



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 03:41 PM UTC

PDB ID : 2MG5 / pdb_00002mg5
BMRB ID : 19586
Title : Solution Structure of Calmodulin bound to the target peptide of Endothelial Nitrogen Oxide Synthase phosphorylated at Thr495
Authors : Piazza, M.; Dieckmann, T.
Deposited on : 2013-10-28

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

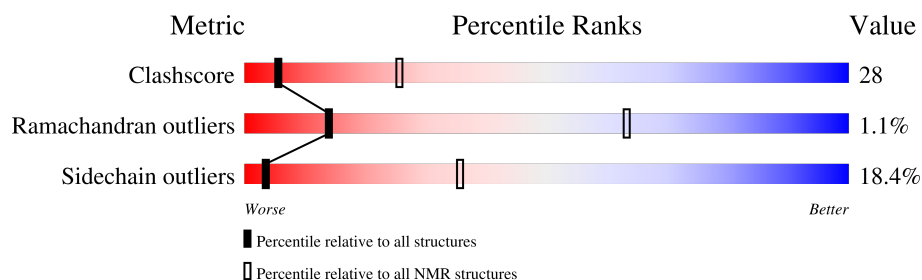
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 71%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	148	
2	B	16	

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:6-A:148, B:496-B:510 (158)	1.18	18

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 4 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2511 atoms, of which 1226 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms						Trace
1	A	148	Total	C	H	N	O	S	0
			2263	714	1097	188	255	9	

- Molecule 2 is a protein called target peptide.

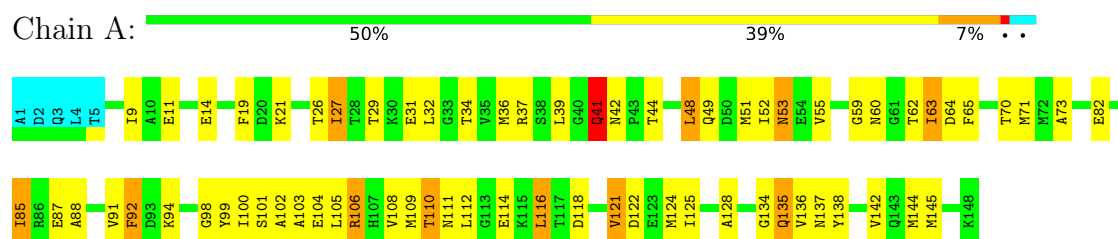
Mol	Chain	Residues	Atoms						Trace
2	B	16	Total	C	H	N	O	S	0
			248	76	129	19	23	1	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Calmodulin



• Molecule 2: target peptide

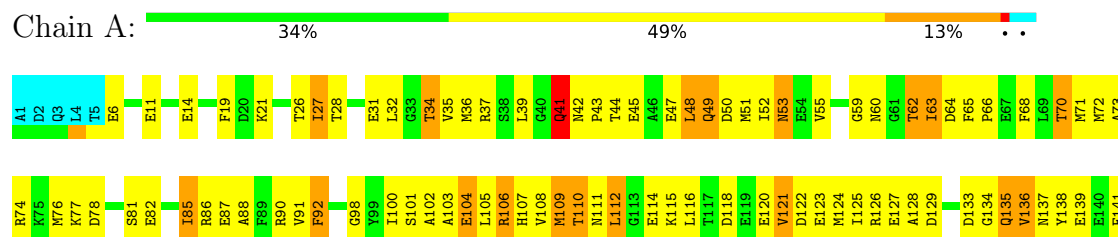


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Calmodulin



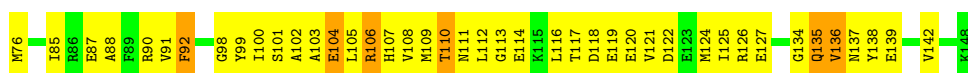
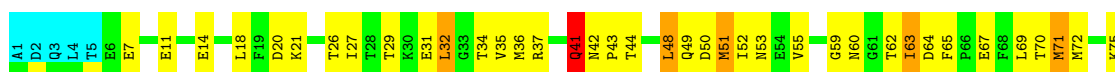


- Molecule 2: target peptide



4.2.2 Score per residue for model 2

- Molecule 1: Calmodulin

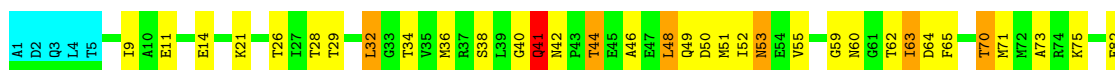


- Molecule 2: target peptide

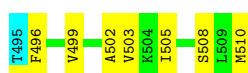


4.2.3 Score per residue for model 3

- Molecule 1: Calmodulin

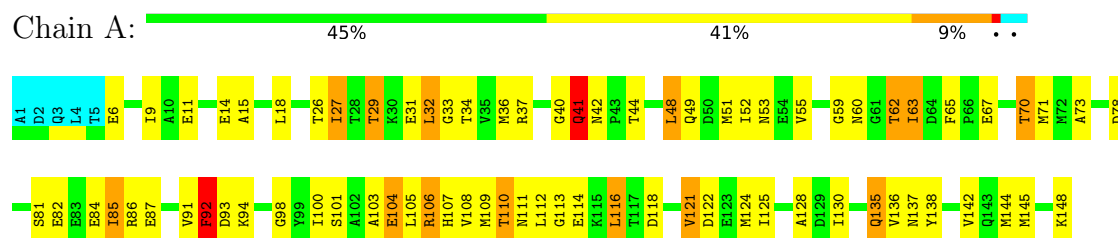


- Molecule 2: target peptide

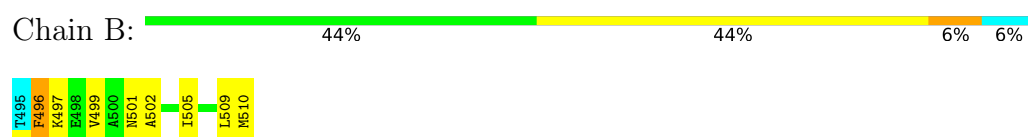


4.2.4 Score per residue for model 4

- Molecule 1: Calmodulin

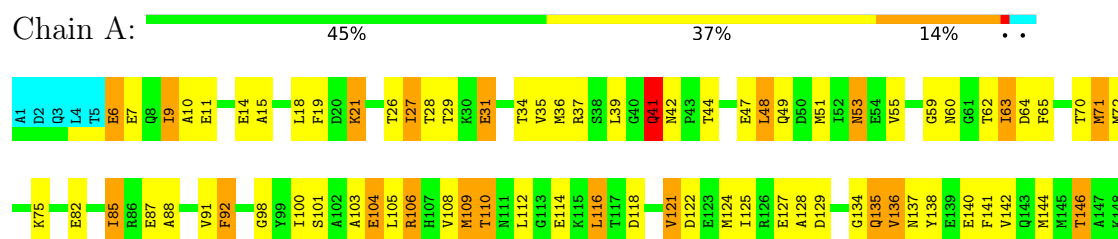


- Molecule 2: target peptide



4.2.5 Score per residue for model 5

- Molecule 1: Calmodulin

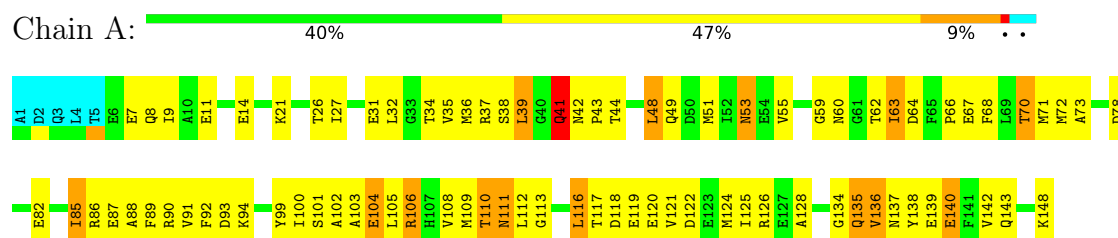


- Molecule 2: target peptide



4.2.6 Score per residue for model 6

- Molecule 1: Calmodulin

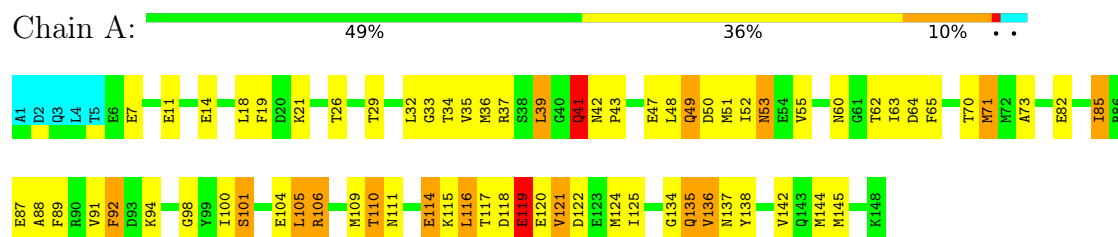


- Molecule 2: target peptide

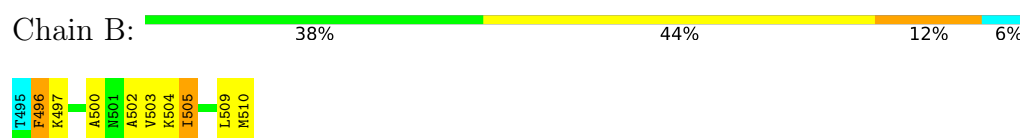


4.2.7 Score per residue for model 7

- Molecule 1: Calmodulin

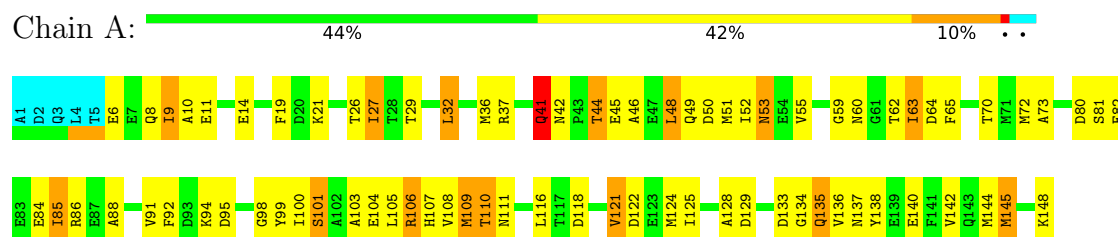


- Molecule 2: target peptide



4.2.8 Score per residue for model 8

- Molecule 1: Calmodulin

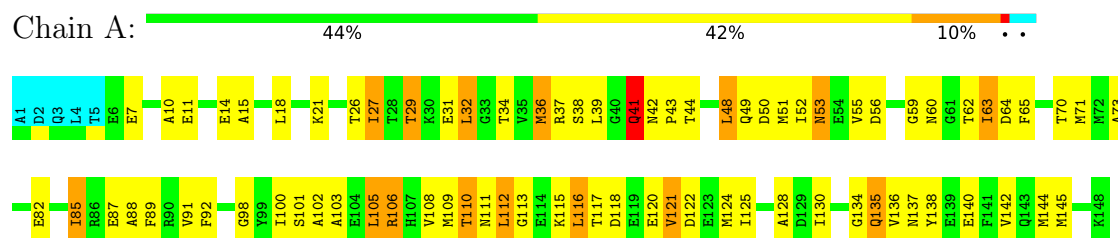


- Molecule 2: target peptide

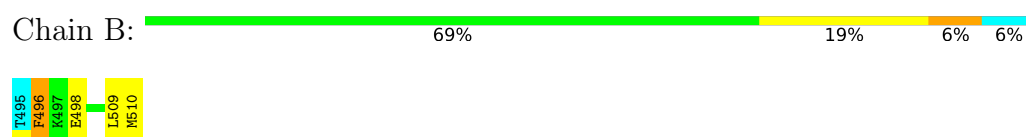


4.2.9 Score per residue for model 9

- Molecule 1: Calmodulin

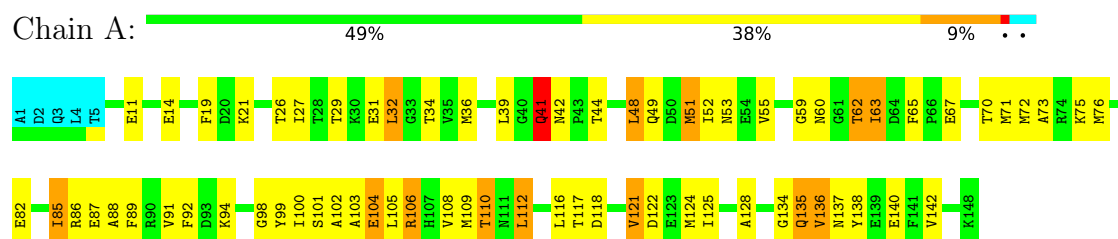


- Molecule 2: target peptide

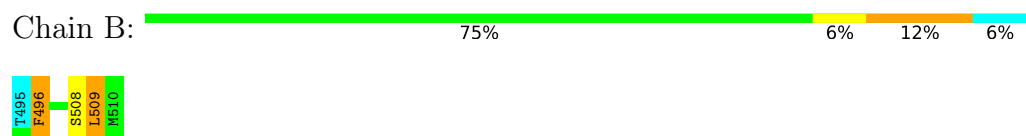


4.2.10 Score per residue for model 10

- Molecule 1: Calmodulin

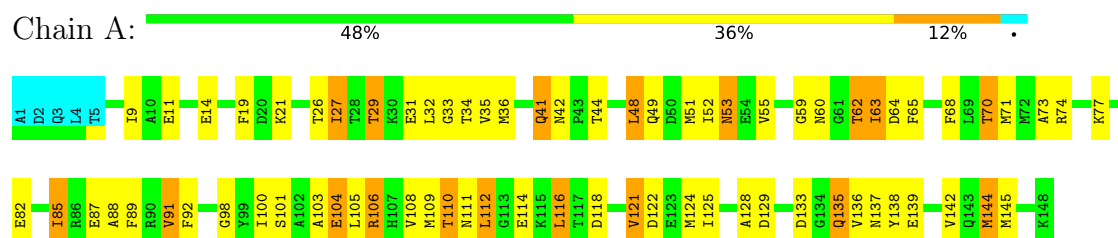


- Molecule 2: target peptide

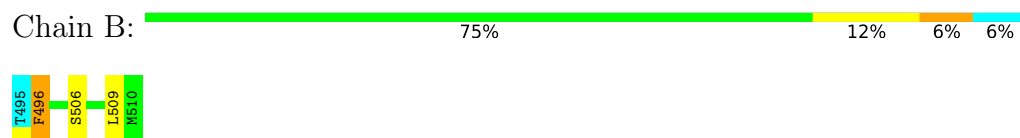


4.2.11 Score per residue for model 11

- Molecule 1: Calmodulin

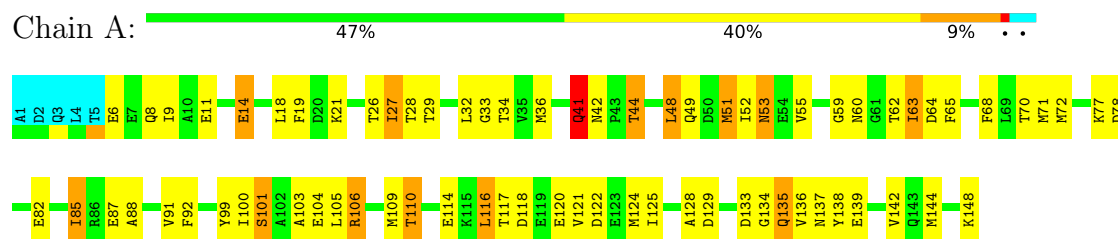


- Molecule 2: target peptide



4.2.12 Score per residue for model 12

- Molecule 1: Calmodulin

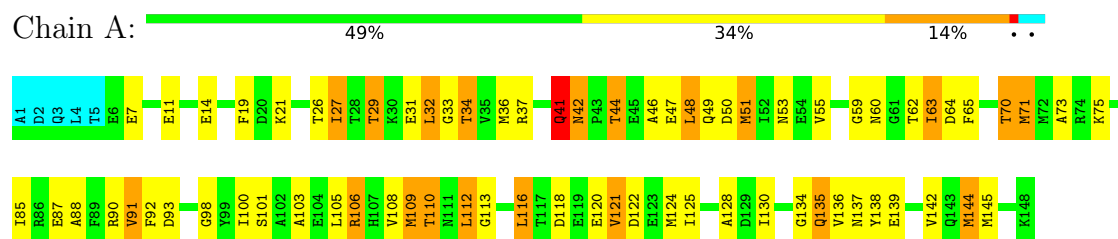


- Molecule 2: target peptide



4.2.13 Score per residue for model 13

- Molecule 1: Calmodulin

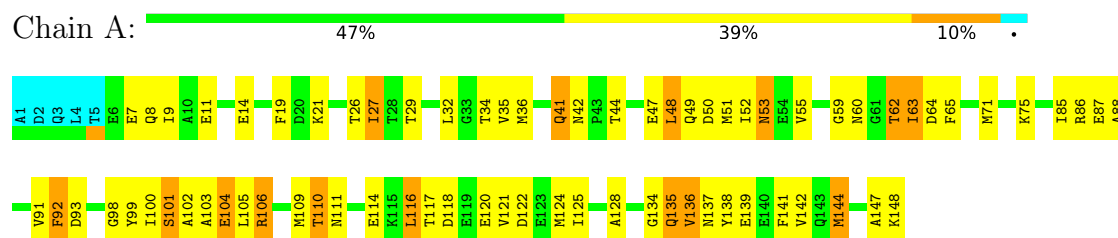


- Molecule 2: target peptide

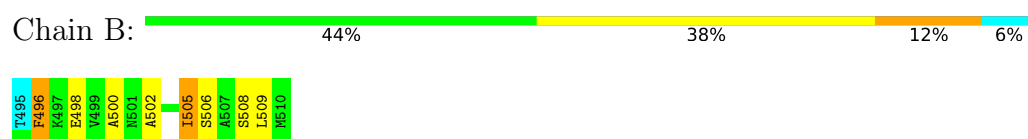


4.2.14 Score per residue for model 14

- Molecule 1: Calmodulin

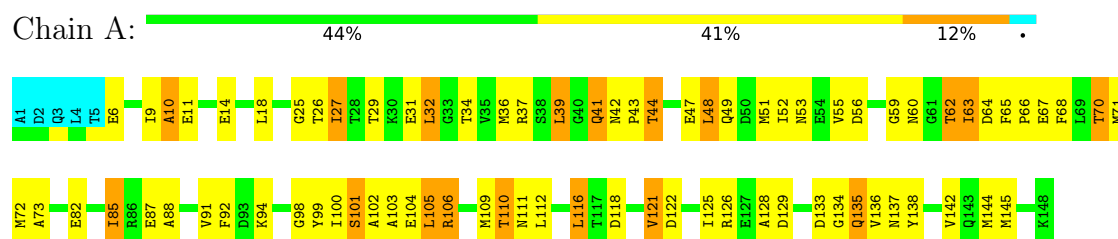


- Molecule 2: target peptide



4.2.15 Score per residue for model 15

- Molecule 1: Calmodulin

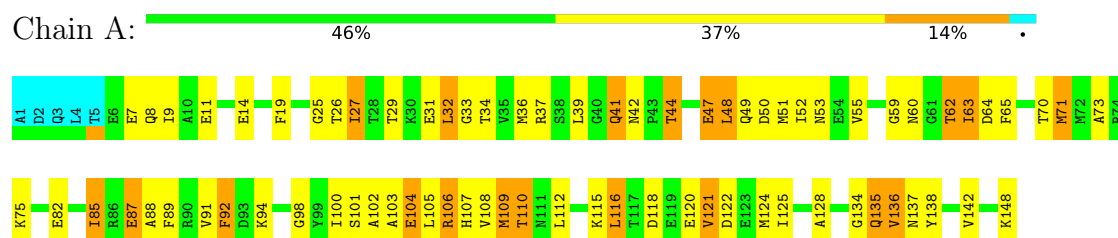


- Molecule 2: target peptide



4.2.16 Score per residue for model 16

- Molecule 1: Calmodulin

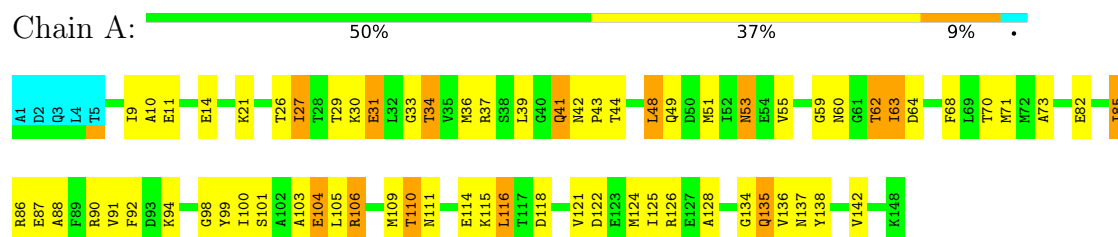


- Molecule 2: target peptide



4.2.17 Score per residue for model 17

- Molecule 1: Calmodulin

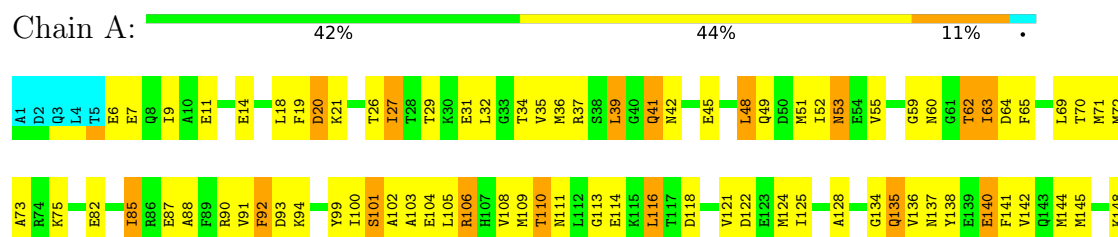


- Molecule 2: target peptide

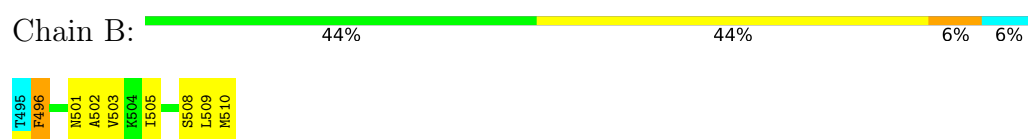


4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Calmodulin

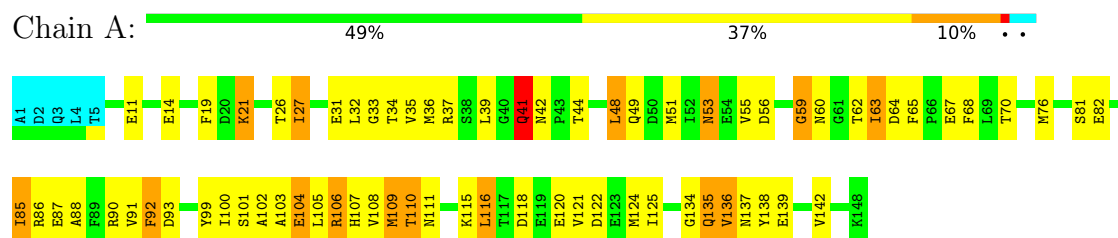


- Molecule 2: target peptide

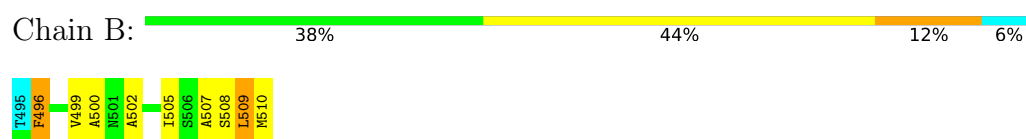


4.2.19 Score per residue for model 19

- Molecule 1: Calmodulin

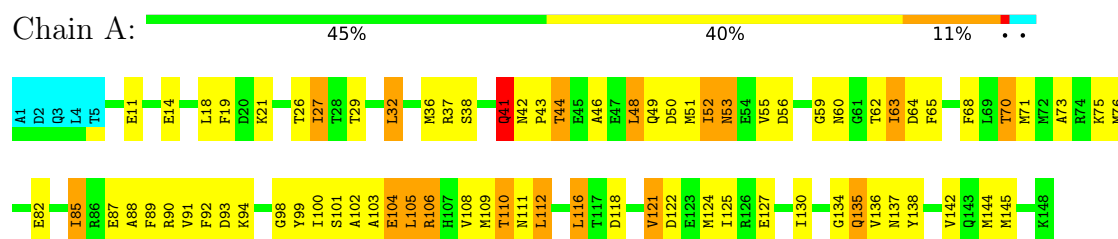


- Molecule 2: target peptide



4.2.20 Score per residue for model 20

- Molecule 1: Calmodulin



- Molecule 2: target peptide



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
CNSSOLVE	structure solution	
CNSSOLVE	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	1523
Number of shifts mapped to atoms	1523
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	0.71±0.01	0±0/1141 (0.0± 0.0%)	1.05±0.02	2±1/1529 (0.1± 0.1%)
2	B	0.81±0.02	0±0/112 (0.0± 0.0%)	0.92±0.06	0±0/147 (0.2± 0.3%)
All	All	0.72	9/25060 (0.0%)	1.04	40/33520 (0.1%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	62	THR	N-CA	-6.00	1.41	1.46	15	9

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	41	GLN	CB-CA-C	-6.71	106.01	114.40	13	14
1	A	119	GLU	N-CA-C	5.89	117.37	111.07	7	1
2	B	496	PHE	CA-CB-CG	5.83	119.62	113.80	8	5
1	A	92	PHE	CA-CB-CG	5.70	119.50	113.80	4	1
1	A	136	VAL	N-CA-C	5.50	116.03	107.28	6	9
1	A	39	LEU	N-CA-C	-5.38	106.58	112.72	15	1
1	A	139	GLU	N-CA-C	5.35	116.81	110.97	13	5
1	A	49	GLN	N-CA-C	-5.32	105.53	112.23	1	2
1	A	146	THR	N-CA-C	-5.29	106.78	113.18	5	1
1	A	14	GLU	N-CA-C	-5.04	107.26	113.41	12	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1129	1060	1059	66±5
2	B	112	121	121	7±2
All	All	24820	23620	23600	1335

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:GLN:O	1:A:53:ASN:HB2	1.23	1.32	3	20
1:A:88:ALA:O	1:A:92:PHE:HB2	1.02	1.53	10	19
1:A:49:GLN:O	1:A:53:ASN:HB3	1.00	1.54	15	4
1:A:49:GLN:O	1:A:53:ASN:CB	0.92	2.15	15	19
1:A:51:MET:O	1:A:55:VAL:HG22	0.91	1.64	7	20
1:A:144:MET:HG3	2:B:496:PHE:O	0.90	1.66	14	3
1:A:106:ARG:O	1:A:110:THR:HB	0.88	1.67	9	20
1:A:48:LEU:H	1:A:48:LEU:HD13	0.83	1.34	19	9
1:A:100:ILE:HG13	1:A:136:VAL:O	0.82	1.72	4	5
1:A:29:THR:HG22	1:A:48:LEU:HD23	0.77	1.55	11	1
1:A:139:GLU:O	1:A:142:VAL:HG12	0.77	1.80	1	2
1:A:100:ILE:HD12	1:A:136:VAL:O	0.76	1.80	3	9
1:A:118:ASP:O	1:A:122:ASP:HB2	0.76	1.79	7	3
1:A:56:ASP:HA	1:A:68:PHE:CE2	0.75	2.16	15	1
1:A:138:TYR:O	1:A:142:VAL:HB	0.74	1.83	1	2
1:A:27:ILE:O	1:A:62:THR:HB	0.73	1.82	9	14
1:A:101:SER:O	1:A:104:GLU:HG3	0.73	1.83	14	2
1:A:26:THR:HB	1:A:62:THR:OG1	0.73	1.84	2	18
1:A:144:MET:SD	2:B:500:ALA:HB2	0.72	2.25	1	3
1:A:36:MET:O	1:A:41:GLN:HB2	0.71	1.85	1	20
1:A:144:MET:SD	2:B:497:LYS:HG2	0.71	2.26	4	4
1:A:100:ILE:O	1:A:135:GLN:HG2	0.70	1.85	12	20
1:A:29:THR:HG23	1:A:52:ILE:HD12	0.70	1.64	11	1
1:A:100:ILE:N	1:A:136:VAL:O	0.69	2.25	8	20
1:A:32:LEU:HD23	1:A:52:ILE:HD12	0.69	1.63	2	2
1:A:103:ALA:HA	1:A:106:ARG:HD3	0.69	1.64	13	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:VAL:HA	1:A:124:MET:SD	0.69	2.28	19	11
1:A:29:THR:HA	1:A:32:LEU:HD11	0.68	1.64	20	4
1:A:32:LEU:HD13	1:A:48:LEU:HG	0.68	1.65	16	5
1:A:93:ASP:HB2	1:A:100:ILE:HG12	0.68	1.66	19	1
1:A:11:GLU:HA	1:A:14:GLU:HB2	0.67	1.64	2	16
1:A:60:ASN:C	1:A:62:THR:H	0.67	1.98	1	18
1:A:26:THR:HG22	1:A:63:ILE:O	0.67	1.89	12	12
1:A:21:LYS:HZ3	1:A:28:THR:H	0.67	1.31	12	1
1:A:32:LEU:HD22	1:A:48:LEU:HG	0.67	1.65	4	4
1:A:32:LEU:HD22	1:A:48:LEU:HB2	0.64	1.68	2	2
1:A:105:LEU:HD21	2:B:499:VAL:HG11	0.64	1.70	15	1
1:A:112:LEU:HD22	1:A:112:LEU:O	0.64	1.93	1	4
1:A:40:GLY:HA2	1:A:94:LYS:HZ3	0.64	1.52	3	2
1:A:32:LEU:HD13	1:A:52:ILE:HD11	0.63	1.68	14	3
1:A:136:VAL:HG21	2:B:496:PHE:CE1	0.63	2.29	20	12
1:A:128:ALA:HB1	1:A:136:VAL:HG13	0.63	1.69	12	14
1:A:124:MET:O	2:B:496:PHE:HB2	0.63	1.94	10	7
1:A:106:ARG:N	1:A:121:VAL:HG11	0.62	2.10	2	15
1:A:105:LEU:O	1:A:109:MET:HB2	0.62	1.95	12	11
1:A:138:TYR:O	1:A:142:VAL:HG22	0.61	1.94	2	18
1:A:128:ALA:O	1:A:140:GLU:HB3	0.61	1.96	5	2
1:A:105:LEU:HD13	1:A:124:MET:SD	0.61	2.36	10	5
1:A:118:ASP:HA	1:A:121:VAL:HG22	0.60	1.72	12	19
1:A:72:MET:SD	2:B:508:SER:HB2	0.60	2.37	8	2
1:A:122:ASP:HA	1:A:125:ILE:HG12	0.60	1.74	7	16
1:A:52:ILE:HG23	1:A:62:THR:O	0.60	1.97	9	7
1:A:36:MET:SD	2:B:510:MET:HG2	0.59	2.37	9	1
1:A:26:THR:HA	1:A:63:ILE:O	0.59	1.98	15	12
1:A:44:THR:O	1:A:48:LEU:HB3	0.59	1.98	3	3
1:A:38:SER:H	1:A:111:ASN:HD22	0.59	1.40	9	1
1:A:33:GLY:O	1:A:37:ARG:HB2	0.59	1.98	4	3
1:A:36:MET:HG2	2:B:510:MET:SD	0.59	2.38	16	2
1:A:124:MET:HE3	2:B:499:VAL:HG21	0.59	1.75	19	1
1:A:142:VAL:HA	1:A:145:MET:SD	0.58	2.37	8	1
1:A:144:MET:SD	2:B:497:LYS:HB3	0.58	2.38	20	1
1:A:98:GLY:O	1:A:137:ASN:HA	0.58	1.99	13	16
1:A:32:LEU:O	1:A:35:VAL:HG23	0.58	1.98	19	1
1:A:118:ASP:O	1:A:122:ASP:N	0.58	2.35	18	18
1:A:48:LEU:H	1:A:48:LEU:CD1	0.58	2.10	11	8
1:A:109:MET:SD	1:A:112:LEU:HD22	0.58	2.38	6	1
1:A:119:GLU:HG3	1:A:120:GLU:H	0.58	1.59	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:MET:O	1:A:39:LEU:HB2	0.57	1.99	15	4
1:A:63:ILE:HD13	1:A:64:ASP:H	0.57	1.60	12	5
1:A:103:ALA:HB1	1:A:106:ARG:NE	0.56	2.15	5	12
1:A:55:VAL:O	1:A:67:GLU:HB3	0.56	2.00	19	4
1:A:37:ARG:C	1:A:39:LEU:H	0.56	2.07	9	3
1:A:120:GLU:O	1:A:124:MET:HG2	0.56	2.00	1	1
1:A:51:MET:SD	1:A:71:MET:HG3	0.56	2.39	2	2
1:A:87:GLU:O	2:B:504:LYS:HA	0.56	1.99	5	2
1:A:87:GLU:C	1:A:91:VAL:HG21	0.56	2.26	18	19
1:A:48:LEU:O	1:A:51:MET:HG2	0.56	2.00	8	1
1:A:36:MET:HE3	2:B:510:MET:SD	0.55	2.41	9	2
1:A:121:VAL:O	1:A:125:ILE:N	0.55	2.40	20	17
1:A:37:ARG:HB3	1:A:111:ASN:OD1	0.55	2.02	17	3
1:A:121:VAL:O	1:A:124:MET:HB2	0.55	2.01	16	16
2:B:502:ALA:O	2:B:505:ILE:HG22	0.55	2.01	1	11
1:A:64:ASP:HB3	1:A:68:PHE:CE1	0.55	2.37	15	1
1:A:29:THR:C	1:A:32:LEU:HG	0.54	2.28	16	7
1:A:32:LEU:HD12	1:A:48:LEU:HD12	0.54	1.77	20	2
1:A:48:LEU:O	1:A:52:ILE:N	0.54	2.34	18	1
1:A:103:ALA:HA	1:A:106:ARG:CD	0.54	2.33	10	7
1:A:47:GLU:O	1:A:50:ASP:HB2	0.54	2.03	7	2
1:A:33:GLY:HA3	1:A:48:LEU:HD12	0.54	1.79	19	3
1:A:35:VAL:HG11	2:B:509:LEU:HB3	0.54	1.80	19	1
1:A:28:THR:O	1:A:31:GLU:HB2	0.54	2.03	5	1
1:A:56:ASP:HA	1:A:68:PHE:CD2	0.54	2.37	15	1
1:A:27:ILE:HG22	1:A:31:GLU:OE1	0.53	2.04	19	1
1:A:106:ARG:HG2	1:A:117:THR:C	0.53	2.28	12	4
1:A:35:VAL:HG23	1:A:36:MET:SD	0.53	2.44	7	2
1:A:72:MET:SD	2:B:505:ILE:HG13	0.53	2.43	1	2
1:A:87:GLU:OE1	2:B:508:SER:HA	0.53	2.04	19	2
1:A:11:GLU:O	1:A:14:GLU:HB2	0.53	2.04	11	17
1:A:72:MET:SD	2:B:505:ILE:HG22	0.53	2.43	2	1
1:A:82:GLU:HA	1:A:85:ILE:HB	0.53	1.81	19	17
1:A:119:GLU:HG3	1:A:120:GLU:N	0.53	2.19	7	2
1:A:122:ASP:O	1:A:126:ARG:HB2	0.52	2.04	6	5
1:A:15:ALA:HA	1:A:18:LEU:HD12	0.52	1.81	4	3
1:A:88:ALA:O	1:A:92:PHE:CB	0.52	2.56	13	4
1:A:72:MET:O	1:A:76:MET:HB2	0.52	2.04	1	2
1:A:100:ILE:HB	1:A:136:VAL:HB	0.52	1.80	12	17
1:A:38:SER:HA	1:A:108:VAL:HG13	0.52	1.82	3	2
1:A:14:GLU:O	1:A:18:LEU:HG	0.52	2.04	5	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:PHE:CE1	1:A:105:LEU:HD21	0.52	2.40	16	6
1:A:41:GLN:CD	1:A:42:ASN:H	0.52	2.13	13	1
1:A:124:MET:SD	2:B:499:VAL:HG11	0.52	2.45	20	1
1:A:60:ASN:ND2	1:A:64:ASP:HB3	0.51	2.20	18	2
1:A:64:ASP:OD2	1:A:66:PRO:HD2	0.51	2.06	1	1
1:A:39:LEU:HG	1:A:91:VAL:HG13	0.51	1.82	10	3
1:A:102:ALA:HB2	1:A:134:GLY:O	0.51	2.05	19	12
1:A:60:ASN:C	1:A:62:THR:N	0.51	2.68	13	17
1:A:105:LEU:O	1:A:109:MET:N	0.51	2.44	1	10
1:A:63:ILE:HD13	1:A:64:ASP:N	0.51	2.21	6	4
1:A:34:THR:HB	1:A:111:ASN:O	0.51	2.05	18	5
1:A:100:ILE:O	1:A:135:GLN:CG	0.51	2.57	12	20
1:A:104:GLU:O	1:A:108:VAL:HG23	0.51	2.06	2	10
1:A:29:THR:HA	1:A:32:LEU:HD12	0.51	1.82	18	1
1:A:19:PHE:O	1:A:21:LYS:HG3	0.51	2.06	8	11
1:A:25:GLY:O	1:A:64:ASP:HA	0.50	2.07	15	2
1:A:29:THR:HA	1:A:32:LEU:CD1	0.50	2.36	7	2
1:A:34:THR:HA	1:A:111:ASN:HD21	0.50	1.64	15	1
1:A:51:MET:HG3	1:A:71:MET:SD	0.50	2.47	16	1
1:A:122:ASP:HA	1:A:125:ILE:CG1	0.50	2.36	1	18
1:A:124:MET:SD	2:B:499:VAL:HG21	0.50	2.46	20	3
1:A:34:THR:HA	1:A:111:ASN:ND2	0.50	2.21	15	2
1:A:136:VAL:HG21	2:B:496:PHE:CZ	0.50	2.42	14	2
1:A:32:LEU:C	1:A:34:THR:H	0.50	2.14	13	14
1:A:38:SER:H	1:A:111:ASN:ND2	0.50	2.03	9	1
1:A:63:ILE:HG23	1:A:64:ASP:N	0.50	2.21	9	1
1:A:60:ASN:ND2	1:A:64:ASP:HB2	0.50	2.21	19	5
1:A:38:SER:O	1:A:91:VAL:O	0.50	2.30	6	1
1:A:55:VAL:HG11	1:A:71:MET:HB3	0.50	1.84	15	1
1:A:31:GLU:OE1	1:A:113:GLY:HA2	0.50	2.07	4	3
1:A:102:ALA:O	1:A:121:VAL:HG21	0.50	2.06	2	3
1:A:125:ILE:HD12	1:A:134:GLY:HA2	0.50	1.84	18	12
1:A:33:GLY:N	1:A:48:LEU:HD11	0.50	2.22	7	1
1:A:44:THR:O	1:A:48:LEU:HD13	0.50	2.07	15	1
1:A:21:LYS:HE3	1:A:31:GLU:OE2	0.50	2.07	17	1
1:A:74:ARG:O	1:A:77:LYS:HD3	0.50	2.07	1	2
1:A:7:GLU:O	1:A:11:GLU:HB2	0.50	2.06	9	3
1:A:93:ASP:HB3	1:A:100:ILE:HG12	0.50	1.84	6	3
2:B:504:LYS:HE2	2:B:504:LYS:O	0.50	2.07	6	1
1:A:101:SER:HB2	1:A:104:GLU:OE2	0.49	2.07	18	2
1:A:109:MET:HA	1:A:112:LEU:HD12	0.49	1.84	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:MET:HA	2:B:496:PHE:N	0.49	2.22	13	1
1:A:144:MET:HE2	2:B:500:ALA:N	0.49	2.22	13	1
1:A:64:ASP:O	1:A:68:PHE:HB2	0.49	2.06	15	3
1:A:34:THR:HG23	1:A:111:ASN:ND2	0.49	2.22	19	1
1:A:29:THR:OG1	1:A:48:LEU:HD23	0.49	2.07	18	2
1:A:19:PHE:O	1:A:27:ILE:HG23	0.49	2.07	20	3
1:A:32:LEU:CD2	1:A:48:LEU:HG	0.49	2.37	9	4
1:A:75:LYS:HG2	2:B:508:SER:O	0.49	2.07	14	8
1:A:21:LYS:NZ	1:A:28:THR:H	0.49	2.04	12	1
1:A:100:ILE:HG23	1:A:104:GLU:OE1	0.49	2.07	15	2
1:A:72:MET:O	1:A:76:MET:HG2	0.49	2.08	10	1
1:A:44:THR:O	1:A:48:LEU:CD1	0.49	2.61	12	1
1:A:34:THR:HG22	1:A:111:ASN:OD1	0.49	2.07	17	1
1:A:60:ASN:OD1	1:A:64:ASP:HB2	0.49	2.07	3	6
1:A:36:MET:SD	1:A:44:THR:HG23	0.49	2.48	3	2
1:A:114:GLU:O	1:A:116:LEU:HG	0.49	2.08	11	7
1:A:39:LEU:HA	1:A:90:ARG:O	0.49	2.08	19	1
1:A:34:THR:HA	1:A:111:ASN:OD1	0.48	2.07	7	2
1:A:45:GLU:HA	1:A:48:LEU:HD11	0.48	1.85	18	1
1:A:129:ASP:HA	1:A:140:GLU:OE2	0.48	2.07	5	1
1:A:104:GLU:OE1	1:A:105:LEU:HG	0.48	2.08	1	1
1:A:48:LEU:HD22	1:A:48:LEU:N	0.48	2.24	13	5
1:A:100:ILE:HD12	1:A:136:VAL:HB	0.48	1.86	4	2
1:A:31:GLU:HB3	1:A:111:ASN:O	0.48	2.08	11	2
1:A:39:LEU:HB3	1:A:41:GLN:OE1	0.48	2.08	7	2
1:A:144:MET:HG2	2:B:496:PHE:CE2	0.48	2.43	8	1
1:A:68:PHE:O	1:A:71:MET:HG3	0.48	2.07	20	2
1:A:106:ARG:HB2	1:A:116:LEU:O	0.48	2.08	15	2
1:A:148:LYS:NZ	2:B:501:ASN:HD22	0.48	2.06	18	1
1:A:137:ASN:ND2	1:A:139:GLU:HB2	0.48	2.23	14	1
1:A:68:PHE:N	1:A:68:PHE:CD1	0.48	2.81	15	1
1:A:21:LYS:HZ3	1:A:28:THR:N	0.48	2.06	12	1
1:A:37:ARG:NE	1:A:43:PRO:HG3	0.48	2.24	17	7
1:A:31:GLU:OE2	1:A:113:GLY:HA2	0.48	2.08	9	2
1:A:107:HIS:O	1:A:110:THR:HG22	0.48	2.08	2	6
1:A:112:LEU:HD13	1:A:112:LEU:C	0.48	2.34	11	2
2:B:500:ALA:O	2:B:504:LYS:HB2	0.48	2.09	15	3
1:A:26:THR:HB	1:A:62:THR:HG1	0.48	1.67	7	2
2:B:499:VAL:O	2:B:503:VAL:HG12	0.48	2.09	13	2
1:A:71:MET:SD	2:B:509:LEU:HD11	0.48	2.48	5	1
1:A:105:LEU:HD22	1:A:109:MET:SD	0.48	2.49	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:VAL:HG12	2:B:506:SER:O	0.47	2.09	2	1
1:A:94:LYS:HB2	1:A:104:GLU:CD	0.47	2.34	20	5
1:A:32:LEU:HD22	1:A:48:LEU:CG	0.47	2.39	13	2
1:A:120:GLU:O	1:A:124:MET:HG3	0.47	2.09	14	2
1:A:68:PHE:O	1:A:71:MET:HG2	0.47	2.10	1	3
1:A:91:VAL:HG11	2:B:507:ALA:HB2	0.47	1.86	6	2
1:A:99:TYR:HA	1:A:136:VAL:O	0.47	2.09	3	1
1:A:35:VAL:HA	2:B:506:SER:O	0.47	2.08	11	2
1:A:119:GLU:OE1	1:A:120:GLU:HG3	0.47	2.09	7	1
1:A:86:ARG:HG2	1:A:90:ARG:NH1	0.47	2.24	6	2
1:A:11:GLU:OE2	2:B:498:GLU:HA	0.47	2.10	9	1
1:A:37:ARG:NH2	1:A:43:PRO:HB3	0.47	2.25	2	1
1:A:82:GLU:O	1:A:86:ARG:HG2	0.47	2.09	8	5
1:A:75:LYS:NZ	2:B:509:LEU:HA	0.47	2.24	10	2
1:A:21:LYS:NZ	1:A:31:GLU:H	0.47	2.08	9	1
1:A:109:MET:HE3	1:A:114:GLU:OE1	0.47	2.09	1	1
1:A:29:THR:O	1:A:32:LEU:HG	0.47	2.10	9	4
1:A:118:ASP:O	1:A:121:VAL:HG22	0.46	2.09	3	7
1:A:142:VAL:CG1	1:A:143:GLN:N	0.46	2.78	1	2
1:A:38:SER:HB3	1:A:111:ASN:OD1	0.46	2.10	6	1
1:A:29:THR:HG23	1:A:62:THR:HG22	0.46	1.86	2	1
1:A:35:VAL:HA	2:B:506:SER:OG	0.46	2.10	14	1
1:A:93:ASP:CG	1:A:100:ILE:HA	0.46	2.35	19	2
1:A:104:GLU:OE2	1:A:105:LEU:HG	0.46	2.10	8	1
1:A:128:ALA:HB1	1:A:136:VAL:CG1	0.46	2.40	12	2
1:A:92:PHE:CD1	2:B:503:VAL:HG11	0.46	2.44	7	3
1:A:8:GLN:HA	1:A:148:LYS:O	0.46	2.10	8	1
1:A:110:THR:OG1	1:A:115:LYS:HA	0.46	2.11	9	3
1:A:21:LYS:HD2	1:A:28:THR:OG1	0.46	2.10	3	1
1:A:66:PRO:HB2	1:A:67:GLU:OE2	0.46	2.11	6	1
1:A:29:THR:O	1:A:48:LEU:HG	0.46	2.10	14	3
1:A:99:TYR:CE2	1:A:137:ASN:HB3	0.46	2.45	15	8
1:A:47:GLU:HG3	1:A:51:MET:SD	0.46	2.50	5	1
1:A:6:GLU:O	1:A:10:ALA:HB3	0.46	2.10	15	2
1:A:101:SER:O	1:A:104:GLU:HB3	0.46	2.11	7	1
1:A:92:PHE:CE2	1:A:105:LEU:HD11	0.45	2.46	8	2
1:A:37:ARG:HB3	1:A:111:ASN:HD21	0.45	1.71	17	2
1:A:124:MET:O	2:B:496:PHE:HB3	0.45	2.10	12	2
1:A:141:PHE:O	1:A:144:MET:HB3	0.45	2.10	14	1
1:A:94:LYS:NZ	1:A:108:VAL:HG22	0.45	2.26	8	1
1:A:129:ASP:CG	1:A:133:ASP:H	0.45	2.19	12	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:ALA:HB3	1:A:145:MET:SD	0.45	2.52	13	1
1:A:108:VAL:O	1:A:112:LEU:HD12	0.45	2.11	10	2
1:A:144:MET:O	1:A:148:LYS:HA	0.45	2.11	14	1
1:A:92:PHE:CE1	1:A:105:LEU:HG	0.45	2.47	4	1
1:A:48:LEU:HD22	1:A:49:GLN:N	0.45	2.27	17	4
1:A:44:THR:HB	1:A:47:GLU:HB2	0.45	1.87	13	2
1:A:46:ALA:O	1:A:50:ASP:HB2	0.45	2.12	8	4
1:A:117:THR:HG22	1:A:118:ASP:H	0.45	1.72	3	2
1:A:32:LEU:CD1	1:A:48:LEU:HG	0.45	2.39	13	4
1:A:37:ARG:HB3	1:A:111:ASN:ND2	0.45	2.27	19	3
1:A:103:ALA:HB1	1:A:106:ARG:NH1	0.45	2.26	17	4
1:A:99:TYR:CE1	1:A:137:ASN:HB3	0.45	2.46	12	1
1:A:32:LEU:HD21	1:A:52:ILE:HD11	0.45	1.89	20	1
1:A:127:GLU:O	1:A:144:MET:HE3	0.45	2.12	20	1
1:A:18:LEU:HA	1:A:114:GLU:OE2	0.45	2.12	2	1
1:A:56:ASP:OD2	1:A:60:ASN:N	0.45	2.46	9	1
1:A:141:PHE:CE2	1:A:144:MET:SD	0.44	3.10	1	1
1:A:34:THR:OG1	1:A:112:LEU:HA	0.44	2.12	4	1
1:A:144:MET:SD	2:B:497:LYS:CG	0.44	3.04	8	2
1:A:116:LEU:HB3	1:A:120:GLU:OE2	0.44	2.12	12	6
1:A:105:LEU:O	1:A:109:MET:CB	0.44	2.66	6	3
1:A:122:ASP:OD2	1:A:125:ILE:HD11	0.44	2.12	7	1
1:A:101:SER:OG	1:A:104:GLU:HB3	0.44	2.13	1	3
1:A:70:THR:O	1:A:73:ALA:HB3	0.44	2.12	6	15
1:A:92:PHE:CD1	1:A:105:LEU:HG	0.44	2.47	4	1
1:A:72:MET:HG2	2:B:508:SER:OG	0.44	2.11	18	1
1:A:90:ARG:HA	1:A:93:ASP:OD2	0.44	2.12	20	2
1:A:38:SER:OG	2:B:503:VAL:HG23	0.44	2.12	20	1
1:A:7:GLU:HB3	1:A:148:LYS:O	0.44	2.13	6	2
1:A:92:PHE:CZ	1:A:105:LEU:HD21	0.44	2.47	16	1
1:A:136:VAL:HG11	2:B:496:PHE:CE2	0.44	2.48	18	7
1:A:86:ARG:O	1:A:91:VAL:HG23	0.44	2.13	8	3
2:B:496:PHE:CD1	2:B:497:LYS:HG3	0.44	2.48	4	3
1:A:92:PHE:CZ	1:A:105:LEU:HD11	0.44	2.47	8	3
1:A:116:LEU:HD23	1:A:120:GLU:HB3	0.44	1.88	7	1
1:A:99:TYR:CD2	1:A:137:ASN:HB3	0.44	2.48	19	6
1:A:144:MET:SD	2:B:496:PHE:CZ	0.44	3.11	11	2
1:A:47:GLU:OE1	2:B:509:LEU:HD22	0.44	2.13	14	1
1:A:141:PHE:O	1:A:145:MET:HG2	0.44	2.12	18	1
1:A:110:THR:HA	1:A:114:GLU:O	0.43	2.12	7	1
1:A:94:LYS:H	1:A:104:GLU:CD	0.43	2.21	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ILE:HD11	1:A:68:PHE:CE2	0.43	2.48	19	1
1:A:71:MET:HE1	1:A:75:LYS:NZ	0.43	2.28	5	1
1:A:7:GLU:OE2	1:A:147:ALA:HB1	0.43	2.13	14	1
1:A:35:VAL:HB	2:B:506:SER:OG	0.43	2.13	1	1
1:A:21:LYS:HE2	1:A:113:GLY:O	0.43	2.13	6	2
1:A:84:GLU:O	1:A:145:MET:HE3	0.43	2.12	3	1
1:A:91:VAL:HG12	2:B:503:VAL:HG22	0.43	1.89	15	1
1:A:93:ASP:HA	1:A:104:GLU:OE1	0.43	2.13	18	1
1:A:136:VAL:HG11	1:A:141:PHE:HB2	0.43	1.91	3	1
1:A:29:THR:CG2	1:A:52:ILE:HD12	0.43	2.41	11	1
1:A:148:LYS:HE2	2:B:501:ASN:ND2	0.43	2.28	12	1
1:A:117:THR:O	1:A:121:VAL:HB	0.43	2.13	7	1
1:A:87:GLU:OE2	2:B:508:SER:HA	0.43	2.13	10	1
1:A:32:LEU:CG	1:A:48:LEU:HG	0.43	2.43	13	1
1:A:92:PHE:CG	1:A:105:LEU:HD21	0.43	2.48	19	1
1:A:116:LEU:HD12	1:A:116:LEU:N	0.43	2.28	7	1
1:A:31:GLU:OE2	1:A:111:ASN:HA	0.43	2.13	11	1
1:A:33:GLY:CA	1:A:48:LEU:HD12	0.43	2.44	11	1
1:A:104:GLU:CD	1:A:105:LEU:HG	0.43	2.38	12	1
1:A:20:ASP:N	1:A:27:ILE:HG22	0.43	2.29	2	1
1:A:93:ASP:HA	1:A:100:ILE:HG23	0.43	1.89	4	1
1:A:29:THR:OG1	1:A:52:ILE:HG13	0.43	2.14	7	1
1:A:117:THR:HB	1:A:119:GLU:HG2	0.43	1.90	2	1
1:A:109:MET:HE2	1:A:114:GLU:OE1	0.43	2.13	7	1
1:A:80:ASP:HB2	1:A:84:GLU:OE1	0.43	2.14	8	1
1:A:148:LYS:OXT	2:B:498:GLU:HA	0.43	2.14	14	1
1:A:108:VAL:O	1:A:112:LEU:HD23	0.43	2.14	5	1
1:A:51:MET:SD	1:A:71:MET:HG2	0.43	2.54	20	1
1:A:148:LYS:HD3	2:B:501:ASN:OD1	0.42	2.13	4	1
1:A:31:GLU:CD	1:A:113:GLY:HA2	0.42	2.39	13	1
2:B:496:PHE:O	2:B:500:ALA:HB2	0.42	2.14	19	1
1:A:36:MET:C	1:A:41:GLN:HB2	0.42	2.39	1	1
1:A:92:PHE:CD1	1:A:100:ILE:HG21	0.42	2.49	4	1
1:A:45:GLU:O	1:A:48:LEU:HD23	0.42	2.14	8	1
1:A:34:THR:HG22	1:A:111:ASN:ND2	0.42	2.29	1	1
1:A:48:LEU:HD23	1:A:48:LEU:N	0.42	2.29	1	1
1:A:32:LEU:HB2	1:A:48:LEU:HD12	0.42	1.90	3	1
1:A:34:THR:OG1	1:A:112:LEU:HD22	0.42	2.14	3	2
1:A:10:ALA:O	1:A:14:GLU:HG3	0.42	2.14	17	3
1:A:92:PHE:CE1	2:B:496:PHE:CZ	0.42	3.07	6	2
1:A:37:ARG:HB3	1:A:111:ASN:O	0.42	2.13	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:THR:OG1	1:A:115:LYS:HD3	0.42	2.14	7	4
1:A:35:VAL:HG11	2:B:509:LEU:HB2	0.42	1.90	5	1
1:A:109:MET:SD	1:A:124:MET:SD	0.42	3.18	3	1
1:A:116:LEU:HD23	1:A:120:GLU:CB	0.42	2.45	7	1
1:A:11:GLU:CA	1:A:14:GLU:HB2	0.42	2.39	2	1
1:A:116:LEU:HD22	1:A:121:VAL:HG23	0.42	1.90	7	1
1:A:48:LEU:HG	1:A:49:GLN:N	0.42	2.28	8	1
1:A:109:MET:HE1	1:A:124:MET:HE1	0.42	1.90	20	1
1:A:35:VAL:HG23	1:A:36:MET:H	0.42	1.75	2	1
1:A:109:MET:HA	1:A:112:LEU:HD13	0.42	1.89	6	1
1:A:21:LYS:HZ1	1:A:31:GLU:H	0.42	1.56	9	1
1:A:11:GLU:OE1	2:B:498:GLU:HG3	0.42	2.14	14	1
1:A:27:ILE:HD11	1:A:68:PHE:CZ	0.42	2.50	19	1
1:A:108:VAL:HA	1:A:111:ASN:ND2	0.42	2.30	4	1
2:B:496:PHE:CE1	2:B:497:LYS:HG3	0.42	2.50	8	3
1:A:141:PHE:O	1:A:144:MET:HE2	0.42	2.15	1	1
1:A:100:ILE:H	1:A:136:VAL:C	0.42	2.23	10	2
1:A:120:GLU:O	1:A:124:MET:SD	0.42	2.78	12	1
1:A:63:ILE:HA	1:A:68:PHE:CD2	0.42	2.50	15	1
1:A:73:ALA:O	1:A:76:MET:HG3	0.42	2.15	20	1
1:A:140:GLU:O	1:A:144:MET:SD	0.41	2.78	18	2
1:A:21:LYS:NZ	1:A:31:GLU:HB2	0.41	2.30	10	1
1:A:52:ILE:O	1:A:56:ASP:CG	0.41	2.63	20	1
1:A:92:PHE:CE1	1:A:100:ILE:HG21	0.41	2.51	13	1
1:A:95:ASP:OD1	1:A:101:SER:HB3	0.41	2.15	8	1
1:A:51:MET:HB3	1:A:71:MET:SD	0.41	2.55	13	1
1:A:84:GLU:O	1:A:145:MET:HE1	0.41	2.15	4	1
1:A:37:ARG:C	1:A:39:LEU:N	0.41	2.78	9	1
1:A:77:LYS:O	1:A:77:LYS:HG3	0.41	2.15	12	1
1:A:51:MET:SD	1:A:71:MET:SD	0.41	3.19	15	1
1:A:148:LYS:O	1:A:148:LYS:HD2	0.41	2.15	6	1
1:A:137:ASN:OD1	1:A:139:GLU:HB2	0.41	2.15	2	1
1:A:37:ARG:HD3	1:A:111:ASN:ND2	0.41	2.31	18	1
1:A:32:LEU:O	1:A:35:VAL:HG22	0.41	2.15	1	1
1:A:106:ARG:O	1:A:110:THR:CB	0.41	2.56	9	1
1:A:52:ILE:HD13	1:A:62:THR:HA	0.41	1.93	3	1
1:A:38:SER:O	1:A:108:VAL:HG13	0.41	2.15	9	1
1:A:32:LEU:HD13	1:A:48:LEU:CG	0.41	2.44	10	1
1:A:86:ARG:C	1:A:88:ALA:H	0.41	2.24	14	1
1:A:144:MET:HE3	2:B:496:PHE:O	0.41	2.15	14	1
1:A:92:PHE:CZ	2:B:499:VAL:HG12	0.41	2.51	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:PHE:CD1	1:A:105:LEU:HD21	0.40	2.51	19	1
1:A:123:GLU:O	1:A:127:GLU:HG3	0.40	2.15	1	1
1:A:127:GLU:O	1:A:144:MET:HE2	0.40	2.16	5	1
1:A:32:LEU:O	1:A:48:LEU:HD12	0.40	2.17	9	1
1:A:28:THR:HB	1:A:31:GLU:OE1	0.40	2.16	1	1
1:A:92:PHE:CE1	1:A:105:LEU:HD11	0.40	2.52	6	1
1:A:56:ASP:CG	1:A:60:ASN:H	0.40	2.24	9	1
1:A:56:ASP:HB2	1:A:59:GLY:HA2	0.40	1.93	19	1
1:A:127:GLU:O	2:B:497:LYS:HE3	0.40	2.16	1	1
1:A:106:ARG:HG3	1:A:121:VAL:HG11	0.40	1.93	10	1
1:A:30:LYS:O	1:A:34:THR:OG1	0.40	2.40	17	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	
1	A	142/148 (96%)	122±3 (86±2%)	18±3 (13±2%)	2±1 (1±1%)	13	61
2	B	14/16 (88%)	14±1 (97±4%)	0±1 (2±4%)	0±0 (0±2%)	31	76
All	All	3120/3280 (95%)	2713 (87%)	372 (12%)	35 (1%)	14	63

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	59	GLY	19
1	A	78	ASP	4
1	A	81	SER	4
1	A	6	GLU	1
1	A	35	VAL	1
2	B	505	ILE	1
1	A	29	THR	1
1	A	10	ALA	1
1	A	66	PRO	1
1	A	20	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	21	LYS	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	
1	A	122/126 (97%)	100±3 (82±2%)	22±3 (18±2%)	3	36
2	B	12/12 (100%)	10±1 (82±8%)	2±1 (18±8%)	3	36
All	All	2680/2760 (97%)	2188 (82%)	492 (18%)	3	36

All 65 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	41	GLN	20
1	A	42	ASN	20
1	A	63	ILE	20
1	A	85	ILE	20
1	A	106	ARG	20
1	A	110	THR	20
1	A	116	LEU	20
1	A	135	GLN	20
1	A	48	LEU	19
1	A	44	THR	18
1	A	65	PHE	18
1	A	101	SER	18
1	A	27	ILE	16
2	B	509	LEU	16
1	A	53	ASN	14
1	A	121	VAL	13
1	A	70	THR	12
1	A	104	GLU	12
1	A	71	MET	12
2	B	496	PHE	11
1	A	32	LEU	10
1	A	9	ILE	10
1	A	92	PHE	9

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Mol	Chain	Res	Type	Models (Total)
1	A	109	MET	9
1	A	112	LEU	9
2	B	510	MET	8
1	A	89	PHE	7
1	A	144	MET	6
1	A	145	MET	6
1	A	31	GLU	5
1	A	39	LEU	5
1	A	50	ASP	4
1	A	51	MET	4
1	A	130	ILE	4
1	A	140	GLU	4
1	A	105	LEU	4
1	A	34	THR	3
2	B	505	ILE	3
1	A	21	LYS	3
1	A	90	ARG	3
1	A	29	THR	3
2	B	497	LYS	3
1	A	69	LEU	2
1	A	119	GLU	2
1	A	7	GLU	2
1	A	72	MET	2
2	B	504	LYS	2
1	A	52	ILE	2
1	A	91	VAL	2
1	A	47	GLU	2
1	A	6	GLU	1
1	A	45	GLU	1
1	A	37	ARG	1
1	A	141	PHE	1
1	A	146	THR	1
1	A	111	ASN	1
1	A	94	LYS	1
1	A	114	GLU	1
1	A	36	MET	1
1	A	67	GLU	1
2	B	498	GLU	1
1	A	19	PHE	1
1	A	87	GLU	1
1	A	20	ASP	1
1	A	76	MET	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	TPO	B	495	2	5,6,11	0.56±0.05	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	TPO	B	495	2	5,7,16	0.89±0.04	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	B	495	2	-	0±0,5,6,13	-

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 71% for the well-defined parts and 71% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	1523
Number of shifts mapped to atoms	1523
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
$^{13}\text{C}_\alpha$	144	2.51 ± 0.12	Should be checked
$^{13}\text{C}_\beta$	130	2.85 ± 0.11	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	145	0.41 ± 0.25	None needed (< 0.5 ppm)

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 71%, i.e. 1479 atoms were assigned a chemical shift out of a possible 2082. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	602/797 (76%)	321/325 (99%)	140/316 (44%)	141/156 (90%)
Sidechain	847/1169 (72%)	601/750 (80%)	246/379 (65%)	0/40 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	30/116 (26%)	30/57 (53%)	0/57 (0%)	0/2 (0%)
Overall	1479/2082 (71%)	952/1132 (84%)	386/752 (51%)	141/198 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 1517 atoms were assigned a chemical shift out of a possible 2144. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	618/822 (75%)	329/335 (98%)	144/326 (44%)	145/161 (90%)
Sidechain	869/1206 (72%)	616/774 (80%)	253/391 (65%)	0/41 (0%)
Aromatic	30/116 (26%)	30/57 (53%)	0/57 (0%)	0/2 (0%)
Overall	1517/2144 (71%)	975/1166 (84%)	397/774 (51%)	145/204 (71%)

7.1.4 Statistically unusual chemical shifts ⓘ

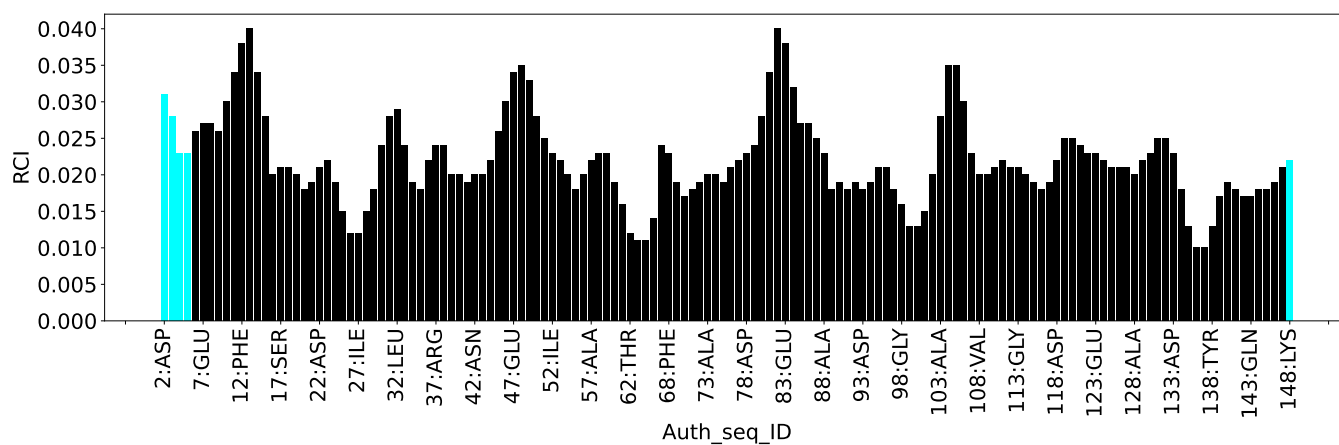
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	125	ILE	CG1	13.60	19.24 – 36.26	-8.3
1	A	125	ILE	CG2	24.79	10.93 – 24.12	5.5

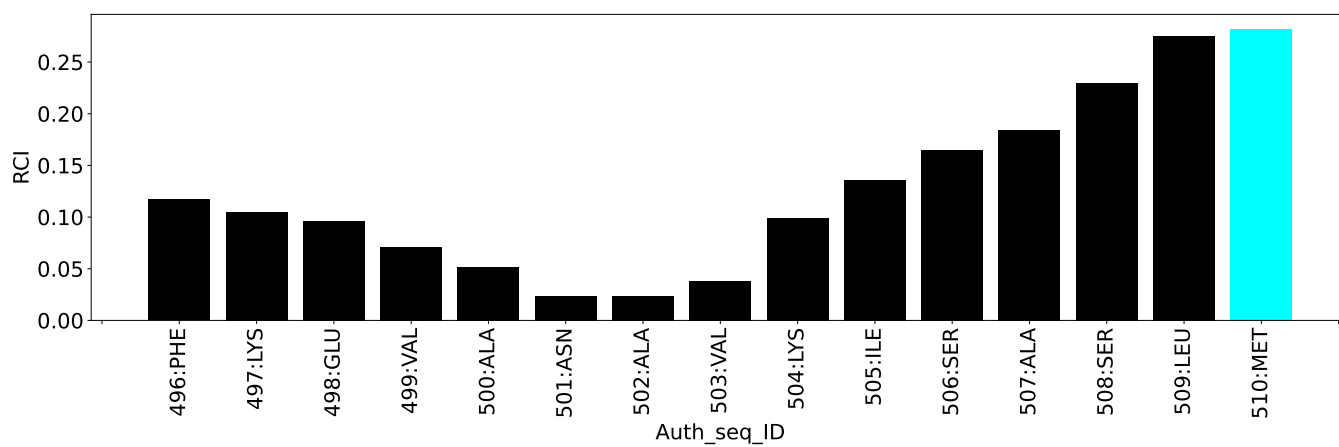
7.1.5 Random Coil Index (RCI) plots ⓘ

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 A:



Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1461
Intra-residue ($ i-j =0$)	864
Sequential ($ i-j =1$)	285
Medium range ($ i-j >1$ and $ i-j <5$)	192
Long range ($ i-j \geq 5$)	120
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	293
Number of unmapped restraints	0
Number of restraints per residue	10.7
Number of long range restraints per residue ¹	0.7

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)	104.3	0.2
0.2-0.5 (Medium)	63.9	0.5
>0.5 (Large)	1.0	1.13

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)	49.4	9.43
10.0-20.0 (Medium)	1.6	19.91
>20.0 (Large)	3.8	145.96

9 Distance violation analysis ⓘ

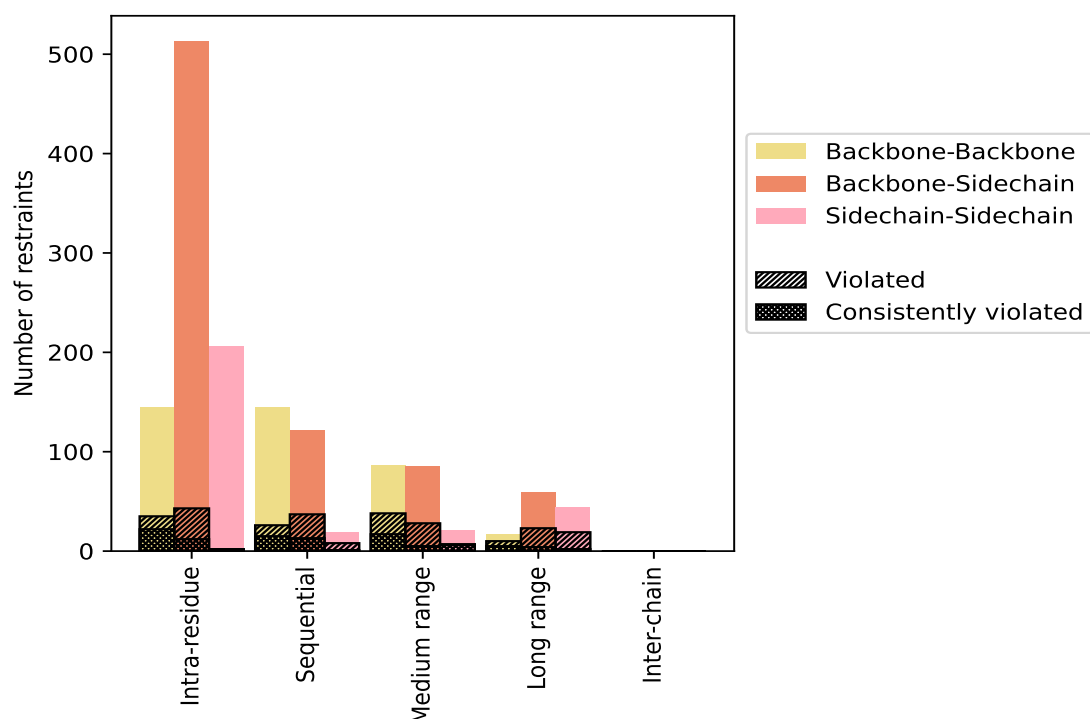
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	864	59.1	80	9.3	5.5	36	4.2	2.5
Backbone-Backbone	145	9.9	35	24.1	2.4	22	15.2	1.5
Backbone-Sidechain	513	35.1	43	8.4	2.9	12	2.3	0.8
Sidechain-Sidechain	206	14.1	2	1.0	0.1	2	1.0	0.1
Sequential (i-j =1)	285	19.5	71	24.9	4.9	29	10.2	2.0
Backbone-Backbone	145	9.9	26	17.9	1.8	15	10.3	1.0
Backbone-Sidechain	121	8.3	37	30.6	2.5	13	10.7	0.9
Sidechain-Sidechain	19	1.3	8	42.1	0.5	1	5.3	0.1
Medium range (i-j >1 & i-j <5)	192	13.1	73	38.0	5.0	28	14.6	1.9
Backbone-Backbone	86	5.9	38	44.2	2.6	17	19.8	1.2
Backbone-Sidechain	85	5.8	28	32.9	1.9	5	5.9	0.3
Sidechain-Sidechain	21	1.4	7	33.3	0.5	6	28.6	0.4
Long range (i-j ≥5)	120	8.2	52	43.3	3.6	11	9.2	0.8
Backbone-Backbone	17	1.2	10	58.8	0.7	5	29.4	0.3
Backbone-Sidechain	59	4.0	23	39.0	1.6	4	6.8	0.3
Sidechain-Sidechain	44	3.0	19	43.2	1.3	2	4.5	0.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1461	100.0	276	18.9	18.9	104	7.1	7.1
Backbone-Backbone	393	26.9	109	27.7	7.5	59	15.0	4.0
Backbone-Sidechain	778	53.3	131	16.8	9.0	34	4.4	2.3
Sidechain-Sidechain	290	19.8	36	12.4	2.5	11	3.8	0.8

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	58	48	53	25	0	184	0.2	0.84	0.1	0.17
2	54	40	49	26	0	169	0.21	0.82	0.1	0.18
3	56	43	45	25	0	169	0.21	0.83	0.1	0.18
4	54	44	47	24	0	169	0.2	0.86	0.1	0.18
5	55	47	50	25	0	177	0.21	1.11	0.11	0.18
6	53	49	52	23	0	177	0.2	1.08	0.11	0.17
7	53	43	49	26	0	171	0.21	1.13	0.11	0.18
8	58	48	44	22	0	172	0.21	0.82	0.1	0.18
9	61	44	45	25	0	175	0.21	0.99	0.1	0.18
10	58	44	44	29	0	175	0.2	0.84	0.1	0.17

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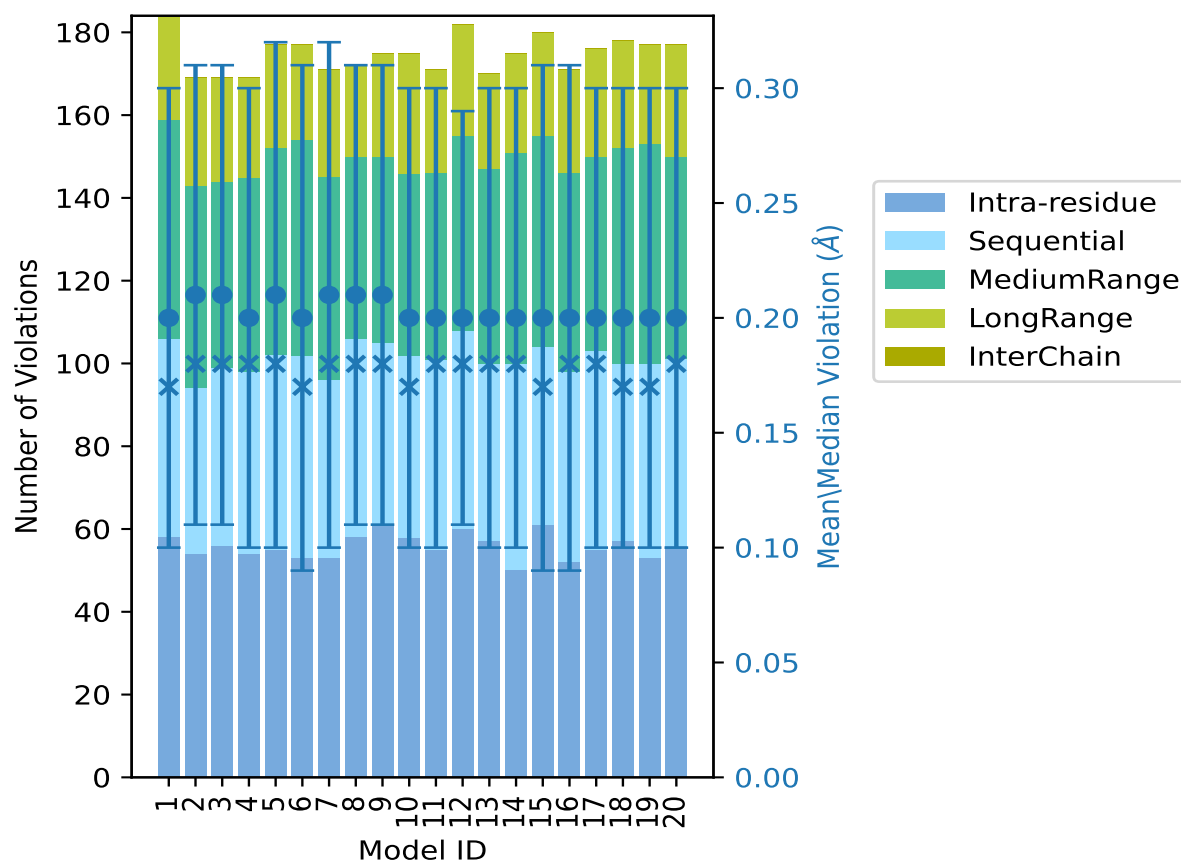
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	55	46	45	25	0	171	0.2	0.86	0.1	0.18
12	60	48	47	27	0	182	0.2	0.84	0.09	0.18
13	57	43	47	23	0	170	0.2	0.9	0.1	0.18
14	50	50	51	24	0	175	0.2	0.85	0.1	0.18
15	61	43	51	25	0	180	0.2	1.03	0.11	0.17
16	52	46	48	25	0	171	0.2	1.12	0.11	0.18
17	55	48	47	26	0	176	0.2	0.9	0.1	0.18
18	57	43	52	26	0	178	0.2	1.0	0.1	0.17
19	53	47	53	24	0	177	0.2	0.83	0.1	0.17
20	56	45	49	27	0	177	0.2	0.83	0.1	0.18

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

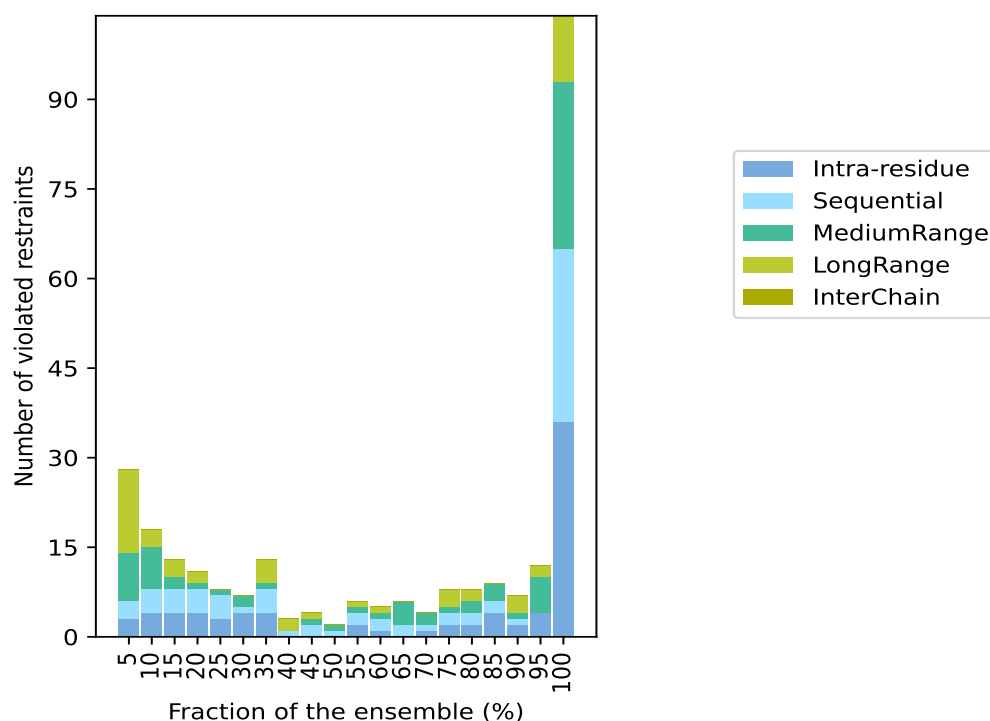
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1185(IR:784, SQ:214, MR:119, LR:68, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
3	3	8	14	0	28	1	5.0
4	4	7	3	0	18	2	10.0
4	4	2	3	0	13	3	15.0
4	4	1	2	0	11	4	20.0
3	4	1	0	0	8	5	25.0
4	1	2	0	0	7	6	30.0
4	4	1	4	0	13	7	35.0
0	1	0	2	0	3	8	40.0
0	2	1	1	0	4	9	45.0
0	1	1	0	0	2	10	50.0
2	2	1	1	0	6	11	55.0
1	2	1	1	0	5	12	60.0
0	2	4	0	0	6	13	65.0
1	1	2	0	0	4	14	70.0
2	2	1	3	0	8	15	75.0
2	2	2	2	0	8	16	80.0
4	2	3	0	0	9	17	85.0
2	1	1	3	0	7	18	90.0
4	0	6	2	0	12	19	95.0
36	29	28	11	0	104	20	100.0

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

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

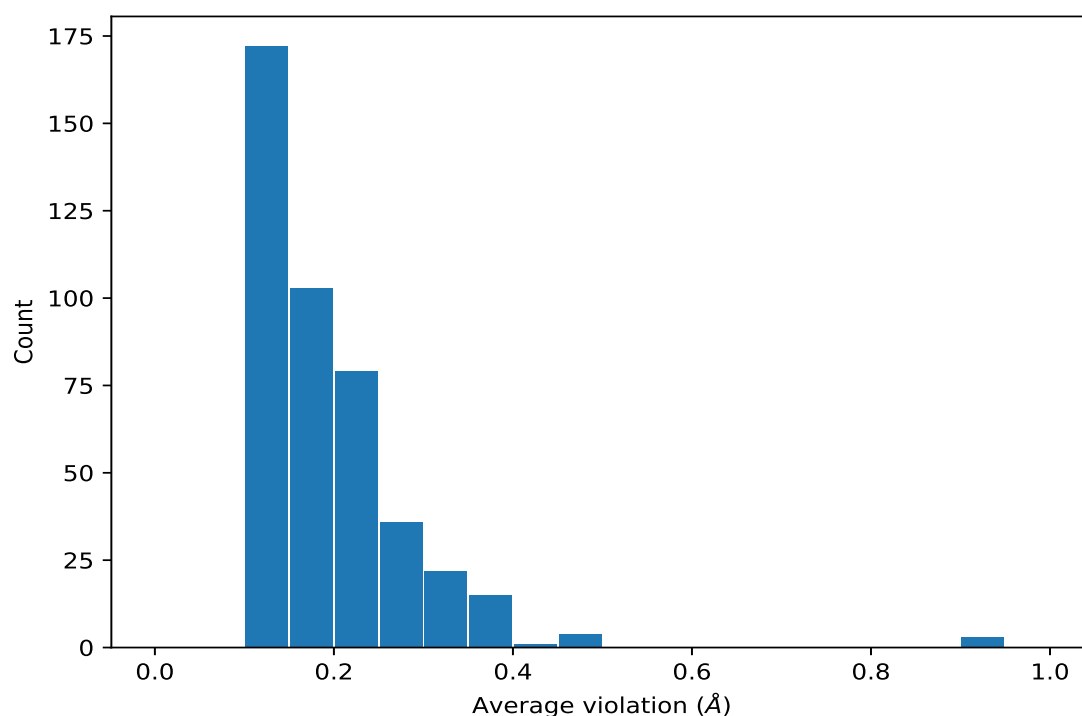
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	20	0.92	0.11	0.86
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	20	0.92	0.11	0.86
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	20	0.92	0.11	0.86
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	20	0.47	0.02	0.48
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	20	0.47	0.02	0.48
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	20	0.46	0.02	0.46
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	20	0.46	0.03	0.47
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	20	0.43	0.02	0.43
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	20	0.38	0.07	0.42
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	20	0.38	0.07	0.42
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	20	0.38	0.07	0.42
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	20	0.38	0.07	0.42
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	20	0.38	0.05	0.4
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	20	0.38	0.05	0.4
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	20	0.38	0.05	0.4
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	20	0.37	0.02	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	20	0.37	0.02	0.37
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	20	0.37	0.02	0.37
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	20	0.36	0.03	0.36
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	20	0.36	0.03	0.36
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	20	0.35	0.09	0.32
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	20	0.35	0.09	0.32
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	20	0.35	0.03	0.34
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	20	0.35	0.03	0.34
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	20	0.34	0.05	0.36
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	20	0.34	0.05	0.36
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	20	0.34	0.05	0.36
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	20	0.33	0.0	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	20	0.33	0.0	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	20	0.33	0.0	0.33
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	20	0.33	0.01	0.32
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	20	0.32	0.06	0.35
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	20	0.32	0.06	0.35
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	20	0.32	0.02	0.32
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	20	0.32	0.01	0.32
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	20	0.32	0.02	0.32
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	20	0.3	0.04	0.29
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	20	0.29	0.02	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	20	0.29	0.02	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	20	0.29	0.02	0.3
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	20	0.29	0.03	0.29
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	20	0.29	0.02	0.28
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	20	0.29	0.02	0.28
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	20	0.27	0.01	0.27
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	20	0.27	0.01	0.27
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	20	0.26	0.03	0.25
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	20	0.26	0.02	0.25
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	20	0.26	0.03	0.25
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	20	0.25	0.1	0.22
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	20	0.25	0.02	0.24
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	20	0.25	0.02	0.24
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	20	0.25	0.07	0.26
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	20	0.25	0.02	0.25
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	20	0.25	0.02	0.25
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	20	0.25	0.02	0.25
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	20	0.24	0.02	0.24
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	20	0.24	0.06	0.24
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	20	0.24	0.06	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	20	0.24	0.06	0.24
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	20	0.24	0.02	0.24
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	20	0.24	0.03	0.24
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	20	0.24	0.03	0.24
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	20	0.23	0.01	0.24
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	20	0.23	0.02	0.24
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	20	0.23	0.02	0.24
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	20	0.23	0.04	0.22
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	20	0.23	0.04	0.22
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	20	0.23	0.04	0.22
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	20	0.23	0.04	0.22
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	20	0.22	0.02	0.23
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	20	0.22	0.02	0.22
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	20	0.22	0.02	0.22
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	20	0.22	0.02	0.23
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	20	0.22	0.02	0.22
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	20	0.22	0.02	0.22
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	20	0.22	0.02	0.22
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	20	0.22	0.03	0.21
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	20	0.22	0.03	0.21
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	20	0.22	0.0	0.22
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	20	0.22	0.03	0.22
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	20	0.22	0.03	0.22
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	20	0.21	0.01	0.22
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	20	0.21	0.06	0.2
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	20	0.21	0.03	0.2
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	20	0.2	0.03	0.2
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	20	0.2	0.02	0.19
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	20	0.2	0.06	0.2
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	20	0.2	0.06	0.2
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	20	0.2	0.01	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	20	0.2	0.0	0.2
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	20	0.2	0.03	0.19
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	20	0.2	0.03	0.19
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	20	0.2	0.03	0.19
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	20	0.2	0.01	0.2
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	20	0.2	0.03	0.2
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	20	0.2	0.06	0.18
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	20	0.2	0.01	0.19
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	20	0.19	0.03	0.18
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	20	0.19	0.08	0.16
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	20	0.19	0.02	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	20	0.19	0.02	0.18
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	20	0.19	0.05	0.18
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	20	0.19	0.05	0.18
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	20	0.19	0.05	0.18
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	20	0.19	0.05	0.18
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	20	0.19	0.05	0.18
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	20	0.19	0.05	0.18
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	20	0.19	0.05	0.18
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	20	0.19	0.05	0.18
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	20	0.19	0.05	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	20	0.18	0.0	0.18
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	20	0.18	0.01	0.19
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	20	0.18	0.01	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	20	0.18	0.0	0.18
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	20	0.18	0.01	0.18
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	20	0.18	0.03	0.18
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	20	0.17	0.02	0.18
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	20	0.17	0.01	0.17
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	20	0.17	0.03	0.16
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	20	0.17	0.03	0.16
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	20	0.17	0.02	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	20	0.17	0.02	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	20	0.17	0.02	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	20	0.17	0.02	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	20	0.17	0.02	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	20	0.17	0.02	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	20	0.17	0.0	0.17
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	20	0.17	0.04	0.16
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	20	0.17	0.01	0.17
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	20	0.16	0.01	0.17
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	20	0.16	0.0	0.16
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	20	0.16	0.02	0.16
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	20	0.16	0.02	0.16
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	20	0.16	0.02	0.16
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	20	0.16	0.02	0.16
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	20	0.16	0.02	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	20	0.15	0.0	0.15
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	20	0.15	0.02	0.16
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	20	0.15	0.0	0.15
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	20	0.15	0.02	0.15
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	20	0.15	0.01	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	20	0.15	0.01	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	20	0.15	0.01	0.15
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	20	0.15	0.02	0.15
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	20	0.15	0.01	0.15
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	20	0.14	0.01	0.14
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	20	0.13	0.01	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	20	0.13	0.0	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	20	0.13	0.0	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	20	0.13	0.0	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	20	0.13	0.0	0.13
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	20	0.13	0.01	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	20	0.13	0.0	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	20	0.13	0.0	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	20	0.13	0.0	0.13
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	20	0.13	0.0	0.13
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	20	0.12	0.02	0.12
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	20	0.12	0.02	0.12
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	20	0.11	0.01	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	20	0.11	0.01	0.11
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	20	0.11	0.01	0.11
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	20	0.11	0.01	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	20	0.11	0.0	0.11
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	19	0.25	0.09	0.25
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	19	0.23	0.05	0.25
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	19	0.23	0.03	0.23
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	19	0.23	0.03	0.23
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	19	0.23	0.03	0.23
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	19	0.21	0.04	0.21
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	19	0.21	0.04	0.21
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	19	0.2	0.05	0.2
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	19	0.2	0.05	0.2
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	19	0.2	0.05	0.2
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	19	0.2	0.05	0.2
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	19	0.2	0.05	0.2
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	19	0.2	0.05	0.2
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	19	0.17	0.03	0.16
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	19	0.17	0.03	0.16
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	19	0.17	0.04	0.17
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	19	0.17	0.04	0.17
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	19	0.17	0.04	0.17
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	19	0.16	0.03	0.16
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	19	0.16	0.03	0.16
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	19	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	19	0.14	0.02	0.13
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	19	0.13	0.01	0.13
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	19	0.12	0.01	0.12
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	19	0.11	0.0	0.11
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	18	0.28	0.01	0.28
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	18	0.27	0.05	0.25
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	18	0.18	0.02	0.18
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	18	0.17	0.03	0.18
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	18	0.16	0.03	0.16
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	18	0.16	0.03	0.16
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	18	0.16	0.03	0.16
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	18	0.15	0.04	0.15
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	18	0.13	0.02	0.12
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	17	0.31	0.09	0.31
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	17	0.25	0.06	0.27
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	17	0.25	0.06	0.27
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	17	0.25	0.06	0.27
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	17	0.24	0.06	0.24
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	17	0.24	0.06	0.24
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	17	0.22	0.01	0.22
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	17	0.21	0.01	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	17	0.21	0.01	0.21
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	17	0.21	0.1	0.14
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	17	0.21	0.1	0.14
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	17	0.2	0.05	0.18
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	17	0.13	0.01	0.13
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	17	0.12	0.0	0.12
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	16	0.17	0.06	0.15
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	16	0.17	0.06	0.15
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	16	0.16	0.05	0.15
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	16	0.16	0.05	0.15
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	16	0.16	0.05	0.15
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	16	0.16	0.05	0.15
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	16	0.16	0.05	0.15
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	16	0.16	0.05	0.15
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	16	0.15	0.04	0.15
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	16	0.15	0.02	0.16
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	16	0.15	0.03	0.15
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	16	0.15	0.03	0.15
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	16	0.15	0.03	0.15
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	16	0.15	0.03	0.15
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	16	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	16	0.15	0.03	0.15
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	16	0.13	0.02	0.12
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	16	0.13	0.01	0.13
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	16	0.12	0.01	0.12
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	15	0.19	0.01	0.2
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	15	0.16	0.05	0.14
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	15	0.16	0.05	0.14
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	15	0.16	0.05	0.14
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	15	0.15	0.02	0.16
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	15	0.13	0.02	0.13
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	15	0.13	0.02	0.12
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	15	0.13	0.01	0.13
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	15	0.13	0.01	0.13
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	15	0.12	0.02	0.12
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	15	0.12	0.02	0.12
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	15	0.11	0.01	0.11
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	14	0.31	0.12	0.38
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	14	0.13	0.02	0.12
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	14	0.13	0.02	0.12
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	14	0.13	0.02	0.12
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	14	0.12	0.02	0.12
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	14	0.11	0.01	0.11
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	13	0.28	0.02	0.27
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	13	0.28	0.02	0.27
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	13	0.17	0.08	0.13
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	13	0.16	0.04	0.15
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	13	0.16	0.04	0.15
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	13	0.16	0.04	0.15
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	13	0.16	0.04	0.15
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	13	0.16	0.04	0.15
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	13	0.16	0.04	0.15
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	13	0.13	0.03	0.13
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	13	0.13	0.03	0.12
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	13	0.12	0.01	0.11
(1,367)	1:31:A:GLU:HA	1:32:A:LEU:HG	12	0.19	0.06	0.19
(1,1149)	1:100:A:ILE:HG21	1:93:A:ASP:HB2	12	0.14	0.02	0.15
(1,1149)	1:100:A:ILE:HG22	1:93:A:ASP:HB2	12	0.14	0.02	0.15
(1,1149)	1:100:A:ILE:HG23	1:93:A:ASP:HB2	12	0.14	0.02	0.15
(1,1249)	1:67:A:GLU:HA	1:67:A:GLU:H	12	0.13	0.02	0.14
(1,899)	1:125:A:ILE:HG12	1:122:A:ASP:HA	12	0.12	0.02	0.11
(1,899)	1:125:A:ILE:HG13	1:122:A:ASP:HA	12	0.12	0.02	0.11
(1,1370)	1:58:A:ASP:HA	1:57:A:ALA:H	12	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG21	11	0.15	0.04	0.13
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG22	11	0.15	0.04	0.13
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG23	11	0.15	0.04	0.13
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG21	11	0.15	0.04	0.13
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG22	11	0.15	0.04	0.13
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG23	11	0.15	0.04	0.13
(1,1411)	1:41:A:GLN:HB2	1:37:A:ARG:HA	11	0.14	0.02	0.13
(1,1411)	1:41:A:GLN:HB3	1:37:A:ARG:HA	11	0.14	0.02	0.13
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG2	11	0.14	0.06	0.12
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG3	11	0.14	0.06	0.12
(1,1304)	1:136:A:VAL:HB	1:136:A:VAL:H	11	0.13	0.03	0.11
(1,1319)	1:33:A:GLY:HA2	1:33:A:GLY:H	11	0.12	0.0	0.12
(1,476)	1:142:A:VAL:HG11	1:141:A:PHE:HA	11	0.11	0.01	0.11
(1,476)	1:142:A:VAL:HG12	1:141:A:PHE:HA	11	0.11	0.01	0.11
(1,476)	1:142:A:VAL:HG13	1:141:A:PHE:HA	11	0.11	0.01	0.11
(1,11)	1:27:A:ILE:HD11	1:28:A:THR:HB	10	0.15	0.03	0.15
(1,11)	1:27:A:ILE:HD12	1:28:A:THR:HB	10	0.15	0.03	0.15
(1,11)	1:27:A:ILE:HD13	1:28:A:THR:HB	10	0.15	0.03	0.15
(1,503)	1:110:A:THR:HB	1:112:A:LEU:H	10	0.11	0.01	0.11
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB2	9	0.16	0.02	0.16
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB3	9	0.16	0.02	0.16
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB2	9	0.13	0.02	0.12
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB3	9	0.13	0.02	0.12
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG2	9	0.12	0.02	0.12
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG3	9	0.12	0.02	0.12
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG2	9	0.12	0.02	0.12
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG3	9	0.12	0.02	0.12
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG2	9	0.12	0.02	0.12
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG3	9	0.12	0.02	0.12
(1,1321)	1:61:A:GLY:HA2	1:60:A:ASN:HA	9	0.11	0.01	0.11
(1,1171)	1:9:A:ILE:HB	1:8:A:GLN:HA	8	0.25	0.02	0.25
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD11	8	0.24	0.06	0.27
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD12	8	0.24	0.06	0.27
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD13	8	0.24	0.06	0.27
(1,759)	1:26:A:THR:HG21	1:62:A:THR:HA	8	0.14	0.02	0.13
(1,759)	1:26:A:THR:HG22	1:62:A:THR:HA	8	0.14	0.02	0.13
(1,759)	1:26:A:THR:HG23	1:62:A:THR:HA	8	0.14	0.02	0.13
(1,1118)	1:29:A:THR:HB	1:28:A:THR:HA	7	0.28	0.13	0.39
(1,789)	1:52:A:ILE:HB	1:29:A:THR:HA	7	0.2	0.06	0.19
(1,1071)	1:106:A:ARG:HD3	1:107:A:HIS:H	7	0.19	0.01	0.19
(1,1067)	1:106:A:ARG:HD3	1:106:A:ARG:H	7	0.17	0.02	0.17
(1,1107)	1:44:A:THR:HG21	1:44:A:THR:H	7	0.16	0.02	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1107)	1:44:A:THR:HG22	1:44:A:THR:H	7	0.16	0.02	0.17
(1,1107)	1:44:A:THR:HG23	1:44:A:THR:H	7	0.16	0.02	0.17
(1,1277)	1:51:A:MET:HB2	1:50:A:ASP:HA	7	0.15	0.02	0.15
(1,1277)	1:51:A:MET:HB3	1:50:A:ASP:HA	7	0.15	0.02	0.15
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG12	7	0.14	0.03	0.13
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG13	7	0.14	0.03	0.13
(1,680)	1:27:A:ILE:HB	1:63:A:ILE:H	7	0.14	0.03	0.13
(1,766)	1:20:A:ASP:HA	1:26:A:THR:HB	7	0.13	0.02	0.12
(1,1138)	1:34:A:THR:HA	1:37:A:ARG:H	7	0.12	0.01	0.12
(1,749)	1:55:A:VAL:HA	1:56:A:ASP:H	7	0.12	0.01	0.12
(1,1180)	1:64:A:ASP:HB3	1:64:A:ASP:H	7	0.12	0.0	0.12
(1,1273)	1:94:A:LYS:HG2	1:94:A:LYS:H	7	0.12	0.02	0.11
(1,1103)	1:48:A:LEU:HD11	1:48:A:LEU:HA	6	0.31	0.13	0.36
(1,1103)	1:48:A:LEU:HD12	1:48:A:LEU:HA	6	0.31	0.13	0.36
(1,1103)	1:48:A:LEU:HD13	1:48:A:LEU:HA	6	0.31	0.13	0.36
(1,95)	1:48:A:LEU:HD21	1:50:A:ASP:HA	6	0.22	0.08	0.18
(1,95)	1:48:A:LEU:HD22	1:50:A:ASP:HA	6	0.22	0.08	0.18
(1,95)	1:48:A:LEU:HD23	1:50:A:ASP:HA	6	0.22	0.08	0.18
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD11	6	0.21	0.04	0.2
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD12	6	0.21	0.04	0.2
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD13	6	0.21	0.04	0.2
(1,1190)	1:91:A:VAL:HG21	1:88:A:ALA:HA	6	0.13	0.02	0.14
(1,1190)	1:91:A:VAL:HG22	1:88:A:ALA:HA	6	0.13	0.02	0.14
(1,1190)	1:91:A:VAL:HG23	1:88:A:ALA:HA	6	0.13	0.02	0.14
(1,1351)	1:110:A:THR:HG21	1:110:A:THR:H	6	0.13	0.02	0.13
(1,1351)	1:110:A:THR:HG22	1:110:A:THR:H	6	0.13	0.02	0.13
(1,1351)	1:110:A:THR:HG23	1:110:A:THR:H	6	0.13	0.02	0.13
(1,1252)	1:48:A:LEU:HA	1:48:A:LEU:H	6	0.12	0.01	0.13
(1,1364)	1:74:A:ARG:HA	1:74:A:ARG:H	6	0.1	0.0	0.1
(1,1038)	1:5:A:THR:HB	1:5:A:THR:H	5	0.32	0.05	0.35
(1,1332)	1:38:A:SER:HB2	1:38:A:SER:H	5	0.22	0.09	0.28
(1,1332)	1:38:A:SER:HB3	1:38:A:SER:H	5	0.22	0.09	0.28
(1,130)	1:34:A:THR:HB	1:31:A:GLU:H	5	0.14	0.01	0.14
(1,1204)	1:52:A:ILE:HG12	1:52:A:ILE:H	5	0.14	0.02	0.14
(1,1204)	1:52:A:ILE:HG13	1:52:A:ILE:H	5	0.14	0.02	0.14
(1,994)	1:29:A:THR:HA	1:30:A:LYS:H	5	0.13	0.02	0.12
(1,1460)	1:88:A:ALA:HA	1:89:A:PHE:H	5	0.12	0.01	0.12
(1,1437)	1:91:A:VAL:HB	1:92:A:PHE:H	5	0.11	0.01	0.11
(1,1130)	1:111:A:ASN:HA	1:112:A:LEU:H	5	0.1	0.0	0.1
(1,1037)	1:5:A:THR:HB	1:6:A:GLU:HG2	4	0.26	0.08	0.3
(1,1037)	1:5:A:THR:HB	1:6:A:GLU:HG3	4	0.26	0.08	0.3
(1,1000)	1:103:A:ALA:HA	1:104:A:GLU:HB2	4	0.2	0.05	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1000)	1:103:A:ALA:HA	1:104:A:GLU:HB3	4	0.2	0.05	0.18
(1,1335)	1:146:A:THR:HB	1:146:A:THR:H	4	0.18	0.14	0.11
(1,1361)	1:76:A:MET:HA	1:77:A:LYS:H	4	0.18	0.06	0.18
(1,1114)	1:29:A:THR:HB	1:29:A:THR:H	4	0.17	0.01	0.17
(1,1228)	1:112:A:LEU:HD11	1:112:A:LEU:H	4	0.17	0.01	0.16
(1,1228)	1:112:A:LEU:HD12	1:112:A:LEU:H	4	0.17	0.01	0.16
(1,1228)	1:112:A:LEU:HD13	1:112:A:LEU:H	4	0.17	0.01	0.16
(1,1228)	1:112:A:LEU:HD21	1:112:A:LEU:H	4	0.17	0.01	0.16
(1,1228)	1:112:A:LEU:HD22	1:112:A:LEU:H	4	0.17	0.01	0.16
(1,1228)	1:112:A:LEU:HD23	1:112:A:LEU:H	4	0.17	0.01	0.16
(1,1429)	1:32:A:LEU:HB2	1:32:A:LEU:H	4	0.13	0.01	0.12
(1,1429)	1:32:A:LEU:HB3	1:32:A:LEU:H	4	0.13	0.01	0.12
(1,151)	1:107:A:HIS:HA	1:94:A:LYS:HG3	4	0.12	0.01	0.12
(1,678)	1:27:A:ILE:HB	1:21:A:LYS:HD2	4	0.11	0.01	0.12
(1,678)	1:27:A:ILE:HB	1:21:A:LYS:HD3	4	0.11	0.01	0.12
(1,1281)	1:13:A:LYS:HA	1:16:A:PHE:HB2	4	0.11	0.01	0.11
(1,1281)	1:13:A:LYS:HA	1:16:A:PHE:HB3	4	0.11	0.01	0.11
(1,860)	1:142:A:VAL:HB	1:143:A:GLN:H	4	0.11	0.0	0.11
(1,1089)	1:77:A:LYS:HG2	1:77:A:LYS:H	3	0.27	0.04	0.27
(1,1089)	1:77:A:LYS:HG3	1:77:A:LYS:H	3	0.27	0.04	0.27
(1,1021)	1:6:A:GLU:HB2	1:3:A:GLN:HA	3	0.19	0.0	0.19
(1,1021)	1:6:A:GLU:HB3	1:3:A:GLN:HA	3	0.19	0.0	0.19
(1,427)	1:39:A:LEU:HA	1:38:A:SER:H	3	0.19	0.02	0.18
(1,856)	1:93:A:ASP:HB3	1:100:A:ILE:HG21	3	0.18	0.0	0.18
(1,856)	1:93:A:ASP:HB3	1:100:A:ILE:HG22	3	0.18	0.0	0.18
(1,856)	1:93:A:ASP:HB3	1:100:A:ILE:HG23	3	0.18	0.0	0.18
(1,1216)	1:144:A:MET:HA	1:144:A:MET:HG2	3	0.14	0.01	0.13
(1,1216)	1:144:A:MET:HA	1:144:A:MET:HG3	3	0.14	0.01	0.13
(1,1377)	1:52:A:ILE:HD11	1:62:A:THR:H	3	0.13	0.02	0.12
(1,1377)	1:52:A:ILE:HD12	1:62:A:THR:H	3	0.13	0.02	0.12
(1,1377)	1:52:A:ILE:HD13	1:62:A:THR:H	3	0.13	0.02	0.12
(1,1397)	1:111:A:ASN:HB3	1:111:A:ASN:H	3	0.13	0.0	0.13
(1,590)	1:27:A:ILE:HA	1:63:A:ILE:H	3	0.13	0.01	0.12
(1,1111)	1:36:A:MET:HA	1:39:A:LEU:HB2	3	0.12	0.02	0.11
(1,1111)	1:36:A:MET:HA	1:39:A:LEU:HB3	3	0.12	0.02	0.11
(1,780)	1:94:A:LYS:HG3	1:94:A:LYS:H	3	0.12	0.0	0.12
(1,9)	1:17:A:SER:HB2	1:16:A:PHE:HA	3	0.11	0.0	0.11
(1,9)	1:17:A:SER:HB3	1:16:A:PHE:HA	3	0.11	0.0	0.11
(1,1263)	1:17:A:SER:HB2	1:16:A:PHE:HA	3	0.11	0.0	0.11
(1,1263)	1:17:A:SER:HB3	1:16:A:PHE:HA	3	0.11	0.0	0.11
(1,847)	1:33:A:GLY:HA3	1:34:A:THR:H	3	0.1	0.0	0.1
(1,1046)	1:142:A:VAL:HG21	1:143:A:GLN:H	2	0.36	0.01	0.36

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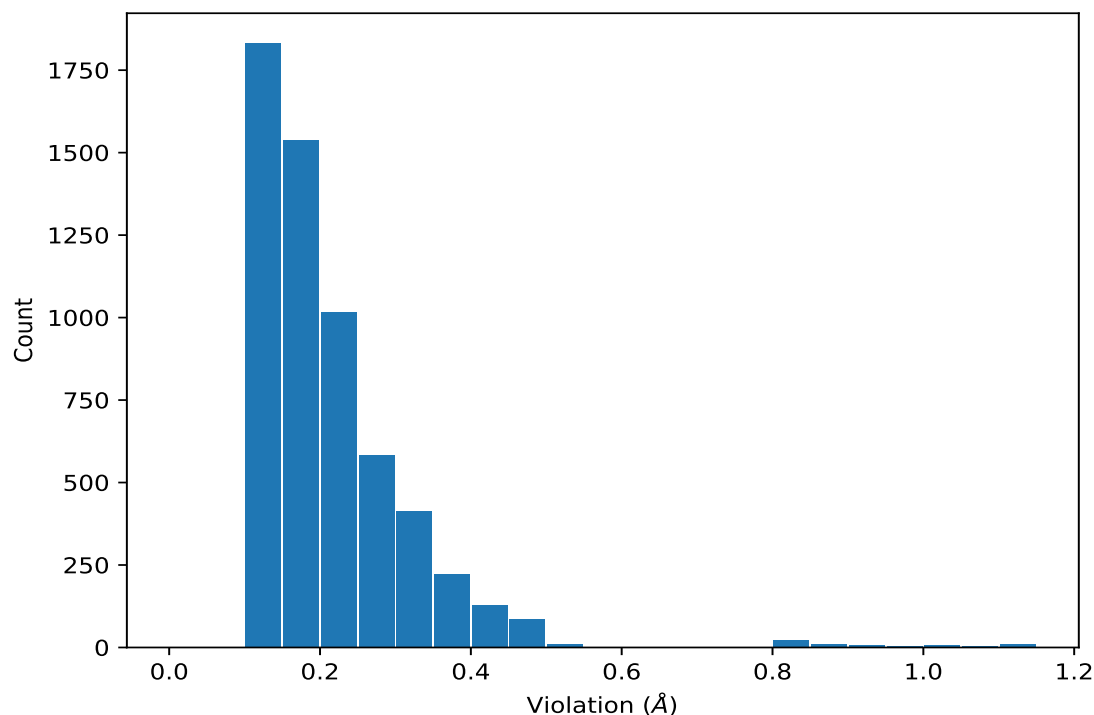
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1046)	1:142:A:VAL:HG22	1:143:A:GLN:H	2	0.36	0.01	0.36
(1,1046)	1:142:A:VAL:HG23	1:143:A:GLN:H	2	0.36	0.01	0.36
(1,1047)	1:142:A:VAL:HG21	1:142:A:VAL:H	2	0.3	0.01	0.3
(1,1047)	1:142:A:VAL:HG22	1:142:A:VAL:H	2	0.3	0.01	0.3
(1,1047)	1:142:A:VAL:HG23	1:142:A:VAL:H	2	0.3	0.01	0.3
(1,1048)	1:142:A:VAL:HG21	1:139:A:GLU:HA	2	0.2	0.0	0.2
(1,1048)	1:142:A:VAL:HG22	1:139:A:GLU:HA	2	0.2	0.0	0.2
(1,1048)	1:142:A:VAL:HG23	1:139:A:GLU:HA	2	0.2	0.0	0.2
(1,819)	1:80:A:ASP:HB2	1:83:A:GLU:H	2	0.18	0.01	0.18
(1,819)	1:80:A:ASP:HB3	1:83:A:GLU:H	2	0.18	0.01	0.18
(1,1082)	1:90:A:ARG:HB2	1:91:A:VAL:HG21	2	0.18	0.01	0.18
(1,1082)	1:90:A:ARG:HB2	1:91:A:VAL:HG22	2	0.18	0.01	0.18
(1,1082)	1:90:A:ARG:HB2	1:91:A:VAL:HG23	2	0.18	0.01	0.18
(1,1082)	1:90:A:ARG:HB3	1:91:A:VAL:HG21	2	0.18	0.01	0.18
(1,1082)	1:90:A:ARG:HB3	1:91:A:VAL:HG22	2	0.18	0.01	0.18
(1,1082)	1:90:A:ARG:HB3	1:91:A:VAL:HG23	2	0.18	0.01	0.18
(1,1246)	1:77:A:LYS:HA	1:78:A:ASP:H	2	0.18	0.04	0.18
(1,497)	1:114:A:GLU:HB2	1:21:A:LYS:HG2	2	0.14	0.0	0.14
(1,497)	1:114:A:GLU:HB3	1:21:A:LYS:HG2	2	0.14	0.0	0.14
(1,1168)	1:85:A:ILE:HB	1:82:A:GLU:HA	2	0.14	0.0	0.14
(1,1432)	1:63:A:ILE:HB	1:63:A:ILE:H	2	0.14	0.02	0.14
(1,1441)	1:61:A:GLY:HA3	1:52:A:ILE:HG21	2	0.13	0.01	0.13
(1,1441)	1:61:A:GLY:HA3	1:52:A:ILE:HG22	2	0.13	0.01	0.13
(1,1441)	1:61:A:GLY:HA3	1:52:A:ILE:HG23	2	0.13	0.01	0.13
(1,357)	1:53:A:ASN:HA	1:56:A:ASP:HB2	2	0.12	0.0	0.12
(1,395)	1:37:A:ARG:HA	1:34:A:THR:HA	2	0.12	0.0	0.12
(1,1236)	1:106:A:ARG:HA	1:121:A:VAL:HG11	2	0.12	0.0	0.12
(1,1236)	1:106:A:ARG:HA	1:121:A:VAL:HG12	2	0.12	0.0	0.12
(1,1236)	1:106:A:ARG:HA	1:121:A:VAL:HG13	2	0.12	0.0	0.12
(1,943)	1:37:A:ARG:HG2	1:37:A:ARG:H	2	0.11	0.0	0.11
(1,943)	1:37:A:ARG:HG3	1:37:A:ARG:H	2	0.11	0.0	0.11
(1,1187)	1:91:A:VAL:HG21	1:88:A:ALA:H	2	0.11	0.01	0.11
(1,1187)	1:91:A:VAL:HG22	1:88:A:ALA:H	2	0.11	0.01	0.11
(1,1187)	1:91:A:VAL:HG23	1:88:A:ALA:H	2	0.11	0.01	0.11
(1,1447)	1:55:A:VAL:HG11	1:55:A:VAL:H	2	0.11	0.0	0.11
(1,1447)	1:55:A:VAL:HG12	1:55:A:VAL:H	2	0.11	0.0	0.11
(1,1447)	1:55:A:VAL:HG13	1:55:A:VAL:H	2	0.11	0.0	0.11
(1,679)	1:27:A:ILE:HB	1:28:A:THR:HB	2	0.11	0.0	0.11
(1,473)	1:142:A:VAL:HG11	1:145:A:MET:H	2	0.1	0.0	0.1
(1,473)	1:142:A:VAL:HG12	1:145:A:MET:H	2	0.1	0.0	0.1
(1,473)	1:142:A:VAL:HG13	1:145:A:MET:H	2	0.1	0.0	0.1

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)
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	7	1.13
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	7	1.13
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	7	1.13
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	16	1.12
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	16	1.12
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	16	1.12
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	5	1.11
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	5	1.11
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	5	1.11
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	6	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	6	1.08
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	6	1.08
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	15	1.03
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	15	1.03
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	15	1.03
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	18	1.0
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	18	1.0
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	18	1.0
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	9	0.99
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	9	0.99
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	9	0.99
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	13	0.9
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	13	0.9
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	13	0.9
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	17	0.9
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	17	0.9
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	17	0.9
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	4	0.86
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	4	0.86
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	4	0.86
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	11	0.86
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	11	0.86
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	11	0.86
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	14	0.85
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	14	0.85
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	14	0.85
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	1	0.84
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	1	0.84
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	1	0.84
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	10	0.84
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	10	0.84
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	10	0.84
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	12	0.84
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	12	0.84
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	12	0.84
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	3	0.83
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	3	0.83
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	3	0.83
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	19	0.83
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	19	0.83
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	19	0.83
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	20	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	20	0.83
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	20	0.83
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	2	0.82
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	2	0.82
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	2	0.82
(1,841)	1:39:A:LEU:HD21	1:39:A:LEU:H	8	0.82
(1,841)	1:39:A:LEU:HD22	1:39:A:LEU:H	8	0.82
(1,841)	1:39:A:LEU:HD23	1:39:A:LEU:H	8	0.82
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	1	0.5
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	13	0.5
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	17	0.5
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	8	0.5
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	8	0.5
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	10	0.5
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	10	0.5
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	10	0.5
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	19	0.5
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	19	0.5
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	14	0.49
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	14	0.49
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	15	0.49
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	15	0.49
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	19	0.49
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	19	0.49
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	20	0.49
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	20	0.49
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	2	0.49
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	6	0.49
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	17	0.49
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	1	0.49
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	1	0.49
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	7	0.48
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	11	0.48
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	1	0.48
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	1	0.48
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	6	0.48
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	6	0.48
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	11	0.48
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	11	0.48
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	12	0.48
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	12	0.48
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	19	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	20	0.48
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	7	0.48
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	7	0.48
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	7	0.48
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	7	0.48
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	17	0.48
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	17	0.48
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	2	0.47
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	5	0.47
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	15	0.47
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	18	0.47
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	19	0.47
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	2	0.47
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	2	0.47
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	3	0.47
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	3	0.47
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	9	0.47
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	9	0.47
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	17	0.47
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	17	0.47
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	5	0.47
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	9	0.47
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	15	0.47
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	16	0.47
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	18	0.47
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	2	0.47
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	2	0.47
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	2	0.47
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	2	0.47
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	12	0.47
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	12	0.47
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	14	0.47
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	14	0.47
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	17	0.46
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	6	0.46
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	14	0.46
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	4	0.46
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	4	0.46
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	5	0.46
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	5	0.46
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	3	0.46
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	8	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	12	0.46
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	3	0.46
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	3	0.46
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	3	0.46
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	3	0.46
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	5	0.45
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	12	0.45
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	16	0.45
(1,1103)	1:48:A:LEU:HD11	1:48:A:LEU:HA	3	0.45
(1,1103)	1:48:A:LEU:HD12	1:48:A:LEU:HA	3	0.45
(1,1103)	1:48:A:LEU:HD13	1:48:A:LEU:HA	3	0.45
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	11	0.45
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	11	0.45
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	11	0.45
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	12	0.45
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	12	0.45
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	12	0.45
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	16	0.45
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	16	0.45
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	11	0.45
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	13	0.45
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	1	0.44
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	6	0.44
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	7	0.44
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	9	0.44
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	16	0.44
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	17	0.44
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	3	0.44
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	4	0.44
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	9	0.44
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	10	0.44
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	5	0.44
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	13	0.44
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	13	0.44
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	18	0.44
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	18	0.44
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	7	0.44
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	1	0.44
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	1	0.44
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	1	0.44
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	1	0.44
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	5	0.44
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	3	0.43
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	4	0.43
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	10	0.43
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	12	0.43
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	15	0.43
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	20	0.43
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	1	0.43
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	8	0.43
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	8	0.43
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	8	0.43
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	4	0.43
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	4	0.43
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	17	0.43
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	17	0.43
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	17	0.43
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	17	0.43
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	18	0.43
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	18	0.43
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	18	0.43
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	18	0.43
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	2	0.42
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	8	0.42
(1,1335)	1:146:A:THR:HB	1:146:A:THR:H	5	0.42
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	8	0.42
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	8	0.42
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	8	0.42
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	8	0.42
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	2	0.42
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	2	0.42
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	2	0.42
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	19	0.42
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	19	0.42
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	19	0.42
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	6	0.42
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	6	0.42
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG12	7	0.42
(1,808)	1:122:A:ASP:HB2	1:125:A:ILE:HG13	7	0.42
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	1	0.42
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	5	0.42
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	5	0.42
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	5	0.42
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	6	0.42
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	6	0.42
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	6	0.42
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	6	0.42
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	9	0.42
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	9	0.42
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	9	0.42
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	9	0.42
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	19	0.42
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	19	0.42
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	19	0.42
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	19	0.42
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	4	0.42
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	9	0.42
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	6	0.42
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	6	0.42
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	15	0.41
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	15	0.41
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	11	0.41
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	18	0.41
(1,1239)	1:104:A:GLU:HA	1:107:A:HIS:H	20	0.41
(1,1118)	1:29:A:THR:HB	1:28:A:THR:HA	2	0.41
(1,1103)	1:48:A:LEU:HD11	1:48:A:LEU:HA	20	0.41
(1,1103)	1:48:A:LEU:HD12	1:48:A:LEU:HA	20	0.41
(1,1103)	1:48:A:LEU:HD13	1:48:A:LEU:HA	20	0.41
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	17	0.41
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	17	0.41
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	17	0.41
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	4	0.41
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	4	0.41
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	4	0.41
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	6	0.41
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	6	0.41
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	6	0.41
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	14	0.41
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	14	0.41
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	14	0.41
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	13	0.41
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	13	0.41
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	13	0.41
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	13	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	10	0.41
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	13	0.4
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	14	0.4
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	19	0.4
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	14	0.4
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	14	0.4
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	14	0.4
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	2	0.4
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	20	0.4
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	15	0.4
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	2	0.4
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	2	0.4
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	3	0.4
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	3	0.4
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	3	0.4
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	13	0.4
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	13	0.4
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	13	0.4
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	17	0.4
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	17	0.4
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	17	0.4
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	14	0.4
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	3	0.4
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	4	0.39
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	6	0.39
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	11	0.39
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	13	0.39
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	15	0.39
(1,1341)	1:139:A:GLU:HA	1:140:A:GLU:HA	19	0.39
(1,1118)	1:29:A:THR:HB	1:28:A:THR:HA	10	0.39
(1,1118)	1:29:A:THR:HB	1:28:A:THR:HA	15	0.39
(1,1118)	1:29:A:THR:HB	1:28:A:THR:HA	16	0.39
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	12	0.39
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	12	0.39
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	12	0.39
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	7	0.39
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	19	0.39
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	15	0.39
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	15	0.39
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	10	0.39
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	10	0.39
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	17	0.39
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	17	0.39
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	17	0.39
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	18	0.39
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	18	0.39
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	18	0.39
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	7	0.39
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	7	0.39
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	13	0.39
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	13	0.39
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	18	0.39
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	18	0.39
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	16	0.39
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	16	0.39
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	16	0.39
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	16	0.39
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	2	0.39
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	16	0.39
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	1	0.38
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	5	0.38
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	10	0.38
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	16	0.38
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	18	0.38
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	19	0.38
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	20	0.38
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	1	0.38
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	1	0.38
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	9	0.38
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	9	0.38
(1,1103)	1:48:A:LEU:HD11	1:48:A:LEU:HA	8	0.38
(1,1103)	1:48:A:LEU:HD12	1:48:A:LEU:HA	8	0.38
(1,1103)	1:48:A:LEU:HD13	1:48:A:LEU:HA	8	0.38
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	2	0.38
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	2	0.38
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	2	0.38
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	4	0.38
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	4	0.38
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	4	0.38
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	19	0.38
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	19	0.38
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	19	0.38
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	11	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	3	0.38
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	3	0.38
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	20	0.38
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	20	0.38
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	18	0.38
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	18	0.38
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	19	0.38
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	19	0.38
(1,802)	1:100:A:ILE:HA	1:136:A:VAL:H	4	0.38
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	6	0.38
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	6	0.38
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	9	0.38
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	9	0.38
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	14	0.38
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	14	0.38
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	15	0.38
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	15	0.38
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	16	0.38
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	16	0.38
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	11	0.38
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	8	0.38
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	8	0.38
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	2	0.37
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	8	0.37
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	9	0.37
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	14	0.37
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	17	0.37
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	20	0.37
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	20	0.37
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	20	0.37
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	11	0.37
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	11	0.37
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	11	0.37
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	18	0.37
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	18	0.37
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	18	0.37
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	9	0.37
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	10	0.37
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	10	0.37
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	10	0.37
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	2	0.37
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	5	0.37
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	5	0.37
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	7	0.37
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	7	0.37
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	8	0.37
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	8	0.37
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	9	0.37
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	9	0.37
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	11	0.37
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	11	0.37
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	16	0.37
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	16	0.37
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	17	0.37
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	17	0.37
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	20	0.37
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	20	0.37
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	3	0.37
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	20	0.37
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	20	0.37
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	8	0.37
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	8	0.37
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	7	0.37
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	15	0.37
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	20	0.37
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	20	0.37
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	2	0.37
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	4	0.37
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	9	0.37
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	16	0.37
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	12	0.36
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	7	0.36
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	7	0.36
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	17	0.36
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	17	0.36
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	3	0.36
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	8	0.36
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	8	0.36
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	19	0.36
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	5	0.36
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	5	0.36
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	5	0.36
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	14	0.36
(1,1046)	1:142:A:VAL:HG21	1:143:A:GLN:H	1	0.36
(1,1046)	1:142:A:VAL:HG22	1:143:A:GLN:H	1	0.36
(1,1046)	1:142:A:VAL:HG23	1:143:A:GLN:H	1	0.36
(1,1038)	1:5:A:THR:HB	1:5:A:THR:H	1	0.36
(1,1038)	1:5:A:THR:HB	1:5:A:THR:H	13	0.36
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	16	0.36
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	17	0.36
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	8	0.36
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	8	0.36
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	11	0.36
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	11	0.36
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	5	0.36
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	5	0.36
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	5	0.36
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	3	0.36
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	3	0.36
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	10	0.36
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	10	0.36
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	12	0.36
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	12	0.36
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	15	0.36
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	15	0.36
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	2	0.36
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	2	0.36
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	10	0.36
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	10	0.36
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	11	0.36
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	11	0.36
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	17	0.36
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	17	0.36
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	13	0.36
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	3	0.35
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	3	0.35
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	4	0.35
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	4	0.35
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	5	0.35
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	5	0.35
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	6	0.35
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	6	0.35
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	8	0.35
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	15	0.35
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	15	0.35
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	8	0.35
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	19	0.35
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	1	0.35
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	1	0.35
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	1	0.35
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	18	0.35
(1,1046)	1:142:A:VAL:HG21	1:143:A:GLN:H	6	0.35
(1,1046)	1:142:A:VAL:HG22	1:143:A:GLN:H	6	0.35
(1,1046)	1:142:A:VAL:HG23	1:143:A:GLN:H	6	0.35
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	4	0.35
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	14	0.35
(1,1038)	1:5:A:THR:HB	1:5:A:THR:H	3	0.35
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	4	0.35
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	4	0.35
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	7	0.35
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	7	0.35
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	1	0.35
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	5	0.35
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	14	0.35
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	1	0.35
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	1	0.35
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	1	0.35
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	4	0.35
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	4	0.35
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	4	0.35
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	3	0.35
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	3	0.35
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	19	0.35
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	19	0.35
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	12	0.35
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	12	0.35
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	12	0.35
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	12	0.35
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	10	0.34
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	10	0.34
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	13	0.34
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	13	0.34
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	18	0.34
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	18	0.34
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	2	0.34
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	3	0.34
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	15	0.34
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	20	0.34
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	13	0.34
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	13	0.34
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	6	0.34
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	6	0.34
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	6	0.34
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	3	0.34
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	14	0.34
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	14	0.34
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	16	0.34
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	16	0.34
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	14	0.34
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	12	0.34
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	17	0.34
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	20	0.34
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	1	0.34
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	1	0.34
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	14	0.34
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	14	0.34
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	1	0.34
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	1	0.34
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	1	0.34
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	1	0.34
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	1	0.34
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	2	0.34
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	2	0.34
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	2	0.34
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	8	0.34
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	8	0.34
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	8	0.34
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	11	0.34
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	11	0.34
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	11	0.34
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	15	0.34
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	15	0.34
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	15	0.34
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	17	0.34
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	17	0.34
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	17	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	12	0.34
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	12	0.34
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	3	0.33
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	2	0.33
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	2	0.33
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	12	0.33
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	12	0.33
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	4	0.33
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	11	0.33
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	12	0.33
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	14	0.33
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	17	0.33
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	9	0.33
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	15	0.33
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	20	0.33
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	1	0.33
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	1	0.33
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	1	0.33
(1,1103)	1:48:A:LEU:HD11	1:48:A:LEU:HA	7	0.33
(1,1103)	1:48:A:LEU:HD12	1:48:A:LEU:HA	7	0.33
(1,1103)	1:48:A:LEU:HD13	1:48:A:LEU:HA	7	0.33
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	3	0.33
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	3	0.33
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	3	0.33
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	5	0.33
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	6	0.33
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	1	0.33
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	8	0.33
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	9	0.33
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	11	0.33
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	12	0.33
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	15	0.33
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG2	13	0.33
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG3	13	0.33
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	9	0.33
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	7	0.33
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	5	0.33
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	5	0.33
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	6	0.33
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	6	0.33
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	9	0.33
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	17	0.33
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	17	0.33
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	19	0.33
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	19	0.33
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	2	0.33
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	8	0.33
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	13	0.33
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	19	0.33
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	9	0.33
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	9	0.33
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	9	0.33
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	16	0.33
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	16	0.33
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	16	0.33
(1,885)	1:143:A:GLN:HB2	1:142:A:VAL:H	13	0.33
(1,885)	1:143:A:GLN:HB3	1:142:A:VAL:H	13	0.33
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	8	0.33
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	8	0.33
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	8	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	3	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	3	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	3	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	4	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	4	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	4	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	5	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	5	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	5	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	6	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	6	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	6	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	7	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	7	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	7	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	9	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	9	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	9	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	10	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	10	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	10	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	12	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	12	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	13	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	13	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	13	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	14	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	14	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	14	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	16	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	16	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	16	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	18	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	18	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	18	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	19	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	19	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	19	0.33
(1,784)	1:147:A:ALA:HB1	1:148:A:LYS:H	20	0.33
(1,784)	1:147:A:ALA:HB2	1:148:A:LYS:H	20	0.33
(1,784)	1:147:A:ALA:HB3	1:148:A:LYS:H	20	0.33
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	6	0.33
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	6	0.33
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	6	0.33
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	7	0.33
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	7	0.33
(1,1442)	1:61:A:GLY:HA3	1:62:A:THR:HA	7	0.32
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	1	0.32
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	4	0.32
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	17	0.32
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	17	0.32
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	1	0.32
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	6	0.32
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	7	0.32
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	8	0.32
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	13	0.32
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	15	0.32
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	16	0.32
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	18	0.32
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	20	0.32
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	4	0.32
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	5	0.32
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	7	0.32
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	11	0.32
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	14	0.32
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	17	0.32
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	15	0.32
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	19	0.32
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	8	0.32
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	19	0.32
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	19	0.32
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	4	0.32
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	4	0.32
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	4	0.32
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD11	13	0.32
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD12	13	0.32
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD13	13	0.32
(1,1089)	1:77:A:LYS:HG2	1:77:A:LYS:H	11	0.32
(1,1089)	1:77:A:LYS:HG3	1:77:A:LYS:H	11	0.32
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	10	0.32
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	10	0.32
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	10	0.32
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	2	0.32
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	15	0.32
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	2	0.32
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	13	0.32
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	17	0.32
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	19	0.32
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	18	0.32
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	18	0.32
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	3	0.32
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	4	0.32
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	7	0.32
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	9	0.32
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	10	0.32
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	15	0.32
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	16	0.32
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	18	0.32
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	1	0.32
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	1	0.32
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	1	0.32
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	8	0.32
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	8	0.32
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	8	0.32
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	6	0.32
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	5	0.32
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	5	0.32
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	8	0.32
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	8	0.32
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	7	0.32
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	7	0.32
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	7	0.32
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	7	0.32
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	7	0.32
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	7	0.32
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	10	0.32
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	10	0.32
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	10	0.32
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	10	0.32
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	14	0.32
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	14	0.32
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	14	0.32
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	14	0.32
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	17	0.32
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	17	0.32
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	17	0.32
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	1	0.32
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	1	0.32
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	11	0.32
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	11	0.32
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	15	0.32
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	15	0.32
(1,95)	1:48:A:LEU:HD21	1:50:A:ASP:HA	1	0.32
(1,95)	1:48:A:LEU:HD22	1:50:A:ASP:HA	1	0.32
(1,95)	1:48:A:LEU:HD23	1:50:A:ASP:HA	1	0.32
(1,95)	1:48:A:LEU:HD21	1:50:A:ASP:HA	7	0.32
(1,95)	1:48:A:LEU:HD22	1:50:A:ASP:HA	7	0.32
(1,95)	1:48:A:LEU:HD23	1:50:A:ASP:HA	7	0.32
(1,1332)	1:38:A:SER:HB2	1:38:A:SER:H	6	0.31
(1,1332)	1:38:A:SER:HB3	1:38:A:SER:H	6	0.31
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	2	0.31
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	3	0.31
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	5	0.31
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	9	0.31
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	1	0.31
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	13	0.31
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	5	0.31
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	10	0.31
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	9	0.31
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	9	0.31
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	13	0.31
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	13	0.31
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	13	0.31
(1,1047)	1:142:A:VAL:HG21	1:142:A:VAL:H	1	0.31
(1,1047)	1:142:A:VAL:HG22	1:142:A:VAL:H	1	0.31
(1,1047)	1:142:A:VAL:HG23	1:142:A:VAL:H	1	0.31
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	7	0.31
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	10	0.31
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	20	0.31
(1,1037)	1:5:A:THR:HB	1:6:A:GLU:HG2	13	0.31
(1,1037)	1:5:A:THR:HB	1:6:A:GLU:HG3	13	0.31
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	7	0.31
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	18	0.31
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	1	0.31
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	1	0.31
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	12	0.31
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	12	0.31
(1,983)	1:53:A:ASN:HB2	1:52:A:ILE:H	13	0.31
(1,983)	1:53:A:ASN:HB3	1:52:A:ILE:H	13	0.31
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	11	0.31
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	7	0.31
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	7	0.31
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	7	0.31
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	15	0.31
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	15	0.31
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	15	0.31
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	4	0.31
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	4	0.31
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	4	0.31
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	12	0.31
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	12	0.31
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	12	0.31
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	7	0.31
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	15	0.31
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	16	0.31
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	10	0.31
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	15	0.31
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	19	0.31
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB2	12	0.31
(1,801)	1:100:A:ILE:HA	1:101:A:SER:HB3	12	0.31
(1,789)	1:52:A:ILE:HB	1:29:A:THR:HA	9	0.31
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	15	0.31
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	15	0.31
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	15	0.31
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	15	0.31
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	20	0.31
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	20	0.31
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	20	0.31
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	20	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	5	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	5	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	5	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	9	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	9	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	9	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	12	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	12	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	12	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	14	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	14	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	14	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	18	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	18	0.31
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	18	0.31
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	6	0.31
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	6	0.31
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	20	0.31
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	20	0.31
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	3	0.31
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	20	0.31
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	11	0.31
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	11	0.31
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	18	0.31
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	18	0.31
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	18	0.3
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	9	0.3
(1,1332)	1:38:A:SER:HB2	1:38:A:SER:H	15	0.3
(1,1332)	1:38:A:SER:HB3	1:38:A:SER:H	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	5	0.3
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	20	0.3
(1,1279)	1:13:A:LYS:HA	1:14:A:GLU:H	19	0.3
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	3	0.3
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	12	0.3
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	18	0.3
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	2	0.3
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	9	0.3
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	1	0.3
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	1	0.3
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	5	0.3
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	5	0.3
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	7	0.3
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	7	0.3
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	8	0.3
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	8	0.3
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	16	0.3
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	16	0.3
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	16	0.3
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	16	0.3
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	16	0.3
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	16	0.3
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	6	0.3
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	16	0.3
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	18	0.3
(1,1037)	1:5:A:THR:HB	1:6:A:GLU:HG2	1	0.3
(1,1037)	1:5:A:THR:HB	1:6:A:GLU:HG3	1	0.3
(1,1037)	1:5:A:THR:HB	1:6:A:GLU:HG2	3	0.3
(1,1037)	1:5:A:THR:HB	1:6:A:GLU:HG3	3	0.3
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	3	0.3
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	8	0.3
(1,936)	1:65:A:PHE:HA	1:65:A:PHE:HZ	6	0.3
(1,914)	1:105:A:LEU:HD11	1:105:A:LEU:HA	20	0.3
(1,914)	1:105:A:LEU:HD12	1:105:A:LEU:HA	20	0.3
(1,914)	1:105:A:LEU:HD13	1:105:A:LEU:HA	20	0.3
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	3	0.3
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	3	0.3
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	3	0.3
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	8	0.3
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	12	0.3
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	13	0.3
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	4	0.3
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	4	0.3
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	4	0.3
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	6	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	4	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	4	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	4	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	11	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	11	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	11	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	15	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	15	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	15	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	19	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	19	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	19	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	20	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	20	0.3
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	20	0.3
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	4	0.3
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	4	0.3
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	17	0.3
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	17	0.3
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	20	0.3
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	20	0.3
(1,367)	1:31:A:GLU:HA	1:32:A:LEU:HG	18	0.3
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	8	0.3
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	10	0.3
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	12	0.29
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	6	0.29
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	7	0.29
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	4	0.29
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	4	0.29
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	13	0.29
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	13	0.29
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	6	0.29
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	10	0.29
(1,1267)	1:14:A:GLU:HA	1:11:A:GLU:HA	16	0.29
(1,1171)	1:9:A:ILE:HB	1:8:A:GLN:HA	5	0.29
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	1	0.29
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	15	0.29
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	18	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	2	0.29
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	2	0.29
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	13	0.29
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	13	0.29
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	20	0.29
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	20	0.29
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD11	4	0.29
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD12	4	0.29
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD13	4	0.29
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	11	0.29
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	11	0.29
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	11	0.29
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	4	0.29
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	12	0.29
(1,1047)	1:142:A:VAL:HG21	1:142:A:VAL:H	6	0.29
(1,1047)	1:142:A:VAL:HG22	1:142:A:VAL:H	6	0.29
(1,1047)	1:142:A:VAL:HG23	1:142:A:VAL:H	6	0.29
(1,1041)	1:145:A:MET:HA	1:148:A:LYS:H	5	0.29
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	6	0.29
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	9	0.29
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	9	0.29
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	20	0.29
(1,1000)	1:103:A:ALA:HA	1:104:A:GLU:HB2	14	0.29
(1,1000)	1:103:A:ALA:HA	1:104:A:GLU:HB3	14	0.29
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	20	0.29
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	20	0.29
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	20	0.29
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	2	0.29
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	14	0.29
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	17	0.29
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	2	0.29
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	2	0.29
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	2	0.29
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	1	0.29
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	14	0.29
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	8	0.29
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	8	0.29
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	8	0.29
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	8	0.29
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	8	0.29
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	8	0.29
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	10	0.29
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	10	0.29
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	10	0.29
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	16	0.29
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	16	0.29
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	16	0.29
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	3	0.29
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	3	0.29
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	8	0.29
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	8	0.29
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	6	0.29
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	15	0.29
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	15	0.29
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	5	0.28
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	14	0.28
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	2	0.28
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	2	0.28
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	17	0.28
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	17	0.28
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	4	0.28
(1,1332)	1:38:A:SER:HB2	1:38:A:SER:H	9	0.28
(1,1332)	1:38:A:SER:HB3	1:38:A:SER:H	9	0.28
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	19	0.28
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	19	0.28
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	6	0.28
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	20	0.28
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	20	0.28
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	4	0.28
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	4	0.28
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	6	0.28
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	6	0.28
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	10	0.28
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	10	0.28
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	11	0.28
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	11	0.28
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	16	0.28
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	16	0.28
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	18	0.28
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	18	0.28
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD11	9	0.28
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD12	9	0.28
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD13	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD11	16	0.28
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD12	16	0.28
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD13	16	0.28
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	8	0.28
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	8	0.28
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	8	0.28
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	9	0.28
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	9	0.28
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	9	0.28
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	15	0.28
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	15	0.28
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	15	0.28
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	1	0.28
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	9	0.28
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	11	0.28
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	13	0.28
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	19	0.28
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	20	0.28
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	20	0.28
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	20	0.28
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	13	0.28
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	14	0.28
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	19	0.28
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	19	0.28
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	12	0.28
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	7	0.28
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	7	0.28
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	7	0.28
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	18	0.28
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	18	0.28
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	18	0.28
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	3	0.28
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	4	0.28
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	5	0.28
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	7	0.28
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	10	0.28
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	13	0.28
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	19	0.28
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	20	0.28
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	10	0.28
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	10	0.28
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	11	0.28
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	17	0.28
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	20	0.28
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	6	0.28
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	6	0.28
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	8	0.28
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	8	0.28
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	14	0.28
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	14	0.28
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	17	0.28
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	17	0.28
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	19	0.28
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	19	0.28
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	2	0.28
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	18	0.28
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	5	0.28
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	1	0.28
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	1	0.28
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	1	0.28
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	2	0.28
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	2	0.28
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	2	0.28
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	10	0.28
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	10	0.28
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD11	3	0.28
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD12	3	0.28
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD13	3	0.28
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	2	0.28
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	2	0.28
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	14	0.28
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	16	0.27
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	19	0.27
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	19	0.27
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	3	0.27
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	5	0.27
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	10	0.27
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	10	0.27
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	10	0.27
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	10	0.27
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	10	0.27
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	10	0.27
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	16	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	16	0.27
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	16	0.27
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	16	0.27
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	16	0.27
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	16	0.27
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	12	0.27
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	14	0.27
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	7	0.27
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	7	0.27
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	17	0.27
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	17	0.27
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	18	0.27
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	14	0.27
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	17	0.27
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	19	0.27
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	3	0.27
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	3	0.27
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	14	0.27
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	14	0.27
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	17	0.27
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	17	0.27
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	20	0.27
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	20	0.27
(1,1089)	1:77:A:LYS:HG2	1:77:A:LYS:H	1	0.27
(1,1089)	1:77:A:LYS:HG3	1:77:A:LYS:H	1	0.27
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	4	0.27
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	4	0.27
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	4	0.27
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	15	0.27
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	15	0.27
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	15	0.27
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	20	0.27
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	20	0.27
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	20	0.27
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	8	0.27
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	17	0.27
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	20	0.27
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	1	0.27
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	1	0.27
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	1	0.27
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	4	0.27
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	4	0.27
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	10	0.27
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	10	0.27
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	10	0.27
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	16	0.27
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	16	0.27
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	16	0.27
(1,1038)	1:5:A:THR:HB	1:5:A:THR:H	4	0.27
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	16	0.27
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	16	0.27
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	7	0.27
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	20	0.27
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	5	0.27
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	5	0.27
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	14	0.27
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	14	0.27
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	1	0.27
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	2	0.27
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	2	0.27
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	2	0.27
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	11	0.27
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	11	0.27
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	11	0.27
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	8	0.27
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	9	0.27
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	11	0.27
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	12	0.27
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	16	0.27
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	18	0.27
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	1	0.27
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	1	0.27
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	1	0.27
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	5	0.27
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	5	0.27
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	5	0.27
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	17	0.27
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	17	0.27
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	17	0.27
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	18	0.27
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	18	0.27
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	18	0.27
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	18	0.27
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	1	0.27
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	1	0.27
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	2	0.27
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	2	0.27
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	5	0.27
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	5	0.27
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	7	0.27
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	7	0.27
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	9	0.27
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	9	0.27
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	20	0.27
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	20	0.27
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	10	0.27
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	16	0.27
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG2	11	0.27
(1,774)	1:116:A:LEU:HB2	1:119:A:GLU:HG3	11	0.27
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG2	11	0.27
(1,774)	1:116:A:LEU:HB3	1:119:A:GLU:HG3	11	0.27
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	3	0.27
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	7	0.27
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	11	0.27
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	19	0.27
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	7	0.27
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	13	0.27
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	13	0.27
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	1	0.27
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	1	0.27
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	2	0.27
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	2	0.27
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	12	0.27
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	12	0.27
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	4	0.27
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	4	0.27
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	16	0.27
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	16	0.27
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	6	0.27
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	13	0.27
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	13	0.27
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	13	0.27
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	13	0.27
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	13	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	13	0.27
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	13	0.27
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	13	0.27
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	13	0.27
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	6	0.26
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	17	0.26
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	10	0.26
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	13	0.26
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	18	0.26
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	18	0.26
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	15	0.26
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	17	0.26
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	20	0.26
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	2	0.26
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	2	0.26
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	1	0.26
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	11	0.26
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	12	0.26
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	14	0.26
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	8	0.26
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	8	0.26
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	8	0.26
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	5	0.26
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	5	0.26
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	7	0.26
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	7	0.26
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	12	0.26
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	12	0.26
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	12	0.26
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA2	15	0.26
(1,1155)	1:56:A:ASP:HA	1:59:A:GLY:HA3	15	0.26
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	5	0.26
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	6	0.26
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	17	0.26
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	19	0.26
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD11	2	0.26
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD12	2	0.26
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD13	2	0.26
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	1	0.26
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	1	0.26
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	10	0.26
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	13	0.26
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	13	0.26
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	13	0.26
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	20	0.26
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	20	0.26
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	20	0.26
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	7	0.26
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	7	0.26
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	7	0.26
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	1	0.26
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	1	0.26
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	1	0.26
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	9	0.26
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	9	0.26
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	9	0.26
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	10	0.26
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	10	0.26
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	10	0.26
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	16	0.26
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	16	0.26
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	16	0.26
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	16	0.26
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	8	0.26
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	8	0.26
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	8	0.26
(1,1038)	1:5:A:THR:HB	1:5:A:THR:H	5	0.26
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	18	0.26
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	2	0.26
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	2	0.26
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	5	0.26
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	10	0.26
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	1	0.26
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	1	0.26
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	2	0.26
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	2	0.26
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	6	0.26
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	6	0.26
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	11	0.26
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	11	0.26
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	16	0.26
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	16	0.26
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	18	0.26
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	19	0.26
(1,862)	1:142:A:VAL:HB	1:142:A:VAL:H	15	0.26
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	15	0.26
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	15	0.26
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	15	0.26
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	3	0.26
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	3	0.26
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	11	0.26
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	11	0.26
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	12	0.26
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	12	0.26
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	15	0.26
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	15	0.26
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	3	0.26
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	14	0.26
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	17	0.26
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	7	0.26
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	7	0.26
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	7	0.26
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	13	0.26
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	13	0.26
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	13	0.26
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	1	0.26
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	1	0.26
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	9	0.26
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	9	0.26
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	10	0.26
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	10	0.26
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	14	0.26
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	14	0.26
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	17	0.26
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	17	0.26
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	5	0.26
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	5	0.26
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	7	0.26
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	7	0.26
(1,367)	1:31:A:GLU:HA	1:32:A:LEU:HG	7	0.26
(1,367)	1:31:A:GLU:HA	1:32:A:LEU:HG	11	0.26
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	10	0.26
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	10	0.26
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	13	0.26
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	3	0.26
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	8	0.26
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	8	0.26
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	8	0.26
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	8	0.26
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	8	0.26
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	8	0.26
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	8	0.26
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	8	0.26
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	8	0.26
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	12	0.26
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	12	0.26
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	12	0.26
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	12	0.26
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	12	0.26
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	12	0.26
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	12	0.26
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	12	0.26
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	12	0.26
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	9	0.25
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	3	0.25
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	9	0.25
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	10	0.25
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	15	0.25
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	19	0.25
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	1	0.25
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	1	0.25
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	4	0.25
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	9	0.25
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	9	0.25
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	16	0.25
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	7	0.25
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	7	0.25
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	5	0.25
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	6	0.25
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	11	0.25
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	18	0.25
(1,1361)	1:76:A:MET:HA	1:77:A:LYS:H	11	0.25
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	3	0.25
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	3	0.25
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	3	0.25
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	3	0.25
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	3	0.25
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	14	0.25
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	14	0.25
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	14	0.25
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	14	0.25
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	14	0.25
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	14	0.25
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	1	0.25
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	1	0.25
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	5	0.25
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	5	0.25
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	11	0.25
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	11	0.25
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	12	0.25
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	12	0.25
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	15	0.25
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	2	0.25
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	5	0.25
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	5	0.25
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	12	0.25
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	1	0.25
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	1	0.25
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	1	0.25
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	1	0.25
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	15	0.25
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	15	0.25
(1,1171)	1:9:A:ILE:HB	1:8:A:GLN:HA	3	0.25
(1,1171)	1:9:A:ILE:HB	1:8:A:GLN:HA	12	0.25
(1,1171)	1:9:A:ILE:HB	1:8:A:GLN:HA	14	0.25
(1,1171)	1:9:A:ILE:HB	1:8:A:GLN:HA	15	0.25
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	3	0.25
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	4	0.25
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	5	0.25
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	10	0.25
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	13	0.25
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	16	0.25
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	8	0.25
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	8	0.25
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	3	0.25
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	3	0.25
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD21	20	0.25
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD22	20	0.25
(1,1072)	1:105:A:LEU:HA	1:105:A:LEU:HD23	20	0.25
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	5	0.25
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	5	0.25
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	5	0.25
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	7	0.25
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	7	0.25
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	7	0.25
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	14	0.25
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	14	0.25
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	14	0.25
(1,1063)	1:110:A:THR:HA	1:113:A:GLY:H	10	0.25
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	15	0.25
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	15	0.25
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	15	0.25
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	1	0.25
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	4	0.25
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	4	0.25
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	10	0.25
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	10	0.25
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	18	0.25
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	7	0.25
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	7	0.25
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	15	0.25
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	5	0.25
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	5	0.25
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	5	0.25
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	9	0.25
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	9	0.25
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	9	0.25
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	2	0.25
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	5	0.25
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	6	0.25
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	4	0.25
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	4	0.25
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	13	0.25
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	13	0.25
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	16	0.25
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	16	0.25
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG2	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,806)	1:122:A:ASP:HB2	1:119:A:GLU:HG3	18	0.25
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	12	0.25
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	17	0.25
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	20	0.25
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	2	0.25
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	12	0.25
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	14	0.25
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	3	0.25
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	3	0.25
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	7	0.25
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	7	0.25
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	8	0.25
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	8	0.25
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	18	0.25
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	18	0.25
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	1	0.25
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	1	0.25
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	4	0.25
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	4	0.25
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	14	0.25
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	14	0.25
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	13	0.25
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	13	0.25
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	20	0.25
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	8	0.24
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	1	0.24
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	10	0.24
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	14	0.24
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	16	0.24
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	17	0.24
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	18	0.24
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	5	0.24
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	5	0.24
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	14	0.24
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	14	0.24
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	16	0.24
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	16	0.24
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	3	0.24
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	3	0.24
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	6	0.24
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	6	0.24
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	10	0.24
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	16	0.24
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	16	0.24
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	2	0.24
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	3	0.24
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	4	0.24
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	8	0.24
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	10	0.24
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	13	0.24
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	14	0.24
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	16	0.24
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	19	0.24
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	13	0.24
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	13	0.24
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	13	0.24
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	13	0.24
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	13	0.24
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	13	0.24
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	4	0.24
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	4	0.24
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	9	0.24
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	9	0.24
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	10	0.24
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	10	0.24
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	16	0.24
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	16	0.24
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	3	0.24
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	7	0.24
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	9	0.24
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	10	0.24
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	11	0.24
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	12	0.24
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	13	0.24
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	15	0.24
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	16	0.24
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	17	0.24
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	20	0.24
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	6	0.24
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	11	0.24
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	19	0.24
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	4	0.24
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	4	0.24
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	6	0.24
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	6	0.24
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	6	0.24
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	14	0.24
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	14	0.24
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	14	0.24
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	11	0.24
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	11	0.24
(1,1171)	1:9:A:ILE:HB	1:8:A:GLN:HA	6	0.24
(1,1171)	1:9:A:ILE:HB	1:8:A:GLN:HA	11	0.24
(1,1171)	1:9:A:ILE:HB	1:8:A:GLN:HA	16	0.24
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	2	0.24
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	6	0.24
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	20	0.24
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	12	0.24
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	14	0.24
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	4	0.24
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	4	0.24
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	10	0.24
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	10	0.24
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	10	0.24
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	18	0.24
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	18	0.24
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	18	0.24
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	2	0.24
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	13	0.24
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	13	0.24
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	13	0.24
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	8	0.24
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	5	0.24
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	12	0.24
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	17	0.24
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	4	0.24
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	4	0.24
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	17	0.24
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	17	0.24
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	2	0.24
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	5	0.24
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	11	0.24
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	16	0.24
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	15	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	15	0.24
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	15	0.24
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	3	0.24
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	3	0.24
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	3	0.24
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	13	0.24
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	13	0.24
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	13	0.24
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	3	0.24
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	3	0.24
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	3	0.24
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	6	0.24
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	6	0.24
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	6	0.24
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	19	0.24
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	19	0.24
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	19	0.24
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	1	0.24
(1,815)	1:99:A:TYR:HA	1:137:A:ASN:H	19	0.24
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	8	0.24
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	11	0.24
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	13	0.24
(1,789)	1:52:A:ILE:HB	1:29:A:THR:HA	13	0.24
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	6	0.24
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	9	0.24
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	11	0.24
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	17	0.24
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	20	0.24
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	15	0.24
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	18	0.24
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	20	0.24
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	12	0.24
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	6	0.24
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	6	0.24
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	15	0.24
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	15	0.24
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	20	0.24
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	20	0.24
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	7	0.24
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	7	0.24
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	13	0.24
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB2	18	0.24
(1,398)	1:37:A:ARG:HA	1:38:A:SER:HB3	18	0.24
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD11	8	0.24
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD12	8	0.24
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD13	8	0.24
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	3	0.24
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	3	0.24
(1,149)	1:31:A:GLU:HB2	1:33:A:GLY:HA2	9	0.24
(1,149)	1:31:A:GLU:HB3	1:33:A:GLY:HA2	9	0.24
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	15	0.24
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	6	0.24
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	6	0.24
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	10	0.24
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	10	0.24
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	10	0.24
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	10	0.24
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	10	0.24
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	10	0.24
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	10	0.24
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	10	0.24
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	10	0.24
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	14	0.24
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	14	0.24
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	14	0.24
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	14	0.24
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	14	0.24
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	14	0.24
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	14	0.24
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	14	0.24
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	14	0.24
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	8	0.24
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	8	0.24
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	8	0.24
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	8	0.24
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	8	0.24
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	8	0.24
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	12	0.24
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	12	0.24
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	12	0.24
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	12	0.24
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	12	0.24
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	10	0.23
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	13	0.23
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	16	0.23
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	13	0.23
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	2	0.23
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	9	0.23
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	12	0.23
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	15	0.23
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	20	0.23
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	10	0.23
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	10	0.23
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	12	0.23
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	12	0.23
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	7	0.23
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	9	0.23
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	9	0.23
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	12	0.23
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	12	0.23
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	13	0.23
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	13	0.23
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	12	0.23
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	10	0.23
(1,1361)	1:76:A:MET:HA	1:77:A:LYS:H	1	0.23
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	11	0.23
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	11	0.23
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	6	0.23
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	6	0.23
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	6	0.23
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	6	0.23
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	6	0.23
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	6	0.23
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	15	0.23
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	15	0.23
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	15	0.23
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	15	0.23
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	15	0.23
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	15	0.23
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	14	0.23
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	14	0.23
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	2	0.23
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	3	0.23
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	6	0.23
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	8	0.23
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	19	0.23
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	14	0.23
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	8	0.23
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	13	0.23
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	18	0.23
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	3	0.23
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	3	0.23
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	3	0.23
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	5	0.23
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	5	0.23
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	5	0.23
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	12	0.23
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	12	0.23
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	12	0.23
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	2	0.23
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	2	0.23
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	9	0.23
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	9	0.23
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	10	0.23
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	10	0.23
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	7	0.23
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	8	0.23
(1,1160)	1:60:A:ASN:HB2	1:63:A:ILE:HB	11	0.23
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	14	0.23
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	14	0.23
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	14	0.23
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	11	0.23
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD11	10	0.23
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD12	10	0.23
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD13	10	0.23
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	2	0.23
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	2	0.23
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	3	0.23
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	3	0.23
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	9	0.23
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	9	0.23
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	9	0.23
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	15	0.23
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	15	0.23
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	18	0.23
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	18	0.23
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	18	0.23
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	3	0.23
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	3	0.23
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	3	0.23
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	6	0.23
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	6	0.23
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	6	0.23
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	8	0.23
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	8	0.23
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	8	0.23
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	19	0.23
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	19	0.23
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	19	0.23
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	9	0.23
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	9	0.23
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	9	0.23
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	9	0.23
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	18	0.23
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	18	0.23
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	18	0.23
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	7	0.23
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	12	0.23
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	6	0.23
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	6	0.23
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	13	0.23
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	13	0.23
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	2	0.23
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	9	0.23
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	13	0.23
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	14	0.23
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	16	0.23
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	19	0.23
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	20	0.23
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	8	0.23
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	8	0.23
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	8	0.23
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	10	0.23
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	10	0.23
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	15	0.23
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	20	0.23
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	20	0.23
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	2	0.23
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	5	0.23
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	8	0.23
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	17	0.23
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	18	0.23
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	4	0.23
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	4	0.23
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	4	0.23
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	7	0.23
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	14	0.23
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	14	0.23
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	14	0.23
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	14	0.23
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	14	0.23
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	14	0.23
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	1	0.23
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	1	0.23
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	1	0.23
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	8	0.23
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	8	0.23
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	8	0.23
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	17	0.23
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	17	0.23
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	17	0.23
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	13	0.23
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	13	0.23
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	13	0.23
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	18	0.23
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	1	0.23
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	5	0.23
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	9	0.23
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	1	0.23
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	2	0.23
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	5	0.23
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	7	0.23
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	8	0.23
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	10	0.23
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	14	0.23
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	1	0.23
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG21	3	0.23
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG22	3	0.23
(1,744)	1:62:A:THR:HA	1:62:A:THR:HG23	3	0.23
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	12	0.23
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	12	0.23
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	8	0.23
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	8	0.23
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	8	0.23
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	5	0.23
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	5	0.23
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	5	0.23
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	5	0.23
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	5	0.23
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	5	0.23
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	2	0.22
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	7	0.22
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	11	0.22
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	13	0.22
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	19	0.22
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	19	0.22
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	19	0.22
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	2	0.22
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	9	0.22
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	1	0.22
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	1	0.22
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	1	0.22
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	2	0.22
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	14	0.22
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	16	0.22
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	14	0.22
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	14	0.22
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	19	0.22
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	19	0.22
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	11	0.22
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	11	0.22
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	11	0.22
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	11	0.22
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	11	0.22
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	11	0.22
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	20	0.22
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	20	0.22
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	20	0.22
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	20	0.22
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	20	0.22
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	3	0.22
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	3	0.22
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	3	0.22
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	6	0.22
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	6	0.22
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	18	0.22
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	18	0.22
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	6	0.22
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	19	0.22
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	20	0.22
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	7	0.22
(1,1246)	1:77:A:LYS:HA	1:78:A:ASP:H	19	0.22
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	1	0.22
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	4	0.22
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	14	0.22
(1,1241)	1:88:A:ALA:HA	1:87:A:GLU:HA	18	0.22
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	4	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	1	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	2	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	3	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	4	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	5	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	7	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	9	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	10	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	11	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	12	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	14	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	15	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	16	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	17	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	19	0.22
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	20	0.22
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	7	0.22
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	7	0.22
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	7	0.22
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	9	0.22
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	9	0.22
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	10	0.22
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	10	0.22
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	10	0.22
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	16	0.22
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	16	0.22
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	16	0.22
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	19	0.22
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	19	0.22
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	19	0.22
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	13	0.22
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	13	0.22
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	18	0.22
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	18	0.22
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	17	0.22
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	17	0.22
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	6	0.22
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	6	0.22
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	6	0.22
(1,1089)	1:77:A:LYS:HG2	1:77:A:LYS:H	12	0.22
(1,1089)	1:77:A:LYS:HG3	1:77:A:LYS:H	12	0.22
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	12	0.22
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	12	0.22
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	12	0.22
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	7	0.22
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	12	0.22
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	3	0.22
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	3	0.22
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	3	0.22
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	5	0.22
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	5	0.22
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	5	0.22
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	6	0.22
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	6	0.22
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	6	0.22
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	11	0.22
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	11	0.22
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	11	0.22
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	14	0.22
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	14	0.22
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	14	0.22
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	19	0.22
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	19	0.22
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	1	0.22
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	2	0.22
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	3	0.22
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	4	0.22
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	10	0.22
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	11	0.22
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	13	0.22
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	14	0.22
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	16	0.22
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	11	0.22
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	8	0.22
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	8	0.22
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	19	0.22
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	19	0.22
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	1	0.22
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	12	0.22
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	4	0.22
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	8	0.22
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	3	0.22
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	3	0.22
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	9	0.22
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	9	0.22
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	12	0.22
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	12	0.22
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG2	13	0.22
(1,980)	1:102:A:ALA:HA	1:135:A:GLN:HG3	13	0.22
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	4	0.22
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	11	0.22
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	16	0.22
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	20	0.22
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	4	0.22
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	6	0.22
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	9	0.22
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	10	0.22
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	20	0.22
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	4	0.22
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	8	0.22
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	11	0.22
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	15	0.22
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	20	0.22
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	4	0.22
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	6	0.22
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	6	0.22
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	14	0.22
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	14	0.22
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	16	0.22
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	16	0.22
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	18	0.22
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	18	0.22
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	19	0.22
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	19	0.22
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	15	0.22
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	15	0.22
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	15	0.22
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	11	0.22
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	11	0.22
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	11	0.22
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	9	0.22
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	9	0.22
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	9	0.22
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	9	0.22
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	7	0.22
(1,789)	1:52:A:ILE:HB	1:29:A:THR:HA	4	0.22
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	4	0.22
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	12	0.22
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	15	0.22
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	16	0.22
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	18	0.22
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	16	0.22
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	16	0.22
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	6	0.22
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	6	0.22
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	9	0.22
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	9	0.22
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	11	0.22
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	11	0.22
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	12	0.22
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	12	0.22
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	15	0.22
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	15	0.22
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	19	0.22
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD11	7	0.22
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD12	7	0.22
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD13	7	0.22
(1,367)	1:31:A:GLU:HA	1:32:A:LEU:HG	12	0.22
(1,367)	1:31:A:GLU:HA	1:32:A:LEU:HG	17	0.22
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	4	0.22
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	4	0.22
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	4	0.22
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	4	0.22
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	4	0.22
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	4	0.22
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	4	0.22
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	4	0.22
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	4	0.22
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	16	0.22
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	16	0.22
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	16	0.22
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	16	0.22
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	16	0.22
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	16	0.22
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	16	0.22
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	16	0.22
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	16	0.22
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	2	0.21
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	4	0.21
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	20	0.21
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	11	0.21
(1,1436)	1:91:A:VAL:HB	1:87:A:GLU:HA	20	0.21
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	11	0.21
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	11	0.21
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	8	0.21
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	8	0.21
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	14	0.21
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	14	0.21
(1,1373)	1:58:A:ASP:HA	1:59:A:GLY:H	7	0.21
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	7	0.21
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	18	0.21
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	11	0.21
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	8	0.21
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	8	0.21
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	13	0.21
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	17	0.21
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	17	0.21
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	20	0.21
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	20	0.21
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	9	0.21
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	9	0.21
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	2	0.21
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	9	0.21
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	12	0.21
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	13	0.21
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	17	0.21
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	18	0.21
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	1	0.21
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	5	0.21
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	6	0.21
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	8	0.21
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	7	0.21
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	11	0.21
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	14	0.21
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	19	0.21
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	9	0.21
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	13	0.21
(1,1200)	1:129:A:ASP:HB3	1:129:A:ASP:HA	6	0.21
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	2	0.21
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	2	0.21
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	2	0.21
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	11	0.21
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	11	0.21
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	11	0.21
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	18	0.21
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	18	0.21
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	18	0.21
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG21	1	0.21
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG22	1	0.21
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG23	1	0.21
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG21	1	0.21
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG22	1	0.21
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG23	1	0.21
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	3	0.21
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	3	0.21
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	8	0.21
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	16	0.21
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	16	0.21
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	9	0.21
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	4	0.21
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	4	0.21
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	4	0.21
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	17	0.21
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	17	0.21
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	17	0.21
(1,1071)	1:106:A:ARG:HD3	1:107:A:HIS:H	13	0.21
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	2	0.21
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	2	0.21
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	2	0.21
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	13	0.21
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	13	0.21
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	13	0.21
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG11	17	0.21
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG12	17	0.21
(1,1068)	1:106:A:ARG:HD3	1:121:A:VAL:HG13	17	0.21
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	6	0.21
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	10	0.21
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	12	0.21
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	12	0.21
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	12	0.21
(1,1048)	1:142:A:VAL:HG21	1:139:A:GLU:HA	1	0.21
(1,1048)	1:142:A:VAL:HG22	1:139:A:GLU:HA	1	0.21
(1,1048)	1:142:A:VAL:HG23	1:139:A:GLU:HA	1	0.21
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	5	0.21
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	6	0.21
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	8	0.21
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	15	0.21
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	17	0.21
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	18	0.21
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	5	0.21
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	5	0.21
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	12	0.21
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	12	0.21
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	14	0.21
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	14	0.21
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	15	0.21
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	15	0.21
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	20	0.21
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	15	0.21
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	2	0.21
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	3	0.21
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	6	0.21
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	7	0.21
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	15	0.21
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	18	0.21
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	3	0.21
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	8	0.21
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	13	0.21
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	14	0.21
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	17	0.21
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	18	0.21
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	6	0.21
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	7	0.21
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	9	0.21
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	12	0.21
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	13	0.21
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	5	0.21
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	5	0.21
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	5	0.21
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	10	0.21
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	12	0.21
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	14	0.21
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	8	0.21
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	10	0.21
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	12	0.21
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	13	0.21
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	18	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	2	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	2	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	5	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	5	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	7	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	7	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	9	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	9	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	10	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	10	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	11	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	12	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	12	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	15	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	15	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	17	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	17	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	20	0.21
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	20	0.21
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	4	0.21
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	4	0.21
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	4	0.21
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	19	0.21
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	19	0.21
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	19	0.21
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	15	0.21
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	15	0.21
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	15	0.21
(1,803)	1:100:A:ILE:HA	1:93:A:ASP:HA	4	0.21
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	15	0.21
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	15	0.21
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	15	0.21
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	15	0.21
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	15	0.21
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	15	0.21
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	4	0.21
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	11	0.21
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	14	0.21
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	16	0.21
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	19	0.21
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	5	0.21
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	5	0.21
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	10	0.21
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	10	0.21
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	10	0.21
(1,427)	1:39:A:LEU:HA	1:38:A:SER:H	6	0.21
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	2	0.21
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	2	0.21
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	3	0.21
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	3	0.21
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	5	0.21
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	5	0.21
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	16	0.21
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	17	0.21
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	17	0.21
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	18	0.21
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	18	0.21
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	20	0.21
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	20	0.21
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	5	0.21
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	11	0.21
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	15	0.21
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	19	0.21
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	7	0.21
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	7	0.21
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	16	0.21
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	16	0.21
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	17	0.21
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	17	0.21
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	17	0.21
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	17	0.21
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	17	0.21
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	17	0.21
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	17	0.21
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	17	0.21
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	17	0.21
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	18	0.21
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	18	0.21
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	18	0.21
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	18	0.21
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	18	0.21
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	18	0.21
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	18	0.21
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	18	0.21
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	18	0.21
(1,11)	1:27:A:ILE:HD11	1:28:A:THR:HB	13	0.21
(1,11)	1:27:A:ILE:HD12	1:28:A:THR:HB	13	0.21
(1,11)	1:27:A:ILE:HD13	1:28:A:THR:HB	13	0.21
(1,11)	1:27:A:ILE:HD11	1:28:A:THR:HB	18	0.21
(1,11)	1:27:A:ILE:HD12	1:28:A:THR:HB	18	0.21
(1,11)	1:27:A:ILE:HD13	1:28:A:THR:HB	18	0.21
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	7	0.2
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	8	0.2
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	8	0.2
(1,1422)	1:82:A:GLU:HA	1:85:A:ILE:H	8	0.2
(1,1411)	1:41:A:GLN:HB2	1:37:A:ARG:HA	19	0.2
(1,1411)	1:41:A:GLN:HB3	1:37:A:ARG:HA	19	0.2
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	6	0.2
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	6	0.2
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	2	0.2
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	2	0.2
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	4	0.2
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	4	0.2
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	5	0.2
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	5	0.2
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	11	0.2
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	11	0.2
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	15	0.2
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	15	0.2
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	9	0.2
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	18	0.2
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	18	0.2
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	18	0.2
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	18	0.2
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	18	0.2
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	18	0.2
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	9	0.2
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	10	0.2
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	10	0.2
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	5	0.2
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	9	0.2
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	11	0.2
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	14	0.2
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	17	0.2
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	4	0.2
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	5	0.2
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	6	0.2
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	10	0.2
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	14	0.2
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	16	0.2
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	3	0.2
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	9	0.2
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	13	0.2
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	18	0.2
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	14	0.2
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	5	0.2
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	6	0.2
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	12	0.2
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	17	0.2
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	18	0.2
(1,1212)	1:48:A:LEU:HG	1:48:A:LEU:H	16	0.2
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	13	0.2
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	13	0.2
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	13	0.2
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	15	0.2
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	15	0.2
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	15	0.2
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	9	0.2
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	9	0.2
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	12	0.2
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	12	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	1	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	2	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	3	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	4	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	5	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	6	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	7	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	8	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	9	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	10	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	11	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	12	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	13	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	14	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	15	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	16	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	17	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	19	0.2
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	20	0.2
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	11	0.2
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	13	0.2
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	16	0.2
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	5	0.2
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	5	0.2
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	9	0.2
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	7	0.2
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	18	0.2
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	11	0.2
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	11	0.2
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	11	0.2
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	12	0.2
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	12	0.2
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	12	0.2
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	14	0.2
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	14	0.2
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	14	0.2
(1,1071)	1:106:A:ARG:HD3	1:107:A:HIS:H	10	0.2
(1,1067)	1:106:A:ARG:HD3	1:106:A:ARG:H	9	0.2
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	17	0.2
(1,1048)	1:142:A:VAL:HG21	1:139:A:GLU:HA	6	0.2
(1,1048)	1:142:A:VAL:HG22	1:139:A:GLU:HA	6	0.2
(1,1048)	1:142:A:VAL:HG23	1:139:A:GLU:HA	6	0.2
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	9	0.2
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	20	0.2
(1,1021)	1:6:A:GLU:HB2	1:3:A:GLN:HA	3	0.2
(1,1021)	1:6:A:GLU:HB3	1:3:A:GLN:HA	3	0.2
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	1	0.2
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	1	0.2
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	3	0.2
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	3	0.2
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	7	0.2
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	7	0.2
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	11	0.2
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	11	0.2
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	6	0.2
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	14	0.2
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	18	0.2
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	18	0.2
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	18	0.2
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	18	0.2
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	18	0.2
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	18	0.2
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	3	0.2
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	6	0.2
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	7	0.2
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB2	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB3	5	0.2
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	2	0.2
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	9	0.2
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	10	0.2
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	17	0.2
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	10	0.2
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	16	0.2
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	1	0.2
(1,917)	1:93:A:ASP:HB2	1:93:A:ASP:H	3	0.2
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	17	0.2
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	17	0.2
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	17	0.2
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	12	0.2
(1,899)	1:125:A:ILE:HG12	1:122:A:ASP:HA	7	0.2
(1,899)	1:125:A:ILE:HG13	1:122:A:ASP:HA	7	0.2
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	1	0.2
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	3	0.2
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	4	0.2
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	7	0.2
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	9	0.2
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	14	0.2
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	16	0.2
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	17	0.2
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	19	0.2
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	20	0.2
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	6	0.2
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	6	0.2
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	6	0.2
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	10	0.2
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	10	0.2
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	10	0.2
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	18	0.2
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	18	0.2
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	18	0.2
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG12	7	0.2
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG13	7	0.2
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	3	0.2
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	13	0.2
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	8	0.2
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	8	0.2
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	8	0.2
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	8	0.2
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	8	0.2
(1,759)	1:26:A:THR:HG21	1:62:A:THR:HA	9	0.2
(1,759)	1:26:A:THR:HG22	1:62:A:THR:HA	9	0.2
(1,759)	1:26:A:THR:HG23	1:62:A:THR:HA	9	0.2
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	1	0.2
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	1	0.2
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	1	0.2
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	1	0.2
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	1	0.2
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	1	0.2
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	2	0.2
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	6	0.2
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	10	0.2
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	20	0.2
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	19	0.2
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	19	0.2
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	13	0.2
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	13	0.2
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	13	0.2
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	14	0.2
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	14	0.2
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	14	0.2
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG2	10	0.2
(1,403)	1:136:A:VAL:HA	1:135:A:GLN:HG3	10	0.2
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	3	0.2
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	12	0.2
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	17	0.2
(1,95)	1:48:A:LEU:HD21	1:50:A:ASP:HA	8	0.2
(1,95)	1:48:A:LEU:HD22	1:50:A:ASP:HA	8	0.2
(1,95)	1:48:A:LEU:HD23	1:50:A:ASP:HA	8	0.2
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	14	0.2
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	14	0.2
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	6	0.19
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	15	0.19
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	4	0.19
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	19	0.19
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	14	0.19
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	8	0.19
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	4	0.19
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	17	0.19
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	8	0.19
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	12	0.19
(1,1333)	1:38:A:SER:HB2	1:40:A:GLY:H	16	0.19
(1,1333)	1:38:A:SER:HB3	1:40:A:GLY:H	16	0.19
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	12	0.19
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	12	0.19
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	12	0.19
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	12	0.19
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	12	0.19
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	12	0.19
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	17	0.19
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	17	0.19
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	17	0.19
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	17	0.19
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	17	0.19
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	17	0.19
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	7	0.19
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	15	0.19
(1,1304)	1:136:A:VAL:HB	1:136:A:VAL:H	8	0.19
(1,1304)	1:136:A:VAL:HB	1:136:A:VAL:H	12	0.19
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	8	0.19
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	12	0.19
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	19	0.19
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	4	0.19
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	7	0.19
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	12	0.19
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	11	0.19
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	15	0.19
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	20	0.19
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	2	0.19
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	4	0.19
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	7	0.19
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	10	0.19
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	11	0.19
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	12	0.19
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	14	0.19
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	15	0.19
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	16	0.19
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	17	0.19
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	20	0.19
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	16	0.19
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	9	0.19
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	10	0.19
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	12	0.19
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	13	0.19
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	17	0.19
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	18	0.19
(1,1228)	1:112:A:LEU:HD11	1:112:A:LEU:H	20	0.19
(1,1228)	1:112:A:LEU:HD12	1:112:A:LEU:H	20	0.19
(1,1228)	1:112:A:LEU:HD13	1:112:A:LEU:H	20	0.19
(1,1228)	1:112:A:LEU:HD21	1:112:A:LEU:H	20	0.19
(1,1228)	1:112:A:LEU:HD22	1:112:A:LEU:H	20	0.19
(1,1228)	1:112:A:LEU:HD23	1:112:A:LEU:H	20	0.19
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	2	0.19
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	17	0.19
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	17	0.19
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	17	0.19
(1,1189)	1:91:A:VAL:HG21	1:90:A:ARG:H	20	0.19
(1,1189)	1:91:A:VAL:HG22	1:90:A:ARG:H	20	0.19
(1,1189)	1:91:A:VAL:HG23	1:90:A:ARG:H	20	0.19
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	2	0.19
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	5	0.19
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	6	0.19
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	9	0.19
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	10	0.19
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	14	0.19
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	16	0.19
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	17	0.19
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	18	0.19
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	19	0.19
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	20	0.19
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	7	0.19
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG21	5	0.19
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG22	5	0.19
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG23	5	0.19
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG21	5	0.19
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG22	5	0.19
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG23	5	0.19
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	8	0.19
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	8	0.19
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	12	0.19
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	12	0.19
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	3	0.19
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	5	0.19
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	15	0.19
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	4	0.19
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	1	0.19
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	7	0.19
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	8	0.19
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	15	0.19
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	18	0.19
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	16	0.19
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	16	0.19
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	4	0.19
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	12	0.19
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	15	0.19
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	5	0.19
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	5	0.19
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	5	0.19
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	19	0.19
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	19	0.19
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	19	0.19
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	4	0.19
(1,1082)	1:90:A:ARG:HB2	1:91:A:VAL:HG21	17	0.19
(1,1082)	1:90:A:ARG:HB2	1:91:A:VAL:HG22	17	0.19
(1,1082)	1:90:A:ARG:HB2	1:91:A:VAL:HG23	17	0.19
(1,1082)	1:90:A:ARG:HB3	1:91:A:VAL:HG21	17	0.19
(1,1082)	1:90:A:ARG:HB3	1:91:A:VAL:HG22	17	0.19
(1,1082)	1:90:A:ARG:HB3	1:91:A:VAL:HG23	17	0.19
(1,1071)	1:106:A:ARG:HD3	1:107:A:HIS:H	9	0.19
(1,1071)	1:106:A:ARG:HD3	1:107:A:HIS:H	17	0.19
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	1	0.19
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	3	0.19
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	15	0.19
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	4	0.19
(1,1036)	1:60:A:ASN:HB3	1:60:A:ASN:H	19	0.19
(1,1021)	1:6:A:GLU:HB2	1:3:A:GLN:HA	1	0.19
(1,1021)	1:6:A:GLU:HB3	1:3:A:GLN:HA	1	0.19
(1,1021)	1:6:A:GLU:HB2	1:3:A:GLN:HA	13	0.19
(1,1021)	1:6:A:GLU:HB3	1:3:A:GLN:HA	13	0.19
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	4	0.19
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	11	0.19
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	7	0.19
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	7	0.19
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	7	0.19
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	7	0.19
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	7	0.19
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	1	0.19
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	3	0.19
(1,978)	1:102:A:ALA:HA	1:104:A:GLU:H	13	0.19
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	2	0.19
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	3	0.19
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	11	0.19
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	19	0.19
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	5	0.19
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	20	0.19
(1,933)	1:70:A:THR:HG21	1:70:A:THR:H	15	0.19
(1,933)	1:70:A:THR:HG22	1:70:A:THR:H	15	0.19
(1,933)	1:70:A:THR:HG23	1:70:A:THR:H	15	0.19
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	8	0.19
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	8	0.19
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	8	0.19
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	20	0.19
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	20	0.19
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	20	0.19
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	1	0.19
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	2	0.19
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	3	0.19
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	5	0.19
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	6	0.19
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	16	0.19
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	17	0.19
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	18	0.19
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	19	0.19
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	2	0.19
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	5	0.19
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	6	0.19
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	11	0.19
(1,891)	1:129:A:ASP:HB2	1:128:A:ALA:HA	15	0.19
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB2	8	0.19
(1,878)	1:5:A:THR:HA	1:6:A:GLU:HB3	8	0.19
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	12	0.19
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	12	0.19
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	12	0.19
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	13	0.19
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	13	0.19
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	15	0.19
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	15	0.19
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	15	0.19
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	5	0.19
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	5	0.19
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	5	0.19
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	12	0.19
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	12	0.19
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	12	0.19
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	14	0.19
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	14	0.19
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	14	0.19
(1,856)	1:93:A:ASP:HB3	1:100:A:ILE:HG21	14	0.19
(1,856)	1:93:A:ASP:HB3	1:100:A:ILE:HG22	14	0.19
(1,856)	1:93:A:ASP:HB3	1:100:A:ILE:HG23	14	0.19
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	14	0.19
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	14	0.19
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	14	0.19
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	11	0.19
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	12	0.19
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	14	0.19
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	16	0.19
(1,819)	1:80:A:ASP:HB2	1:83:A:GLU:H	19	0.19
(1,819)	1:80:A:ASP:HB3	1:83:A:GLU:H	19	0.19
(1,789)	1:52:A:ILE:HB	1:29:A:THR:HA	10	0.19
(1,789)	1:52:A:ILE:HB	1:29:A:THR:HA	16	0.19
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	11	0.19
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	11	0.19
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	11	0.19
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	11	0.19
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	11	0.19
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	11	0.19
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	10	0.19
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	5	0.19
(1,680)	1:27:A:ILE:HB	1:63:A:ILE:H	9	0.19
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	4	0.19
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	4	0.19
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	11	0.19
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	11	0.19
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	9	0.19
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	9	0.19
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	16	0.19
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	16	0.19
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	16	0.19
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	18	0.19
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	18	0.19
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	18	0.19
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	20	0.19
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	20	0.19
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	20	0.19
(1,367)	1:31:A:GLU:HA	1:32:A:LEU:HG	1	0.19
(1,367)	1:31:A:GLU:HA	1:32:A:LEU:HG	14	0.19
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	7	0.19
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	12	0.19
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	8	0.19
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	20	0.19
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	9	0.19
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	9	0.19
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	20	0.19
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	20	0.19
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	3	0.18
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	1	0.18
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	3	0.18
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	14	0.18
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	17	0.18
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	18	0.18
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	20	0.18
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	7	0.18
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	7	0.18
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	5	0.18
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	17	0.18
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	17	0.18
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	17	0.18
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	2	0.18
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	15	0.18
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	19	0.18
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	20	0.18
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	5	0.18
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	13	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	1	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	3	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	4	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	5	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	6	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	9	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	10	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	11	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	13	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	14	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	15	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	16	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	17	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	18	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	19	0.18
(1,1343)	1:129:A:ASP:HA	1:129:A:ASP:H	20	0.18
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	18	0.18
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	7	0.18
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	6	0.18
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	6	0.18
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	15	0.18
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	15	0.18
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	1	0.18
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	6	0.18
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	8	0.18
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	16	0.18
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	8	0.18
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	19	0.18
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	1	0.18
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	3	0.18
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	8	0.18
(1,1271)	1:116:A:LEU:HA	1:116:A:LEU:H	19	0.18
(1,1269)	1:3:A:GLN:HA	1:3:A:GLN:H	19	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	1	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	2	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	3	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	4	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	5	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	6	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	7	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	8	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	9	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	11	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	12	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	13	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	14	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	15	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	16	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	17	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	18	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	19	0.18
(1,1266)	1:14:A:GLU:HA	1:14:A:GLU:H	20	0.18
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	2	0.18
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	11	0.18
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	18	0.18
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	1	0.18
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	2	0.18
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	4	0.18
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	7	0.18
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	11	0.18
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	19	0.18
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	4	0.18
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	9	0.18
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	13	0.18
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	15	0.18
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	16	0.18
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	1	0.18
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	11	0.18
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	15	0.18
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	5	0.18
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG21	19	0.18
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG22	19	0.18
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG23	19	0.18
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG21	19	0.18
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG22	19	0.18
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG23	19	0.18
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	7	0.18
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	7	0.18
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	13	0.18
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	13	0.18
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	17	0.18
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	17	0.18
(1,1170)	1:97:A:ASN:HA	1:97:A:ASN:H	18	0.18
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	4	0.18
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	9	0.18
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	12	0.18
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	13	0.18
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	17	0.18
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	10	0.18
(1,1149)	1:100:A:ILE:HG21	1:93:A:ASP:HB2	20	0.18
(1,1149)	1:100:A:ILE:HG22	1:93:A:ASP:HB2	20	0.18
(1,1149)	1:100:A:ILE:HG23	1:93:A:ASP:HB2	20	0.18
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	3	0.18
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	20	0.18
(1,1114)	1:29:A:THR:HB	1:29:A:THR:H	2	0.18
(1,1114)	1:29:A:THR:HB	1:29:A:THR:H	16	0.18
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	12	0.18
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	12	0.18
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	3	0.18
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	5	0.18
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	6	0.18
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	11	0.18
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	14	0.18
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	19	0.18
(1,1107)	1:44:A:THR:HG21	1:44:A:THR:H	11	0.18
(1,1107)	1:44:A:THR:HG22	1:44:A:THR:H	11	0.18
(1,1107)	1:44:A:THR:HG23	1:44:A:THR:H	11	0.18
(1,1107)	1:44:A:THR:HG21	1:44:A:THR:H	19	0.18
(1,1107)	1:44:A:THR:HG22	1:44:A:THR:H	19	0.18
(1,1107)	1:44:A:THR:HG23	1:44:A:THR:H	19	0.18
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	2	0.18
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	2	0.18
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	2	0.18
(1,1071)	1:106:A:ARG:HD3	1:107:A:HIS:H	14	0.18
(1,1071)	1:106:A:ARG:HD3	1:107:A:HIS:H	18	0.18
(1,1067)	1:106:A:ARG:HD3	1:106:A:ARG:H	18	0.18
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	4	0.18
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	5	0.18
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	11	0.18
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	13	0.18
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	14	0.18
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	20	0.18
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	2	0.18
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	7	0.18
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	17	0.18
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	17	0.18
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB2	18	0.18
(1,1019)	1:42:A:ASN:HB2	1:41:A:GLN:HB3	18	0.18
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	16	0.18
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	20	0.18
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	13	0.18
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	17	0.18
(1,1000)	1:103:A:ALA:HA	1:104:A:GLU:HB2	8	0.18
(1,1000)	1:103:A:ALA:HA	1:104:A:GLU:HB3	8	0.18
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	11	0.18
(1,999)	1:103:A:ALA:HA	1:106:A:ARG:H	15	0.18
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB2	19	0.18
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB3	19	0.18
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	5	0.18
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	17	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	1	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	4	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	5	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	6	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	8	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	9	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	10	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	12	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	13	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	15	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	16	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	17	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	18	0.18
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	20	0.18
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	11	0.18
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	19	0.18
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	12	0.18
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	12	0.18
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	12	0.18
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	16	0.18
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	16	0.18
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	16	0.18
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	9	0.18
(1,907)	1:119:A:GLU:HA	1:120:A:GLU:H	13	0.18
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	7	0.18
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	12	0.18
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	12	0.18
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	1	0.18
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	1	0.18
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	1	0.18
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	4	0.18
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	4	0.18
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	4	0.18
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	4	0.18
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	4	0.18
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	4	0.18
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	10	0.18
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	10	0.18
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	10	0.18
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	19	0.18
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	19	0.18
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	19	0.18
(1,856)	1:93:A:ASP:HB3	1:100:A:ILE:HG21	4	0.18
(1,856)	1:93:A:ASP:HB3	1:100:A:ILE:HG22	4	0.18
(1,856)	1:93:A:ASP:HB3	1:100:A:ILE:HG23	4	0.18
(1,856)	1:93:A:ASP:HB3	1:100:A:ILE:HG21	19	0.18
(1,856)	1:93:A:ASP:HB3	1:100:A:ILE:HG22	19	0.18
(1,856)	1:93:A:ASP:HB3	1:100:A:ILE:HG23	19	0.18
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	5	0.18
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	8	0.18
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	20	0.18
(1,819)	1:80:A:ASP:HB2	1:83:A:GLU:H	8	0.18
(1,819)	1:80:A:ASP:HB3	1:83:A:GLU:H	8	0.18
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	19	0.18
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	20	0.18
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	17	0.18
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	17	0.18
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	17	0.18
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	17	0.18
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	17	0.18
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	17	0.18
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	8	0.18
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	8	0.18
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	8	0.18
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	8	0.18
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	8	0.18
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	12	0.18
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	12	0.18
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	12	0.18
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	12	0.18
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	12	0.18
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	12	0.18
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	3	0.18
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	8	0.18
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	15	0.18
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	18	0.18
(1,680)	1:27:A:ILE:HB	1:63:A:ILE:H	7	0.18
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB2	2	0.18
(1,501)	1:110:A:THR:HB	1:107:A:HIS:HB3	2	0.18
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	4	0.18
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	4	0.18
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	4	0.18
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	17	0.18
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	17	0.18
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	17	0.18
(1,427)	1:39:A:LEU:HA	1:38:A:SER:H	9	0.18
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD11	18	0.18
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD12	18	0.18
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD13	18	0.18
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	2	0.18
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	6	0.18
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	1	0.18
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	1	0.18
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	11	0.18
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	11	0.18
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	11	0.18
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	11	0.18
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	11	0.18
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	11	0.18
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	11	0.18
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	11	0.18
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	11	0.18
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	2	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	4	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	5	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	6	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	8	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	10	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	11	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	13	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	14	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	15	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	16	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	17	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	18	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	19	0.17
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	20	0.17
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	7	0.17
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	11	0.17
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	19	0.17
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	2	0.17
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	2	0.17
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	5	0.17
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	9	0.17
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	15	0.17
(1,1411)	1:41:A:GLN:HB2	1:37:A:ARG:HA	11	0.17
(1,1411)	1:41:A:GLN:HB3	1:37:A:ARG:HA	11	0.17
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	15	0.17
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	18	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	1	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	3	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	4	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	5	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	6	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	7	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	8	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	10	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	11	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	12	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	13	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	14	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	16	0.17
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	18	0.17
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	1	0.17
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	8	0.17
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	8	0.17
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	8	0.17
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	8	0.17
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	8	0.17
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	8	0.17
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	10	0.17
(1,1314)	1:39:A:LEU:HB2	1:42:A:ASN:H	15	0.17
(1,1314)	1:39:A:LEU:HB3	1:42:A:ASN:H	15	0.17
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	4	0.17
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	4	0.17
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	14	0.17
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	14	0.17
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	16	0.17
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	16	0.17
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	20	0.17
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	20	0.17
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	4	0.17
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	11	0.17
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	10	0.17
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	18	0.17
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	2	0.17
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	4	0.17
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	5	0.17
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	7	0.17
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	13	0.17
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	14	0.17
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	15	0.17
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	17	0.17
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	2	0.17
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	4	0.17
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	9	0.17
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	14	0.17
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	20	0.17
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	1	0.17
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	2	0.17
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	4	0.17
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	6	0.17
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	7	0.17
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	11	0.17
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	12	0.17
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	13	0.17
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	14	0.17
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	19	0.17
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	20	0.17
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	9	0.17
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	10	0.17
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	13	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	2	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	3	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	4	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	5	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	6	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	9	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	10	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	13	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	14	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	15	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	16	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	17	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	18	0.17
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	20	0.17
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	3	0.17
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	5	0.17
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	6	0.17
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	8	0.17
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	15	0.17
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	20	0.17
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	3	0.17
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	4	0.17
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	8	0.17
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	12	0.17
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	13	0.17
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG21	2	0.17
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG22	2	0.17
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG23	2	0.17
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG21	2	0.17
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG22	2	0.17
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG23	2	0.17
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	1	0.17
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	1	0.17
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	4	0.17
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	4	0.17
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	10	0.17
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	10	0.17
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	17	0.17
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	14	0.17
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	14	0.17
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	6	0.17
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	10	0.17
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	14	0.17
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	18	0.17
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	20	0.17
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	5	0.17
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	7	0.17
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	14	0.17
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	17	0.17
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	20	0.17
(1,1149)	1:100:A:ILE:HG21	1:93:A:ASP:HB2	11	0.17
(1,1149)	1:100:A:ILE:HG22	1:93:A:ASP:HB2	11	0.17
(1,1149)	1:100:A:ILE:HG23	1:93:A:ASP:HB2	11	0.17
(1,1149)	1:100:A:ILE:HG21	1:93:A:ASP:HB2	17	0.17
(1,1149)	1:100:A:ILE:HG22	1:93:A:ASP:HB2	17	0.17
(1,1149)	1:100:A:ILE:HG23	1:93:A:ASP:HB2	17	0.17
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	4	0.17
(1,1120)	1:29:A:THR:HB	1:52:A:ILE:HD11	11	0.17
(1,1120)	1:29:A:THR:HB	1:52:A:ILE:HD12	11	0.17
(1,1120)	1:29:A:THR:HB	1:52:A:ILE:HD13	11	0.17
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	7	0.17
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	7	0.17
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	18	0.17
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	18	0.17
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	2	0.17
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	9	0.17
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	17	0.17
(1,1107)	1:44:A:THR:HG21	1:44:A:THR:H	12	0.17
(1,1107)	1:44:A:THR:HG22	1:44:A:THR:H	12	0.17
(1,1107)	1:44:A:THR:HG23	1:44:A:THR:H	12	0.17
(1,1107)	1:44:A:THR:HG21	1:44:A:THR:H	17	0.17
(1,1107)	1:44:A:THR:HG22	1:44:A:THR:H	17	0.17
(1,1107)	1:44:A:THR:HG23	1:44:A:THR:H	17	0.17
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	10	0.17
(1,1082)	1:90:A:ARG:HB2	1:91:A:VAL:HG21	13	0.17
(1,1082)	1:90:A:ARG:HB2	1:91:A:VAL:HG22	13	0.17
(1,1082)	1:90:A:ARG:HB2	1:91:A:VAL:HG23	13	0.17
(1,1082)	1:90:A:ARG:HB3	1:91:A:VAL:HG21	13	0.17
(1,1082)	1:90:A:ARG:HB3	1:91:A:VAL:HG22	13	0.17
(1,1082)	1:90:A:ARG:HB3	1:91:A:VAL:HG23	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:106:A:ARG:HD3	1:106:A:ARG:H	10	0.17
(1,1067)	1:106:A:ARG:HD3	1:106:A:ARG:H	13	0.17
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	16	0.17
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	18	0.17
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	19	0.17
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	3	0.17
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	17	0.17
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	17	0.17
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	17	0.17
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	9	0.17
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	17	0.17
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	19	0.17
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	3	0.17
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	10	0.17
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	14	0.17
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	18	0.17
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	9	0.17
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	14	0.17
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	14	0.17
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	14	0.17
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	14	0.17
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	14	0.17
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	14	0.17
(1,1000)	1:103:A:ALA:HA	1:104:A:GLU:HB2	12	0.17
(1,1000)	1:103:A:ALA:HA	1:104:A:GLU:HB3	12	0.17
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB2	6	0.17
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB3	6	0.17
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB2	12	0.17
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB3	12	0.17
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	10	0.17
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	7	0.17
(1,977)	1:102:A:ALA:HA	1:103:A:ALA:H	14	0.17
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	7	0.17
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	2	0.17
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	2	0.17
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	2	0.17
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	11	0.17
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	11	0.17
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	11	0.17
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	2	0.17
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	11	0.17
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	11	0.17
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	3	0.17
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	3	0.17
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	3	0.17
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	2	0.17
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	2	0.17
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	2	0.17
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	13	0.17
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	13	0.17
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	13	0.17
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	16	0.17
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	16	0.17
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	16	0.17
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	20	0.17
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	20	0.17
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	20	0.17
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	6	0.17
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	6	0.17
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	6	0.17
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	9	0.17
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	9	0.17
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	9	0.17
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	10	0.17
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG12	19	0.17
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG13	19	0.17
(1,783)	1:94:A:LYS:HG3	1:94:A:LYS:HA	19	0.17
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	20	0.17
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	20	0.17
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	20	0.17
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	20	0.17
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	20	0.17
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	20	0.17
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	3	0.17
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	7	0.17
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	19	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	2	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	2	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	2	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	2	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	2	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	2	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	9	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	9	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	9	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	9	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	9	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	10	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	10	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	10	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	10	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	10	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	10	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	11	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	11	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	11	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	11	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	11	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	11	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	14	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	14	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	14	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	14	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	14	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	14	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	17	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	17	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	17	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	17	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	17	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	17	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	18	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	18	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	18	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	18	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	18	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	18	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	20	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	20	0.17
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	20	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	20	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	20	0.17
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	20	0.17
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	17	0.17
(1,427)	1:39:A:LEU:HA	1:38:A:SER:H	15	0.17
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD11	11	0.17
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD12	11	0.17
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD13	11	0.17
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD11	20	0.17
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD12	20	0.17
(1,368)	1:31:A:GLU:HA	1:32:A:LEU:HD13	20	0.17
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	5	0.17
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	17	0.17
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	16	0.17
(1,95)	1:48:A:LEU:HD21	1:50:A:ASP:HA	3	0.17
(1,95)	1:48:A:LEU:HD22	1:50:A:ASP:HA	3	0.17
(1,95)	1:48:A:LEU:HD23	1:50:A:ASP:HA	3	0.17
(1,95)	1:48:A:LEU:HD21	1:50:A:ASP:HA	20	0.17
(1,95)	1:48:A:LEU:HD22	1:50:A:ASP:HA	20	0.17
(1,95)	1:48:A:LEU:HD23	1:50:A:ASP:HA	20	0.17
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	11	0.17
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	11	0.17
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	5	0.17
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	5	0.17
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	5	0.17
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	5	0.17
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	5	0.17
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	5	0.17
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	5	0.17
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	5	0.17
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	5	0.17
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	6	0.16
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	8	0.16
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	1	0.16
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	3	0.16
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	7	0.16
(1,1444)	1:61:A:GLY:HA3	1:61:A:GLY:H	12	0.16
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	5	0.16
(1,1438)	1:42:A:ASN:HB3	1:42:A:ASN:H	12	0.16
(1,1432)	1:63:A:ILE:HB	1:63:A:ILE:H	15	0.16
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	5	0.16
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	5	0.16
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	15	0.16
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	15	0.16
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	16	0.16
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	10	0.16
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	17	0.16
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	19	0.16
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	6	0.16
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	11	0.16
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	14	0.16
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	16	0.16
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	18	0.16
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	19	0.16
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	19	0.16
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	19	0.16
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE1	20	0.16
(1,1388)	1:16:A:PHE:HA	1:16:A:PHE:HE2	20	0.16
(1,1377)	1:52:A:ILE:HD11	1:62:A:THR:H	13	0.16
(1,1377)	1:52:A:ILE:HD12	1:62:A:THR:H	13	0.16
(1,1377)	1:52:A:ILE:HD13	1:62:A:THR:H	13	0.16
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	9	0.16
(1,1372)	1:58:A:ASP:HA	1:58:A:ASP:H	17	0.16
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	12	0.16
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	3	0.16
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	10	0.16
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	19	0.16
(1,1351)	1:110:A:THR:HG21	1:110:A:THR:H	9	0.16
(1,1351)	1:110:A:THR:HG22	1:110:A:THR:H	9	0.16
(1,1351)	1:110:A:THR:HG23	1:110:A:THR:H	9	0.16
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	18	0.16
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	4	0.16
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	4	0.16
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	4	0.16
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	4	0.16
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	4	0.16
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	4	0.16
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	19	0.16
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	19	0.16
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	19	0.16
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	19	0.16
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	19	0.16
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	19	0.16
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	7	0.16
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	7	0.16
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	18	0.16
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	7	0.16
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	1	0.16
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	3	0.16
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	6	0.16
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	8	0.16
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	9	0.16
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	10	0.16
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	11	0.16
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	12	0.16
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	16	0.16
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	18	0.16
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	19	0.16
(1,1285)	1:52:A:ILE:HA	1:52:A:ILE:H	20	0.16
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	1	0.16
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	5	0.16
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	13	0.16
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	15	0.16
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	16	0.16
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	17	0.16
(1,1277)	1:51:A:MET:HB2	1:50:A:ASP:HA	9	0.16
(1,1277)	1:51:A:MET:HB3	1:50:A:ASP:HA	9	0.16
(1,1277)	1:51:A:MET:HB2	1:50:A:ASP:HA	19	0.16
(1,1277)	1:51:A:MET:HB3	1:50:A:ASP:HA	19	0.16
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	3	0.16
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	5	0.16
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	8	0.16
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	9	0.16
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	10	0.16
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	16	0.16
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	17	0.16
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	18	0.16
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	7	0.16
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	12	0.16
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	7	0.16
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	8	0.16
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	12	0.16
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	19	0.16
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	20	0.16
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	1	0.16
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	8	0.16
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	19	0.16
(1,1237)	1:106:A:ARG:HA	1:107:A:HIS:H	16	0.16
(1,1228)	1:112:A:LEU:HD11	1:112:A:LEU:H	1	0.16
(1,1228)	1:112:A:LEU:HD12	1:112:A:LEU:H	1	0.16
(1,1228)	1:112:A:LEU:HD13	1:112:A:LEU:H	1	0.16
(1,1228)	1:112:A:LEU:HD21	1:112:A:LEU:H	1	0.16
(1,1228)	1:112:A:LEU:HD22	1:112:A:LEU:H	1	0.16
(1,1228)	1:112:A:LEU:HD23	1:112:A:LEU:H	1	0.16
(1,1228)	1:112:A:LEU:HD11	1:112:A:LEU:H	9	0.16
(1,1228)	1:112:A:LEU:HD12	1:112:A:LEU:H	9	0.16
(1,1228)	1:112:A:LEU:HD13	1:112:A:LEU:H	9	0.16
(1,1228)	1:112:A:LEU:HD21	1:112:A:LEU:H	9	0.16
(1,1228)	1:112:A:LEU:HD22	1:112:A:LEU:H	9	0.16
(1,1228)	1:112:A:LEU:HD23	1:112:A:LEU:H	9	0.16
(1,1228)	1:112:A:LEU:HD11	1:112:A:LEU:H	11	0.16
(1,1228)	1:112:A:LEU:HD12	1:112:A:LEU:H	11	0.16
(1,1228)	1:112:A:LEU:HD13	1:112:A:LEU:H	11	0.16
(1,1228)	1:112:A:LEU:HD21	1:112:A:LEU:H	11	0.16
(1,1228)	1:112:A:LEU:HD22	1:112:A:LEU:H	11	0.16
(1,1228)	1:112:A:LEU:HD23	1:112:A:LEU:H	11	0.16
(1,1214)	1:48:A:LEU:HG	1:48:A:LEU:HA	10	0.16
(1,1204)	1:52:A:ILE:HG12	1:52:A:ILE:H	9	0.16
(1,1204)	1:52:A:ILE:HG13	1:52:A:ILE:H	9	0.16
(1,1190)	1:91:A:VAL:HG21	1:88:A:ALA:HA	18	0.16
(1,1190)	1:91:A:VAL:HG22	1:88:A:ALA:HA	18	0.16
(1,1190)	1:91:A:VAL:HG23	1:88:A:ALA:HA	18	0.16
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	9	0.16
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	16	0.16
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	17	0.16
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG21	6	0.16
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG22	6	0.16
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG23	6	0.16
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG21	6	0.16
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG22	6	0.16
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG23	6	0.16
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	6	0.16
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	6	0.16
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	14	0.16
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	14	0.16
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	18	0.16
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	18	0.16
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	1	0.16
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	5	0.16
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	7	0.16
(1,1164)	1:85:A:ILE:HB	1:82:A:GLU:H	16	0.16
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	1	0.16
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	2	0.16
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	3	0.16
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	11	0.16
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	13	0.16
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	15	0.16
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	16	0.16
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	18	0.16
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	3	0.16
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	3	0.16
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	3	0.16
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	11	0.16
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	11	0.16
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	11	0.16
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	18	0.16
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	18	0.16
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	18	0.16
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	19	0.16
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	19	0.16
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	19	0.16
(1,1149)	1:100:A:ILE:HG21	1:93:A:ASP:HB2	16	0.16
(1,1149)	1:100:A:ILE:HG22	1:93:A:ASP:HB2	16	0.16
(1,1149)	1:100:A:ILE:HG23	1:93:A:ASP:HB2	16	0.16
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	2	0.16
(1,1147)	1:49:A:GLN:HA	1:51:A:MET:H	10	0.16
(1,1143)	1:49:A:GLN:HA	1:52:A:ILE:H	2	0.16
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD11	15	0.16
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD12	15	0.16
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD13	15	0.16
(1,1114)	1:29:A:THR:HB	1:29:A:THR:H	10	0.16
(1,1114)	1:29:A:THR:HB	1:29:A:THR:H	15	0.16
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	1	0.16
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	13	0.16
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	16	0.16
(1,1107)	1:44:A:THR:HG21	1:44:A:THR:H	10	0.16
(1,1107)	1:44:A:THR:HG22	1:44:A:THR:H	10	0.16
(1,1107)	1:44:A:THR:HG23	1:44:A:THR:H	10	0.16
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	8	0.16
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	17	0.16
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	19	0.16
(1,1071)	1:106:A:ARG:HD3	1:107:A:HIS:H	12	0.16
(1,1067)	1:106:A:ARG:HD3	1:106:A:ARG:H	12	0.16
(1,1067)	1:106:A:ARG:HD3	1:106:A:ARG:H	14	0.16
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	5	0.16
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	7	0.16
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	11	0.16
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	12	0.16
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	15	0.16
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	18	0.16
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	5	0.16
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	14	0.16
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	16	0.16
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	18	0.16
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	8	0.16
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	11	0.16
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	12	0.16
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	10	0.16
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	4	0.16
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	4	0.16
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	4	0.16
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	4	0.16
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	4	0.16
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	4	0.16
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	6	0.16
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	6	0.16
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	6	0.16
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	6	0.16
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	6	0.16
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	6	0.16
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB2	17	0.16
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB3	17	0.16
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	1	0.16
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	12	0.16
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	14	0.16
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	14	0.16
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	14	0.16
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	18	0.16
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	18	0.16
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	19	0.16
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	19	0.16
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	19	0.16
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	10	0.16
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	14	0.16
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	15	0.16
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	8	0.16
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	8	0.16
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	8	0.16
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	17	0.16
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	17	0.16
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	17	0.16
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	20	0.16
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	20	0.16
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	20	0.16
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	10	0.16
(1,789)	1:52:A:ILE:HB	1:29:A:THR:HA	2	0.16
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	5	0.16
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	5	0.16
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	5	0.16
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	17	0.16
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	17	0.16
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	17	0.16
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	10	0.16
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	10	0.16
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	10	0.16
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	10	0.16
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	10	0.16
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	10	0.16
(1,766)	1:20:A:ASP:HA	1:26:A:THR:HB	12	0.16
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	6	0.16
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	6	0.16
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	6	0.16
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	6	0.16
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	6	0.16
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	6	0.16
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	7	0.16
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	7	0.16
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	7	0.16
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	7	0.16
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	7	0.16
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	19	0.16
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	19	0.16
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	19	0.16
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	19	0.16
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	19	0.16
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	19	0.16
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	1	0.16
(1,698)	1:121:A:VAL:HA	1:118:A:ASP:HA	9	0.16
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	19	0.16
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB2	9	0.16
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB3	9	0.16
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB2	13	0.16
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB3	13	0.16
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	2	0.16
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	2	0.16
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	20	0.16
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	20	0.16
(1,367)	1:31:A:GLU:HA	1:32:A:LEU:HG	6	0.16
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	1	0.16
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	3	0.16
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	17	0.16
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	18	0.16
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	20	0.16
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	1	0.16
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	9	0.16
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	3	0.16
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	3	0.16
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	15	0.16
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	15	0.16
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	18	0.16
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	18	0.16
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	19	0.16
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	19	0.16
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	3	0.16
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	3	0.16
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	3	0.16
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	3	0.16
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	3	0.16
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	3	0.16
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	3	0.16
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	3	0.16
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	9	0.16
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	9	0.16
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	9	0.16
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	9	0.16
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	9	0.16
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	9	0.16
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	9	0.16
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	9	0.16
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	9	0.16
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	19	0.16
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	19	0.16
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	19	0.16
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	19	0.16
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	19	0.16
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	19	0.16
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	19	0.16
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	19	0.16
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	19	0.16
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	11	0.16
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	11	0.16
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	11	0.16
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	11	0.16
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	11	0.16
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	11	0.16
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	15	0.16
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	15	0.16
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	15	0.16
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	15	0.16
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	15	0.16
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	15	0.16
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	2	0.15
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	10	0.15
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	20	0.15
(1,1429)	1:32:A:LEU:HB2	1:32:A:LEU:H	20	0.15
(1,1429)	1:32:A:LEU:HB3	1:32:A:LEU:H	20	0.15
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	1	0.15
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	2	0.15
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	4	0.15
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	7	0.15
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	11	0.15
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	13	0.15
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	17	0.15
(1,1411)	1:41:A:GLN:HB2	1:37:A:ARG:HA	5	0.15
(1,1411)	1:41:A:GLN:HB3	1:37:A:ARG:HA	5	0.15
(1,1410)	1:137:A:ASN:HB2	1:138:A:TYR:H	5	0.15
(1,1410)	1:137:A:ASN:HB3	1:138:A:TYR:H	5	0.15
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	6	0.15
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	11	0.15
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	12	0.15
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	20	0.15
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	20	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	2	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	3	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	4	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	5	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	7	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	8	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	9	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	12	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	13	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	14	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	15	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	16	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	17	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	18	0.15
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	20	0.15
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	1	0.15
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	4	0.15
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	8	0.15
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	10	0.15
(1,1304)	1:136:A:VAL:HB	1:136:A:VAL:H	3	0.15
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	2	0.15
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	2	0.15
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	11	0.15
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	11	0.15
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	13	0.15
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	13	0.15
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	9	0.15
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	20	0.15
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	1	0.15
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	15	0.15
(1,1294)	1:122:A:ASP:HA	1:125:A:ILE:H	13	0.15
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	11	0.15
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	18	0.15
(1,1277)	1:51:A:MET:HB2	1:50:A:ASP:HA	5	0.15
(1,1277)	1:51:A:MET:HB3	1:50:A:ASP:HA	5	0.15
(1,1277)	1:51:A:MET:HB2	1:50:A:ASP:HA	8	0.15
(1,1277)	1:51:A:MET:HB3	1:50:A:ASP:HA	8	0.15
(1,1277)	1:51:A:MET:HB2	1:50:A:ASP:HA	16	0.15
(1,1277)	1:51:A:MET:HB3	1:50:A:ASP:HA	16	0.15
(1,1276)	1:147:A:ALA:HA	1:147:A:ALA:H	15	0.15
(1,1273)	1:94:A:LYS:HG2	1:94:A:LYS:H	3	0.15
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	1	0.15
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	14	0.15
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	15	0.15
(1,1249)	1:67:A:GLU:HA	1:67:A:GLU:H	6	0.15
(1,1249)	1:67:A:GLU:HA	1:67:A:GLU:H	13	0.15
(1,1249)	1:67:A:GLU:HA	1:67:A:GLU:H	17	0.15
(1,1249)	1:67:A:GLU:HA	1:67:A:GLU:H	19	0.15
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	1	0.15
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	2	0.15
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	7	0.15
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	9	0.15
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	10	0.15
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	13	0.15
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	15	0.15
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	16	0.15
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	17	0.15
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	19	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	2	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	3	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	4	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	5	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	6	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	7	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	9	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	10	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	11	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	12	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	15	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	16	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	17	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	18	0.15
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1216)	1:144:A:MET:HA	1:144:A:MET:HG2	13	0.15
(1,1216)	1:144:A:MET:HA	1:144:A:MET:HG3	13	0.15
(1,1190)	1:91:A:VAL:HG21	1:88:A:ALA:HA	1	0.15
(1,1190)	1:91:A:VAL:HG22	1:88:A:ALA:HA	1	0.15
(1,1190)	1:91:A:VAL:HG23	1:88:A:ALA:HA	1	0.15
(1,1190)	1:91:A:VAL:HG21	1:88:A:ALA:HA	14	0.15
(1,1190)	1:91:A:VAL:HG22	1:88:A:ALA:HA	14	0.15
(1,1190)	1:91:A:VAL:HG23	1:88:A:ALA:HA	14	0.15
(1,1186)	1:128:A:ALA:HA	1:128:A:ALA:H	7	0.15
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	6	0.15
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	15	0.15
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	18	0.15
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	20	0.15
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	3	0.15
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	3	0.15
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	15	0.15
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	15	0.15
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	16	0.15
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	16	0.15
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	19	0.15
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	19	0.15
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	20	0.15
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	20	0.15
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	5	0.15
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	5	0.15
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	4	0.15
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	6	0.15
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	9	0.15
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	5	0.15
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	5	0.15
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	5	0.15
(1,1149)	1:100:A:ILE:HG21	1:93:A:ASP:HB2	10	0.15
(1,1149)	1:100:A:ILE:HG22	1:93:A:ASP:HB2	10	0.15
(1,1149)	1:100:A:ILE:HG23	1:93:A:ASP:HB2	10	0.15
(1,1149)	1:100:A:ILE:HG21	1:93:A:ASP:HB2	15	0.15
(1,1149)	1:100:A:ILE:HG22	1:93:A:ASP:HB2	15	0.15
(1,1149)	1:100:A:ILE:HG23	1:93:A:ASP:HB2	15	0.15
(1,1111)	1:36:A:MET:HA	1:39:A:LEU:HB2	9	0.15
(1,1111)	1:36:A:MET:HA	1:39:A:LEU:HB3	9	0.15
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	8	0.15
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	10	0.15
(1,1107)	1:44:A:THR:HG21	1:44:A:THR:H	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	1:44:A:THR:HG22	1:44:A:THR:H	5	0.15
(1,1107)	1:44:A:THR:HG23	1:44:A:THR:H	5	0.15
(1,1106)	1:44:A:THR:HG21	1:45:A:GLU:H	7	0.15
(1,1106)	1:44:A:THR:HG22	1:45:A:GLU:H	7	0.15
(1,1106)	1:44:A:THR:HG23	1:45:A:GLU:H	7	0.15
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	6	0.15
(1,1067)	1:106:A:ARG:HD3	1:106:A:ARG:H	17	0.15
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	6	0.15
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	14	0.15
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	19	0.15
(1,1058)	1:121:A:VAL:HG11	1:124:A:MET:HA	2	0.15
(1,1058)	1:121:A:VAL:HG12	1:124:A:MET:HA	2	0.15
(1,1058)	1:121:A:VAL:HG13	1:124:A:MET:HA	2	0.15
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	3	0.15
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	4	0.15
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	8	0.15
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	11	0.15
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	13	0.15
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	13	0.15
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	20	0.15
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG2	9	0.15
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG3	9	0.15
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	13	0.15
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	19	0.15
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	16	0.15
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	18	0.15
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	2	0.15
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	2	0.15
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	2	0.15
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	2	0.15
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	2	0.15
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	2	0.15
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	9	0.15
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	9	0.15
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	9	0.15
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	9	0.15
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	9	0.15
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	9	0.15
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	16	0.15
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	16	0.15
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	16	0.15
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	16	0.15
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	16	0.15
(1,1000)	1:103:A:ALA:HA	1:104:A:GLU:HB2	1	0.15
(1,1000)	1:103:A:ALA:HA	1:104:A:GLU:HB3	1	0.15
(1,994)	1:29:A:THR:HA	1:30:A:LYS:H	5	0.15
(1,994)	1:29:A:THR:HA	1:30:A:LYS:H	12	0.15
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB2	20	0.15
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB3	20	0.15
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	1	0.15
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	6	0.15
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	2	0.15
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	8	0.15
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	8	0.15
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	8	0.15
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	1	0.15
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	9	0.15
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	11	0.15
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	13	0.15
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	19	0.15
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	4	0.15
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	19	0.15
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	6	0.15
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	6	0.15
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	6	0.15
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	4	0.15
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	4	0.15
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	4	0.15
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	4	0.15
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	4	0.15
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	4	0.15
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	9	0.15
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	9	0.15
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	9	0.15
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	9	0.15
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	9	0.15
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	9	0.15
(1,766)	1:20:A:ASP:HA	1:26:A:THR:HB	18	0.15
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	1	0.15
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	5	0.15
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	8	0.15
(1,759)	1:26:A:THR:HG21	1:62:A:THR:HA	16	0.15
(1,759)	1:26:A:THR:HG22	1:62:A:THR:HA	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,759)	1:26:A:THR:HG23	1:62:A:THR:HA	16	0.15
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	4	0.15
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	16	0.15
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	7	0.15
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	7	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	3	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	3	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	3	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	3	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	3	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	3	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	4	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	4	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	4	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	4	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	4	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	4	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	5	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	5	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	5	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	5	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	5	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	5	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	13	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	13	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	13	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	13	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	13	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	13	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB1	16	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB2	16	0.15
(1,736)	1:71:A:MET:HB2	1:73:A:ALA:HB3	16	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB1	16	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB2	16	0.15
(1,736)	1:71:A:MET:HB3	1:73:A:ALA:HB3	16	0.15
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	1	0.15
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	12	0.15
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	13	0.15
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG2	3	0.15
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG3	3	0.15
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG2	3	0.15
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG3	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG2	3	0.15
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG3	3	0.15
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB2	10	0.15
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB3	10	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	1	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	1	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	3	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	3	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	4	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	4	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	5	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	5	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	6	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	6	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	7	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	7	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	8	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	8	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	9	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	9	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	12	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	12	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	13	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	13	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	14	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	14	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	18	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	18	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	19	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	19	0.15
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	20	0.15
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	20	0.15
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	10	0.15
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	10	0.15
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	17	0.15
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	17	0.15
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	10	0.15
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	10	0.15
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	19	0.15
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	19	0.15
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	1	0.15
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	1	0.15
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	2	0.15
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	2	0.15
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	2	0.15
(1,367)	1:31:A:GLU:HA	1:32:A:LEU:HG	19	0.15
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	18	0.15
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	5	0.15
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	12	0.15
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	15	0.15
(1,313)	1:26:A:THR:HA	1:16:A:PHE:HZ	6	0.15
(1,130)	1:34:A:THR:HB	1:31:A:GLU:H	14	0.15
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	11	0.15
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	2	0.15
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	4	0.15
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	10	0.15
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	14	0.15
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	2	0.15
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	2	0.15
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	5	0.15
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	5	0.15
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	12	0.15
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	12	0.15
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	7	0.15
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	7	0.15
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	7	0.15
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	7	0.15
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	7	0.15
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	7	0.15
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	7	0.15
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	7	0.15
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	7	0.15
(1,11)	1:27:A:ILE:HD11	1:28:A:THR:HB	1	0.15
(1,11)	1:27:A:ILE:HD12	1:28:A:THR:HB	1	0.15
(1,11)	1:27:A:ILE:HD13	1:28:A:THR:HB	1	0.15
(1,11)	1:27:A:ILE:HD11	1:28:A:THR:HB	8	0.15
(1,11)	1:27:A:ILE:HD12	1:28:A:THR:HB	8	0.15
(1,11)	1:27:A:ILE:HD13	1:28:A:THR:HB	8	0.15
(1,11)	1:27:A:ILE:HD11	1:28:A:THR:HB	17	0.15
(1,11)	1:27:A:ILE:HD12	1:28:A:THR:HB	17	0.15
(1,11)	1:27:A:ILE:HD13	1:28:A:THR:HB	17	0.15
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	2	0.15
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	2	0.15
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	2	0.15
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	2	0.15
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	2	0.15
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	3	0.15
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	3	0.15
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	3	0.15
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	3	0.15
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	3	0.15
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	3	0.15
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	16	0.15
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	16	0.15
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	16	0.15
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	16	0.15
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	16	0.15
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	16	0.15
(1,1460)	1:88:A:ALA:HA	1:89:A:PHE:H	4	0.14
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	7	0.14
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	13	0.14
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	5	0.14
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	14	0.14
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	18	0.14
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	6	0.14
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	8	0.14
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	11	0.14
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	19	0.14
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	20	0.14
(1,1441)	1:61:A:GLY:HA3	1:52:A:ILE:HG21	7	0.14
(1,1441)	1:61:A:GLY:HA3	1:52:A:ILE:HG22	7	0.14
(1,1441)	1:61:A:GLY:HA3	1:52:A:ILE:HG23	7	0.14
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	4	0.14
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	4	0.14
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	6	0.14
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	6	0.14
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	6	0.14
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	12	0.14
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	15	0.14
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	1	0.14
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	5	0.14
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	6	0.14
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	7	0.14
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	11	0.14
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	12	0.14
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	17	0.14
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	19	0.14
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	2	0.14
(1,1411)	1:41:A:GLN:HB2	1:37:A:ARG:HA	12	0.14
(1,1411)	1:41:A:GLN:HB3	1:37:A:ARG:HA	12	0.14
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	18	0.14
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	18	0.14
(1,1397)	1:111:A:ASN:HB3	1:111:A:ASN:H	13	0.14
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	6	0.14
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	11	0.14
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	4	0.14
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	7	0.14
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	9	0.14
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	10	0.14
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	14	0.14
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	16	0.14
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	17	0.14
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	19	0.14
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	6	0.14
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	11	0.14
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	19	0.14
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	1	0.14
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	6	0.14
(1,1362)	1:76:A:MET:HA	1:76:A:MET:H	11	0.14
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	5	0.14
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	6	0.14
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	12	0.14
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	15	0.14
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	5	0.14
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	5	0.14
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	5	0.14
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	5	0.14
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	5	0.14
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	5	0.14
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	7	0.14
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	7	0.14
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	7	0.14
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	7	0.14
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	7	0.14
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	2	0.14
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	13	0.14
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	16	0.14
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	11	0.14
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	12	0.14
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	14	0.14
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	20	0.14
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	15	0.14
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	15	0.14
(1,1304)	1:136:A:VAL:HB	1:136:A:VAL:H	1	0.14
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	1	0.14
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	1	0.14
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	3	0.14
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	3	0.14
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	5	0.14
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	5	0.14
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	12	0.14
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	12	0.14
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	2	0.14
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	3	0.14
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	5	0.14
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	10	0.14
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	13	0.14
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	14	0.14
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	15	0.14
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	16	0.14
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	17	0.14
(1,1300)	1:80:A:ASP:HA	1:80:A:ASP:H	18	0.14
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	6	0.14
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	11	0.14
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	19	0.14
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	4	0.14
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	9	0.14
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	13	0.14
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	16	0.14
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	3	0.14
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	10	0.14
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	12	0.14
(1,1277)	1:51:A:MET:HB2	1:50:A:ASP:HA	6	0.14
(1,1277)	1:51:A:MET:HB3	1:50:A:ASP:HA	6	0.14
(1,1273)	1:94:A:LYS:HG2	1:94:A:LYS:H	13	0.14
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	10	0.14
(1,1252)	1:48:A:LEU:HA	1:48:A:LEU:H	1	0.14
(1,1249)	1:67:A:GLU:HA	1:67:A:GLU:H	1	0.14
(1,1249)	1:67:A:GLU:HA	1:67:A:GLU:H	5	0.14
(1,1249)	1:67:A:GLU:HA	1:67:A:GLU:H	18	0.14
(1,1247)	1:77:A:LYS:HA	1:77:A:LYS:H	11	0.14
(1,1246)	1:77:A:LYS:HA	1:78:A:ASP:H	8	0.14
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	1	0.14
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	3	0.14
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	4	0.14
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	5	0.14
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	6	0.14
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	8	0.14
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	11	0.14
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	12	0.14
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	14	0.14
(1,1240)	1:88:A:ALA:HA	1:88:A:ALA:H	18	0.14
(1,1238)	1:104:A:GLU:HA	1:104:A:GLU:H	13	0.14
(1,1204)	1:52:A:ILE:HG12	1:52:A:ILE:H	2	0.14
(1,1204)	1:52:A:ILE:HG13	1:52:A:ILE:H	2	0.14
(1,1204)	1:52:A:ILE:HG12	1:52:A:ILE:H	8	0.14
(1,1204)	1:52:A:ILE:HG13	1:52:A:ILE:H	8	0.14
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	2	0.14
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	2	0.14
(1,1182)	1:101:A:SER:HB2	1:102:A:ALA:H	11	0.14
(1,1182)	1:101:A:SER:HB3	1:102:A:ALA:H	11	0.14
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	11	0.14
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	13	0.14
(1,1168)	1:85:A:ILE:HB	1:82:A:GLU:HA	8	0.14
(1,1168)	1:85:A:ILE:HB	1:82:A:GLU:HA	19	0.14
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	12	0.14
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	6	0.14
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	6	0.14
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	6	0.14
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	17	0.14
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	17	0.14
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	17	0.14
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	20	0.14
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	20	0.14
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	20	0.14
(1,1149)	1:100:A:ILE:HG21	1:93:A:ASP:HB2	3	0.14
(1,1149)	1:100:A:ILE:HG22	1:93:A:ASP:HB2	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1149)	1:100:A:ILE:HG23	1:93:A:ASP:HB2	3	0.14
(1,1149)	1:100:A:ILE:HG21	1:93:A:ASP:HB2	5	0.14
(1,1149)	1:100:A:ILE:HG22	1:93:A:ASP:HB2	5	0.14
(1,1149)	1:100:A:ILE:HG23	1:93:A:ASP:HB2	5	0.14
(1,1138)	1:34:A:THR:HA	1:37:A:ARG:H	9	0.14
(1,1118)	1:29:A:THR:HB	1:28:A:THR:HA	13	0.14
(1,1109)	1:36:A:MET:HA	1:37:A:ARG:H	20	0.14
(1,1103)	1:48:A:LEU:HD11	1:48:A:LEU:HA	10	0.14
(1,1103)	1:48:A:LEU:HD12	1:48:A:LEU:HA	10	0.14
(1,1103)	1:48:A:LEU:HD13	1:48:A:LEU:HA	10	0.14
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	1	0.14
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	5	0.14
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	2	0.14
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	10	0.14
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	13	0.14
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	16	0.14
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	20	0.14
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	9	0.14
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	10	0.14
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	12	0.14
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	14	0.14
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	17	0.14
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	18	0.14
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	20	0.14
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	3	0.14
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	4	0.14
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	11	0.14
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	8	0.14
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG2	16	0.14
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG3	16	0.14
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	1	0.14
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	5	0.14
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	19	0.14
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	5	0.14
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	5	0.14
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	5	0.14
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	5	0.14
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	5	0.14
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	5	0.14
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	10	0.14
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	10	0.14
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	10	0.14
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	10	0.14
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	10	0.14
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB2	14	0.14
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB3	14	0.14
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	14	0.14
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	15	0.14
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	19	0.14
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	6	0.14
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	6	0.14
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	12	0.14
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	12	0.14
(1,940)	1:54:A:GLU:HA	1:55:A:VAL:H	15	0.14
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	19	0.14
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	19	0.14
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	19	0.14
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	5	0.14
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	6	0.14
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	17	0.14
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	18	0.14
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	6	0.14
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	6	0.14
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	6	0.14
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	10	0.14
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	10	0.14
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	10	0.14
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	16	0.14
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	16	0.14
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	16	0.14
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	2	0.14
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	3	0.14
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	8	0.14
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	9	0.14
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	11	0.14
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	15	0.14
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	16	0.14
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	18	0.14
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG12	1	0.14
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG13	1	0.14
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	2	0.14
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	2	0.14
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	9	0.14
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	9	0.14
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	9	0.14
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	12	0.14
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	12	0.14
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	12	0.14
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	12	0.14
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	12	0.14
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	12	0.14
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	18	0.14
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	18	0.14
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	18	0.14
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	18	0.14
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	18	0.14
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	18	0.14
(1,766)	1:20:A:ASP:HA	1:26:A:THR:HB	1	0.14
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	11	0.14
(1,759)	1:26:A:THR:HG21	1:62:A:THR:HA	14	0.14
(1,759)	1:26:A:THR:HG22	1:62:A:THR:HA	14	0.14
(1,759)	1:26:A:THR:HG23	1:62:A:THR:HA	14	0.14
(1,749)	1:55:A:VAL:HA	1:56:A:ASP:H	9	0.14
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	17	0.14
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	17	0.14
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	10	0.14
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	10	0.14
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	11	0.14
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	11	0.14
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	15	0.14
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	15	0.14
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	16	0.14
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	16	0.14
(1,642)	1:13:A:LYS:HB2	1:12:A:PHE:HA	17	0.14
(1,642)	1:13:A:LYS:HB3	1:12:A:PHE:HA	17	0.14
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	1	0.14
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	1	0.14
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	5	0.14
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	5	0.14
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	13	0.14
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	13	0.14
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	18	0.14
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	18	0.14
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	19	0.14
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	6	0.14
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	6	0.14
(1,590)	1:27:A:ILE:HA	1:63:A:ILE:H	20	0.14
(1,497)	1:114:A:GLU:HB2	1:21:A:LYS:HG2	4	0.14
(1,497)	1:114:A:GLU:HB3	1:21:A:LYS:HG2	4	0.14
(1,497)	1:114:A:GLU:HB2	1:21:A:LYS:HG2	20	0.14
(1,497)	1:114:A:GLU:HB3	1:21:A:LYS:HG2	20	0.14
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	6	0.14
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	6	0.14
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	6	0.14
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	12	0.14
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	12	0.14
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	12	0.14
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	19	0.14
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	19	0.14
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	19	0.14
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	6	0.14
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	6	0.14
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	7	0.14
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	7	0.14
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	15	0.14
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	15	0.14
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	19	0.14
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	19	0.14
(1,476)	1:142:A:VAL:HG11	1:141:A:PHE:HA	15	0.14
(1,476)	1:142:A:VAL:HG12	1:141:A:PHE:HA	15	0.14
(1,476)	1:142:A:VAL:HG13	1:141:A:PHE:HA	15	0.14
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	6	0.14
(1,130)	1:34:A:THR:HB	1:31:A:GLU:H	11	0.14
(1,130)	1:34:A:THR:HB	1:31:A:GLU:H	12	0.14
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	19	0.14
(1,97)	1:44:A:THR:HA	1:46:A:ALA:HA	13	0.14
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	15	0.14
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	15	0.14
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	15	0.14
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	15	0.14
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	15	0.14
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	15	0.14
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	15	0.14
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	15	0.14
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	20	0.14
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	20	0.14
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	20	0.14
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	20	0.14
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	20	0.14
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	20	0.14
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	20	0.14
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	20	0.14
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	20	0.14
(1,11)	1:27:A:ILE:HD11	1:28:A:THR:HB	5	0.14
(1,11)	1:27:A:ILE:HD12	1:28:A:THR:HB	5	0.14
(1,11)	1:27:A:ILE:HD13	1:28:A:THR:HB	5	0.14
(1,11)	1:27:A:ILE:HD11	1:28:A:THR:HB	6	0.14
(1,11)	1:27:A:ILE:HD12	1:28:A:THR:HB	6	0.14
(1,11)	1:27:A:ILE:HD13	1:28:A:THR:HB	6	0.14
(1,11)	1:27:A:ILE:HD11	1:28:A:THR:HB	14	0.14
(1,11)	1:27:A:ILE:HD12	1:28:A:THR:HB	14	0.14
(1,11)	1:27:A:ILE:HD13	1:28:A:THR:HB	14	0.14
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	20	0.14
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	20	0.14
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	20	0.14
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	20	0.14
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	20	0.14
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	20	0.14
(1,1460)	1:88:A:ALA:HA	1:89:A:PHE:H	19	0.13
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	19	0.13
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	2	0.13
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	7	0.13
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	11	0.13
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	12	0.13
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	2	0.13
(1,1437)	1:91:A:VAL:HB	1:92:A:PHE:H	6	0.13
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	12	0.13
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	12	0.13
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	20	0.13
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	20	0.13
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	3	0.13
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	8	0.13
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	14	0.13
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	2	0.13
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	3	0.13
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	9	0.13
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	13	0.13
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	14	0.13
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	15	0.13
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	16	0.13
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	18	0.13
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	20	0.13
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	5	0.13
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	8	0.13
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	20	0.13
(1,1411)	1:41:A:GLN:HB2	1:37:A:ARG:HA	2	0.13
(1,1411)	1:41:A:GLN:HB3	1:37:A:ARG:HA	2	0.13
(1,1411)	1:41:A:GLN:HB2	1:37:A:ARG:HA	4	0.13
(1,1411)	1:41:A:GLN:HB3	1:37:A:ARG:HA	4	0.13
(1,1411)	1:41:A:GLN:HB2	1:37:A:ARG:HA	15	0.13
(1,1411)	1:41:A:GLN:HB3	1:37:A:ARG:HA	15	0.13
(1,1411)	1:41:A:GLN:HB2	1:37:A:ARG:HA	16	0.13
(1,1411)	1:41:A:GLN:HB3	1:37:A:ARG:HA	16	0.13
(1,1397)	1:111:A:ASN:HB3	1:111:A:ASN:H	9	0.13
(1,1397)	1:111:A:ASN:HB3	1:111:A:ASN:H	10	0.13
(1,1370)	1:58:A:ASP:HA	1:57:A:ALA:H	6	0.13
(1,1370)	1:58:A:ASP:HA	1:57:A:ALA:H	13	0.13
(1,1370)	1:58:A:ASP:HA	1:57:A:ALA:H	19	0.13
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	1	0.13
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	7	0.13
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	19	0.13
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	2	0.13
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	3	0.13
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	6	0.13
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	8	0.13
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	12	0.13
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	18	0.13
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	20	0.13
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	12	0.13
(1,1366)	1:70:A:THR:HA	1:73:A:ALA:HA	15	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	1	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	2	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	3	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	4	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	6	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	7	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	9	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	10	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	11	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	12	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	13	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	14	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	15	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	16	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	17	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	18	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	19	0.13
(1,1358)	1:87:A:GLU:HA	1:87:A:GLU:H	20	0.13
(1,1351)	1:110:A:THR:HG21	1:110:A:THR:H	10	0.13
(1,1351)	1:110:A:THR:HG22	1:110:A:THR:H	10	0.13
(1,1351)	1:110:A:THR:HG23	1:110:A:THR:H	10	0.13
(1,1351)	1:110:A:THR:HG21	1:110:A:THR:H	13	0.13
(1,1351)	1:110:A:THR:HG22	1:110:A:THR:H	13	0.13
(1,1351)	1:110:A:THR:HG23	1:110:A:THR:H	13	0.13
(1,1351)	1:110:A:THR:HG21	1:110:A:THR:H	17	0.13
(1,1351)	1:110:A:THR:HG22	1:110:A:THR:H	17	0.13
(1,1351)	1:110:A:THR:HG23	1:110:A:THR:H	17	0.13
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	2	0.13
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	7	0.13
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	9	0.13
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	19	0.13
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	3	0.13
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	4	0.13
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	9	0.13
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	11	0.13
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	1	0.13
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	1	0.13
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	1	0.13
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	1	0.13
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	1	0.13
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	1	0.13
(1,1321)	1:61:A:GLY:HA2	1:60:A:ASN:HA	1	0.13
(1,1321)	1:61:A:GLY:HA2	1:60:A:ASN:HA	13	0.13
(1,1320)	1:33:A:GLY:HA2	1:34:A:THR:H	4	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	1	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	1	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	2	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	3	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	3	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	4	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	4	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	5	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	5	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	7	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	7	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	8	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	8	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	9	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	9	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	10	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	10	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	11	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	11	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	12	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	12	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	13	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	13	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	14	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	14	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	16	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	16	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	17	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	17	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	18	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	18	0.13
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	20	0.13
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	20	0.13
(1,1304)	1:136:A:VAL:HB	1:136:A:VAL:H	13	0.13
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	19	0.13
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	19	0.13
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	5	0.13
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	7	0.13
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	8	0.13
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	9	0.13
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	13	0.13
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	16	0.13
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	17	0.13
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	20	0.13
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	2	0.13
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	3	0.13
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	8	0.13
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	10	0.13
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	15	0.13
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	20	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	1	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	2	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	3	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	4	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	5	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	6	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	7	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	8	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	9	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	10	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	12	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	13	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	14	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	15	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	16	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	17	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	18	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	19	0.13
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	20	0.13
(1,1252)	1:48:A:LEU:HA	1:48:A:LEU:H	3	0.13
(1,1252)	1:48:A:LEU:HA	1:48:A:LEU:H	8	0.13
(1,1252)	1:48:A:LEU:HA	1:48:A:LEU:H	20	0.13
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	5	0.13
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	6	0.13
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	16	0.13
(1,1216)	1:144:A:MET:HA	1:144:A:MET:HG2	1	0.13
(1,1216)	1:144:A:MET:HA	1:144:A:MET:HG3	1	0.13
(1,1216)	1:144:A:MET:HA	1:144:A:MET:HG2	7	0.13
(1,1216)	1:144:A:MET:HA	1:144:A:MET:HG3	7	0.13
(1,1204)	1:52:A:ILE:HG12	1:52:A:ILE:H	3	0.13
(1,1204)	1:52:A:ILE:HG13	1:52:A:ILE:H	3	0.13
(1,1190)	1:91:A:VAL:HG21	1:88:A:ALA:HA	4	0.13
(1,1190)	1:91:A:VAL:HG22	1:88:A:ALA:HA	4	0.13
(1,1190)	1:91:A:VAL:HG23	1:88:A:ALA:HA	4	0.13
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	10	0.13
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG21	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG22	16	0.13
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG23	16	0.13
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG21	16	0.13
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG22	16	0.13
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG23	16	0.13
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG21	18	0.13
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG22	18	0.13
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG23	18	0.13
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG21	18	0.13
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG22	18	0.13
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG23	18	0.13
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	6	0.13
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	6	0.13
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	2	0.13
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	3	0.13
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	4	0.13
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	8	0.13
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	10	0.13
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	11	0.13
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	12	0.13
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	13	0.13
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	15	0.13
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	17	0.13
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	20	0.13
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	3	0.13
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	10	0.13
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	10	0.13
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	10	0.13
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	13	0.13
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	13	0.13
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	13	0.13
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	15	0.13
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	15	0.13
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	15	0.13
(1,1149)	1:100:A:ILE:HG21	1:93:A:ASP:HB2	2	0.13
(1,1149)	1:100:A:ILE:HG22	1:93:A:ASP:HB2	2	0.13
(1,1149)	1:100:A:ILE:HG23	1:93:A:ASP:HB2	2	0.13
(1,1138)	1:34:A:THR:HA	1:37:A:ARG:H	10	0.13
(1,1138)	1:34:A:THR:HA	1:37:A:ARG:H	15	0.13
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD11	18	0.13
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD12	18	0.13
(1,1119)	1:29:A:THR:HB	1:48:A:LEU:HD13	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	11	0.13
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	11	0.13
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	14	0.13
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	14	0.13
(1,1096)	1:55:A:VAL:HG21	1:71:A:MET:HB2	7	0.13
(1,1096)	1:55:A:VAL:HG21	1:71:A:MET:HB3	7	0.13
(1,1096)	1:55:A:VAL:HG22	1:71:A:MET:HB2	7	0.13
(1,1096)	1:55:A:VAL:HG22	1:71:A:MET:HB3	7	0.13
(1,1096)	1:55:A:VAL:HG23	1:71:A:MET:HB2	7	0.13
(1,1096)	1:55:A:VAL:HG23	1:71:A:MET:HB3	7	0.13
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	3	0.13
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	20	0.13
(1,1066)	1:110:A:THR:HA	1:116:A:LEU:H	8	0.13
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	9	0.13
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	2	0.13
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	5	0.13
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	6	0.13
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	15	0.13
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	16	0.13
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	19	0.13
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	12	0.13
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	15	0.13
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG2	17	0.13
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG3	17	0.13
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	6	0.13
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	7	0.13
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	17	0.13
(1,1012)	1:63:A:ILE:HA	1:56:A:ASP:HA	4	0.13
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	12	0.13
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	12	0.13
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	12	0.13
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	12	0.13
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	12	0.13
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	12	0.13
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	13	0.13
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	13	0.13
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	13	0.13
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	13	0.13
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	13	0.13
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	13	0.13
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB2	1	0.13
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB3	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB2	7	0.13
(1,993)	1:29:A:THR:HA	1:30:A:LYS:HB3	7	0.13
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	12	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	1	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	1	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	2	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	2	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	3	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	3	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	4	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	4	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	5	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	5	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	7	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	7	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	8	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	8	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	9	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	9	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	10	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	10	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	11	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	11	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	13	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	13	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	14	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	14	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	15	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	15	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	16	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	16	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	17	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	17	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	18	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	18	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	19	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	19	0.13
(1,950)	1:16:A:PHE:HB2	1:16:A:PHE:HZ	20	0.13
(1,950)	1:16:A:PHE:HB3	1:16:A:PHE:HZ	20	0.13
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	12	0.13
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	12	0.13
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	3	0.13
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	3	0.13
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	3	0.13
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	6	0.13
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	6	0.13
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	6	0.13
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	3	0.13
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	4	0.13
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	8	0.13
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	16	0.13
(1,899)	1:125:A:ILE:HG12	1:122:A:ASP:HA	19	0.13
(1,899)	1:125:A:ILE:HG13	1:122:A:ASP:HA	19	0.13
(1,898)	1:125:A:ILE:HG12	1:134:A:GLY:HA2	7	0.13
(1,898)	1:125:A:ILE:HG13	1:134:A:GLY:HA2	7	0.13
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	2	0.13
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	2	0.13
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	2	0.13
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	7	0.13
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	7	0.13
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	7	0.13
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	9	0.13
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	9	0.13
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	9	0.13
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	18	0.13
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	18	0.13
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	18	0.13
(1,840)	1:39:A:LEU:HD21	1:39:A:LEU:HA	11	0.13
(1,840)	1:39:A:LEU:HD22	1:39:A:LEU:HA	11	0.13
(1,840)	1:39:A:LEU:HD23	1:39:A:LEU:HA	11	0.13
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	7	0.13
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	13	0.13
(1,832)	1:64:A:ASP:HA	1:27:A:ILE:H	17	0.13
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	1	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	1	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	2	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	3	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	4	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	5	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	6	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	7	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	8	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	12	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	13	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	14	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	17	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	19	0.13
(1,794)	1:57:A:ALA:HA	1:58:A:ASP:H	20	0.13
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG12	5	0.13
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG13	5	0.13
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG12	12	0.13
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG13	12	0.13
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	13	0.13
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	13	0.13
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	13	0.13
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	18	0.13
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	18	0.13
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	18	0.13
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	1	0.13
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	1	0.13
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	1	0.13
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	1	0.13
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	1	0.13
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	1	0.13
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	14	0.13
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	14	0.13
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	14	0.13
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	14	0.13
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	14	0.13
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	14	0.13
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	13	0.13
(1,759)	1:26:A:THR:HG21	1:62:A:THR:HA	2	0.13
(1,759)	1:26:A:THR:HG22	1:62:A:THR:HA	2	0.13
(1,759)	1:26:A:THR:HG23	1:62:A:THR:HA	2	0.13
(1,759)	1:26:A:THR:HG21	1:62:A:THR:HA	4	0.13
(1,759)	1:26:A:THR:HG22	1:62:A:THR:HA	4	0.13
(1,759)	1:26:A:THR:HG23	1:62:A:THR:HA	4	0.13
(1,759)	1:26:A:THR:HG21	1:62:A:THR:HA	10	0.13
(1,759)	1:26:A:THR:HG22	1:62:A:THR:HA	10	0.13
(1,759)	1:26:A:THR:HG23	1:62:A:THR:HA	10	0.13
(1,759)	1:26:A:THR:HG21	1:62:A:THR:HA	12	0.13
(1,759)	1:26:A:THR:HG22	1:62:A:THR:HA	12	0.13
(1,759)	1:26:A:THR:HG23	1:62:A:THR:HA	12	0.13
(1,749)	1:55:A:VAL:HA	1:56:A:ASP:H	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	16	0.13
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	16	0.13
(1,699)	1:121:A:VAL:HA	1:125:A:ILE:HG12	7	0.13
(1,699)	1:121:A:VAL:HA	1:125:A:ILE:HG13	7	0.13
(1,680)	1:27:A:ILE:HB	1:63:A:ILE:H	3	0.13
(1,680)	1:27:A:ILE:HB	1:63:A:ILE:H	10	0.13
(1,675)	1:27:A:ILE:HB	1:26:A:THR:HA	14	0.13
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG2	6	0.13
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG3	6	0.13
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG2	6	0.13
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG3	6	0.13
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG2	6	0.13
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG3	6	0.13
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG2	16	0.13
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG3	16	0.13
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG2	16	0.13
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG3	16	0.13
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG2	16	0.13
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG3	16	0.13
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG2	19	0.13
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG3	19	0.13
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG2	19	0.13
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG3	19	0.13
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG2	19	0.13
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG3	19	0.13
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB2	18	0.13
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB3	18	0.13
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	11	0.13
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	11	0.13
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	1	0.13
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	1	0.13
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	2	0.13
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	2	0.13
(1,503)	1:110:A:THR:HB	1:112:A:LEU:H	15	0.13
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	8	0.13
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	8	0.13
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	8	0.13
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	1	0.13
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	1	0.13
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	5	0.13
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	5	0.13
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	10	0.13
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	14	0.13
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	14	0.13
(1,476)	1:142:A:VAL:HG11	1:141:A:PHE:HA	8	0.13
(1,476)	1:142:A:VAL:HG12	1:141:A:PHE:HA	8	0.13
(1,476)	1:142:A:VAL:HG13	1:141:A:PHE:HA	8	0.13
(1,367)	1:31:A:GLU:HA	1:32:A:LEU:HG	20	0.13
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	7	0.13
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	8	0.13
(1,222)	1:19:A:PHE:HA	1:31:A:GLU:HB2	8	0.13
(1,222)	1:19:A:PHE:HA	1:31:A:GLU:HB3	8	0.13
(1,151)	1:107:A:HIS:HA	1:94:A:LYS:HG3	8	0.13
(1,130)	1:34:A:THR:HB	1:31:A:GLU:H	6	0.13
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	1	0.13
(1,101)	1:44:A:THR:HA	1:47:A:GLU:HA	18	0.13
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	4	0.13
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	4	0.13
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	10	0.13
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	10	0.13
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	13	0.13
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	13	0.13
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	2	0.13
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	2	0.13
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	2	0.13
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	2	0.13
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	2	0.13
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	2	0.13
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	2	0.13
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	2	0.13
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	2	0.13
(1,11)	1:27:A:ILE:HD11	1:28:A:THR:HB	12	0.13
(1,11)	1:27:A:ILE:HD12	1:28:A:THR:HB	12	0.13
(1,11)	1:27:A:ILE:HD13	1:28:A:THR:HB	12	0.13
(1,11)	1:27:A:ILE:HD11	1:28:A:THR:HB	20	0.13
(1,11)	1:27:A:ILE:HD12	1:28:A:THR:HB	20	0.13
(1,11)	1:27:A:ILE:HD13	1:28:A:THR:HB	20	0.13
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	10	0.13
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	10	0.13
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	10	0.13
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	10	0.13
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	10	0.13
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1460)	1:88:A:ALA:HA	1:89:A:PHE:H	1	0.12
(1,1460)	1:88:A:ALA:HA	1:89:A:PHE:H	14	0.12
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	1	0.12
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	4	0.12
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	9	0.12
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	10	0.12
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	20	0.12
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	1	0.12
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	3	0.12
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	4	0.12
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	19	0.12
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	4	0.12
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	5	0.12
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	10	0.12
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	15	0.12
(1,1441)	1:61:A:GLY:HA3	1:52:A:ILE:HG21	3	0.12
(1,1441)	1:61:A:GLY:HA3	1:52:A:ILE:HG22	3	0.12
(1,1441)	1:61:A:GLY:HA3	1:52:A:ILE:HG23	3	0.12
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	2	0.12
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	6	0.12
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	9	0.12
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	14	0.12
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	15	0.12
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	16	0.12
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	18	0.12
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	19	0.12
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	20	0.12
(1,1437)	1:91:A:VAL:HB	1:92:A:PHE:H	11	0.12
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	9	0.12
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	9	0.12
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	10	0.12
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	10	0.12
(1,1429)	1:32:A:LEU:HB2	1:32:A:LEU:H	2	0.12
(1,1429)	1:32:A:LEU:HB3	1:32:A:LEU:H	2	0.12
(1,1429)	1:32:A:LEU:HB2	1:32:A:LEU:H	8	0.12
(1,1429)	1:32:A:LEU:HB3	1:32:A:LEU:H	8	0.12
(1,1429)	1:32:A:LEU:HB2	1:32:A:LEU:H	15	0.12
(1,1429)	1:32:A:LEU:HB3	1:32:A:LEU:H	15	0.12
(1,1427)	1:12:A:PHE:HA	1:15:A:ALA:HA	16	0.12
(1,1424)	1:12:A:PHE:HA	1:12:A:PHE:H	4	0.12
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	10	0.12
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1411)	1:41:A:GLN:HB2	1:37:A:ARG:HA	14	0.12
(1,1411)	1:41:A:GLN:HB3	1:37:A:ARG:HA	14	0.12
(1,1411)	1:41:A:GLN:HB2	1:37:A:ARG:HA	18	0.12
(1,1411)	1:41:A:GLN:HB3	1:37:A:ARG:HA	18	0.12
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	2	0.12
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB2	1	0.12
(1,1405)	1:50:A:ASP:HA	1:53:A:ASN:HB3	1	0.12
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	10	0.12
(1,1377)	1:52:A:ILE:HD11	1:62:A:THR:H	10	0.12
(1,1377)	1:52:A:ILE:HD12	1:62:A:THR:H	10	0.12
(1,1377)	1:52:A:ILE:HD13	1:62:A:THR:H	10	0.12
(1,1377)	1:52:A:ILE:HD11	1:62:A:THR:H	16	0.12
(1,1377)	1:52:A:ILE:HD12	1:62:A:THR:H	16	0.12
(1,1377)	1:52:A:ILE:HD13	1:62:A:THR:H	16	0.12
(1,1370)	1:58:A:ASP:HA	1:57:A:ALA:H	1	0.12
(1,1370)	1:58:A:ASP:HA	1:57:A:ALA:H	7	0.12
(1,1370)	1:58:A:ASP:HA	1:57:A:ALA:H	8	0.12
(1,1370)	1:58:A:ASP:HA	1:57:A:ALA:H	14	0.12
(1,1370)	1:58:A:ASP:HA	1:57:A:ALA:H	17	0.12
(1,1370)	1:58:A:ASP:HA	1:57:A:ALA:H	18	0.12
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	1	0.12
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	5	0.12
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	11	0.12
(1,1361)	1:76:A:MET:HA	1:77:A:LYS:H	4	0.12
(1,1346)	1:125:A:ILE:HG21	1:122:A:ASP:H	7	0.12
(1,1346)	1:125:A:ILE:HG22	1:122:A:ASP:H	7	0.12
(1,1346)	1:125:A:ILE:HG23	1:122:A:ASP:H	7	0.12
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	1	0.12
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	4	0.12
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	5	0.12
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	6	0.12
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	17	0.12
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	2	0.12
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	8	0.12
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	16	0.12
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	17	0.12
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	20	0.12
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD21	2	0.12
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD22	2	0.12
(1,1331)	1:38:A:SER:HB2	1:105:A:LEU:HD23	2	0.12
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD21	2	0.12
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD22	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1331)	1:38:A:SER:HB3	1:105:A:LEU:HD23	2	0.12
(1,1319)	1:33:A:GLY:HA2	1:33:A:GLY:H	2	0.12
(1,1319)	1:33:A:GLY:HA2	1:33:A:GLY:H	4	0.12
(1,1319)	1:33:A:GLY:HA2	1:33:A:GLY:H	9	0.12
(1,1319)	1:33:A:GLY:HA2	1:33:A:GLY:H	10	0.12
(1,1319)	1:33:A:GLY:HA2	1:33:A:GLY:H	13	0.12
(1,1319)	1:33:A:GLY:HA2	1:33:A:GLY:H	16	0.12
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	13	0.12
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	15	0.12
(1,1310)	1:68:A:PHE:HB2	1:63:A:ILE:HD11	15	0.12
(1,1310)	1:68:A:PHE:HB2	1:63:A:ILE:HD12	15	0.12
(1,1310)	1:68:A:PHE:HB2	1:63:A:ILE:HD13	15	0.12
(1,1310)	1:68:A:PHE:HB3	1:63:A:ILE:HD11	15	0.12
(1,1310)	1:68:A:PHE:HB3	1:63:A:ILE:HD12	15	0.12
(1,1310)	1:68:A:PHE:HB3	1:63:A:ILE:HD13	15	0.12
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	6	0.12
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	6	0.12
(1,1305)	1:68:A:PHE:HB2	1:68:A:PHE:HZ	19	0.12
(1,1305)	1:68:A:PHE:HB3	1:68:A:PHE:HZ	19	0.12
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	8	0.12
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	8	0.12
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	2	0.12
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	3	0.12
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	4	0.12
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	10	0.12
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	12	0.12
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	14	0.12
(1,1296)	1:40:A:GLY:HA3	1:40:A:GLY:H	18	0.12
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	7	0.12
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	11	0.12
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	18	0.12
(1,1282)	1:13:A:LYS:HA	1:13:A:LYS:H	11	0.12
(1,1281)	1:13:A:LYS:HA	1:16:A:PHE:HB2	19	0.12
(1,1281)	1:13:A:LYS:HA	1:16:A:PHE:HB3	19	0.12
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	5	0.12
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	1	0.12
(1,1256)	1:48:A:LEU:HA	1:51:A:MET:H	4	0.12
(1,1252)	1:48:A:LEU:HA	1:48:A:LEU:H	7	0.12
(1,1249)	1:67:A:GLU:HA	1:67:A:GLU:H	8	0.12
(1,1249)	1:67:A:GLU:HA	1:67:A:GLU:H	11	0.12
(1,1236)	1:106:A:ARG:HA	1:121:A:VAL:HG11	7	0.12
(1,1236)	1:106:A:ARG:HA	1:121:A:VAL:HG12	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	1:106:A:ARG:HA	1:121:A:VAL:HG13	7	0.12
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	2	0.12
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	4	0.12
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	6	0.12
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	8	0.12
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	12	0.12
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	13	0.12
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	2	0.12
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	7	0.12
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	9	0.12
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	10	0.12
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	15	0.12
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	17	0.12
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	18	0.12
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	19	0.12
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	20	0.12
(1,1187)	1:91:A:VAL:HG21	1:88:A:ALA:H	1	0.12
(1,1187)	1:91:A:VAL:HG22	1:88:A:ALA:H	1	0.12
(1,1187)	1:91:A:VAL:HG23	1:88:A:ALA:H	1	0.12
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	2	0.12
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	3	0.12
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG21	17	0.12
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG22	17	0.12
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG23	17	0.12
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG21	17	0.12
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG22	17	0.12
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG23	17	0.12
(1,1180)	1:64:A:ASP:HB3	1:64:A:ASP:H	9	0.12
(1,1180)	1:64:A:ASP:HB3	1:64:A:ASP:H	12	0.12
(1,1180)	1:64:A:ASP:HB3	1:64:A:ASP:H	14	0.12
(1,1180)	1:64:A:ASP:HB3	1:64:A:ASP:H	15	0.12
(1,1180)	1:64:A:ASP:HB3	1:64:A:ASP:H	17	0.12
(1,1180)	1:64:A:ASP:HB3	1:64:A:ASP:H	18	0.12
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB2	19	0.12
(1,1178)	1:89:A:PHE:HA	1:92:A:PHE:HB3	19	0.12
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	1	0.12
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	5	0.12
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	6	0.12
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	7	0.12
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	9	0.12
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	14	0.12
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	18	0.12
(1,1175)	1:89:A:PHE:HA	1:89:A:PHE:H	19	0.12
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	19	0.12
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	20	0.12
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	2	0.12
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	2	0.12
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	2	0.12
(1,1150)	1:100:A:ILE:HG21	1:136:A:VAL:H	16	0.12
(1,1150)	1:100:A:ILE:HG22	1:136:A:VAL:H	16	0.12
(1,1150)	1:100:A:ILE:HG23	1:136:A:VAL:H	16	0.12
(1,1149)	1:100:A:ILE:HG21	1:93:A:ASP:HB2	9	0.12
(1,1149)	1:100:A:ILE:HG22	1:93:A:ASP:HB2	9	0.12
(1,1149)	1:100:A:ILE:HG23	1:93:A:ASP:HB2	9	0.12
(1,1138)	1:34:A:THR:HA	1:37:A:ARG:H	4	0.12
(1,1138)	1:34:A:THR:HA	1:37:A:ARG:H	13	0.12
(1,1138)	1:34:A:THR:HA	1:37:A:ARG:H	16	0.12
(1,1118)	1:29:A:THR:HB	1:28:A:THR:HA	9	0.12
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	6	0.12
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	6	0.12
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	15	0.12
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	15	0.12
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG2	19	0.12
(1,1110)	1:36:A:MET:HA	1:41:A:GLN:HG3	19	0.12
(1,1103)	1:48:A:LEU:HD11	1:48:A:LEU:HA	15	0.12
(1,1103)	1:48:A:LEU:HD12	1:48:A:LEU:HA	15	0.12
(1,1103)	1:48:A:LEU:HD13	1:48:A:LEU:HA	15	0.12
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	2	0.12
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	12	0.12
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	14	0.12
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	16	0.12
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	1	0.12
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	1	0.12
(1,1053)	1:125:A:ILE:HA	1:126:A:ARG:H	7	0.12
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	1	0.12
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	8	0.12
(1,1028)	1:141:A:PHE:HA	1:145:A:MET:H	1	0.12
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG2	10	0.12
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG3	10	0.12
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG2	20	0.12
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG3	20	0.12
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	17	0.12
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	17	0.12
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	17	0.12
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	17	0.12
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	17	0.12
(1,994)	1:29:A:THR:HA	1:30:A:LYS:H	19	0.12
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	4	0.12
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	9	0.12
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	16	0.12
(1,937)	1:65:A:PHE:HA	1:67:A:GLU:H	15	0.12
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	7	0.12
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	7	0.12
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	7	0.12
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	13	0.12
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	13	0.12
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	13	0.12
(1,904)	1:119:A:GLU:HA	1:122:A:ASP:H	20	0.12
(1,899)	1:125:A:ILE:HG12	1:122:A:ASP:HA	1	0.12
(1,899)	1:125:A:ILE:HG13	1:122:A:ASP:HA	1	0.12
(1,899)	1:125:A:ILE:HG12	1:122:A:ASP:HA	6	0.12
(1,899)	1:125:A:ILE:HG13	1:122:A:ASP:HA	6	0.12
(1,899)	1:125:A:ILE:HG12	1:122:A:ASP:HA	15	0.12
(1,899)	1:125:A:ILE:HG13	1:122:A:ASP:HA	15	0.12
(1,865)	1:116:A:LEU:HD11	1:116:A:LEU:HA	7	0.12
(1,865)	1:116:A:LEU:HD12	1:116:A:LEU:HA	7	0.12
(1,865)	1:116:A:LEU:HD13	1:116:A:LEU:HA	7	0.12
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	4	0.12
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	5	0.12
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	12	0.12
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG12	14	0.12
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG13	14	0.12
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG12	17	0.12
(1,790)	1:52:A:ILE:HB	1:63:A:ILE:HG13	17	0.12
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	7	0.12
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	7	0.12
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	7	0.12
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	10	0.12
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	10	0.12
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	10	0.12
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	14	0.12
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	14	0.12
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	14	0.12
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	16	0.12
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	16	0.12
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	20	0.12
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	20	0.12
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	20	0.12
(1,780)	1:94:A:LYS:HG3	1:94:A:LYS:H	8	0.12
(1,780)	1:94:A:LYS:HG3	1:94:A:LYS:H	12	0.12
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	3	0.12
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	3	0.12
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	3	0.12
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	3	0.12
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	3	0.12
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	3	0.12
(1,766)	1:20:A:ASP:HA	1:26:A:THR:HB	5	0.12
(1,766)	1:20:A:ASP:HA	1:26:A:THR:HB	20	0.12
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	6	0.12
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	10	0.12
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	18	0.12
(1,759)	1:26:A:THR:HG21	1:62:A:THR:HA	11	0.12
(1,759)	1:26:A:THR:HG22	1:62:A:THR:HA	11	0.12
(1,759)	1:26:A:THR:HG23	1:62:A:THR:HA	11	0.12
(1,749)	1:55:A:VAL:HA	1:56:A:ASP:H	5	0.12
(1,749)	1:55:A:VAL:HA	1:56:A:ASP:H	12	0.12
(1,749)	1:55:A:VAL:HA	1:56:A:ASP:H	20	0.12
(1,745)	1:55:A:VAL:HA	1:51:A:MET:HA	13	0.12
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	4	0.12
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	4	0.12
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	10	0.12
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	10	0.12
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	14	0.12
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	14	0.12
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	18	0.12
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	18	0.12
(1,680)	1:27:A:ILE:HB	1:63:A:ILE:H	2	0.12
(1,678)	1:27:A:ILE:HB	1:21:A:LYS:HD2	5	0.12
(1,678)	1:27:A:ILE:HB	1:21:A:LYS:HD3	5	0.12
(1,678)	1:27:A:ILE:HB	1:21:A:LYS:HD2	19	0.12
(1,678)	1:27:A:ILE:HB	1:21:A:LYS:HD3	19	0.12
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG2	13	0.12
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG3	13	0.12
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG2	13	0.12
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG3	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG2	13	0.12
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG3	13	0.12
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB2	20	0.12
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB3	20	0.12
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	3	0.12
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	3	0.12
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	8	0.12
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	8	0.12
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	12	0.12
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	12	0.12
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	15	0.12
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	15	0.12
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	16	0.12
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	16	0.12
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	5	0.12
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	5	0.12
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	9	0.12
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	9	0.12
(1,590)	1:27:A:ILE:HA	1:63:A:ILE:H	8	0.12
(1,590)	1:27:A:ILE:HA	1:63:A:ILE:H	19	0.12
(1,503)	1:110:A:THR:HB	1:112:A:LEU:H	6	0.12
(1,503)	1:110:A:THR:HB	1:112:A:LEU:H	14	0.12
(1,503)	1:110:A:THR:HB	1:112:A:LEU:H	18	0.12
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	5	0.12
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	5	0.12
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	5	0.12
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	15	0.12
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	15	0.12
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	15	0.12
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	9	0.12
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	9	0.12
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	11	0.12
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	11	0.12
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	16	0.12
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	16	0.12
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	18	0.12
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	18	0.12
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	20	0.12
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	20	0.12
(1,476)	1:142:A:VAL:HG11	1:141:A:PHE:HA	11	0.12
(1,476)	1:142:A:VAL:HG12	1:141:A:PHE:HA	11	0.12
(1,476)	1:142:A:VAL:HG13	1:141:A:PHE:HA	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,476)	1:142:A:VAL:HG11	1:141:A:PHE:HA	12	0.12
(1,476)	1:142:A:VAL:HG12	1:141:A:PHE:HA	12	0.12
(1,476)	1:142:A:VAL:HG13	1:141:A:PHE:HA	12	0.12
(1,395)	1:37:A:ARG:HA	1:34:A:THR:HA	18	0.12
(1,367)	1:31:A:GLU:HA	1:32:A:LEU:HG	5	0.12
(1,367)	1:31:A:GLU:HA	1:32:A:LEU:HG	8	0.12
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	5	0.12
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	9	0.12
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	14	0.12
(1,357)	1:53:A:ASN:HA	1:56:A:ASP:HB2	20	0.12
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	4	0.12
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	9	0.12
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	19	0.12
(1,151)	1:107:A:HIS:HA	1:94:A:LYS:HG3	12	0.12
(1,130)	1:34:A:THR:HB	1:31:A:GLU:H	18	0.12
(1,95)	1:48:A:LEU:HD21	1:50:A:ASP:HA	18	0.12
(1,95)	1:48:A:LEU:HD22	1:50:A:ASP:HA	18	0.12
(1,95)	1:48:A:LEU:HD23	1:50:A:ASP:HA	18	0.12
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	17	0.12
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	17	0.12
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	17	0.12
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	17	0.12
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	17	0.12
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	17	0.12
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	19	0.12
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	19	0.12
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	19	0.12
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	19	0.12
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	19	0.12
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	19	0.12
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	3	0.11
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	5	0.11
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	12	0.11
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	8	0.11
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	9	0.11
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	17	0.11
(1,1447)	1:55:A:VAL:HG11	1:55:A:VAL:H	6	0.11
(1,1447)	1:55:A:VAL:HG12	1:55:A:VAL:H	6	0.11
(1,1447)	1:55:A:VAL:HG13	1:55:A:VAL:H	6	0.11
(1,1447)	1:55:A:VAL:HG11	1:55:A:VAL:H	7	0.11
(1,1447)	1:55:A:VAL:HG12	1:55:A:VAL:H	7	0.11
(1,1447)	1:55:A:VAL:HG13	1:55:A:VAL:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1446)	1:55:A:VAL:HG11	1:71:A:MET:H	15	0.11
(1,1446)	1:55:A:VAL:HG12	1:71:A:MET:H	15	0.11
(1,1446)	1:55:A:VAL:HG13	1:71:A:MET:H	15	0.11
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	12	0.11
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	14	0.11
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	16	0.11
(1,1443)	1:61:A:GLY:HA3	1:62:A:THR:H	17	0.11
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	4	0.11
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	5	0.11
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	7	0.11
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	8	0.11
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	10	0.11
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	11	0.11
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	12	0.11
(1,1439)	1:6:A:GLU:HA	1:6:A:GLU:H	17	0.11
(1,1437)	1:91:A:VAL:HB	1:92:A:PHE:H	5	0.11
(1,1437)	1:91:A:VAL:HB	1:92:A:PHE:H	18	0.11
(1,1432)	1:63:A:ILE:HB	1:63:A:ILE:H	9	0.11
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	13	0.11
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	13	0.11
(1,1430)	1:32:A:LEU:HB2	1:34:A:THR:H	14	0.11
(1,1430)	1:32:A:LEU:HB3	1:34:A:THR:H	14	0.11
(1,1411)	1:41:A:GLN:HB2	1:37:A:ARG:HA	6	0.11
(1,1411)	1:41:A:GLN:HB3	1:37:A:ARG:HA	6	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	4	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	5	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	6	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	9	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	10	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	11	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	12	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	13	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	14	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	15	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	16	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	18	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	19	0.11
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	20	0.11
(1,1404)	1:50:A:ASP:HA	1:47:A:GLU:HA	1	0.11
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	1	0.11
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	2	0.11
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	5	0.11
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	7	0.11
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	12	0.11
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	14	0.11
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	18	0.11
(1,1370)	1:58:A:ASP:HA	1:57:A:ALA:H	3	0.11
(1,1370)	1:58:A:ASP:HA	1:57:A:ALA:H	4	0.11
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	15	0.11
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	16	0.11
(1,1367)	1:70:A:THR:HA	1:70:A:THR:H	13	0.11
(1,1364)	1:74:A:ARG:HA	1:74:A:ARG:H	4	0.11
(1,1364)	1:74:A:ARG:HA	1:74:A:ARG:H	12	0.11
(1,1361)	1:76:A:MET:HA	1:77:A:LYS:H	9	0.11
(1,1351)	1:110:A:THR:HG21	1:110:A:THR:H	1	0.11
(1,1351)	1:110:A:THR:HG22	1:110:A:THR:H	1	0.11
(1,1351)	1:110:A:THR:HG23	1:110:A:THR:H	1	0.11
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	3	0.11
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	5	0.11
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	14	0.11
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	15	0.11
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	18	0.11
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	20	0.11
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	3	0.11
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	7	0.11
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	9	0.11
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	10	0.11
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	12	0.11
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	16	0.11
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	18	0.11
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	5	0.11
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	7	0.11
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	13	0.11
(1,1338)	1:143:A:GLN:HA	1:145:A:MET:H	19	0.11
(1,1335)	1:146:A:THR:HB	1:146:A:THR:H	15	0.11
(1,1332)	1:38:A:SER:HB2	1:38:A:SER:H	14	0.11
(1,1332)	1:38:A:SER:HB3	1:38:A:SER:H	14	0.11
(1,1332)	1:38:A:SER:HB2	1:38:A:SER:H	16	0.11
(1,1332)	1:38:A:SER:HB3	1:38:A:SER:H	16	0.11
(1,1321)	1:61:A:GLY:HA2	1:60:A:ASN:HA	6	0.11
(1,1321)	1:61:A:GLY:HA2	1:60:A:ASN:HA	8	0.11
(1,1321)	1:61:A:GLY:HA2	1:60:A:ASN:HA	12	0.11
(1,1321)	1:61:A:GLY:HA2	1:60:A:ASN:HA	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1321)	1:61:A:GLY:HA2	1:60:A:ASN:HA	20	0.11
(1,1319)	1:33:A:GLY:HA2	1:33:A:GLY:H	3	0.11
(1,1319)	1:33:A:GLY:HA2	1:33:A:GLY:H	7	0.11
(1,1319)	1:33:A:GLY:HA2	1:33:A:GLY:H	11	0.11
(1,1319)	1:33:A:GLY:HA2	1:33:A:GLY:H	15	0.11
(1,1319)	1:33:A:GLY:HA2	1:33:A:GLY:H	18	0.11
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	3	0.11
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	6	0.11
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	9	0.11
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	16	0.11
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	17	0.11
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	18	0.11
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	19	0.11
(1,1304)	1:136:A:VAL:HB	1:136:A:VAL:H	4	0.11
(1,1304)	1:136:A:VAL:HB	1:136:A:VAL:H	5	0.11
(1,1304)	1:136:A:VAL:HB	1:136:A:VAL:H	9	0.11
(1,1303)	1:37:A:ARG:HB2	1:36:A:MET:HA	17	0.11
(1,1303)	1:37:A:ARG:HB3	1:36:A:MET:HA	17	0.11
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	6	0.11
(1,1291)	1:30:A:LYS:HA	1:30:A:LYS:H	19	0.11
(1,1283)	1:13:A:LYS:HA	1:16:A:PHE:HA	6	0.11
(1,1281)	1:13:A:LYS:HA	1:16:A:PHE:HB2	15	0.11
(1,1281)	1:13:A:LYS:HA	1:16:A:PHE:HB3	15	0.11
(1,1277)	1:51:A:MET:HB2	1:50:A:ASP:HA	17	0.11
(1,1277)	1:51:A:MET:HB3	1:50:A:ASP:HA	17	0.11
(1,1273)	1:94:A:LYS:HG2	1:94:A:LYS:H	12	0.11
(1,1273)	1:94:A:LYS:HG2	1:94:A:LYS:H	15	0.11
(1,1273)	1:94:A:LYS:HG2	1:94:A:LYS:H	18	0.11
(1,1273)	1:94:A:LYS:HG2	1:94:A:LYS:H	19	0.11
(1,1263)	1:17:A:SER:HB2	1:16:A:PHE:HA	6	0.11
(1,1263)	1:17:A:SER:HB3	1:16:A:PHE:HA	6	0.11
(1,1263)	1:17:A:SER:HB2	1:16:A:PHE:HA	19	0.11
(1,1263)	1:17:A:SER:HB3	1:16:A:PHE:HA	19	0.11
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	17	0.11
(1,1261)	1:26:A:THR:HB	1:63:A:ILE:H	18	0.11
(1,1249)	1:67:A:GLU:HA	1:67:A:GLU:H	3	0.11
(1,1249)	1:67:A:GLU:HA	1:67:A:GLU:H	12	0.11
(1,1249)	1:67:A:GLU:HA	1:67:A:GLU:H	15	0.11
(1,1236)	1:106:A:ARG:HA	1:121:A:VAL:HG11	18	0.11
(1,1236)	1:106:A:ARG:HA	1:121:A:VAL:HG12	18	0.11
(1,1236)	1:106:A:ARG:HA	1:121:A:VAL:HG13	18	0.11
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	3	0.11
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	5	0.11
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	7	0.11
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	9	0.11
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	10	0.11
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	11	0.11
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	14	0.11
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	15	0.11
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	16	0.11
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	17	0.11
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	18	0.11
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	19	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	1	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	2	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	3	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	4	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	5	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	6	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	7	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	8	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	9	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	10	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	11	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	12	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	13	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	14	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	15	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	16	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	17	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	18	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	19	0.11
(1,1220)	1:140:A:GLU:HA	1:140:A:GLU:H	20	0.11
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	1	0.11
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	3	0.11
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	4	0.11
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	8	0.11
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	11	0.11
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	12	0.11
(1,1217)	1:144:A:MET:HA	1:144:A:MET:H	13	0.11
(1,1204)	1:52:A:ILE:HG12	1:52:A:ILE:H	20	0.11
(1,1204)	1:52:A:ILE:HG13	1:52:A:ILE:H	20	0.11
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	19	0.11
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG21	10	0.11
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG22	10	0.11
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG23	10	0.11
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG21	10	0.11
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG22	10	0.11
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG23	10	0.11
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG21	20	0.11
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG22	20	0.11
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG23	20	0.11
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG21	20	0.11
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG22	20	0.11
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG23	20	0.11
(1,1180)	1:64:A:ASP:HB3	1:64:A:ASP:H	1	0.11
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	2	0.11
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	6	0.11
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	10	0.11
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	16	0.11
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	17	0.11
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	8	0.11
(1,1163)	1:85:A:ILE:HB	1:86:A:ARG:H	19	0.11
(1,1149)	1:100:A:ILE:HG21	1:93:A:ASP:HB2	6	0.11
(1,1149)	1:100:A:ILE:HG22	1:93:A:ASP:HB2	6	0.11
(1,1149)	1:100:A:ILE:HG23	1:93:A:ASP:HB2	6	0.11
(1,1149)	1:100:A:ILE:HG21	1:93:A:ASP:HB2	18	0.11
(1,1149)	1:100:A:ILE:HG22	1:93:A:ASP:HB2	18	0.11
(1,1149)	1:100:A:ILE:HG23	1:93:A:ASP:HB2	18	0.11
(1,1130)	1:111:A:ASN:HA	1:112:A:LEU:H	1	0.11
(1,1118)	1:29:A:THR:HB	1:28:A:THR:HA	4	0.11
(1,1115)	1:29:A:THR:HB	1:62:A:THR:HA	15	0.11
(1,1111)	1:36:A:MET:HA	1:39:A:LEU:HB2	6	0.11
(1,1111)	1:36:A:MET:HA	1:39:A:LEU:HB3	6	0.11
(1,1111)	1:36:A:MET:HA	1:39:A:LEU:HB2	15	0.11
(1,1111)	1:36:A:MET:HA	1:39:A:LEU:HB3	15	0.11
(1,1107)	1:44:A:THR:HG21	1:44:A:THR:H	1	0.11
(1,1107)	1:44:A:THR:HG22	1:44:A:THR:H	1	0.11
(1,1107)	1:44:A:THR:HG23	1:44:A:THR:H	1	0.11
(1,1104)	1:48:A:LEU:HD11	1:33:A:GLY:HA2	20	0.11
(1,1104)	1:48:A:LEU:HD12	1:33:A:GLY:HA2	20	0.11
(1,1104)	1:48:A:LEU:HD13	1:33:A:GLY:HA2	20	0.11
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	9	0.11
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	15	0.11
(1,1085)	1:83:A:GLU:HA	1:86:A:ARG:H	18	0.11
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	17	0.11
(1,1037)	1:5:A:THR:HB	1:6:A:GLU:HG2	8	0.11
(1,1037)	1:5:A:THR:HB	1:6:A:GLU:HG3	8	0.11
(1,1030)	1:141:A:PHE:HA	1:142:A:VAL:H	6	0.11
(1,1027)	1:141:A:PHE:HA	1:141:A:PHE:HZ	12	0.11
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG2	1	0.11
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG3	1	0.11
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG2	8	0.11
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG3	8	0.11
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG2	11	0.11
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG3	11	0.11
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG2	14	0.11
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG3	14	0.11
(1,1013)	1:63:A:ILE:HA	1:56:A:ASP:HB3	2	0.11
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	11	0.11
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	11	0.11
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	11	0.11
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	11	0.11
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	11	0.11
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	11	0.11
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	15	0.11
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	15	0.11
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	15	0.11
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	15	0.11
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	15	0.11
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	15	0.11
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB2	19	0.11
(1,1005)	1:46:A:ALA:HB1	1:45:A:GLU:HB3	19	0.11
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB2	19	0.11
(1,1005)	1:46:A:ALA:HB2	1:45:A:GLU:HB3	19	0.11
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB2	19	0.11
(1,1005)	1:46:A:ALA:HB3	1:45:A:GLU:HB3	19	0.11
(1,994)	1:29:A:THR:HA	1:30:A:LYS:H	14	0.11
(1,992)	1:29:A:THR:HA	1:62:A:THR:HA	11	0.11
(1,943)	1:37:A:ARG:HG2	1:37:A:ARG:H	17	0.11
(1,943)	1:37:A:ARG:HG3	1:37:A:ARG:H	17	0.11
(1,943)	1:37:A:ARG:HG2	1:37:A:ARG:H	19	0.11
(1,943)	1:37:A:ARG:HG3	1:37:A:ARG:H	19	0.11
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	1	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	1	0.11
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	2	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	2	0.11
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	2	0.11
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	3	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	3	0.11
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	3	0.11
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	4	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	4	0.11
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	4	0.11
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	5	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	5	0.11
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	5	0.11
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	6	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	6	0.11
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	6	0.11
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	7	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	7	0.11
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	7	0.11
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	9	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	9	0.11
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	9	0.11
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	10	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	10	0.11
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	10	0.11
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	11	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	11	0.11
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	11	0.11
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	13	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	13	0.11
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	13	0.11
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	16	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	16	0.11
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	16	0.11
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	20	0.11
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	20	0.11
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	20	0.11
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	1	0.11
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	1	0.11
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	1	0.11
(1,915)	1:105:A:LEU:HD11	1:105:A:LEU:H	9	0.11
(1,915)	1:105:A:LEU:HD12	1:105:A:LEU:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,915)	1:105:A:LEU:HD13	1:105:A:LEU:H	9	0.11
(1,899)	1:125:A:ILE:HG12	1:122:A:ASP:HA	2	0.11
(1,899)	1:125:A:ILE:HG13	1:122:A:ASP:HA	2	0.11
(1,899)	1:125:A:ILE:HG12	1:122:A:ASP:HA	5	0.11
(1,899)	1:125:A:ILE:HG13	1:122:A:ASP:HA	5	0.11
(1,899)	1:125:A:ILE:HG12	1:122:A:ASP:HA	14	0.11
(1,899)	1:125:A:ILE:HG13	1:122:A:ASP:HA	14	0.11
(1,899)	1:125:A:ILE:HG12	1:122:A:ASP:HA	16	0.11
(1,899)	1:125:A:ILE:HG13	1:122:A:ASP:HA	16	0.11
(1,899)	1:125:A:ILE:HG12	1:122:A:ASP:HA	18	0.11
(1,899)	1:125:A:ILE:HG13	1:122:A:ASP:HA	18	0.11
(1,899)	1:125:A:ILE:HG12	1:122:A:ASP:HA	20	0.11
(1,899)	1:125:A:ILE:HG13	1:122:A:ASP:HA	20	0.11
(1,870)	1:136:A:VAL:HG21	1:141:A:PHE:HA	19	0.11
(1,870)	1:136:A:VAL:HG22	1:141:A:PHE:HA	19	0.11
(1,870)	1:136:A:VAL:HG23	1:141:A:PHE:HA	19	0.11
(1,860)	1:142:A:VAL:HB	1:143:A:GLN:H	8	0.11
(1,860)	1:142:A:VAL:HB	1:143:A:GLN:H	11	0.11
(1,847)	1:33:A:GLY:HA3	1:34:A:THR:H	16	0.11
(1,826)	1:69:A:LEU:HA	1:72:A:MET:H	15	0.11
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	2	0.11
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	14	0.11
(1,789)	1:52:A:ILE:HB	1:29:A:THR:HA	6	0.11
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	19	0.11
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	19	0.11
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	19	0.11
(1,780)	1:94:A:LYS:HG3	1:94:A:LYS:H	1	0.11
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	13	0.11
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	13	0.11
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	13	0.11
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	13	0.11
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	13	0.11
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	13	0.11
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	15	0.11
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	15	0.11
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	15	0.11
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	15	0.11
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	15	0.11
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	15	0.11
(1,766)	1:20:A:ASP:HA	1:26:A:THR:HB	17	0.11
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	14	0.11
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:48:A:LEU:HB2	1:32:A:LEU:HD11	1	0.11
(1,755)	1:48:A:LEU:HB2	1:32:A:LEU:HD12	1	0.11
(1,755)	1:48:A:LEU:HB2	1:32:A:LEU:HD13	1	0.11
(1,755)	1:48:A:LEU:HB3	1:32:A:LEU:HD11	1	0.11
(1,755)	1:48:A:LEU:HB3	1:32:A:LEU:HD12	1	0.11
(1,755)	1:48:A:LEU:HB3	1:32:A:LEU:HD13	1	0.11
(1,749)	1:55:A:VAL:HA	1:56:A:ASP:H	7	0.11
(1,740)	1:67:A:GLU:HB2	1:55:A:VAL:HG21	15	0.11
(1,740)	1:67:A:GLU:HB2	1:55:A:VAL:HG22	15	0.11
(1,740)	1:67:A:GLU:HB2	1:55:A:VAL:HG23	15	0.11
(1,740)	1:67:A:GLU:HB3	1:55:A:VAL:HG21	15	0.11
(1,740)	1:67:A:GLU:HB3	1:55:A:VAL:HG22	15	0.11
(1,740)	1:67:A:GLU:HB3	1:55:A:VAL:HG23	15	0.11
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	3	0.11
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	3	0.11
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	9	0.11
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	9	0.11
(1,680)	1:27:A:ILE:HB	1:63:A:ILE:H	11	0.11
(1,680)	1:27:A:ILE:HB	1:63:A:ILE:H	16	0.11
(1,679)	1:27:A:ILE:HB	1:28:A:THR:HB	9	0.11
(1,678)	1:27:A:ILE:HB	1:21:A:LYS:HD2	12	0.11
(1,678)	1:27:A:ILE:HB	1:21:A:LYS:HD3	12	0.11
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG2	1	0.11
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG3	1	0.11
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG2	1	0.11
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG3	1	0.11
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG2	1	0.11
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG3	1	0.11
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG2	5	0.11
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG3	5	0.11
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG2	5	0.11
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG3	5	0.11
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG2	5	0.11
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG3	5	0.11
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB2	5	0.11
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB3	5	0.11
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB2	17	0.11
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB3	17	0.11
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	2	0.11
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	2	0.11
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	4	0.11
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	9	0.11
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	9	0.11
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	14	0.11
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	14	0.11
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	20	0.11
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	20	0.11
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	7	0.11
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	7	0.11
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	8	0.11
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	8	0.11
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	13	0.11
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	13	0.11
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	17	0.11
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	17	0.11
(1,503)	1:110:A:THR:HB	1:112:A:LEU:H	3	0.11
(1,503)	1:110:A:THR:HB	1:112:A:LEU:H	7	0.11
(1,503)	1:110:A:THR:HB	1:112:A:LEU:H	12	0.11
(1,503)	1:110:A:THR:HB	1:112:A:LEU:H	16	0.11
(1,495)	1:121:A:VAL:HG21	1:105:A:LEU:HG	3	0.11
(1,495)	1:121:A:VAL:HG22	1:105:A:LEU:HG	3	0.11
(1,495)	1:121:A:VAL:HG23	1:105:A:LEU:HG	3	0.11
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	2	0.11
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	2	0.11
(1,476)	1:142:A:VAL:HG11	1:141:A:PHE:HA	1	0.11
(1,476)	1:142:A:VAL:HG12	1:141:A:PHE:HA	1	0.11
(1,476)	1:142:A:VAL:HG13	1:141:A:PHE:HA	1	0.11
(1,476)	1:142:A:VAL:HG11	1:141:A:PHE:HA	20	0.11
(1,476)	1:142:A:VAL:HG12	1:141:A:PHE:HA	20	0.11
(1,476)	1:142:A:VAL:HG13	1:141:A:PHE:HA	20	0.11
(1,395)	1:37:A:ARG:HA	1:34:A:THR:HA	17	0.11
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	12	0.11
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	19	0.11
(1,357)	1:53:A:ASN:HA	1:56:A:ASP:HB2	14	0.11
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	13	0.11
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	14	0.11
(1,151)	1:107:A:HIS:HA	1:94:A:LYS:HG3	1	0.11
(1,151)	1:107:A:HIS:HA	1:94:A:LYS:HG3	3	0.11
(1,143)	1:100:A:ILE:HB	1:136:A:VAL:HB	12	0.11
(1,116)	1:116:A:LEU:HG	1:121:A:VAL:HG11	7	0.11
(1,116)	1:116:A:LEU:HG	1:121:A:VAL:HG12	7	0.11
(1,116)	1:116:A:LEU:HG	1:121:A:VAL:HG13	7	0.11
(1,63)	1:86:A:ARG:HB2	1:89:A:PHE:HA	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:86:A:ARG:HB3	1:89:A:PHE:HA	17	0.11
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	6	0.11
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	6	0.11
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	6	0.11
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	6	0.11
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	6	0.11
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	6	0.11
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	6	0.11
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	6	0.11
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	6	0.11
(1,9)	1:17:A:SER:HB2	1:16:A:PHE:HA	6	0.11
(1,9)	1:17:A:SER:HB3	1:16:A:PHE:HA	6	0.11
(1,9)	1:17:A:SER:HB2	1:16:A:PHE:HA	19	0.11
(1,9)	1:17:A:SER:HB3	1:16:A:PHE:HA	19	0.11
(1,1460)	1:88:A:ALA:HA	1:89:A:PHE:H	6	0.1
(1,1456)	1:85:A:ILE:HA	1:88:A:ALA:H	15	0.1
(1,1451)	1:18:A:LEU:HA	1:15:A:ALA:HA	13	0.1
(1,1437)	1:91:A:VAL:HB	1:92:A:PHE:H	3	0.1
(1,1417)	1:93:A:ASP:HA	1:93:A:ASP:H	3	0.1
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	1	0.1
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	3	0.1
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	8	0.1
(1,1406)	1:50:A:ASP:HA	1:50:A:ASP:H	17	0.1
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	4	0.1
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	9	0.1
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	13	0.1
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	19	0.1
(1,1387)	1:16:A:PHE:HA	1:16:A:PHE:H	20	0.1
(1,1370)	1:58:A:ASP:HA	1:57:A:ALA:H	16	0.1
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	4	0.1
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	14	0.1
(1,1368)	1:70:A:THR:HA	1:73:A:ALA:H	17	0.1
(1,1364)	1:74:A:ARG:HA	1:74:A:ARG:H	9	0.1
(1,1364)	1:74:A:ARG:HA	1:74:A:ARG:H	10	0.1
(1,1364)	1:74:A:ARG:HA	1:74:A:ARG:H	18	0.1
(1,1364)	1:74:A:ARG:HA	1:74:A:ARG:H	20	0.1
(1,1354)	1:105:A:LEU:HG	1:105:A:LEU:H	12	0.1
(1,1351)	1:110:A:THR:HG21	1:110:A:THR:H	8	0.1
(1,1351)	1:110:A:THR:HG22	1:110:A:THR:H	8	0.1
(1,1351)	1:110:A:THR:HG23	1:110:A:THR:H	8	0.1
(1,1348)	1:123:A:GLU:HA	1:127:A:GLU:H	16	0.1
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	15	0.1
(1,1339)	1:139:A:GLU:HA	1:139:A:GLU:H	20	0.1
(1,1335)	1:146:A:THR:HB	1:146:A:THR:H	4	0.1
(1,1335)	1:146:A:THR:HB	1:146:A:THR:H	8	0.1
(1,1321)	1:61:A:GLY:HA2	1:60:A:ASN:HA	4	0.1
(1,1321)	1:61:A:GLY:HA2	1:60:A:ASN:HA	5	0.1
(1,1318)	1:118:A:ASP:HB3	1:119:A:GLU:H	2	0.1
(1,1304)	1:136:A:VAL:HB	1:136:A:VAL:H	7	0.1
(1,1304)	1:136:A:VAL:HB	1:136:A:VAL:H	11	0.1
(1,1304)	1:136:A:VAL:HB	1:136:A:VAL:H	15	0.1
(1,1281)	1:13:A:LYS:HA	1:16:A:PHE:HB2	17	0.1
(1,1281)	1:13:A:LYS:HA	1:16:A:PHE:HB3	17	0.1
(1,1281)	1:13:A:LYS:HA	1:16:A:PHE:HB2	20	0.1
(1,1281)	1:13:A:LYS:HA	1:16:A:PHE:HB3	20	0.1
(1,1273)	1:94:A:LYS:HG2	1:94:A:LYS:H	7	0.1
(1,1263)	1:17:A:SER:HB2	1:16:A:PHE:HA	17	0.1
(1,1263)	1:17:A:SER:HB3	1:16:A:PHE:HA	17	0.1
(1,1252)	1:48:A:LEU:HA	1:48:A:LEU:H	15	0.1
(1,1232)	1:109:A:MET:HA	1:109:A:MET:H	20	0.1
(1,1225)	1:124:A:MET:HA	1:124:A:MET:H	20	0.1
(1,1190)	1:91:A:VAL:HG21	1:88:A:ALA:HA	7	0.1
(1,1190)	1:91:A:VAL:HG22	1:88:A:ALA:HA	7	0.1
(1,1190)	1:91:A:VAL:HG23	1:88:A:ALA:HA	7	0.1
(1,1190)	1:91:A:VAL:HG21	1:88:A:ALA:HA	11	0.1
(1,1190)	1:91:A:VAL:HG22	1:88:A:ALA:HA	11	0.1
(1,1190)	1:91:A:VAL:HG23	1:88:A:ALA:HA	11	0.1
(1,1187)	1:91:A:VAL:HG21	1:88:A:ALA:H	18	0.1
(1,1187)	1:91:A:VAL:HG22	1:88:A:ALA:H	18	0.1
(1,1187)	1:91:A:VAL:HG23	1:88:A:ALA:H	18	0.1
(1,1185)	1:128:A:ALA:HA	1:141:A:PHE:H	8	0.1
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG21	11	0.1
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG22	11	0.1
(1,1183)	1:101:A:SER:HB2	1:136:A:VAL:HG23	11	0.1
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG21	11	0.1
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG22	11	0.1
(1,1183)	1:101:A:SER:HB3	1:136:A:VAL:HG23	11	0.1
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	15	0.1
(1,1169)	1:97:A:ASN:HA	1:99:A:TYR:H	18	0.1
(1,1138)	1:34:A:THR:HA	1:37:A:ARG:H	6	0.1
(1,1130)	1:111:A:ASN:HA	1:112:A:LEU:H	9	0.1
(1,1130)	1:111:A:ASN:HA	1:112:A:LEU:H	10	0.1
(1,1130)	1:111:A:ASN:HA	1:112:A:LEU:H	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1130)	1:111:A:ASN:HA	1:112:A:LEU:H	20	0.1
(1,1062)	1:110:A:THR:HA	1:111:A:ASN:H	8	0.1
(1,1056)	1:125:A:ILE:HA	1:128:A:ALA:H	7	0.1
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG2	4	0.1
(1,1018)	1:42:A:ASN:HB2	1:41:A:GLN:HG3	4	0.1
(1,994)	1:29:A:THR:HA	1:30:A:LYS:H	17	0.1
(1,990)	1:29:A:THR:HA	1:32:A:LEU:H	13	0.1
(1,957)	1:8:A:GLN:HG2	1:7:A:GLU:HA	3	0.1
(1,957)	1:8:A:GLN:HG3	1:7:A:GLU:HA	3	0.1
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	14	0.1
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	14	0.1
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	14	0.1
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	15	0.1
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	15	0.1
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	15	0.1
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	17	0.1
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	17	0.1
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	17	0.1
(1,921)	1:85:A:ILE:HG21	1:85:A:ILE:H	18	0.1
(1,921)	1:85:A:ILE:HG22	1:85:A:ILE:H	18	0.1
(1,921)	1:85:A:ILE:HG23	1:85:A:ILE:H	18	0.1
(1,899)	1:125:A:ILE:HG12	1:122:A:ASP:HA	17	0.1
(1,899)	1:125:A:ILE:HG13	1:122:A:ASP:HA	17	0.1
(1,880)	1:5:A:THR:HA	1:6:A:GLU:HG2	14	0.1
(1,880)	1:5:A:THR:HA	1:6:A:GLU:HG3	14	0.1
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD21	16	0.1
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD22	16	0.1
(1,874)	1:38:A:SER:HA	1:105:A:LEU:HD23	16	0.1
(1,860)	1:142:A:VAL:HB	1:143:A:GLN:H	14	0.1
(1,860)	1:142:A:VAL:HB	1:143:A:GLN:H	15	0.1
(1,851)	1:25:A:GLY:HA2	1:23:A:GLY:H	2	0.1
(1,847)	1:33:A:GLY:HA3	1:34:A:THR:H	2	0.1
(1,847)	1:33:A:GLY:HA3	1:34:A:THR:H	4	0.1
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	7	0.1
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	11	0.1
(1,798)	1:73:A:ALA:HA	1:76:A:MET:H	13	0.1
(1,785)	1:147:A:ALA:HB1	1:144:A:MET:HA	1	0.1
(1,785)	1:147:A:ALA:HB2	1:144:A:MET:HA	1	0.1
(1,785)	1:147:A:ALA:HB3	1:144:A:MET:HA	1	0.1
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG11	6	0.1
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG12	6	0.1
(1,777)	1:116:A:LEU:HB2	1:121:A:VAL:HG13	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG11	6	0.1
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG12	6	0.1
(1,777)	1:116:A:LEU:HB3	1:121:A:VAL:HG13	6	0.1
(1,766)	1:20:A:ASP:HA	1:26:A:THR:HB	11	0.1
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	12	0.1
(1,764)	1:20:A:ASP:HA	1:21:A:LYS:HG2	15	0.1
(1,749)	1:55:A:VAL:HA	1:56:A:ASP:H	1	0.1
(1,739)	1:71:A:MET:HB2	1:70:A:THR:HA	19	0.1
(1,739)	1:71:A:MET:HB3	1:70:A:THR:HA	19	0.1
(1,679)	1:27:A:ILE:HB	1:28:A:THR:HB	10	0.1
(1,678)	1:27:A:ILE:HB	1:21:A:LYS:HD2	14	0.1
(1,678)	1:27:A:ILE:HB	1:21:A:LYS:HD3	14	0.1
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG2	17	0.1
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG3	17	0.1
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG2	17	0.1
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG3	17	0.1
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG2	17	0.1
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG3	17	0.1
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG2	18	0.1
(1,673)	1:117:A:THR:HG21	1:120:A:GLU:HG3	18	0.1
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG2	18	0.1
(1,673)	1:117:A:THR:HG22	1:120:A:GLU:HG3	18	0.1
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG2	18	0.1
(1,673)	1:117:A:THR:HG23	1:120:A:GLU:HG3	18	0.1
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB2	12	0.1
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB3	12	0.1
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB2	14	0.1
(1,654)	1:42:A:ASN:HA	1:37:A:ARG:HB3	14	0.1
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	6	0.1
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	6	0.1
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB2	7	0.1
(1,608)	1:10:A:ALA:HA	1:11:A:GLU:HB3	7	0.1
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	3	0.1
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	3	0.1
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	11	0.1
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	11	0.1
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG12	12	0.1
(1,598)	1:135:A:GLN:HA	1:125:A:ILE:HG13	12	0.1
(1,503)	1:110:A:THR:HB	1:112:A:LEU:H	4	0.1
(1,503)	1:110:A:THR:HB	1:112:A:LEU:H	5	0.1
(1,486)	1:127:A:GLU:HG2	1:126:A:ARG:HA	17	0.1
(1,486)	1:127:A:GLU:HG3	1:126:A:ARG:HA	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,476)	1:142:A:VAL:HG11	1:141:A:PHE:HA	3	0.1
(1,476)	1:142:A:VAL:HG12	1:141:A:PHE:HA	3	0.1
(1,476)	1:142:A:VAL:HG13	1:141:A:PHE:HA	3	0.1
(1,476)	1:142:A:VAL:HG11	1:141:A:PHE:HA	4	0.1
(1,476)	1:142:A:VAL:HG12	1:141:A:PHE:HA	4	0.1
(1,476)	1:142:A:VAL:HG13	1:141:A:PHE:HA	4	0.1
(1,476)	1:142:A:VAL:HG11	1:141:A:PHE:HA	5	0.1
(1,476)	1:142:A:VAL:HG12	1:141:A:PHE:HA	5	0.1
(1,476)	1:142:A:VAL:HG13	1:141:A:PHE:HA	5	0.1
(1,476)	1:142:A:VAL:HG11	1:141:A:PHE:HA	14	0.1
(1,476)	1:142:A:VAL:HG12	1:141:A:PHE:HA	14	0.1
(1,476)	1:142:A:VAL:HG13	1:141:A:PHE:HA	14	0.1
(1,476)	1:142:A:VAL:HG11	1:141:A:PHE:HA	16	0.1
(1,476)	1:142:A:VAL:HG12	1:141:A:PHE:HA	16	0.1
(1,476)	1:142:A:VAL:HG13	1:141:A:PHE:HA	16	0.1
(1,473)	1:142:A:VAL:HG11	1:145:A:MET:H	14	0.1
(1,473)	1:142:A:VAL:HG12	1:145:A:MET:H	14	0.1
(1,473)	1:142:A:VAL:HG13	1:145:A:MET:H	14	0.1
(1,473)	1:142:A:VAL:HG11	1:145:A:MET:H	18	0.1
(1,473)	1:142:A:VAL:HG12	1:145:A:MET:H	18	0.1
(1,473)	1:142:A:VAL:HG13	1:145:A:MET:H	18	0.1
(1,360)	1:53:A:ASN:HA	1:49:A:GLN:HA	11	0.1
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	1	0.1
(1,316)	1:26:A:THR:HA	1:62:A:THR:HA	10	0.1
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD11	1	0.1
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD12	1	0.1
(1,16)	1:136:A:VAL:HG11	1:125:A:ILE:HD13	1	0.1
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD11	1	0.1
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD12	1	0.1
(1,16)	1:136:A:VAL:HG12	1:125:A:ILE:HD13	1	0.1
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD11	1	0.1
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD12	1	0.1
(1,16)	1:136:A:VAL:HG13	1:125:A:ILE:HD13	1	0.1
(1,9)	1:17:A:SER:HB2	1:16:A:PHE:HA	17	0.1
(1,9)	1:17:A:SER:HB3	1:16:A:PHE:HA	17	0.1
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB2	13	0.1
(1,4)	1:100:A:ILE:HD11	1:101:A:SER:HB3	13	0.1
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB2	13	0.1
(1,4)	1:100:A:ILE:HD12	1:101:A:SER:HB3	13	0.1
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB2	13	0.1
(1,4)	1:100:A:ILE:HD13	1:101:A:SER:HB3	13	0.1

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

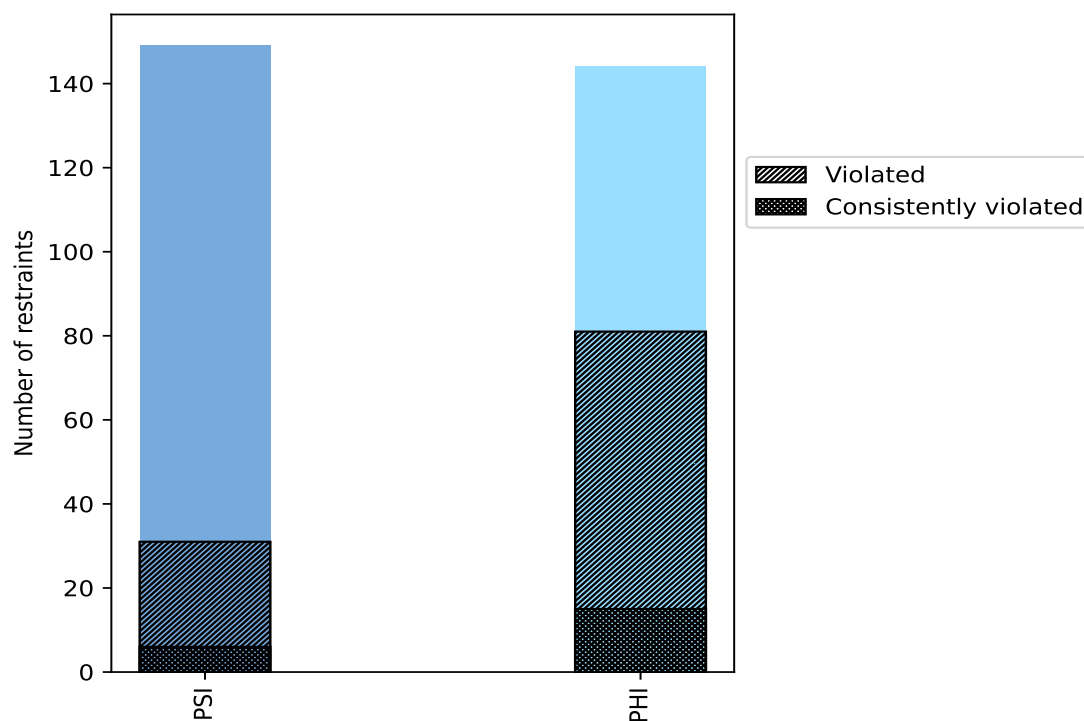
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	149	50.9	31	20.8	10.6	6	4.0	2.0
PHI	144	49.1	81	56.2	27.6	15	10.4	5.1
Total	293	100.0	112	38.2	38.2	21	7.2	7.2

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

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



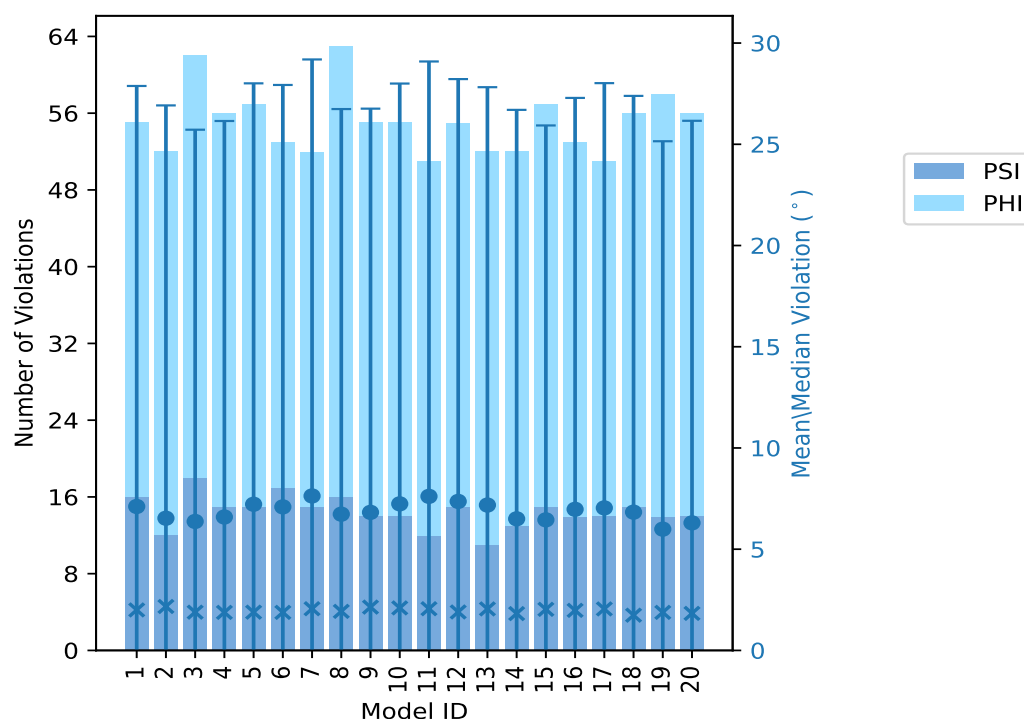
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	16	39	55	7.11	140.21	20.77	2.0
2	12	40	52	6.53	143.53	20.39	2.17
3	18	44	62	6.37	144.23	19.35	1.89
4	15	41	56	6.59	141.56	19.56	1.88
5	15	42	57	7.22	142.27	20.79	1.89
6	17	36	53	7.09	145.96	20.84	1.88
7	15	37	52	7.63	142.12	21.56	2.06
8	16	47	63	6.73	142.85	20.01	1.93
9	14	41	55	6.82	141.14	19.94	2.14
10	14	41	55	7.24	142.69	20.76	2.1
11	12	39	51	7.61	142.72	21.48	2.06
12	15	40	55	7.36	141.41	20.86	1.9
13	11	41	52	7.18	144.42	20.64	2.05
14	13	39	52	6.5	142.25	20.2	1.82
15	15	42	57	6.45	142.29	19.48	2.03
16	14	39	53	6.97	142.7	20.32	1.98
17	14	37	51	7.04	143.37	20.98	2.05
18	15	41	56	6.83	141.3	20.56	1.74
19	14	44	58	5.99	141.55	19.16	1.88
20	14	42	56	6.3	144.58	19.86	1.83

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
4	13	17	1	5.0
5	10	15	2	10.0
2	4	6	3	15.0
1	3	4	4	20.0
0	2	2	5	25.0
2	4	6	6	30.0
1	3	4	7	35.0
3	3	6	8	40.0
1	2	3	9	45.0
0	0	0	10	50.0
2	2	4	11	55.0

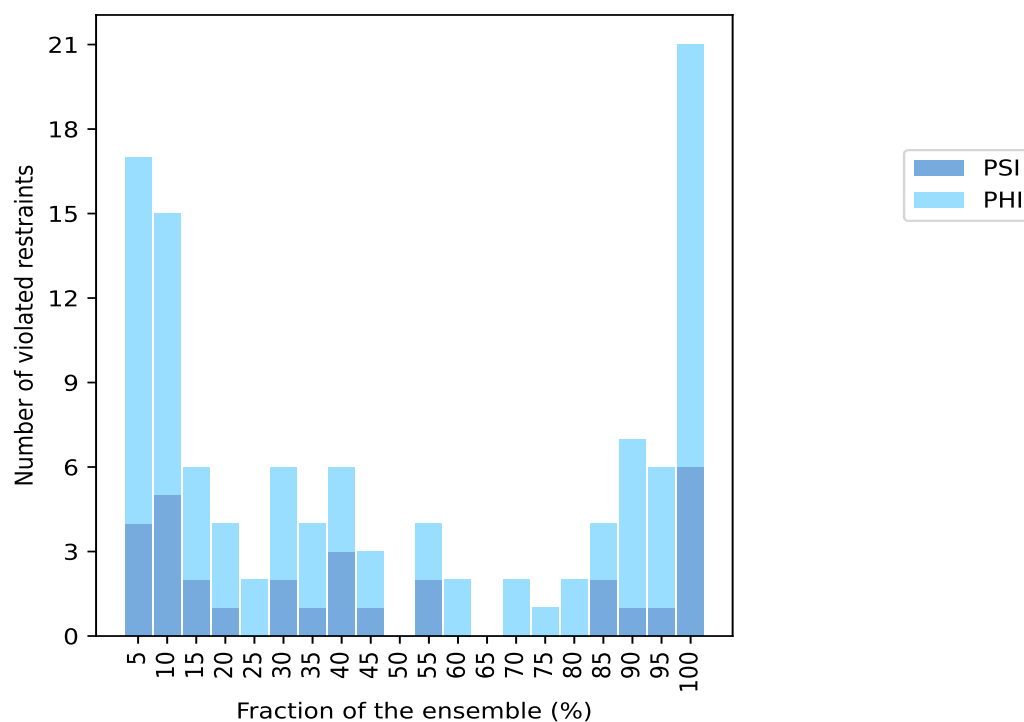
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	2	2	12	60.0
0	0	0	13	65.0
0	2	2	14	70.0
0	1	1	15	75.0
0	2	2	16	80.0
2	2	4	17	85.0
1	6	7	18	90.0
1	5	6	19	95.0
6	15	21	20	100.0

¹ Number of models with violations

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

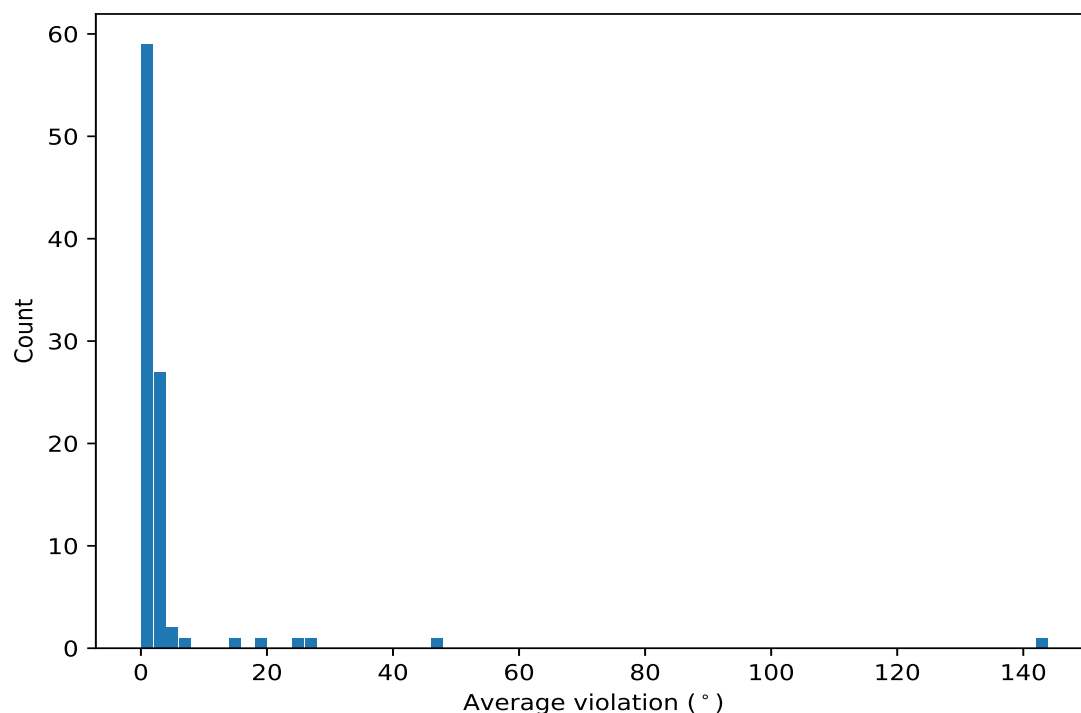


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	20	142.66	1.35	142.49
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	20	46.0	1.32	45.74
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	20	27.31	12.12	22.8
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	20	25.59	14.19	20.4
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	20	14.84	7.04	13.02
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	20	4.28	0.3	4.31
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	20	4.16	0.33	4.18
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	20	3.89	0.39	3.88
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	20	3.32	0.59	3.3
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	20	3.3	0.58	3.24
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	20	3.01	1.0	3.06
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	20	3.0	0.61	2.87
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	20	2.49	1.0	2.41
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	20	2.39	0.28	2.4
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	20	2.37	0.55	2.42
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	20	2.3	0.3	2.35
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	20	2.24	0.49	2.3
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	20	2.18	0.12	2.18
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	20	1.79	0.31	1.78
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	20	1.76	0.42	1.63

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	20	1.57	0.14	1.56
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	19	19.19	18.39	13.63
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	19	2.77	0.68	2.74
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	19	2.63	0.87	2.48
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	19	1.61	0.58	1.4
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	19	1.44	0.23	1.46
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	19	1.43	0.27	1.38
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	18	3.49	1.08	4.03
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	18	2.22	0.64	2.0
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	18	1.83	0.41	1.92
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	18	1.66	0.27	1.66
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	18	1.58	0.24	1.65
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	18	1.43	0.27	1.38
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	18	1.31	0.17	1.3
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	17	2.61	0.83	2.39
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	17	1.95	0.46	1.88
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	17	1.76	0.45	1.68
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	17	1.34	0.19	1.33
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	16	2.28	0.45	2.33
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	16	1.74	0.78	1.45
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	15	1.5	0.4	1.39
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	14	2.64	0.8	2.38
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	14	1.87	0.5	1.84
(1,34)	1:29:A:THR:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	12	1.78	0.49	1.84
(1,21)	1:16:A:PHE:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	12	1.23	0.19	1.12
(1,48)	1:44:A:THR:C	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	11	2.08	0.65	2.05
(1,92)	1:90:A:ARG:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	11	1.37	0.2	1.32
(1,270)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	11	1.22	0.13	1.19
(1,277)	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	1:132:A:GLY:N	11	1.11	0.18	1.04
(1,77)	1:74:A:ARG:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	9	1.38	0.53	1.13
(1,56)	1:53:A:ASN:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	9	1.25	0.29	1.05
(1,280)	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	1:135:A:GLN:N	9	1.2	0.17	1.13
(1,36)	1:31:A:GLU:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	8	3.54	1.12	4.04
(1,287)	1:141:A:PHE:N	1:141:A:PHE:CA	1:141:A:PHE:C	1:142:A:VAL:N	8	2.03	0.74	2.06
(1,256)	1:109:A:MET:N	1:109:A:MET:CA	1:109:A:MET:C	1:110:A:THR:N	8	1.61	0.31	1.62
(1,143)	1:143:A:GLN:C	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	8	1.42	0.23	1.45
(1,9)	1:7:A:GLU:C	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	8	1.36	0.19	1.37
(1,275)	1:128:A:ALA:N	1:128:A:ALA:CA	1:128:A:ALA:C	1:129:A:ASP:N	8	1.35	0.17	1.37
(1,180)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:LEU:N	7	3.27	1.08	3.36
(1,54)	1:51:A:MET:C	1:52:A:ILE:N	1:52:A:ILE:CA	1:52:A:ILE:C	7	1.81	0.6	1.77
(1,46)	1:42:A:ASN:C	1:43:A:PRO:N	1:43:A:PRO:CA	1:43:A:PRO:C	7	1.35	0.23	1.38
(1,70)	1:67:A:GLU:C	1:68:A:PHE:N	1:68:A:PHE:CA	1:68:A:PHE:C	7	1.22	0.34	1.09
(1,55)	1:52:A:ILE:C	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	6	2.0	0.76	1.6
(1,264)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:ASP:N	6	1.5	0.3	1.44
(1,124)	1:123:A:GLU:C	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	6	1.42	0.26	1.38
(1,91)	1:89:A:PHE:C	1:90:A:ARG:N	1:90:A:ARG:CA	1:90:A:ARG:C	6	1.32	0.28	1.28
(1,255)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:MET:N	6	1.27	0.16	1.25
(1,89)	1:86:A:ARG:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	6	1.25	0.18	1.27
(1,33)	1:28:A:THR:C	1:29:A:THR:N	1:29:A:THR:CA	1:29:A:THR:C	5	1.28	0.22	1.13
(1,11)	1:10:A:ALA:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	5	1.13	0.07	1.11
(1,51)	1:47:A:GLU:C	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	4	1.5	0.04	1.49

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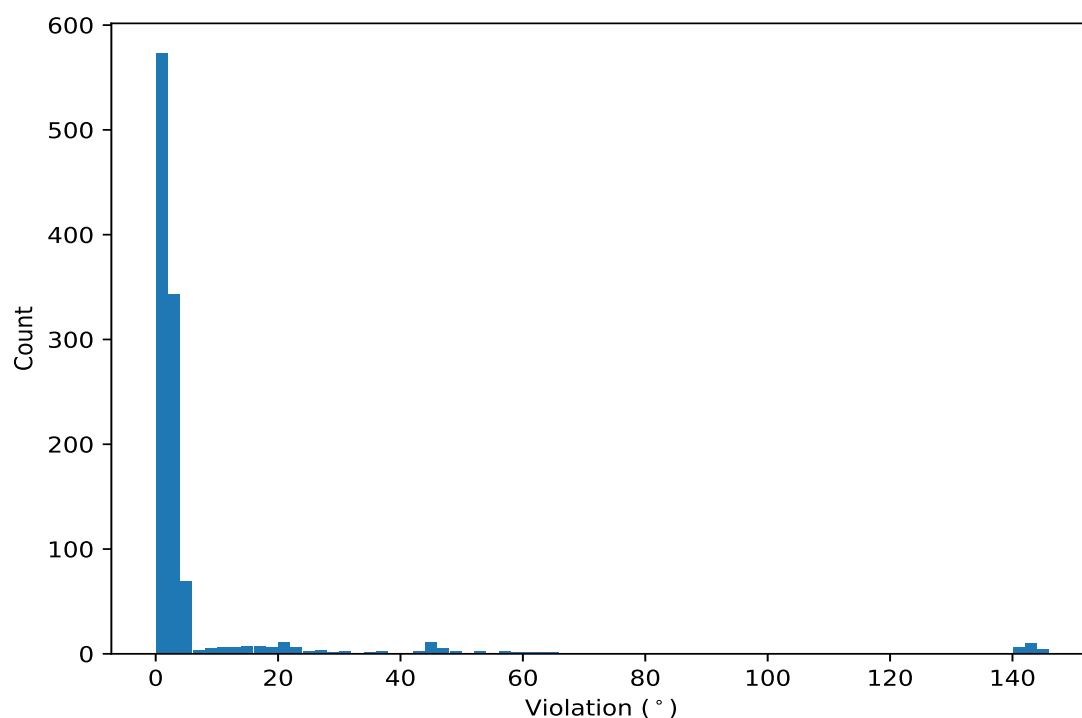
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,235)	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	1:88:A:ALA:N	4	1.4	0.29	1.39
(1,119)	1:118:A:ASP:C	1:119:A:GLU:N	1:119:A:GLU:CA	1:119:A:GLU:C	4	1.25	0.22	1.25
(1,17)	1:14:A:GLU:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	4	1.08	0.05	1.07
(1,145)	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	1:4:A:LEU:N	3	1.86	0.06	1.87
(1,6)	2:499:B:VAL:C	2:500:B:ALA:N	2:500:B:ALA:CA	2:500:B:ALA:C	3	1.78	0.4	1.69
(1,78)	1:75:A:LYS:C	1:76:A:MET:N	1:76:A:MET:CA	1:76:A:MET:C	3	1.5	0.27	1.67
(1,93)	1:91:A:VAL:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	3	1.34	0.16	1.43
(1,265)	1:118:A:ASP:N	1:118:A:ASP:CA	1:118:A:ASP:C	1:119:A:GLU:N	3	1.27	0.03	1.27
(1,71)	1:68:A:PHE:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	3	1.17	0.15	1.09
(1,4)	2:497:B:LYS:C	2:498:B:GLU:N	2:498:B:GLU:CA	2:498:B:GLU:C	2	6.69	4.8	6.69
(1,82)	1:79:A:THR:C	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	2	2.9	0.01	2.9
(1,227)	1:79:A:THR:N	1:79:A:THR:CA	1:79:A:THR:C	1:80:A:ASP:N	2	2.62	0.14	2.62
(1,285)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:GLU:N	2	2.56	0.07	2.56
(1,80)	1:77:A:LYS:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	2	2.22	0.28	2.22
(1,81)	1:78:A:ASP:C	1:79:A:THR:N	1:79:A:THR:CA	1:79:A:THR:C	2	1.82	0.07	1.82
(1,226)	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	1:79:A:THR:N	2	1.54	0.12	1.54
(1,258)	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	1:112:A:LEU:N	2	1.33	0.26	1.33
(1,251)	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	1:105:A:LEU:N	2	1.27	0.19	1.27
(1,84)	1:81:A:SER:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	2	1.25	0.15	1.25
(1,87)	1:84:A:GLU:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	2	1.11	0.01	1.11
(1,121)	1:120:A:GLU:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	2	1.08	0.04	1.08
(1,5)	1:5:A:THR:C	1:6:A:GLU:N	1:6:A:GLU:CA	1:6:A:GLU:C	2	1.07	0.04	1.07
(1,83)	1:80:A:ASP:C	1:81:A:SER:N	1:81:A:SER:CA	1:81:A:SER:C	2	1.06	0.03	1.06
(1,31)	1:26:A:THR:C	1:27:A:ILE:N	1:27:A:ILE:CA	1:27:A:ILE:C	2	1.04	0.02	1.04

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 (°)
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	6	145.96
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	20	144.58
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	13	144.42
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	3	144.23
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	2	143.53
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	17	143.37
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	8	142.85
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	11	142.72
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	16	142.7
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	10	142.69
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	15	142.29
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	5	142.27
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	14	142.25
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	7	142.12
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	4	141.56
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	19	141.55
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	12	141.41
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	18	141.3
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	9	141.14
(1,146)	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2:498:B:GLU:N	1	140.21
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	8	65.82

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	1	62.41
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	7	61.12
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	18	59.01
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	12	57.29
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	5	56.15
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	11	53.62
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	10	52.13
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	3	48.73
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	17	48.46
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	9	47.96
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	2	47.3
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	5	46.71
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	13	46.65
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	10	46.55
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	4	45.88
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	11	45.74
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	20	45.74
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	15	45.73
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	19	45.71
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	12	45.66
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	16	45.39
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	8	45.35
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	7	45.07
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	6	45.04
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	18	44.75
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	1	43.83
(1,2)	2:496:B:PHE:C	2:497:B:LYS:N	2:497:B:LYS:CA	2:497:B:LYS:C	14	43.74
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	17	37.53
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	5	36.99
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	9	34.0
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	6	31.83
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	16	31.8
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	3	29.45
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	3	27.66
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	7	26.18
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	15	26.15
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	8	25.96
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	1	24.68
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	20	23.76
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	10	23.65
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	13	23.18
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	3	22.94
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	12	22.17
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	14	22.16
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	9	21.95
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	4	21.6
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	19	21.55
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	13	21.39
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	6	21.33
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	12	21.29
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	19	21.28

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	11	20.48
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	4	20.33
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	16	20.27
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	15	20.23
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	2	19.91
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	14	19.91
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	6	19.78
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	12	19.43
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	4	18.95
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	18	18.87
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	10	17.69
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	5	17.43
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	13	16.76
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	2	16.14
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	7	16.09
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	16	16.03
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	6	16.0
(1,20)	2:509:B:LEU:C	2:510:B:MET:N	2:510:B:MET:CA	2:510:B:MET:C	11	15.7
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	8	15.69
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	11	15.53
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	20	14.93
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	15	14.74
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	18	14.68
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	10	14.62
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	20	13.87
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	4	13.63
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	9	12.68
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	17	12.32
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	3	12.18
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	17	12.05
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	14	11.97
(1,4)	2:497:B:LYS:C	2:498:B:GLU:N	2:498:B:GLU:CA	2:498:B:GLU:C	13	11.49
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	17	11.24
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	13	11.13
(1,14)	2:505:B:ILE:C	2:506:B:SER:N	2:506:B:SER:CA	2:506:B:SER:C	9	10.98
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	5	10.69
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	20	9.43
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	1	9.36
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	15	9.15
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	16	8.51
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	1	8.21
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	2	7.94
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	8	7.34
(1,18)	2:508:B:SER:C	2:509:B:LEU:N	2:509:B:LEU:CA	2:509:B:LEU:C	19	6.84
(1,36)	1:31:A:GLU:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	4	4.85
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	14	4.84
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	20	4.78
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	7	4.78
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	8	4.76
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	9	4.73
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	5	4.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	19	4.68
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	19	4.67
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	2	4.66
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	16	4.61
(1,180)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:LEU:N	9	4.58
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	11	4.55
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	16	4.55
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	6	4.54
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	2	4.54
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	15	4.53
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	1	4.51
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	19	4.49
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	7	4.48
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	18	4.47
(1,180)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:LEU:N	4	4.46
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	19	4.45
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	2	4.44
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	5	4.44
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	9	4.43
(1,36)	1:31:A:GLU:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	9	4.42
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	4	4.4
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	4	4.39
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	7	4.38
(1,266)	1:119:A:GLU:N	1:119:A:GLU:CA	1:119:A:GLU:C	1:120:A:GLU:N	7	4.38
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	10	4.38
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	4	4.37
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	11	4.37
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	13	4.37
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	10	4.36
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	7	4.35
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	12	4.32
(1,36)	1:31:A:GLU:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	16	4.32
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	13	4.3
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	15	4.3
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	13	4.3
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	8	4.26
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	9	4.25
(1,36)	1:31:A:GLU:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	13	4.25
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	11	4.24
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	17	4.24
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	13	4.22
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	18	4.22
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	16	4.21
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	20	4.18
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	2	4.17
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	8	4.16
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	15	4.15
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	16	4.13
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	13	4.13
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	17	4.13
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	16	4.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	17	4.1
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	2	4.09
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	1	4.08
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	14	4.08
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	6	4.06
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	16	4.05
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	12	4.03
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	1	4.01
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	17	4.0
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1	4.0
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	18	4.0
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	20	3.99
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	10	3.97
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	20	3.96
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	5	3.95
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	18	3.94
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	1	3.94
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	15	3.91
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	3	3.9
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	3	3.9
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	12	3.89
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	1	3.88
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	8	3.88
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	20	3.87
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	18	3.85
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	11	3.84
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	18	3.83
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	14	3.83
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	15	3.83
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	19	3.82
(1,36)	1:31:A:GLU:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	10	3.82
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	6	3.81
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	14	3.79
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	9	3.78
(1,180)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:LEU:N	13	3.78
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	8	3.78
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	12	3.78
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	19	3.77
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	11	3.77
(1,293)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:LYS:N	5	3.76
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	2	3.75
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	4	3.75
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	1	3.73
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	15	3.72
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	6	3.72
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	8	3.71
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	3	3.7
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	11	3.69
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	20	3.69
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	14	3.67
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	20	3.66

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	9	3.66
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	3	3.64
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	18	3.63
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	7	3.62
(1,48)	1:44:A:THR:C	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	1	3.62
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	4	3.59
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	9	3.59
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	2	3.59
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	18	3.57
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	3	3.56
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	8	3.56
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	7	3.56
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	16	3.56
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	5	3.55
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	20	3.55
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	7	3.51
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	14	3.5
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	10	3.5
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	17	3.49
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	8	3.49
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	11	3.48
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	8	3.48
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	18	3.47
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	19	3.46
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	3	3.46
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	6	3.46
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	8	3.45
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	15	3.42
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	17	3.41
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	11	3.41
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	2	3.41
(1,101)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	5	3.38
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	7	3.37
(1,180)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:LEU:N	16	3.36
(1,55)	1:52:A:ILE:C	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	9	3.36
(1,287)	1:141:A:PHE:N	1:141:A:PHE:CA	1:141:A:PHE:C	1:142:A:VAL:N	6	3.31
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	7	3.3
(1,180)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:LEU:N	10	3.24
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	5	3.24
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	16	3.24
(1,268)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:ASP:N	10	3.22
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	6	3.22
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	12	3.2
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	17	3.19
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	4	3.16
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	8	3.16
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	17	3.14
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	4	3.13
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	14	3.13
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	5	3.13
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	3	3.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	15	3.1
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	6	3.1
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	5	3.09
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	15	3.08
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	14	3.05
(1,36)	1:31:A:GLU:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	2	3.05
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	4	3.04
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	19	3.04
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	7	3.03
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	4	3.02
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	14	3.02
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	13	3.01
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	10	3.01
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	19	3.0
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	2	3.0
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	20	2.98
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	20	2.97
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	15	2.97
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	9	2.94
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	16	2.94
(1,287)	1:141:A:PHE:N	1:141:A:PHE:CA	1:141:A:PHE:C	1:142:A:VAL:N	1	2.91
(1,82)	1:79:A:THR:C	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	8	2.91
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	3	2.91
(1,82)	1:79:A:THR:C	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	19	2.89
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	12	2.89
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	20	2.88
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	11	2.88
(1,54)	1:51:A:MET:C	1:52:A:ILE:N	1:52:A:ILE:CA	1:52:A:ILE:C	15	2.86
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	18	2.85
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	3	2.85
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	12	2.85
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	14	2.84
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	6	2.83
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	7	2.82
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	8	2.82
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	2	2.81
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	18	2.8
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	19	2.8
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	11	2.8
(1,77)	1:74:A:ARG:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	1	2.8
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	4	2.79
(1,48)	1:44:A:THR:C	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	8	2.79
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	17	2.78
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	6	2.78
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	15	2.78
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	13	2.77
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	13	2.77
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	14	2.76
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	5	2.76
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	5	2.76
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	6	2.76

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,227)	1:79:A:THR:N	1:79:A:THR:CA	1:79:A:THR:C	1:80:A:ASP:N	8	2.75
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	17	2.75
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	6	2.74
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	14	2.74
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	12	2.73
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	17	2.73
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	8	2.72
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	8	2.72
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	10	2.72
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	20	2.7
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	5	2.7
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	18	2.7
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	16	2.69
(1,55)	1:52:A:ILE:C	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	4	2.69
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	17	2.68
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	3	2.67
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	19	2.67
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	8	2.67
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	4	2.67
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	1	2.66
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	12	2.65
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	9	2.65
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	15	2.65
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	14	2.64
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	8	2.64
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	6	2.64
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	19	2.64
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	7	2.64
(1,285)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:GLU:N	1	2.63
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	11	2.62
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	13	2.62
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	2	2.61
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	10	2.61
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	12	2.6
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	15	2.6
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	12	2.59
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	13	2.58
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	12	2.58
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	12	2.58
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	18	2.57
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	15	2.57
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	18	2.56
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	11	2.55
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	6	2.55
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	9	2.54
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	4	2.54
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	2	2.54
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	17	2.54
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	5	2.53
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	9	2.53
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	13	2.53

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	16	2.52
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	2	2.51
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	1	2.5
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	13	2.5
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	3	2.5
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	3	2.5
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	9	2.5
(1,285)	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	1:140:A:GLU:N	6	2.49
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	8	2.49
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	1	2.49
(1,80)	1:77:A:LYS:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	7	2.49
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	11	2.49
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	18	2.49
(1,227)	1:79:A:THR:N	1:79:A:THR:CA	1:79:A:THR:C	1:80:A:ASP:N	19	2.48
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	16	2.48
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	2	2.48
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	10	2.48
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	20	2.48
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	7	2.46
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	12	2.46
(1,34)	1:29:A:THR:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	15	2.46
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	20	2.45
(1,103)	1:102:A:ALA:C	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	9	2.45
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	3	2.45
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	3	2.44
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	7	2.44
(1,54)	1:51:A:MET:C	1:52:A:ILE:N	1:52:A:ILE:CA	1:52:A:ILE:C	2	2.44
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	19	2.42
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	14	2.42
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	16	2.42
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	2	2.42
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	9	2.41
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	6	2.41
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	4	2.4
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	3	2.4
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	12	2.4
(1,34)	1:29:A:THR:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	13	2.4
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	17	2.39
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	2	2.39
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	14	2.39
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	12	2.38
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	16	2.37
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	17	2.36
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	9	2.36
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	14	2.36
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	19	2.36
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	10	2.35
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	19	2.35
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	4	2.33
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	18	2.32
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	9	2.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	2	2.31
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	20	2.31
(1,6)	2:499:B:VAL:C	2:500:B:ALA:N	2:500:B:ALA:CA	2:500:B:ALA:C	1	2.31
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	7	2.3
(1,113)	1:112:A:LEU:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	10	2.3
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	8	2.3
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	3	2.29
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	7	2.29
(1,34)	1:29:A:THR:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	10	2.29
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	13	2.29
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	1	2.28
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	11	2.28
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	1	2.28
(1,48)	1:44:A:THR:C	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	3	2.28
(1,48)	1:44:A:THR:C	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	20	2.28
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	2	2.27
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	18	2.27
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	1	2.26
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	10	2.26
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	12	2.25
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	10	2.25
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	10	2.24
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	7	2.24
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	8	2.24
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	17	2.24
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	13	2.23
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	14	2.23
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	1	2.23
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	16	2.23
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	16	2.22
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	5	2.22
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	11	2.22
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	9	2.22
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	9	2.21
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	17	2.21
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	19	2.21
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	2	2.21
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	10	2.2
(1,287)	1:141:A:PHE:N	1:141:A:PHE:CA	1:141:A:PHE:C	1:142:A:VAL:N	8	2.19
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	4	2.19
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	8	2.18
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	11	2.18
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	1	2.17
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	19	2.17
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	9	2.17
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	3	2.17
(1,256)	1:109:A:MET:N	1:109:A:MET:CA	1:109:A:MET:C	1:110:A:THR:N	5	2.16
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	14	2.16
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	10	2.16
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	17	2.15
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	1	2.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	15	2.15
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	13	2.15
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	5	2.15
(1,287)	1:141:A:PHE:N	1:141:A:PHE:CA	1:141:A:PHE:C	1:142:A:VAL:N	15	2.14
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	9	2.14
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	15	2.14
(1,34)	1:29:A:THR:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	20	2.14
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	2	2.14
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	10	2.13
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	6	2.13
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	18	2.13
(1,65)	1:62:A:THR:C	1:63:A:ILE:N	1:63:A:ILE:CA	1:63:A:ILE:C	20	2.13
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	7	2.13
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	3	2.12
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	11	2.11
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	2	2.11
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	11	2.11
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	10	2.1
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	17	2.1
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	15	2.1
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	5	2.1
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	12	2.1
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	10	2.1
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	15	2.1
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	11	2.09
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	13	2.09
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	4	2.08
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	5	2.07
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	7	2.07
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	16	2.07
(1,48)	1:44:A:THR:C	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	11	2.06
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	7	2.06
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	19	2.05
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	12	2.05
(1,70)	1:67:A:GLU:C	1:68:A:PHE:N	1:68:A:PHE:CA	1:68:A:PHE:C	15	2.05
(1,48)	1:44:A:THR:C	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	17	2.05
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	14	2.05
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	6	2.04
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	6	2.04
(1,36)	1:31:A:GLU:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	15	2.03
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	4	2.02
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	9	2.02
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	19	2.01
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	13	2.01
(1,67)	1:64:A:ASP:C	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	15	2.01
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	3	2.0
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	3	2.0
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	1	2.0
(1,34)	1:29:A:THR:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	16	1.99
(1,15)	1:12:A:PHE:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	12	1.99
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	16	1.98

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,287)	1:141:A:PHE:N	1:141:A:PHE:CA	1:141:A:PHE:C	1:142:A:VAL:N	12	1.97
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	16	1.97
(1,34)	1:29:A:THR:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	9	1.97
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	11	1.97
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	2	1.96
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	9	1.96
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	16	1.96
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	16	1.96
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	19	1.96
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	3	1.96
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	20	1.95
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	7	1.95
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	3	1.95
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1	1.95
(1,264)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:ASP:N	8	1.94
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	10	1.94
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	5	1.94
(1,80)	1:77:A:LYS:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	15	1.94
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	5	1.94
(1,145)	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	1:4:A:LEU:N	3	1.93
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	7	1.93
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	4	1.93
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	8	1.93
(1,48)	1:44:A:THR:C	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	19	1.93
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	14	1.93
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	5	1.92
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	5	1.92
(1,124)	1:123:A:GLU:C	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	13	1.91
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	1	1.91
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	17	1.91
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	13	1.91
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	6	1.9
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	12	1.9
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	7	1.9
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	18	1.9
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	13	1.9
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	10	1.89
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	5	1.89
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	18	1.89
(1,180)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:LEU:N	2	1.89
(1,81)	1:78:A:ASP:C	1:79:A:THR:N	1:79:A:THR:CA	1:79:A:THR:C	19	1.89
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	3	1.89
(1,56)	1:53:A:ASN:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	20	1.89
(1,4)	2:497:B:LYS:C	2:498:B:GLU:N	2:498:B:GLU:CA	2:498:B:GLU:C	3	1.89
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	7	1.88
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	19	1.88
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	6	1.88
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	3	1.88
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	20	1.88
(1,91)	1:89:A:PHE:C	1:90:A:ARG:N	1:90:A:ARG:CA	1:90:A:ARG:C	4	1.88
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	19	1.87

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	19	1.87
(1,145)	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	1:4:A:LEU:N	13	1.87
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	18	1.87
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	4	1.87
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	16	1.85
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	5	1.85
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	3	1.84
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	16	1.84
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	19	1.84
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	14	1.83
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	15	1.83
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	20	1.83
(1,54)	1:51:A:MET:C	1:52:A:ILE:N	1:52:A:ILE:CA	1:52:A:ILE:C	7	1.83
(1,16)	2:506:B:SER:C	2:507:B:ALA:N	2:507:B:ALA:CA	2:507:B:ALA:C	7	1.83
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	10	1.82
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	20	1.82
(1,256)	1:109:A:MET:N	1:109:A:MET:CA	1:109:A:MET:C	1:110:A:THR:N	14	1.81
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	8	1.81
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	7	1.81
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	11	1.81
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	4	1.8
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	2	1.8
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	7	1.8
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	17	1.79
(1,145)	1:3:A:GLN:N	1:3:A:GLN:CA	1:3:A:GLN:C	1:4:A:LEU:N	1	1.79
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	17	1.79
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	12	1.79
(1,256)	1:109:A:MET:N	1:109:A:MET:CA	1:109:A:MET:C	1:110:A:THR:N	3	1.78
(1,143)	1:143:A:GLN:C	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	15	1.78
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	6	1.78
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	18	1.78
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	9	1.77
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	14	1.77
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	15	1.77
(1,54)	1:51:A:MET:C	1:52:A:ILE:N	1:52:A:ILE:CA	1:52:A:ILE:C	14	1.77
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	12	1.77
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	15	1.77
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1	1.77
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	19	1.77
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	2	1.76
(1,264)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:ASP:N	11	1.76
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	19	1.76
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	18	1.76
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	6	1.75
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	2	1.75
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	7	1.74
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	9	1.74
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	7	1.74
(1,90)	1:88:A:ALA:C	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	4	1.74
(1,81)	1:78:A:ASP:C	1:79:A:THR:N	1:79:A:THR:CA	1:79:A:THR:C	8	1.74
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	5	1.74

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	13	1.74
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	8	1.73
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	10	1.73
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	13	1.73
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	15	1.72
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	6	1.72
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	7	1.72
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	15	1.72
(1,235)	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	1:88:A:ALA:N	18	1.72
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	19	1.72
(1,34)	1:29:A:THR:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	4	1.72
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	14	1.71
(1,78)	1:75:A:LYS:C	1:76:A:MET:N	1:76:A:MET:CA	1:76:A:MET:C	10	1.71
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	3	1.7
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	2	1.69
(1,48)	1:44:A:THR:C	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	15	1.69
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	16	1.69
(1,6)	2:499:B:VAL:C	2:500:B:ALA:N	2:500:B:ALA:CA	2:500:B:ALA:C	14	1.69
(1,256)	1:109:A:MET:N	1:109:A:MET:CA	1:109:A:MET:C	1:110:A:THR:N	6	1.68
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	2	1.68
(1,46)	1:42:A:ASN:C	1:43:A:PRO:N	1:43:A:PRO:CA	1:43:A:PRO:C	1	1.68
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	13	1.68
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	17	1.68
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	18	1.67
(1,92)	1:90:A:ARG:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	5	1.67
(1,78)	1:75:A:LYS:C	1:76:A:MET:N	1:76:A:MET:CA	1:76:A:MET:C	8	1.67
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	14	1.67
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	16	1.67
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	3	1.67
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	10	1.67
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	12	1.67
(1,277)	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	1:132:A:GLY:N	14	1.66
(1,226)	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	1:79:A:THR:N	19	1.66
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	9	1.66
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	12	1.66
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	1	1.66
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	10	1.66
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	16	1.66
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	5	1.65
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	1	1.65
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	18	1.65
(1,235)	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	1:88:A:ALA:N	14	1.65
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	12	1.65
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	10	1.65
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	19	1.65
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	11	1.65
(1,21)	1:16:A:PHE:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	19	1.65
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	14	1.64
(1,120)	1:119:A:GLU:C	1:120:A:GLU:N	1:120:A:GLU:CA	1:120:A:GLU:C	7	1.64
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	17	1.64
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	9	1.64

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	14	1.64
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	10	1.64
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	2	1.64
(1,143)	1:143:A:GLN:C	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	11	1.63
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	13	1.63
(1,55)	1:52:A:ILE:C	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	16	1.63
(1,48)	1:44:A:THR:C	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	18	1.62
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	5	1.62
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	8	1.62
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	7	1.61
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	15	1.61
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	17	1.61
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	10	1.61
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	12	1.6
(1,92)	1:90:A:ARG:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	4	1.6
(1,46)	1:42:A:ASN:C	1:43:A:PRO:N	1:43:A:PRO:CA	1:43:A:PRO:C	13	1.6
(1,275)	1:128:A:ALA:N	1:128:A:ALA:CA	1:128:A:ALA:C	1:129:A:ASP:N	1	1.59
(1,258)	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	1:112:A:LEU:N	15	1.59
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	20	1.59
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	16	1.59
(1,33)	1:28:A:THR:C	1:29:A:THR:N	1:29:A:THR:CA	1:29:A:THR:C	5	1.59
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	6	1.59
(1,9)	1:7:A:GLU:C	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	4	1.59
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	20	1.58
(1,275)	1:128:A:ALA:N	1:128:A:ALA:CA	1:128:A:ALA:C	1:129:A:ASP:N	6	1.58
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	5	1.58
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	15	1.58
(1,92)	1:90:A:ARG:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	6	1.58
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	9	1.58
(1,9)	1:7:A:GLU:C	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	8	1.58
(1,180)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:LEU:N	3	1.57
(1,143)	1:143:A:GLN:C	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	12	1.57
(1,77)	1:74:A:ARG:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	2	1.57
(1,51)	1:47:A:GLU:C	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	3	1.57
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	6	1.57
(1,21)	1:16:A:PHE:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	17	1.57
(1,256)	1:109:A:MET:N	1:109:A:MET:CA	1:109:A:MET:C	1:110:A:THR:N	12	1.56
(1,255)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:MET:N	3	1.56
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	2	1.56
(1,55)	1:52:A:ILE:C	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	13	1.56
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	4	1.56
(1,36)	1:31:A:GLU:C	1:32:A:LEU:N	1:32:A:LEU:CA	1:32:A:LEU:C	3	1.56
(1,9)	1:7:A:GLU:C	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	9	1.56
(1,252)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:ARG:N	20	1.55
(1,89)	1:86:A:ARG:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	8	1.55
(1,54)	1:51:A:MET:C	1:52:A:ILE:N	1:52:A:ILE:CA	1:52:A:ILE:C	17	1.55
(1,34)	1:29:A:THR:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	8	1.55
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	18	1.55
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	10	1.54
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	8	1.54
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	8	1.53

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	1	1.53
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	11	1.53
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	18	1.53
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	13	1.53
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	12	1.53
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	11	1.53
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	13	1.53
(1,34)	1:29:A:THR:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	2	1.53
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	15	1.53
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	16	1.52
(1,264)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:ASP:N	15	1.52
(1,190)	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1:42:A:ASN:N	16	1.52
(1,124)	1:123:A:GLU:C	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	12	1.52
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	1	1.52
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	12	1.52
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	11	1.52
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	16	1.52
(1,280)	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	1:135:A:GLN:N	3	1.51
(1,256)	1:109:A:MET:N	1:109:A:MET:CA	1:109:A:MET:C	1:110:A:THR:N	18	1.51
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	11	1.51
(1,92)	1:90:A:ARG:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	10	1.51
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	6	1.51
(1,56)	1:53:A:ASN:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	3	1.51
(1,51)	1:47:A:GLU:C	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	20	1.51
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	5	1.51
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	19	1.51
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	4	1.5
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	4	1.5
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	9	1.5
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	16	1.5
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	20	1.5
(1,280)	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	1:135:A:GLN:N	4	1.49
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	17	1.49
(1,55)	1:52:A:ILE:C	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	10	1.49
(1,53)	1:49:A:GLN:C	1:50:A:ASP:N	1:50:A:ASP:CA	1:50:A:ASP:C	20	1.49
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	7	1.49
(1,33)	1:28:A:THR:C	1:29:A:THR:N	1:29:A:THR:CA	1:29:A:THR:C	13	1.49
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	17	1.49
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	10	1.48
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	9	1.48
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	12	1.48
(1,143)	1:143:A:GLN:C	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	8	1.48
(1,124)	1:123:A:GLU:C	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	4	1.48
(1,119)	1:118:A:ASP:C	1:119:A:GLU:N	1:119:A:GLU:CA	1:119:A:GLU:C	20	1.48
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	4	1.48
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	6	1.48
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	1	1.47
(1,93)	1:91:A:VAL:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	12	1.47
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	18	1.47
(1,51)	1:47:A:GLU:C	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	8	1.47
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	13	1.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	12	1.47
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	14	1.47
(1,287)	1:141:A:PHE:N	1:141:A:PHE:CA	1:141:A:PHE:C	1:142:A:VAL:N	3	1.46
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	17	1.46
(1,251)	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	1:105:A:LEU:N	13	1.46
(1,119)	1:118:A:ASP:C	1:119:A:GLU:N	1:119:A:GLU:CA	1:119:A:GLU:C	10	1.46
(1,51)	1:47:A:GLU:C	1:48:A:LEU:N	1:48:A:LEU:CA	1:48:A:LEU:C	1	1.46
(1,46)	1:42:A:ASN:C	1:43:A:PRO:N	1:43:A:PRO:CA	1:43:A:PRO:C	16	1.46
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	7	1.46
(1,270)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	16	1.45
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	14	1.45
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	9	1.45
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	3	1.45
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	5	1.45
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	15	1.45
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	13	1.45
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	2	1.44
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	12	1.44
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	14	1.44
(1,270)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	20	1.43
(1,226)	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	1:79:A:THR:N	8	1.43
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	7	1.43
(1,93)	1:91:A:VAL:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	1	1.43
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	10	1.42
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	18	1.42
(1,216)	1:67:A:GLU:N	1:67:A:GLU:CA	1:67:A:GLU:C	1:68:A:PHE:N	19	1.42
(1,143)	1:143:A:GLN:C	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	3	1.42
(1,92)	1:90:A:ARG:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	15	1.42
(1,77)	1:74:A:ARG:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	5	1.42
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	18	1.42
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	12	1.42
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	11	1.41
(1,275)	1:128:A:ALA:N	1:128:A:ALA:CA	1:128:A:ALA:C	1:129:A:ASP:N	5	1.41
(1,49)	1:45:A:GLU:C	1:46:A:ALA:N	1:46:A:ALA:CA	1:46:A:ALA:C	14	1.41
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	14	1.41
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	17	1.41
(1,141)	1:141:A:PHE:C	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	15	1.4
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	17	1.4
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	6	1.4
(1,84)	1:81:A:SER:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	19	1.4
(1,21)	1:16:A:PHE:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	15	1.4
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	12	1.39
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	11	1.39
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	2	1.39
(1,275)	1:128:A:ALA:N	1:128:A:ALA:CA	1:128:A:ALA:C	1:129:A:ASP:N	3	1.38
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	11	1.38
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	18	1.38
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	16	1.38
(1,71)	1:68:A:PHE:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	17	1.38
(1,46)	1:42:A:ASN:C	1:43:A:PRO:N	1:43:A:PRO:CA	1:43:A:PRO:C	6	1.38
(1,9)	1:7:A:GLU:C	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	3	1.38

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,264)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:ASP:N	4	1.37
(1,264)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:ASP:N	20	1.37
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	17	1.37
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	15	1.37
(1,56)	1:53:A:ASN:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	8	1.37
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	5	1.37
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	4	1.36
(1,275)	1:128:A:ALA:N	1:128:A:ALA:CA	1:128:A:ALA:C	1:129:A:ASP:N	9	1.36
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	4	1.36
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	18	1.36
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	20	1.36
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	4	1.36
(1,9)	1:7:A:GLU:C	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	18	1.36
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	6	1.35
(1,255)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:MET:N	6	1.35
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	11	1.35
(1,48)	1:44:A:THR:C	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	5	1.35
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	17	1.35
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	4	1.35
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	9	1.34
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	14	1.34
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	2	1.34
(1,89)	1:86:A:ARG:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	10	1.34
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	15	1.34
(1,56)	1:53:A:ASN:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	19	1.34
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	18	1.34
(1,6)	2:499:B:VAL:C	2:500:B:ALA:N	2:500:B:ALA:CA	2:500:B:ALA:C	20	1.34
(1,286)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:PHE:N	8	1.33
(1,270)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	9	1.33
(1,250)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:ALA:N	9	1.33
(1,144)	1:144:A:MET:C	1:145:A:MET:N	1:145:A:MET:CA	1:145:A:MET:C	18	1.33
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	13	1.33
(1,91)	1:89:A:PHE:C	1:90:A:ARG:N	1:90:A:ARG:CA	1:90:A:ARG:C	3	1.33
(1,89)	1:86:A:ARG:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	4	1.33
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	1	1.33
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	8	1.33
(1,256)	1:109:A:MET:N	1:109:A:MET:CA	1:109:A:MET:C	1:110:A:THR:N	4	1.32
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	2	1.32
(1,92)	1:90:A:ARG:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	11	1.32
(1,92)	1:90:A:ARG:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	19	1.32
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	17	1.32
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	18	1.32
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	10	1.32
(1,265)	1:118:A:ASP:N	1:118:A:ASP:CA	1:118:A:ASP:C	1:119:A:GLU:N	20	1.31
(1,143)	1:143:A:GLN:C	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	4	1.31
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	18	1.31
(1,92)	1:90:A:ARG:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	2	1.31
(1,91)	1:89:A:PHE:C	1:90:A:ARG:N	1:90:A:ARG:CA	1:90:A:ARG:C	8	1.31
(1,270)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	18	1.3
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	19	1.3
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	4	1.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	6	1.29
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	9	1.29
(1,124)	1:123:A:GLU:C	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	11	1.28
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	3	1.28
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	16	1.28
(1,34)	1:29:A:THR:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	3	1.28
(1,27)	1:22:A:ASP:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	1	1.28
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	11	1.27
(1,265)	1:118:A:ASP:N	1:118:A:ASP:CA	1:118:A:ASP:C	1:119:A:GLU:N	4	1.27
(1,255)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:MET:N	7	1.27
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	5	1.27
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	15	1.26
(1,91)	1:89:A:PHE:C	1:90:A:ARG:N	1:90:A:ARG:CA	1:90:A:ARG:C	14	1.26
(1,77)	1:74:A:ARG:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	15	1.26
(1,21)	1:16:A:PHE:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	6	1.26
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	15	1.25
(1,137)	1:137:A:ASN:C	1:138:A:TYR:N	1:138:A:TYR:CA	1:138:A:TYR:C	5	1.25
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	11	1.25
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	10	1.25
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	9	1.25
(1,22)	1:17:A:SER:C	1:18:A:LEU:N	1:18:A:LEU:CA	1:18:A:LEU:C	19	1.25
(1,9)	1:7:A:GLU:C	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	13	1.25
(1,280)	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	1:135:A:GLN:N	15	1.24
(1,270)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	14	1.24
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	5	1.24
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	16	1.24
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	20	1.24
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	2	1.24
(1,55)	1:52:A:ILE:C	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	20	1.24
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	3	1.23
(1,265)	1:118:A:ASP:N	1:118:A:ASP:CA	1:118:A:ASP:C	1:119:A:GLU:N	8	1.23
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	9	1.23
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	6	1.23
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	5	1.23
(1,11)	1:10:A:ALA:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	19	1.23
(1,255)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:MET:N	14	1.22
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	16	1.22
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	13	1.22
(1,48)	1:44:A:THR:C	1:45:A:GLU:N	1:45:A:GLU:CA	1:45:A:GLU:C	12	1.22
(1,287)	1:141:A:PHE:N	1:141:A:PHE:CA	1:141:A:PHE:C	1:142:A:VAL:N	11	1.21
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	1	1.21
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	13	1.21
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	20	1.21
(1,92)	1:90:A:ARG:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	16	1.21
(1,69)	1:66:A:PRO:C	1:67:A:GLU:N	1:67:A:GLU:CA	1:67:A:GLU:C	6	1.21
(1,11)	1:10:A:ALA:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	18	1.21
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	4	1.2
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	13	1.2
(1,275)	1:128:A:ALA:N	1:128:A:ALA:CA	1:128:A:ALA:C	1:129:A:ASP:N	17	1.2
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	8	1.2
(1,89)	1:86:A:ARG:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	17	1.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,21)	1:16:A:PHE:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	2	1.2
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	20	1.19
(1,270)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	5	1.19
(1,255)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:MET:N	5	1.19
(1,124)	1:123:A:GLU:C	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	8	1.19
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	15	1.19
(1,46)	1:42:A:ASN:C	1:43:A:PRO:N	1:43:A:PRO:CA	1:43:A:PRO:C	7	1.19
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	1	1.19
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	2	1.19
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	3	1.19
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	4	1.18
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	10	1.18
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	11	1.18
(1,290)	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	1:145:A:MET:N	18	1.17
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	3	1.17
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	19	1.17
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	20	1.17
(1,270)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	19	1.16
(1,124)	1:123:A:GLU:C	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	3	1.16
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	13	1.16
(1,54)	1:51:A:MET:C	1:52:A:ILE:N	1:52:A:ILE:CA	1:52:A:ILE:C	5	1.16
(1,46)	1:42:A:ASN:C	1:43:A:PRO:N	1:43:A:PRO:CA	1:43:A:PRO:C	17	1.16
(1,277)	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	1:132:A:GLY:N	16	1.15
(1,275)	1:128:A:ALA:N	1:128:A:ALA:CA	1:128:A:ALA:C	1:129:A:ASP:N	12	1.15
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	2	1.15
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	14	1.15
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	8	1.15
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	14	1.15
(1,17)	1:14:A:GLU:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	11	1.15
(1,280)	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	1:135:A:GLN:N	14	1.14
(1,275)	1:128:A:ALA:N	1:128:A:ALA:CA	1:128:A:ALA:C	1:129:A:ASP:N	15	1.14
(1,272)	1:125:A:ILE:N	1:125:A:ILE:CA	1:125:A:ILE:C	1:126:A:ARG:N	3	1.14
(1,143)	1:143:A:GLN:C	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	20	1.14
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	8	1.14
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	6	1.14
(1,111)	1:110:A:THR:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	8	1.14
(1,68)	1:65:A:PHE:C	1:66:A:PRO:N	1:66:A:PRO:CA	1:66:A:PRO:C	5	1.14
(1,280)	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	1:135:A:GLN:N	20	1.13
(1,270)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	10	1.13
(1,270)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	17	1.13
(1,235)	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	1:88:A:ALA:N	17	1.13
(1,121)	1:120:A:GLU:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	9	1.13
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1	1.13
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	18	1.13
(1,77)	1:74:A:ARG:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	13	1.13
(1,74)	1:71:A:MET:C	1:72:A:MET:N	1:72:A:MET:CA	1:72:A:MET:C	10	1.13
(1,70)	1:67:A:GLU:C	1:68:A:PHE:N	1:68:A:PHE:CA	1:68:A:PHE:C	10	1.13
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	4	1.13
(1,33)	1:28:A:THR:C	1:29:A:THR:N	1:29:A:THR:CA	1:29:A:THR:C	9	1.13
(1,21)	1:16:A:PHE:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	5	1.13
(1,9)	1:7:A:GLU:C	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	7	1.13

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,191)	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	1:43:A:PRO:N	10	1.12
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	9	1.12
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	17	1.12
(1,92)	1:90:A:ARG:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	7	1.12
(1,87)	1:84:A:GLU:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	8	1.12
(1,78)	1:75:A:LYS:C	1:76:A:MET:N	1:76:A:MET:CA	1:76:A:MET:C	19	1.12
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	20	1.12
(1,21)	1:16:A:PHE:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	8	1.12
(1,21)	1:16:A:PHE:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	13	1.12
(1,93)	1:91:A:VAL:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	3	1.11
(1,70)	1:67:A:GLU:C	1:68:A:PHE:N	1:68:A:PHE:CA	1:68:A:PHE:C	3	1.11
(1,40)	1:35:A:VAL:C	1:36:A:MET:N	1:36:A:MET:CA	1:36:A:MET:C	8	1.11
(1,23)	1:18:A:LEU:C	1:19:A:PHE:N	1:19:A:PHE:CA	1:19:A:PHE:C	2	1.11
(1,21)	1:16:A:PHE:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	9	1.11
(1,21)	1:16:A:PHE:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	16	1.11
(1,11)	1:10:A:ALA:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	12	1.11
(1,5)	1:5:A:THR:C	1:6:A:GLU:N	1:6:A:GLU:CA	1:6:A:GLU:C	19	1.11
(1,235)	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	1:88:A:ALA:N	1	1.1
(1,118)	1:117:A:THR:C	1:118:A:ASP:N	1:118:A:ASP:CA	1:118:A:ASP:C	8	1.1
(1,107)	1:106:A:ARG:C	1:107:A:HIS:N	1:107:A:HIS:CA	1:107:A:HIS:C	20	1.1
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	5	1.1
(1,91)	1:89:A:PHE:C	1:90:A:ARG:N	1:90:A:ARG:CA	1:90:A:ARG:C	6	1.1
(1,87)	1:84:A:GLU:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	19	1.1
(1,84)	1:81:A:SER:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	8	1.1
(1,77)	1:74:A:ARG:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	11	1.1
(1,33)	1:28:A:THR:C	1:29:A:THR:N	1:29:A:THR:CA	1:29:A:THR:C	4	1.1
(1,21)	1:16:A:PHE:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	1	1.1
(1,280)	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	1:135:A:GLN:N	8	1.09
(1,280)	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	1:135:A:GLN:N	13	1.09
(1,277)	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	1:132:A:GLY:N	7	1.09
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1	1.09
(1,83)	1:80:A:ASP:C	1:81:A:SER:N	1:81:A:SER:CA	1:81:A:SER:C	8	1.09
(1,71)	1:68:A:PHE:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	1	1.09
(1,70)	1:67:A:GLU:C	1:68:A:PHE:N	1:68:A:PHE:CA	1:68:A:PHE:C	18	1.09
(1,37)	1:32:A:LEU:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	9	1.09
(1,17)	1:14:A:GLU:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	20	1.09
(1,287)	1:141:A:PHE:N	1:141:A:PHE:CA	1:141:A:PHE:C	1:142:A:VAL:N	4	1.08
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	8	1.08
(1,279)	1:133:A:ASP:N	1:133:A:ASP:CA	1:133:A:ASP:C	1:134:A:GLY:N	12	1.08
(1,277)	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	1:132:A:GLY:N	10	1.08
(1,277)	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	1:132:A:GLY:N	17	1.08
(1,77)	1:74:A:ARG:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	20	1.08
(1,33)	1:28:A:THR:C	1:29:A:THR:N	1:29:A:THR:CA	1:29:A:THR:C	3	1.08
(1,11)	1:10:A:ALA:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	5	1.08
(1,270)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	1	1.07
(1,251)	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	1:105:A:LEU:N	3	1.07
(1,143)	1:143:A:GLN:C	1:144:A:MET:N	1:144:A:MET:CA	1:144:A:MET:C	6	1.07
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	10	1.07
(1,104)	1:103:A:ALA:C	1:104:A:GLU:N	1:104:A:GLU:CA	1:104:A:GLU:C	20	1.07
(1,89)	1:86:A:ARG:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	19	1.07
(1,77)	1:74:A:ARG:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	14	1.07

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,54)	1:51:A:MET:C	1:52:A:ILE:N	1:52:A:ILE:CA	1:52:A:ILE:C	18	1.07
(1,25)	1:20:A:ASP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	2	1.07
(1,9)	1:7:A:GLU:C	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	17	1.07
(1,280)	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	1:135:A:GLN:N	11	1.06
(1,258)	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	1:112:A:LEU:N	12	1.06
(1,135)	1:135:A:GLN:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	15	1.06
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	7	1.06
(1,31)	1:26:A:THR:C	1:27:A:ILE:N	1:27:A:ILE:CA	1:27:A:ILE:C	12	1.06
(1,280)	1:134:A:GLY:N	1:134:A:GLY:CA	1:134:A:GLY:C	1:135:A:GLN:N	1	1.05
(1,256)	1:109:A:MET:N	1:109:A:MET:CA	1:109:A:MET:C	1:110:A:THR:N	7	1.05
(1,70)	1:67:A:GLU:C	1:68:A:PHE:N	1:68:A:PHE:CA	1:68:A:PHE:C	11	1.05
(1,56)	1:53:A:ASN:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	6	1.05
(1,35)	1:30:A:LYS:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	14	1.05
(1,17)	1:14:A:GLU:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	19	1.05
(1,277)	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	1:132:A:GLY:N	6	1.04
(1,255)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:MET:N	18	1.04
(1,253)	1:106:A:ARG:N	1:106:A:ARG:CA	1:106:A:ARG:C	1:107:A:HIS:N	16	1.04
(1,121)	1:120:A:GLU:C	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	19	1.04
(1,119)	1:118:A:ASP:C	1:119:A:GLU:N	1:119:A:GLU:CA	1:119:A:GLU:C	18	1.04
(1,102)	1:101:A:SER:C	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	10	1.04
(1,71)	1:68:A:PHE:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	12	1.04
(1,70)	1:67:A:GLU:C	1:68:A:PHE:N	1:68:A:PHE:CA	1:68:A:PHE:C	14	1.04
(1,70)	1:67:A:GLU:C	1:68:A:PHE:N	1:68:A:PHE:CA	1:68:A:PHE:C	20	1.04
(1,44)	1:40:A:GLY:C	1:41:A:GLN:N	1:41:A:GLN:CA	1:41:A:GLN:C	11	1.04
(1,11)	1:10:A:ALA:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	3	1.04
(1,277)	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	1:132:A:GLY:N	2	1.03
(1,277)	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	1:132:A:GLY:N	18	1.03
(1,270)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	6	1.03
(1,83)	1:80:A:ASP:C	1:81:A:SER:N	1:81:A:SER:CA	1:81:A:SER:C	19	1.03
(1,77)	1:74:A:ARG:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	6	1.03
(1,57)	1:54:A:GLU:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	9	1.03
(1,56)	1:53:A:ASN:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	11	1.03
(1,34)	1:29:A:THR:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	7	1.03
(1,31)	1:26:A:THR:C	1:27:A:ILE:N	1:27:A:ILE:CA	1:27:A:ILE:C	1	1.03
(1,5)	1:5:A:THR:C	1:6:A:GLU:N	1:6:A:GLU:CA	1:6:A:GLU:C	5	1.03
(1,277)	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	1:132:A:GLY:N	5	1.02
(1,92)	1:90:A:ARG:C	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	12	1.02
(1,89)	1:86:A:ARG:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	3	1.02
(1,86)	1:83:A:GLU:C	1:84:A:GLU:N	1:84:A:GLU:CA	1:84:A:GLU:C	4	1.02
(1,56)	1:53:A:ASN:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	2	1.02
(1,56)	1:53:A:ASN:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	5	1.02
(1,21)	1:16:A:PHE:C	1:17:A:SER:N	1:17:A:SER:CA	1:17:A:SER:C	20	1.02
(1,17)	1:14:A:GLU:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	5	1.02
(1,277)	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	1:132:A:GLY:N	9	1.01
(1,277)	1:131:A:ASP:N	1:131:A:ASP:CA	1:131:A:ASP:C	1:132:A:GLY:N	12	1.01
(1,264)	1:117:A:THR:N	1:117:A:THR:CA	1:117:A:THR:C	1:118:A:ASP:N	7	1.01
(1,139)	1:139:A:GLU:C	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	6	1.01
(1,136)	1:136:A:VAL:C	1:137:A:ASN:N	1:137:A:ASN:CA	1:137:A:ASN:C	20	1.01
(1,119)	1:118:A:ASP:C	1:119:A:GLU:N	1:119:A:GLU:CA	1:119:A:GLU:C	9	1.01
(1,91)	1:89:A:PHE:C	1:90:A:ARG:N	1:90:A:ARG:CA	1:90:A:ARG:C	1	1.01
(1,56)	1:53:A:ASN:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	14	1.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,52)	1:48:A:LEU:C	1:49:A:GLN:N	1:49:A:GLN:CA	1:49:A:GLN:C	1	1.01
(1,50)	1:46:A:ALA:C	1:47:A:GLU:N	1:47:A:GLU:CA	1:47:A:GLU:C	15	1.01
(1,38)	1:33:A:GLY:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	16	1.01
(1,34)	1:29:A:THR:C	1:30:A:LYS:N	1:30:A:LYS:CA	1:30:A:LYS:C	18	1.01
(1,128)	1:128:A:ALA:C	1:129:A:ASP:N	1:129:A:ASP:CA	1:129:A:ASP:C	19	1.0
(1,114)	1:113:A:GLY:C	1:114:A:GLU:N	1:114:A:GLU:CA	1:114:A:GLU:C	18	1.0
(1,108)	1:107:A:HIS:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	12	1.0
(1,46)	1:42:A:ASN:C	1:43:A:PRO:N	1:43:A:PRO:CA	1:43:A:PRO:C	19	1.0
(1,41)	1:36:A:MET:C	1:37:A:ARG:N	1:37:A:ARG:CA	1:37:A:ARG:C	16	1.0