Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 10:49 AM EDT

PDB ID	:	2NB1
BMRB ID	:	25958
Title	:	P63/p73 hetero-tetramerisation domain
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Deposited on	:	2016-01-19

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 (i) 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 (i)) were used in the production of this report:

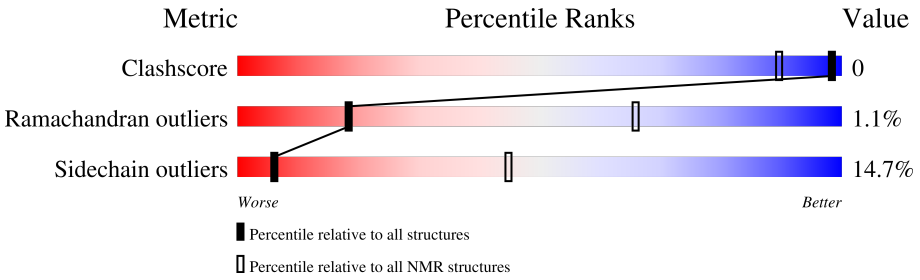
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 86%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	60	65% · 32%
1	C	60	67% · 32%
2	B	50	82% · 14%
2	D	50	78% 8% 14%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:4-A:32, B:98-B:140, C:1004-C:1032, D:1098-D:1140 (144)	0.84	3
2	A:35-A:46 (12)	0.30	17
3	C:1035-C:1046 (12)	0.32	3

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3732 atoms, of which 1862 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tumor protein 63.

Mol	Chain	Residues	Atoms						Trace
1	A	60	Total	C	H	N	O	S	0
			1016	320	503	89	102	2	
1	C	60	Total	C	H	N	O	S	0
			1016	320	503	89	102	2	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9H3D4
A	21	GLU	LYS	engineered mutation	UNP Q9H3D4
C	1001	SER	-	expression tag	UNP Q9H3D4
C	1021	GLU	LYS	engineered mutation	UNP Q9H3D4

- Molecule 2 is a protein called Tumor protein p73.

Mol	Chain	Residues	Atoms						Trace
2	B	50	Total	C	H	N	O	S	0
			850	266	428	73	81	2	
2	D	50	Total	C	H	N	O	S	0
			850	266	428	73	81	2	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	93	GLY	-	expression tag	UNP O15350
B	94	SER	-	expression tag	UNP O15350
B	107	LYS	GLU	engineered mutation	UNP O15350
D	1093	GLY	-	expression tag	UNP O15350
D	1094	SER	-	expression tag	UNP O15350
D	1107	LYS	GLU	engineered mutation	UNP O15350

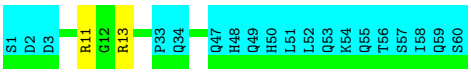
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

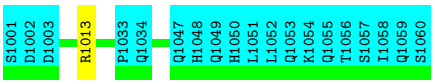
• Molecule 1: Tumor protein 63

Chain A:



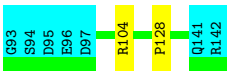
• Molecule 1: Tumor protein 63

Chain C:



• Molecule 2: Tumor protein p73

Chain B:



• Molecule 2: Tumor protein p73

Chain D:

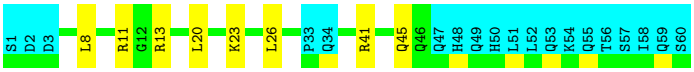
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

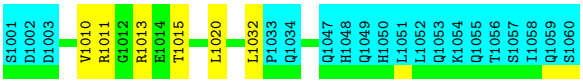
• Molecule 1: Tumor protein 63

Chain A:



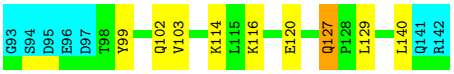
• Molecule 1: Tumor protein 63

Chain C:



• Molecule 2: Tumor protein p73

Chain B:



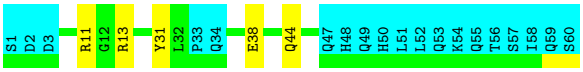
• Molecule 2: Tumor protein p73

Chain D:

4.2.2 Score per residue for model 2

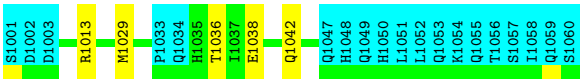
• Molecule 1: Tumor protein 63

Chain A:



• Molecule 1: Tumor protein 63

Chain C:



• Molecule 2: Tumor protein p73

Chain B:

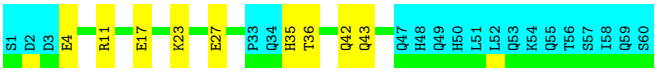
• Molecule 2: Tumor protein p73

Chain D:

4.2.3 Score per residue for model 3 (medoid)

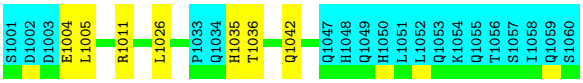
• Molecule 1: Tumor protein 63

Chain A:



• Molecule 1: Tumor protein 63

Chain C:



• Molecule 2: Tumor protein p73

Chain B:

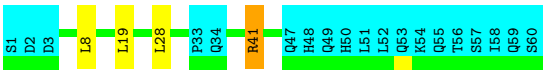
• Molecule 2: Tumor protein p73

Chain D:

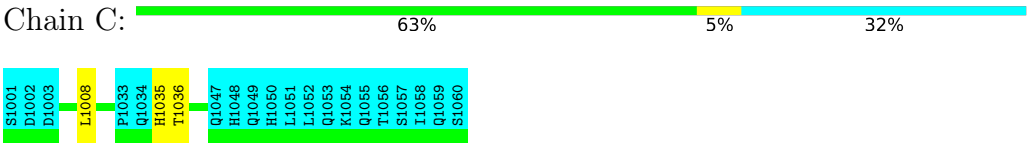
4.2.4 Score per residue for model 4

• Molecule 1: Tumor protein 63

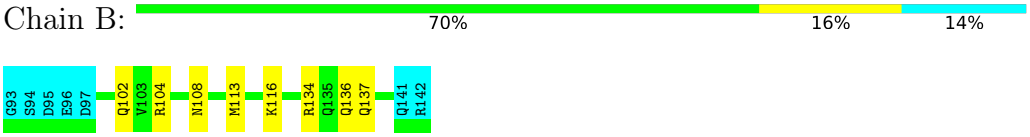
Chain A:



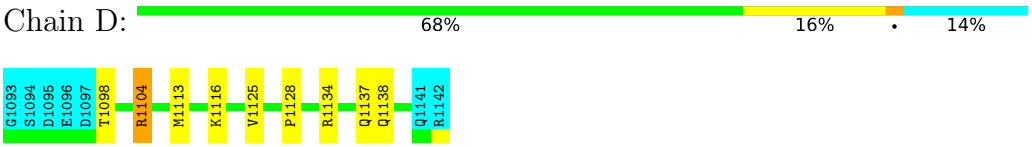
• Molecule 1: Tumor protein 63



• Molecule 2: Tumor protein p73

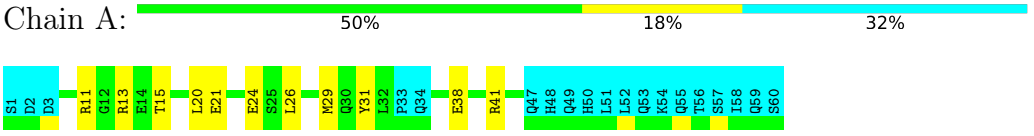


• Molecule 2: Tumor protein p73

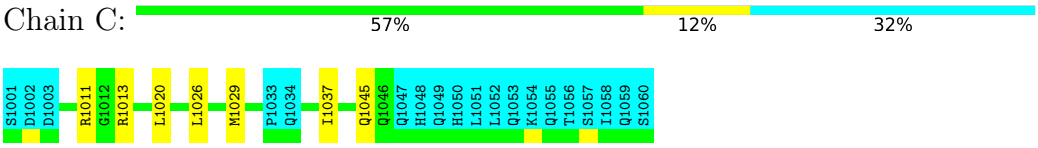


4.2.5 Score per residue for model 5

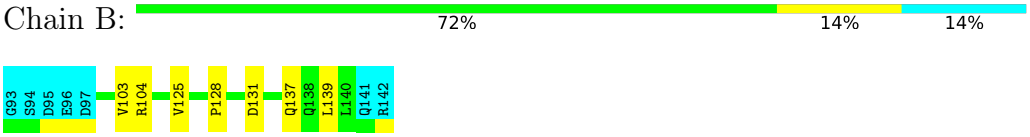
• Molecule 1: Tumor protein 63



• Molecule 1: Tumor protein 63

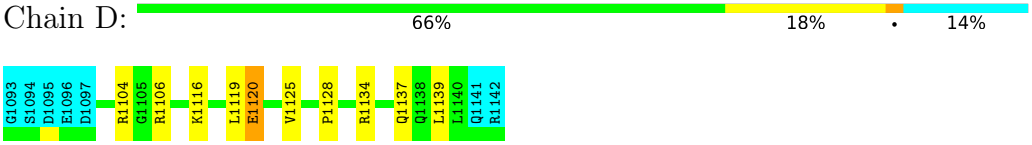


• Molecule 2: Tumor protein p73



• Molecule 2: Tumor protein p73

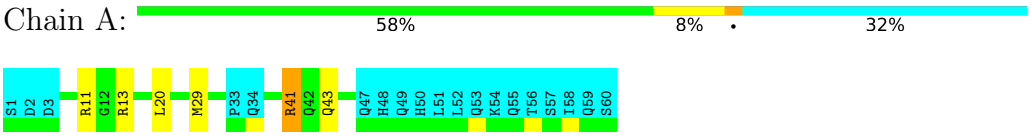
Chain D:



4.2.6 Score per residue for model 6

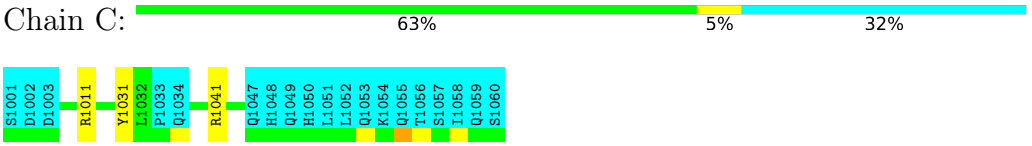
• Molecule 1: Tumor protein 63

Chain A:



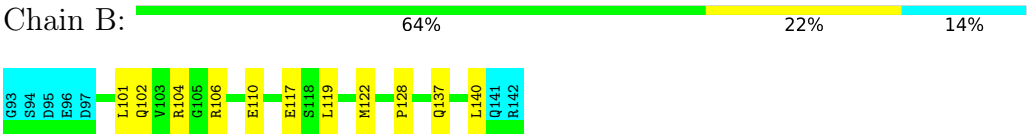
• Molecule 1: Tumor protein 63

Chain C:



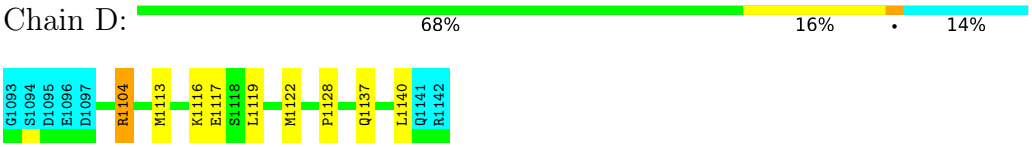
• Molecule 2: Tumor protein p73

Chain B:



• Molecule 2: Tumor protein p73

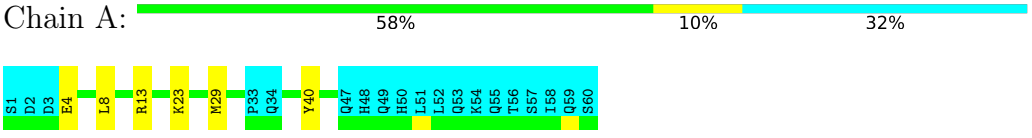
Chain D:



4.2.7 Score per residue for model 7

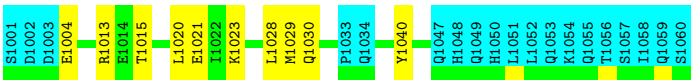
• Molecule 1: Tumor protein 63

Chain A:



• Molecule 1: Tumor protein 63

Chain C:



• Molecule 2: Tumor protein p73

Chain B:

• Molecule 2: Tumor protein p73

Chain D:

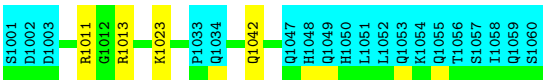
4.2.8 Score per residue for model 8

• Molecule 1: Tumor protein 63

Chain A:

• Molecule 1: Tumor protein 63

Chain C:

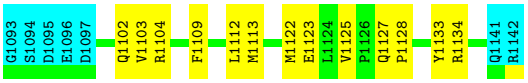


• Molecule 2: Tumor protein p73

Chain B:

• Molecule 2: Tumor protein p73

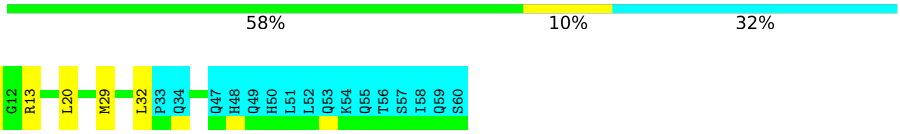
Chain D:



4.2.9 Score per residue for model 9

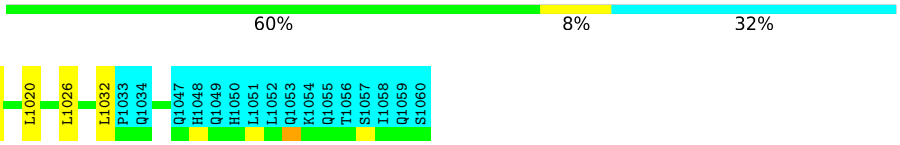
• Molecule 1: Tumor protein 63

Chain A:



• Molecule 1: Tumor protein 63

Chain C:



• Molecule 2: Tumor protein p73

Chain B:

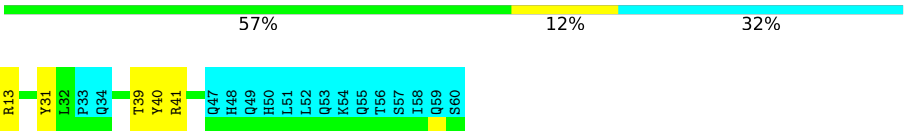
• Molecule 2: Tumor protein p73

Chain D:

4.2.10 Score per residue for model 10

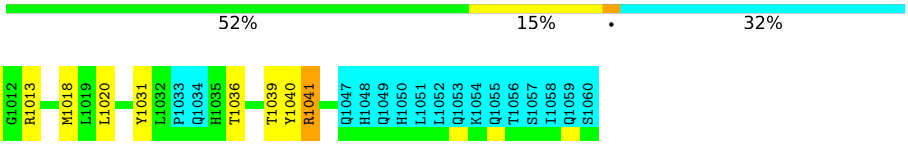
• Molecule 1: Tumor protein 63

Chain A:



• Molecule 1: Tumor protein 63

Chain C:



• Molecule 2: Tumor protein p73

Chain B:

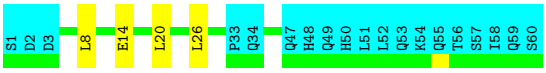
• Molecule 2: Tumor protein p73

Chain D:

4.2.11 Score per residue for model 11

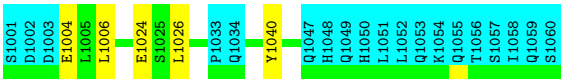
• Molecule 1: Tumor protein 63

Chain A:



• Molecule 1: Tumor protein 63

Chain C:

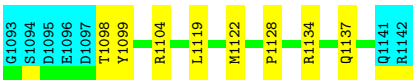


• Molecule 2: Tumor protein p73

Chain B:

• Molecule 2: Tumor protein p73

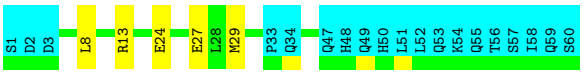
Chain D:



4.2.12 Score per residue for model 12

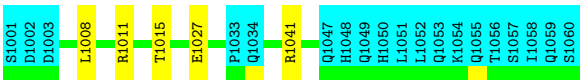
• Molecule 1: Tumor protein 63

Chain A:



• Molecule 1: Tumor protein 63

Chain C:

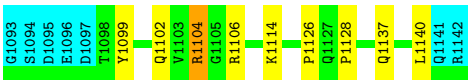


• Molecule 2: Tumor protein p73

Chain B:

• Molecule 2: Tumor protein p73

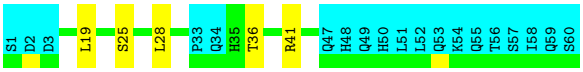
Chain D:



4.2.13 Score per residue for model 13

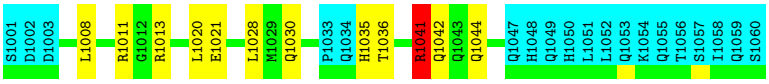
• Molecule 1: Tumor protein 63

Chain A:



• Molecule 1: Tumor protein 63

Chain C:

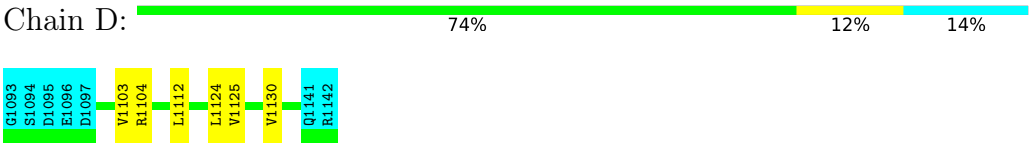


• Molecule 2: Tumor protein p73

Chain B:

• Molecule 2: Tumor protein p73

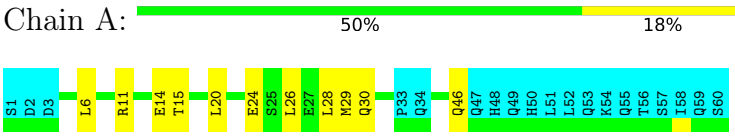
Chain D:



4.2.14 Score per residue for model 14

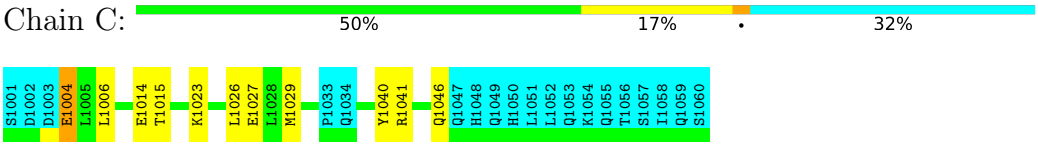
• Molecule 1: Tumor protein 63

Chain A:



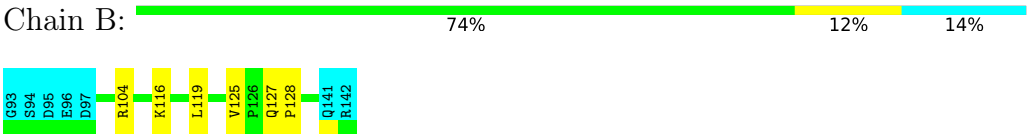
• Molecule 1: Tumor protein 63

Chain C:



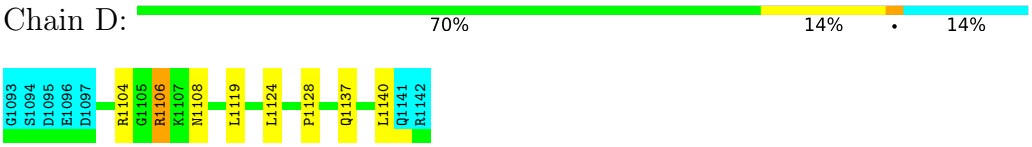
• Molecule 2: Tumor protein p73

Chain B:



• Molecule 2: Tumor protein p73

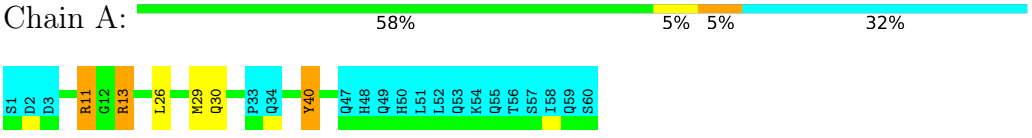
Chain D:



4.2.15 Score per residue for model 15

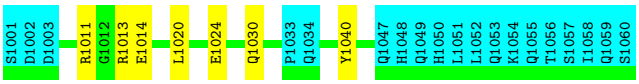
• Molecule 1: Tumor protein 63

Chain A:



• Molecule 1: Tumor protein 63

Chain C:



• Molecule 2: Tumor protein p73

Chain B:

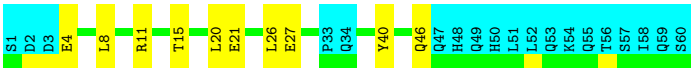
• Molecule 2: Tumor protein p73

Chain D:

4.2.16 Score per residue for model 16

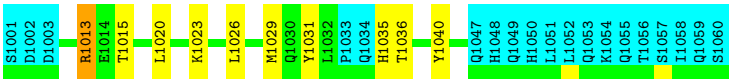
• Molecule 1: Tumor protein 63

Chain A:



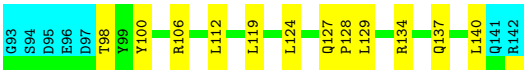
• Molecule 1: Tumor protein 63

Chain C:



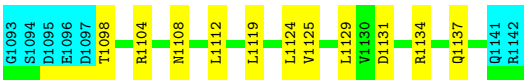
• Molecule 2: Tumor protein p73

Chain B:



• Molecule 2: Tumor protein p73

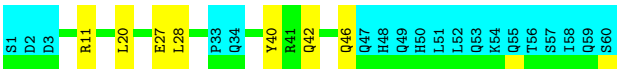
Chain D:



4.2.17 Score per residue for model 17

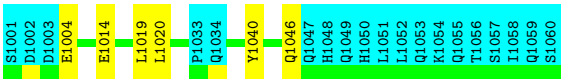
• Molecule 1: Tumor protein 63

Chain A:



• Molecule 1: Tumor protein 63

Chain C:

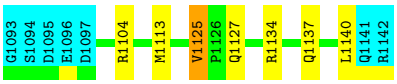


• Molecule 2: Tumor protein p73

Chain B:

• Molecule 2: Tumor protein p73

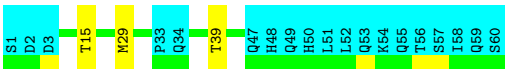
Chain D:



4.2.18 Score per residue for model 18

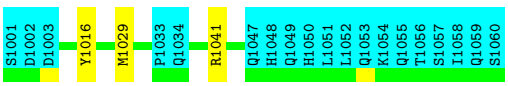
• Molecule 1: Tumor protein 63

Chain A:



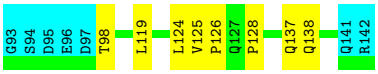
• Molecule 1: Tumor protein 63

Chain C:



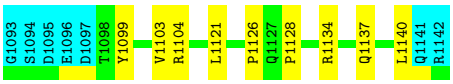
• Molecule 2: Tumor protein p73

Chain B:



• Molecule 2: Tumor protein p73

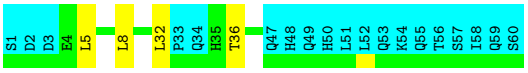
Chain D:



4.2.19 Score per residue for model 19

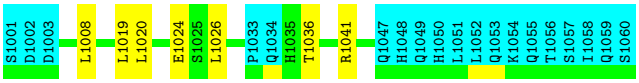
• Molecule 1: Tumor protein 63

Chain A:



• Molecule 1: Tumor protein 63

Chain C:

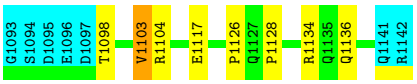


• Molecule 2: Tumor protein p73

Chain B:

• Molecule 2: Tumor protein p73

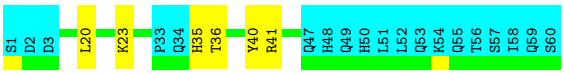
Chain D:



4.2.20 Score per residue for model 20

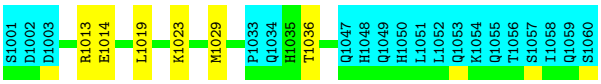
• Molecule 1: Tumor protein 63

Chain A:



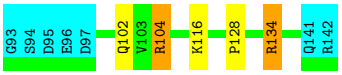
• Molecule 1: Tumor protein 63

Chain C:



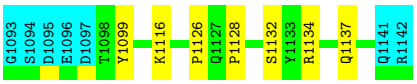
• Molecule 2: Tumor protein p73

Chain B:



• Molecule 2: Tumor protein p73

Chain D:



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	3.97
OPALp	refinement	1.4

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2706
Number of shifts mapped to atoms	2706
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.64±0.01	0±0/364 (0.0± 0.0%)	0.95±0.04	0±0/492 (0.0± 0.1%)
1	C	0.64±0.01	0±0/364 (0.0± 0.0%)	0.96±0.04	0±1/492 (0.1± 0.1%)
2	B	0.63±0.01	0±0/373 (0.0± 0.0%)	0.99±0.04	0±0/502 (0.1± 0.1%)
2	D	0.63±0.01	0±0/373 (0.0± 0.0%)	0.98±0.05	0±1/502 (0.1± 0.1%)
All	All	0.64	0/29480 (0.0%)	0.97	26/39760 (0.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.7±0.7
1	C	0.0±0.0	0.5±0.6
2	B	0.0±0.0	0.5±0.6
2	D	0.0±0.0	0.6±0.7
All	All	0	45

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	104	ARG	NE-CZ-NH2	-7.33	116.63	120.30	12	3
2	D	1104	ARG	NE-CZ-NH2	-7.27	116.67	120.30	4	4
2	B	106	ARG	NE-CZ-NH2	-6.52	117.04	120.30	6	1
2	D	1125	VAL	CA-CB-CG1	6.03	119.95	110.90	13	2
1	C	1011	ARG	NE-CZ-NH2	-5.66	117.47	120.30	12	1
1	A	41	ARG	NE-CZ-NH2	-5.51	117.55	120.30	20	1
2	B	133	TYR	CB-CG-CD1	-5.49	117.71	121.00	8	1
1	C	1013	ARG	NE-CZ-NH2	-5.38	117.61	120.30	16	3
2	D	1106	ARG	NE-CZ-NH2	-5.36	117.62	120.30	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	C	1041	ARG	NE-CZ-NH1	5.36	122.98	120.30	13	1
2	D	1133	TYR	CB-CG-CD1	-5.21	117.87	121.00	1	2
2	B	100	TYR	CB-CG-CD1	-5.13	117.92	121.00	13	1
1	A	11	ARG	NE-CZ-NH2	-5.10	117.75	120.30	2	1
1	C	1011	ARG	NE-CZ-NH1	5.09	122.85	120.30	12	1
1	A	13	ARG	NE-CZ-NH2	-5.09	117.75	120.30	15	1
1	A	41	ARG	NE-CZ-NH1	5.01	122.81	120.30	4	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	11	ARG	Sidechain	5
2	B	99	TYR	Sidechain	4
2	D	1099	TYR	Sidechain	4
2	B	106	ARG	Sidechain	3
1	C	1013	ARG	Sidechain	3
2	D	1106	ARG	Sidechain	3
1	A	13	ARG	Sidechain	3
1	A	40	TYR	Sidechain	3
1	C	1041	ARG	Sidechain	3
1	A	41	ARG	Sidechain	2
2	D	1104	ARG	Sidechain	2
1	C	1040	TYR	Sidechain	2
2	B	134	ARG	Sidechain	2
2	D	1134	ARG	Sidechain	1
1	C	1011	ARG	Sidechain	1
1	A	7	TYR	Sidechain	1
2	D	1133	TYR	Sidechain	1
2	B	100	TYR	Sidechain	1
1	C	1016	TYR	Sidechain	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	358	358	358	0±0
1	C	358	358	358	0±0
2	D	367	385	385	0±0
2	B	367	385	385	0±0
All	All	29000	29720	29720	11

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:119:LEU:HD12	2:D:1108:ASN:HD21	0.49	1.67	14	1
1:C:1037:ILE:H	1:C:1037:ILE:HD12	0.47	1.70	5	1
2:B:101:LEU:HD22	2:D:1116:LYS:HE2	0.46	1.87	6	1
1:C:1028:LEU:HD22	2:D:1130:VAL:HG23	0.46	1.86	13	1
1:C:1036:THR:HG23	2:D:1125:VAL:HG21	0.46	1.87	10	1
2:D:1116:LYS:HZ1	2:D:1120:GLU:CG	0.44	2.26	5	1
2:B:103:VAL:HG11	2:D:1116:LYS:HE3	0.43	1.90	3	1
2:B:99:TYR:HB3	2:D:1109:PHE:CD2	0.42	2.49	8	1
1:A:23:LYS:HE2	1:C:1010:VAL:HG11	0.42	1.92	1	1
1:A:8:LEU:HD21	1:C:1023:LYS:HE2	0.41	1.93	7	1
2:B:116:LYS:HD2	2:D:1103:VAL:HG11	0.40	1.93	19	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	41/60 (68%)	39±1 (95±2%)	2±1 (5±2%)	0±0 (0±1%)	54	85
1	C	41/60 (68%)	39±1 (96±2%)	2±1 (4±2%)	0±0 (0±1%)	54	85
2	B	43/50 (86%)	40±1 (93±2%)	2±1 (5±2%)	1±1 (2±2%)	10	50
2	D	43/50 (86%)	40±1 (93±2%)	2±1 (5±2%)	1±1 (2±2%)	11	52
All	All	3360/4400 (76%)	3166 (94%)	157 (5%)	37 (1%)	18	66

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occur-

rence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	128	PRO	13
2	D	1128	PRO	12
2	B	126	PRO	4
2	D	1126	PRO	4
2	B	127	GLN	1
2	D	1127	GLN	1
1	A	4	GLU	1
1	C	1004	GLU	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	40/59 (68%)	34±2 (86±6%)	6±2 (14±6%)	7	47
1	C	40/59 (68%)	34±3 (86±6%)	6±3 (14±6%)	6	45
2	B	42/48 (88%)	36±2 (86±5%)	6±2 (14±5%)	6	46
2	D	42/48 (88%)	35±2 (84±5%)	7±2 (16±5%)	5	42
All	All	3280/4280 (77%)	2799 (85%)	481 (15%)	6	45

All 128 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	D	1104	ARG	14
2	D	1134	ARG	11
2	B	102	GLN	10
1	C	1020	LEU	10
2	D	1137	GLN	10
1	A	20	LEU	9
2	D	1140	LEU	9
1	C	1011	ARG	8
2	B	104	ARG	8
2	D	1119	LEU	8
2	D	1125	VAL	8
1	A	29	MET	8
1	A	13	ARG	7

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Mol	Chain	Res	Type	Models (Total)
2	B	119	LEU	7
2	B	124	LEU	7
1	C	1029	MET	7
1	C	1036	THR	7
2	B	134	ARG	7
1	C	1026	LEU	7
2	B	137	GLN	7
1	A	8	LEU	6
1	A	11	ARG	6
1	A	26	LEU	6
2	B	140	LEU	6
1	C	1015	THR	6
2	D	1098	THR	6
2	B	125	VAL	6
1	C	1041	ARG	6
2	B	116	LYS	5
2	B	127	GLN	5
1	C	1013	ARG	5
2	D	1103	VAL	5
2	D	1113	MET	5
1	C	1004	GLU	5
2	D	1122	MET	5
1	A	41	ARG	5
1	C	1008	LEU	5
2	B	98	THR	5
1	C	1040	TYR	5
2	B	103	VAL	4
2	D	1101	LEU	4
2	B	101	LEU	4
2	B	122	MET	4
1	C	1042	GLN	4
2	D	1120	GLU	4
1	A	23	LYS	4
1	A	27	GLU	4
1	A	36	THR	4
1	C	1035	HIS	4
1	A	28	LEU	4
1	A	15	THR	4
2	D	1102	GLN	4
1	C	1023	LYS	4
2	D	1124	LEU	4
1	A	40	TYR	4

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Mol	Chain	Res	Type	Models (Total)
1	C	1014	GLU	4
2	B	120	GLU	3
2	B	129	LEU	3
2	D	1106	ARG	3
2	D	1129	LEU	3
1	A	31	TYR	3
1	A	38	GLU	3
2	D	1116	LYS	3
1	A	4	GLU	3
2	B	108	ASN	3
2	B	136	GLN	3
1	A	24	GLU	3
2	B	110	GLU	3
2	B	117	GLU	3
1	C	1031	TYR	3
2	D	1117	GLU	3
1	C	1030	GLN	3
2	D	1112	LEU	3
2	D	1127	GLN	3
2	D	1132	SER	3
1	C	1024	GLU	3
1	A	46	GLN	3
1	C	1019	LEU	3
1	C	1032	LEU	2
2	D	1114	LYS	2
1	A	44	GLN	2
2	D	1121	LEU	2
2	D	1131	ASP	2
1	A	35	HIS	2
1	A	42	GLN	2
1	A	43	GLN	2
2	D	1110	GLU	2
1	A	19	LEU	2
2	B	113	MET	2
1	A	21	GLU	2
2	B	139	LEU	2
2	D	1139	LEU	2
1	C	1021	GLU	2
2	D	1136	GLN	2
2	B	112	LEU	2
1	A	32	LEU	2
1	A	39	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	14	GLU	2
1	C	1006	LEU	2
2	B	132	SER	2
1	C	1027	GLU	2
1	A	30	GLN	2
1	C	1046	GLN	2
1	A	45	GLN	1
2	B	114	LYS	1
2	B	121	LEU	1
1	C	1038	GLU	1
1	A	17	GLU	1
2	B	107	LYS	1
1	C	1005	LEU	1
2	D	1107	LYS	1
2	D	1138	GLN	1
2	B	131	ASP	1
1	C	1045	GLN	1
1	C	1028	LEU	1
2	D	1123	GLU	1
1	C	1018	MET	1
1	C	1039	THR	1
2	D	1118	SER	1
2	B	135	GLN	1
1	A	25	SER	1
2	B	133	TYR	1
1	C	1044	GLN	1
1	A	6	LEU	1
2	B	106	ARG	1
2	D	1108	ASN	1
2	B	138	GLN	1
1	A	5	LEU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides 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 86% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	2706
Number of shifts mapped to atoms	2706
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	214	-0.52 ± 0.04	Should be checked
$^{13}C_{\beta}$	212	0.09 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	210	-0.17 ± 0.10	None needed (< 0.5 ppm)
^{15}N	202	-0.49 ± 0.21	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 86%, i.e. 2214 atoms were assigned a chemical shift out of a possible 2582. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	832/832 (100%)	334/334 (100%)	336/336 (100%)	162/162 (100%)
Sidechain	1280/1590 (81%)	866/1028 (84%)	398/492 (81%)	16/70 (23%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	102/160 (64%)	68/74 (92%)	34/84 (40%)	0/2 (0%)
Overall	2214/2582 (86%)	1268/1436 (88%)	768/912 (84%)	178/234 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 2706 atoms were assigned a chemical shift out of a possible 3260. 0 out of 46 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1044/1090 (96%)	418/438 (95%)	424/440 (96%)	202/212 (95%)
Sidechain	1552/1982 (78%)	1048/1272 (82%)	488/618 (79%)	16/92 (17%)
Aromatic	110/188 (59%)	72/90 (80%)	38/92 (41%)	0/6 (0%)
Overall	2706/3260 (83%)	1538/1800 (85%)	950/1150 (83%)	218/310 (70%)

7.1.4 Statistically unusual chemical shifts (i)

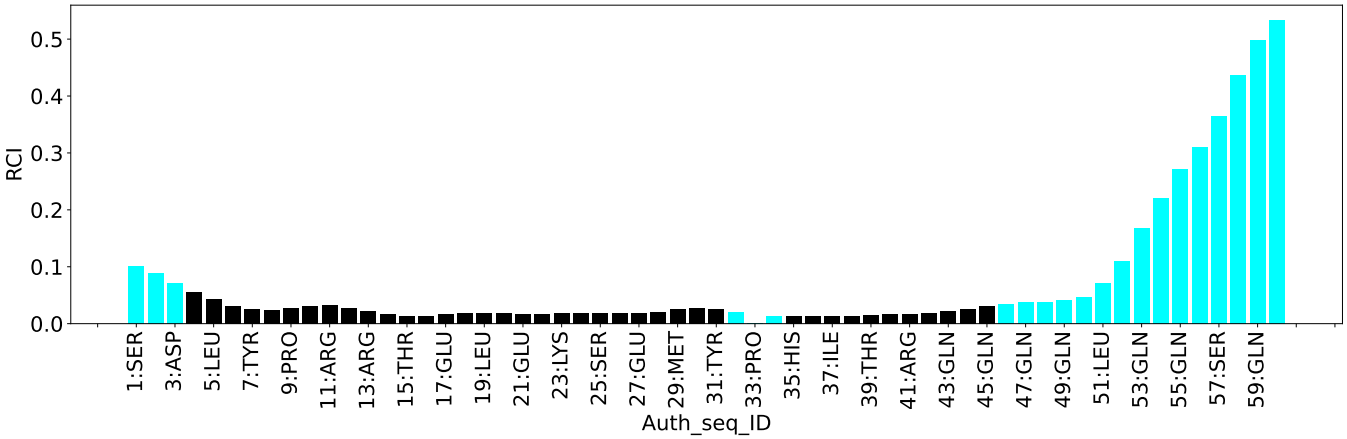
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	41	ARG	NE	136.90	76.53 – 92.65	32.5
1	C	1041	ARG	NE	136.90	76.53 – 92.65	32.5
1	B	104	ARG	NE	136.28	76.53 – 92.65	32.1
1	D	1104	ARG	NE	136.28	76.53 – 92.65	32.1
1	B	134	ARG	NE	135.12	76.53 – 92.65	31.4
1	D	1134	ARG	NE	135.12	76.53 – 92.65	31.4
1	A	11	ARG	NE	134.86	76.53 – 92.65	31.2
1	C	1011	ARG	NE	134.86	76.53 – 92.65	31.2
1	A	13	ARG	NE	134.05	76.53 – 92.65	30.7
1	C	1013	ARG	NE	134.05	76.53 – 92.65	30.7

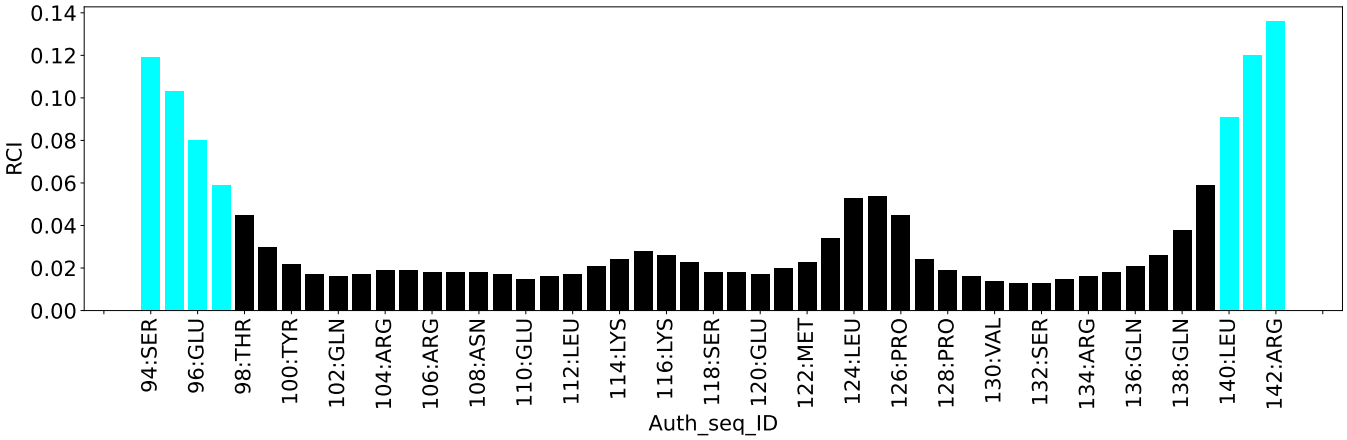
7.1.5 Random Coil Index (RCI) plots (i)

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

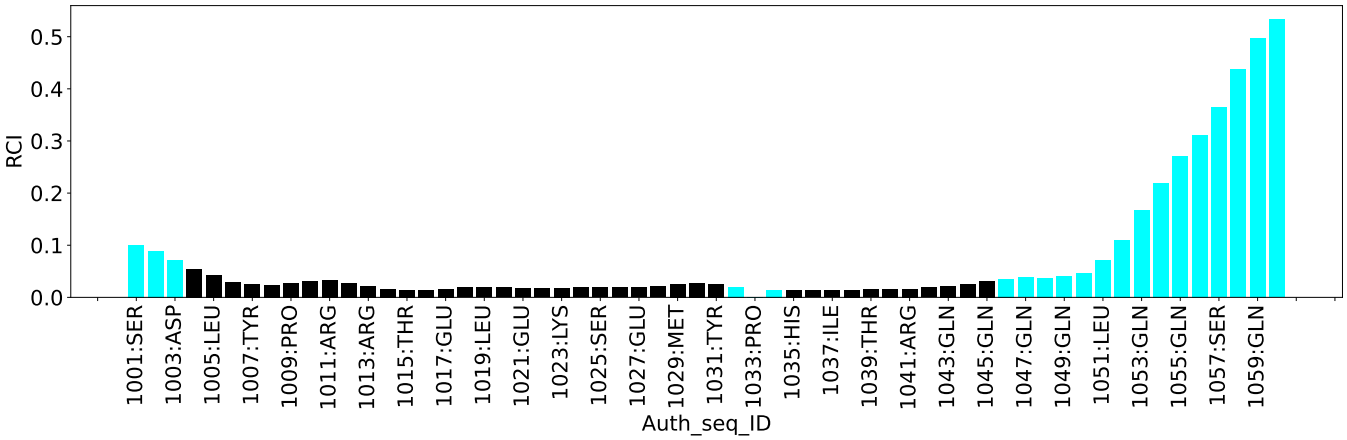
Random coil index (RCI) for chain A:



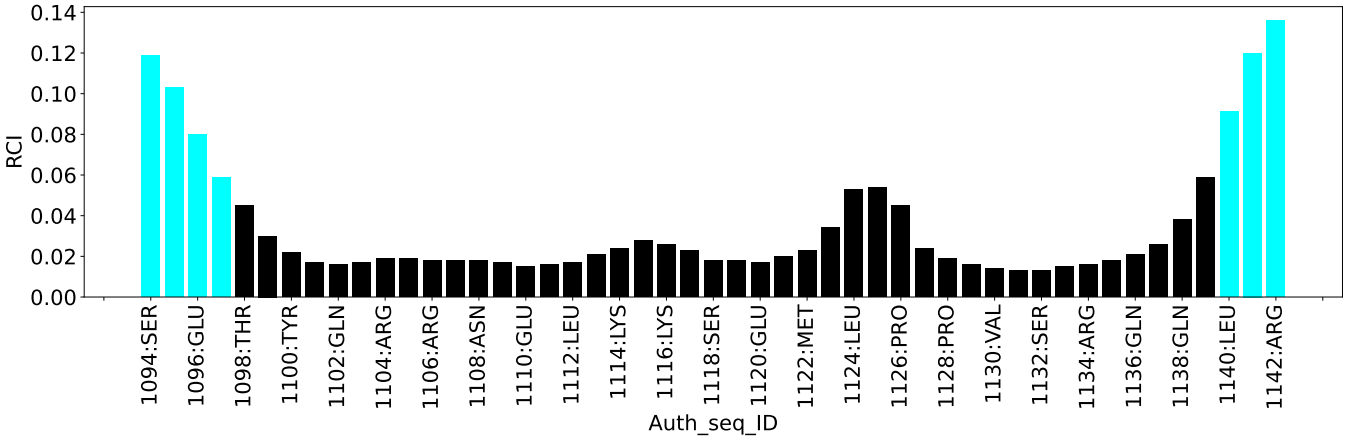
Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:



Random coil index (RCI) for chain D:


RCI
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
1094:SER
1096:GLU
1098:THR
1100:TYR
1102:GLN
1104:ARG
1106:ARG
1108:ASN
1110:GLU
1112:LEU
1114:LYS
1116:LYS
1118:SER
1120:GLU
1122:MET
1124:LEU
1126:PRO
1128:PRO
1130:VAL
1132:SER
1134:ARG
1136:GLN
1138:GLN
1140:LEU
1142:ARG
Auth_seq_ID

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	3020
Intra-residue (|i-j|=0)	412
Sequential (|i-j|=1)	706
Medium range (|i-j|>1 and |i-j|<5)	614
Long range (|i-j|≥5)	52
Inter-chain	796
Hydrogen bond restraints	440
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	13.7
Number of long range restraints per residue[1]	0.2

[1]Long 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)	38.0	0.2
0.2-0.5 (Medium)	56.3	0.5
>0.5 (Large)	13.8	0.58

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

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

9 Distance violation analysis (i)

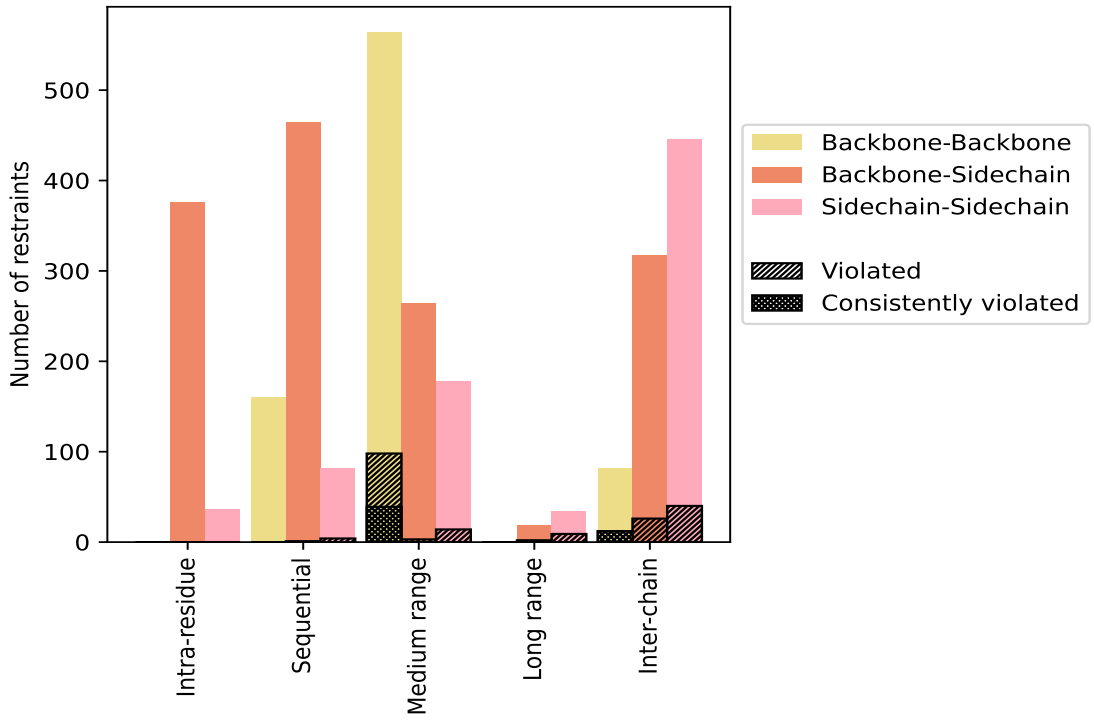
9.1 Summary of distance violations (i)

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)	412	13.6	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	376	12.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	36	1.2	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	706	23.4	5	0.7	0.2	0	0.0	0.0
Backbone-Backbone	160	5.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	464	15.4	1	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	82	2.7	4	4.9	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	614	20.3	17	2.8	0.6	0	0.0	0.0
Backbone-Backbone	172	5.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	264	8.7	3	1.1	0.1	0	0.0	0.0
Sidechain-Sidechain	178	5.9	14	7.9	0.5	0	0.0	0.0
Long range (|i-j|≥5)	52	1.7	11	21.2	0.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	18	0.6	2	11.1	0.1	0	0.0	0.0
Sidechain-Sidechain	34	1.1	9	26.5	0.3	0	0.0	0.0
Inter-chain	796	26.4	66	8.3	2.2	0	0.0	0.0
Backbone-Backbone	34	1.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	317	10.5	26	8.2	0.9	0	0.0	0.0
Sidechain-Sidechain	445	14.7	40	9.0	1.3	0	0.0	0.0
Hydrogen bond	440	14.6	110	25.0	3.6	51	11.6	1.7
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3020	100.0	209	6.9	6.9	51	1.7	1.7
Backbone-Backbone	806	26.7	110	13.6	3.6	51	6.3	1.7
Backbone-Sidechain	1439	47.6	32	2.2	1.1	0	0.0	0.0
Sidechain-Sidechain	775	25.7	67	8.6	2.2	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

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	0	2	83	0	22	107	0.28	0.57	0.15	0.24
2	0	0	88	1	18	107	0.32	0.57	0.15	0.3
3	0	0	90	1	15	106	0.29	0.58	0.13	0.29
4	0	0	84	1	18	103	0.29	0.58	0.13	0.27
5	0	0	88	0	17	105	0.3	0.57	0.15	0.28
6	0	0	89	1	20	110	0.28	0.57	0.14	0.25
7	0	0	93	1	23	117	0.29	0.57	0.15	0.26
8	0	1	88	2	19	110	0.28	0.58	0.13	0.25
9	0	1	89	0	22	112	0.3	0.57	0.15	0.25
10	0	0	86	1	19	106	0.32	0.56	0.15	0.32
11	0	0	90	0	16	106	0.33	0.58	0.15	0.3

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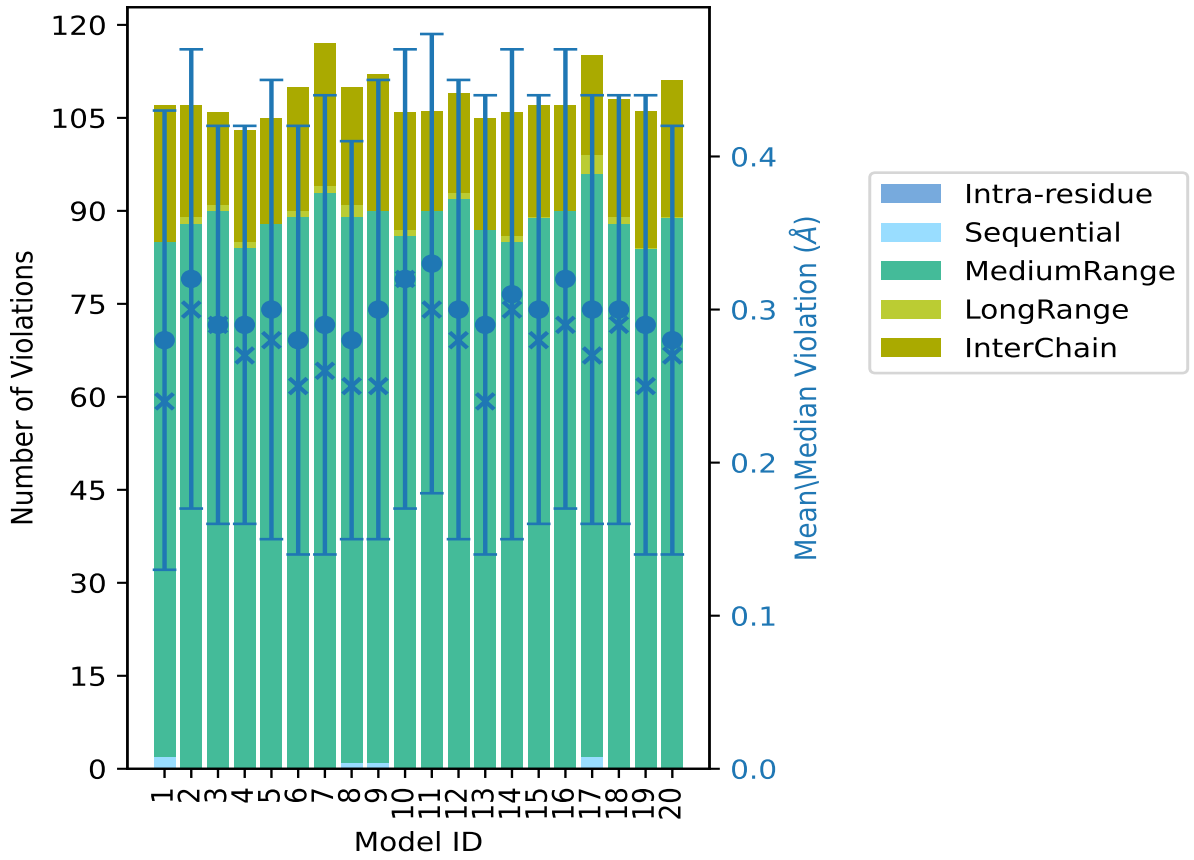
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	92	1	16	109	0.3	0.58	0.15	0.28
13	0	0	87	0	18	105	0.29	0.58	0.15	0.24
14	0	0	85	1	20	106	0.31	0.58	0.16	0.3
15	0	0	89	0	18	107	0.3	0.58	0.14	0.28
16	0	0	90	0	17	107	0.32	0.58	0.15	0.29
17	0	2	94	3	16	115	0.3	0.58	0.14	0.27
18	0	0	88	1	19	108	0.3	0.58	0.14	0.29
19	0	0	84	0	22	106	0.29	0.58	0.15	0.25
20	0	0	89	0	22	111	0.28	0.58	0.14	0.27

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard 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

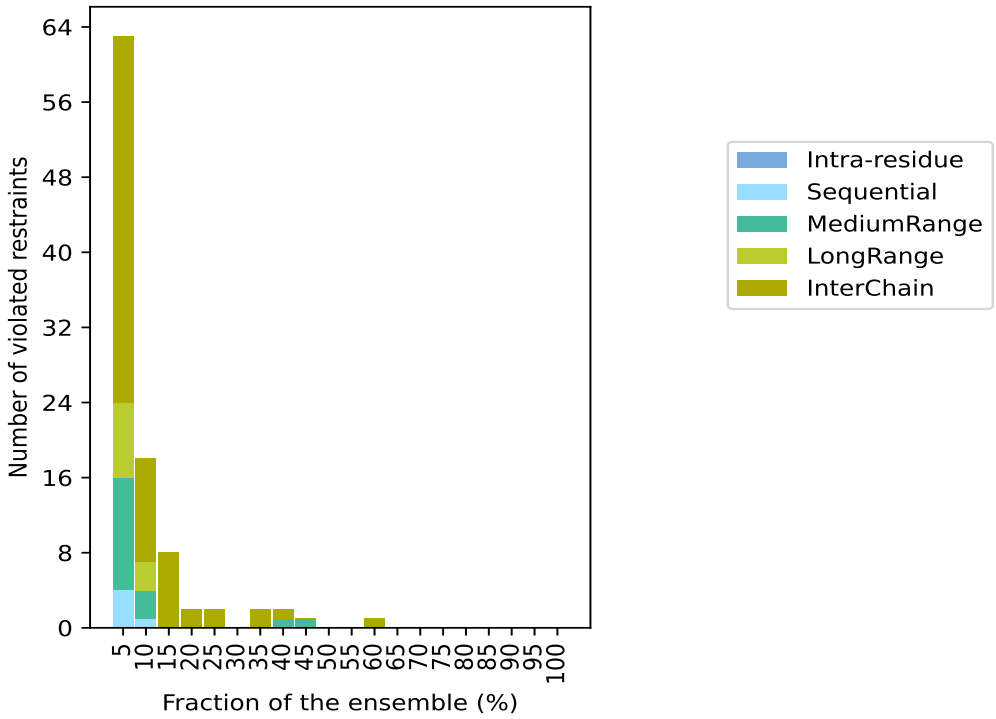
9.3 Distance violation statistics for the ensemble (i)

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, 2481(IR:412, SQ:701, MR:597, LR:41, IC:730) 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]	%
0	4	12	8	39	63	1	5.0
0	1	3	3	11	18	2	10.0
0	0	0	0	8	8	3	15.0
0	0	0	0	2	2	4	20.0
0	0	0	0	2	2	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	2	2	7	35.0
0	0	1	0	1	2	8	40.0
0	0	1	0	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	1	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

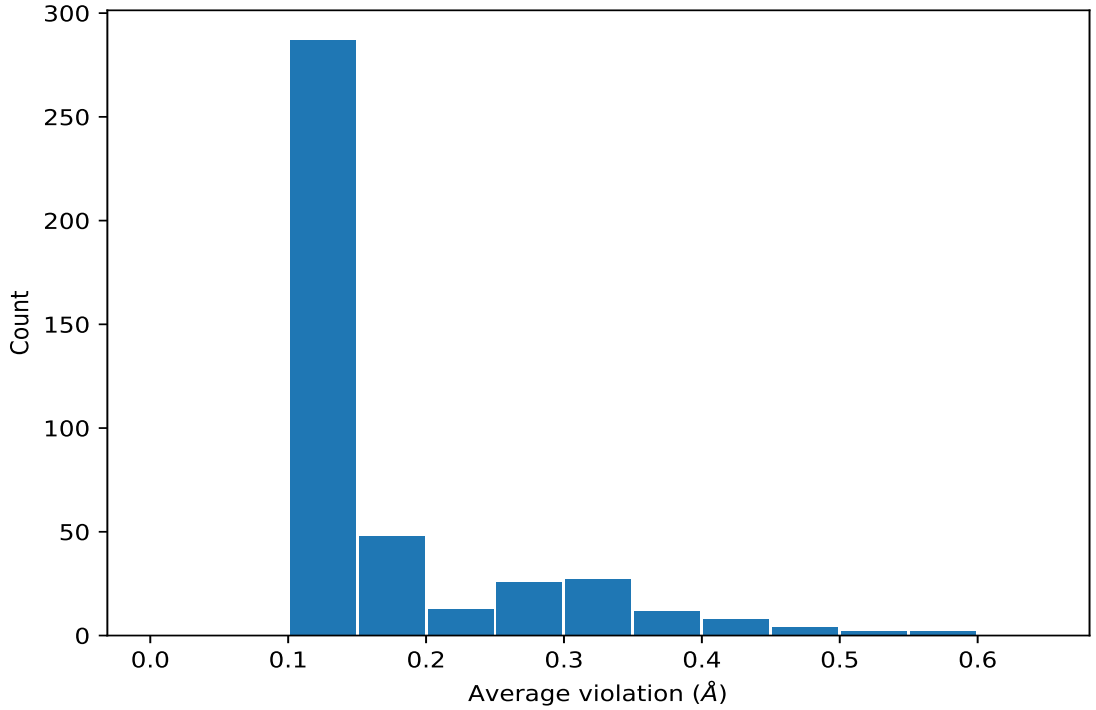
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance 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



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)
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	20	0.56	0.02	0.56
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	20	0.55	0.04	0.56
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	20	0.52	0.06	0.55
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	20	0.51	0.09	0.56
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	20	0.49	0.05	0.5
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	20	0.47	0.11	0.53
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	20	0.46	0.1	0.48
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	20	0.46	0.08	0.49
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	20	0.43	0.12	0.45
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	20	0.43	0.13	0.46
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	20	0.42	0.11	0.44
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	20	0.42	0.1	0.42
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	20	0.42	0.09	0.43
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	20	0.41	0.14	0.46
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	20	0.4	0.08	0.4
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	20	0.4	0.13	0.39

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	20	0.39	0.11	0.43
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	20	0.39	0.1	0.4
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	20	0.38	0.12	0.4
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	20	0.38	0.14	0.37
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	20	0.38	0.13	0.36
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	20	0.37	0.09	0.4
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	20	0.37	0.13	0.42
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	20	0.37	0.12	0.38
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	20	0.36	0.12	0.33
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	20	0.35	0.14	0.34
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	20	0.35	0.09	0.38
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	20	0.35	0.11	0.36
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	20	0.34	0.13	0.34
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	20	0.34	0.16	0.34
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	20	0.34	0.11	0.34
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	20	0.34	0.09	0.34
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	20	0.33	0.09	0.32
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	20	0.33	0.13	0.32
(4,22)	1:A:25:SER:O	1:A:29:MET:N	20	0.33	0.1	0.29
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	20	0.32	0.11	0.32
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	20	0.32	0.15	0.27
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	20	0.32	0.14	0.28
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	20	0.32	0.12	0.28
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	20	0.31	0.09	0.31
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	20	0.31	0.12	0.32
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	20	0.3	0.11	0.29
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	20	0.3	0.07	0.3
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	20	0.3	0.12	0.28
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	20	0.29	0.13	0.26
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	20	0.29	0.1	0.27
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	20	0.29	0.09	0.26
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	20	0.28	0.07	0.27
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	20	0.27	0.13	0.22
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	20	0.27	0.13	0.24
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	20	0.26	0.1	0.24
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	19	0.34	0.13	0.35
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	19	0.33	0.11	0.31
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	19	0.32	0.12	0.34
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	19	0.3	0.15	0.26
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	19	0.3	0.13	0.27
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	19	0.3	0.11	0.26
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	19	0.29	0.09	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	19	0.27	0.12	0.22
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	19	0.26	0.12	0.24
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	19	0.26	0.14	0.2
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	19	0.22	0.07	0.2
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	18	0.37	0.12	0.39
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	18	0.36	0.08	0.38
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	18	0.36	0.13	0.39
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	18	0.35	0.17	0.36
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	18	0.34	0.09	0.32
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	18	0.34	0.12	0.34
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	18	0.33	0.15	0.32
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	18	0.32	0.13	0.28
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	18	0.32	0.12	0.3
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	18	0.31	0.16	0.24
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	18	0.28	0.13	0.22
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	18	0.27	0.1	0.24
(4,83)	2:B:118:SER:O	2:B:122:MET:N	18	0.23	0.09	0.21
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	18	0.21	0.06	0.22
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	18	0.2	0.08	0.18
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	18	0.18	0.05	0.17
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	18	0.17	0.05	0.18
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	17	0.29	0.14	0.25
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	17	0.28	0.11	0.29
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	17	0.27	0.12	0.23
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	17	0.26	0.14	0.22
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	17	0.25	0.09	0.25
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	17	0.23	0.09	0.2
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	17	0.23	0.09	0.2
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	17	0.22	0.12	0.2
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	17	0.19	0.1	0.16
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	17	0.18	0.06	0.18
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	16	0.3	0.13	0.27
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	16	0.18	0.07	0.16
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	15	0.35	0.17	0.35
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	15	0.22	0.11	0.17
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	15	0.22	0.09	0.21
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	15	0.2	0.07	0.17
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	15	0.16	0.05	0.15
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	14	0.3	0.1	0.3
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	14	0.2	0.1	0.18
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	14	0.19	0.09	0.16
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	14	0.19	0.07	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	14	0.15	0.03	0.15
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	13	0.23	0.11	0.22
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	13	0.2	0.08	0.17
(4,17)	1:A:20:LEU:O	1:A:24:GLU:N	12	0.18	0.08	0.16
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG11	12	0.12	0.01	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG12	12	0.12	0.01	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG13	12	0.12	0.01	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG21	12	0.12	0.01	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG22	12	0.12	0.01	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG23	12	0.12	0.01	0.12
(4,68)	2:B:133:TYR:O	2:B:137:GLN:N	11	0.13	0.02	0.13
(4,98)	2:D:1109:PHE:O	2:D:1113:MET:N	10	0.14	0.03	0.14
(4,101)	2:D:1112:LEU:O	2:D:1116:LYS:N	9	0.16	0.06	0.13
(2,165)	2:B:124:LEU:HD11	2:B:126:PRO:HB3	9	0.11	0.0	0.11
(2,165)	2:B:124:LEU:HD12	2:B:126:PRO:HB3	9	0.11	0.0	0.11
(2,165)	2:B:124:LEU:HD13	2:B:126:PRO:HB3	9	0.11	0.0	0.11
(2,165)	2:B:124:LEU:HD21	2:B:126:PRO:HB3	9	0.11	0.0	0.11
(2,165)	2:B:124:LEU:HD22	2:B:126:PRO:HB3	9	0.11	0.0	0.11
(2,165)	2:B:124:LEU:HD23	2:B:126:PRO:HB3	9	0.11	0.0	0.11
(4,88)	2:D:1129:LEU:O	2:D:1133:TYR:N	8	0.15	0.06	0.12
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE1	8	0.12	0.01	0.12
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE2	8	0.12	0.01	0.12
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE1	8	0.12	0.01	0.12
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE2	8	0.12	0.01	0.12
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE1	8	0.12	0.01	0.12
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE2	8	0.12	0.01	0.12
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE1	8	0.12	0.01	0.12
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE2	8	0.12	0.01	0.12
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE1	8	0.12	0.01	0.12
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE2	8	0.12	0.01	0.12
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE1	8	0.12	0.01	0.12
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE2	8	0.12	0.01	0.12
(2,166)	2:D:1124:LEU:HD11	2:D:1126:PRO:HB3	8	0.11	0.0	0.11
(2,166)	2:D:1124:LEU:HD12	2:D:1126:PRO:HB3	8	0.11	0.0	0.11
(2,166)	2:D:1124:LEU:HD13	2:D:1126:PRO:HB3	8	0.11	0.0	0.11
(2,166)	2:D:1124:LEU:HD21	2:D:1126:PRO:HB3	8	0.11	0.0	0.11
(2,166)	2:D:1124:LEU:HD22	2:D:1126:PRO:HB3	8	0.11	0.0	0.11
(2,166)	2:D:1124:LEU:HD23	2:D:1126:PRO:HB3	8	0.11	0.0	0.11
(4,64)	2:B:129:LEU:O	2:B:133:TYR:N	7	0.17	0.12	0.13
(2,725)	1:A:28:LEU:HD11	2:B:122:MET:HA	7	0.12	0.01	0.12
(2,725)	1:A:28:LEU:HD12	2:B:122:MET:HA	7	0.12	0.01	0.12
(2,725)	1:A:28:LEU:HD13	2:B:122:MET:HA	7	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,725)	1:A:28:LEU:HD21	2:B:122:MET:HA	7	0.12	0.01	0.12
(2,725)	1:A:28:LEU:HD22	2:B:122:MET:HA	7	0.12	0.01	0.12
(2,725)	1:A:28:LEU:HD23	2:B:122:MET:HA	7	0.12	0.01	0.12
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG11	7	0.11	0.0	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG12	7	0.11	0.0	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG13	7	0.11	0.0	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG21	7	0.11	0.0	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG22	7	0.11	0.0	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG23	7	0.11	0.0	0.11
(4,92)	2:D:1133:TYR:O	2:D:1137:GLN:N	6	0.18	0.03	0.16
(2,726)	1:C:1028:LEU:HD11	2:D:1122:MET:HA	5	0.12	0.01	0.12
(2,726)	1:C:1028:LEU:HD12	2:D:1122:MET:HA	5	0.12	0.01	0.12
(2,726)	1:C:1028:LEU:HD13	2:D:1122:MET:HA	5	0.12	0.01	0.12
(2,726)	1:C:1028:LEU:HD21	2:D:1122:MET:HA	5	0.12	0.01	0.12
(2,726)	1:C:1028:LEU:HD22	2:D:1122:MET:HA	5	0.12	0.01	0.12
(2,726)	1:C:1028:LEU:HD23	2:D:1122:MET:HA	5	0.12	0.01	0.12
(2,879)	2:B:104:ARG:HB2	2:D:1120:GLU:HG2	5	0.11	0.0	0.11
(2,879)	2:B:104:ARG:HB2	2:D:1120:GLU:HG3	5	0.11	0.0	0.11
(2,879)	2:B:104:ARG:HB3	2:D:1120:GLU:HG2	5	0.11	0.0	0.11
(2,879)	2:B:104:ARG:HB3	2:D:1120:GLU:HG3	5	0.11	0.0	0.11
(2,868)	1:C:1020:LEU:HD11	2:D:1133:TYR:HE1	4	0.12	0.0	0.12
(2,868)	1:C:1020:LEU:HD11	2:D:1133:TYR:HE2	4	0.12	0.0	0.12
(2,868)	1:C:1020:LEU:HD12	2:D:1133:TYR:HE1	4	0.12	0.0	0.12
(2,868)	1:C:1020:LEU:HD12	2:D:1133:TYR:HE2	4	0.12	0.0	0.12
(2,868)	1:C:1020:LEU:HD13	2:D:1133:TYR:HE1	4	0.12	0.0	0.12
(2,868)	1:C:1020:LEU:HD13	2:D:1133:TYR:HE2	4	0.12	0.0	0.12
(2,868)	1:C:1020:LEU:HD21	2:D:1133:TYR:HE1	4	0.12	0.0	0.12
(2,868)	1:C:1020:LEU:HD21	2:D:1133:TYR:HE2	4	0.12	0.0	0.12
(2,868)	1:C:1020:LEU:HD22	2:D:1133:TYR:HE1	4	0.12	0.0	0.12
(2,868)	1:C:1020:LEU:HD22	2:D:1133:TYR:HE2	4	0.12	0.0	0.12
(2,868)	1:C:1020:LEU:HD23	2:D:1133:TYR:HE1	4	0.12	0.0	0.12
(2,868)	1:C:1020:LEU:HD23	2:D:1133:TYR:HE2	4	0.12	0.0	0.12
(2,652)	1:C:1005:LEU:HD11	2:D:1140:LEU:HA	4	0.12	0.0	0.12
(2,652)	1:C:1005:LEU:HD12	2:D:1140:LEU:HA	4	0.12	0.0	0.12
(2,652)	1:C:1005:LEU:HD13	2:D:1140:LEU:HA	4	0.12	0.0	0.12
(2,652)	1:C:1005:LEU:HD21	2:D:1140:LEU:HA	4	0.12	0.0	0.12
(2,652)	1:C:1005:LEU:HD22	2:D:1140:LEU:HA	4	0.12	0.0	0.12
(2,652)	1:C:1005:LEU:HD23	2:D:1140:LEU:HA	4	0.12	0.0	0.12
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD11	3	0.12	0.01	0.12
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD12	3	0.12	0.01	0.12
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD13	3	0.12	0.01	0.12
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD21	3	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD22	3	0.12	0.01	0.12
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD23	3	0.12	0.01	0.12
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD11	3	0.12	0.01	0.12
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD12	3	0.12	0.01	0.12
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD13	3	0.12	0.01	0.12
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD21	3	0.12	0.01	0.12
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD22	3	0.12	0.01	0.12
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD23	3	0.12	0.01	0.12
(2,871)	2:B:140:LEU:HD11	1:C:1011:ARG:HD2	3	0.12	0.0	0.12
(2,871)	2:B:140:LEU:HD11	1:C:1011:ARG:HD3	3	0.12	0.0	0.12
(2,871)	2:B:140:LEU:HD12	1:C:1011:ARG:HD2	3	0.12	0.0	0.12
(2,871)	2:B:140:LEU:HD12	1:C:1011:ARG:HD3	3	0.12	0.0	0.12
(2,871)	2:B:140:LEU:HD13	1:C:1011:ARG:HD2	3	0.12	0.0	0.12
(2,871)	2:B:140:LEU:HD13	1:C:1011:ARG:HD3	3	0.12	0.0	0.12
(2,871)	2:B:140:LEU:HD21	1:C:1011:ARG:HD2	3	0.12	0.0	0.12
(2,871)	2:B:140:LEU:HD21	1:C:1011:ARG:HD3	3	0.12	0.0	0.12
(2,871)	2:B:140:LEU:HD22	1:C:1011:ARG:HD2	3	0.12	0.0	0.12
(2,871)	2:B:140:LEU:HD22	1:C:1011:ARG:HD3	3	0.12	0.0	0.12
(2,871)	2:B:140:LEU:HD23	1:C:1011:ARG:HD2	3	0.12	0.0	0.12
(2,871)	2:B:140:LEU:HD23	1:C:1011:ARG:HD3	3	0.12	0.0	0.12
(1,1074)	1:A:6:LEU:HD21	1:C:1013:ARG:HD2	3	0.12	0.0	0.12
(1,1074)	1:A:6:LEU:HD21	1:C:1013:ARG:HD3	3	0.12	0.0	0.12
(1,1074)	1:A:6:LEU:HD22	1:C:1013:ARG:HD2	3	0.12	0.0	0.12
(1,1074)	1:A:6:LEU:HD22	1:C:1013:ARG:HD3	3	0.12	0.0	0.12
(1,1074)	1:A:6:LEU:HD23	1:C:1013:ARG:HD2	3	0.12	0.0	0.12
(1,1074)	1:A:6:LEU:HD23	1:C:1013:ARG:HD3	3	0.12	0.0	0.12
(1,1505)	1:A:26:LEU:HD11	2:B:115:LEU:HA	3	0.12	0.0	0.12
(1,1505)	1:A:26:LEU:HD12	2:B:115:LEU:HA	3	0.12	0.0	0.12
(1,1505)	1:A:26:LEU:HD13	2:B:115:LEU:HA	3	0.12	0.0	0.12
(1,1505)	1:A:26:LEU:HD21	2:B:115:LEU:HA	3	0.12	0.0	0.12
(1,1505)	1:A:26:LEU:HD22	2:B:115:LEU:HA	3	0.12	0.0	0.12
(1,1505)	1:A:26:LEU:HD23	2:B:115:LEU:HA	3	0.12	0.0	0.12
(1,1515)	1:A:26:LEU:HD11	2:B:118:SER:HA	3	0.12	0.0	0.12
(1,1515)	1:A:26:LEU:HD12	2:B:118:SER:HA	3	0.12	0.0	0.12
(1,1515)	1:A:26:LEU:HD13	2:B:118:SER:HA	3	0.12	0.0	0.12
(1,1515)	1:A:26:LEU:HD21	2:B:118:SER:HA	3	0.12	0.0	0.12
(1,1515)	1:A:26:LEU:HD22	2:B:118:SER:HA	3	0.12	0.0	0.12
(1,1515)	1:A:26:LEU:HD23	2:B:118:SER:HA	3	0.12	0.0	0.12
(2,683)	1:A:7:TYR:HE1	2:B:140:LEU:HB2	3	0.12	0.0	0.12
(2,683)	1:A:7:TYR:HE1	2:B:140:LEU:HB3	3	0.12	0.0	0.12
(2,683)	1:A:7:TYR:HE2	2:B:140:LEU:HB2	3	0.12	0.0	0.12
(2,683)	1:A:7:TYR:HE2	2:B:140:LEU:HB3	3	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,332)	2:B:112:LEU:HB2	1:C:1022:ILE:HD11	3	0.11	0.0	0.11
(2,332)	2:B:112:LEU:HB2	1:C:1022:ILE:HD12	3	0.11	0.0	0.11
(2,332)	2:B:112:LEU:HB2	1:C:1022:ILE:HD13	3	0.11	0.0	0.11
(2,332)	2:B:112:LEU:HB3	1:C:1022:ILE:HD11	3	0.11	0.0	0.11
(2,332)	2:B:112:LEU:HB3	1:C:1022:ILE:HD12	3	0.11	0.0	0.11
(2,332)	2:B:112:LEU:HB3	1:C:1022:ILE:HD13	3	0.11	0.0	0.11
(2,331)	1:A:22:ILE:HD11	2:D:1112:LEU:HB2	3	0.11	0.0	0.11
(2,331)	1:A:22:ILE:HD11	2:D:1112:LEU:HB3	3	0.11	0.0	0.11
(2,331)	1:A:22:ILE:HD12	2:D:1112:LEU:HB2	3	0.11	0.0	0.11
(2,331)	1:A:22:ILE:HD12	2:D:1112:LEU:HB3	3	0.11	0.0	0.11
(2,331)	1:A:22:ILE:HD13	2:D:1112:LEU:HB2	3	0.11	0.0	0.11
(2,331)	1:A:22:ILE:HD13	2:D:1112:LEU:HB3	3	0.11	0.0	0.11
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD11	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD12	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD13	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD21	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD22	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD23	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD11	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD12	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD13	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD21	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD22	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD23	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD11	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD12	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD13	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD21	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD22	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD23	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD11	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD12	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD13	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD21	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD22	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD23	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD11	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD12	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD13	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD21	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD22	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD23	2	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD11	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD12	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD13	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD21	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD22	2	0.16	0.01	0.16
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD23	2	0.16	0.01	0.16
(2,781)	2:B:103:VAL:HG11	2:B:109:PHE:HE1	2	0.12	0.02	0.12
(2,781)	2:B:103:VAL:HG11	2:B:109:PHE:HE2	2	0.12	0.02	0.12
(2,781)	2:B:103:VAL:HG12	2:B:109:PHE:HE1	2	0.12	0.02	0.12
(2,781)	2:B:103:VAL:HG12	2:B:109:PHE:HE2	2	0.12	0.02	0.12
(2,781)	2:B:103:VAL:HG13	2:B:109:PHE:HE1	2	0.12	0.02	0.12
(2,781)	2:B:103:VAL:HG13	2:B:109:PHE:HE2	2	0.12	0.02	0.12
(2,781)	2:B:103:VAL:HG21	2:B:109:PHE:HE1	2	0.12	0.02	0.12
(2,781)	2:B:103:VAL:HG21	2:B:109:PHE:HE2	2	0.12	0.02	0.12
(2,781)	2:B:103:VAL:HG22	2:B:109:PHE:HE1	2	0.12	0.02	0.12
(2,781)	2:B:103:VAL:HG22	2:B:109:PHE:HE2	2	0.12	0.02	0.12
(2,781)	2:B:103:VAL:HG23	2:B:109:PHE:HE1	2	0.12	0.02	0.12
(2,781)	2:B:103:VAL:HG23	2:B:109:PHE:HE2	2	0.12	0.02	0.12
(1,594)	1:A:20:LEU:HD11	1:A:23:LYS:HE2	2	0.12	0.01	0.12
(1,594)	1:A:20:LEU:HD11	1:A:23:LYS:HE3	2	0.12	0.01	0.12
(1,594)	1:A:20:LEU:HD12	1:A:23:LYS:HE2	2	0.12	0.01	0.12
(1,594)	1:A:20:LEU:HD12	1:A:23:LYS:HE3	2	0.12	0.01	0.12
(1,594)	1:A:20:LEU:HD13	1:A:23:LYS:HE2	2	0.12	0.01	0.12
(1,594)	1:A:20:LEU:HD13	1:A:23:LYS:HE3	2	0.12	0.01	0.12
(1,594)	1:A:20:LEU:HD21	1:A:23:LYS:HE2	2	0.12	0.01	0.12
(1,594)	1:A:20:LEU:HD21	1:A:23:LYS:HE3	2	0.12	0.01	0.12
(1,594)	1:A:20:LEU:HD22	1:A:23:LYS:HE2	2	0.12	0.01	0.12
(1,594)	1:A:20:LEU:HD22	1:A:23:LYS:HE3	2	0.12	0.01	0.12
(1,594)	1:A:20:LEU:HD23	1:A:23:LYS:HE2	2	0.12	0.01	0.12
(1,594)	1:A:20:LEU:HD23	1:A:23:LYS:HE3	2	0.12	0.01	0.12
(1,1232)	1:C:1036:THR:HG21	1:C:1037:ILE:HD11	2	0.12	0.0	0.12
(1,1232)	1:C:1036:THR:HG21	1:C:1037:ILE:HD12	2	0.12	0.0	0.12
(1,1232)	1:C:1036:THR:HG21	1:C:1037:ILE:HD13	2	0.12	0.0	0.12
(1,1232)	1:C:1036:THR:HG22	1:C:1037:ILE:HD11	2	0.12	0.0	0.12
(1,1232)	1:C:1036:THR:HG22	1:C:1037:ILE:HD12	2	0.12	0.0	0.12
(1,1232)	1:C:1036:THR:HG22	1:C:1037:ILE:HD13	2	0.12	0.0	0.12
(1,1232)	1:C:1036:THR:HG23	1:C:1037:ILE:HD11	2	0.12	0.0	0.12
(1,1232)	1:C:1036:THR:HG23	1:C:1037:ILE:HD12	2	0.12	0.0	0.12
(1,1232)	1:C:1036:THR:HG23	1:C:1037:ILE:HD13	2	0.12	0.0	0.12
(1,1282)	1:C:1010:VAL:HG11	1:C:1015:THR:HG21	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG11	1:C:1015:THR:HG22	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG11	1:C:1015:THR:HG23	2	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1282)	1:C:1010:VAL:HG12	1:C:1015:THR:HG21	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG12	1:C:1015:THR:HG22	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG12	1:C:1015:THR:HG23	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG13	1:C:1015:THR:HG21	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG13	1:C:1015:THR:HG22	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG13	1:C:1015:THR:HG23	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG21	1:C:1015:THR:HG21	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG21	1:C:1015:THR:HG22	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG21	1:C:1015:THR:HG23	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG22	1:C:1015:THR:HG21	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG22	1:C:1015:THR:HG22	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG22	1:C:1015:THR:HG23	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG23	1:C:1015:THR:HG21	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG23	1:C:1015:THR:HG22	2	0.12	0.01	0.12
(1,1282)	1:C:1010:VAL:HG23	1:C:1015:THR:HG23	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD11	1:C:1029:MET:HE1	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD11	1:C:1029:MET:HE2	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD11	1:C:1029:MET:HE3	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD12	1:C:1029:MET:HE1	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD12	1:C:1029:MET:HE2	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD12	1:C:1029:MET:HE3	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD13	1:C:1029:MET:HE1	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD13	1:C:1029:MET:HE2	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD13	1:C:1029:MET:HE3	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD21	1:C:1029:MET:HE1	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD21	1:C:1029:MET:HE2	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD21	1:C:1029:MET:HE3	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD22	1:C:1029:MET:HE1	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD22	1:C:1029:MET:HE2	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD22	1:C:1029:MET:HE3	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD23	1:C:1029:MET:HE1	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD23	1:C:1029:MET:HE2	2	0.12	0.01	0.12
(1,1496)	1:C:1026:LEU:HD23	1:C:1029:MET:HE3	2	0.12	0.01	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD11	2	0.12	0.0	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD12	2	0.12	0.0	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD13	2	0.12	0.0	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD21	2	0.12	0.0	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD22	2	0.12	0.0	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD23	2	0.12	0.0	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD11	2	0.12	0.0	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD12	2	0.12	0.0	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD13	2	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD21	2	0.12	0.0	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD22	2	0.12	0.0	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD23	2	0.12	0.0	0.12
(1,1423)	1:A:6:LEU:HD11	1:C:1013:ARG:HA	2	0.12	0.0	0.12
(1,1423)	1:A:6:LEU:HD12	1:C:1013:ARG:HA	2	0.12	0.0	0.12
(1,1423)	1:A:6:LEU:HD13	1:C:1013:ARG:HA	2	0.12	0.0	0.12
(1,1423)	1:A:6:LEU:HD21	1:C:1013:ARG:HA	2	0.12	0.0	0.12
(1,1423)	1:A:6:LEU:HD22	1:C:1013:ARG:HA	2	0.12	0.0	0.12
(1,1423)	1:A:6:LEU:HD23	1:C:1013:ARG:HA	2	0.12	0.0	0.12
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD11	2	0.12	0.0	0.12
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD12	2	0.12	0.0	0.12
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD13	2	0.12	0.0	0.12
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD21	2	0.12	0.0	0.12
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD22	2	0.12	0.0	0.12
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD23	2	0.12	0.0	0.12
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD11	2	0.12	0.0	0.12
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD12	2	0.12	0.0	0.12
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD13	2	0.12	0.0	0.12
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD21	2	0.12	0.0	0.12
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD22	2	0.12	0.0	0.12
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD23	2	0.12	0.0	0.12
(2,655)	1:A:36:THR:HG21	2:B:124:LEU:HA	2	0.12	0.0	0.12
(2,655)	1:A:36:THR:HG22	2:B:124:LEU:HA	2	0.12	0.0	0.12
(2,655)	1:A:36:THR:HG23	2:B:124:LEU:HA	2	0.12	0.0	0.12
(2,656)	1:C:1036:THR:HG21	2:D:1124:LEU:HA	2	0.12	0.0	0.12
(2,656)	1:C:1036:THR:HG22	2:D:1124:LEU:HA	2	0.12	0.0	0.12
(2,656)	1:C:1036:THR:HG23	2:D:1124:LEU:HA	2	0.12	0.0	0.12
(2,880)	2:B:120:GLU:HG2	2:D:1104:ARG:HB2	2	0.12	0.0	0.12
(2,880)	2:B:120:GLU:HG2	2:D:1104:ARG:HB3	2	0.12	0.0	0.12
(2,880)	2:B:120:GLU:HG3	2:D:1104:ARG:HB2	2	0.12	0.0	0.12
(2,880)	2:B:120:GLU:HG3	2:D:1104:ARG:HB3	2	0.12	0.0	0.12
(1,749)	1:C:1020:LEU:HD11	2:D:1122:MET:HE1	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD11	2:D:1122:MET:HE2	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD11	2:D:1122:MET:HE3	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD12	2:D:1122:MET:HE1	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD12	2:D:1122:MET:HE2	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD12	2:D:1122:MET:HE3	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD13	2:D:1122:MET:HE1	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD13	2:D:1122:MET:HE2	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD13	2:D:1122:MET:HE3	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD21	2:D:1122:MET:HE1	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD21	2:D:1122:MET:HE2	2	0.11	0.0	0.11

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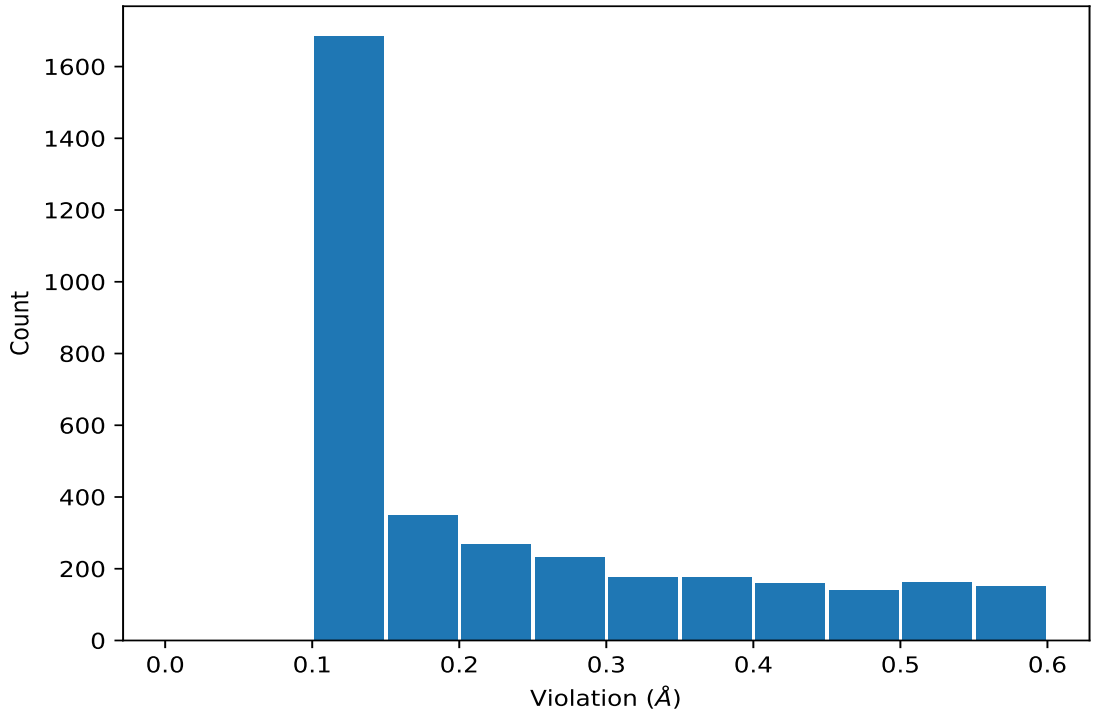
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,749)	1:C:1020:LEU:HD21	2:D:1122:MET:HE3	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD22	2:D:1122:MET:HE1	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD22	2:D:1122:MET:HE2	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD22	2:D:1122:MET:HE3	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD23	2:D:1122:MET:HE1	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD23	2:D:1122:MET:HE2	2	0.11	0.0	0.11
(1,749)	1:C:1020:LEU:HD23	2:D:1122:MET:HE3	2	0.11	0.0	0.11
(1,1075)	1:A:13:ARG:HD2	1:C:1006:LEU:HD21	2	0.11	0.0	0.11
(1,1075)	1:A:13:ARG:HD2	1:C:1006:LEU:HD22	2	0.11	0.0	0.11
(1,1075)	1:A:13:ARG:HD2	1:C:1006:LEU:HD23	2	0.11	0.0	0.11
(1,1075)	1:A:13:ARG:HD3	1:C:1006:LEU:HD21	2	0.11	0.0	0.11
(1,1075)	1:A:13:ARG:HD3	1:C:1006:LEU:HD22	2	0.11	0.0	0.11
(1,1075)	1:A:13:ARG:HD3	1:C:1006:LEU:HD23	2	0.11	0.0	0.11
(1,1506)	1:C:1026:LEU:HD11	2:D:1115:LEU:HA	2	0.11	0.0	0.11
(1,1506)	1:C:1026:LEU:HD12	2:D:1115:LEU:HA	2	0.11	0.0	0.11
(1,1506)	1:C:1026:LEU:HD13	2:D:1115:LEU:HA	2	0.11	0.0	0.11
(1,1506)	1:C:1026:LEU:HD21	2:D:1115:LEU:HA	2	0.11	0.0	0.11
(1,1506)	1:C:1026:LEU:HD22	2:D:1115:LEU:HA	2	0.11	0.0	0.11
(1,1506)	1:C:1026:LEU:HD23	2:D:1115:LEU:HA	2	0.11	0.0	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD11	2	0.11	0.0	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD12	2	0.11	0.0	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD13	2	0.11	0.0	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD21	2	0.11	0.0	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD22	2	0.11	0.0	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD23	2	0.11	0.0	0.11
(1,1574)	2:D:1103:VAL:HG11	2:D:1109:PHE:H	2	0.11	0.0	0.11
(1,1574)	2:D:1103:VAL:HG12	2:D:1109:PHE:H	2	0.11	0.0	0.11
(1,1574)	2:D:1103:VAL:HG13	2:D:1109:PHE:H	2	0.11	0.0	0.11
(1,1574)	2:D:1103:VAL:HG21	2:D:1109:PHE:H	2	0.11	0.0	0.11
(1,1574)	2:D:1103:VAL:HG22	2:D:1109:PHE:H	2	0.11	0.0	0.11
(1,1574)	2:D:1103:VAL:HG23	2:D:1109:PHE:H	2	0.11	0.0	0.11
(2,684)	1:C:1007:TYR:HE1	2:D:1140:LEU:HB2	2	0.11	0.0	0.11
(2,684)	1:C:1007:TYR:HE1	2:D:1140:LEU:HB3	2	0.11	0.0	0.11
(2,684)	1:C:1007:TYR:HE2	2:D:1140:LEU:HB2	2	0.11	0.0	0.11
(2,684)	1:C:1007:TYR:HE2	2:D:1140:LEU:HB3	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard 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)
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	15	0.58
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	4	0.58
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	8	0.58
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	13	0.58
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	14	0.58
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	15	0.58
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	20	0.58
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	14	0.58
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	19	0.58
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	18	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	3	0.58
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	11	0.58
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	12	0.58
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	16	0.58
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	18	0.58
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	11	0.58
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	18	0.58
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	19	0.58
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	13	0.58
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	17	0.58
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	1	0.57
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	12	0.57
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	17	0.57
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	18	0.57
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	9	0.57
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	13	0.57
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	5	0.57
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	11	0.57
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	20	0.57
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	2	0.57
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	6	0.57
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	14	0.57
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	15	0.57
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	19	0.57
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	20	0.57
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	12	0.57
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	15	0.57
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	16	0.57
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	15	0.57
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	5	0.57
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	16	0.57
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	5	0.57
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	2	0.57
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	20	0.57
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	20	0.57
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	5	0.57
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	7	0.57
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	14	0.57
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	19	0.57
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	1	0.56
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	2	0.56
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	19	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	2	0.56
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	5	0.56
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	9	0.56
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	10	0.56
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	1	0.56
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	16	0.56
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	8	0.56
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	9	0.56
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	18	0.56
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	19	0.56
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	1	0.56
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	5	0.56
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	9	0.56
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	13	0.56
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	17	0.56
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	11	0.56
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	9	0.56
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	6	0.56
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	8	0.56
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	9	0.56
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	14	0.56
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	1	0.56
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	5	0.56
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	11	0.56
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	11	0.56
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	17	0.56
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	11	0.56
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	3	0.56
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	11	0.56
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	12	0.56
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	13	0.56
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	5	0.56
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	8	0.56
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	11	0.56
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	5	0.56
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	15	0.56
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	14	0.56
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	3	0.56
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	1	0.56
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	2	0.56
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	6	0.56
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	9	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	12	0.56
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	2	0.56
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	4	0.56
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	11	0.56
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	16	0.56
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	2	0.56
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	16	0.56
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	17	0.56
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	1	0.56
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	11	0.56
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	6	0.56
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	1	0.56
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	9	0.56
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	10	0.56
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	6	0.56
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	7	0.56
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	3	0.55
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	7	0.55
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	10	0.55
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	11	0.55
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	2	0.55
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	7	0.55
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	12	0.55
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	16	0.55
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	14	0.55
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	6	0.55
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	11	0.55
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	16	0.55
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	4	0.55
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	10	0.55
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	19	0.55
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	12	0.55
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	6	0.55
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	19	0.55
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	4	0.55
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	10	0.55
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	12	0.55
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	2	0.55
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	7	0.55
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	2	0.55
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	8	0.55
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	7	0.55
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	1	0.55
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	17	0.55
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	10	0.55
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	14	0.55
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	14	0.55
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	5	0.55
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	19	0.55
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	6	0.55
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	9	0.55
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	10	0.55
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	17	0.55
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	9	0.55
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	10	0.55
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	8	0.55
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	5	0.55
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	14	0.55
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	12	0.54
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	6	0.54
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	16	0.54
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	10	0.54
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	13	0.54
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	1	0.54
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	13	0.54
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	17	0.54
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	17	0.54
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	5	0.54
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	20	0.54
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	9	0.54
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	19	0.54
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	10	0.54
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	7	0.54
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	9	0.54
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	12	0.54
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	4	0.54
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	10	0.54
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	14	0.54
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	2	0.54
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	10	0.54
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	17	0.54
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	11	0.54
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	14	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	7	0.54
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	13	0.54
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	2	0.54
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	5	0.54
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	17	0.54
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	14	0.54
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	7	0.54
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	15	0.54
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	12	0.54
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	11	0.54
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	12	0.54
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	16	0.54
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	16	0.54
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	11	0.53
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	18	0.53
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	9	0.53
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	19	0.53
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	5	0.53
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	13	0.53
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	19	0.53
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	4	0.53
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	10	0.53
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	2	0.53
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	15	0.53
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	7	0.53
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	17	0.53
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	2	0.53
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	14	0.53
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	10	0.53
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	17	0.53
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	17	0.53
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	20	0.53
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	2	0.53
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	1	0.53
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	19	0.53
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	2	0.53
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	11	0.53
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	8	0.53
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	16	0.53
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	20	0.53
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	2	0.53
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	14	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	8	0.53
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	14	0.52
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	18	0.52
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	6	0.52
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	1	0.52
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	5	0.52
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	3	0.52
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	3	0.52
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	6	0.52
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	5	0.52
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	10	0.52
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	9	0.52
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	2	0.52
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	3	0.52
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	11	0.52
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	4	0.52
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	1	0.52
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	16	0.52
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	10	0.52
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	1	0.52
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	7	0.52
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	14	0.52
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	20	0.52
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	10	0.52
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	10	0.52
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	9	0.52
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	20	0.52
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	16	0.51
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	5	0.51
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	12	0.51
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	17	0.51
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	11	0.51
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	14	0.51
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	20	0.51
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	16	0.51
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	12	0.51
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	10	0.51
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	12	0.51
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	6	0.51
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	7	0.51
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	16	0.51
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	15	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	11	0.51
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	9	0.51
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	6	0.51
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	1	0.51
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	8	0.51
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	19	0.51
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	13	0.51
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	6	0.51
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	14	0.51
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	19	0.51
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	12	0.51
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	9	0.51
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	20	0.51
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	11	0.51
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	16	0.5
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	8	0.5
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	9	0.5
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	2	0.5
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	3	0.5
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	14	0.5
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	18	0.5
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	2	0.5
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	7	0.5
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	3	0.5
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	20	0.5
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	2	0.5
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	14	0.5
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	1	0.5
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	2	0.5
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	19	0.5
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	2	0.5
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	11	0.5
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	13	0.5
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	9	0.5
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	18	0.5
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	15	0.5
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	16	0.5
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	1	0.5
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	5	0.5
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	5	0.5
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	2	0.5
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	19	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	7	0.5
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	16	0.5
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	10	0.5
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	16	0.5
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	16	0.5
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	13	0.5
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	14	0.5
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	13	0.5
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	2	0.5
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	20	0.5
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	16	0.5
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	7	0.49
(4,95)	2:D:1106:ARG:O	2:D:1110:GLU:N	19	0.49
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	4	0.49
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	11	0.49
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	12	0.49
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	12	0.49
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	19	0.49
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	12	0.49
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	15	0.49
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	8	0.49
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	16	0.49
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	17	0.49
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	11	0.49
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	13	0.49
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	3	0.49
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	17	0.49
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	13	0.49
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	14	0.49
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	8	0.49
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	9	0.49
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	3	0.49
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	19	0.49
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	9	0.49
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	18	0.49
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	11	0.49
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	6	0.49
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	12	0.49
(4,22)	1:A:25:SER:O	1:A:29:MET:N	11	0.49
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	15	0.49
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	12	0.49
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	15	0.48
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	4	0.48
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	4	0.48
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	18	0.48
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	9	0.48
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	18	0.48
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	15	0.48
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	18	0.48
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	18	0.48
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	19	0.48
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	13	0.48
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	8	0.48
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	19	0.48
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	11	0.48
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	3	0.48
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	6	0.48
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	11	0.48
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	12	0.48
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	14	0.48
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	4	0.48
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	17	0.48
(4,22)	1:A:25:SER:O	1:A:29:MET:N	8	0.48
(4,22)	1:A:25:SER:O	1:A:29:MET:N	14	0.48
(4,22)	1:A:25:SER:O	1:A:29:MET:N	16	0.48
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	7	0.48
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	12	0.48
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	13	0.48
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	13	0.48
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	1	0.47
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	16	0.47
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	16	0.47
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	7	0.47
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	16	0.47
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	16	0.47
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	18	0.47
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	6	0.47
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	20	0.47
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	6	0.47
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	4	0.47
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	5	0.47
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	6	0.47
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	12	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	18	0.47
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	9	0.47
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	8	0.47
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	15	0.47
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	18	0.47
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	8	0.47
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	19	0.47
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	20	0.47
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	7	0.47
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	10	0.47
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	4	0.47
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	17	0.47
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	13	0.47
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	4	0.47
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	16	0.46
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	20	0.46
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	15	0.46
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	1	0.46
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	9	0.46
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	7	0.46
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	13	0.46
(4,64)	2:B:129:LEU:O	2:B:133:TYR:N	17	0.46
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	5	0.46
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	11	0.46
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	13	0.46
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	18	0.46
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	3	0.46
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	7	0.46
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	13	0.46
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	17	0.46
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	7	0.46
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	11	0.46
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	15	0.46
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	20	0.46
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	4	0.46
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	13	0.46
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	5	0.46
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	10	0.46
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	18	0.46
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	3	0.46
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	5	0.46
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	3	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	3	0.45
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	20	0.45
(4,71)	2:B:106:ARG:O	2:B:110:GLU:N	2	0.45
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	5	0.45
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	11	0.45
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	8	0.45
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	16	0.45
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	17	0.45
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	16	0.45
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	13	0.45
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	12	0.45
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	6	0.45
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	3	0.45
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	7	0.45
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	14	0.45
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	7	0.45
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	11	0.45
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	2	0.45
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	16	0.45
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	20	0.45
(4,22)	1:A:25:SER:O	1:A:29:MET:N	20	0.45
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	19	0.45
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	2	0.45
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	9	0.45
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	9	0.45
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	15	0.45
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	7	0.44
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	1	0.44
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	15	0.44
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	16	0.44
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	9	0.44
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	7	0.44
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	12	0.44
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	18	0.44
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	6	0.44
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	2	0.44
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	13	0.44
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	15	0.44
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	6	0.44
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	9	0.44
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	7	0.44
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	9	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	14	0.44
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	4	0.44
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	8	0.44
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	14	0.44
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	8	0.44
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	12	0.44
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	10	0.44
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	10	0.44
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	9	0.44
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	2	0.44
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	18	0.44
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	7	0.44
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	10	0.44
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	3	0.44
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	20	0.44
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	5	0.43
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	6	0.43
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	11	0.43
(4,83)	2:B:118:SER:O	2:B:122:MET:N	4	0.43
(4,83)	2:B:118:SER:O	2:B:122:MET:N	11	0.43
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	14	0.43
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	12	0.43
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	16	0.43
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	17	0.43
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	2	0.43
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	2	0.43
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	7	0.43
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	9	0.43
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	11	0.43
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	2	0.43
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	17	0.43
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	20	0.43
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	5	0.43
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	19	0.43
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	16	0.43
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	14	0.43
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	4	0.43
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	7	0.43
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	10	0.43
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	3	0.43
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	19	0.43
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	14	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	18	0.43
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	5	0.43
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	7	0.43
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	1	0.43
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	3	0.43
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	19	0.43
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	5	0.43
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	15	0.43
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	8	0.43
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	14	0.43
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	6	0.43
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	15	0.43
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	13	0.42
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	11	0.42
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	15	0.42
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	5	0.42
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	1	0.42
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	3	0.42
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	3	0.42
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	9	0.42
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	2	0.42
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	10	0.42
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	18	0.42
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	10	0.42
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	5	0.42
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	16	0.42
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	13	0.42
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	14	0.42
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	18	0.42
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	8	0.42
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	18	0.42
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	4	0.42
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	4	0.42
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	10	0.42
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	15	0.42
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	16	0.42
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	10	0.42
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	10	0.42
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	3	0.42
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	4	0.42
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	12	0.42
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	17	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	7	0.42
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	17	0.42
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	17	0.41
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	14	0.41
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	4	0.41
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	12	0.41
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	20	0.41
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	1	0.41
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	17	0.41
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	19	0.41
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	16	0.41
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	4	0.41
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	1	0.41
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	4	0.41
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	2	0.41
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	2	0.41
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	1	0.41
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	18	0.41
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	17	0.41
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	3	0.41
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	17	0.41
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	2	0.41
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	15	0.41
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	12	0.41
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	4	0.4
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	13	0.4
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	14	0.4
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	6	0.4
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	17	0.4
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	16	0.4
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	1	0.4
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	12	0.4
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	4	0.4
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	7	0.4
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	14	0.4
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	1	0.4
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	17	0.4
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	2	0.4
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	1	0.4
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	7	0.4
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	6	0.4
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	12	0.4
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	5	0.4
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	2	0.4
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	6	0.4
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	8	0.4
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	10	0.4
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	4	0.4
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	3	0.4
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	18	0.4
(4,22)	1:A:25:SER:O	1:A:29:MET:N	5	0.4
(4,22)	1:A:25:SER:O	1:A:29:MET:N	10	0.4
(4,17)	1:A:20:LEU:O	1:A:24:GLU:N	14	0.4
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	12	0.4
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	1	0.4
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	15	0.4
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	11	0.4
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	11	0.4
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	18	0.4
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	4	0.39
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	6	0.39
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	11	0.39
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	12	0.39
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	15	0.39
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	2	0.39
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	8	0.39
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	20	0.39
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	13	0.39
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	3	0.39
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	13	0.39
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	14	0.39
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	5	0.39
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	8	0.39
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	15	0.39
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	18	0.39
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	20	0.39
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	3	0.39
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	18	0.39
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	8	0.39
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	1	0.39
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	12	0.39
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	15	0.39
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	17	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	19	0.39
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	9	0.39
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	17	0.39
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	19	0.39
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	5	0.39
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	9	0.39
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	16	0.39
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	19	0.39
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	18	0.39
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	20	0.39
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	4	0.39
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	14	0.39
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	15	0.39
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	18	0.39
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	1	0.39
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	7	0.39
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	4	0.39
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	18	0.39
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	5	0.39
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	13	0.38
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	9	0.38
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	11	0.38
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	14	0.38
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	7	0.38
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	7	0.38
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	17	0.38
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	13	0.38
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	5	0.38
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	10	0.38
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	4	0.38
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	8	0.38
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	13	0.38
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	7	0.38
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	10	0.38
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	11	0.38
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	2	0.38
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	6	0.38
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	7	0.38
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	8	0.38
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	15	0.38
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	2	0.38
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	16	0.38
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	10	0.38
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	19	0.37
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	20	0.37
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	16	0.37
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	8	0.37
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	18	0.37
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	12	0.37
(4,70)	2:B:135:GLN:O	2:B:139:LEU:N	8	0.37
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	18	0.37
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	3	0.37
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	20	0.37
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	20	0.37
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	16	0.37
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	17	0.37
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	4	0.37
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	19	0.37
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	14	0.37
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	20	0.37
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	18	0.37
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	17	0.37
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	10	0.37
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	16	0.37
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	15	0.37
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	17	0.37
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	4	0.37
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	10	0.37
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	6	0.37
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	8	0.37
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	9	0.37
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	14	0.37
(4,22)	1:A:25:SER:O	1:A:29:MET:N	3	0.37
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	15	0.37
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	17	0.37
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	18	0.37
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	19	0.37
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	17	0.37
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	2	0.37
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	14	0.37
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	9	0.36
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	10	0.36
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	17	0.36
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	2	0.36
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	11	0.36
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	10	0.36
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	2	0.36
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	20	0.36
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	10	0.36
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	14	0.36
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	16	0.36
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	18	0.36
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	18	0.36
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	11	0.36
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	15	0.36
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	4	0.36
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	16	0.36
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	18	0.36
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	20	0.36
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	7	0.36
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	20	0.36
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	3	0.36
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	17	0.36
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	14	0.36
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	1	0.36
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	5	0.36
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	1	0.36
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	3	0.36
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	17	0.36
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	7	0.36
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	13	0.36
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	15	0.36
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	2	0.36
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	17	0.35
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	1	0.35
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	6	0.35
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	10	0.35
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	7	0.35
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	10	0.35
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	8	0.35
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	4	0.35
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	15	0.35
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	9	0.35
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	10	0.35
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	20	0.35
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	10	0.35
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	3	0.35
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	8	0.35
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	12	0.35
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	10	0.35
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	6	0.35
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	18	0.35
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	14	0.35
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	10	0.35
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	16	0.35
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	3	0.35
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	15	0.35
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	12	0.35
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	3	0.35
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	6	0.35
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	16	0.35
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	3	0.35
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	18	0.35
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	7	0.35
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	3	0.35
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	17	0.35
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	20	0.35
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	17	0.35
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	15	0.35
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	1	0.34
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	8	0.34
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	13	0.34
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	8	0.34
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	15	0.34
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	2	0.34
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	1	0.34
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	9	0.34
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	7	0.34
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	17	0.34
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	5	0.34
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	16	0.34
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	4	0.34
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	15	0.34
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	7	0.34
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	16	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	9	0.34
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	15	0.34
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	19	0.34
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	20	0.34
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	12	0.34
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	12	0.34
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	17	0.34
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	13	0.34
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	3	0.34
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	12	0.34
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	5	0.34
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	14	0.34
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	9	0.34
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	9	0.33
(4,87)	2:D:1128:PRO:O	2:D:1132:SER:N	10	0.33
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	18	0.33
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	5	0.33
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	10	0.33
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	17	0.33
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	15	0.33
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	13	0.33
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	5	0.33
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	19	0.33
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	16	0.33
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	10	0.33
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	14	0.33
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	20	0.33
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	11	0.33
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	6	0.33
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	7	0.33
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	2	0.33
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	11	0.33
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	12	0.33
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	9	0.33
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	12	0.33
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	8	0.33
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	19	0.33
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	5	0.33
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	6	0.33
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	19	0.33
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	8	0.33
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,22)	1:A:25:SER:O	1:A:29:MET:N	4	0.33
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	19	0.33
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	18	0.33
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	6	0.33
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	17	0.33
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	4	0.33
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	4	0.33
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	14	0.33
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	15	0.33
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	5	0.32
(4,83)	2:B:118:SER:O	2:B:122:MET:N	6	0.32
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	2	0.32
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	20	0.32
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	4	0.32
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	10	0.32
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	8	0.32
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	6	0.32
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	8	0.32
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	19	0.32
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	11	0.32
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	3	0.32
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	6	0.32
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	7	0.32
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	12	0.32
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	3	0.32
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	5	0.32
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	12	0.32
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	3	0.32
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	1	0.32
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	17	0.32
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	11	0.32
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	9	0.32
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	2	0.32
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	6	0.32
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	10	0.32
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	6	0.32
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	9	0.32
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	9	0.32
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	3	0.32
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	15	0.32
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	12	0.32
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	19	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	12	0.32
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	15	0.32
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	15	0.32
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	19	0.32
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	16	0.32
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	19	0.32
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	2	0.32
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	2	0.31
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	15	0.31
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	4	0.31
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	11	0.31
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	3	0.31
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	5	0.31
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	11	0.31
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	8	0.31
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	11	0.31
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	13	0.31
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	9	0.31
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	11	0.31
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	10	0.31
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	14	0.31
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	18	0.31
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	12	0.31
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	10	0.31
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	14	0.31
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	18	0.31
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	20	0.31
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	12	0.31
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	8	0.31
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	15	0.31
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	20	0.31
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	4	0.31
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	17	0.31
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	5	0.31
(4,22)	1:A:25:SER:O	1:A:29:MET:N	2	0.31
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	11	0.31
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	10	0.31
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	3	0.31
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	4	0.31
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	1	0.31
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	9	0.31
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	18	0.31
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	20	0.31
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	1	0.31
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	4	0.31
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	18	0.31
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	6	0.31
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	8	0.3
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	19	0.3
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	20	0.3
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	15	0.3
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	4	0.3
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	7	0.3
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	15	0.3
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	8	0.3
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	18	0.3
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	5	0.3
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	14	0.3
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	4	0.3
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	3	0.3
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	6	0.3
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	17	0.3
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	18	0.3
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	4	0.3
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	14	0.3
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	3	0.3
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	15	0.3
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	10	0.3
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	4	0.3
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	18	0.3
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	6	0.3
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	18	0.3
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	7	0.3
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	2	0.3
(4,101)	2:D:1112:LEU:O	2:D:1116:LYS:N	10	0.3
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	2	0.3
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	3	0.29
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	16	0.29
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	3	0.29
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	8	0.29
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	3	0.29
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	14	0.29
(4,88)	2:D:1129:LEU:O	2:D:1133:TYR:N	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	2	0.29
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	4	0.29
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	13	0.29
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	9	0.29
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	11	0.29
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	7	0.29
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	8	0.29
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	11	0.29
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	16	0.29
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	18	0.29
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	13	0.29
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	20	0.29
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	13	0.29
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	16	0.29
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	1	0.29
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	5	0.29
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	5	0.29
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	19	0.29
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	2	0.29
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	12	0.29
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	1	0.29
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	11	0.29
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	1	0.29
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	11	0.29
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	9	0.29
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	1	0.29
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	20	0.29
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	13	0.29
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	1	0.29
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	11	0.29
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	3	0.29
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	5	0.29
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	11	0.29
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	18	0.29
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	8	0.29
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	3	0.29
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	11	0.29
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	10	0.29
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	12	0.29
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	3	0.29
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	8	0.29
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	6	0.29
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	8	0.29
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	4	0.29
(4,10)	1:A:13:ARG:O	1:A:17:GLU:N	20	0.29
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	12	0.29
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	20	0.28
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	15	0.28
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	20	0.28
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	7	0.28
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	3	0.28
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	5	0.28
(4,83)	2:B:118:SER:O	2:B:122:MET:N	8	0.28
(4,83)	2:B:118:SER:O	2:B:122:MET:N	10	0.28
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	16	0.28
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	1	0.28
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	6	0.28
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	17	0.28
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	20	0.28
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	19	0.28
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	3	0.28
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	17	0.28
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	9	0.28
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	19	0.28
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	1	0.28
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	11	0.28
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	16	0.28
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	11	0.28
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	3	0.28
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	4	0.28
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	11	0.28
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	9	0.28
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	12	0.28
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	5	0.28
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	11	0.28
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	16	0.28
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	6	0.28
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	10	0.28
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	12	0.28
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	20	0.28
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	13	0.28
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	16	0.28
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	9	0.28
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	6	0.28
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	15	0.28
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	18	0.28
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	20	0.28
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	1	0.28
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	19	0.28
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	8	0.28
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	2	0.27
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	13	0.27
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	4	0.27
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	17	0.27
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	18	0.27
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	3	0.27
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	20	0.27
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	8	0.27
(4,83)	2:B:118:SER:O	2:B:122:MET:N	19	0.27
(4,83)	2:B:118:SER:O	2:B:122:MET:N	20	0.27
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	17	0.27
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	18	0.27
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	10	0.27
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	6	0.27
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	12	0.27
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	19	0.27
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	9	0.27
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	1	0.27
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	13	0.27
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	14	0.27
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	15	0.27
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	5	0.27
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	8	0.27
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	14	0.27
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	17	0.27
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	6	0.27
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	20	0.27
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	13	0.27
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	2	0.27
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	3	0.27
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	6	0.27
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	1	0.27
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	7	0.27
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	2	0.27
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	18	0.27
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	12	0.27
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	2	0.27
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	17	0.27
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	1	0.27
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	17	0.27
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	20	0.27
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	15	0.27
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	19	0.27
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	13	0.27
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	10	0.27
(4,22)	1:A:25:SER:O	1:A:29:MET:N	1	0.27
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	7	0.27
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	16	0.27
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	14	0.27
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	4	0.27
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	10	0.27
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	20	0.27
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	3	0.27
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	14	0.26
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	15	0.26
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	17	0.26
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	18	0.26
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	6	0.26
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	10	0.26
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	13	0.26
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	7	0.26
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	17	0.26
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	7	0.26
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	15	0.26
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	7	0.26
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	7	0.26
(4,60)	2:D:1099:TYR:O	2:B:103:VAL:N	4	0.26
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	20	0.26
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	3	0.26
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	9	0.26
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	15	0.26
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	12	0.26
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	18	0.26
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	8	0.26
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	18	0.26
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	17	0.26
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	13	0.26
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	7	0.26
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	17	0.26
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	2	0.26
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	20	0.26
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	12	0.26
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	8	0.26
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	6	0.26
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	16	0.26
(4,22)	1:A:25:SER:O	1:A:29:MET:N	13	0.26
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	11	0.26
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	7	0.26
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	12	0.26
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	11	0.26
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	10	0.26
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	16	0.26
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	20	0.26
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	18	0.25
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	19	0.25
(4,94)	2:D:1135:GLN:O	2:D:1139:LEU:N	7	0.25
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	9	0.25
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	14	0.25
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	6	0.25
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	15	0.25
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	15	0.25
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	6	0.25
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	17	0.25
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	16	0.25
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	16	0.25
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	8	0.25
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	8	0.25
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	14	0.25
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	12	0.25
(4,57)	2:B:99:TYR:O	2:D:1103:VAL:N	20	0.25
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	4	0.25
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	2	0.25
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	6	0.25
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	19	0.25
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	8	0.25
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	8	0.25
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	16	0.25
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	2	0.25
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	13	0.25
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	6	0.25
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	13	0.25
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	17	0.25
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	2	0.25
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	7	0.25
(4,22)	1:A:25:SER:O	1:A:29:MET:N	19	0.25
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	4	0.25
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	18	0.25
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	19	0.25
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	14	0.25
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	7	0.25
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	10	0.25
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	19	0.25
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	11	0.24
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	15	0.24
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	9	0.24
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	8	0.24
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	11	0.24
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	13	0.24
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	17	0.24
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	20	0.24
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	12	0.24
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	3	0.24
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	14	0.24
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	2	0.24
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	7	0.24
(4,58)	2:B:101:LEU:O	2:D:1101:LEU:N	15	0.24
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	13	0.24
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	12	0.24
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	14	0.24
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	15	0.24
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	8	0.24
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	6	0.24
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	13	0.24
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	12	0.24
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	17	0.24
(4,44)	1:C:1022:ILE:O	1:C:1026:LEU:N	1	0.24
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	8	0.24
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	17	0.24
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	6	0.24
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	4	0.24
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	17	0.24
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	19	0.24
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	20	0.24
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	5	0.24
(4,22)	1:A:25:SER:O	1:A:29:MET:N	6	0.24
(4,22)	1:A:25:SER:O	1:A:29:MET:N	12	0.24
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	4	0.24
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	8	0.24
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	17	0.24
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	8	0.24
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	9	0.24
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	7	0.24
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	7	0.24
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	9	0.24
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	16	0.24
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	18	0.24
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	15	0.23
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	11	0.23
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	9	0.23
(4,83)	2:B:118:SER:O	2:B:122:MET:N	14	0.23
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	16	0.23
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	19	0.23
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	3	0.23
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	20	0.23
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	15	0.23
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	4	0.23
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	10	0.23
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	1	0.23
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	9	0.23
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	17	0.23
(4,61)	2:D:1101:LEU:O	2:B:101:LEU:N	4	0.23
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	10	0.23
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	16	0.23
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	4	0.23
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	6	0.23
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	2	0.23
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	12	0.23
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	3	0.23
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	20	0.23
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	4	0.23
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	6	0.23
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	7	0.23
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	15	0.23
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	18	0.23
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	16	0.23
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	13	0.23
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	9	0.23
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	2	0.23
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	16	0.23
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	9	0.23
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	13	0.23
(4,22)	1:A:25:SER:O	1:A:29:MET:N	15	0.23
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	4	0.23
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	8	0.23
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	17	0.23
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	20	0.23
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	5	0.23
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	12	0.23
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	10	0.23
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	3	0.22
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	12	0.22
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	10	0.22
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	12	0.22
(4,92)	2:D:1133:TYR:O	2:D:1137:GLN:N	7	0.22
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	1	0.22
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	6	0.22
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	9	0.22
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	1	0.22
(4,83)	2:B:118:SER:O	2:B:122:MET:N	16	0.22
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	19	0.22
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	8	0.22
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	10	0.22
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	4	0.22
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	7	0.22
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	11	0.22
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	3	0.22
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	4	0.22
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	16	0.22
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,63)	2:B:128:PRO:O	2:B:132:SER:N	1	0.22
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	11	0.22
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	1	0.22
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	1	0.22
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	15	0.22
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	1	0.22
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	5	0.22
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	9	0.22
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	2	0.22
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	9	0.22
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	11	0.22
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	4	0.22
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	6	0.22
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	16	0.22
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	18	0.22
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	8	0.22
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	7	0.22
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	16	0.22
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	18	0.22
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	9	0.22
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	17	0.22
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	11	0.22
(4,22)	1:A:25:SER:O	1:A:29:MET:N	7	0.22
(4,22)	1:A:25:SER:O	1:A:29:MET:N	18	0.22
(4,19)	1:A:22:ILE:O	1:A:26:LEU:N	4	0.22
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	15	0.22
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	2	0.22
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	7	0.22
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	16	0.22
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	19	0.22
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	5	0.22
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	20	0.22
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	8	0.22
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	17	0.22
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	19	0.22
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	5	0.22
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	6	0.22
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	8	0.22
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	5	0.22
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	6	0.22
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	13	0.22
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	17	0.22
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	11	0.22
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	6	0.21
(4,92)	2:D:1133:TYR:O	2:D:1137:GLN:N	19	0.21
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	6	0.21
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	8	0.21
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	2	0.21
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	15	0.21
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	5	0.21
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	17	0.21
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	2	0.21
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	18	0.21
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	13	0.21
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	3	0.21
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	13	0.21
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	6	0.21
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	9	0.21
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	11	0.21
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	8	0.21
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	19	0.21
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	15	0.21
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	13	0.21
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	1	0.21
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	19	0.21
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	9	0.21
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	10	0.21
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	18	0.21
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	9	0.21
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	17	0.21
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	8	0.21
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	15	0.21
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	1	0.21
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	17	0.21
(4,22)	1:A:25:SER:O	1:A:29:MET:N	17	0.21
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	2	0.21
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	13	0.21
(4,17)	1:A:20:LEU:O	1:A:24:GLU:N	13	0.21
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	16	0.21
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	4	0.21
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	9	0.21
(4,109)	2:D:1120:GLU:O	2:D:1124:LEU:N	5	0.21
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	20	0.21
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	12	0.21
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	4	0.21
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	10	0.21
(4,101)	2:D:1112:LEU:O	2:D:1116:LYS:N	4	0.21
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	13	0.21
(4,98)	2:D:1109:PHE:O	2:D:1113:MET:N	19	0.2
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	9	0.2
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	20	0.2
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	2	0.2
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	3	0.2
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	4	0.2
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	5	0.2
(4,83)	2:B:118:SER:O	2:B:122:MET:N	13	0.2
(4,83)	2:B:118:SER:O	2:B:122:MET:N	15	0.2
(4,8)	1:A:41:ARG:O	1:A:45:GLN:N	7	0.2
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	5	0.2
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	19	0.2
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	13	0.2
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	14	0.2
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	8	0.2
(4,75)	2:B:110:GLU:O	2:B:114:LYS:N	3	0.2
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	11	0.2
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	12	0.2
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	3	0.2
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	12	0.2
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	14	0.2
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	9	0.2
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	20	0.2
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	5	0.2
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	7	0.2
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	11	0.2
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	18	0.2
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	8	0.2
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	2	0.2
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	9	0.2
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	5	0.2
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	6	0.2
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	18	0.2
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	9	0.2
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	17	0.2
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	3	0.2
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	5	0.2
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	15	0.2
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	2	0.2
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	14	0.2
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	13	0.2
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	14	0.2
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	20	0.2
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	3	0.2
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	18	0.2
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	7	0.2
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	7	0.2
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	19	0.2
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	20	0.2
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	3	0.2
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	8	0.2
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	10	0.2
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	16	0.2
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	17	0.2
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	5	0.2
(4,17)	1:A:20:LEU:O	1:A:24:GLU:N	7	0.2
(4,17)	1:A:20:LEU:O	1:A:24:GLU:N	18	0.2
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	8	0.2
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	9	0.2
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	16	0.2
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	18	0.2
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	2	0.2
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	7	0.2
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	13	0.2
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	18	0.2
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	5	0.2
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	2	0.2
(4,101)	2:D:1112:LEU:O	2:D:1116:LYS:N	1	0.2
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	11	0.2
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	5	0.19
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	6	0.19
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	14	0.19
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	17	0.19
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	12	0.19
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	18	0.19
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	4	0.19
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	11	0.19
(4,83)	2:B:118:SER:O	2:B:122:MET:N	3	0.19
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	7	0.19
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	12	0.19
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	6	0.19
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	14	0.19
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	8	0.19
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	10	0.19
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	6	0.19
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	17	0.19
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	20	0.19
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	13	0.19
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	4	0.19
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	3	0.19
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	4	0.19
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	14	0.19
(4,56)	1:C:1006:LEU:O	1:A:10:VAL:N	16	0.19
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	10	0.19
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	16	0.19
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	20	0.19
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	3	0.19
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	8	0.19
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	12	0.19
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	13	0.19
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	20	0.19
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	10	0.19
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	15	0.19
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	17	0.19
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	10	0.19
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	14	0.19
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	18	0.19
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	4	0.19
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	9	0.19
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	19	0.19
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	13	0.19
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	12	0.19
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	15	0.19
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	16	0.19
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	3	0.19
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	4	0.19
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	5	0.19
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	12	0.19
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	11	0.19
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	16	0.19
(4,22)	1:A:25:SER:O	1:A:29:MET:N	9	0.19
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	11	0.19
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	15	0.19
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	20	0.19
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	19	0.19
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	20	0.19
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	11	0.19
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	2	0.19
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	11	0.19
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	13	0.19
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	4	0.19
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	19	0.19
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	18	0.19
(4,99)	2:D:1110:GLU:O	2:D:1114:LYS:N	8	0.18
(4,98)	2:D:1109:PHE:O	2:D:1113:MET:N	7	0.18
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	14	0.18
(4,91)	2:D:1132:SER:O	2:D:1136:GLN:N	15	0.18
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	8	0.18
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	7	0.18
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	7	0.18
(4,83)	2:B:118:SER:O	2:B:122:MET:N	7	0.18
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	20	0.18
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	5	0.18
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	10	0.18
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	1	0.18
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	8	0.18
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	18	0.18
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	18	0.18
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	20	0.18
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	20	0.18
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	5	0.18
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	6	0.18
(4,66)	2:B:131:ASP:O	2:B:135:GLN:N	12	0.18
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	5	0.18
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	17	0.18
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	20	0.18
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	1	0.18
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	12	0.18
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	16	0.18
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	9	0.18
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	18	0.18
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	11	0.18
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	12	0.18
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	14	0.18
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	6	0.18
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	6	0.18
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	19	0.18
(4,17)	1:A:20:LEU:O	1:A:24:GLU:N	12	0.18
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	3	0.18
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	12	0.18
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	14	0.18
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	1	0.18
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	3	0.18
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	17	0.18
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	19	0.18
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	3	0.17
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	4	0.17
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	6	0.17
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	12	0.17
(4,83)	2:B:118:SER:O	2:B:122:MET:N	9	0.17
(4,83)	2:B:118:SER:O	2:B:122:MET:N	18	0.17
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	5	0.17
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	16	0.17
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	8	0.17
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	14	0.17
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	13	0.17
(4,72)	2:B:107:LYS:O	2:B:111:ILE:N	6	0.17
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	1	0.17
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	3	0.17
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	19	0.17
(4,68)	2:B:133:TYR:O	2:B:137:GLN:N	8	0.17
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	1	0.17
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	7	0.17
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	19	0.17
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	3	0.17
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	18	0.17
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	18	0.17
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	19	0.17
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	2	0.17
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	13	0.17
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	18	0.17
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	11	0.17
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	20	0.17
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	11	0.17
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	1	0.17
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	13	0.17
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	5	0.17
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	8	0.17
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	14	0.17
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	1	0.17
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	7	0.17
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	19	0.17
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	2	0.17
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	8	0.17
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	18	0.17
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	10	0.17
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	14	0.17
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	2	0.17
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	9	0.17
(4,17)	1:A:20:LEU:O	1:A:24:GLU:N	2	0.17
(4,15)	1:A:18:MET:O	1:A:22:ILE:N	6	0.17
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	8	0.17
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	15	0.17
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	2	0.17
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	13	0.17
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD11	9	0.17
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD12	9	0.17
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD13	9	0.17
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD21	9	0.17
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD22	9	0.17
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD23	9	0.17
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD11	9	0.17
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD12	9	0.17
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD13	9	0.17
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD21	9	0.17
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD22	9	0.17
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD23	9	0.17
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD11	9	0.17
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD12	9	0.17
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD13	9	0.17
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD21	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD22	9	0.17
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD23	9	0.17
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD11	9	0.17
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD12	9	0.17
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD13	9	0.17
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD21	9	0.17
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD22	9	0.17
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD23	9	0.17
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD11	9	0.17
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD12	9	0.17
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD13	9	0.17
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD21	9	0.17
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD22	9	0.17
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD23	9	0.17
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD11	9	0.17
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD12	9	0.17
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD13	9	0.17
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD21	9	0.17
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD22	9	0.17
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD23	9	0.17
(4,98)	2:D:1109:PHE:O	2:D:1113:MET:N	18	0.16
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	2	0.16
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	7	0.16
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	10	0.16
(4,96)	2:D:1107:LYS:O	2:D:1111:ILE:N	8	0.16
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	16	0.16
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	19	0.16
(4,92)	2:D:1133:TYR:O	2:D:1137:GLN:N	8	0.16
(4,92)	2:D:1133:TYR:O	2:D:1137:GLN:N	17	0.16
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	19	0.16
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	11	0.16
(4,85)	2:B:120:GLU:O	2:B:124:LEU:N	4	0.16
(4,78)	2:B:113:MET:O	2:B:117:GLU:N	1	0.16
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	13	0.16
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	19	0.16
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	15	0.16
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	18	0.16
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	9	0.16
(4,68)	2:B:133:TYR:O	2:B:137:GLN:N	19	0.16
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	12	0.16
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	19	0.16
(4,64)	2:B:129:LEU:O	2:B:133:TYR:N	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	4	0.16
(4,62)	2:D:1103:VAL:O	2:B:99:TYR:N	15	0.16
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	5	0.16
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	10	0.16
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	17	0.16
(4,52)	1:A:8:LEU:O	1:C:1008:LEU:N	10	0.16
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	1	0.16
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	4	0.16
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	14	0.16
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	1	0.16
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	6	0.16
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	15	0.16
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	19	0.16
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	15	0.16
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	6	0.16
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	14	0.16
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	14	0.16
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	18	0.16
(4,35)	1:C:1013:ARG:O	1:C:1017:GLU:N	15	0.16
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	15	0.16
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	9	0.16
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	20	0.16
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	6	0.16
(4,17)	1:A:20:LEU:O	1:A:24:GLU:N	17	0.16
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	2	0.16
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	7	0.16
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	6	0.16
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	8	0.16
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	9	0.16
(4,103)	2:D:1114:LYS:O	2:D:1118:SER:N	17	0.16
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	14	0.16
(4,98)	2:D:1109:PHE:O	2:D:1113:MET:N	1	0.15
(4,98)	2:D:1109:PHE:O	2:D:1113:MET:N	9	0.15
(4,92)	2:D:1133:TYR:O	2:D:1137:GLN:N	11	0.15
(4,92)	2:D:1133:TYR:O	2:D:1137:GLN:N	14	0.15
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	18	0.15
(4,88)	2:D:1129:LEU:O	2:D:1133:TYR:N	3	0.15
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	20	0.15
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	4	0.15
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	11	0.15
(4,81)	2:B:116:LYS:O	2:B:120:GLU:N	19	0.15
(4,80)	2:B:115:LEU:O	2:B:119:LEU:N	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	12	0.15
(4,76)	2:B:111:ILE:O	2:B:115:LEU:N	19	0.15
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	1	0.15
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	9	0.15
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	10	0.15
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	12	0.15
(4,68)	2:B:133:TYR:O	2:B:137:GLN:N	7	0.15
(4,68)	2:B:133:TYR:O	2:B:137:GLN:N	9	0.15
(4,68)	2:B:133:TYR:O	2:B:137:GLN:N	13	0.15
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	4	0.15
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	15	0.15
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	1	0.15
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	12	0.15
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	20	0.15
(4,54)	1:C:1010:VAL:O	1:A:6:LEU:N	12	0.15
(4,53)	1:A:6:LEU:O	1:C:1010:VAL:N	1	0.15
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	15	0.15
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	1	0.15
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	14	0.15
(4,48)	1:C:1026:LEU:O	1:C:1030:GLN:N	7	0.15
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	3	0.15
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	6	0.15
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	14	0.15
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	13	0.15
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	4	0.15
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	10	0.15
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	11	0.15
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	17	0.15
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	20	0.15
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	12	0.15
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	5	0.15
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	14	0.15
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	8	0.15
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	1	0.15
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	18	0.15
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	2	0.15
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	6	0.15
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	7	0.15
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	2	0.15
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	5	0.15
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	16	0.15
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	18	0.15
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	5	0.15
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	13	0.15
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	20	0.15
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	6	0.15
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	10	0.15
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	19	0.15
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	13	0.15
(4,101)	2:D:1112:LEU:O	2:D:1116:LYS:N	12	0.15
(4,100)	2:D:1111:ILE:O	2:D:1115:LEU:N	1	0.15
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	10	0.15
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD11	13	0.15
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD12	13	0.15
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD13	13	0.15
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD21	13	0.15
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD22	13	0.15
(1,1404)	1:A:19:LEU:HD11	2:D:1115:LEU:HD23	13	0.15
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD11	13	0.15
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD12	13	0.15
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD13	13	0.15
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD21	13	0.15
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD22	13	0.15
(1,1404)	1:A:19:LEU:HD12	2:D:1115:LEU:HD23	13	0.15
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD11	13	0.15
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD12	13	0.15
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD13	13	0.15
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD21	13	0.15
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD22	13	0.15
(1,1404)	1:A:19:LEU:HD13	2:D:1115:LEU:HD23	13	0.15
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD11	13	0.15
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD12	13	0.15
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD13	13	0.15
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD21	13	0.15
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD22	13	0.15
(1,1404)	1:A:19:LEU:HD21	2:D:1115:LEU:HD23	13	0.15
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD11	13	0.15
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD12	13	0.15
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD13	13	0.15
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD21	13	0.15
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD22	13	0.15
(1,1404)	1:A:19:LEU:HD22	2:D:1115:LEU:HD23	13	0.15
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD11	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD12	13	0.15
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD13	13	0.15
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD21	13	0.15
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD22	13	0.15
(1,1404)	1:A:19:LEU:HD23	2:D:1115:LEU:HD23	13	0.15
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	10	0.14
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	17	0.14
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	3	0.14
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	5	0.14
(4,88)	2:D:1129:LEU:O	2:D:1133:TYR:N	7	0.14
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	2	0.14
(4,83)	2:B:118:SER:O	2:B:122:MET:N	5	0.14
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	17	0.14
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	11	0.14
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	12	0.14
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	14	0.14
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	5	0.14
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	6	0.14
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	2	0.14
(4,7)	1:A:40:TYR:O	1:A:44:GLN:N	2	0.14
(4,55)	1:C:1008:LEU:O	1:A:8:LEU:N	19	0.14
(4,51)	1:A:10:VAL:O	1:C:1006:LEU:N	14	0.14
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	19	0.14
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	8	0.14
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	12	0.14
(4,43)	1:C:1021:GLU:O	1:C:1025:SER:N	20	0.14
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	12	0.14
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	6	0.14
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	1	0.14
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	1	0.14
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	12	0.14
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	5	0.14
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	15	0.14
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	1	0.14
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	4	0.14
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	13	0.14
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	3	0.14
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	20	0.14
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	3	0.14
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	6	0.14
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	18	0.14
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	7	0.14
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	9	0.14
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	12	0.14
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	14	0.14
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	7	0.14
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	15	0.14
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	5	0.14
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	11	0.14
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	10	0.14
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	7	0.14
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	6	0.14
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	8	0.14
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	11	0.14
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	5	0.14
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	16	0.14
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	18	0.14
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	5	0.14
(4,102)	2:D:1113:MET:O	2:D:1117:GLU:N	16	0.14
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE1	7	0.14
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE2	7	0.14
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE1	7	0.14
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE2	7	0.14
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE1	7	0.14
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE2	7	0.14
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE1	7	0.14
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE2	7	0.14
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE1	7	0.14
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE2	7	0.14
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE1	7	0.14
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE2	7	0.14
(2,781)	2:B:103:VAL:HG11	2:B:109:PHE:HE1	3	0.14
(2,781)	2:B:103:VAL:HG11	2:B:109:PHE:HE2	3	0.14
(2,781)	2:B:103:VAL:HG12	2:B:109:PHE:HE1	3	0.14
(2,781)	2:B:103:VAL:HG12	2:B:109:PHE:HE2	3	0.14
(2,781)	2:B:103:VAL:HG13	2:B:109:PHE:HE1	3	0.14
(2,781)	2:B:103:VAL:HG13	2:B:109:PHE:HE2	3	0.14
(2,781)	2:B:103:VAL:HG21	2:B:109:PHE:HE1	3	0.14
(2,781)	2:B:103:VAL:HG21	2:B:109:PHE:HE2	3	0.14
(2,781)	2:B:103:VAL:HG22	2:B:109:PHE:HE1	3	0.14
(2,781)	2:B:103:VAL:HG22	2:B:109:PHE:HE2	3	0.14
(2,781)	2:B:103:VAL:HG23	2:B:109:PHE:HE1	3	0.14
(2,781)	2:B:103:VAL:HG23	2:B:109:PHE:HE2	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG11	4	0.14
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG12	4	0.14
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG13	4	0.14
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG21	4	0.14
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG22	4	0.14
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG23	4	0.14
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD11	19	0.14
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD12	19	0.14
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD13	19	0.14
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD21	19	0.14
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD22	19	0.14
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD23	19	0.14
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD11	19	0.14
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD12	19	0.14
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD13	19	0.14
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD21	19	0.14
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD22	19	0.14
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD23	19	0.14
(1,1617)	2:B:121:LEU:HB2	2:B:124:LEU:HD11	11	0.14
(1,1617)	2:B:121:LEU:HB2	2:B:124:LEU:HD12	11	0.14
(1,1617)	2:B:121:LEU:HB2	2:B:124:LEU:HD13	11	0.14
(1,1617)	2:B:121:LEU:HB2	2:B:124:LEU:HD21	11	0.14
(1,1617)	2:B:121:LEU:HB2	2:B:124:LEU:HD22	11	0.14
(1,1617)	2:B:121:LEU:HB2	2:B:124:LEU:HD23	11	0.14
(1,1617)	2:B:121:LEU:HB3	2:B:124:LEU:HD11	11	0.14
(1,1617)	2:B:121:LEU:HB3	2:B:124:LEU:HD12	11	0.14
(1,1617)	2:B:121:LEU:HB3	2:B:124:LEU:HD13	11	0.14
(1,1617)	2:B:121:LEU:HB3	2:B:124:LEU:HD21	11	0.14
(1,1617)	2:B:121:LEU:HB3	2:B:124:LEU:HD22	11	0.14
(1,1617)	2:B:121:LEU:HB3	2:B:124:LEU:HD23	11	0.14
(1,1222)	1:C:1015:THR:HG21	1:C:1019:LEU:HD11	9	0.14
(1,1222)	1:C:1015:THR:HG21	1:C:1019:LEU:HD12	9	0.14
(1,1222)	1:C:1015:THR:HG21	1:C:1019:LEU:HD13	9	0.14
(1,1222)	1:C:1015:THR:HG21	1:C:1019:LEU:HD21	9	0.14
(1,1222)	1:C:1015:THR:HG21	1:C:1019:LEU:HD22	9	0.14
(1,1222)	1:C:1015:THR:HG21	1:C:1019:LEU:HD23	9	0.14
(1,1222)	1:C:1015:THR:HG22	1:C:1019:LEU:HD11	9	0.14
(1,1222)	1:C:1015:THR:HG22	1:C:1019:LEU:HD12	9	0.14
(1,1222)	1:C:1015:THR:HG22	1:C:1019:LEU:HD13	9	0.14
(1,1222)	1:C:1015:THR:HG22	1:C:1019:LEU:HD21	9	0.14
(1,1222)	1:C:1015:THR:HG22	1:C:1019:LEU:HD22	9	0.14
(1,1222)	1:C:1015:THR:HG22	1:C:1019:LEU:HD23	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:C:1015:THR:HG23	1:C:1019:LEU:HD11	9	0.14
(1,1222)	1:C:1015:THR:HG23	1:C:1019:LEU:HD12	9	0.14
(1,1222)	1:C:1015:THR:HG23	1:C:1019:LEU:HD13	9	0.14
(1,1222)	1:C:1015:THR:HG23	1:C:1019:LEU:HD21	9	0.14
(1,1222)	1:C:1015:THR:HG23	1:C:1019:LEU:HD22	9	0.14
(1,1222)	1:C:1015:THR:HG23	1:C:1019:LEU:HD23	9	0.14
(1,1221)	1:A:15:THR:HG21	1:A:19:LEU:HD11	5	0.14
(1,1221)	1:A:15:THR:HG21	1:A:19:LEU:HD12	5	0.14
(1,1221)	1:A:15:THR:HG21	1:A:19:LEU:HD13	5	0.14
(1,1221)	1:A:15:THR:HG21	1:A:19:LEU:HD21	5	0.14
(1,1221)	1:A:15:THR:HG21	1:A:19:LEU:HD22	5	0.14
(1,1221)	1:A:15:THR:HG21	1:A:19:LEU:HD23	5	0.14
(1,1221)	1:A:15:THR:HG22	1:A:19:LEU:HD11	5	0.14
(1,1221)	1:A:15:THR:HG22	1:A:19:LEU:HD12	5	0.14
(1,1221)	1:A:15:THR:HG22	1:A:19:LEU:HD13	5	0.14
(1,1221)	1:A:15:THR:HG22	1:A:19:LEU:HD21	5	0.14
(1,1221)	1:A:15:THR:HG22	1:A:19:LEU:HD22	5	0.14
(1,1221)	1:A:15:THR:HG22	1:A:19:LEU:HD23	5	0.14
(1,1221)	1:A:15:THR:HG23	1:A:19:LEU:HD11	5	0.14
(1,1221)	1:A:15:THR:HG23	1:A:19:LEU:HD12	5	0.14
(1,1221)	1:A:15:THR:HG23	1:A:19:LEU:HD13	5	0.14
(1,1221)	1:A:15:THR:HG23	1:A:19:LEU:HD21	5	0.14
(1,1221)	1:A:15:THR:HG23	1:A:19:LEU:HD22	5	0.14
(1,1221)	1:A:15:THR:HG23	1:A:19:LEU:HD23	5	0.14
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	13	0.13
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	11	0.13
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	17	0.13
(4,88)	2:D:1129:LEU:O	2:D:1133:TYR:N	2	0.13
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	6	0.13
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	1	0.13
(4,82)	2:B:117:GLU:O	2:B:121:LEU:N	2	0.13
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	2	0.13
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	5	0.13
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	3	0.13
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	3	0.13
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	5	0.13
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	20	0.13
(4,68)	2:B:133:TYR:O	2:B:137:GLN:N	4	0.13
(4,67)	2:B:132:SER:O	2:B:136:GLN:N	13	0.13
(4,64)	2:B:129:LEU:O	2:B:133:TYR:N	5	0.13
(4,64)	2:B:129:LEU:O	2:B:133:TYR:N	16	0.13
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	20	0.13
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	9	0.13
(4,5)	1:A:38:GLU:O	1:A:42:GLN:N	10	0.13
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	2	0.13
(4,47)	1:C:1025:SER:O	1:C:1029:MET:N	19	0.13
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	10	0.13
(4,45)	1:C:1023:LYS:O	1:C:1027:GLU:N	20	0.13
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	19	0.13
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	5	0.13
(4,39)	1:C:1017:GLU:O	1:C:1021:GLU:N	7	0.13
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	9	0.13
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	19	0.13
(4,36)	1:C:1014:GLU:O	1:C:1018:MET:N	5	0.13
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	3	0.13
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	20	0.13
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	3	0.13
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	16	0.13
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	10	0.13
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	12	0.13
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	3	0.13
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	17	0.13
(4,18)	1:A:21:GLU:O	1:A:25:SER:N	1	0.13
(4,17)	1:A:20:LEU:O	1:A:24:GLU:N	15	0.13
(4,17)	1:A:20:LEU:O	1:A:24:GLU:N	16	0.13
(4,14)	1:A:17:GLU:O	1:A:21:GLU:N	13	0.13
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	4	0.13
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	9	0.13
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	1	0.13
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	16	0.13
(4,110)	2:D:1121:LEU:O	2:D:1125:VAL:N	16	0.13
(4,11)	1:A:14:GLU:O	1:A:18:MET:N	13	0.13
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	14	0.13
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	6	0.13
(4,104)	2:D:1115:LEU:O	2:D:1119:LEU:N	8	0.13
(4,101)	2:D:1112:LEU:O	2:D:1116:LYS:N	7	0.13
(4,101)	2:D:1112:LEU:O	2:D:1116:LYS:N	18	0.13
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE1	20	0.13
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE2	20	0.13
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE1	20	0.13
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE2	20	0.13
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE1	20	0.13
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE2	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE1	20	0.13
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE2	20	0.13
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE1	20	0.13
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE2	20	0.13
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE1	20	0.13
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE2	20	0.13
(2,726)	1:C:1028:LEU:HD11	2:D:1122:MET:HA	11	0.13
(2,726)	1:C:1028:LEU:HD12	2:D:1122:MET:HA	11	0.13
(2,726)	1:C:1028:LEU:HD13	2:D:1122:MET:HA	11	0.13
(2,726)	1:C:1028:LEU:HD21	2:D:1122:MET:HA	11	0.13
(2,726)	1:C:1028:LEU:HD22	2:D:1122:MET:HA	11	0.13
(2,726)	1:C:1028:LEU:HD23	2:D:1122:MET:HA	11	0.13
(2,725)	1:A:28:LEU:HD11	2:B:122:MET:HA	15	0.13
(2,725)	1:A:28:LEU:HD12	2:B:122:MET:HA	15	0.13
(2,725)	1:A:28:LEU:HD13	2:B:122:MET:HA	15	0.13
(2,725)	1:A:28:LEU:HD21	2:B:122:MET:HA	15	0.13
(2,725)	1:A:28:LEU:HD22	2:B:122:MET:HA	15	0.13
(2,725)	1:A:28:LEU:HD23	2:B:122:MET:HA	15	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG11	3	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG12	3	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG13	3	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG21	3	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG22	3	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG23	3	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG11	9	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG12	9	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG13	9	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG21	9	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG22	9	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG23	9	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG11	19	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG12	19	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG13	19	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG21	19	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG22	19	0.13
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG23	19	0.13
(1,594)	1:A:20:LEU:HD11	1:A:23:LYS:HE2	17	0.13
(1,594)	1:A:20:LEU:HD11	1:A:23:LYS:HE3	17	0.13
(1,594)	1:A:20:LEU:HD12	1:A:23:LYS:HE2	17	0.13
(1,594)	1:A:20:LEU:HD12	1:A:23:LYS:HE3	17	0.13
(1,594)	1:A:20:LEU:HD13	1:A:23:LYS:HE2	17	0.13
(1,594)	1:A:20:LEU:HD13	1:A:23:LYS:HE3	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:A:20:LEU:HD21	1:A:23:LYS:HE2	17	0.13
(1,594)	1:A:20:LEU:HD21	1:A:23:LYS:HE3	17	0.13
(1,594)	1:A:20:LEU:HD22	1:A:23:LYS:HE2	17	0.13
(1,594)	1:A:20:LEU:HD22	1:A:23:LYS:HE3	17	0.13
(1,594)	1:A:20:LEU:HD23	1:A:23:LYS:HE2	17	0.13
(1,594)	1:A:20:LEU:HD23	1:A:23:LYS:HE3	17	0.13
(1,1626)	2:D:1128:PRO:HD2	2:D:1130:VAL:HG11	13	0.13
(1,1626)	2:D:1128:PRO:HD2	2:D:1130:VAL:HG12	13	0.13
(1,1626)	2:D:1128:PRO:HD2	2:D:1130:VAL:HG13	13	0.13
(1,1626)	2:D:1128:PRO:HD2	2:D:1130:VAL:HG21	13	0.13
(1,1626)	2:D:1128:PRO:HD2	2:D:1130:VAL:HG22	13	0.13
(1,1626)	2:D:1128:PRO:HD2	2:D:1130:VAL:HG23	13	0.13
(1,1626)	2:D:1128:PRO:HD3	2:D:1130:VAL:HG11	13	0.13
(1,1626)	2:D:1128:PRO:HD3	2:D:1130:VAL:HG12	13	0.13
(1,1626)	2:D:1128:PRO:HD3	2:D:1130:VAL:HG13	13	0.13
(1,1626)	2:D:1128:PRO:HD3	2:D:1130:VAL:HG21	13	0.13
(1,1626)	2:D:1128:PRO:HD3	2:D:1130:VAL:HG22	13	0.13
(1,1626)	2:D:1128:PRO:HD3	2:D:1130:VAL:HG23	13	0.13
(1,1523)	1:A:28:LEU:HD11	2:B:133:TYR:HB2	7	0.13
(1,1523)	1:A:28:LEU:HD11	2:B:133:TYR:HB3	7	0.13
(1,1523)	1:A:28:LEU:HD12	2:B:133:TYR:HB2	7	0.13
(1,1523)	1:A:28:LEU:HD12	2:B:133:TYR:HB3	7	0.13
(1,1523)	1:A:28:LEU:HD13	2:B:133:TYR:HB2	7	0.13
(1,1523)	1:A:28:LEU:HD13	2:B:133:TYR:HB3	7	0.13
(1,1523)	1:A:28:LEU:HD21	2:B:133:TYR:HB2	7	0.13
(1,1523)	1:A:28:LEU:HD21	2:B:133:TYR:HB3	7	0.13
(1,1523)	1:A:28:LEU:HD22	2:B:133:TYR:HB2	7	0.13
(1,1523)	1:A:28:LEU:HD22	2:B:133:TYR:HB3	7	0.13
(1,1523)	1:A:28:LEU:HD23	2:B:133:TYR:HB2	7	0.13
(1,1523)	1:A:28:LEU:HD23	2:B:133:TYR:HB3	7	0.13
(1,1496)	1:C:1026:LEU:HD11	1:C:1029:MET:HE1	20	0.13
(1,1496)	1:C:1026:LEU:HD11	1:C:1029:MET:HE2	20	0.13
(1,1496)	1:C:1026:LEU:HD11	1:C:1029:MET:HE3	20	0.13
(1,1496)	1:C:1026:LEU:HD12	1:C:1029:MET:HE1	20	0.13
(1,1496)	1:C:1026:LEU:HD12	1:C:1029:MET:HE2	20	0.13
(1,1496)	1:C:1026:LEU:HD12	1:C:1029:MET:HE3	20	0.13
(1,1496)	1:C:1026:LEU:HD13	1:C:1029:MET:HE1	20	0.13
(1,1496)	1:C:1026:LEU:HD13	1:C:1029:MET:HE2	20	0.13
(1,1496)	1:C:1026:LEU:HD13	1:C:1029:MET:HE3	20	0.13
(1,1496)	1:C:1026:LEU:HD21	1:C:1029:MET:HE1	20	0.13
(1,1496)	1:C:1026:LEU:HD21	1:C:1029:MET:HE2	20	0.13
(1,1496)	1:C:1026:LEU:HD21	1:C:1029:MET:HE3	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1496)	1:C:1026:LEU:HD22	1:C:1029:MET:HE1	20	0.13
(1,1496)	1:C:1026:LEU:HD22	1:C:1029:MET:HE2	20	0.13
(1,1496)	1:C:1026:LEU:HD22	1:C:1029:MET:HE3	20	0.13
(1,1496)	1:C:1026:LEU:HD23	1:C:1029:MET:HE1	20	0.13
(1,1496)	1:C:1026:LEU:HD23	1:C:1029:MET:HE2	20	0.13
(1,1496)	1:C:1026:LEU:HD23	1:C:1029:MET:HE3	20	0.13
(1,1495)	1:A:26:LEU:HD11	1:A:29:MET:HE1	9	0.13
(1,1495)	1:A:26:LEU:HD11	1:A:29:MET:HE2	9	0.13
(1,1495)	1:A:26:LEU:HD11	1:A:29:MET:HE3	9	0.13
(1,1495)	1:A:26:LEU:HD12	1:A:29:MET:HE1	9	0.13
(1,1495)	1:A:26:LEU:HD12	1:A:29:MET:HE2	9	0.13
(1,1495)	1:A:26:LEU:HD12	1:A:29:MET:HE3	9	0.13
(1,1495)	1:A:26:LEU:HD13	1:A:29:MET:HE1	9	0.13
(1,1495)	1:A:26:LEU:HD13	1:A:29:MET:HE2	9	0.13
(1,1495)	1:A:26:LEU:HD13	1:A:29:MET:HE3	9	0.13
(1,1495)	1:A:26:LEU:HD21	1:A:29:MET:HE1	9	0.13
(1,1495)	1:A:26:LEU:HD21	1:A:29:MET:HE2	9	0.13
(1,1495)	1:A:26:LEU:HD21	1:A:29:MET:HE3	9	0.13
(1,1495)	1:A:26:LEU:HD22	1:A:29:MET:HE1	9	0.13
(1,1495)	1:A:26:LEU:HD22	1:A:29:MET:HE2	9	0.13
(1,1495)	1:A:26:LEU:HD22	1:A:29:MET:HE3	9	0.13
(1,1495)	1:A:26:LEU:HD23	1:A:29:MET:HE1	9	0.13
(1,1495)	1:A:26:LEU:HD23	1:A:29:MET:HE2	9	0.13
(1,1495)	1:A:26:LEU:HD23	1:A:29:MET:HE3	9	0.13
(1,1282)	1:C:1010:VAL:HG11	1:C:1015:THR:HG21	12	0.13
(1,1282)	1:C:1010:VAL:HG11	1:C:1015:THR:HG22	12	0.13
(1,1282)	1:C:1010:VAL:HG11	1:C:1015:THR:HG23	12	0.13
(1,1282)	1:C:1010:VAL:HG12	1:C:1015:THR:HG21	12	0.13
(1,1282)	1:C:1010:VAL:HG12	1:C:1015:THR:HG22	12	0.13
(1,1282)	1:C:1010:VAL:HG12	1:C:1015:THR:HG23	12	0.13
(1,1282)	1:C:1010:VAL:HG13	1:C:1015:THR:HG21	12	0.13
(1,1282)	1:C:1010:VAL:HG13	1:C:1015:THR:HG22	12	0.13
(1,1282)	1:C:1010:VAL:HG13	1:C:1015:THR:HG23	12	0.13
(1,1282)	1:C:1010:VAL:HG21	1:C:1015:THR:HG21	12	0.13
(1,1282)	1:C:1010:VAL:HG21	1:C:1015:THR:HG22	12	0.13
(1,1282)	1:C:1010:VAL:HG21	1:C:1015:THR:HG23	12	0.13
(1,1282)	1:C:1010:VAL:HG22	1:C:1015:THR:HG21	12	0.13
(1,1282)	1:C:1010:VAL:HG22	1:C:1015:THR:HG22	12	0.13
(1,1282)	1:C:1010:VAL:HG22	1:C:1015:THR:HG23	12	0.13
(1,1282)	1:C:1010:VAL:HG23	1:C:1015:THR:HG21	12	0.13
(1,1282)	1:C:1010:VAL:HG23	1:C:1015:THR:HG22	12	0.13
(1,1282)	1:C:1010:VAL:HG23	1:C:1015:THR:HG23	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,98)	2:D:1109:PHE:O	2:D:1113:MET:N	4	0.12
(4,98)	2:D:1109:PHE:O	2:D:1113:MET:N	5	0.12
(4,98)	2:D:1109:PHE:O	2:D:1113:MET:N	14	0.12
(4,98)	2:D:1109:PHE:O	2:D:1113:MET:N	15	0.12
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	6	0.12
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	11	0.12
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	7	0.12
(4,90)	2:D:1131:ASP:O	2:D:1135:GLN:N	20	0.12
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	12	0.12
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	19	0.12
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	12	0.12
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	15	0.12
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	17	0.12
(4,88)	2:D:1129:LEU:O	2:D:1133:TYR:N	12	0.12
(4,88)	2:D:1129:LEU:O	2:D:1133:TYR:N	13	0.12
(4,88)	2:D:1129:LEU:O	2:D:1133:TYR:N	20	0.12
(4,86)	2:B:121:LEU:O	2:B:125:VAL:N	17	0.12
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	3	0.12
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	4	0.12
(4,84)	2:B:119:LEU:O	2:B:123:GLU:N	7	0.12
(4,83)	2:B:118:SER:O	2:B:122:MET:N	17	0.12
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	9	0.12
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	18	0.12
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	7	0.12
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	9	0.12
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	13	0.12
(4,73)	2:B:108:ASN:O	2:B:112:LEU:N	4	0.12
(4,68)	2:B:133:TYR:O	2:B:137:GLN:N	6	0.12
(4,68)	2:B:133:TYR:O	2:B:137:GLN:N	15	0.12
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	7	0.12
(4,65)	2:B:130:VAL:O	2:B:134:ARG:N	16	0.12
(4,64)	2:B:129:LEU:O	2:B:133:TYR:N	3	0.12
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	13	0.12
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	15	0.12
(4,50)	1:C:1028:LEU:O	1:C:1032:LEU:N	7	0.12
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	15	0.12
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	15	0.12
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	7	0.12
(4,40)	1:C:1018:MET:O	1:C:1022:ILE:N	16	0.12
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	2	0.12
(4,4)	1:A:37:ILE:O	1:A:41:ARG:N	16	0.12
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,37)	1:C:1015:THR:O	1:C:1019:LEU:N	16	0.12
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	6	0.12
(4,34)	1:C:1042:GLN:O	1:C:1046:GLN:N	17	0.12
(4,33)	1:C:1041:ARG:O	1:C:1045:GLN:N	11	0.12
(4,31)	1:C:1039:THR:O	1:C:1043:GLN:N	1	0.12
(4,30)	1:C:1038:GLU:O	1:C:1042:GLN:N	9	0.12
(4,28)	1:C:1036:THR:O	1:C:1040:TYR:N	12	0.12
(4,27)	1:C:1035:HIS:O	1:C:1039:THR:N	11	0.12
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	18	0.12
(4,26)	1:C:1034:GLN:O	1:C:1038:GLU:N	19	0.12
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	14	0.12
(4,23)	1:A:26:LEU:O	1:A:30:GLN:N	19	0.12
(4,20)	1:A:23:LYS:O	1:A:27:GLU:N	19	0.12
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	6	0.12
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	14	0.12
(4,16)	1:A:19:LEU:O	1:A:23:LYS:N	11	0.12
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	1	0.12
(4,13)	1:A:16:TYR:O	1:A:20:LEU:N	17	0.12
(4,12)	1:A:15:THR:O	1:A:19:LEU:N	3	0.12
(4,108)	2:D:1119:LEU:O	2:D:1123:GLU:N	10	0.12
(4,101)	2:D:1112:LEU:O	2:D:1116:LYS:N	13	0.12
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	13	0.12
(4,1)	1:A:34:GLN:O	1:A:38:GLU:N	20	0.12
(2,880)	2:B:120:GLU:HG2	2:D:1104:ARG:HB2	12	0.12
(2,880)	2:B:120:GLU:HG2	2:D:1104:ARG:HB3	12	0.12
(2,880)	2:B:120:GLU:HG3	2:D:1104:ARG:HB2	12	0.12
(2,880)	2:B:120:GLU:HG3	2:D:1104:ARG:HB3	12	0.12
(2,872)	1:A:11:ARG:HD2	2:D:1140:LEU:HD11	8	0.12
(2,872)	1:A:11:ARG:HD2	2:D:1140:LEU:HD12	8	0.12
(2,872)	1:A:11:ARG:HD2	2:D:1140:LEU:HD13	8	0.12
(2,872)	1:A:11:ARG:HD2	2:D:1140:LEU:HD21	8	0.12
(2,872)	1:A:11:ARG:HD2	2:D:1140:LEU:HD22	8	0.12
(2,872)	1:A:11:ARG:HD2	2:D:1140:LEU:HD23	8	0.12
(2,872)	1:A:11:ARG:HD3	2:D:1140:LEU:HD11	8	0.12
(2,872)	1:A:11:ARG:HD3	2:D:1140:LEU:HD12	8	0.12
(2,872)	1:A:11:ARG:HD3	2:D:1140:LEU:HD13	8	0.12
(2,872)	1:A:11:ARG:HD3	2:D:1140:LEU:HD21	8	0.12
(2,872)	1:A:11:ARG:HD3	2:D:1140:LEU:HD22	8	0.12
(2,872)	1:A:11:ARG:HD3	2:D:1140:LEU:HD23	8	0.12
(2,871)	2:B:140:LEU:HD11	1:C:1011:ARG:HD2	8	0.12
(2,871)	2:B:140:LEU:HD11	1:C:1011:ARG:HD3	8	0.12
(2,871)	2:B:140:LEU:HD12	1:C:1011:ARG:HD2	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,871)	2:B:140:LEU:HD12	1:C:1011:ARG:HD3	8	0.12
(2,871)	2:B:140:LEU:HD13	1:C:1011:ARG:HD2	8	0.12
(2,871)	2:B:140:LEU:HD13	1:C:1011:ARG:HD3	8	0.12
(2,871)	2:B:140:LEU:HD21	1:C:1011:ARG:HD2	8	0.12
(2,871)	2:B:140:LEU:HD21	1:C:1011:ARG:HD3	8	0.12
(2,871)	2:B:140:LEU:HD22	1:C:1011:ARG:HD2	8	0.12
(2,871)	2:B:140:LEU:HD22	1:C:1011:ARG:HD3	8	0.12
(2,871)	2:B:140:LEU:HD23	1:C:1011:ARG:HD2	8	0.12
(2,871)	2:B:140:LEU:HD23	1:C:1011:ARG:HD3	8	0.12
(2,871)	2:B:140:LEU:HD11	1:C:1011:ARG:HD2	10	0.12
(2,871)	2:B:140:LEU:HD11	1:C:1011:ARG:HD3	10	0.12
(2,871)	2:B:140:LEU:HD12	1:C:1011:ARG:HD2	10	0.12
(2,871)	2:B:140:LEU:HD12	1:C:1011:ARG:HD3	10	0.12
(2,871)	2:B:140:LEU:HD13	1:C:1011:ARG:HD2	10	0.12
(2,871)	2:B:140:LEU:HD13	1:C:1011:ARG:HD3	10	0.12
(2,871)	2:B:140:LEU:HD21	1:C:1011:ARG:HD2	10	0.12
(2,871)	2:B:140:LEU:HD21	1:C:1011:ARG:HD3	10	0.12
(2,871)	2:B:140:LEU:HD22	1:C:1011:ARG:HD2	10	0.12
(2,871)	2:B:140:LEU:HD22	1:C:1011:ARG:HD3	10	0.12
(2,871)	2:B:140:LEU:HD23	1:C:1011:ARG:HD2	10	0.12
(2,871)	2:B:140:LEU:HD23	1:C:1011:ARG:HD3	10	0.12
(2,871)	2:B:140:LEU:HD11	1:C:1011:ARG:HD2	20	0.12
(2,871)	2:B:140:LEU:HD11	1:C:1011:ARG:HD3	20	0.12
(2,871)	2:B:140:LEU:HD12	1:C:1011:ARG:HD2	20	0.12
(2,871)	2:B:140:LEU:HD12	1:C:1011:ARG:HD3	20	0.12
(2,871)	2:B:140:LEU:HD13	1:C:1011:ARG:HD2	20	0.12
(2,871)	2:B:140:LEU:HD13	1:C:1011:ARG:HD3	20	0.12
(2,871)	2:B:140:LEU:HD21	1:C:1011:ARG:HD2	20	0.12
(2,871)	2:B:140:LEU:HD21	1:C:1011:ARG:HD3	20	0.12
(2,871)	2:B:140:LEU:HD22	1:C:1011:ARG:HD2	20	0.12
(2,871)	2:B:140:LEU:HD22	1:C:1011:ARG:HD3	20	0.12
(2,871)	2:B:140:LEU:HD23	1:C:1011:ARG:HD2	20	0.12
(2,871)	2:B:140:LEU:HD23	1:C:1011:ARG:HD3	20	0.12
(2,868)	1:C:1020:LEU:HD11	2:D:1133:TYR:HE1	6	0.12
(2,868)	1:C:1020:LEU:HD11	2:D:1133:TYR:HE2	6	0.12
(2,868)	1:C:1020:LEU:HD12	2:D:1133:TYR:HE1	6	0.12
(2,868)	1:C:1020:LEU:HD12	2:D:1133:TYR:HE2	6	0.12
(2,868)	1:C:1020:LEU:HD13	2:D:1133:TYR:HE1	6	0.12
(2,868)	1:C:1020:LEU:HD13	2:D:1133:TYR:HE2	6	0.12
(2,868)	1:C:1020:LEU:HD21	2:D:1133:TYR:HE1	6	0.12
(2,868)	1:C:1020:LEU:HD21	2:D:1133:TYR:HE2	6	0.12
(2,868)	1:C:1020:LEU:HD22	2:D:1133:TYR:HE1	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,868)	1:C:1020:LEU:HD22	2:D:1133:TYR:HE2	6	0.12
(2,868)	1:C:1020:LEU:HD23	2:D:1133:TYR:HE1	6	0.12
(2,868)	1:C:1020:LEU:HD23	2:D:1133:TYR:HE2	6	0.12
(2,868)	1:C:1020:LEU:HD11	2:D:1133:TYR:HE1	13	0.12
(2,868)	1:C:1020:LEU:HD11	2:D:1133:TYR:HE2	13	0.12
(2,868)	1:C:1020:LEU:HD12	2:D:1133:TYR:HE1	13	0.12
(2,868)	1:C:1020:LEU:HD12	2:D:1133:TYR:HE2	13	0.12
(2,868)	1:C:1020:LEU:HD13	2:D:1133:TYR:HE1	13	0.12
(2,868)	1:C:1020:LEU:HD13	2:D:1133:TYR:HE2	13	0.12
(2,868)	1:C:1020:LEU:HD21	2:D:1133:TYR:HE1	13	0.12
(2,868)	1:C:1020:LEU:HD21	2:D:1133:TYR:HE2	13	0.12
(2,868)	1:C:1020:LEU:HD22	2:D:1133:TYR:HE1	13	0.12
(2,868)	1:C:1020:LEU:HD22	2:D:1133:TYR:HE2	13	0.12
(2,868)	1:C:1020:LEU:HD23	2:D:1133:TYR:HE1	13	0.12
(2,868)	1:C:1020:LEU:HD23	2:D:1133:TYR:HE2	13	0.12
(2,868)	1:C:1020:LEU:HD11	2:D:1133:TYR:HE1	19	0.12
(2,868)	1:C:1020:LEU:HD11	2:D:1133:TYR:HE2	19	0.12
(2,868)	1:C:1020:LEU:HD12	2:D:1133:TYR:HE1	19	0.12
(2,868)	1:C:1020:LEU:HD12	2:D:1133:TYR:HE2	19	0.12
(2,868)	1:C:1020:LEU:HD13	2:D:1133:TYR:HE1	19	0.12
(2,868)	1:C:1020:LEU:HD13	2:D:1133:TYR:HE2	19	0.12
(2,868)	1:C:1020:LEU:HD21	2:D:1133:TYR:HE1	19	0.12
(2,868)	1:C:1020:LEU:HD21	2:D:1133:TYR:HE2	19	0.12
(2,868)	1:C:1020:LEU:HD22	2:D:1133:TYR:HE1	19	0.12
(2,868)	1:C:1020:LEU:HD22	2:D:1133:TYR:HE2	19	0.12
(2,868)	1:C:1020:LEU:HD23	2:D:1133:TYR:HE1	19	0.12
(2,868)	1:C:1020:LEU:HD23	2:D:1133:TYR:HE2	19	0.12
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE1	6	0.12
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE2	6	0.12
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE1	6	0.12
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE2	6	0.12
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE1	6	0.12
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE2	6	0.12
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE1	6	0.12
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE2	6	0.12
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE1	6	0.12
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE2	6	0.12
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE1	6	0.12
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE2	6	0.12
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE1	11	0.12
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE2	11	0.12
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE1	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE2	11	0.12
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE1	11	0.12
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE2	11	0.12
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE1	11	0.12
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE2	11	0.12
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE1	11	0.12
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE2	11	0.12
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE1	11	0.12
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE2	11	0.12
(2,782)	2:D:1103:VAL:HG11	2:D:1109:PHE:HE1	10	0.12
(2,782)	2:D:1103:VAL:HG11	2:D:1109:PHE:HE2	10	0.12
(2,782)	2:D:1103:VAL:HG12	2:D:1109:PHE:HE1	10	0.12
(2,782)	2:D:1103:VAL:HG12	2:D:1109:PHE:HE2	10	0.12
(2,782)	2:D:1103:VAL:HG13	2:D:1109:PHE:HE1	10	0.12
(2,782)	2:D:1103:VAL:HG13	2:D:1109:PHE:HE2	10	0.12
(2,782)	2:D:1103:VAL:HG21	2:D:1109:PHE:HE1	10	0.12
(2,782)	2:D:1103:VAL:HG21	2:D:1109:PHE:HE2	10	0.12
(2,782)	2:D:1103:VAL:HG22	2:D:1109:PHE:HE1	10	0.12
(2,782)	2:D:1103:VAL:HG22	2:D:1109:PHE:HE2	10	0.12
(2,782)	2:D:1103:VAL:HG23	2:D:1109:PHE:HE1	10	0.12
(2,782)	2:D:1103:VAL:HG23	2:D:1109:PHE:HE2	10	0.12
(2,749)	1:A:37:ILE:HG12	2:B:124:LEU:HD11	4	0.12
(2,749)	1:A:37:ILE:HG12	2:B:124:LEU:HD12	4	0.12
(2,749)	1:A:37:ILE:HG12	2:B:124:LEU:HD13	4	0.12
(2,749)	1:A:37:ILE:HG12	2:B:124:LEU:HD21	4	0.12
(2,749)	1:A:37:ILE:HG12	2:B:124:LEU:HD22	4	0.12
(2,749)	1:A:37:ILE:HG12	2:B:124:LEU:HD23	4	0.12
(2,749)	1:A:37:ILE:HG13	2:B:124:LEU:HD11	4	0.12
(2,749)	1:A:37:ILE:HG13	2:B:124:LEU:HD12	4	0.12
(2,749)	1:A:37:ILE:HG13	2:B:124:LEU:HD13	4	0.12
(2,749)	1:A:37:ILE:HG13	2:B:124:LEU:HD21	4	0.12
(2,749)	1:A:37:ILE:HG13	2:B:124:LEU:HD22	4	0.12
(2,749)	1:A:37:ILE:HG13	2:B:124:LEU:HD23	4	0.12
(2,726)	1:C:1028:LEU:HD11	2:D:1122:MET:HA	9	0.12
(2,726)	1:C:1028:LEU:HD12	2:D:1122:MET:HA	9	0.12
(2,726)	1:C:1028:LEU:HD13	2:D:1122:MET:HA	9	0.12
(2,726)	1:C:1028:LEU:HD21	2:D:1122:MET:HA	9	0.12
(2,726)	1:C:1028:LEU:HD22	2:D:1122:MET:HA	9	0.12
(2,726)	1:C:1028:LEU:HD23	2:D:1122:MET:HA	9	0.12
(2,726)	1:C:1028:LEU:HD11	2:D:1122:MET:HA	20	0.12
(2,726)	1:C:1028:LEU:HD12	2:D:1122:MET:HA	20	0.12
(2,726)	1:C:1028:LEU:HD13	2:D:1122:MET:HA	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,726)	1:C:1028:LEU:HD21	2:D:1122:MET:HA	20	0.12
(2,726)	1:C:1028:LEU:HD22	2:D:1122:MET:HA	20	0.12
(2,726)	1:C:1028:LEU:HD23	2:D:1122:MET:HA	20	0.12
(2,725)	1:A:28:LEU:HD11	2:B:122:MET:HA	5	0.12
(2,725)	1:A:28:LEU:HD12	2:B:122:MET:HA	5	0.12
(2,725)	1:A:28:LEU:HD13	2:B:122:MET:HA	5	0.12
(2,725)	1:A:28:LEU:HD21	2:B:122:MET:HA	5	0.12
(2,725)	1:A:28:LEU:HD22	2:B:122:MET:HA	5	0.12
(2,725)	1:A:28:LEU:HD23	2:B:122:MET:HA	5	0.12
(2,725)	1:A:28:LEU:HD11	2:B:122:MET:HA	14	0.12
(2,725)	1:A:28:LEU:HD12	2:B:122:MET:HA	14	0.12
(2,725)	1:A:28:LEU:HD13	2:B:122:MET:HA	14	0.12
(2,725)	1:A:28:LEU:HD21	2:B:122:MET:HA	14	0.12
(2,725)	1:A:28:LEU:HD22	2:B:122:MET:HA	14	0.12
(2,725)	1:A:28:LEU:HD23	2:B:122:MET:HA	14	0.12
(2,725)	1:A:28:LEU:HD11	2:B:122:MET:HA	20	0.12
(2,725)	1:A:28:LEU:HD12	2:B:122:MET:HA	20	0.12
(2,725)	1:A:28:LEU:HD13	2:B:122:MET:HA	20	0.12
(2,725)	1:A:28:LEU:HD21	2:B:122:MET:HA	20	0.12
(2,725)	1:A:28:LEU:HD22	2:B:122:MET:HA	20	0.12
(2,725)	1:A:28:LEU:HD23	2:B:122:MET:HA	20	0.12
(2,694)	1:C:1029:MET:HA	2:D:1129:LEU:HD11	1	0.12
(2,694)	1:C:1029:MET:HA	2:D:1129:LEU:HD12	1	0.12
(2,694)	1:C:1029:MET:HA	2:D:1129:LEU:HD13	1	0.12
(2,694)	1:C:1029:MET:HA	2:D:1129:LEU:HD21	1	0.12
(2,694)	1:C:1029:MET:HA	2:D:1129:LEU:HD22	1	0.12
(2,694)	1:C:1029:MET:HA	2:D:1129:LEU:HD23	1	0.12
(2,683)	1:A:7:TYR:HE1	2:B:140:LEU:HB2	4	0.12
(2,683)	1:A:7:TYR:HE1	2:B:140:LEU:HB3	4	0.12
(2,683)	1:A:7:TYR:HE2	2:B:140:LEU:HB2	4	0.12
(2,683)	1:A:7:TYR:HE2	2:B:140:LEU:HB3	4	0.12
(2,683)	1:A:7:TYR:HE1	2:B:140:LEU:HB2	14	0.12
(2,683)	1:A:7:TYR:HE1	2:B:140:LEU:HB3	14	0.12
(2,683)	1:A:7:TYR:HE2	2:B:140:LEU:HB2	14	0.12
(2,683)	1:A:7:TYR:HE2	2:B:140:LEU:HB3	14	0.12
(2,656)	1:C:1036:THR:HG21	2:D:1124:LEU:HA	20	0.12
(2,656)	1:C:1036:THR:HG22	2:D:1124:LEU:HA	20	0.12
(2,656)	1:C:1036:THR:HG23	2:D:1124:LEU:HA	20	0.12
(2,655)	1:A:36:THR:HG21	2:B:124:LEU:HA	3	0.12
(2,655)	1:A:36:THR:HG22	2:B:124:LEU:HA	3	0.12
(2,655)	1:A:36:THR:HG23	2:B:124:LEU:HA	3	0.12
(2,652)	1:C:1005:LEU:HD11	2:D:1140:LEU:HA	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,652)	1:C:1005:LEU:HD12	2:D:1140:LEU:HA	13	0.12
(2,652)	1:C:1005:LEU:HD13	2:D:1140:LEU:HA	13	0.12
(2,652)	1:C:1005:LEU:HD21	2:D:1140:LEU:HA	13	0.12
(2,652)	1:C:1005:LEU:HD22	2:D:1140:LEU:HA	13	0.12
(2,652)	1:C:1005:LEU:HD23	2:D:1140:LEU:HA	13	0.12
(2,652)	1:C:1005:LEU:HD11	2:D:1140:LEU:HA	14	0.12
(2,652)	1:C:1005:LEU:HD12	2:D:1140:LEU:HA	14	0.12
(2,652)	1:C:1005:LEU:HD13	2:D:1140:LEU:HA	14	0.12
(2,652)	1:C:1005:LEU:HD21	2:D:1140:LEU:HA	14	0.12
(2,652)	1:C:1005:LEU:HD22	2:D:1140:LEU:HA	14	0.12
(2,652)	1:C:1005:LEU:HD23	2:D:1140:LEU:HA	14	0.12
(2,651)	1:A:5:LEU:HD11	2:B:140:LEU:HA	5	0.12
(2,651)	1:A:5:LEU:HD12	2:B:140:LEU:HA	5	0.12
(2,651)	1:A:5:LEU:HD13	2:B:140:LEU:HA	5	0.12
(2,651)	1:A:5:LEU:HD21	2:B:140:LEU:HA	5	0.12
(2,651)	1:A:5:LEU:HD22	2:B:140:LEU:HA	5	0.12
(2,651)	1:A:5:LEU:HD23	2:B:140:LEU:HA	5	0.12
(2,637)	1:A:20:LEU:HD11	2:B:134:ARG:HA	2	0.12
(2,637)	1:A:20:LEU:HD12	2:B:134:ARG:HA	2	0.12
(2,637)	1:A:20:LEU:HD13	2:B:134:ARG:HA	2	0.12
(2,637)	1:A:20:LEU:HD21	2:B:134:ARG:HA	2	0.12
(2,637)	1:A:20:LEU:HD22	2:B:134:ARG:HA	2	0.12
(2,637)	1:A:20:LEU:HD23	2:B:134:ARG:HA	2	0.12
(2,591)	1:A:31:TYR:HD1	2:B:130:VAL:HG11	18	0.12
(2,591)	1:A:31:TYR:HD1	2:B:130:VAL:HG12	18	0.12
(2,591)	1:A:31:TYR:HD1	2:B:130:VAL:HG13	18	0.12
(2,591)	1:A:31:TYR:HD1	2:B:130:VAL:HG21	18	0.12
(2,591)	1:A:31:TYR:HD1	2:B:130:VAL:HG22	18	0.12
(2,591)	1:A:31:TYR:HD1	2:B:130:VAL:HG23	18	0.12
(2,591)	1:A:31:TYR:HD2	2:B:130:VAL:HG11	18	0.12
(2,591)	1:A:31:TYR:HD2	2:B:130:VAL:HG12	18	0.12
(2,591)	1:A:31:TYR:HD2	2:B:130:VAL:HG13	18	0.12
(2,591)	1:A:31:TYR:HD2	2:B:130:VAL:HG21	18	0.12
(2,591)	1:A:31:TYR:HD2	2:B:130:VAL:HG22	18	0.12
(2,591)	1:A:31:TYR:HD2	2:B:130:VAL:HG23	18	0.12
(2,332)	2:B:112:LEU:HB2	1:C:1022:ILE:HD11	20	0.12
(2,332)	2:B:112:LEU:HB2	1:C:1022:ILE:HD12	20	0.12
(2,332)	2:B:112:LEU:HB2	1:C:1022:ILE:HD13	20	0.12
(2,332)	2:B:112:LEU:HB3	1:C:1022:ILE:HD11	20	0.12
(2,332)	2:B:112:LEU:HB3	1:C:1022:ILE:HD12	20	0.12
(2,332)	2:B:112:LEU:HB3	1:C:1022:ILE:HD13	20	0.12
(2,301)	1:A:31:TYR:HA	2:B:129:LEU:HD11	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,301)	1:A:31:TYR:HA	2:B:129:LEU:HD12	8	0.12
(2,301)	1:A:31:TYR:HA	2:B:129:LEU:HD13	8	0.12
(2,301)	1:A:31:TYR:HA	2:B:129:LEU:HD21	8	0.12
(2,301)	1:A:31:TYR:HA	2:B:129:LEU:HD22	8	0.12
(2,301)	1:A:31:TYR:HA	2:B:129:LEU:HD23	8	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG11	5	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG12	5	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG13	5	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG21	5	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG22	5	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG23	5	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG11	7	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG12	7	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG13	7	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG21	7	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG22	7	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG23	7	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG11	10	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG12	10	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG13	10	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG21	10	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG22	10	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG23	10	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG11	14	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG12	14	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG13	14	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG21	14	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG22	14	0.12
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG23	14	0.12
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG11	10	0.12
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG12	10	0.12
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG13	10	0.12
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG21	10	0.12
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG22	10	0.12
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG23	10	0.12
(2,275)	1:A:23:LYS:HE2	2:B:133:TYR:HE1	14	0.12
(2,275)	1:A:23:LYS:HE2	2:B:133:TYR:HE2	14	0.12
(2,275)	1:A:23:LYS:HE3	2:B:133:TYR:HE1	14	0.12
(2,275)	1:A:23:LYS:HE3	2:B:133:TYR:HE2	14	0.12
(2,2)	2:D:1140:LEU:HD11	2:D:1142:ARG:H	10	0.12
(2,2)	2:D:1140:LEU:HD12	2:D:1142:ARG:H	10	0.12
(2,2)	2:D:1140:LEU:HD13	2:D:1142:ARG:H	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	2:D:1140:LEU:HD21	2:D:1142:ARG:H	10	0.12
(2,2)	2:D:1140:LEU:HD22	2:D:1142:ARG:H	10	0.12
(2,2)	2:D:1140:LEU:HD23	2:D:1142:ARG:H	10	0.12
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD11	7	0.12
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD12	7	0.12
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD13	7	0.12
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD21	7	0.12
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD22	7	0.12
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD23	7	0.12
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD11	7	0.12
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD12	7	0.12
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD13	7	0.12
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD21	7	0.12
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD22	7	0.12
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD23	7	0.12
(2,193)	1:A:7:TYR:HD1	2:B:140:LEU:HD11	19	0.12
(2,193)	1:A:7:TYR:HD1	2:B:140:LEU:HD12	19	0.12
(2,193)	1:A:7:TYR:HD1	2:B:140:LEU:HD13	19	0.12
(2,193)	1:A:7:TYR:HD1	2:B:140:LEU:HD21	19	0.12
(2,193)	1:A:7:TYR:HD1	2:B:140:LEU:HD22	19	0.12
(2,193)	1:A:7:TYR:HD1	2:B:140:LEU:HD23	19	0.12
(2,193)	1:A:7:TYR:HD2	2:B:140:LEU:HD11	19	0.12
(2,193)	1:A:7:TYR:HD2	2:B:140:LEU:HD12	19	0.12
(2,193)	1:A:7:TYR:HD2	2:B:140:LEU:HD13	19	0.12
(2,193)	1:A:7:TYR:HD2	2:B:140:LEU:HD21	19	0.12
(2,193)	1:A:7:TYR:HD2	2:B:140:LEU:HD22	19	0.12
(2,193)	1:A:7:TYR:HD2	2:B:140:LEU:HD23	19	0.12
(2,166)	2:D:1124:LEU:HD11	2:D:1126:PRO:HB3	10	0.12
(2,166)	2:D:1124:LEU:HD12	2:D:1126:PRO:HB3	10	0.12
(2,166)	2:D:1124:LEU:HD13	2:D:1126:PRO:HB3	10	0.12
(2,166)	2:D:1124:LEU:HD21	2:D:1126:PRO:HB3	10	0.12
(2,166)	2:D:1124:LEU:HD22	2:D:1126:PRO:HB3	10	0.12
(2,166)	2:D:1124:LEU:HD23	2:D:1126:PRO:HB3	10	0.12
(2,165)	2:B:124:LEU:HD11	2:B:126:PRO:HB3	5	0.12
(2,165)	2:B:124:LEU:HD12	2:B:126:PRO:HB3	5	0.12
(2,165)	2:B:124:LEU:HD13	2:B:126:PRO:HB3	5	0.12
(2,165)	2:B:124:LEU:HD21	2:B:126:PRO:HB3	5	0.12
(2,165)	2:B:124:LEU:HD22	2:B:126:PRO:HB3	5	0.12
(2,165)	2:B:124:LEU:HD23	2:B:126:PRO:HB3	5	0.12
(2,165)	2:B:124:LEU:HD11	2:B:126:PRO:HB3	10	0.12
(2,165)	2:B:124:LEU:HD12	2:B:126:PRO:HB3	10	0.12
(2,165)	2:B:124:LEU:HD13	2:B:126:PRO:HB3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,165)	2:B:124:LEU:HD21	2:B:126:PRO:HB3	10	0.12
(2,165)	2:B:124:LEU:HD22	2:B:126:PRO:HB3	10	0.12
(2,165)	2:B:124:LEU:HD23	2:B:126:PRO:HB3	10	0.12
(2,152)	2:D:1134:ARG:HD2	2:D:1137:GLN:HB2	9	0.12
(2,152)	2:D:1134:ARG:HD2	2:D:1137:GLN:HB3	9	0.12
(2,152)	2:D:1134:ARG:HD3	2:D:1137:GLN:HB2	9	0.12
(2,152)	2:D:1134:ARG:HD3	2:D:1137:GLN:HB3	9	0.12
(1,755)	1:C:1028:LEU:HD11	2:D:1122:MET:HE1	7	0.12
(1,755)	1:C:1028:LEU:HD11	2:D:1122:MET:HE2	7	0.12
(1,755)	1:C:1028:LEU:HD11	2:D:1122:MET:HE3	7	0.12
(1,755)	1:C:1028:LEU:HD12	2:D:1122:MET:HE1	7	0.12
(1,755)	1:C:1028:LEU:HD12	2:D:1122:MET:HE2	7	0.12
(1,755)	1:C:1028:LEU:HD12	2:D:1122:MET:HE3	7	0.12
(1,755)	1:C:1028:LEU:HD13	2:D:1122:MET:HE1	7	0.12
(1,755)	1:C:1028:LEU:HD13	2:D:1122:MET:HE2	7	0.12
(1,755)	1:C:1028:LEU:HD13	2:D:1122:MET:HE3	7	0.12
(1,755)	1:C:1028:LEU:HD21	2:D:1122:MET:HE1	7	0.12
(1,755)	1:C:1028:LEU:HD21	2:D:1122:MET:HE2	7	0.12
(1,755)	1:C:1028:LEU:HD21	2:D:1122:MET:HE3	7	0.12
(1,755)	1:C:1028:LEU:HD22	2:D:1122:MET:HE1	7	0.12
(1,755)	1:C:1028:LEU:HD22	2:D:1122:MET:HE2	7	0.12
(1,755)	1:C:1028:LEU:HD22	2:D:1122:MET:HE3	7	0.12
(1,755)	1:C:1028:LEU:HD23	2:D:1122:MET:HE1	7	0.12
(1,755)	1:C:1028:LEU:HD23	2:D:1122:MET:HE2	7	0.12
(1,755)	1:C:1028:LEU:HD23	2:D:1122:MET:HE3	7	0.12
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD11	6	0.12
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD12	6	0.12
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD13	6	0.12
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD21	6	0.12
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD22	6	0.12
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD23	6	0.12
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD11	6	0.12
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD12	6	0.12
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD13	6	0.12
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD21	6	0.12
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD22	6	0.12
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD23	6	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD11	1	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD12	1	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD13	1	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD21	1	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD22	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD23	1	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD11	1	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD12	1	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD13	1	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD21	1	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD22	1	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD23	1	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD11	4	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD12	4	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD13	4	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD21	4	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD22	4	0.12
(1,1528)	1:C:1029:MET:HB2	2:D:1121:LEU:HD23	4	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD11	4	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD12	4	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD13	4	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD21	4	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD22	4	0.12
(1,1528)	1:C:1029:MET:HB3	2:D:1121:LEU:HD23	4	0.12
(1,1515)	1:A:26:LEU:HD11	2:B:118:SER:HA	9	0.12
(1,1515)	1:A:26:LEU:HD12	2:B:118:SER:HA	9	0.12
(1,1515)	1:A:26:LEU:HD13	2:B:118:SER:HA	9	0.12
(1,1515)	1:A:26:LEU:HD21	2:B:118:SER:HA	9	0.12
(1,1515)	1:A:26:LEU:HD22	2:B:118:SER:HA	9	0.12
(1,1515)	1:A:26:LEU:HD23	2:B:118:SER:HA	9	0.12
(1,1515)	1:A:26:LEU:HD11	2:B:118:SER:HA	20	0.12
(1,1515)	1:A:26:LEU:HD12	2:B:118:SER:HA	20	0.12
(1,1515)	1:A:26:LEU:HD13	2:B:118:SER:HA	20	0.12
(1,1515)	1:A:26:LEU:HD21	2:B:118:SER:HA	20	0.12
(1,1515)	1:A:26:LEU:HD22	2:B:118:SER:HA	20	0.12
(1,1515)	1:A:26:LEU:HD23	2:B:118:SER:HA	20	0.12
(1,1505)	1:A:26:LEU:HD11	2:B:115:LEU:HA	6	0.12
(1,1505)	1:A:26:LEU:HD12	2:B:115:LEU:HA	6	0.12
(1,1505)	1:A:26:LEU:HD13	2:B:115:LEU:HA	6	0.12
(1,1505)	1:A:26:LEU:HD21	2:B:115:LEU:HA	6	0.12
(1,1505)	1:A:26:LEU:HD22	2:B:115:LEU:HA	6	0.12
(1,1505)	1:A:26:LEU:HD23	2:B:115:LEU:HA	6	0.12
(1,1505)	1:A:26:LEU:HD11	2:B:115:LEU:HA	8	0.12
(1,1505)	1:A:26:LEU:HD12	2:B:115:LEU:HA	8	0.12
(1,1505)	1:A:26:LEU:HD13	2:B:115:LEU:HA	8	0.12
(1,1505)	1:A:26:LEU:HD21	2:B:115:LEU:HA	8	0.12
(1,1505)	1:A:26:LEU:HD22	2:B:115:LEU:HA	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1505)	1:A:26:LEU:HD23	2:B:115:LEU:HA	8	0.12
(1,1464)	1:C:1021:GLU:HG2	2:D:1119:LEU:HD11	12	0.12
(1,1464)	1:C:1021:GLU:HG2	2:D:1119:LEU:HD12	12	0.12
(1,1464)	1:C:1021:GLU:HG2	2:D:1119:LEU:HD13	12	0.12
(1,1464)	1:C:1021:GLU:HG2	2:D:1119:LEU:HD21	12	0.12
(1,1464)	1:C:1021:GLU:HG2	2:D:1119:LEU:HD22	12	0.12
(1,1464)	1:C:1021:GLU:HG2	2:D:1119:LEU:HD23	12	0.12
(1,1464)	1:C:1021:GLU:HG3	2:D:1119:LEU:HD11	12	0.12
(1,1464)	1:C:1021:GLU:HG3	2:D:1119:LEU:HD12	12	0.12
(1,1464)	1:C:1021:GLU:HG3	2:D:1119:LEU:HD13	12	0.12
(1,1464)	1:C:1021:GLU:HG3	2:D:1119:LEU:HD21	12	0.12
(1,1464)	1:C:1021:GLU:HG3	2:D:1119:LEU:HD22	12	0.12
(1,1464)	1:C:1021:GLU:HG3	2:D:1119:LEU:HD23	12	0.12
(1,1463)	1:A:21:GLU:HG2	2:B:119:LEU:HD11	7	0.12
(1,1463)	1:A:21:GLU:HG2	2:B:119:LEU:HD12	7	0.12
(1,1463)	1:A:21:GLU:HG2	2:B:119:LEU:HD13	7	0.12
(1,1463)	1:A:21:GLU:HG2	2:B:119:LEU:HD21	7	0.12
(1,1463)	1:A:21:GLU:HG2	2:B:119:LEU:HD22	7	0.12
(1,1463)	1:A:21:GLU:HG2	2:B:119:LEU:HD23	7	0.12
(1,1463)	1:A:21:GLU:HG3	2:B:119:LEU:HD11	7	0.12
(1,1463)	1:A:21:GLU:HG3	2:B:119:LEU:HD12	7	0.12
(1,1463)	1:A:21:GLU:HG3	2:B:119:LEU:HD13	7	0.12
(1,1463)	1:A:21:GLU:HG3	2:B:119:LEU:HD21	7	0.12
(1,1463)	1:A:21:GLU:HG3	2:B:119:LEU:HD22	7	0.12
(1,1463)	1:A:21:GLU:HG3	2:B:119:LEU:HD23	7	0.12
(1,1423)	1:A:6:LEU:HD11	1:C:1013:ARG:HA	11	0.12
(1,1423)	1:A:6:LEU:HD12	1:C:1013:ARG:HA	11	0.12
(1,1423)	1:A:6:LEU:HD13	1:C:1013:ARG:HA	11	0.12
(1,1423)	1:A:6:LEU:HD21	1:C:1013:ARG:HA	11	0.12
(1,1423)	1:A:6:LEU:HD22	1:C:1013:ARG:HA	11	0.12
(1,1423)	1:A:6:LEU:HD23	1:C:1013:ARG:HA	11	0.12
(1,1385)	2:B:114:LYS:HE2	1:C:1018:MET:HE1	10	0.12
(1,1385)	2:B:114:LYS:HE2	1:C:1018:MET:HE2	10	0.12
(1,1385)	2:B:114:LYS:HE2	1:C:1018:MET:HE3	10	0.12
(1,1385)	2:B:114:LYS:HE3	1:C:1018:MET:HE1	10	0.12
(1,1385)	2:B:114:LYS:HE3	1:C:1018:MET:HE2	10	0.12
(1,1385)	2:B:114:LYS:HE3	1:C:1018:MET:HE3	10	0.12
(1,1232)	1:C:1036:THR:HG21	1:C:1037:ILE:HD11	8	0.12
(1,1232)	1:C:1036:THR:HG21	1:C:1037:ILE:HD12	8	0.12
(1,1232)	1:C:1036:THR:HG21	1:C:1037:ILE:HD13	8	0.12
(1,1232)	1:C:1036:THR:HG22	1:C:1037:ILE:HD11	8	0.12
(1,1232)	1:C:1036:THR:HG22	1:C:1037:ILE:HD12	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1232)	1:C:1036:THR:HG22	1:C:1037:ILE:HD13	8	0.12
(1,1232)	1:C:1036:THR:HG23	1:C:1037:ILE:HD11	8	0.12
(1,1232)	1:C:1036:THR:HG23	1:C:1037:ILE:HD12	8	0.12
(1,1232)	1:C:1036:THR:HG23	1:C:1037:ILE:HD13	8	0.12
(1,1232)	1:C:1036:THR:HG21	1:C:1037:ILE:HD11	9	0.12
(1,1232)	1:C:1036:THR:HG21	1:C:1037:ILE:HD12	9	0.12
(1,1232)	1:C:1036:THR:HG21	1:C:1037:ILE:HD13	9	0.12
(1,1232)	1:C:1036:THR:HG22	1:C:1037:ILE:HD11	9	0.12
(1,1232)	1:C:1036:THR:HG22	1:C:1037:ILE:HD12	9	0.12
(1,1232)	1:C:1036:THR:HG22	1:C:1037:ILE:HD13	9	0.12
(1,1232)	1:C:1036:THR:HG23	1:C:1037:ILE:HD11	9	0.12
(1,1232)	1:C:1036:THR:HG23	1:C:1037:ILE:HD12	9	0.12
(1,1232)	1:C:1036:THR:HG23	1:C:1037:ILE:HD13	9	0.12
(1,1231)	1:A:36:THR:HG21	1:A:37:ILE:HD11	17	0.12
(1,1231)	1:A:36:THR:HG21	1:A:37:ILE:HD12	17	0.12
(1,1231)	1:A:36:THR:HG21	1:A:37:ILE:HD13	17	0.12
(1,1231)	1:A:36:THR:HG22	1:A:37:ILE:HD11	17	0.12
(1,1231)	1:A:36:THR:HG22	1:A:37:ILE:HD12	17	0.12
(1,1231)	1:A:36:THR:HG22	1:A:37:ILE:HD13	17	0.12
(1,1231)	1:A:36:THR:HG23	1:A:37:ILE:HD11	17	0.12
(1,1231)	1:A:36:THR:HG23	1:A:37:ILE:HD12	17	0.12
(1,1231)	1:A:36:THR:HG23	1:A:37:ILE:HD13	17	0.12
(1,1082)	1:A:11:ARG:HD2	1:C:1003:ASP:HB2	15	0.12
(1,1082)	1:A:11:ARG:HD2	1:C:1003:ASP:HB3	15	0.12
(1,1082)	1:A:11:ARG:HD3	1:C:1003:ASP:HB2	15	0.12
(1,1082)	1:A:11:ARG:HD3	1:C:1003:ASP:HB3	15	0.12
(1,1074)	1:A:6:LEU:HD21	1:C:1013:ARG:HD2	7	0.12
(1,1074)	1:A:6:LEU:HD21	1:C:1013:ARG:HD3	7	0.12
(1,1074)	1:A:6:LEU:HD22	1:C:1013:ARG:HD2	7	0.12
(1,1074)	1:A:6:LEU:HD22	1:C:1013:ARG:HD3	7	0.12
(1,1074)	1:A:6:LEU:HD23	1:C:1013:ARG:HD2	7	0.12
(1,1074)	1:A:6:LEU:HD23	1:C:1013:ARG:HD3	7	0.12
(1,1074)	1:A:6:LEU:HD21	1:C:1013:ARG:HD2	17	0.12
(1,1074)	1:A:6:LEU:HD21	1:C:1013:ARG:HD3	17	0.12
(1,1074)	1:A:6:LEU:HD22	1:C:1013:ARG:HD2	17	0.12
(1,1074)	1:A:6:LEU:HD22	1:C:1013:ARG:HD3	17	0.12
(1,1074)	1:A:6:LEU:HD23	1:C:1013:ARG:HD2	17	0.12
(1,1074)	1:A:6:LEU:HD23	1:C:1013:ARG:HD3	17	0.12
(4,98)	2:D:1109:PHE:O	2:D:1113:MET:N	10	0.11
(4,97)	2:D:1108:ASN:O	2:D:1112:LEU:N	19	0.11
(4,93)	2:D:1134:ARG:O	2:D:1138:GLN:N	9	0.11
(4,9)	1:A:42:GLN:O	1:A:46:GLN:N	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,89)	2:D:1130:VAL:O	2:D:1134:ARG:N	14	0.11
(4,88)	2:D:1129:LEU:O	2:D:1133:TYR:N	1	0.11
(4,83)	2:B:118:SER:O	2:B:122:MET:N	1	0.11
(4,79)	2:B:114:LYS:O	2:B:118:SER:N	4	0.11
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	9	0.11
(4,77)	2:B:112:LEU:O	2:B:116:LYS:N	16	0.11
(4,74)	2:B:109:PHE:O	2:B:113:MET:N	15	0.11
(4,69)	2:B:134:ARG:O	2:B:138:GLN:N	11	0.11
(4,68)	2:B:133:TYR:O	2:B:137:GLN:N	2	0.11
(4,68)	2:B:133:TYR:O	2:B:137:GLN:N	5	0.11
(4,68)	2:B:133:TYR:O	2:B:137:GLN:N	17	0.11
(4,64)	2:B:129:LEU:O	2:B:133:TYR:N	7	0.11
(4,64)	2:B:129:LEU:O	2:B:133:TYR:N	12	0.11
(4,6)	1:A:39:THR:O	1:A:43:GLN:N	8	0.11
(4,59)	2:B:103:VAL:O	2:D:1099:TYR:N	4	0.11
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	13	0.11
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	16	0.11
(4,49)	1:C:1027:GLU:O	1:C:1031:TYR:N	20	0.11
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	2	0.11
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	4	0.11
(4,46)	1:C:1024:GLU:O	1:C:1028:LEU:N	16	0.11
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	3	0.11
(4,42)	1:C:1020:LEU:O	1:C:1024:GLU:N	5	0.11
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	3	0.11
(4,41)	1:C:1019:LEU:O	1:C:1023:LYS:N	14	0.11
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	6	0.11
(4,38)	1:C:1016:TYR:O	1:C:1020:LEU:N	8	0.11
(4,32)	1:C:1040:TYR:O	1:C:1044:GLN:N	13	0.11
(4,3)	1:A:36:THR:O	1:A:40:TYR:N	8	0.11
(4,29)	1:C:1037:ILE:O	1:C:1041:ARG:N	17	0.11
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	5	0.11
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	13	0.11
(4,25)	1:A:28:LEU:O	1:A:32:LEU:N	18	0.11
(4,24)	1:A:27:GLU:O	1:A:31:TYR:N	3	0.11
(4,21)	1:A:24:GLU:O	1:A:28:LEU:N	18	0.11
(4,2)	1:A:35:HIS:O	1:A:39:THR:N	15	0.11
(4,17)	1:A:20:LEU:O	1:A:24:GLU:N	5	0.11
(4,17)	1:A:20:LEU:O	1:A:24:GLU:N	8	0.11
(4,17)	1:A:20:LEU:O	1:A:24:GLU:N	20	0.11
(4,107)	2:D:1118:SER:O	2:D:1122:MET:N	12	0.11
(4,106)	2:D:1117:GLU:O	2:D:1121:LEU:N	7	0.11
(4,105)	2:D:1116:LYS:O	2:D:1120:GLU:N	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,101)	2:D:1112:LEU:O	2:D:1116:LYS:N	2	0.11
(4,101)	2:D:1112:LEU:O	2:D:1116:LYS:N	16	0.11
(2,880)	2:B:120:GLU:HG2	2:D:1104:ARG:HB2	14	0.11
(2,880)	2:B:120:GLU:HG2	2:D:1104:ARG:HB3	14	0.11
(2,880)	2:B:120:GLU:HG3	2:D:1104:ARG:HB2	14	0.11
(2,880)	2:B:120:GLU:HG3	2:D:1104:ARG:HB3	14	0.11
(2,879)	2:B:104:ARG:HB2	2:D:1120:GLU:HG2	9	0.11
(2,879)	2:B:104:ARG:HB2	2:D:1120:GLU:HG3	9	0.11
(2,879)	2:B:104:ARG:HB3	2:D:1120:GLU:HG2	9	0.11
(2,879)	2:B:104:ARG:HB3	2:D:1120:GLU:HG3	9	0.11
(2,879)	2:B:104:ARG:HB2	2:D:1120:GLU:HG2	13	0.11
(2,879)	2:B:104:ARG:HB2	2:D:1120:GLU:HG3	13	0.11
(2,879)	2:B:104:ARG:HB3	2:D:1120:GLU:HG2	13	0.11
(2,879)	2:B:104:ARG:HB3	2:D:1120:GLU:HG3	13	0.11
(2,879)	2:B:104:ARG:HB2	2:D:1120:GLU:HG2	15	0.11
(2,879)	2:B:104:ARG:HB2	2:D:1120:GLU:HG3	15	0.11
(2,879)	2:B:104:ARG:HB3	2:D:1120:GLU:HG2	15	0.11
(2,879)	2:B:104:ARG:HB3	2:D:1120:GLU:HG3	15	0.11
(2,879)	2:B:104:ARG:HB2	2:D:1120:GLU:HG2	16	0.11
(2,879)	2:B:104:ARG:HB2	2:D:1120:GLU:HG3	16	0.11
(2,879)	2:B:104:ARG:HB3	2:D:1120:GLU:HG2	16	0.11
(2,879)	2:B:104:ARG:HB3	2:D:1120:GLU:HG3	16	0.11
(2,879)	2:B:104:ARG:HB2	2:D:1120:GLU:HG2	18	0.11
(2,879)	2:B:104:ARG:HB2	2:D:1120:GLU:HG3	18	0.11
(2,879)	2:B:104:ARG:HB3	2:D:1120:GLU:HG2	18	0.11
(2,879)	2:B:104:ARG:HB3	2:D:1120:GLU:HG3	18	0.11
(2,878)	2:D:1103:VAL:HB	2:D:1112:LEU:HD11	8	0.11
(2,878)	2:D:1103:VAL:HB	2:D:1112:LEU:HD12	8	0.11
(2,878)	2:D:1103:VAL:HB	2:D:1112:LEU:HD13	8	0.11
(2,878)	2:D:1103:VAL:HB	2:D:1112:LEU:HD21	8	0.11
(2,878)	2:D:1103:VAL:HB	2:D:1112:LEU:HD22	8	0.11
(2,878)	2:D:1103:VAL:HB	2:D:1112:LEU:HD23	8	0.11
(2,877)	2:B:103:VAL:HB	2:B:112:LEU:HD11	2	0.11
(2,877)	2:B:103:VAL:HB	2:B:112:LEU:HD12	2	0.11
(2,877)	2:B:103:VAL:HB	2:B:112:LEU:HD13	2	0.11
(2,877)	2:B:103:VAL:HB	2:B:112:LEU:HD21	2	0.11
(2,877)	2:B:103:VAL:HB	2:B:112:LEU:HD22	2	0.11
(2,877)	2:B:103:VAL:HB	2:B:112:LEU:HD23	2	0.11
(2,868)	1:C:1020:LEU:HD11	2:D:1133:TYR:HE1	8	0.11
(2,868)	1:C:1020:LEU:HD11	2:D:1133:TYR:HE2	8	0.11
(2,868)	1:C:1020:LEU:HD12	2:D:1133:TYR:HE1	8	0.11
(2,868)	1:C:1020:LEU:HD12	2:D:1133:TYR:HE2	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,868)	1:C:1020:LEU:HD13	2:D:1133:TYR:HE1	8	0.11
(2,868)	1:C:1020:LEU:HD13	2:D:1133:TYR:HE2	8	0.11
(2,868)	1:C:1020:LEU:HD21	2:D:1133:TYR:HE1	8	0.11
(2,868)	1:C:1020:LEU:HD21	2:D:1133:TYR:HE2	8	0.11
(2,868)	1:C:1020:LEU:HD22	2:D:1133:TYR:HE1	8	0.11
(2,868)	1:C:1020:LEU:HD22	2:D:1133:TYR:HE2	8	0.11
(2,868)	1:C:1020:LEU:HD23	2:D:1133:TYR:HE1	8	0.11
(2,868)	1:C:1020:LEU:HD23	2:D:1133:TYR:HE2	8	0.11
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE1	1	0.11
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE2	1	0.11
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE1	1	0.11
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE2	1	0.11
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE1	1	0.11
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE2	1	0.11
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE1	1	0.11
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE2	1	0.11
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE1	1	0.11
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE2	1	0.11
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE1	1	0.11
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE2	1	0.11
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE1	5	0.11
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE2	5	0.11
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE1	5	0.11
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE2	5	0.11
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE1	5	0.11
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE2	5	0.11
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE1	5	0.11
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE2	5	0.11
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE1	5	0.11
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE2	5	0.11
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE1	5	0.11
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE2	5	0.11
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE1	10	0.11
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE2	10	0.11
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE1	10	0.11
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE2	10	0.11
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE1	10	0.11
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE2	10	0.11
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE1	10	0.11
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE2	10	0.11
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE1	10	0.11
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE1	10	0.11
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE2	10	0.11
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE1	19	0.11
(2,867)	1:A:20:LEU:HD11	2:B:133:TYR:HE2	19	0.11
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE1	19	0.11
(2,867)	1:A:20:LEU:HD12	2:B:133:TYR:HE2	19	0.11
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE1	19	0.11
(2,867)	1:A:20:LEU:HD13	2:B:133:TYR:HE2	19	0.11
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE1	19	0.11
(2,867)	1:A:20:LEU:HD21	2:B:133:TYR:HE2	19	0.11
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE1	19	0.11
(2,867)	1:A:20:LEU:HD22	2:B:133:TYR:HE2	19	0.11
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE1	19	0.11
(2,867)	1:A:20:LEU:HD23	2:B:133:TYR:HE2	19	0.11
(2,802)	2:B:116:LYS:HD2	2:D:1109:PHE:H	19	0.11
(2,802)	2:B:116:LYS:HD3	2:D:1109:PHE:H	19	0.11
(2,801)	2:B:109:PHE:H	2:D:1116:LYS:HD2	19	0.11
(2,801)	2:B:109:PHE:H	2:D:1116:LYS:HD3	19	0.11
(2,781)	2:B:103:VAL:HG11	2:B:109:PHE:HE1	17	0.11
(2,781)	2:B:103:VAL:HG11	2:B:109:PHE:HE2	17	0.11
(2,781)	2:B:103:VAL:HG12	2:B:109:PHE:HE1	17	0.11
(2,781)	2:B:103:VAL:HG12	2:B:109:PHE:HE2	17	0.11
(2,781)	2:B:103:VAL:HG13	2:B:109:PHE:HE1	17	0.11
(2,781)	2:B:103:VAL:HG13	2:B:109:PHE:HE2	17	0.11
(2,781)	2:B:103:VAL:HG21	2:B:109:PHE:HE1	17	0.11
(2,781)	2:B:103:VAL:HG21	2:B:109:PHE:HE2	17	0.11
(2,781)	2:B:103:VAL:HG22	2:B:109:PHE:HE1	17	0.11
(2,781)	2:B:103:VAL:HG22	2:B:109:PHE:HE2	17	0.11
(2,781)	2:B:103:VAL:HG23	2:B:109:PHE:HE1	17	0.11
(2,781)	2:B:103:VAL:HG23	2:B:109:PHE:HE2	17	0.11
(2,726)	1:C:1028:LEU:HD11	2:D:1122:MET:HA	14	0.11
(2,726)	1:C:1028:LEU:HD12	2:D:1122:MET:HA	14	0.11
(2,726)	1:C:1028:LEU:HD13	2:D:1122:MET:HA	14	0.11
(2,726)	1:C:1028:LEU:HD21	2:D:1122:MET:HA	14	0.11
(2,726)	1:C:1028:LEU:HD22	2:D:1122:MET:HA	14	0.11
(2,726)	1:C:1028:LEU:HD23	2:D:1122:MET:HA	14	0.11
(2,726)	1:C:1028:LEU:HD11	2:D:1122:MET:HA	19	0.11
(2,726)	1:C:1028:LEU:HD12	2:D:1122:MET:HA	19	0.11
(2,726)	1:C:1028:LEU:HD13	2:D:1122:MET:HA	19	0.11
(2,726)	1:C:1028:LEU:HD21	2:D:1122:MET:HA	19	0.11
(2,726)	1:C:1028:LEU:HD22	2:D:1122:MET:HA	19	0.11
(2,726)	1:C:1028:LEU:HD23	2:D:1122:MET:HA	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,725)	1:A:28:LEU:HD11	2:B:122:MET:HA	1	0.11
(2,725)	1:A:28:LEU:HD12	2:B:122:MET:HA	1	0.11
(2,725)	1:A:28:LEU:HD13	2:B:122:MET:HA	1	0.11
(2,725)	1:A:28:LEU:HD21	2:B:122:MET:HA	1	0.11
(2,725)	1:A:28:LEU:HD22	2:B:122:MET:HA	1	0.11
(2,725)	1:A:28:LEU:HD23	2:B:122:MET:HA	1	0.11
(2,725)	1:A:28:LEU:HD11	2:B:122:MET:HA	9	0.11
(2,725)	1:A:28:LEU:HD12	2:B:122:MET:HA	9	0.11
(2,725)	1:A:28:LEU:HD13	2:B:122:MET:HA	9	0.11
(2,725)	1:A:28:LEU:HD21	2:B:122:MET:HA	9	0.11
(2,725)	1:A:28:LEU:HD22	2:B:122:MET:HA	9	0.11
(2,725)	1:A:28:LEU:HD23	2:B:122:MET:HA	9	0.11
(2,725)	1:A:28:LEU:HD11	2:B:122:MET:HA	19	0.11
(2,725)	1:A:28:LEU:HD12	2:B:122:MET:HA	19	0.11
(2,725)	1:A:28:LEU:HD13	2:B:122:MET:HA	19	0.11
(2,725)	1:A:28:LEU:HD21	2:B:122:MET:HA	19	0.11
(2,725)	1:A:28:LEU:HD22	2:B:122:MET:HA	19	0.11
(2,725)	1:A:28:LEU:HD23	2:B:122:MET:HA	19	0.11
(2,684)	1:C:1007:TYR:HE1	2:D:1140:LEU:HB2	1	0.11
(2,684)	1:C:1007:TYR:HE1	2:D:1140:LEU:HB3	1	0.11
(2,684)	1:C:1007:TYR:HE2	2:D:1140:LEU:HB2	1	0.11
(2,684)	1:C:1007:TYR:HE2	2:D:1140:LEU:HB3	1	0.11
(2,684)	1:C:1007:TYR:HE1	2:D:1140:LEU:HB2	18	0.11
(2,684)	1:C:1007:TYR:HE1	2:D:1140:LEU:HB3	18	0.11
(2,684)	1:C:1007:TYR:HE2	2:D:1140:LEU:HB2	18	0.11
(2,684)	1:C:1007:TYR:HE2	2:D:1140:LEU:HB3	18	0.11
(2,683)	1:A:7:TYR:HE1	2:B:140:LEU:HB2	17	0.11
(2,683)	1:A:7:TYR:HE1	2:B:140:LEU:HB3	17	0.11
(2,683)	1:A:7:TYR:HE2	2:B:140:LEU:HB2	17	0.11
(2,683)	1:A:7:TYR:HE2	2:B:140:LEU:HB3	17	0.11
(2,656)	1:C:1036:THR:HG21	2:D:1124:LEU:HA	16	0.11
(2,656)	1:C:1036:THR:HG22	2:D:1124:LEU:HA	16	0.11
(2,656)	1:C:1036:THR:HG23	2:D:1124:LEU:HA	16	0.11
(2,655)	1:A:36:THR:HG21	2:B:124:LEU:HA	20	0.11
(2,655)	1:A:36:THR:HG22	2:B:124:LEU:HA	20	0.11
(2,655)	1:A:36:THR:HG23	2:B:124:LEU:HA	20	0.11
(2,652)	1:C:1005:LEU:HD11	2:D:1140:LEU:HA	6	0.11
(2,652)	1:C:1005:LEU:HD12	2:D:1140:LEU:HA	6	0.11
(2,652)	1:C:1005:LEU:HD13	2:D:1140:LEU:HA	6	0.11
(2,652)	1:C:1005:LEU:HD21	2:D:1140:LEU:HA	6	0.11
(2,652)	1:C:1005:LEU:HD22	2:D:1140:LEU:HA	6	0.11
(2,652)	1:C:1005:LEU:HD23	2:D:1140:LEU:HA	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,652)	1:C:1005:LEU:HD11	2:D:1140:LEU:HA	8	0.11
(2,652)	1:C:1005:LEU:HD12	2:D:1140:LEU:HA	8	0.11
(2,652)	1:C:1005:LEU:HD13	2:D:1140:LEU:HA	8	0.11
(2,652)	1:C:1005:LEU:HD21	2:D:1140:LEU:HA	8	0.11
(2,652)	1:C:1005:LEU:HD22	2:D:1140:LEU:HA	8	0.11
(2,652)	1:C:1005:LEU:HD23	2:D:1140:LEU:HA	8	0.11
(2,638)	1:C:1020:LEU:HD11	2:D:1134:ARG:HA	16	0.11
(2,638)	1:C:1020:LEU:HD12	2:D:1134:ARG:HA	16	0.11
(2,638)	1:C:1020:LEU:HD13	2:D:1134:ARG:HA	16	0.11
(2,638)	1:C:1020:LEU:HD21	2:D:1134:ARG:HA	16	0.11
(2,638)	1:C:1020:LEU:HD22	2:D:1134:ARG:HA	16	0.11
(2,638)	1:C:1020:LEU:HD23	2:D:1134:ARG:HA	16	0.11
(2,332)	2:B:112:LEU:HB2	1:C:1022:ILE:HD11	6	0.11
(2,332)	2:B:112:LEU:HB2	1:C:1022:ILE:HD12	6	0.11
(2,332)	2:B:112:LEU:HB2	1:C:1022:ILE:HD13	6	0.11
(2,332)	2:B:112:LEU:HB3	1:C:1022:ILE:HD11	6	0.11
(2,332)	2:B:112:LEU:HB3	1:C:1022:ILE:HD12	6	0.11
(2,332)	2:B:112:LEU:HB3	1:C:1022:ILE:HD13	6	0.11
(2,332)	2:B:112:LEU:HB2	1:C:1022:ILE:HD11	11	0.11
(2,332)	2:B:112:LEU:HB2	1:C:1022:ILE:HD12	11	0.11
(2,332)	2:B:112:LEU:HB2	1:C:1022:ILE:HD13	11	0.11
(2,332)	2:B:112:LEU:HB3	1:C:1022:ILE:HD11	11	0.11
(2,332)	2:B:112:LEU:HB3	1:C:1022:ILE:HD12	11	0.11
(2,332)	2:B:112:LEU:HB3	1:C:1022:ILE:HD13	11	0.11
(2,331)	1:A:22:ILE:HD11	2:D:1112:LEU:HB2	6	0.11
(2,331)	1:A:22:ILE:HD11	2:D:1112:LEU:HB3	6	0.11
(2,331)	1:A:22:ILE:HD12	2:D:1112:LEU:HB2	6	0.11
(2,331)	1:A:22:ILE:HD12	2:D:1112:LEU:HB3	6	0.11
(2,331)	1:A:22:ILE:HD13	2:D:1112:LEU:HB2	6	0.11
(2,331)	1:A:22:ILE:HD13	2:D:1112:LEU:HB3	6	0.11
(2,331)	1:A:22:ILE:HD11	2:D:1112:LEU:HB2	16	0.11
(2,331)	1:A:22:ILE:HD11	2:D:1112:LEU:HB3	16	0.11
(2,331)	1:A:22:ILE:HD12	2:D:1112:LEU:HB2	16	0.11
(2,331)	1:A:22:ILE:HD12	2:D:1112:LEU:HB3	16	0.11
(2,331)	1:A:22:ILE:HD13	2:D:1112:LEU:HB2	16	0.11
(2,331)	1:A:22:ILE:HD13	2:D:1112:LEU:HB3	16	0.11
(2,331)	1:A:22:ILE:HD11	2:D:1112:LEU:HB2	20	0.11
(2,331)	1:A:22:ILE:HD11	2:D:1112:LEU:HB3	20	0.11
(2,331)	1:A:22:ILE:HD12	2:D:1112:LEU:HB2	20	0.11
(2,331)	1:A:22:ILE:HD12	2:D:1112:LEU:HB3	20	0.11
(2,331)	1:A:22:ILE:HD13	2:D:1112:LEU:HB2	20	0.11
(2,331)	1:A:22:ILE:HD13	2:D:1112:LEU:HB3	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,302)	1:C:1031:TYR:HA	2:D:1129:LEU:HD11	20	0.11
(2,302)	1:C:1031:TYR:HA	2:D:1129:LEU:HD12	20	0.11
(2,302)	1:C:1031:TYR:HA	2:D:1129:LEU:HD13	20	0.11
(2,302)	1:C:1031:TYR:HA	2:D:1129:LEU:HD21	20	0.11
(2,302)	1:C:1031:TYR:HA	2:D:1129:LEU:HD22	20	0.11
(2,302)	1:C:1031:TYR:HA	2:D:1129:LEU:HD23	20	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG11	1	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG12	1	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG13	1	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG21	1	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG22	1	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG23	1	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG11	2	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG12	2	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG13	2	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG21	2	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG22	2	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG23	2	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG11	6	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG12	6	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG13	6	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG21	6	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG22	6	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG23	6	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG11	18	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG12	18	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG13	18	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG21	18	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG22	18	0.11
(2,298)	1:C:1031:TYR:H	2:D:1130:VAL:HG23	18	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG11	1	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG12	1	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG13	1	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG21	1	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG22	1	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG23	1	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG11	4	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG12	4	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG13	4	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG21	4	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG22	4	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG23	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG11	6	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG12	6	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG13	6	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG21	6	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG22	6	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG23	6	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG11	12	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG12	12	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG13	12	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG21	12	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG22	12	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG23	12	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG11	14	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG12	14	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG13	14	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG21	14	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG22	14	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG23	14	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG11	19	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG12	19	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG13	19	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG21	19	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG22	19	0.11
(2,297)	1:A:31:TYR:H	2:B:130:VAL:HG23	19	0.11
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD11	9	0.11
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD12	9	0.11
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD13	9	0.11
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD21	9	0.11
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD22	9	0.11
(2,194)	1:C:1007:TYR:HD1	2:D:1140:LEU:HD23	9	0.11
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD11	9	0.11
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD12	9	0.11
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD13	9	0.11
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD21	9	0.11
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD22	9	0.11
(2,194)	1:C:1007:TYR:HD2	2:D:1140:LEU:HD23	9	0.11
(2,166)	2:D:1124:LEU:HD11	2:D:1126:PRO:HB3	1	0.11
(2,166)	2:D:1124:LEU:HD12	2:D:1126:PRO:HB3	1	0.11
(2,166)	2:D:1124:LEU:HD13	2:D:1126:PRO:HB3	1	0.11
(2,166)	2:D:1124:LEU:HD21	2:D:1126:PRO:HB3	1	0.11
(2,166)	2:D:1124:LEU:HD22	2:D:1126:PRO:HB3	1	0.11
(2,166)	2:D:1124:LEU:HD23	2:D:1126:PRO:HB3	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	2:D:1124:LEU:HD11	2:D:1126:PRO:HB3	5	0.11
(2,166)	2:D:1124:LEU:HD12	2:D:1126:PRO:HB3	5	0.11
(2,166)	2:D:1124:LEU:HD13	2:D:1126:PRO:HB3	5	0.11
(2,166)	2:D:1124:LEU:HD21	2:D:1126:PRO:HB3	5	0.11
(2,166)	2:D:1124:LEU:HD22	2:D:1126:PRO:HB3	5	0.11
(2,166)	2:D:1124:LEU:HD23	2:D:1126:PRO:HB3	5	0.11
(2,166)	2:D:1124:LEU:HD11	2:D:1126:PRO:HB3	6	0.11
(2,166)	2:D:1124:LEU:HD12	2:D:1126:PRO:HB3	6	0.11
(2,166)	2:D:1124:LEU:HD13	2:D:1126:PRO:HB3	6	0.11
(2,166)	2:D:1124:LEU:HD21	2:D:1126:PRO:HB3	6	0.11
(2,166)	2:D:1124:LEU:HD22	2:D:1126:PRO:HB3	6	0.11
(2,166)	2:D:1124:LEU:HD23	2:D:1126:PRO:HB3	6	0.11
(2,166)	2:D:1124:LEU:HD11	2:D:1126:PRO:HB3	8	0.11
(2,166)	2:D:1124:LEU:HD12	2:D:1126:PRO:HB3	8	0.11
(2,166)	2:D:1124:LEU:HD13	2:D:1126:PRO:HB3	8	0.11
(2,166)	2:D:1124:LEU:HD21	2:D:1126:PRO:HB3	8	0.11
(2,166)	2:D:1124:LEU:HD22	2:D:1126:PRO:HB3	8	0.11
(2,166)	2:D:1124:LEU:HD23	2:D:1126:PRO:HB3	8	0.11
(2,166)	2:D:1124:LEU:HD11	2:D:1126:PRO:HB3	11	0.11
(2,166)	2:D:1124:LEU:HD12	2:D:1126:PRO:HB3	11	0.11
(2,166)	2:D:1124:LEU:HD13	2:D:1126:PRO:HB3	11	0.11
(2,166)	2:D:1124:LEU:HD21	2:D:1126:PRO:HB3	11	0.11
(2,166)	2:D:1124:LEU:HD22	2:D:1126:PRO:HB3	11	0.11
(2,166)	2:D:1124:LEU:HD23	2:D:1126:PRO:HB3	11	0.11
(2,166)	2:D:1124:LEU:HD11	2:D:1126:PRO:HB3	13	0.11
(2,166)	2:D:1124:LEU:HD12	2:D:1126:PRO:HB3	13	0.11
(2,166)	2:D:1124:LEU:HD13	2:D:1126:PRO:HB3	13	0.11
(2,166)	2:D:1124:LEU:HD21	2:D:1126:PRO:HB3	13	0.11
(2,166)	2:D:1124:LEU:HD22	2:D:1126:PRO:HB3	13	0.11
(2,166)	2:D:1124:LEU:HD23	2:D:1126:PRO:HB3	13	0.11
(2,166)	2:D:1124:LEU:HD11	2:D:1126:PRO:HB3	20	0.11
(2,166)	2:D:1124:LEU:HD12	2:D:1126:PRO:HB3	20	0.11
(2,166)	2:D:1124:LEU:HD13	2:D:1126:PRO:HB3	20	0.11
(2,166)	2:D:1124:LEU:HD21	2:D:1126:PRO:HB3	20	0.11
(2,166)	2:D:1124:LEU:HD22	2:D:1126:PRO:HB3	20	0.11
(2,166)	2:D:1124:LEU:HD23	2:D:1126:PRO:HB3	20	0.11
(2,165)	2:B:124:LEU:HD11	2:B:126:PRO:HB3	1	0.11
(2,165)	2:B:124:LEU:HD12	2:B:126:PRO:HB3	1	0.11
(2,165)	2:B:124:LEU:HD13	2:B:126:PRO:HB3	1	0.11
(2,165)	2:B:124:LEU:HD21	2:B:126:PRO:HB3	1	0.11
(2,165)	2:B:124:LEU:HD22	2:B:126:PRO:HB3	1	0.11
(2,165)	2:B:124:LEU:HD23	2:B:126:PRO:HB3	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,165)	2:B:124:LEU:HD11	2:B:126:PRO:HB3	4	0.11
(2,165)	2:B:124:LEU:HD12	2:B:126:PRO:HB3	4	0.11
(2,165)	2:B:124:LEU:HD13	2:B:126:PRO:HB3	4	0.11
(2,165)	2:B:124:LEU:HD21	2:B:126:PRO:HB3	4	0.11
(2,165)	2:B:124:LEU:HD22	2:B:126:PRO:HB3	4	0.11
(2,165)	2:B:124:LEU:HD23	2:B:126:PRO:HB3	4	0.11
(2,165)	2:B:124:LEU:HD11	2:B:126:PRO:HB3	7	0.11
(2,165)	2:B:124:LEU:HD12	2:B:126:PRO:HB3	7	0.11
(2,165)	2:B:124:LEU:HD13	2:B:126:PRO:HB3	7	0.11
(2,165)	2:B:124:LEU:HD21	2:B:126:PRO:HB3	7	0.11
(2,165)	2:B:124:LEU:HD22	2:B:126:PRO:HB3	7	0.11
(2,165)	2:B:124:LEU:HD23	2:B:126:PRO:HB3	7	0.11
(2,165)	2:B:124:LEU:HD11	2:B:126:PRO:HB3	8	0.11
(2,165)	2:B:124:LEU:HD12	2:B:126:PRO:HB3	8	0.11
(2,165)	2:B:124:LEU:HD13	2:B:126:PRO:HB3	8	0.11
(2,165)	2:B:124:LEU:HD21	2:B:126:PRO:HB3	8	0.11
(2,165)	2:B:124:LEU:HD22	2:B:126:PRO:HB3	8	0.11
(2,165)	2:B:124:LEU:HD23	2:B:126:PRO:HB3	8	0.11
(2,165)	2:B:124:LEU:HD11	2:B:126:PRO:HB3	12	0.11
(2,165)	2:B:124:LEU:HD12	2:B:126:PRO:HB3	12	0.11
(2,165)	2:B:124:LEU:HD13	2:B:126:PRO:HB3	12	0.11
(2,165)	2:B:124:LEU:HD21	2:B:126:PRO:HB3	12	0.11
(2,165)	2:B:124:LEU:HD22	2:B:126:PRO:HB3	12	0.11
(2,165)	2:B:124:LEU:HD23	2:B:126:PRO:HB3	12	0.11
(2,165)	2:B:124:LEU:HD11	2:B:126:PRO:HB3	14	0.11
(2,165)	2:B:124:LEU:HD12	2:B:126:PRO:HB3	14	0.11
(2,165)	2:B:124:LEU:HD13	2:B:126:PRO:HB3	14	0.11
(2,165)	2:B:124:LEU:HD21	2:B:126:PRO:HB3	14	0.11
(2,165)	2:B:124:LEU:HD22	2:B:126:PRO:HB3	14	0.11
(2,165)	2:B:124:LEU:HD23	2:B:126:PRO:HB3	14	0.11
(2,165)	2:B:124:LEU:HD11	2:B:126:PRO:HB3	15	0.11
(2,165)	2:B:124:LEU:HD12	2:B:126:PRO:HB3	15	0.11
(2,165)	2:B:124:LEU:HD13	2:B:126:PRO:HB3	15	0.11
(2,165)	2:B:124:LEU:HD21	2:B:126:PRO:HB3	15	0.11
(2,165)	2:B:124:LEU:HD22	2:B:126:PRO:HB3	15	0.11
(2,165)	2:B:124:LEU:HD23	2:B:126:PRO:HB3	15	0.11
(2,12)	2:B:102:GLN:H	2:D:1109:PHE:HE1	10	0.11
(2,12)	2:B:102:GLN:H	2:D:1109:PHE:HE2	10	0.11
(2,109)	2:B:118:SER:H	2:D:1112:LEU:HD11	2	0.11
(2,109)	2:B:118:SER:H	2:D:1112:LEU:HD12	2	0.11
(2,109)	2:B:118:SER:H	2:D:1112:LEU:HD13	2	0.11
(2,109)	2:B:118:SER:H	2:D:1112:LEU:HD21	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	2:B:118:SER:H	2:D:1112:LEU:HD22	2	0.11
(2,109)	2:B:118:SER:H	2:D:1112:LEU:HD23	2	0.11
(2,1)	2:B:140:LEU:HD11	2:B:142:ARG:H	6	0.11
(2,1)	2:B:140:LEU:HD12	2:B:142:ARG:H	6	0.11
(2,1)	2:B:140:LEU:HD13	2:B:142:ARG:H	6	0.11
(2,1)	2:B:140:LEU:HD21	2:B:142:ARG:H	6	0.11
(2,1)	2:B:140:LEU:HD22	2:B:142:ARG:H	6	0.11
(2,1)	2:B:140:LEU:HD23	2:B:142:ARG:H	6	0.11
(1,749)	1:C:1020:LEU:HD11	2:D:1122:MET:HE1	2	0.11
(1,749)	1:C:1020:LEU:HD11	2:D:1122:MET:HE2	2	0.11
(1,749)	1:C:1020:LEU:HD11	2:D:1122:MET:HE3	2	0.11
(1,749)	1:C:1020:LEU:HD12	2:D:1122:MET:HE1	2	0.11
(1,749)	1:C:1020:LEU:HD12	2:D:1122:MET:HE2	2	0.11
(1,749)	1:C:1020:LEU:HD12	2:D:1122:MET:HE3	2	0.11
(1,749)	1:C:1020:LEU:HD13	2:D:1122:MET:HE1	2	0.11
(1,749)	1:C:1020:LEU:HD13	2:D:1122:MET:HE2	2	0.11
(1,749)	1:C:1020:LEU:HD13	2:D:1122:MET:HE3	2	0.11
(1,749)	1:C:1020:LEU:HD21	2:D:1122:MET:HE1	2	0.11
(1,749)	1:C:1020:LEU:HD21	2:D:1122:MET:HE2	2	0.11
(1,749)	1:C:1020:LEU:HD21	2:D:1122:MET:HE3	2	0.11
(1,749)	1:C:1020:LEU:HD22	2:D:1122:MET:HE1	2	0.11
(1,749)	1:C:1020:LEU:HD22	2:D:1122:MET:HE2	2	0.11
(1,749)	1:C:1020:LEU:HD22	2:D:1122:MET:HE3	2	0.11
(1,749)	1:C:1020:LEU:HD23	2:D:1122:MET:HE1	2	0.11
(1,749)	1:C:1020:LEU:HD23	2:D:1122:MET:HE2	2	0.11
(1,749)	1:C:1020:LEU:HD23	2:D:1122:MET:HE3	2	0.11
(1,749)	1:C:1020:LEU:HD11	2:D:1122:MET:HE1	18	0.11
(1,749)	1:C:1020:LEU:HD11	2:D:1122:MET:HE2	18	0.11
(1,749)	1:C:1020:LEU:HD11	2:D:1122:MET:HE3	18	0.11
(1,749)	1:C:1020:LEU:HD12	2:D:1122:MET:HE1	18	0.11
(1,749)	1:C:1020:LEU:HD12	2:D:1122:MET:HE2	18	0.11
(1,749)	1:C:1020:LEU:HD12	2:D:1122:MET:HE3	18	0.11
(1,749)	1:C:1020:LEU:HD13	2:D:1122:MET:HE1	18	0.11
(1,749)	1:C:1020:LEU:HD13	2:D:1122:MET:HE2	18	0.11
(1,749)	1:C:1020:LEU:HD13	2:D:1122:MET:HE3	18	0.11
(1,749)	1:C:1020:LEU:HD21	2:D:1122:MET:HE1	18	0.11
(1,749)	1:C:1020:LEU:HD21	2:D:1122:MET:HE2	18	0.11
(1,749)	1:C:1020:LEU:HD21	2:D:1122:MET:HE3	18	0.11
(1,749)	1:C:1020:LEU:HD22	2:D:1122:MET:HE1	18	0.11
(1,749)	1:C:1020:LEU:HD22	2:D:1122:MET:HE2	18	0.11
(1,749)	1:C:1020:LEU:HD22	2:D:1122:MET:HE3	18	0.11
(1,749)	1:C:1020:LEU:HD23	2:D:1122:MET:HE1	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	1:C:1020:LEU:HD23	2:D:1122:MET:HE2	18	0.11
(1,749)	1:C:1020:LEU:HD23	2:D:1122:MET:HE3	18	0.11
(1,748)	1:A:20:LEU:HD11	2:B:122:MET:HE1	18	0.11
(1,748)	1:A:20:LEU:HD11	2:B:122:MET:HE2	18	0.11
(1,748)	1:A:20:LEU:HD11	2:B:122:MET:HE3	18	0.11
(1,748)	1:A:20:LEU:HD12	2:B:122:MET:HE1	18	0.11
(1,748)	1:A:20:LEU:HD12	2:B:122:MET:HE2	18	0.11
(1,748)	1:A:20:LEU:HD12	2:B:122:MET:HE3	18	0.11
(1,748)	1:A:20:LEU:HD13	2:B:122:MET:HE1	18	0.11
(1,748)	1:A:20:LEU:HD13	2:B:122:MET:HE2	18	0.11
(1,748)	1:A:20:LEU:HD13	2:B:122:MET:HE3	18	0.11
(1,748)	1:A:20:LEU:HD21	2:B:122:MET:HE1	18	0.11
(1,748)	1:A:20:LEU:HD21	2:B:122:MET:HE2	18	0.11
(1,748)	1:A:20:LEU:HD21	2:B:122:MET:HE3	18	0.11
(1,748)	1:A:20:LEU:HD22	2:B:122:MET:HE1	18	0.11
(1,748)	1:A:20:LEU:HD22	2:B:122:MET:HE2	18	0.11
(1,748)	1:A:20:LEU:HD22	2:B:122:MET:HE3	18	0.11
(1,748)	1:A:20:LEU:HD23	2:B:122:MET:HE1	18	0.11
(1,748)	1:A:20:LEU:HD23	2:B:122:MET:HE2	18	0.11
(1,748)	1:A:20:LEU:HD23	2:B:122:MET:HE3	18	0.11
(1,685)	1:C:1031:TYR:HD1	2:D:1129:LEU:HD11	7	0.11
(1,685)	1:C:1031:TYR:HD1	2:D:1129:LEU:HD12	7	0.11
(1,685)	1:C:1031:TYR:HD1	2:D:1129:LEU:HD13	7	0.11
(1,685)	1:C:1031:TYR:HD2	2:D:1129:LEU:HD11	7	0.11
(1,685)	1:C:1031:TYR:HD2	2:D:1129:LEU:HD12	7	0.11
(1,685)	1:C:1031:TYR:HD2	2:D:1129:LEU:HD13	7	0.11
(1,684)	1:A:31:TYR:HD1	2:B:129:LEU:HD11	15	0.11
(1,684)	1:A:31:TYR:HD1	2:B:129:LEU:HD12	15	0.11
(1,684)	1:A:31:TYR:HD1	2:B:129:LEU:HD13	15	0.11
(1,684)	1:A:31:TYR:HD2	2:B:129:LEU:HD11	15	0.11
(1,684)	1:A:31:TYR:HD2	2:B:129:LEU:HD12	15	0.11
(1,684)	1:A:31:TYR:HD2	2:B:129:LEU:HD13	15	0.11
(1,679)	2:B:114:LYS:H	1:C:1018:MET:HE1	2	0.11
(1,679)	2:B:114:LYS:H	1:C:1018:MET:HE2	2	0.11
(1,679)	2:B:114:LYS:H	1:C:1018:MET:HE3	2	0.11
(1,663)	1:C:1031:TYR:HD1	2:D:1133:TYR:HE1	15	0.11
(1,663)	1:C:1031:TYR:HD1	2:D:1133:TYR:HE2	15	0.11
(1,663)	1:C:1031:TYR:HD2	2:D:1133:TYR:HE1	15	0.11
(1,663)	1:C:1031:TYR:HD2	2:D:1133:TYR:HE2	15	0.11
(1,620)	1:A:40:TYR:HE1	2:B:117:GLU:HG2	7	0.11
(1,620)	1:A:40:TYR:HE1	2:B:117:GLU:HG3	7	0.11
(1,620)	1:A:40:TYR:HE2	2:B:117:GLU:HG2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,620)	1:A:40:TYR:HE2	2:B:117:GLU:HG3	7	0.11
(1,594)	1:A:20:LEU:HD11	1:A:23:LYS:HE2	1	0.11
(1,594)	1:A:20:LEU:HD11	1:A:23:LYS:HE3	1	0.11
(1,594)	1:A:20:LEU:HD12	1:A:23:LYS:HE2	1	0.11
(1,594)	1:A:20:LEU:HD12	1:A:23:LYS:HE3	1	0.11
(1,594)	1:A:20:LEU:HD13	1:A:23:LYS:HE2	1	0.11
(1,594)	1:A:20:LEU:HD13	1:A:23:LYS:HE3	1	0.11
(1,594)	1:A:20:LEU:HD21	1:A:23:LYS:HE2	1	0.11
(1,594)	1:A:20:LEU:HD21	1:A:23:LYS:HE3	1	0.11
(1,594)	1:A:20:LEU:HD22	1:A:23:LYS:HE2	1	0.11
(1,594)	1:A:20:LEU:HD22	1:A:23:LYS:HE3	1	0.11
(1,594)	1:A:20:LEU:HD23	1:A:23:LYS:HE2	1	0.11
(1,594)	1:A:20:LEU:HD23	1:A:23:LYS:HE3	1	0.11
(1,178)	2:D:1098:THR:HG21	2:D:1100:TYR:H	19	0.11
(1,178)	2:D:1098:THR:HG22	2:D:1100:TYR:H	19	0.11
(1,178)	2:D:1098:THR:HG23	2:D:1100:TYR:H	19	0.11
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD11	17	0.11
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD12	17	0.11
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD13	17	0.11
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD21	17	0.11
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD22	17	0.11
(1,1688)	2:D:1135:GLN:HG2	2:D:1139:LEU:HD23	17	0.11
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD11	17	0.11
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD12	17	0.11
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD13	17	0.11
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD21	17	0.11
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD22	17	0.11
(1,1688)	2:D:1135:GLN:HG3	2:D:1139:LEU:HD23	17	0.11
(1,1684)	2:D:1103:VAL:HG11	2:D:1112:LEU:HB2	6	0.11
(1,1684)	2:D:1103:VAL:HG11	2:D:1112:LEU:HB3	6	0.11
(1,1684)	2:D:1103:VAL:HG12	2:D:1112:LEU:HB2	6	0.11
(1,1684)	2:D:1103:VAL:HG12	2:D:1112:LEU:HB3	6	0.11
(1,1684)	2:D:1103:VAL:HG13	2:D:1112:LEU:HB2	6	0.11
(1,1684)	2:D:1103:VAL:HG13	2:D:1112:LEU:HB3	6	0.11
(1,1684)	2:D:1103:VAL:HG21	2:D:1112:LEU:HB2	6	0.11
(1,1684)	2:D:1103:VAL:HG21	2:D:1112:LEU:HB3	6	0.11
(1,1684)	2:D:1103:VAL:HG22	2:D:1112:LEU:HB2	6	0.11
(1,1684)	2:D:1103:VAL:HG22	2:D:1112:LEU:HB3	6	0.11
(1,1684)	2:D:1103:VAL:HG23	2:D:1112:LEU:HB2	6	0.11
(1,1684)	2:D:1103:VAL:HG23	2:D:1112:LEU:HB3	6	0.11
(1,1683)	2:B:103:VAL:HG11	2:B:112:LEU:HB2	7	0.11
(1,1683)	2:B:103:VAL:HG11	2:B:112:LEU:HB3	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1683)	2:B:103:VAL:HG12	2:B:112:LEU:HB2	7	0.11
(1,1683)	2:B:103:VAL:HG12	2:B:112:LEU:HB3	7	0.11
(1,1683)	2:B:103:VAL:HG13	2:B:112:LEU:HB2	7	0.11
(1,1683)	2:B:103:VAL:HG13	2:B:112:LEU:HB3	7	0.11
(1,1683)	2:B:103:VAL:HG21	2:B:112:LEU:HB2	7	0.11
(1,1683)	2:B:103:VAL:HG21	2:B:112:LEU:HB3	7	0.11
(1,1683)	2:B:103:VAL:HG22	2:B:112:LEU:HB2	7	0.11
(1,1683)	2:B:103:VAL:HG22	2:B:112:LEU:HB3	7	0.11
(1,1683)	2:B:103:VAL:HG23	2:B:112:LEU:HB2	7	0.11
(1,1683)	2:B:103:VAL:HG23	2:B:112:LEU:HB3	7	0.11
(1,1644)	2:D:1134:ARG:HD2	2:D:1135:GLN:HB2	1	0.11
(1,1644)	2:D:1134:ARG:HD2	2:D:1135:GLN:HB3	1	0.11
(1,1644)	2:D:1134:ARG:HD3	2:D:1135:GLN:HB2	1	0.11
(1,1644)	2:D:1134:ARG:HD3	2:D:1135:GLN:HB3	1	0.11
(1,1643)	2:B:134:ARG:HD2	2:B:135:GLN:HB2	1	0.11
(1,1643)	2:B:134:ARG:HD2	2:B:135:GLN:HB3	1	0.11
(1,1643)	2:B:134:ARG:HD3	2:B:135:GLN:HB2	1	0.11
(1,1643)	2:B:134:ARG:HD3	2:B:135:GLN:HB3	1	0.11
(1,1625)	2:B:128:PRO:HD2	2:B:130:VAL:HG11	7	0.11
(1,1625)	2:B:128:PRO:HD2	2:B:130:VAL:HG12	7	0.11
(1,1625)	2:B:128:PRO:HD2	2:B:130:VAL:HG13	7	0.11
(1,1625)	2:B:128:PRO:HD2	2:B:130:VAL:HG21	7	0.11
(1,1625)	2:B:128:PRO:HD2	2:B:130:VAL:HG22	7	0.11
(1,1625)	2:B:128:PRO:HD2	2:B:130:VAL:HG23	7	0.11
(1,1625)	2:B:128:PRO:HD3	2:B:130:VAL:HG11	7	0.11
(1,1625)	2:B:128:PRO:HD3	2:B:130:VAL:HG12	7	0.11
(1,1625)	2:B:128:PRO:HD3	2:B:130:VAL:HG13	7	0.11
(1,1625)	2:B:128:PRO:HD3	2:B:130:VAL:HG21	7	0.11
(1,1625)	2:B:128:PRO:HD3	2:B:130:VAL:HG22	7	0.11
(1,1625)	2:B:128:PRO:HD3	2:B:130:VAL:HG23	7	0.11
(1,1574)	2:D:1103:VAL:HG11	2:D:1109:PHE:H	8	0.11
(1,1574)	2:D:1103:VAL:HG12	2:D:1109:PHE:H	8	0.11
(1,1574)	2:D:1103:VAL:HG13	2:D:1109:PHE:H	8	0.11
(1,1574)	2:D:1103:VAL:HG21	2:D:1109:PHE:H	8	0.11
(1,1574)	2:D:1103:VAL:HG22	2:D:1109:PHE:H	8	0.11
(1,1574)	2:D:1103:VAL:HG23	2:D:1109:PHE:H	8	0.11
(1,1574)	2:D:1103:VAL:HG11	2:D:1109:PHE:H	17	0.11
(1,1574)	2:D:1103:VAL:HG12	2:D:1109:PHE:H	17	0.11
(1,1574)	2:D:1103:VAL:HG13	2:D:1109:PHE:H	17	0.11
(1,1574)	2:D:1103:VAL:HG21	2:D:1109:PHE:H	17	0.11
(1,1574)	2:D:1103:VAL:HG22	2:D:1109:PHE:H	17	0.11
(1,1574)	2:D:1103:VAL:HG23	2:D:1109:PHE:H	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1548)	1:C:1040:TYR:HA	2:D:1121:LEU:HD11	9	0.11
(1,1548)	1:C:1040:TYR:HA	2:D:1121:LEU:HD12	9	0.11
(1,1548)	1:C:1040:TYR:HA	2:D:1121:LEU:HD13	9	0.11
(1,1548)	1:C:1040:TYR:HA	2:D:1121:LEU:HD21	9	0.11
(1,1548)	1:C:1040:TYR:HA	2:D:1121:LEU:HD22	9	0.11
(1,1548)	1:C:1040:TYR:HA	2:D:1121:LEU:HD23	9	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD11	1	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD12	1	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD13	1	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD21	1	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD22	1	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD23	1	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD11	9	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD12	9	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD13	9	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD21	9	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD22	9	0.11
(1,1547)	1:A:40:TYR:HA	2:B:121:LEU:HD23	9	0.11
(1,1515)	1:A:26:LEU:HD11	2:B:118:SER:HA	8	0.11
(1,1515)	1:A:26:LEU:HD12	2:B:118:SER:HA	8	0.11
(1,1515)	1:A:26:LEU:HD13	2:B:118:SER:HA	8	0.11
(1,1515)	1:A:26:LEU:HD21	2:B:118:SER:HA	8	0.11
(1,1515)	1:A:26:LEU:HD22	2:B:118:SER:HA	8	0.11
(1,1515)	1:A:26:LEU:HD23	2:B:118:SER:HA	8	0.11
(1,1506)	1:C:1026:LEU:HD11	2:D:1115:LEU:HA	5	0.11
(1,1506)	1:C:1026:LEU:HD12	2:D:1115:LEU:HA	5	0.11
(1,1506)	1:C:1026:LEU:HD13	2:D:1115:LEU:HA	5	0.11
(1,1506)	1:C:1026:LEU:HD21	2:D:1115:LEU:HA	5	0.11
(1,1506)	1:C:1026:LEU:HD22	2:D:1115:LEU:HA	5	0.11
(1,1506)	1:C:1026:LEU:HD23	2:D:1115:LEU:HA	5	0.11
(1,1506)	1:C:1026:LEU:HD11	2:D:1115:LEU:HA	9	0.11
(1,1506)	1:C:1026:LEU:HD12	2:D:1115:LEU:HA	9	0.11
(1,1506)	1:C:1026:LEU:HD13	2:D:1115:LEU:HA	9	0.11
(1,1506)	1:C:1026:LEU:HD21	2:D:1115:LEU:HA	9	0.11
(1,1506)	1:C:1026:LEU:HD22	2:D:1115:LEU:HA	9	0.11
(1,1506)	1:C:1026:LEU:HD23	2:D:1115:LEU:HA	9	0.11
(1,1505)	1:A:26:LEU:HD11	2:B:115:LEU:HA	16	0.11
(1,1505)	1:A:26:LEU:HD12	2:B:115:LEU:HA	16	0.11
(1,1505)	1:A:26:LEU:HD13	2:B:115:LEU:HA	16	0.11
(1,1505)	1:A:26:LEU:HD21	2:B:115:LEU:HA	16	0.11
(1,1505)	1:A:26:LEU:HD22	2:B:115:LEU:HA	16	0.11
(1,1505)	1:A:26:LEU:HD23	2:B:115:LEU:HA	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1496)	1:C:1026:LEU:HD11	1:C:1029:MET:HE1	8	0.11
(1,1496)	1:C:1026:LEU:HD11	1:C:1029:MET:HE2	8	0.11
(1,1496)	1:C:1026:LEU:HD11	1:C:1029:MET:HE3	8	0.11
(1,1496)	1:C:1026:LEU:HD12	1:C:1029:MET:HE1	8	0.11
(1,1496)	1:C:1026:LEU:HD12	1:C:1029:MET:HE2	8	0.11
(1,1496)	1:C:1026:LEU:HD12	1:C:1029:MET:HE3	8	0.11
(1,1496)	1:C:1026:LEU:HD13	1:C:1029:MET:HE1	8	0.11
(1,1496)	1:C:1026:LEU:HD13	1:C:1029:MET:HE2	8	0.11
(1,1496)	1:C:1026:LEU:HD13	1:C:1029:MET:HE3	8	0.11
(1,1496)	1:C:1026:LEU:HD21	1:C:1029:MET:HE1	8	0.11
(1,1496)	1:C:1026:LEU:HD21	1:C:1029:MET:HE2	8	0.11
(1,1496)	1:C:1026:LEU:HD21	1:C:1029:MET:HE3	8	0.11
(1,1496)	1:C:1026:LEU:HD22	1:C:1029:MET:HE1	8	0.11
(1,1496)	1:C:1026:LEU:HD22	1:C:1029:MET:HE2	8	0.11
(1,1496)	1:C:1026:LEU:HD22	1:C:1029:MET:HE3	8	0.11
(1,1496)	1:C:1026:LEU:HD23	1:C:1029:MET:HE1	8	0.11
(1,1496)	1:C:1026:LEU:HD23	1:C:1029:MET:HE2	8	0.11
(1,1496)	1:C:1026:LEU:HD23	1:C:1029:MET:HE3	8	0.11
(1,1447)	1:A:13:ARG:HD2	1:A:17:GLU:HG2	6	0.11
(1,1447)	1:A:13:ARG:HD2	1:A:17:GLU:HG3	6	0.11
(1,1447)	1:A:13:ARG:HD3	1:A:17:GLU:HG2	6	0.11
(1,1447)	1:A:13:ARG:HD3	1:A:17:GLU:HG3	6	0.11
(1,1442)	1:A:19:LEU:HB2	1:C:1008:LEU:HD11	4	0.11
(1,1442)	1:A:19:LEU:HB2	1:C:1008:LEU:HD12	4	0.11
(1,1442)	1:A:19:LEU:HB2	1:C:1008:LEU:HD13	4	0.11
(1,1442)	1:A:19:LEU:HB2	1:C:1008:LEU:HD21	4	0.11
(1,1442)	1:A:19:LEU:HB2	1:C:1008:LEU:HD22	4	0.11
(1,1442)	1:A:19:LEU:HB2	1:C:1008:LEU:HD23	4	0.11
(1,1442)	1:A:19:LEU:HB3	1:C:1008:LEU:HD11	4	0.11
(1,1442)	1:A:19:LEU:HB3	1:C:1008:LEU:HD12	4	0.11
(1,1442)	1:A:19:LEU:HB3	1:C:1008:LEU:HD13	4	0.11
(1,1442)	1:A:19:LEU:HB3	1:C:1008:LEU:HD21	4	0.11
(1,1442)	1:A:19:LEU:HB3	1:C:1008:LEU:HD22	4	0.11
(1,1442)	1:A:19:LEU:HB3	1:C:1008:LEU:HD23	4	0.11
(1,1424)	1:A:13:ARG:HA	1:C:1006:LEU:HD11	10	0.11
(1,1424)	1:A:13:ARG:HA	1:C:1006:LEU:HD12	10	0.11
(1,1424)	1:A:13:ARG:HA	1:C:1006:LEU:HD13	10	0.11
(1,1424)	1:A:13:ARG:HA	1:C:1006:LEU:HD21	10	0.11
(1,1424)	1:A:13:ARG:HA	1:C:1006:LEU:HD22	10	0.11
(1,1424)	1:A:13:ARG:HA	1:C:1006:LEU:HD23	10	0.11
(1,1423)	1:A:6:LEU:HD11	1:C:1013:ARG:HA	12	0.11
(1,1423)	1:A:6:LEU:HD12	1:C:1013:ARG:HA	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1423)	1:A:6:LEU:HD13	1:C:1013:ARG:HA	12	0.11
(1,1423)	1:A:6:LEU:HD21	1:C:1013:ARG:HA	12	0.11
(1,1423)	1:A:6:LEU:HD22	1:C:1013:ARG:HA	12	0.11
(1,1423)	1:A:6:LEU:HD23	1:C:1013:ARG:HA	12	0.11
(1,1406)	1:C:1036:THR:HG21	2:D:1124:LEU:HD11	13	0.11
(1,1406)	1:C:1036:THR:HG21	2:D:1124:LEU:HD12	13	0.11
(1,1406)	1:C:1036:THR:HG21	2:D:1124:LEU:HD13	13	0.11
(1,1406)	1:C:1036:THR:HG21	2:D:1124:LEU:HD21	13	0.11
(1,1406)	1:C:1036:THR:HG21	2:D:1124:LEU:HD22	13	0.11
(1,1406)	1:C:1036:THR:HG21	2:D:1124:LEU:HD23	13	0.11
(1,1406)	1:C:1036:THR:HG22	2:D:1124:LEU:HD11	13	0.11
(1,1406)	1:C:1036:THR:HG22	2:D:1124:LEU:HD12	13	0.11
(1,1406)	1:C:1036:THR:HG22	2:D:1124:LEU:HD13	13	0.11
(1,1406)	1:C:1036:THR:HG22	2:D:1124:LEU:HD21	13	0.11
(1,1406)	1:C:1036:THR:HG22	2:D:1124:LEU:HD22	13	0.11
(1,1406)	1:C:1036:THR:HG22	2:D:1124:LEU:HD23	13	0.11
(1,1406)	1:C:1036:THR:HG23	2:D:1124:LEU:HD11	13	0.11
(1,1406)	1:C:1036:THR:HG23	2:D:1124:LEU:HD12	13	0.11
(1,1406)	1:C:1036:THR:HG23	2:D:1124:LEU:HD13	13	0.11
(1,1406)	1:C:1036:THR:HG23	2:D:1124:LEU:HD21	13	0.11
(1,1406)	1:C:1036:THR:HG23	2:D:1124:LEU:HD22	13	0.11
(1,1406)	1:C:1036:THR:HG23	2:D:1124:LEU:HD23	13	0.11
(1,1402)	1:A:15:THR:HG21	2:D:1115:LEU:HD11	17	0.11
(1,1402)	1:A:15:THR:HG21	2:D:1115:LEU:HD12	17	0.11
(1,1402)	1:A:15:THR:HG21	2:D:1115:LEU:HD13	17	0.11
(1,1402)	1:A:15:THR:HG21	2:D:1115:LEU:HD21	17	0.11
(1,1402)	1:A:15:THR:HG21	2:D:1115:LEU:HD22	17	0.11
(1,1402)	1:A:15:THR:HG21	2:D:1115:LEU:HD23	17	0.11
(1,1402)	1:A:15:THR:HG22	2:D:1115:LEU:HD11	17	0.11
(1,1402)	1:A:15:THR:HG22	2:D:1115:LEU:HD12	17	0.11
(1,1402)	1:A:15:THR:HG22	2:D:1115:LEU:HD13	17	0.11
(1,1402)	1:A:15:THR:HG22	2:D:1115:LEU:HD21	17	0.11
(1,1402)	1:A:15:THR:HG22	2:D:1115:LEU:HD22	17	0.11
(1,1402)	1:A:15:THR:HG22	2:D:1115:LEU:HD23	17	0.11
(1,1402)	1:A:15:THR:HG23	2:D:1115:LEU:HD11	17	0.11
(1,1402)	1:A:15:THR:HG23	2:D:1115:LEU:HD12	17	0.11
(1,1402)	1:A:15:THR:HG23	2:D:1115:LEU:HD13	17	0.11
(1,1402)	1:A:15:THR:HG23	2:D:1115:LEU:HD21	17	0.11
(1,1402)	1:A:15:THR:HG23	2:D:1115:LEU:HD22	17	0.11
(1,1402)	1:A:15:THR:HG23	2:D:1115:LEU:HD23	17	0.11
(1,1389)	2:B:114:LYS:HD2	1:C:1018:MET:HE1	7	0.11
(1,1389)	2:B:114:LYS:HD2	1:C:1018:MET:HE2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1389)	2:B:114:LYS:HD2	1:C:1018:MET:HE3	7	0.11
(1,1389)	2:B:114:LYS:HD3	1:C:1018:MET:HE1	7	0.11
(1,1389)	2:B:114:LYS:HD3	1:C:1018:MET:HE2	7	0.11
(1,1389)	2:B:114:LYS:HD3	1:C:1018:MET:HE3	7	0.11
(1,1386)	1:A:18:MET:HE1	2:D:1114:LYS:HE2	13	0.11
(1,1386)	1:A:18:MET:HE1	2:D:1114:LYS:HE3	13	0.11
(1,1386)	1:A:18:MET:HE2	2:D:1114:LYS:HE2	13	0.11
(1,1386)	1:A:18:MET:HE2	2:D:1114:LYS:HE3	13	0.11
(1,1386)	1:A:18:MET:HE3	2:D:1114:LYS:HE2	13	0.11
(1,1386)	1:A:18:MET:HE3	2:D:1114:LYS:HE3	13	0.11
(1,1380)	1:A:18:MET:HE1	2:D:1112:LEU:HA	1	0.11
(1,1380)	1:A:18:MET:HE2	2:D:1112:LEU:HA	1	0.11
(1,1380)	1:A:18:MET:HE3	2:D:1112:LEU:HA	1	0.11
(1,1362)	1:C:1028:LEU:HD11	2:D:1133:TYR:HD1	7	0.11
(1,1362)	1:C:1028:LEU:HD11	2:D:1133:TYR:HD2	7	0.11
(1,1362)	1:C:1028:LEU:HD12	2:D:1133:TYR:HD1	7	0.11
(1,1362)	1:C:1028:LEU:HD12	2:D:1133:TYR:HD2	7	0.11
(1,1362)	1:C:1028:LEU:HD13	2:D:1133:TYR:HD1	7	0.11
(1,1362)	1:C:1028:LEU:HD13	2:D:1133:TYR:HD2	7	0.11
(1,1339)	1:A:48:HIS:HD2	1:A:51:LEU:HD11	4	0.11
(1,1339)	1:A:48:HIS:HD2	1:A:51:LEU:HD12	4	0.11
(1,1339)	1:A:48:HIS:HD2	1:A:51:LEU:HD13	4	0.11
(1,1339)	1:A:48:HIS:HD2	1:A:51:LEU:HD21	4	0.11
(1,1339)	1:A:48:HIS:HD2	1:A:51:LEU:HD22	4	0.11
(1,1339)	1:A:48:HIS:HD2	1:A:51:LEU:HD23	4	0.11
(1,1303)	1:A:10:VAL:HB	1:A:16:TYR:HD1	17	0.11
(1,1303)	1:A:10:VAL:HB	1:A:16:TYR:HD2	17	0.11
(1,1282)	1:C:1010:VAL:HG11	1:C:1015:THR:HG21	14	0.11
(1,1282)	1:C:1010:VAL:HG11	1:C:1015:THR:HG22	14	0.11
(1,1282)	1:C:1010:VAL:HG11	1:C:1015:THR:HG23	14	0.11
(1,1282)	1:C:1010:VAL:HG12	1:C:1015:THR:HG21	14	0.11
(1,1282)	1:C:1010:VAL:HG12	1:C:1015:THR:HG22	14	0.11
(1,1282)	1:C:1010:VAL:HG12	1:C:1015:THR:HG23	14	0.11
(1,1282)	1:C:1010:VAL:HG13	1:C:1015:THR:HG21	14	0.11
(1,1282)	1:C:1010:VAL:HG13	1:C:1015:THR:HG22	14	0.11
(1,1282)	1:C:1010:VAL:HG13	1:C:1015:THR:HG23	14	0.11
(1,1282)	1:C:1010:VAL:HG21	1:C:1015:THR:HG21	14	0.11
(1,1282)	1:C:1010:VAL:HG21	1:C:1015:THR:HG22	14	0.11
(1,1282)	1:C:1010:VAL:HG21	1:C:1015:THR:HG23	14	0.11
(1,1282)	1:C:1010:VAL:HG22	1:C:1015:THR:HG21	14	0.11
(1,1282)	1:C:1010:VAL:HG22	1:C:1015:THR:HG22	14	0.11
(1,1282)	1:C:1010:VAL:HG22	1:C:1015:THR:HG23	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1282)	1:C:1010:VAL:HG23	1:C:1015:THR:HG21	14	0.11
(1,1282)	1:C:1010:VAL:HG23	1:C:1015:THR:HG22	14	0.11
(1,1282)	1:C:1010:VAL:HG23	1:C:1015:THR:HG23	14	0.11
(1,1277)	1:A:10:VAL:HG11	1:A:16:TYR:HB3	18	0.11
(1,1277)	1:A:10:VAL:HG12	1:A:16:TYR:HB3	18	0.11
(1,1277)	1:A:10:VAL:HG13	1:A:16:TYR:HB3	18	0.11
(1,1277)	1:A:10:VAL:HG21	1:A:16:TYR:HB3	18	0.11
(1,1277)	1:A:10:VAL:HG22	1:A:16:TYR:HB3	18	0.11
(1,1277)	1:A:10:VAL:HG23	1:A:16:TYR:HB3	18	0.11
(1,1242)	1:C:1010:VAL:HG11	1:C:1016:TYR:H	4	0.11
(1,1242)	1:C:1010:VAL:HG12	1:C:1016:TYR:H	4	0.11
(1,1242)	1:C:1010:VAL:HG13	1:C:1016:TYR:H	4	0.11
(1,1242)	1:C:1010:VAL:HG21	1:C:1016:TYR:H	4	0.11
(1,1242)	1:C:1010:VAL:HG22	1:C:1016:TYR:H	4	0.11
(1,1242)	1:C:1010:VAL:HG23	1:C:1016:TYR:H	4	0.11
(1,1156)	1:A:8:LEU:HD11	1:C:1023:LYS:HE2	3	0.11
(1,1156)	1:A:8:LEU:HD11	1:C:1023:LYS:HE3	3	0.11
(1,1156)	1:A:8:LEU:HD12	1:C:1023:LYS:HE2	3	0.11
(1,1156)	1:A:8:LEU:HD12	1:C:1023:LYS:HE3	3	0.11
(1,1156)	1:A:8:LEU:HD13	1:C:1023:LYS:HE2	3	0.11
(1,1156)	1:A:8:LEU:HD13	1:C:1023:LYS:HE3	3	0.11
(1,1155)	1:A:23:LYS:HE2	1:C:1008:LEU:HD11	1	0.11
(1,1155)	1:A:23:LYS:HE2	1:C:1008:LEU:HD12	1	0.11
(1,1155)	1:A:23:LYS:HE2	1:C:1008:LEU:HD13	1	0.11
(1,1155)	1:A:23:LYS:HE3	1:C:1008:LEU:HD11	1	0.11
(1,1155)	1:A:23:LYS:HE3	1:C:1008:LEU:HD12	1	0.11
(1,1155)	1:A:23:LYS:HE3	1:C:1008:LEU:HD13	1	0.11
(1,1125)	2:D:1137:GLN:HG2	2:D:1138:GLN:HA	17	0.11
(1,1125)	2:D:1137:GLN:HG3	2:D:1138:GLN:HA	17	0.11
(1,1083)	1:A:3:ASP:HB2	1:C:1011:ARG:HD2	15	0.11
(1,1083)	1:A:3:ASP:HB2	1:C:1011:ARG:HD3	15	0.11
(1,1083)	1:A:3:ASP:HB3	1:C:1011:ARG:HD2	15	0.11
(1,1083)	1:A:3:ASP:HB3	1:C:1011:ARG:HD3	15	0.11
(1,1075)	1:A:13:ARG:HD2	1:C:1006:LEU:HD21	2	0.11
(1,1075)	1:A:13:ARG:HD2	1:C:1006:LEU:HD22	2	0.11
(1,1075)	1:A:13:ARG:HD2	1:C:1006:LEU:HD23	2	0.11
(1,1075)	1:A:13:ARG:HD3	1:C:1006:LEU:HD21	2	0.11
(1,1075)	1:A:13:ARG:HD3	1:C:1006:LEU:HD22	2	0.11
(1,1075)	1:A:13:ARG:HD3	1:C:1006:LEU:HD23	2	0.11
(1,1075)	1:A:13:ARG:HD2	1:C:1006:LEU:HD21	17	0.11
(1,1075)	1:A:13:ARG:HD2	1:C:1006:LEU:HD22	17	0.11
(1,1075)	1:A:13:ARG:HD2	1:C:1006:LEU:HD23	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:A:13:ARG:HD3	1:C:1006:LEU:HD21	17	0.11
(1,1075)	1:A:13:ARG:HD3	1:C:1006:LEU:HD22	17	0.11
(1,1075)	1:A:13:ARG:HD3	1:C:1006:LEU:HD23	17	0.11
(1,1074)	1:A:6:LEU:HD21	1:C:1013:ARG:HD2	18	0.11
(1,1074)	1:A:6:LEU:HD21	1:C:1013:ARG:HD3	18	0.11
(1,1074)	1:A:6:LEU:HD22	1:C:1013:ARG:HD2	18	0.11
(1,1074)	1:A:6:LEU:HD22	1:C:1013:ARG:HD3	18	0.11
(1,1074)	1:A:6:LEU:HD23	1:C:1013:ARG:HD2	18	0.11
(1,1074)	1:A:6:LEU:HD23	1:C:1013:ARG:HD3	18	0.11

10 Dihedral-angle violation analysis

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value