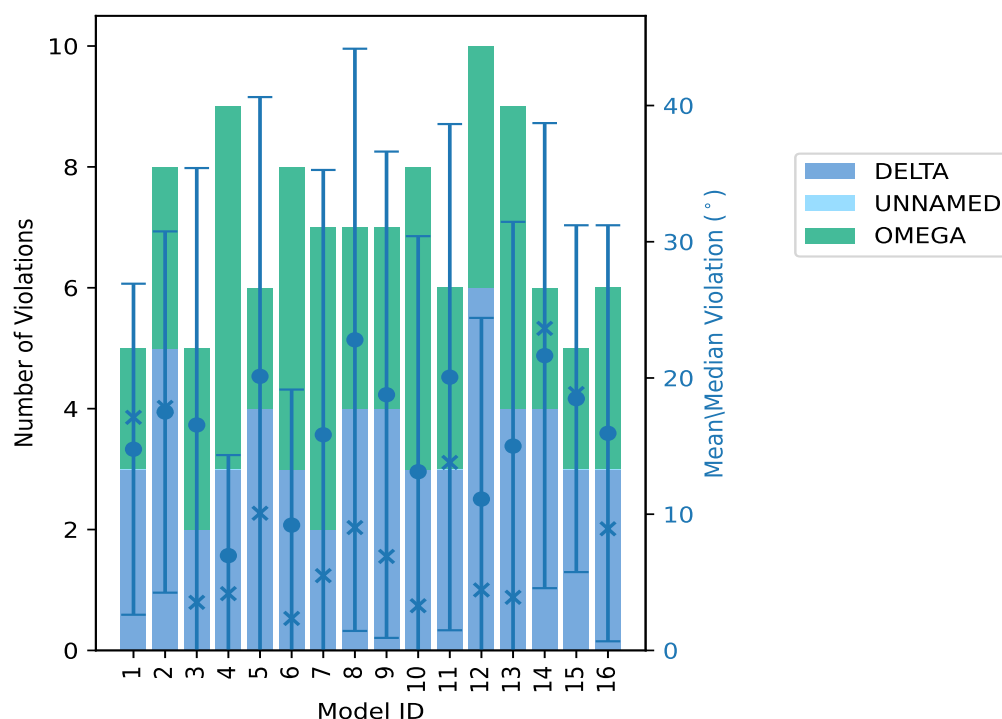
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	DELTA	UNNAMED	OMEGA	Total				
1	3	0	2	5	14.77	34.36	12.15	17.11
2	5	0	3	8	17.5	42.68	13.26	17.84
3	2	0	3	5	16.55	50.38	18.86	3.53
4	3	0	6	9	6.96	25.74	7.38	4.17
5	4	0	2	6	20.12	50.2	20.5	10.07
6	3	0	5	8	9.2	25.9	9.95	2.35
7	2	0	5	7	15.83	48.54	19.44	5.49
8	4	0	3	7	22.8	55.69	21.37	9.02
9	4	0	3	7	18.77	46.08	17.85	6.9
10	3	0	5	8	13.12	50.86	17.29	3.28
11	3	0	3	6	20.06	46.95	18.58	13.8
12	6	0	4	10	11.11	38.21	13.3	4.44
13	4	0	5	9	15.0	50.88	16.46	3.9
14	4	0	2	6	21.64	46.29	17.07	23.64
15	3	0	2	5	18.48	32.91	12.73	18.86
16	3	0	3	6	15.94	45.67	15.27	8.93

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	
DELTA	UNNAMED	OMEGA	Total	Count ¹	%
0	0	7	7	1	6.2
0	0	0	0	2	12.5
1	0	1	2	3	18.8
0	0	0	0	4	25.0
1	0	0	1	5	31.2
0	0	0	0	6	37.5
0	0	1	1	7	43.8
0	0	2	2	8	50.0
0	0	1	1	9	56.2
1	0	0	1	10	62.5
2	0	0	2	11	68.8

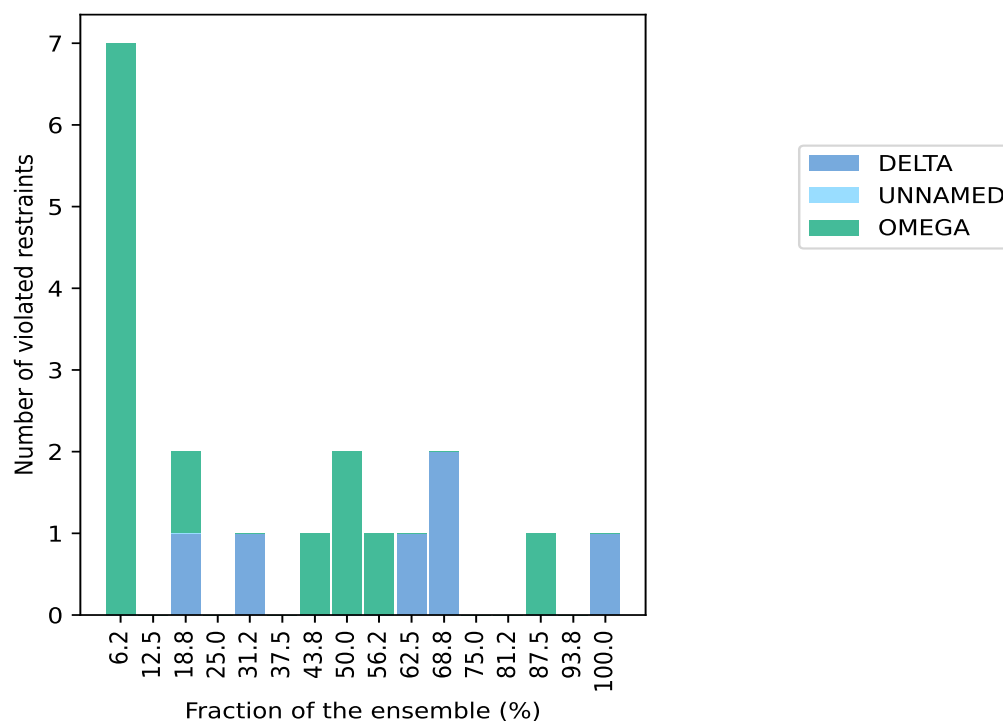
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Number of violated restraints				Fraction of the ensemble	
DELTA	UNNAMED	OMEGA	Total	Count ¹	%
0	0	0	0	12	75.0
0	0	0	0	13	81.2
0	0	1	1	14	87.5
0	0	0	0	15	93.8
1	0	0	1	16	100.0

¹ Number of models with violations

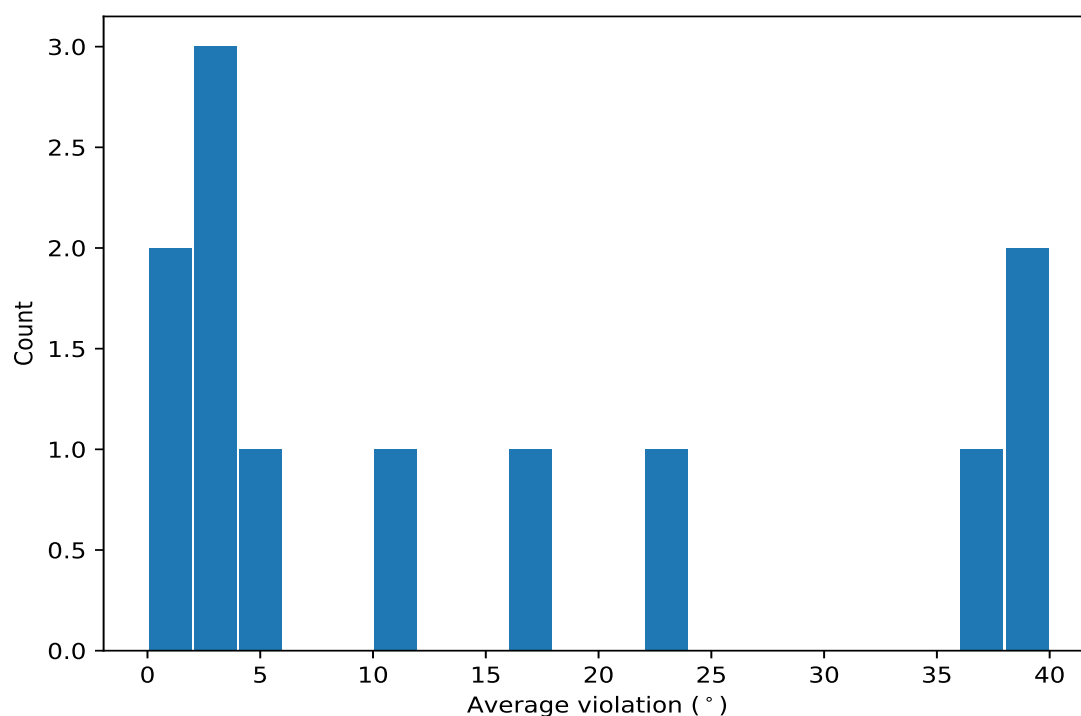
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

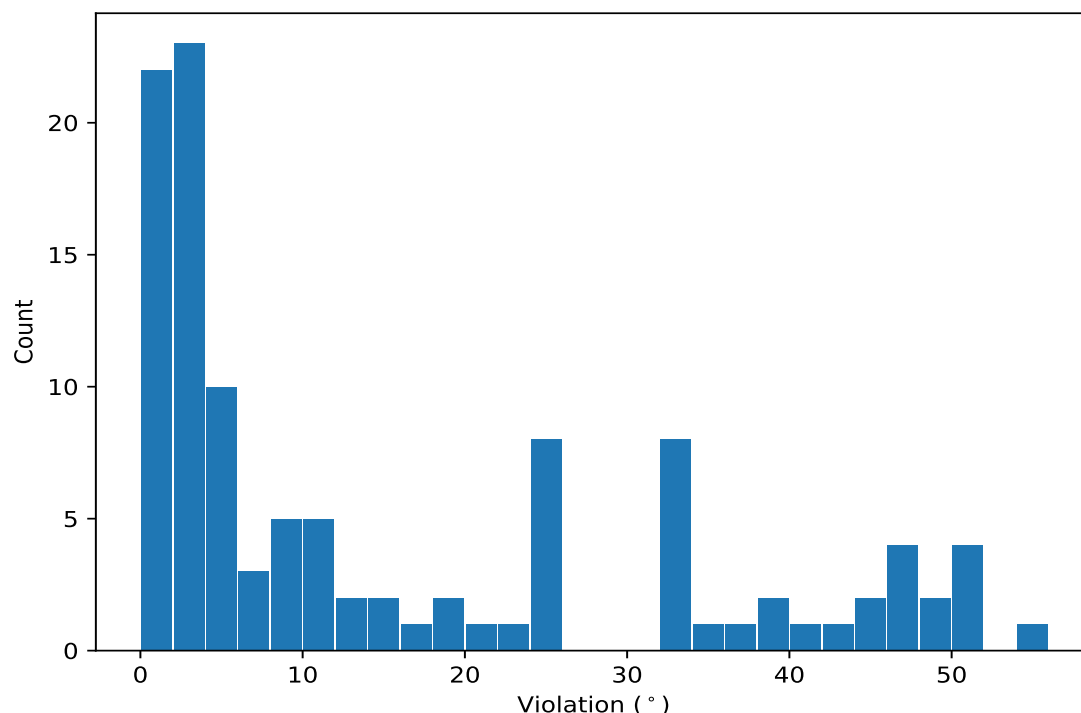
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	16	36.47	8.65	34.09
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	14	3.5	1.2	3.79
(1,1)	1:1:A:U:C5'	1:1:A:U:C4'	1:1:A:U:C3'	1:1:A:U:O3'	11	22.99	11.53	24.15
(1,3)	1:3:A:A:C5'	1:3:A:A:C4'	1:3:A:A:C3'	1:3:A:A:O3'	11	16.52	11.26	14.31
(1,8)	1:8:A:C:C5'	1:8:A:C:C4'	1:8:A:C:C3'	1:8:A:C:O3'	10	39.51	13.39	44.86
(1,310)	2:151:B:ASP:CA	2:151:B:ASP:N	2:150:B:ALA:C	2:150:B:ALA:CA	9	1.93	0.43	1.71
(1,276)	2:117:B:ARG:CA	2:117:B:ARG:N	2:116:B:SER:C	2:116:B:SER:CA	8	4.64	3.23	3.55
(1,335)	2:180:B:PHE:CA	2:180:B:PHE:N	2:179:B:LYS:C	2:179:B:LYS:CA	8	2.05	0.47	2.04
(1,280)	2:121:B:ASN:CA	2:121:B:ASN:N	2:120:B:GLU:C	2:120:B:GLU:CA	7	3.66	2.19	3.83
(1,6)	1:6:A:G:C5'	1:6:A:G:C4'	1:6:A:G:C3'	1:6:A:G:O3'	5	10.46	5.1	8.42
(1,2)	1:2:A:G:C5'	1:2:A:G:C4'	1:2:A:G:C3'	1:2:A:G:O3'	3	38.0	13.83	36.38
(1,331)	2:176:B:ASP:CA	2:176:B:ASP:N	2:175:B:LEU:C	2:175:B:LEU:CA	3	1.71	0.43	1.68

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 (°)
(1,2)	1:2:A:G:C5'	1:2:A:G:C4'	1:2:A:G:C3'	1:2:A:G:O3'	8	55.69
(1,8)	1:8:A:C:C5'	1:8:A:C:C4'	1:8:A:C:C3'	1:8:A:C:O3'	13	50.88
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	10	50.86
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	3	50.38
(1,8)	1:8:A:C:C5'	1:8:A:C:C4'	1:8:A:C:C3'	1:8:A:C:O3'	5	50.2
(1,8)	1:8:A:C:C5'	1:8:A:C:C4'	1:8:A:C:C3'	1:8:A:C:O3'	8	49.85
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	7	48.54
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	5	47.14
(1,8)	1:8:A:C:C5'	1:8:A:C:C4'	1:8:A:C:C3'	1:8:A:C:O3'	11	46.95
(1,1)	1:1:A:U:C5'	1:1:A:U:C4'	1:1:A:U:C3'	1:1:A:U:O3'	14	46.29
(1,3)	1:3:A:A:C5'	1:3:A:A:C4'	1:3:A:A:C3'	1:3:A:A:O3'	9	46.08
(1,8)	1:8:A:C:C5'	1:8:A:C:C4'	1:8:A:C:C3'	1:8:A:C:O3'	16	45.67
(1,8)	1:8:A:C:C5'	1:8:A:C:C4'	1:8:A:C:C3'	1:8:A:C:O3'	7	44.04
(1,8)	1:8:A:C:C5'	1:8:A:C:C4'	1:8:A:C:C3'	1:8:A:C:O3'	2	42.68

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	11	40.88
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	12	38.21
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	9	38.04
(1,2)	1:2:A:G:C5'	1:2:A:G:C4'	1:2:A:G:C3'	1:2:A:G:O3'	12	36.38
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	1	34.36
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	13	33.82
(1,8)	1:8:A:C:C5'	1:8:A:C:C4'	1:8:A:C:C3'	1:8:A:C:O3'	14	33.5
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	8	33.01
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	14	32.96
(1,1)	1:1:A:U:C5'	1:1:A:U:C4'	1:1:A:U:C3'	1:1:A:U:O3'	15	32.91
(1,1)	1:1:A:U:C5'	1:1:A:U:C4'	1:1:A:U:C3'	1:1:A:U:O3'	9	32.43
(1,1)	1:1:A:U:C5'	1:1:A:U:C4'	1:1:A:U:C3'	1:1:A:U:O3'	10	32.32
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	15	32.3
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	2	25.97
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	6	25.9
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	4	25.74
(1,1)	1:1:A:U:C5'	1:1:A:U:C4'	1:1:A:U:C3'	1:1:A:U:O3'	2	25.51
(1,7)	1:7:A:A:C5'	1:7:A:A:C4'	1:7:A:A:C3'	1:7:A:A:O3'	16	25.43
(1,8)	1:8:A:C:C5'	1:8:A:C:C4'	1:8:A:C:C3'	1:8:A:C:O3'	3	24.23
(1,1)	1:1:A:U:C5'	1:1:A:U:C4'	1:1:A:U:C3'	1:1:A:U:O3'	11	24.15
(1,3)	1:3:A:A:C5'	1:3:A:A:C4'	1:3:A:A:C3'	1:3:A:A:O3'	6	24.0
(1,3)	1:3:A:A:C5'	1:3:A:A:C4'	1:3:A:A:C3'	1:3:A:A:O3'	13	22.33
(1,2)	1:2:A:G:C5'	1:2:A:G:C4'	1:2:A:G:C3'	1:2:A:G:O3'	2	21.94
(1,3)	1:3:A:A:C5'	1:3:A:A:C4'	1:3:A:A:C3'	1:3:A:A:O3'	15	18.86
(1,6)	1:6:A:G:C5'	1:6:A:G:C4'	1:6:A:G:C3'	1:6:A:G:O3'	1	18.68
(1,3)	1:3:A:A:C5'	1:3:A:A:C4'	1:3:A:A:C3'	1:3:A:A:O3'	1	17.11
(1,3)	1:3:A:A:C5'	1:3:A:A:C4'	1:3:A:A:C3'	1:3:A:A:O3'	14	14.31
(1,1)	1:1:A:U:C5'	1:1:A:U:C4'	1:1:A:U:C3'	1:1:A:U:O3'	6	14.28
(1,6)	1:6:A:G:C5'	1:6:A:G:C4'	1:6:A:G:C3'	1:6:A:G:O3'	2	13.73
(1,1)	1:1:A:U:C5'	1:1:A:U:C4'	1:1:A:U:C3'	1:1:A:U:O3'	13	13.7
(1,1)	1:1:A:U:C5'	1:1:A:U:C4'	1:1:A:U:C3'	1:1:A:U:O3'	4	11.77
(1,276)	2:117:B:ARG:CA	2:117:B:ARG:N	2:116:B:SER:C	2:116:B:SER:CA	16	10.96
(1,3)	1:3:A:A:C5'	1:3:A:A:C4'	1:3:A:A:C3'	1:3:A:A:O3'	5	10.79
(1,3)	1:3:A:A:C5'	1:3:A:A:C4'	1:3:A:A:C3'	1:3:A:A:O3'	10	10.3
(1,1)	1:1:A:U:C5'	1:1:A:U:C4'	1:1:A:U:C3'	1:1:A:U:O3'	12	10.17
(1,1)	1:1:A:U:C5'	1:1:A:U:C4'	1:1:A:U:C3'	1:1:A:U:O3'	5	9.36
(1,276)	2:117:B:ARG:CA	2:117:B:ARG:N	2:116:B:SER:C	2:116:B:SER:CA	8	9.02
(1,6)	1:6:A:G:C5'	1:6:A:G:C4'	1:6:A:G:C3'	1:6:A:G:O3'	8	8.42
(1,3)	1:3:A:A:C5'	1:3:A:A:C4'	1:3:A:A:C3'	1:3:A:A:O3'	4	8.31
(1,280)	2:121:B:ASN:CA	2:121:B:ASN:N	2:120:B:GLU:C	2:120:B:GLU:CA	7	8.1
(1,8)	1:8:A:C:C5'	1:8:A:C:C4'	1:8:A:C:C3'	1:8:A:C:O3'	12	7.13
(1,6)	1:6:A:G:C5'	1:6:A:G:C4'	1:6:A:G:C3'	1:6:A:G:O3'	9	6.9
(1,3)	1:3:A:A:C5'	1:3:A:A:C4'	1:3:A:A:C3'	1:3:A:A:O3'	16	6.89
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	7	5.49
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	15	4.62
(1,6)	1:6:A:G:C5'	1:6:A:G:C4'	1:6:A:G:C3'	1:6:A:G:O3'	12	4.55
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	9	4.48
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	2	4.43
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	16	4.4
(1,336)	2:181:B:ARG:CA	2:181:B:ARG:N	2:180:B:PHE:C	2:180:B:PHE:CA	12	4.34
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	4	4.27

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,280)	2:121:B:ASN:CA	2:121:B:ASN:N	2:120:B:GLU:C	2:120:B:GLU:CA	4	4.17
(1,280)	2:121:B:ASN:CA	2:121:B:ASN:N	2:120:B:GLU:C	2:120:B:GLU:CA	2	4.01
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	13	3.9
(1,280)	2:121:B:ASN:CA	2:121:B:ASN:N	2:120:B:GLU:C	2:120:B:GLU:CA	13	3.83
(1,276)	2:117:B:ARG:CA	2:117:B:ARG:N	2:116:B:SER:C	2:116:B:SER:CA	15	3.7
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	10	3.68
(1,276)	2:117:B:ARG:CA	2:117:B:ARG:N	2:116:B:SER:C	2:116:B:SER:CA	4	3.57
(1,276)	2:117:B:ARG:CA	2:117:B:ARG:N	2:116:B:SER:C	2:116:B:SER:CA	3	3.53
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	11	3.46
(1,280)	2:121:B:ASN:CA	2:121:B:ASN:N	2:120:B:GLU:C	2:120:B:GLU:CA	11	3.37
(1,335)	2:180:B:PHE:CA	2:180:B:PHE:N	2:179:B:LYS:C	2:179:B:LYS:CA	6	2.99
(1,276)	2:117:B:ARG:CA	2:117:B:ARG:N	2:116:B:SER:C	2:116:B:SER:CA	10	2.87
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	12	2.8
(1,3)	1:3:A:A:C5'	1:3:A:A:C4'	1:3:A:A:C3'	1:3:A:A:O3'	12	2.76
(1,310)	2:151:B:ASP:CA	2:151:B:ASP:N	2:150:B:ALA:C	2:150:B:ALA:CA	12	2.69
(1,310)	2:151:B:ASP:CA	2:151:B:ASP:N	2:150:B:ALA:C	2:150:B:ALA:CA	3	2.52
(1,335)	2:180:B:PHE:CA	2:180:B:PHE:N	2:179:B:LYS:C	2:179:B:LYS:CA	16	2.31
(1,335)	2:180:B:PHE:CA	2:180:B:PHE:N	2:179:B:LYS:C	2:179:B:LYS:CA	13	2.29
(1,276)	2:117:B:ARG:CA	2:117:B:ARG:N	2:116:B:SER:C	2:116:B:SER:CA	9	2.28
(1,331)	2:176:B:ASP:CA	2:176:B:ASP:N	2:175:B:LEU:C	2:175:B:LEU:CA	1	2.25
(1,310)	2:151:B:ASP:CA	2:151:B:ASP:N	2:150:B:ALA:C	2:150:B:ALA:CA	13	2.25
(1,335)	2:180:B:PHE:CA	2:180:B:PHE:N	2:179:B:LYS:C	2:179:B:LYS:CA	10	2.2
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	5	2.11
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	3	2.1
(1,337)	2:182:B:SER:CA	2:182:B:SER:N	2:181:B:ARG:C	2:181:B:ARG:CA	12	2.07
(1,334)	2:179:B:LYS:CA	2:179:B:LYS:N	2:178:B:THR:C	2:178:B:THR:CA	13	1.99
(1,310)	2:151:B:ASP:CA	2:151:B:ASP:N	2:150:B:ALA:C	2:150:B:ALA:CA	8	1.95
(1,335)	2:180:B:PHE:CA	2:180:B:PHE:N	2:179:B:LYS:C	2:179:B:LYS:CA	4	1.88
(1,335)	2:180:B:PHE:CA	2:180:B:PHE:N	2:179:B:LYS:C	2:179:B:LYS:CA	7	1.73
(1,310)	2:151:B:ASP:CA	2:151:B:ASP:N	2:150:B:ALA:C	2:150:B:ALA:CA	6	1.71
(1,310)	2:151:B:ASP:CA	2:151:B:ASP:N	2:150:B:ALA:C	2:150:B:ALA:CA	10	1.71
(1,281)	2:122:B:ARG:CA	2:122:B:ARG:N	2:121:B:ASN:C	2:121:B:ASN:CA	2	1.69
(1,331)	2:176:B:ASP:CA	2:176:B:ASP:N	2:175:B:LEU:C	2:175:B:LEU:CA	6	1.68
(1,310)	2:151:B:ASP:CA	2:151:B:ASP:N	2:150:B:ALA:C	2:150:B:ALA:CA	14	1.66
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	8	1.65
(1,279)	2:120:B:GLU:CA	2:120:B:GLU:N	2:119:B:SER:C	2:119:B:SER:CA	6	1.6
(1,318)	2:161:B:GLU:CA	2:161:B:GLU:N	2:160:B:VAL:C	2:160:B:VAL:CA	4	1.54
(1,335)	2:180:B:PHE:CA	2:180:B:PHE:N	2:179:B:LYS:C	2:179:B:LYS:CA	11	1.53
(1,310)	2:151:B:ASP:CA	2:151:B:ASP:N	2:150:B:ALA:C	2:150:B:ALA:CA	7	1.47
(1,335)	2:180:B:PHE:CA	2:180:B:PHE:N	2:179:B:LYS:C	2:179:B:LYS:CA	1	1.46
(1,301)	2:142:B:ARG:CA	2:142:B:ARG:N	2:141:B:MET:C	2:141:B:MET:CA	6	1.45
(1,287)	2:128:B:LEU:CA	2:128:B:LEU:N	2:127:B:GLY:C	2:127:B:GLY:CA	7	1.45
(1,310)	2:151:B:ASP:CA	2:151:B:ASP:N	2:150:B:ALA:C	2:150:B:ALA:CA	4	1.41
(1,331)	2:176:B:ASP:CA	2:176:B:ASP:N	2:175:B:LEU:C	2:175:B:LEU:CA	9	1.21
(1,276)	2:117:B:ARG:CA	2:117:B:ARG:N	2:116:B:SER:C	2:116:B:SER:CA	14	1.15
(1,280)	2:121:B:ASN:CA	2:121:B:ASN:N	2:120:B:GLU:C	2:120:B:GLU:CA	5	1.14
(1,280)	2:121:B:ASN:CA	2:121:B:ASN:N	2:120:B:GLU:C	2:120:B:GLU:CA	10	1.01