Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2N97
BMRB ID	:	25883
Title	:	DD homodimer
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Deposited on	:	2015-11-07

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:

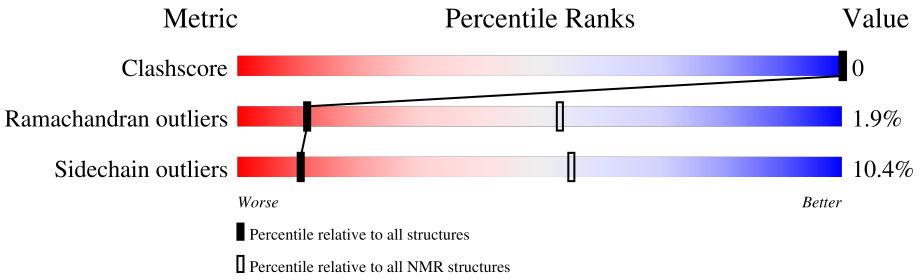
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 39%.

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	98	81% 5% 10% .
1	B	98	83% 5% 8% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:335-A:418, B:334-B:419 (170)	0.50	2

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 and 1 single-model cluster was found.

Cluster number	Models
1	2, 6, 8, 9
2	1, 3, 5
3	4, 10
Single-model clusters	7

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2826 atoms, of which 1398 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tumor necrosis factor receptor superfamily member 16.

Mol	Chain	Residues	Atoms						Trace
1	A	94	Total	C	H	N	O	S	0
			1413	444	699	126	142	2	
1	B	94	Total	C	H	N	O	S	0
			1413	444	699	126	142	2	

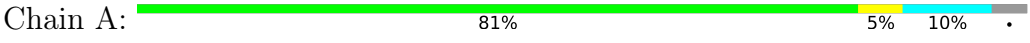
4 Residue-property plots

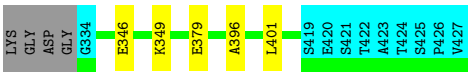
4.1 Average score per residue in the NMR ensemble

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 necrosis factor receptor superfamily member 16

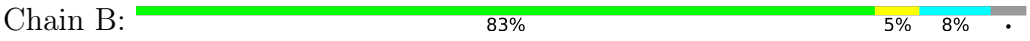
Chain A:





• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain B:



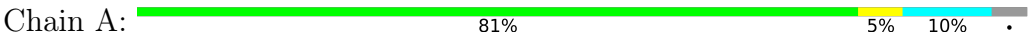
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

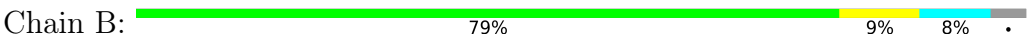
• Molecule 1: Tumor necrosis factor receptor superfamily member 16

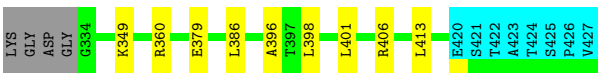
Chain A:



• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain B:





4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain A:

• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain B:

4.2.3 Score per residue for model 3

• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain A:

• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain B:

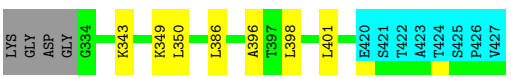
4.2.4 Score per residue for model 4

• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain A:

• Molecule 1: Tumor necrosis factor receptor superfamily member 16

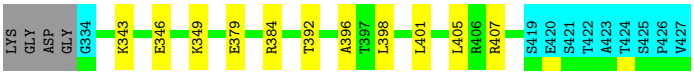
Chain B:



4.2.5 Score per residue for model 5

• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain A:



• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain B:

4.2.6 Score per residue for model 6

• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain A:

• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain B:

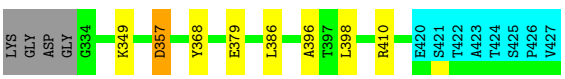
4.2.7 Score per residue for model 7

• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain A:

• Molecule 1: Tumor necrosis factor receptor superfamily member 16

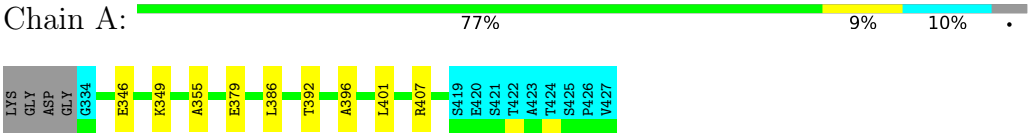
Chain B:



4.2.8 Score per residue for model 8

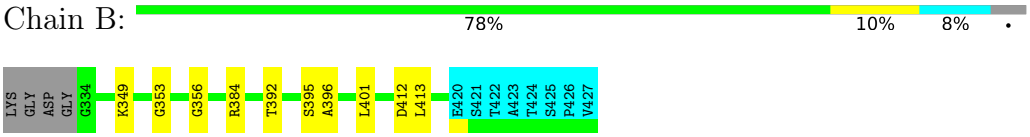
• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain A:



• Molecule 1: Tumor necrosis factor receptor superfamily member 16

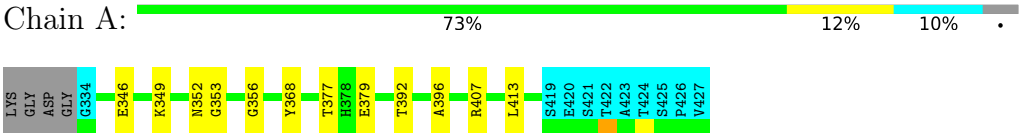
Chain B:



4.2.9 Score per residue for model 9

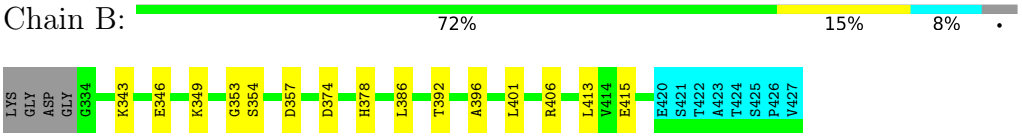
• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain A:



• Molecule 1: Tumor necrosis factor receptor superfamily member 16

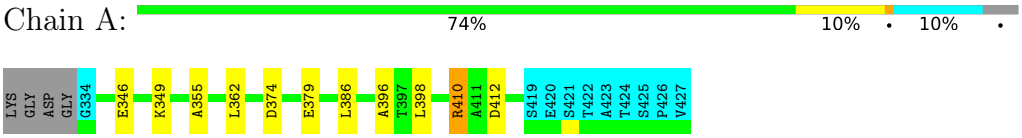
Chain B:



4.2.10 Score per residue for model 10

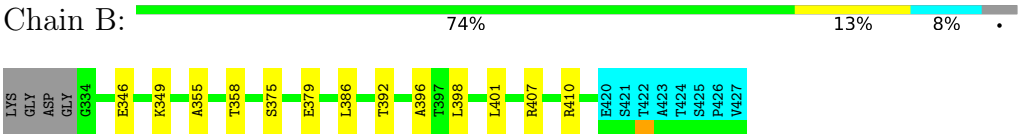
• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain A:



• Molecule 1: Tumor necrosis factor receptor superfamily member 16

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
Amber	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	999
Number of shifts mapped to atoms	969
Number of unparsed shifts	0
Number of shifts with mapping errors	30
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	39%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.70±0.00	0±0/664 (0.0± 0.0%)	0.93±0.01	0±0/905 (0.0± 0.1%)
1	B	0.69±0.01	0±0/674 (0.0± 0.0%)	0.94±0.02	1±1/918 (0.1± 0.1%)
All	All	0.70	0/13380 (0.0%)	0.93	12/18230 (0.1%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	384	ARG	NE-CZ-NH1	7.45	124.03	120.30	3	2
1	B	410	ARG	NE-CZ-NH1	6.45	123.53	120.30	7	3
1	B	407	ARG	NE-CZ-NH1	6.29	123.45	120.30	3	2
1	A	410	ARG	NE-CZ-NH1	5.62	123.11	120.30	6	3
1	B	384	ARG	NE-CZ-NH2	-5.61	117.50	120.30	2	1
1	B	344	ARG	NE-CZ-NH1	5.27	122.94	120.30	6	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	650	640	640	0±0
1	B	660	648	647	0±0
All	All	13100	12880	12870	1

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
1:A:377:THR:HG23	1:B:357:ASP:HB3	0.45	1.88	9	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	84/98 (86%)	81±1 (96±1%)	2±1 (2±1%)	2±1 (2±1%)	12	54
1	B	85/98 (87%)	80±1 (95±2%)	3±1 (3±1%)	2±1 (2±1%)	11	52
All	All	1690/1960 (86%)	1610 (95%)	48 (3%)	32 (2%)	11	53

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	396	ALA	10
1	B	396	ALA	10
1	A	355	ALA	3
1	B	353	GLY	3
1	B	354	SER	1
1	B	357	ASP	1
1	B	356	GLY	1
1	A	353	GLY	1
1	A	356	GLY	1
1	B	355	ALA	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	68/78 (87%)	61±2 (90±3%)	7±2 (10±3%)	12 57
1	B	69/78 (88%)	61±2 (89±3%)	8±2 (11±3%)	9 53
All	All	1370/1560 (88%)	1227 (90%)	143 (10%)	10 55

All 50 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	349	LYS	10
1	B	349	LYS	10
1	B	398	LEU	8
1	B	401	LEU	8
1	A	379	GLU	7
1	A	401	LEU	7
1	B	386	LEU	7
1	A	346	GLU	7
1	A	386	LEU	5
1	B	379	GLU	5
1	B	392	THR	5
1	A	392	THR	4
1	B	346	GLU	4
1	B	413	LEU	3
1	B	352	ASN	3
1	B	343	LYS	3
1	A	407	ARG	3
1	B	406	ARG	2
1	A	352	ASN	2
1	B	368	TYR	2
1	B	350	LEU	2
1	B	384	ARG	2
1	A	362	LEU	2
1	A	410	ARG	2
1	A	384	ARG	2
1	A	398	LEU	2
1	A	413	LEU	2
1	A	374	ASP	2
1	B	360	ARG	1
1	A	338	SER	1
1	B	372	HIS	1
1	A	336	TYR	1
1	A	350	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	343	LYS	1
1	A	405	LEU	1
1	B	405	LEU	1
1	A	406	ARG	1
1	B	399	ASP	1
1	A	360	ARG	1
1	B	357	ASP	1
1	B	395	SER	1
1	B	412	ASP	1
1	A	368	TYR	1
1	B	354	SER	1
1	B	374	ASP	1
1	B	378	HIS	1
1	B	415	GLU	1
1	A	412	ASP	1
1	B	358	THR	1
1	B	375	SER	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

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 39% for the well-defined parts and 40% 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	999
Number of shifts mapped to atoms	969
Number of unparsed shifts	0
Number of shifts with mapping errors	30
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

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

- No matching atom found in the structure. All 30 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	330	LYS	N	122.71	.	1
1	A	330	LYS	H	8.436	.	1
1	A	330	LYS	CA	56.198	.	1
1	A	330	LYS	HA	4.385	.	1
1	A	330	LYS	CB	32.532	.	1
1	A	330	LYS	HB2	1.907	.	2
1	A	330	LYS	HB3	1.816	.	2
1	A	330	LYS	CG	24.308	.	1
1	A	330	LYS	HG2	1.453	.	2
1	A	330	LYS	HG3	1.499	.	2
1	A	330	LYS	CD	28.655	.	1
1	A	330	LYS	HD2	1.713	.	2
1	A	330	LYS	CE	41.753	.	1
1	A	330	LYS	HE2	3.02	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	330	LYS	HE3	3.02	.	2
1	A	331	GLY	N	109.849	.	1
1	A	331	GLY	H	8.394	.	1
1	A	331	GLY	CA	45.051	.	1
1	A	332	ASP	N	120.247	.	1
1	A	332	ASP	H	8.231	.	1
1	A	332	ASP	CA	53.927	.	1
1	A	332	ASP	HA	4.664	.	1
1	A	332	ASP	CB	41.087	.	1
1	A	332	ASP	HB2	2.743	.	2
1	A	332	ASP	HB3	2.743	.	2
1	A	333	GLY	N	108.972	.	1
1	A	333	GLY	H	8.496	.	1
1	A	333	GLY	CA	45.347	.	1
1	A	333	GLY	HA2	4.0	.	2
1	A	333	GLY	HA3	4.0	.	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	97	-0.05 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	90	0.76 ± 0.10	Should be checked
$^{13}C'$	0	—	None (insufficient data)
^{15}N	93	0.62 ± 0.27	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 39%, i.e. 881 atoms were assigned a chemical shift out of a possible 2266. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	321/843 (38%)	158/341 (46%)	83/340 (24%)	80/162 (49%)
Sidechain	540/1277 (42%)	368/836 (44%)	167/393 (42%)	5/48 (10%)
Aromatic	20/146 (14%)	10/74 (14%)	8/62 (13%)	2/10 (20%)
Overall	881/2266 (39%)	536/1251 (43%)	258/795 (32%)	87/220 (40%)

The following table shows the completeness of the chemical shift assignments for the full structure.

The overall completeness is 40%, i.e. 969 atoms were assigned a chemical shift out of a possible 2452. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	359/930 (39%)	177/376 (47%)	93/376 (25%)	89/178 (50%)
Sidechain	590/1376 (43%)	402/902 (45%)	183/426 (43%)	5/48 (10%)
Aromatic	20/146 (14%)	10/74 (14%)	8/62 (13%)	2/10 (20%)
Overall	969/2452 (40%)	589/1352 (44%)	284/864 (33%)	96/236 (41%)

7.1.4 Statistically unusual chemical shifts (i)

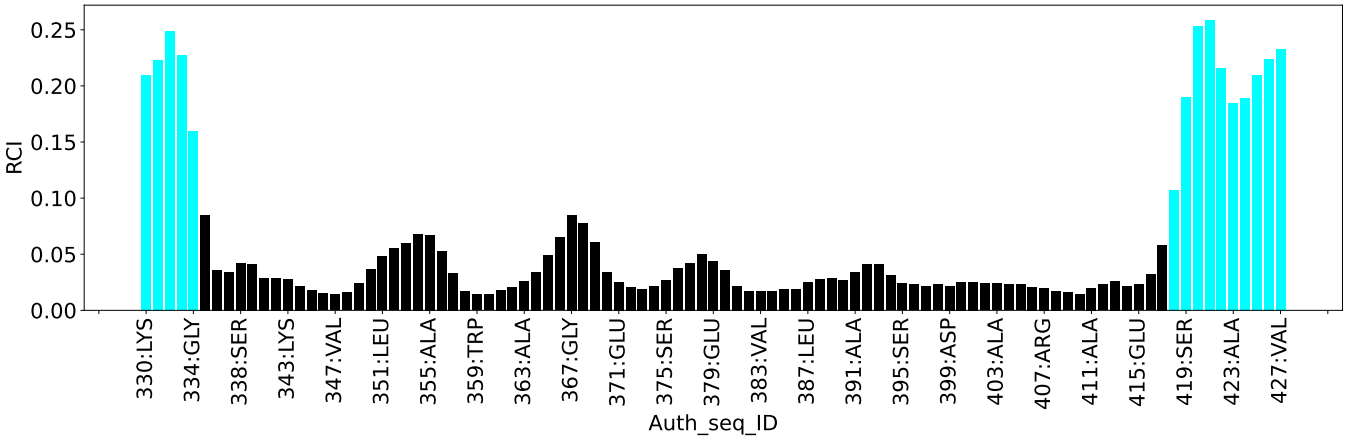
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	382	PRO	HB3	-0.18	0.25 – 3.76	-6.2
1	A	396	ALA	HB1	-0.12	0.14 – 2.58	-6.1
1	A	396	ALA	HB2	-0.12	0.14 – 2.58	-6.1
1	A	396	ALA	HB3	-0.12	0.14 – 2.58	-6.1
1	A	360	ARG	HG2	0.04	0.26 – 2.87	-5.8
1	A	360	ARG	HG3	0.07	0.15 – 2.94	-5.3

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:


RCI
0.25
0.20
0.15
0.10
0.05
0.00
330:LYS
334:GLY
338:SER
343:LYS
347:VAL
351:LEU
355:ALA
359:TRP
363:ALA
367:GLY
371:GLU
375:SER
379:GLU
383:VAL
387:LEU
391:ALA
395:SER
399:ASP
403:ALA
407:ARG
411:ALA
415:GLU
419:SER
423:ALA
427:VAL
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	1688
Intra-residue (|i-j|=0)	364
Sequential (|i-j|=1)	497
Medium range (|i-j|>1 and |i-j|<5)	454
Long range (|i-j|≥5)	373
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	8.6
Number of long range restraints per residue[1]	1.9

[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)	2.6	0.2
0.2-0.5 (Medium)	2.6	0.47
>0.5 (Large)	17.1	5.91

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)

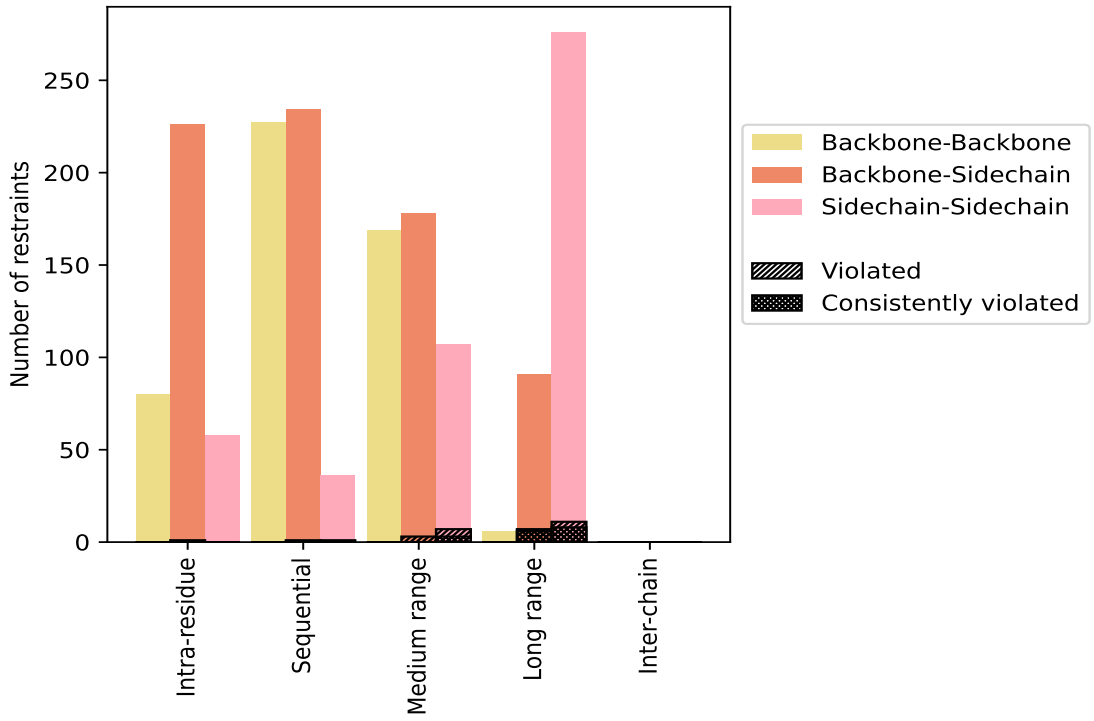
9.1 Summary of distance violations (i)

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)	364	21.6	1	0.3	0.1	0	0.0	0.0
Backbone-Backbone	80	4.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	226	13.4	1	0.4	0.1	0	0.0	0.0
Sidechain-Sidechain	58	3.4	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	497	29.4	2	0.4	0.1	0	0.0	0.0
Backbone-Backbone	227	13.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	234	13.9	1	0.4	0.1	0	0.0	0.0
Sidechain-Sidechain	36	2.1	1	2.8	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	454	26.9	10	2.2	0.6	3	0.7	0.2
Backbone-Backbone	169	10.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	178	10.5	3	1.7	0.2	0	0.0	0.0
Sidechain-Sidechain	107	6.3	7	6.5	0.4	3	2.8	0.2
Long range (|i-j|≥5)	373	22.1	18	4.8	1.1	14	3.8	0.8
Backbone-Backbone	6	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	91	5.4	7	7.7	0.4	6	6.6	0.4
Sidechain-Sidechain	276	16.4	11	4.0	0.7	8	2.9	0.5
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1688	100.0	31	1.8	1.8	17	1.0	1.0
Backbone-Backbone	482	28.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	729	43.2	12	1.6	0.7	6	0.8	0.4
Sidechain-Sidechain	477	28.3	19	4.0	1.1	11	2.3	0.7

[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

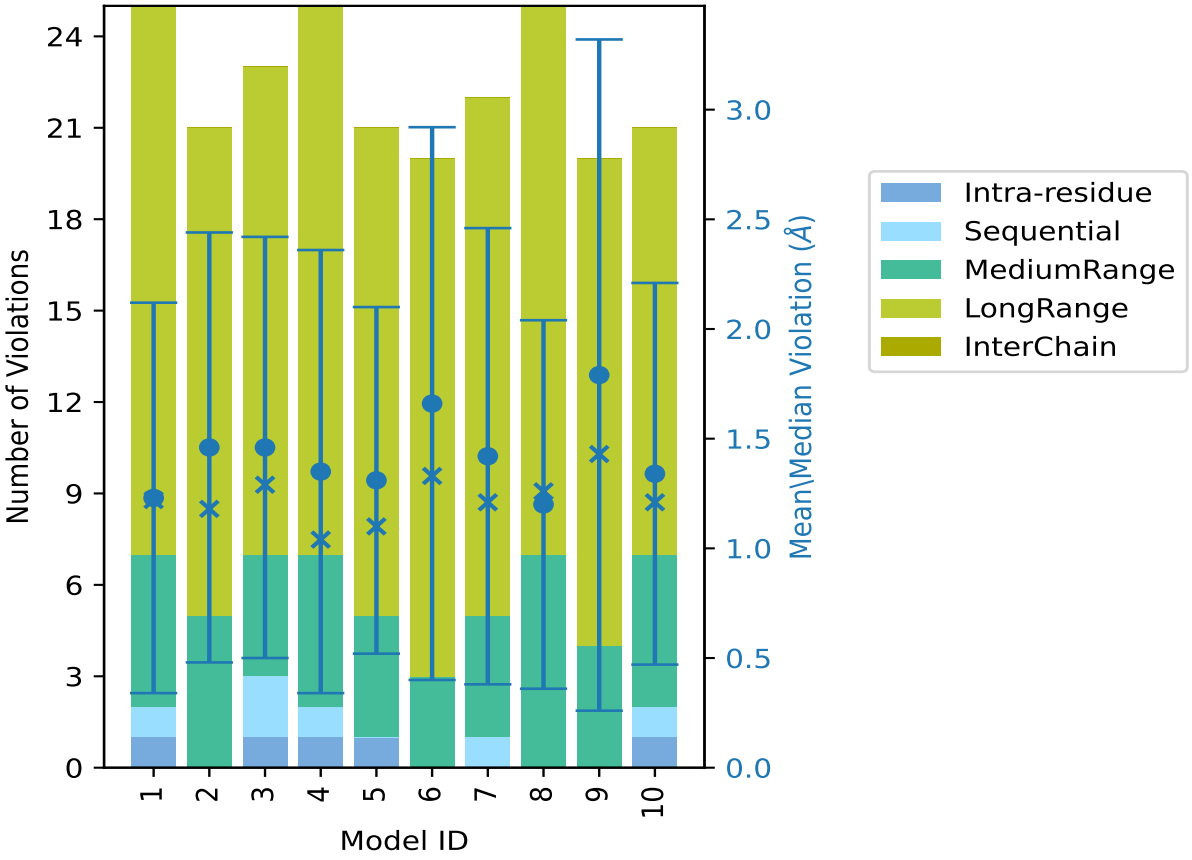
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	1	1	5	18	0	25	1.23	2.93	0.89	1.22
2	0	0	5	16	0	21	1.46	3.75	0.98	1.18
3	1	2	4	16	0	23	1.46	3.35	0.96	1.29
4	1	1	5	18	0	25	1.35	3.53	1.01	1.04
5	1	0	4	16	0	21	1.31	2.53	0.79	1.1
6	0	0	3	17	0	20	1.66	4.78	1.26	1.33
7	0	1	4	17	0	22	1.42	4.14	1.04	1.21
8	0	0	7	18	0	25	1.2	2.46	0.84	1.26
9	0	0	4	16	0	20	1.79	5.91	1.53	1.43
10	1	1	5	14	0	21	1.34	2.95	0.87	1.21

[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

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, 1657(IR:363, SQ:495, MR:444, LR:355, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	2	0	0	2	1	10.0
0	1	3	0	0	4	2	20.0
0	0	1	0	0	1	3	30.0
0	1	0	2	0	3	4	40.0

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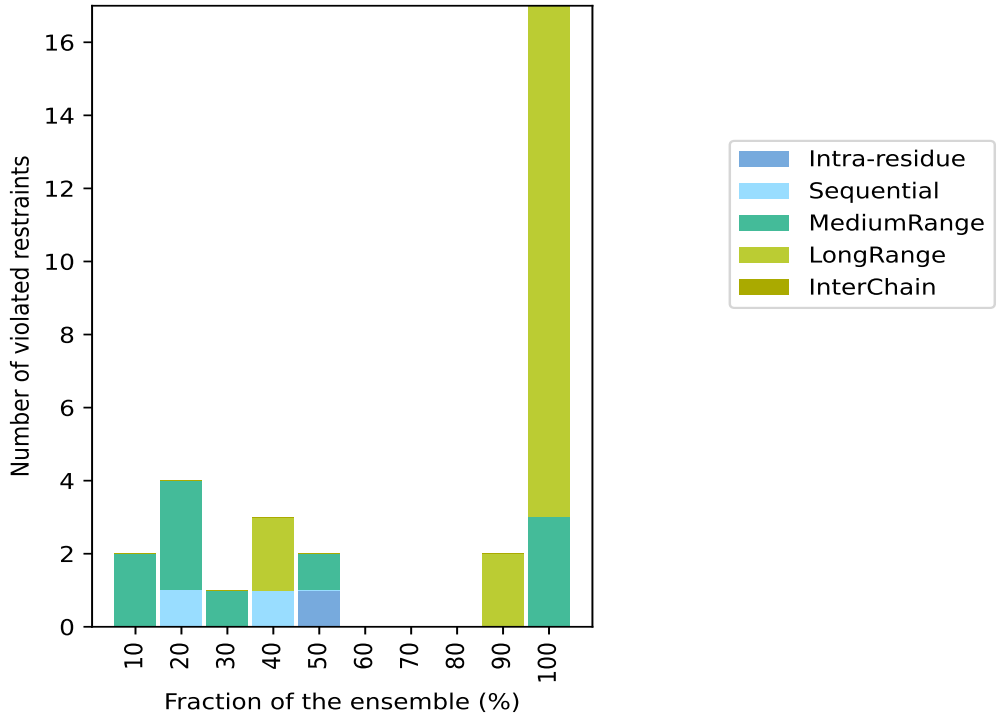
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	0	1	0	0	2	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	2	0	2	9	90.0
0	0	3	14	0	17	10	100.0

[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

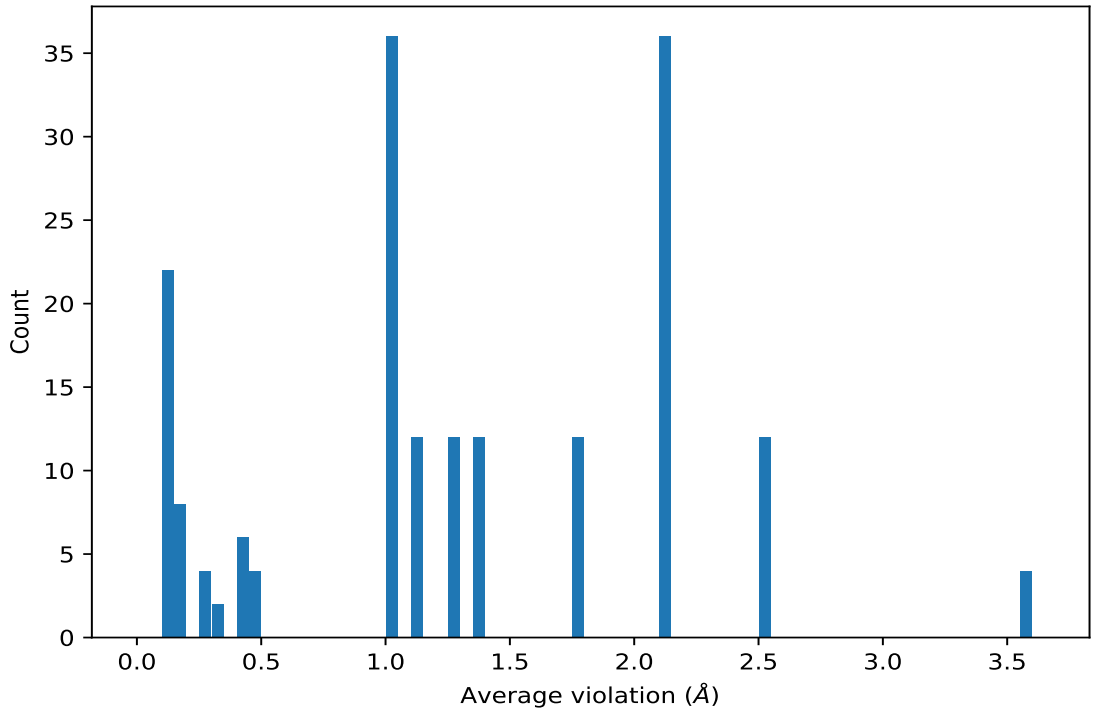
9.3.1 Bar graph : Distance violation statistics for the ensemble



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)
(2,12)	1:B:352:ASN:HD22	1:B:379:GLU:HG3	10	3.58	1.09	3.44
(2,12)	1:A:352:ASN:HD22	1:A:379:GLU:HG3	10	3.58	1.09	3.44
(2,13)	1:B:379:GLU:HG3	1:B:352:ASN:HD22	10	3.58	1.09	3.44
(2,13)	1:A:379:GLU:HG3	1:A:352:ASN:HD22	10	3.58	1.09	3.44
(2,18)	1:B:380:ALA:HB1	1:B:351:LEU:HA	10	2.52	0.21	2.48
(2,18)	1:B:380:ALA:HB2	1:B:351:LEU:HA	10	2.52	0.21	2.48
(2,18)	1:B:380:ALA:HB3	1:B:351:LEU:HA	10	2.52	0.21	2.48
(2,18)	1:A:380:ALA:HB1	1:A:351:LEU:HA	10	2.52	0.21	2.48
(2,18)	1:A:380:ALA:HB2	1:A:351:LEU:HA	10	2.52	0.21	2.48
(2,18)	1:A:380:ALA:HB3	1:A:351:LEU:HA	10	2.52	0.21	2.48
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB1	10	2.52	0.21	2.48
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB2	10	2.52	0.21	2.48
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB3	10	2.52	0.21	2.48
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB1	10	2.52	0.21	2.48
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB2	10	2.52	0.21	2.48
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB3	10	2.52	0.21	2.48

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB1	10	2.11	0.11	2.11
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB2	10	2.11	0.11	2.11
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB3	10	2.11	0.11	2.11
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB1	10	2.11	0.11	2.11
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB2	10	2.11	0.11	2.11
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB3	10	2.11	0.11	2.11
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB1	10	2.11	0.11	2.11
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB2	10	2.11	0.11	2.11
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB3	10	2.11	0.11	2.11
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB1	10	2.11	0.11	2.11
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB2	10	2.11	0.11	2.11
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB3	10	2.11	0.11	2.11
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB1	10	2.11	0.11	2.11
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB2	10	2.11	0.11	2.11
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB3	10	2.11	0.11	2.11
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB1	10	2.11	0.11	2.11
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB2	10	2.11	0.11	2.11
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB3	10	2.11	0.11	2.11
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD11	10	2.11	0.11	2.11
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD12	10	2.11	0.11	2.11
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD13	10	2.11	0.11	2.11
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD11	10	2.11	0.11	2.11
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD12	10	2.11	0.11	2.11
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD13	10	2.11	0.11	2.11
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD11	10	2.11	0.11	2.11
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD12	10	2.11	0.11	2.11
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD13	10	2.11	0.11	2.11
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD11	10	2.11	0.11	2.11
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD12	10	2.11	0.11	2.11
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD13	10	2.11	0.11	2.11
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD11	10	2.11	0.11	2.11
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD12	10	2.11	0.11	2.11
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD13	10	2.11	0.11	2.11
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD11	10	2.11	0.11	2.11
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD12	10	2.11	0.11	2.11
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD13	10	2.11	0.11	2.11
(2,14)	1:B:380:ALA:HB1	1:B:348:GLU:HA	10	1.76	0.09	1.76
(2,14)	1:B:380:ALA:HB2	1:B:348:GLU:HA	10	1.76	0.09	1.76
(2,14)	1:B:380:ALA:HB3	1:B:348:GLU:HA	10	1.76	0.09	1.76
(2,14)	1:A:380:ALA:HB1	1:A:348:GLU:HA	10	1.76	0.09	1.76
(2,14)	1:A:380:ALA:HB2	1:A:348:GLU:HA	10	1.76	0.09	1.76
(2,14)	1:A:380:ALA:HB3	1:A:348:GLU:HA	10	1.76	0.09	1.76

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB1	10	1.76	0.09	1.76
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB2	10	1.76	0.09	1.76
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB3	10	1.76	0.09	1.76
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB1	10	1.76	0.09	1.76
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB2	10	1.76	0.09	1.76
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB3	10	1.76	0.09	1.76
(2,22)	1:B:380:ALA:HB1	1:B:352:ASN:H	10	1.39	0.17	1.38
(2,22)	1:B:380:ALA:HB2	1:B:352:ASN:H	10	1.39	0.17	1.38
(2,22)	1:B:380:ALA:HB3	1:B:352:ASN:H	10	1.39	0.17	1.38
(2,22)	1:A:380:ALA:HB1	1:A:352:ASN:H	10	1.39	0.17	1.38
(2,22)	1:A:380:ALA:HB2	1:A:352:ASN:H	10	1.39	0.17	1.38
(2,22)	1:A:380:ALA:HB3	1:A:352:ASN:H	10	1.39	0.17	1.38
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB1	10	1.39	0.17	1.38
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB2	10	1.39	0.17	1.38
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB3	10	1.39	0.17	1.38
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB1	10	1.39	0.17	1.38
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB2	10	1.39	0.17	1.38
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB3	10	1.39	0.17	1.38
(2,40)	1:B:380:ALA:HB1	1:B:383:VAL:HB	10	1.25	0.04	1.25
(2,40)	1:B:380:ALA:HB2	1:B:383:VAL:HB	10	1.25	0.04	1.25
(2,40)	1:B:380:ALA:HB3	1:B:383:VAL:HB	10	1.25	0.04	1.25
(2,40)	1:A:380:ALA:HB1	1:A:383:VAL:HB	10	1.25	0.04	1.25
(2,40)	1:A:380:ALA:HB2	1:A:383:VAL:HB	10	1.25	0.04	1.25
(2,40)	1:A:380:ALA:HB3	1:A:383:VAL:HB	10	1.25	0.04	1.25
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB1	10	1.25	0.04	1.25
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB2	10	1.25	0.04	1.25
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB3	10	1.25	0.04	1.25
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB1	10	1.25	0.04	1.25
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB2	10	1.25	0.04	1.25
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB3	10	1.25	0.04	1.25
(2,16)	1:B:380:ALA:HB1	1:B:348:GLU:HB3	10	1.12	0.13	1.14
(2,16)	1:B:380:ALA:HB2	1:B:348:GLU:HB3	10	1.12	0.13	1.14
(2,16)	1:B:380:ALA:HB3	1:B:348:GLU:HB3	10	1.12	0.13	1.14
(2,16)	1:A:380:ALA:HB1	1:A:348:GLU:HB3	10	1.12	0.13	1.14
(2,16)	1:A:380:ALA:HB2	1:A:348:GLU:HB3	10	1.12	0.13	1.14
(2,16)	1:A:380:ALA:HB3	1:A:348:GLU:HB3	10	1.12	0.13	1.14
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB1	10	1.12	0.13	1.14
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB2	10	1.12	0.13	1.14
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB3	10	1.12	0.13	1.14
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB1	10	1.12	0.13	1.14
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB2	10	1.12	0.13	1.14
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB3	10	1.12	0.13	1.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD21	10	1.02	0.09	1.04
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD22	10	1.02	0.09	1.04
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD23	10	1.02	0.09	1.04
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD21	10	1.02	0.09	1.04
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD22	10	1.02	0.09	1.04
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD23	10	1.02	0.09	1.04
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD21	10	1.02	0.09	1.04
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD22	10	1.02	0.09	1.04
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD23	10	1.02	0.09	1.04
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD21	10	1.02	0.09	1.04
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD22	10	1.02	0.09	1.04
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD23	10	1.02	0.09	1.04
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD21	10	1.02	0.09	1.04
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD22	10	1.02	0.09	1.04
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD23	10	1.02	0.09	1.04
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD21	10	1.02	0.09	1.04
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD22	10	1.02	0.09	1.04
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD23	10	1.02	0.09	1.04
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB1	10	1.02	0.09	1.04
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB2	10	1.02	0.09	1.04
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB3	10	1.02	0.09	1.04
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB1	10	1.02	0.09	1.04
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB2	10	1.02	0.09	1.04
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB3	10	1.02	0.09	1.04
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB1	10	1.02	0.09	1.04
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB2	10	1.02	0.09	1.04
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB3	10	1.02	0.09	1.04
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB1	10	1.02	0.09	1.04
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB2	10	1.02	0.09	1.04
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB3	10	1.02	0.09	1.04
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB1	10	1.02	0.09	1.04
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB2	10	1.02	0.09	1.04
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB3	10	1.02	0.09	1.04
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB1	10	1.02	0.09	1.04
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB2	10	1.02	0.09	1.04
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB3	10	1.02	0.09	1.04
(2,6)	1:A:394:ASP:HB3	1:A:397:THR:HB	10	0.44	0.13	0.42
(2,6)	1:B:394:ASP:HB3	1:B:397:THR:HB	10	0.44	0.13	0.42
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE1	9	0.45	0.2	0.4
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE2	9	0.45	0.2	0.4
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE1	9	0.45	0.2	0.4
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE2	9	0.45	0.2	0.4

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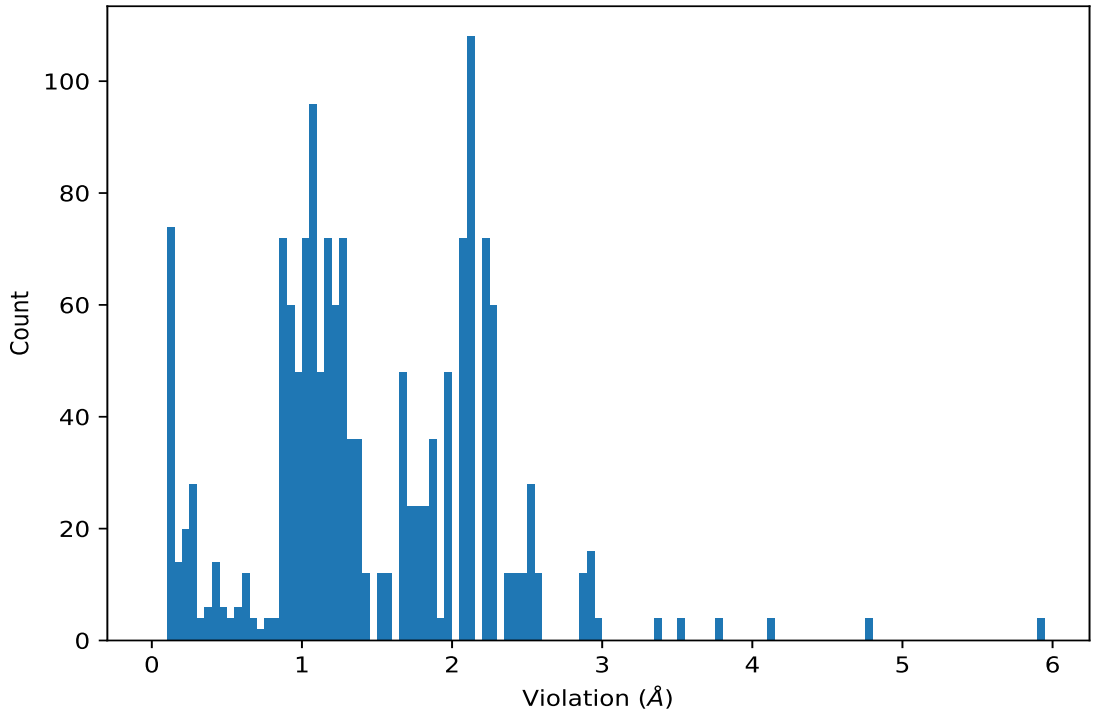
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE1	9	0.43	0.22	0.44
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE2	9	0.43	0.22	0.44
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE1	9	0.43	0.22	0.44
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE2	9	0.43	0.22	0.44
(1,988)	1:A:393:GLN:HG3	1:A:390:TRP:HA	5	0.28	0.05	0.27
(1,988)	1:B:393:GLN:HG3	1:B:390:TRP:HA	5	0.28	0.05	0.27
(1,352)	1:B:361:HIS:HD2	1:B:361:HIS:HA	5	0.18	0.06	0.17
(1,352)	1:A:361:HIS:HD2	1:A:361:HIS:HA	5	0.18	0.06	0.17
(1,538)	1:B:372:HIS:HD2	1:B:371:GLU:HG2	4	0.3	0.19	0.3
(1,538)	1:A:372:HIS:HD2	1:A:371:GLU:HG2	4	0.3	0.19	0.3
(1,675)	1:A:359:TRP:HZ2	1:A:377:THR:HA	4	0.26	0.06	0.28
(1,675)	1:B:359:TRP:HZ2	1:B:377:THR:HA	4	0.26	0.06	0.28
(1,1166)	1:B:401:LEU:HB3	1:B:390:TRP:HH2	4	0.13	0.02	0.12
(1,1166)	1:A:401:LEU:HB3	1:A:390:TRP:HH2	4	0.13	0.02	0.12
(1,240)	1:A:348:GLU:HB2	1:A:351:LEU:HD11	3	0.14	0.02	0.15
(1,240)	1:A:348:GLU:HB2	1:A:351:LEU:HD12	3	0.14	0.02	0.15
(1,240)	1:A:348:GLU:HB2	1:A:351:LEU:HD13	3	0.14	0.02	0.15
(1,240)	1:B:348:GLU:HB2	1:B:351:LEU:HD11	3	0.14	0.02	0.15
(1,240)	1:B:348:GLU:HB2	1:B:351:LEU:HD12	3	0.14	0.02	0.15
(1,240)	1:B:348:GLU:HB2	1:B:351:LEU:HD13	3	0.14	0.02	0.15
(1,686)	1:A:374:ASP:HB2	1:A:377:THR:HG21	2	0.16	0.05	0.16
(1,686)	1:A:374:ASP:HB2	1:A:377:THR:HG22	2	0.16	0.05	0.16
(1,686)	1:A:374:ASP:HB2	1:A:377:THR:HG23	2	0.16	0.05	0.16
(1,686)	1:B:374:ASP:HB2	1:B:377:THR:HG21	2	0.16	0.05	0.16
(1,686)	1:B:374:ASP:HB2	1:B:377:THR:HG22	2	0.16	0.05	0.16
(1,686)	1:B:374:ASP:HB2	1:B:377:THR:HG23	2	0.16	0.05	0.16
(1,301)	1:A:354:SER:HB2	1:A:358:THR:HG21	2	0.13	0.02	0.13
(1,301)	1:A:354:SER:HB2	1:A:358:THR:HG22	2	0.13	0.02	0.13
(1,301)	1:A:354:SER:HB2	1:A:358:THR:HG23	2	0.13	0.02	0.13
(1,301)	1:B:354:SER:HB2	1:B:358:THR:HG21	2	0.13	0.02	0.13
(1,301)	1:B:354:SER:HB2	1:B:358:THR:HG22	2	0.13	0.02	0.13
(1,301)	1:B:354:SER:HB2	1:B:358:THR:HG23	2	0.13	0.02	0.13
(1,302)	1:A:358:THR:HG21	1:A:354:SER:HB2	2	0.13	0.02	0.13
(1,302)	1:A:358:THR:HG22	1:A:354:SER:HB2	2	0.13	0.02	0.13
(1,302)	1:A:358:THR:HG23	1:A:354:SER:HB2	2	0.13	0.02	0.13
(1,302)	1:B:358:THR:HG21	1:B:354:SER:HB2	2	0.13	0.02	0.13
(1,302)	1:B:358:THR:HG22	1:B:354:SER:HB2	2	0.13	0.02	0.13
(1,302)	1:B:358:THR:HG23	1:B:354:SER:HB2	2	0.13	0.02	0.13
(1,318)	1:A:359:TRP:H	1:A:358:THR:HB	2	0.11	0.0	0.11
(1,318)	1:B:359:TRP:H	1:B:358:THR:HB	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)
(2,13)	1:B:379:GLU:HG3	1:B:352:ASN:HD22	9	5.91
(2,13)	1:A:379:GLU:HG3	1:A:352:ASN:HD22	9	5.91
(2,12)	1:B:352:ASN:HD22	1:B:379:GLU:HG3	9	5.91
(2,12)	1:A:352:ASN:HD22	1:A:379:GLU:HG3	9	5.91
(2,13)	1:B:379:GLU:HG3	1:B:352:ASN:HD22	6	4.78
(2,13)	1:A:379:GLU:HG3	1:A:352:ASN:HD22	6	4.78
(2,12)	1:B:352:ASN:HD22	1:B:379:GLU:HG3	6	4.78
(2,12)	1:A:352:ASN:HD22	1:A:379:GLU:HG3	6	4.78
(2,13)	1:B:379:GLU:HG3	1:B:352:ASN:HD22	7	4.14
(2,13)	1:A:379:GLU:HG3	1:A:352:ASN:HD22	7	4.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:B:352:ASN:HD22	1:B:379:GLU:HG3	7	4.14
(2,12)	1:A:352:ASN:HD22	1:A:379:GLU:HG3	7	4.14
(2,13)	1:B:379:GLU:HG3	1:B:352:ASN:HD22	2	3.75
(2,13)	1:A:379:GLU:HG3	1:A:352:ASN:HD22	2	3.75
(2,12)	1:B:352:ASN:HD22	1:B:379:GLU:HG3	2	3.75
(2,12)	1:A:352:ASN:HD22	1:A:379:GLU:HG3	2	3.75
(2,13)	1:B:379:GLU:HG3	1:B:352:ASN:HD22	4	3.53
(2,13)	1:A:379:GLU:HG3	1:A:352:ASN:HD22	4	3.53
(2,12)	1:B:352:ASN:HD22	1:B:379:GLU:HG3	4	3.53
(2,12)	1:A:352:ASN:HD22	1:A:379:GLU:HG3	4	3.53
(2,13)	1:B:379:GLU:HG3	1:B:352:ASN:HD22	3	3.35
(2,13)	1:A:379:GLU:HG3	1:A:352:ASN:HD22	3	3.35
(2,12)	1:B:352:ASN:HD22	1:B:379:GLU:HG3	3	3.35
(2,12)	1:A:352:ASN:HD22	1:A:379:GLU:HG3	3	3.35
(2,13)	1:B:379:GLU:HG3	1:B:352:ASN:HD22	10	2.95
(2,13)	1:A:379:GLU:HG3	1:A:352:ASN:HD22	10	2.95
(2,12)	1:B:352:ASN:HD22	1:B:379:GLU:HG3	10	2.95
(2,12)	1:A:352:ASN:HD22	1:A:379:GLU:HG3	10	2.95
(2,13)	1:B:379:GLU:HG3	1:B:352:ASN:HD22	1	2.93
(2,13)	1:A:379:GLU:HG3	1:A:352:ASN:HD22	1	2.93
(2,12)	1:B:352:ASN:HD22	1:B:379:GLU:HG3	1	2.93
(2,12)	1:A:352:ASN:HD22	1:A:379:GLU:HG3	1	2.93
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB1	4	2.91
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB2	4	2.91
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB3	4	2.91
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB1	4	2.91
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB2	4	2.91
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB3	4	2.91
(2,18)	1:B:380:ALA:HB1	1:B:351:LEU:HA	4	2.91
(2,18)	1:B:380:ALA:HB2	1:B:351:LEU:HA	4	2.91
(2,18)	1:B:380:ALA:HB3	1:B:351:LEU:HA	4	2.91
(2,18)	1:A:380:ALA:HB1	1:A:351:LEU:HA	4	2.91
(2,18)	1:A:380:ALA:HB2	1:A:351:LEU:HA	4	2.91
(2,18)	1:A:380:ALA:HB3	1:A:351:LEU:HA	4	2.91
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB1	3	2.86
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB2	3	2.86
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB3	3	2.86
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB1	3	2.86
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB2	3	2.86
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB3	3	2.86
(2,18)	1:B:380:ALA:HB1	1:B:351:LEU:HA	3	2.86
(2,18)	1:B:380:ALA:HB2	1:B:351:LEU:HA	3	2.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,18)	1:B:380:ALA:HB3	1:B:351:LEU:HA	3	2.86
(2,18)	1:A:380:ALA:HB1	1:A:351:LEU:HA	3	2.86
(2,18)	1:A:380:ALA:HB2	1:A:351:LEU:HA	3	2.86
(2,18)	1:A:380:ALA:HB3	1:A:351:LEU:HA	3	2.86
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB1	6	2.59
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB2	6	2.59
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB3	6	2.59
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB1	6	2.59
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB2	6	2.59
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB3	6	2.59
(2,18)	1:B:380:ALA:HB1	1:B:351:LEU:HA	6	2.59
(2,18)	1:B:380:ALA:HB2	1:B:351:LEU:HA	6	2.59
(2,18)	1:B:380:ALA:HB3	1:B:351:LEU:HA	6	2.59
(2,18)	1:A:380:ALA:HB1	1:A:351:LEU:HA	6	2.59
(2,18)	1:A:380:ALA:HB2	1:A:351:LEU:HA	6	2.59
(2,18)	1:A:380:ALA:HB3	1:A:351:LEU:HA	6	2.59
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB1	1	2.53
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB2	1	2.53
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB3	1	2.53
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB1	1	2.53
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB2	1	2.53
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB3	1	2.53
(2,18)	1:B:380:ALA:HB1	1:B:351:LEU:HA	1	2.53
(2,18)	1:B:380:ALA:HB2	1:B:351:LEU:HA	1	2.53
(2,18)	1:B:380:ALA:HB3	1:B:351:LEU:HA	1	2.53
(2,18)	1:A:380:ALA:HB1	1:A:351:LEU:HA	1	2.53
(2,18)	1:A:380:ALA:HB2	1:A:351:LEU:HA	1	2.53
(2,18)	1:A:380:ALA:HB3	1:A:351:LEU:HA	1	2.53
(2,13)	1:B:379:GLU:HG3	1:B:352:ASN:HD22	5	2.53
(2,13)	1:A:379:GLU:HG3	1:A:352:ASN:HD22	5	2.53
(2,12)	1:B:352:ASN:HD22	1:B:379:GLU:HG3	5	2.53
(2,12)	1:A:352:ASN:HD22	1:A:379:GLU:HG3	5	2.53
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB1	5	2.51
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB2	5	2.51
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB3	5	2.51
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB1	5	2.51
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB2	5	2.51
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB3	5	2.51
(2,18)	1:B:380:ALA:HB1	1:B:351:LEU:HA	5	2.51
(2,18)	1:B:380:ALA:HB2	1:B:351:LEU:HA	5	2.51
(2,18)	1:B:380:ALA:HB3	1:B:351:LEU:HA	5	2.51
(2,18)	1:A:380:ALA:HB1	1:A:351:LEU:HA	5	2.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,18)	1:A:380:ALA:HB2	1:A:351:LEU:HA	5	2.51
(2,18)	1:A:380:ALA:HB3	1:A:351:LEU:HA	5	2.51
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB1	8	2.46
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB2	8	2.46
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB3	8	2.46
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB1	8	2.46
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB2	8	2.46
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB3	8	2.46
(2,18)	1:B:380:ALA:HB1	1:B:351:LEU:HA	8	2.46
(2,18)	1:B:380:ALA:HB2	1:B:351:LEU:HA	8	2.46
(2,18)	1:B:380:ALA:HB3	1:B:351:LEU:HA	8	2.46
(2,18)	1:A:380:ALA:HB1	1:A:351:LEU:HA	8	2.46
(2,18)	1:A:380:ALA:HB2	1:A:351:LEU:HA	8	2.46
(2,18)	1:A:380:ALA:HB3	1:A:351:LEU:HA	8	2.46
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB1	10	2.42
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB2	10	2.42
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB3	10	2.42
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB1	10	2.42
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB2	10	2.42
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB3	10	2.42
(2,18)	1:B:380:ALA:HB1	1:B:351:LEU:HA	10	2.42
(2,18)	1:B:380:ALA:HB2	1:B:351:LEU:HA	10	2.42
(2,18)	1:B:380:ALA:HB3	1:B:351:LEU:HA	10	2.42
(2,18)	1:A:380:ALA:HB1	1:A:351:LEU:HA	10	2.42
(2,18)	1:A:380:ALA:HB2	1:A:351:LEU:HA	10	2.42
(2,18)	1:A:380:ALA:HB3	1:A:351:LEU:HA	10	2.42
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB1	9	2.39
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB2	9	2.39
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB3	9	2.39
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB1	9	2.39
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB2	9	2.39
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB3	9	2.39
(2,18)	1:B:380:ALA:HB1	1:B:351:LEU:HA	9	2.39
(2,18)	1:B:380:ALA:HB2	1:B:351:LEU:HA	9	2.39
(2,18)	1:B:380:ALA:HB3	1:B:351:LEU:HA	9	2.39
(2,18)	1:A:380:ALA:HB1	1:A:351:LEU:HA	9	2.39
(2,18)	1:A:380:ALA:HB2	1:A:351:LEU:HA	9	2.39
(2,18)	1:A:380:ALA:HB3	1:A:351:LEU:HA	9	2.39
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD11	8	2.29
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD12	8	2.29
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD13	8	2.29
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD11	8	2.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD12	8	2.29
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD13	8	2.29
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD11	8	2.29
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD12	8	2.29
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD13	8	2.29
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD11	8	2.29
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD12	8	2.29
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD13	8	2.29
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD11	8	2.29
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD12	8	2.29
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD13	8	2.29
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD11	8	2.29
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD12	8	2.29
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD13	8	2.29
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB1	8	2.29
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB2	8	2.29
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB3	8	2.29
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB1	8	2.29
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB2	8	2.29
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB3	8	2.29
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB1	8	2.29
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB2	8	2.29
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB3	8	2.29
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB1	8	2.29
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB2	8	2.29
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB3	8	2.29
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB1	8	2.29
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB2	8	2.29
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB3	8	2.29
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB1	8	2.29
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB2	8	2.29
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB3	8	2.29
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB1	2	2.26
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB2	2	2.26
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB3	2	2.26
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB1	2	2.26
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB2	2	2.26
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB3	2	2.26
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB1	7	2.26
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB2	7	2.26
(2,19)	1:A:351:LEU:HA	1:A:380:ALA:HB3	7	2.26
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB1	7	2.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB2	7	2.26
(2,19)	1:B:351:LEU:HA	1:B:380:ALA:HB3	7	2.26
(2,18)	1:B:380:ALA:HB1	1:B:351:LEU:HA	2	2.26
(2,18)	1:B:380:ALA:HB2	1:B:351:LEU:HA	2	2.26
(2,18)	1:B:380:ALA:HB3	1:B:351:LEU:HA	2	2.26
(2,18)	1:A:380:ALA:HB1	1:A:351:LEU:HA	2	2.26
(2,18)	1:A:380:ALA:HB2	1:A:351:LEU:HA	2	2.26
(2,18)	1:A:380:ALA:HB3	1:A:351:LEU:HA	2	2.26
(2,18)	1:B:380:ALA:HB1	1:B:351:LEU:HA	7	2.26
(2,18)	1:B:380:ALA:HB2	1:B:351:LEU:HA	7	2.26
(2,18)	1:B:380:ALA:HB3	1:B:351:LEU:HA	7	2.26
(2,18)	1:A:380:ALA:HB1	1:A:351:LEU:HA	7	2.26
(2,18)	1:A:380:ALA:HB2	1:A:351:LEU:HA	7	2.26
(2,18)	1:A:380:ALA:HB3	1:A:351:LEU:HA	7	2.26
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD11	4	2.24
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD12	4	2.24
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD13	4	2.24
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD11	4	2.24
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD12	4	2.24
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD13	4	2.24
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD11	4	2.24
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD12	4	2.24
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD13	4	2.24
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD11	4	2.24
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD12	4	2.24
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD13	4	2.24
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD11	4	2.24
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD12	4	2.24
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD13	4	2.24
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD11	4	2.24
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD12	4	2.24
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD13	4	2.24
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB1	4	2.24
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB2	4	2.24
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB3	4	2.24
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB1	4	2.24
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB2	4	2.24
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB3	4	2.24
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB1	4	2.24
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB2	4	2.24
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB3	4	2.24
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB1	4	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB2	4	2.24
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB3	4	2.24
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB1	4	2.24
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB2	4	2.24
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB3	4	2.24
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB1	4	2.24
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB2	4	2.24
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB3	4	2.24
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD11	3	2.21
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD12	3	2.21
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD13	3	2.21
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD11	3	2.21
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD12	3	2.21
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD13	3	2.21
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD11	3	2.21
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD12	3	2.21
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD13	3	2.21
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD11	3	2.21
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD12	3	2.21
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD13	3	2.21
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD11	3	2.21
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD12	3	2.21
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD13	3	2.21
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD11	3	2.21
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD12	3	2.21
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD13	3	2.21
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB1	3	2.21
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB2	3	2.21
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB3	3	2.21
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB1	3	2.21
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB2	3	2.21
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB3	3	2.21
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB1	3	2.21
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB2	3	2.21
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB3	3	2.21
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB1	3	2.21
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB2	3	2.21
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB3	3	2.21
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB1	3	2.21
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB2	3	2.21
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB3	3	2.21
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB1	3	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB2	3	2.21
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB3	3	2.21
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD11	6	2.13
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD12	6	2.13
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD13	6	2.13
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD11	6	2.13
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD12	6	2.13
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD13	6	2.13
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD11	6	2.13
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD12	6	2.13
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD13	6	2.13
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD11	6	2.13
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD12	6	2.13
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD13	6	2.13
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD11	6	2.13
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD12	6	2.13
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD13	6	2.13
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD11	6	2.13
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD12	6	2.13
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD13	6	2.13
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB1	6	2.13
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB2	6	2.13
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB3	6	2.13
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB1	6	2.13
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB2	6	2.13
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB3	6	2.13
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB1	6	2.13
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB2	6	2.13
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB3	6	2.13
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB1	6	2.13
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB2	6	2.13
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB3	6	2.13
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB1	6	2.13
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB2	6	2.13
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB3	6	2.13
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB1	6	2.13
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB2	6	2.13
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB3	6	2.13
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD11	2	2.11
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD12	2	2.11
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD13	2	2.11
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD11	2	2.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD12	2	2.11
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD13	2	2.11
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD11	2	2.11
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD12	2	2.11
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD13	2	2.11
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD11	2	2.11
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD12	2	2.11
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD13	2	2.11
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD11	2	2.11
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD12	2	2.11
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD13	2	2.11
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD11	2	2.11
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD12	2	2.11
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD13	2	2.11
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD11	9	2.11
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD12	9	2.11
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD13	9	2.11
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD11	9	2.11
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD12	9	2.11
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD13	9	2.11
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD11	9	2.11
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD12	9	2.11
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD13	9	2.11
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD11	9	2.11
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD12	9	2.11
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD13	9	2.11
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD11	9	2.11
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD12	9	2.11
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD13	9	2.11
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD11	9	2.11
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD12	9	2.11
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD13	9	2.11
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB1	2	2.11
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB2	2	2.11
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB3	2	2.11
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB1	2	2.11
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB2	2	2.11
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB3	2	2.11
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB1	2	2.11
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB2	2	2.11
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB3	2	2.11
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB1	2	2.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB2	2	2.11
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB3	2	2.11
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB1	2	2.11
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB2	2	2.11
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB3	2	2.11
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB1	2	2.11
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB2	2	2.11
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB3	2	2.11
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB1	9	2.11
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB2	9	2.11
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB3	9	2.11
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB1	9	2.11
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB2	9	2.11
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB3	9	2.11
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB1	9	2.11
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB2	9	2.11
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB3	9	2.11
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB1	9	2.11
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB2	9	2.11
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB3	9	2.11
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB1	9	2.11
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB2	9	2.11
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB3	9	2.11
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB1	9	2.11
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB2	9	2.11
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB3	9	2.11
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD11	1	2.09
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD12	1	2.09
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD13	1	2.09
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD11	1	2.09
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD12	1	2.09
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD13	1	2.09
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD11	1	2.09
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD12	1	2.09
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD13	1	2.09
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD11	1	2.09
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD12	1	2.09
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD13	1	2.09
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD11	1	2.09
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD12	1	2.09
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD13	1	2.09
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD11	1	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD12	1	2.09
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD13	1	2.09
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB1	1	2.09
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB2	1	2.09
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB3	1	2.09
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB1	1	2.09
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB2	1	2.09
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB3	1	2.09
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB1	1	2.09
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB2	1	2.09
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB3	1	2.09
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB1	1	2.09
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB2	1	2.09
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB3	1	2.09
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB1	1	2.09
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB2	1	2.09
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB3	1	2.09
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB1	1	2.09
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB2	1	2.09
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB3	1	2.09
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD11	10	2.07
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD12	10	2.07
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD13	10	2.07
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD11	10	2.07
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD12	10	2.07
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD13	10	2.07
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD11	10	2.07
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD12	10	2.07
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD13	10	2.07
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD11	10	2.07
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD12	10	2.07
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD13	10	2.07
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD11	10	2.07
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD12	10	2.07
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD13	10	2.07
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD11	10	2.07
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD12	10	2.07
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD13	10	2.07
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB1	10	2.07
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB2	10	2.07
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB3	10	2.07
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB1	10	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB2	10	2.07
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB3	10	2.07
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB1	10	2.07
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB2	10	2.07
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB3	10	2.07
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB1	10	2.07
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB2	10	2.07
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB3	10	2.07
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB1	10	2.07
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB2	10	2.07
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB3	10	2.07
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB1	10	2.07
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB2	10	2.07
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB3	10	2.07
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD11	5	1.98
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD12	5	1.98
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD13	5	1.98
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD11	5	1.98
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD12	5	1.98
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD13	5	1.98
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD11	5	1.98
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD12	5	1.98
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD13	5	1.98
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD11	5	1.98
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD12	5	1.98
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD13	5	1.98
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD11	5	1.98
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD12	5	1.98
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD13	5	1.98
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD11	5	1.98
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD12	5	1.98
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD13	5	1.98
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB1	5	1.98
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB2	5	1.98
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB3	5	1.98
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB1	5	1.98
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB2	5	1.98
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB3	5	1.98
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB1	5	1.98
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB2	5	1.98
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB3	5	1.98
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB1	5	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB2	5	1.98
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB3	5	1.98
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB1	5	1.98
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB2	5	1.98
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB3	5	1.98
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB1	5	1.98
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB2	5	1.98
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB3	5	1.98
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB1	8	1.97
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB2	8	1.97
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB3	8	1.97
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB1	8	1.97
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB2	8	1.97
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB3	8	1.97
(2,14)	1:B:380:ALA:HB1	1:B:348:GLU:HA	8	1.97
(2,14)	1:B:380:ALA:HB2	1:B:348:GLU:HA	8	1.97
(2,14)	1:B:380:ALA:HB3	1:B:348:GLU:HA	8	1.97
(2,14)	1:A:380:ALA:HB1	1:A:348:GLU:HA	8	1.97
(2,14)	1:A:380:ALA:HB2	1:A:348:GLU:HA	8	1.97
(2,14)	1:A:380:ALA:HB3	1:A:348:GLU:HA	8	1.97
(2,13)	1:B:379:GLU:HG3	1:B:352:ASN:HD22	8	1.95
(2,13)	1:A:379:GLU:HG3	1:A:352:ASN:HD22	8	1.95
(2,12)	1:B:352:ASN:HD22	1:B:379:GLU:HG3	8	1.95
(2,12)	1:A:352:ASN:HD22	1:A:379:GLU:HG3	8	1.95
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD11	7	1.88
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD12	7	1.88
(2,33)	1:B:380:ALA:HB1	1:B:351:LEU:HD13	7	1.88
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD11	7	1.88
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD12	7	1.88
(2,33)	1:B:380:ALA:HB2	1:B:351:LEU:HD13	7	1.88
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD11	7	1.88
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD12	7	1.88
(2,33)	1:B:380:ALA:HB3	1:B:351:LEU:HD13	7	1.88
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD11	7	1.88
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD12	7	1.88
(2,33)	1:A:380:ALA:HB1	1:A:351:LEU:HD13	7	1.88
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD11	7	1.88
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD12	7	1.88
(2,33)	1:A:380:ALA:HB2	1:A:351:LEU:HD13	7	1.88
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD11	7	1.88
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD12	7	1.88
(2,33)	1:A:380:ALA:HB3	1:A:351:LEU:HD13	7	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB1	7	1.88
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB2	7	1.88
(2,32)	1:A:351:LEU:HD11	1:A:380:ALA:HB3	7	1.88
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB1	7	1.88
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB2	7	1.88
(2,32)	1:A:351:LEU:HD12	1:A:380:ALA:HB3	7	1.88
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB1	7	1.88
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB2	7	1.88
(2,32)	1:A:351:LEU:HD13	1:A:380:ALA:HB3	7	1.88
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB1	7	1.88
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB2	7	1.88
(2,32)	1:B:351:LEU:HD11	1:B:380:ALA:HB3	7	1.88
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB1	7	1.88
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB2	7	1.88
(2,32)	1:B:351:LEU:HD12	1:B:380:ALA:HB3	7	1.88
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB1	7	1.88
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB2	7	1.88
(2,32)	1:B:351:LEU:HD13	1:B:380:ALA:HB3	7	1.88
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB1	9	1.81
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB2	9	1.81
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB3	9	1.81
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB1	9	1.81
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB2	9	1.81
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB3	9	1.81
(2,14)	1:B:380:ALA:HB1	1:B:348:GLU:HA	9	1.81
(2,14)	1:B:380:ALA:HB2	1:B:348:GLU:HA	9	1.81
(2,14)	1:B:380:ALA:HB3	1:B:348:GLU:HA	9	1.81
(2,14)	1:A:380:ALA:HB1	1:A:348:GLU:HA	9	1.81
(2,14)	1:A:380:ALA:HB2	1:A:348:GLU:HA	9	1.81
(2,14)	1:A:380:ALA:HB3	1:A:348:GLU:HA	9	1.81
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB1	6	1.8
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB2	6	1.8
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB3	6	1.8
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB1	6	1.8
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB2	6	1.8
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB3	6	1.8
(2,14)	1:B:380:ALA:HB1	1:B:348:GLU:HA	6	1.8
(2,14)	1:B:380:ALA:HB2	1:B:348:GLU:HA	6	1.8
(2,14)	1:B:380:ALA:HB3	1:B:348:GLU:HA	6	1.8
(2,14)	1:A:380:ALA:HB1	1:A:348:GLU:HA	6	1.8
(2,14)	1:A:380:ALA:HB2	1:A:348:GLU:HA	6	1.8
(2,14)	1:A:380:ALA:HB3	1:A:348:GLU:HA	6	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB1	3	1.79
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB2	3	1.79
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB3	3	1.79
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB1	3	1.79
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB2	3	1.79
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB3	3	1.79
(2,14)	1:B:380:ALA:HB1	1:B:348:GLU:HA	3	1.79
(2,14)	1:B:380:ALA:HB2	1:B:348:GLU:HA	3	1.79
(2,14)	1:B:380:ALA:HB3	1:B:348:GLU:HA	3	1.79
(2,14)	1:A:380:ALA:HB1	1:A:348:GLU:HA	3	1.79
(2,14)	1:A:380:ALA:HB2	1:A:348:GLU:HA	3	1.79
(2,14)	1:A:380:ALA:HB3	1:A:348:GLU:HA	3	1.79
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB1	1	1.78
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB2	1	1.78
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB3	1	1.78
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB1	1	1.78
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB2	1	1.78
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB3	1	1.78
(2,14)	1:B:380:ALA:HB1	1:B:348:GLU:HA	1	1.78
(2,14)	1:B:380:ALA:HB2	1:B:348:GLU:HA	1	1.78
(2,14)	1:B:380:ALA:HB3	1:B:348:GLU:HA	1	1.78
(2,14)	1:A:380:ALA:HB1	1:A:348:GLU:HA	1	1.78
(2,14)	1:A:380:ALA:HB2	1:A:348:GLU:HA	1	1.78
(2,14)	1:A:380:ALA:HB3	1:A:348:GLU:HA	1	1.78
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB1	4	1.73
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB2	4	1.73
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB3	4	1.73
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB1	4	1.73
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB2	4	1.73
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB3	4	1.73
(2,14)	1:B:380:ALA:HB1	1:B:348:GLU:HA	4	1.73
(2,14)	1:B:380:ALA:HB2	1:B:348:GLU:HA	4	1.73
(2,14)	1:B:380:ALA:HB3	1:B:348:GLU:HA	4	1.73
(2,14)	1:A:380:ALA:HB1	1:A:348:GLU:HA	4	1.73
(2,14)	1:A:380:ALA:HB2	1:A:348:GLU:HA	4	1.73
(2,14)	1:A:380:ALA:HB3	1:A:348:GLU:HA	4	1.73
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB1	2	1.71
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB2	2	1.71
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB3	2	1.71
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB1	2	1.71
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB2	2	1.71
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB3	2	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,14)	1:B:380:ALA:HB1	1:B:348:GLU:HA	2	1.71
(2,14)	1:B:380:ALA:HB2	1:B:348:GLU:HA	2	1.71
(2,14)	1:B:380:ALA:HB3	1:B:348:GLU:HA	2	1.71
(2,14)	1:A:380:ALA:HB1	1:A:348:GLU:HA	2	1.71
(2,14)	1:A:380:ALA:HB2	1:A:348:GLU:HA	2	1.71
(2,14)	1:A:380:ALA:HB3	1:A:348:GLU:HA	2	1.71
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB1	8	1.7
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB2	8	1.7
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB3	8	1.7
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB1	8	1.7
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB2	8	1.7
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB3	8	1.7
(2,22)	1:B:380:ALA:HB1	1:B:352:ASN:H	8	1.7
(2,22)	1:B:380:ALA:HB2	1:B:352:ASN:H	8	1.7
(2,22)	1:B:380:ALA:HB3	1:B:352:ASN:H	8	1.7
(2,22)	1:A:380:ALA:HB1	1:A:352:ASN:H	8	1.7
(2,22)	1:A:380:ALA:HB2	1:A:352:ASN:H	8	1.7
(2,22)	1:A:380:ALA:HB3	1:A:352:ASN:H	8	1.7
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB1	7	1.7
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB2	7	1.7
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB3	7	1.7
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB1	7	1.7
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB2	7	1.7
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB3	7	1.7
(2,14)	1:B:380:ALA:HB1	1:B:348:GLU:HA	7	1.7
(2,14)	1:B:380:ALA:HB2	1:B:348:GLU:HA	7	1.7
(2,14)	1:B:380:ALA:HB3	1:B:348:GLU:HA	7	1.7
(2,14)	1:A:380:ALA:HB1	1:A:348:GLU:HA	7	1.7
(2,14)	1:A:380:ALA:HB2	1:A:348:GLU:HA	7	1.7
(2,14)	1:A:380:ALA:HB3	1:A:348:GLU:HA	7	1.7
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB1	5	1.67
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB2	5	1.67
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB3	5	1.67
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB1	5	1.67
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB2	5	1.67
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB3	5	1.67
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB1	10	1.67
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB2	10	1.67
(2,15)	1:A:348:GLU:HA	1:A:380:ALA:HB3	10	1.67
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB1	10	1.67
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB2	10	1.67
(2,15)	1:B:348:GLU:HA	1:B:380:ALA:HB3	10	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,14)	1:B:380:ALA:HB1	1:B:348:GLU:HA	5	1.67
(2,14)	1:B:380:ALA:HB2	1:B:348:GLU:HA	5	1.67
(2,14)	1:B:380:ALA:HB3	1:B:348:GLU:HA	5	1.67
(2,14)	1:A:380:ALA:HB1	1:A:348:GLU:HA	5	1.67
(2,14)	1:A:380:ALA:HB2	1:A:348:GLU:HA	5	1.67
(2,14)	1:A:380:ALA:HB3	1:A:348:GLU:HA	5	1.67
(2,14)	1:B:380:ALA:HB1	1:B:348:GLU:HA	10	1.67
(2,14)	1:B:380:ALA:HB2	1:B:348:GLU:HA	10	1.67
(2,14)	1:B:380:ALA:HB3	1:B:348:GLU:HA	10	1.67
(2,14)	1:A:380:ALA:HB1	1:A:348:GLU:HA	10	1.67
(2,14)	1:A:380:ALA:HB2	1:A:348:GLU:HA	10	1.67
(2,14)	1:A:380:ALA:HB3	1:A:348:GLU:HA	10	1.67
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB1	9	1.57
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB2	9	1.57
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB3	9	1.57
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB1	9	1.57
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB2	9	1.57
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB3	9	1.57
(2,22)	1:B:380:ALA:HB1	1:B:352:ASN:H	9	1.57
(2,22)	1:B:380:ALA:HB2	1:B:352:ASN:H	9	1.57
(2,22)	1:B:380:ALA:HB3	1:B:352:ASN:H	9	1.57
(2,22)	1:A:380:ALA:HB1	1:A:352:ASN:H	9	1.57
(2,22)	1:A:380:ALA:HB2	1:A:352:ASN:H	9	1.57
(2,22)	1:A:380:ALA:HB3	1:A:352:ASN:H	9	1.57
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB1	3	1.52
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB2	3	1.52
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB3	3	1.52
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB1	3	1.52
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB2	3	1.52
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB3	3	1.52
(2,22)	1:B:380:ALA:HB1	1:B:352:ASN:H	3	1.52
(2,22)	1:B:380:ALA:HB2	1:B:352:ASN:H	3	1.52
(2,22)	1:B:380:ALA:HB3	1:B:352:ASN:H	3	1.52
(2,22)	1:A:380:ALA:HB1	1:A:352:ASN:H	3	1.52
(2,22)	1:A:380:ALA:HB2	1:A:352:ASN:H	3	1.52
(2,22)	1:A:380:ALA:HB3	1:A:352:ASN:H	3	1.52
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB1	6	1.43
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB2	6	1.43
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB3	6	1.43
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB1	6	1.43
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB2	6	1.43
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB3	6	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:B:380:ALA:HB1	1:B:352:ASN:H	6	1.43
(2,22)	1:B:380:ALA:HB2	1:B:352:ASN:H	6	1.43
(2,22)	1:B:380:ALA:HB3	1:B:352:ASN:H	6	1.43
(2,22)	1:A:380:ALA:HB1	1:A:352:ASN:H	6	1.43
(2,22)	1:A:380:ALA:HB2	1:A:352:ASN:H	6	1.43
(2,22)	1:A:380:ALA:HB3	1:A:352:ASN:H	6	1.43
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB1	2	1.38
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB2	2	1.38
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB3	2	1.38
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB1	2	1.38
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB2	2	1.38
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB3	2	1.38
(2,22)	1:B:380:ALA:HB1	1:B:352:ASN:H	2	1.38
(2,22)	1:B:380:ALA:HB2	1:B:352:ASN:H	2	1.38
(2,22)	1:B:380:ALA:HB3	1:B:352:ASN:H	2	1.38
(2,22)	1:A:380:ALA:HB1	1:A:352:ASN:H	2	1.38
(2,22)	1:A:380:ALA:HB2	1:A:352:ASN:H	2	1.38
(2,22)	1:A:380:ALA:HB3	1:A:352:ASN:H	2	1.38
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB1	4	1.37
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB2	4	1.37
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB3	4	1.37
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB1	4	1.37
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB2	4	1.37
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB3	4	1.37
(2,22)	1:B:380:ALA:HB1	1:B:352:ASN:H	4	1.37
(2,22)	1:B:380:ALA:HB2	1:B:352:ASN:H	4	1.37
(2,22)	1:B:380:ALA:HB3	1:B:352:ASN:H	4	1.37
(2,22)	1:A:380:ALA:HB1	1:A:352:ASN:H	4	1.37
(2,22)	1:A:380:ALA:HB2	1:A:352:ASN:H	4	1.37
(2,22)	1:A:380:ALA:HB3	1:A:352:ASN:H	4	1.37
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB1	10	1.35
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB2	10	1.35
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB3	10	1.35
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB1	10	1.35
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB2	10	1.35
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB3	10	1.35
(2,22)	1:B:380:ALA:HB1	1:B:352:ASN:H	10	1.35
(2,22)	1:B:380:ALA:HB2	1:B:352:ASN:H	10	1.35
(2,22)	1:B:380:ALA:HB3	1:B:352:ASN:H	10	1.35
(2,22)	1:A:380:ALA:HB1	1:A:352:ASN:H	10	1.35
(2,22)	1:A:380:ALA:HB2	1:A:352:ASN:H	10	1.35
(2,22)	1:A:380:ALA:HB3	1:A:352:ASN:H	10	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB1	4	1.32
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB2	4	1.32
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB3	4	1.32
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB1	4	1.32
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB2	4	1.32
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB3	4	1.32
(2,40)	1:B:380:ALA:HB1	1:B:383:VAL:HB	4	1.32
(2,40)	1:B:380:ALA:HB2	1:B:383:VAL:HB	4	1.32
(2,40)	1:B:380:ALA:HB3	1:B:383:VAL:HB	4	1.32
(2,40)	1:A:380:ALA:HB1	1:A:383:VAL:HB	4	1.32
(2,40)	1:A:380:ALA:HB2	1:A:383:VAL:HB	4	1.32
(2,40)	1:A:380:ALA:HB3	1:A:383:VAL:HB	4	1.32
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB1	1	1.32
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB2	1	1.32
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB3	1	1.32
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB1	1	1.32
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB2	1	1.32
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB3	1	1.32
(2,22)	1:B:380:ALA:HB1	1:B:352:ASN:H	1	1.32
(2,22)	1:B:380:ALA:HB2	1:B:352:ASN:H	1	1.32
(2,22)	1:B:380:ALA:HB3	1:B:352:ASN:H	1	1.32
(2,22)	1:A:380:ALA:HB1	1:A:352:ASN:H	1	1.32
(2,22)	1:A:380:ALA:HB2	1:A:352:ASN:H	1	1.32
(2,22)	1:A:380:ALA:HB3	1:A:352:ASN:H	1	1.32
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB1	8	1.32
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB2	8	1.32
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB3	8	1.32
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB1	8	1.32
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB2	8	1.32
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB3	8	1.32
(2,16)	1:B:380:ALA:HB1	1:B:348:GLU:HB3	8	1.32
(2,16)	1:B:380:ALA:HB2	1:B:348:GLU:HB3	8	1.32
(2,16)	1:B:380:ALA:HB3	1:B:348:GLU:HB3	8	1.32
(2,16)	1:A:380:ALA:HB1	1:A:348:GLU:HB3	8	1.32
(2,16)	1:A:380:ALA:HB2	1:A:348:GLU:HB3	8	1.32
(2,16)	1:A:380:ALA:HB3	1:A:348:GLU:HB3	8	1.32
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB1	3	1.29
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB2	3	1.29
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB3	3	1.29
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB1	3	1.29
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB2	3	1.29
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB3	3	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB1	5	1.29
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB2	5	1.29
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB3	5	1.29
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB1	5	1.29
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB2	5	1.29
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB3	5	1.29
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB1	9	1.29
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB2	9	1.29
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB3	9	1.29
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB1	9	1.29
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB2	9	1.29
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB3	9	1.29
(2,40)	1:B:380:ALA:HB1	1:B:383:VAL:HB	3	1.29
(2,40)	1:B:380:ALA:HB2	1:B:383:VAL:HB	3	1.29
(2,40)	1:B:380:ALA:HB3	1:B:383:VAL:HB	3	1.29
(2,40)	1:A:380:ALA:HB1	1:A:383:VAL:HB	3	1.29
(2,40)	1:A:380:ALA:HB2	1:A:383:VAL:HB	3	1.29
(2,40)	1:A:380:ALA:HB3	1:A:383:VAL:HB	3	1.29
(2,40)	1:B:380:ALA:HB1	1:B:383:VAL:HB	5	1.29
(2,40)	1:B:380:ALA:HB2	1:B:383:VAL:HB	5	1.29
(2,40)	1:B:380:ALA:HB3	1:B:383:VAL:HB	5	1.29
(2,40)	1:A:380:ALA:HB1	1:A:383:VAL:HB	5	1.29
(2,40)	1:A:380:ALA:HB2	1:A:383:VAL:HB	5	1.29
(2,40)	1:A:380:ALA:HB3	1:A:383:VAL:HB	5	1.29
(2,40)	1:B:380:ALA:HB1	1:B:383:VAL:HB	9	1.29
(2,40)	1:B:380:ALA:HB2	1:B:383:VAL:HB	9	1.29
(2,40)	1:B:380:ALA:HB3	1:B:383:VAL:HB	9	1.29
(2,40)	1:A:380:ALA:HB1	1:A:383:VAL:HB	9	1.29
(2,40)	1:A:380:ALA:HB2	1:A:383:VAL:HB	9	1.29
(2,40)	1:A:380:ALA:HB3	1:A:383:VAL:HB	9	1.29
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB1	8	1.26
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB2	8	1.26
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB3	8	1.26
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB1	8	1.26
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB2	8	1.26
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB3	8	1.26
(2,40)	1:B:380:ALA:HB1	1:B:383:VAL:HB	8	1.26
(2,40)	1:B:380:ALA:HB2	1:B:383:VAL:HB	8	1.26
(2,40)	1:B:380:ALA:HB3	1:B:383:VAL:HB	8	1.26
(2,40)	1:A:380:ALA:HB1	1:A:383:VAL:HB	8	1.26
(2,40)	1:A:380:ALA:HB2	1:A:383:VAL:HB	8	1.26
(2,40)	1:A:380:ALA:HB3	1:A:383:VAL:HB	8	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB1	7	1.25
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB2	7	1.25
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB3	7	1.25
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB1	7	1.25
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB2	7	1.25
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB3	7	1.25
(2,40)	1:B:380:ALA:HB1	1:B:383:VAL:HB	7	1.25
(2,40)	1:B:380:ALA:HB2	1:B:383:VAL:HB	7	1.25
(2,40)	1:B:380:ALA:HB3	1:B:383:VAL:HB	7	1.25
(2,40)	1:A:380:ALA:HB1	1:A:383:VAL:HB	7	1.25
(2,40)	1:A:380:ALA:HB2	1:A:383:VAL:HB	7	1.25
(2,40)	1:A:380:ALA:HB3	1:A:383:VAL:HB	7	1.25
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB1	3	1.25
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB2	3	1.25
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB3	3	1.25
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB1	3	1.25
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB2	3	1.25
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB3	3	1.25
(2,16)	1:B:380:ALA:HB1	1:B:348:GLU:HB3	3	1.25
(2,16)	1:B:380:ALA:HB2	1:B:348:GLU:HB3	3	1.25
(2,16)	1:B:380:ALA:HB3	1:B:348:GLU:HB3	3	1.25
(2,16)	1:A:380:ALA:HB1	1:A:348:GLU:HB3	3	1.25
(2,16)	1:A:380:ALA:HB2	1:A:348:GLU:HB3	3	1.25
(2,16)	1:A:380:ALA:HB3	1:A:348:GLU:HB3	3	1.25
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB1	6	1.23
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB2	6	1.23
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB3	6	1.23
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB1	6	1.23
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB2	6	1.23
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB3	6	1.23
(2,40)	1:B:380:ALA:HB1	1:B:383:VAL:HB	6	1.23
(2,40)	1:B:380:ALA:HB2	1:B:383:VAL:HB	6	1.23
(2,40)	1:B:380:ALA:HB3	1:B:383:VAL:HB	6	1.23
(2,40)	1:A:380:ALA:HB1	1:A:383:VAL:HB	6	1.23
(2,40)	1:A:380:ALA:HB2	1:A:383:VAL:HB	6	1.23
(2,40)	1:A:380:ALA:HB3	1:A:383:VAL:HB	6	1.23
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB1	1	1.22
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB2	1	1.22
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB3	1	1.22
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB1	1	1.22
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB2	1	1.22
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB3	1	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,40)	1:B:380:ALA:HB1	1:B:383:VAL:HB	1	1.22
(2,40)	1:B:380:ALA:HB2	1:B:383:VAL:HB	1	1.22
(2,40)	1:B:380:ALA:HB3	1:B:383:VAL:HB	1	1.22
(2,40)	1:A:380:ALA:HB1	1:A:383:VAL:HB	1	1.22
(2,40)	1:A:380:ALA:HB2	1:A:383:VAL:HB	1	1.22
(2,40)	1:A:380:ALA:HB3	1:A:383:VAL:HB	1	1.22
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB1	1	1.22
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB2	1	1.22
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB3	1	1.22
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB1	1	1.22
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB2	1	1.22
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB3	1	1.22
(2,16)	1:B:380:ALA:HB1	1:B:348:GLU:HB3	1	1.22
(2,16)	1:B:380:ALA:HB2	1:B:348:GLU:HB3	1	1.22
(2,16)	1:B:380:ALA:HB3	1:B:348:GLU:HB3	1	1.22
(2,16)	1:A:380:ALA:HB1	1:A:348:GLU:HB3	1	1.22
(2,16)	1:A:380:ALA:HB2	1:A:348:GLU:HB3	1	1.22
(2,16)	1:A:380:ALA:HB3	1:A:348:GLU:HB3	1	1.22
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB1	10	1.21
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB2	10	1.21
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB3	10	1.21
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB1	10	1.21
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB2	10	1.21
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB3	10	1.21
(2,40)	1:B:380:ALA:HB1	1:B:383:VAL:HB	10	1.21
(2,40)	1:B:380:ALA:HB2	1:B:383:VAL:HB	10	1.21
(2,40)	1:B:380:ALA:HB3	1:B:383:VAL:HB	10	1.21
(2,40)	1:A:380:ALA:HB1	1:A:383:VAL:HB	10	1.21
(2,40)	1:A:380:ALA:HB2	1:A:383:VAL:HB	10	1.21
(2,40)	1:A:380:ALA:HB3	1:A:383:VAL:HB	10	1.21
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB1	7	1.21
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB2	7	1.21
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB3	7	1.21
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB1	7	1.21
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB2	7	1.21
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB3	7	1.21
(2,22)	1:B:380:ALA:HB1	1:B:352:ASN:H	7	1.21
(2,22)	1:B:380:ALA:HB2	1:B:352:ASN:H	7	1.21
(2,22)	1:B:380:ALA:HB3	1:B:352:ASN:H	7	1.21
(2,22)	1:A:380:ALA:HB1	1:A:352:ASN:H	7	1.21
(2,22)	1:A:380:ALA:HB2	1:A:352:ASN:H	7	1.21
(2,22)	1:A:380:ALA:HB3	1:A:352:ASN:H	7	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB1	8	1.19
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB2	8	1.19
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB3	8	1.19
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB1	8	1.19
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB2	8	1.19
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB3	8	1.19
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB1	8	1.19
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB2	8	1.19
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB3	8	1.19
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB1	8	1.19
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB2	8	1.19
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB3	8	1.19
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB1	8	1.19
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB2	8	1.19
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB3	8	1.19
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB1	8	1.19
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB2	8	1.19
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB3	8	1.19
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD21	8	1.19
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD22	8	1.19
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD23	8	1.19
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD21	8	1.19
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD22	8	1.19
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD23	8	1.19
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD21	8	1.19
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD22	8	1.19
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD23	8	1.19
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD21	8	1.19
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD22	8	1.19
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD23	8	1.19
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD21	8	1.19
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD22	8	1.19
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD23	8	1.19
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD21	8	1.19
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD22	8	1.19
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD23	8	1.19
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB1	2	1.18
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB2	2	1.18
(2,41)	1:B:383:VAL:HB	1:B:380:ALA:HB3	2	1.18
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB1	2	1.18
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB2	2	1.18
(2,41)	1:A:383:VAL:HB	1:A:380:ALA:HB3	2	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,40)	1:B:380:ALA:HB1	1:B:383:VAL:HB	2	1.18
(2,40)	1:B:380:ALA:HB2	1:B:383:VAL:HB	2	1.18
(2,40)	1:B:380:ALA:HB3	1:B:383:VAL:HB	2	1.18
(2,40)	1:A:380:ALA:HB1	1:A:383:VAL:HB	2	1.18
(2,40)	1:A:380:ALA:HB2	1:A:383:VAL:HB	2	1.18
(2,40)	1:A:380:ALA:HB3	1:A:383:VAL:HB	2	1.18
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB1	6	1.18
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB2	6	1.18
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB3	6	1.18
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB1	6	1.18
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB2	6	1.18
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB3	6	1.18
(2,16)	1:B:380:ALA:HB1	1:B:348:GLU:HB3	6	1.18
(2,16)	1:B:380:ALA:HB2	1:B:348:GLU:HB3	6	1.18
(2,16)	1:B:380:ALA:HB3	1:B:348:GLU:HB3	6	1.18
(2,16)	1:A:380:ALA:HB1	1:A:348:GLU:HB3	6	1.18
(2,16)	1:A:380:ALA:HB2	1:A:348:GLU:HB3	6	1.18
(2,16)	1:A:380:ALA:HB3	1:A:348:GLU:HB3	6	1.18
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB1	9	1.17
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB2	9	1.17
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB3	9	1.17
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB1	9	1.17
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB2	9	1.17
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB3	9	1.17
(2,16)	1:B:380:ALA:HB1	1:B:348:GLU:HB3	9	1.17
(2,16)	1:B:380:ALA:HB2	1:B:348:GLU:HB3	9	1.17
(2,16)	1:B:380:ALA:HB3	1:B:348:GLU:HB3	9	1.17
(2,16)	1:A:380:ALA:HB1	1:A:348:GLU:HB3	9	1.17
(2,16)	1:A:380:ALA:HB2	1:A:348:GLU:HB3	9	1.17
(2,16)	1:A:380:ALA:HB3	1:A:348:GLU:HB3	9	1.17
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB1	3	1.12
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB2	3	1.12
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB3	3	1.12
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB1	3	1.12
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB2	3	1.12
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB3	3	1.12
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB1	3	1.12
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB2	3	1.12
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB3	3	1.12
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB1	3	1.12
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB2	3	1.12
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB3	3	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB1	3	1.12
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB2	3	1.12
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB3	3	1.12
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB1	3	1.12
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB2	3	1.12
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB3	3	1.12
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD21	3	1.12
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD22	3	1.12
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD23	3	1.12
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD21	3	1.12
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD22	3	1.12
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD23	3	1.12
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD21	3	1.12
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD22	3	1.12
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD23	3	1.12
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD21	3	1.12
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD22	3	1.12
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD23	3	1.12
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD21	3	1.12
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD22	3	1.12
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD23	3	1.12
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD21	3	1.12
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD22	3	1.12
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD23	3	1.12
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB1	5	1.1
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB2	5	1.1
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB3	5	1.1
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB1	5	1.1
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB2	5	1.1
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB3	5	1.1
(2,16)	1:B:380:ALA:HB1	1:B:348:GLU:HB3	5	1.1
(2,16)	1:B:380:ALA:HB2	1:B:348:GLU:HB3	5	1.1
(2,16)	1:B:380:ALA:HB3	1:B:348:GLU:HB3	5	1.1
(2,16)	1:A:380:ALA:HB1	1:A:348:GLU:HB3	5	1.1
(2,16)	1:A:380:ALA:HB2	1:A:348:GLU:HB3	5	1.1
(2,16)	1:A:380:ALA:HB3	1:A:348:GLU:HB3	5	1.1
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB1	9	1.09
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB2	9	1.09
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB3	9	1.09
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB1	9	1.09
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB2	9	1.09
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB3	9	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB1	9	1.09
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB2	9	1.09
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB3	9	1.09
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB1	9	1.09
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB2	9	1.09
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB3	9	1.09
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB1	9	1.09
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB2	9	1.09
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB3	9	1.09
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB1	9	1.09
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB2	9	1.09
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB3	9	1.09
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD21	9	1.09
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD22	9	1.09
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD23	9	1.09
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD21	9	1.09
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD22	9	1.09
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD23	9	1.09
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD21	9	1.09
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD22	9	1.09
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD23	9	1.09
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD21	9	1.09
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD22	9	1.09
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD23	9	1.09
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD21	9	1.09
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD22	9	1.09
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD23	9	1.09
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD21	9	1.09
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD22	9	1.09
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD23	9	1.09
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB1	2	1.09
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB2	2	1.09
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB3	2	1.09
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB1	2	1.09
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB2	2	1.09
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB3	2	1.09
(2,16)	1:B:380:ALA:HB1	1:B:348:GLU:HB3	2	1.09
(2,16)	1:B:380:ALA:HB2	1:B:348:GLU:HB3	2	1.09
(2,16)	1:B:380:ALA:HB3	1:B:348:GLU:HB3	2	1.09
(2,16)	1:A:380:ALA:HB1	1:A:348:GLU:HB3	2	1.09
(2,16)	1:A:380:ALA:HB2	1:A:348:GLU:HB3	2	1.09
(2,16)	1:A:380:ALA:HB3	1:A:348:GLU:HB3	2	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB1	5	1.08
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB2	5	1.08
(2,23)	1:B:352:ASN:H	1:B:380:ALA:HB3	5	1.08
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB1	5	1.08
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB2	5	1.08
(2,23)	1:A:352:ASN:H	1:A:380:ALA:HB3	5	1.08
(2,22)	1:B:380:ALA:HB1	1:B:352:ASN:H	5	1.08
(2,22)	1:B:380:ALA:HB2	1:B:352:ASN:H	5	1.08
(2,22)	1:B:380:ALA:HB3	1:B:352:ASN:H	5	1.08
(2,22)	1:A:380:ALA:HB1	1:A:352:ASN:H	5	1.08
(2,22)	1:A:380:ALA:HB2	1:A:352:ASN:H	5	1.08
(2,22)	1:A:380:ALA:HB3	1:A:352:ASN:H	5	1.08
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB1	2	1.05
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB2	2	1.05
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB3	2	1.05
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB1	2	1.05
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB2	2	1.05
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB3	2	1.05
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB1	2	1.05
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB2	2	1.05
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB3	2	1.05
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB1	2	1.05
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB2	2	1.05
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB3	2	1.05
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB1	2	1.05
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB2	2	1.05
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB3	2	1.05
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB1	2	1.05
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB2	2	1.05
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB3	2	1.05
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD21	2	1.05
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD22	2	1.05
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD23	2	1.05
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD21	2	1.05
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD22	2	1.05
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD23	2	1.05
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD21	2	1.05
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD22	2	1.05
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD23	2	1.05
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD21	2	1.05
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD22	2	1.05
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD23	2	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD21	2	1.05
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD22	2	1.05
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD23	2	1.05
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD21	2	1.05
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD22	2	1.05
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD23	2	1.05
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB1	4	1.04
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB2	4	1.04
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB3	4	1.04
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB1	4	1.04
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB2	4	1.04
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB3	4	1.04
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB1	4	1.04
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB2	4	1.04
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB3	4	1.04
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB1	4	1.04
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB2	4	1.04
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB3	4	1.04
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB1	4	1.04
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB2	4	1.04
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB3	4	1.04
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB1	4	1.04
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB2	4	1.04
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB3	4	1.04
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD21	4	1.04
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD22	4	1.04
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD23	4	1.04
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD21	4	1.04
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD22	4	1.04
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD23	4	1.04
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD21	4	1.04
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD22	4	1.04
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD23	4	1.04
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD21	4	1.04
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD22	4	1.04
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD23	4	1.04
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD21	4	1.04
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD22	4	1.04
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD23	4	1.04
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD21	4	1.04
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD22	4	1.04
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD23	4	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB1	10	1.03
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB2	10	1.03
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB3	10	1.03
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB1	10	1.03
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB2	10	1.03
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB3	10	1.03
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB1	10	1.03
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB2	10	1.03
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB3	10	1.03
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB1	10	1.03
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB2	10	1.03
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB3	10	1.03
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB1	10	1.03
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB2	10	1.03
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB3	10	1.03
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB1	10	1.03
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB2	10	1.03
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB3	10	1.03
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD21	10	1.03
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD22	10	1.03
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD23	10	1.03
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD21	10	1.03
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD22	10	1.03
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD23	10	1.03
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD21	10	1.03
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD22	10	1.03
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD23	10	1.03
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD21	10	1.03
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD22	10	1.03
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD23	10	1.03
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD21	10	1.03
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD22	10	1.03
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD23	10	1.03
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD21	10	1.03
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD22	10	1.03
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD23	10	1.03
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB1	6	0.99
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB2	6	0.99
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB3	6	0.99
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB1	6	0.99
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB2	6	0.99
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB3	6	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB1	6	0.99
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB2	6	0.99
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB3	6	0.99
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB1	6	0.99
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB2	6	0.99
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB3	6	0.99
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB1	6	0.99
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB2	6	0.99
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB3	6	0.99
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB1	6	0.99
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB2	6	0.99
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB3	6	0.99
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD21	6	0.99
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD22	6	0.99
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD23	6	0.99
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD21	6	0.99
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD22	6	0.99
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD23	6	0.99
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD21	6	0.99
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD22	6	0.99
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD23	6	0.99
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD21	6	0.99
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD22	6	0.99
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD23	6	0.99
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD21	6	0.99
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD22	6	0.99
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD23	6	0.99
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD21	6	0.99
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD22	6	0.99
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD23	6	0.99
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB1	7	0.97
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB2	7	0.97
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB3	7	0.97
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB1	7	0.97
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB2	7	0.97
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB3	7	0.97
(2,16)	1:B:380:ALA:HB1	1:B:348:GLU:HB3	7	0.97
(2,16)	1:B:380:ALA:HB2	1:B:348:GLU:HB3	7	0.97
(2,16)	1:B:380:ALA:HB3	1:B:348:GLU:HB3	7	0.97
(2,16)	1:A:380:ALA:HB1	1:A:348:GLU:HB3	7	0.97
(2,16)	1:A:380:ALA:HB2	1:A:348:GLU:HB3	7	0.97
(2,16)	1:A:380:ALA:HB3	1:A:348:GLU:HB3	7	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB1	1	0.95
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB2	1	0.95
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB3	1	0.95
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB1	1	0.95
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB2	1	0.95
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB3	1	0.95
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB1	1	0.95
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB2	1	0.95
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB3	1	0.95
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB1	1	0.95
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB2	1	0.95
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB3	1	0.95
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB1	1	0.95
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB2	1	0.95
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB3	1	0.95
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB1	1	0.95
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB2	1	0.95
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB3	1	0.95
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD21	1	0.95
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD22	1	0.95
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD23	1	0.95
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD21	1	0.95
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD22	1	0.95
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD23	1	0.95
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD21	1	0.95
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD22	1	0.95
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD23	1	0.95
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD21	1	0.95
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD22	1	0.95
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD23	1	0.95
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD21	1	0.95
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD22	1	0.95
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD23	1	0.95
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD21	1	0.95
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD22	1	0.95
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD23	1	0.95
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB1	10	0.93
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB2	10	0.93
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB3	10	0.93
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB1	10	0.93
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB2	10	0.93
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB3	10	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,16)	1:B:380:ALA:HB1	1:B:348:GLU:HB3	10	0.93
(2,16)	1:B:380:ALA:HB2	1:B:348:GLU:HB3	10	0.93
(2,16)	1:B:380:ALA:HB3	1:B:348:GLU:HB3	10	0.93
(2,16)	1:A:380:ALA:HB1	1:A:348:GLU:HB3	10	0.93
(2,16)	1:A:380:ALA:HB2	1:A:348:GLU:HB3	10	0.93
(2,16)	1:A:380:ALA:HB3	1:A:348:GLU:HB3	10	0.93
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB1	4	0.92
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB2	4	0.92
(2,17)	1:A:348:GLU:HB3	1:A:380:ALA:HB3	4	0.92
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB1	4	0.92
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB2	4	0.92
(2,17)	1:B:348:GLU:HB3	1:B:380:ALA:HB3	4	0.92
(2,16)	1:B:380:ALA:HB1	1:B:348:GLU:HB3	4	0.92
(2,16)	1:B:380:ALA:HB2	1:B:348:GLU:HB3	4	0.92
(2,16)	1:B:380:ALA:HB3	1:B:348:GLU:HB3	4	0.92
(2,16)	1:A:380:ALA:HB1	1:A:348:GLU:HB3	4	0.92
(2,16)	1:A:380:ALA:HB2	1:A:348:GLU:HB3	4	0.92
(2,16)	1:A:380:ALA:HB3	1:A:348:GLU:HB3	4	0.92
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB1	7	0.89
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB2	7	0.89
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB3	7	0.89
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB1	7	0.89
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB2	7	0.89
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB3	7	0.89
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB1	7	0.89
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB2	7	0.89
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB3	7	0.89
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB1	7	0.89
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB2	7	0.89
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB3	7	0.89
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB1	7	0.89
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB2	7	0.89
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB3	7	0.89
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB1	7	0.89
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB2	7	0.89
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB3	7	0.89
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD21	7	0.89
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD22	7	0.89
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD23	7	0.89
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD21	7	0.89
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD22	7	0.89
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD23	7	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD21	7	0.89
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD22	7	0.89
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD23	7	0.89
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD21	7	0.89
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD22	7	0.89
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD23	7	0.89
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD21	7	0.89
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD22	7	0.89
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD23	7	0.89
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD21	7	0.89
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD22	7	0.89
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD23	7	0.89
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB1	5	0.88
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB2	5	0.88
(2,21)	1:A:351:LEU:HD21	1:A:380:ALA:HB3	5	0.88
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB1	5	0.88
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB2	5	0.88
(2,21)	1:A:351:LEU:HD22	1:A:380:ALA:HB3	5	0.88
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB1	5	0.88
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB2	5	0.88
(2,21)	1:A:351:LEU:HD23	1:A:380:ALA:HB3	5	0.88
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB1	5	0.88
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB2	5	0.88
(2,21)	1:B:351:LEU:HD21	1:B:380:ALA:HB3	5	0.88
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB1	5	0.88
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB2	5	0.88
(2,21)	1:B:351:LEU:HD22	1:B:380:ALA:HB3	5	0.88
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB1	5	0.88
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB2	5	0.88
(2,21)	1:B:351:LEU:HD23	1:B:380:ALA:HB3	5	0.88
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD21	5	0.88
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD22	5	0.88
(2,20)	1:B:380:ALA:HB1	1:B:351:LEU:HD23	5	0.88
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD21	5	0.88
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD22	5	0.88
(2,20)	1:B:380:ALA:HB2	1:B:351:LEU:HD23	5	0.88
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD21	5	0.88
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD22	5	0.88
(2,20)	1:B:380:ALA:HB3	1:B:351:LEU:HD23	5	0.88
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD21	5	0.88
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD22	5	0.88
(2,20)	1:A:380:ALA:HB1	1:A:351:LEU:HD23	5	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD21	5	0.88
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD22	5	0.88
(2,20)	1:A:380:ALA:HB2	1:A:351:LEU:HD23	5	0.88
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD21	5	0.88
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD22	5	0.88
(2,20)	1:A:380:ALA:HB3	1:A:351:LEU:HD23	5	0.88
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE1	4	0.8
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE2	4	0.8
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE1	4	0.8
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE2	4	0.8
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE1	4	0.77
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE2	4	0.77
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE1	4	0.77
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE2	4	0.77
(2,6)	1:A:394:ASP:HB3	1:A:397:THR:HB	4	0.74
(2,6)	1:B:394:ASP:HB3	1:B:397:THR:HB	4	0.74
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE1	7	0.7
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE2	7	0.7
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE1	7	0.7
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE2	7	0.7
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE1	1	0.63
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE2	1	0.63
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE1	1	0.63
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE2	1	0.63
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE1	3	0.63
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE2	3	0.63
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE1	3	0.63
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE2	3	0.63
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE1	3	0.62
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE2	3	0.62
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE1	3	0.62
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE2	3	0.62
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE1	7	0.57
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE2	7	0.57
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE1	7	0.57
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE2	7	0.57
(2,6)	1:A:394:ASP:HB3	1:A:397:THR:HB	2	0.55
(2,6)	1:B:394:ASP:HB3	1:B:397:THR:HB	2	0.55
(2,6)	1:A:394:ASP:HB3	1:A:397:THR:HB	3	0.51
(2,6)	1:B:394:ASP:HB3	1:B:397:THR:HB	3	0.51
(1,538)	1:B:372:HIS:HD2	1:B:371:GLU:HG2	3	0.51
(1,538)	1:A:372:HIS:HD2	1:A:371:GLU:HG2	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE1	1	0.47
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE2	1	0.47
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE1	1	0.47
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE2	1	0.47
(1,538)	1:B:372:HIS:HD2	1:B:371:GLU:HG2	7	0.47
(1,538)	1:A:372:HIS:HD2	1:A:371:GLU:HG2	7	0.47
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE1	5	0.44
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE2	5	0.44
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE1	5	0.44
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE2	5	0.44
(2,6)	1:A:394:ASP:HB3	1:A:397:THR:HB	8	0.43
(2,6)	1:B:394:ASP:HB3	1:B:397:THR:HB	8	0.43
(2,6)	1:A:394:ASP:HB3	1:A:397:THR:HB	1	0.42
(2,6)	1:B:394:ASP:HB3	1:B:397:THR:HB	1	0.42
(2,6)	1:A:394:ASP:HB3	1:A:397:THR:HB	6	0.42
(2,6)	1:B:394:ASP:HB3	1:B:397:THR:HB	6	0.42
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE1	2	0.4
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE2	2	0.4
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE1	2	0.4
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE2	2	0.4
(2,6)	1:A:394:ASP:HB3	1:A:397:THR:HB	9	0.37
(2,6)	1:B:394:ASP:HB3	1:B:397:THR:HB	9	0.37
(1,988)	1:A:393:GLN:HG3	1:A:390:TRP:HA	4	0.37
(1,988)	1:B:393:GLN:HG3	1:B:390:TRP:HA	4	0.37
(2,6)	1:A:394:ASP:HB3	1:A:397:THR:HB	5	0.36
(2,6)	1:B:394:ASP:HB3	1:B:397:THR:HB	5	0.36
(2,6)	1:A:394:ASP:HB3	1:A:397:THR:HB	7	0.34
(2,6)	1:B:394:ASP:HB3	1:B:397:THR:HB	7	0.34
(1,675)	1:A:359:TRP:HZ2	1:A:377:THR:HA	1	0.33
(1,675)	1:B:359:TRP:HZ2	1:B:377:THR:HA	1	0.33
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE1	2	0.3
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE2	2	0.3
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE1	2	0.3
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE2	2	0.3
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE1	6	0.3
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE2	6	0.3
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE1	6	0.3
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE2	6	0.3
(1,675)	1:A:359:TRP:HZ2	1:A:377:THR:HA	4	0.3
(1,675)	1:B:359:TRP:HZ2	1:B:377:THR:HA	4	0.3
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE1	9	0.29
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE2	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE1	9	0.29
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE2	9	0.29
(1,352)	1:B:361:HIS:HD2	1:B:361:HIS:HA	3	0.29
(1,352)	1:A:361:HIS:HD2	1:A:361:HIS:HA	3	0.29
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE1	5	0.28
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE2	5	0.28
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE1	5	0.28
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE2	5	0.28
(1,988)	1:A:393:GLN:HG3	1:A:390:TRP:HA	7	0.27
(1,988)	1:B:393:GLN:HG3	1:B:390:TRP:HA	7	0.27
(1,988)	1:A:393:GLN:HG3	1:A:390:TRP:HA	8	0.27
(1,988)	1:B:393:GLN:HG3	1:B:390:TRP:HA	8	0.27
(1,988)	1:A:393:GLN:HG3	1:A:390:TRP:HA	10	0.27
(1,988)	1:B:393:GLN:HG3	1:B:390:TRP:HA	10	0.27
(1,675)	1:A:359:TRP:HZ2	1:A:377:THR:HA	7	0.25
(1,675)	1:B:359:TRP:HZ2	1:B:377:THR:HA	7	0.25
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE1	9	0.23
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE2	9	0.23
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE1	9	0.23
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE2	9	0.23
(2,6)	1:A:394:ASP:HB3	1:A:397:THR:HB	10	0.22
(2,6)	1:B:394:ASP:HB3	1:B:397:THR:HB	10	0.22
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE1	8	0.22
(1,982)	1:A:393:GLN:HE21	1:A:368:TYR:HE2	8	0.22
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE1	8	0.22
(1,982)	1:B:393:GLN:HE21	1:B:368:TYR:HE2	8	0.22
(1,686)	1:A:374:ASP:HB2	1:A:377:THR:HG21	1	0.21
(1,686)	1:A:374:ASP:HB2	1:A:377:THR:HG22	1	0.21
(1,686)	1:A:374:ASP:HB2	1:A:377:THR:HG23	1	0.21
(1,686)	1:B:374:ASP:HB2	1:B:377:THR:HG21	1	0.21
(1,686)	1:B:374:ASP:HB2	1:B:377:THR:HG22	1	0.21
(1,686)	1:B:374:ASP:HB2	1:B:377:THR:HG23	1	0.21
(1,988)	1:A:393:GLN:HG3	1:A:390:TRP:HA	5	0.2
(1,988)	1:B:393:GLN:HG3	1:B:390:TRP:HA	5	0.2
(1,352)	1:B:361:HIS:HD2	1:B:361:HIS:HA	4	0.2
(1,352)	1:A:361:HIS:HD2	1:A:361:HIS:HA	4	0.2
(1,898)	1:A:386:LEU:HA	1:A:389:SER:HB2	9	0.17
(1,898)	1:B:386:LEU:HA	1:B:389:SER:HB2	9	0.17
(1,675)	1:A:359:TRP:HZ2	1:A:377:THR:HA	8	0.17
(1,675)	1:B:359:TRP:HZ2	1:B:377:THR:HA	8	0.17
(1,352)	1:B:361:HIS:HD2	1:B:361:HIS:HA	1	0.17
(1,352)	1:A:361:HIS:HD2	1:A:361:HIS:HA	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,240)	1:A:348:GLU:HB2	1:A:351:LEU:HD11	4	0.16
(1,240)	1:A:348:GLU:HB2	1:A:351:LEU:HD12	4	0.16
(1,240)	1:A:348:GLU:HB2	1:A:351:LEU:HD13	4	0.16
(1,240)	1:B:348:GLU:HB2	1:B:351:LEU:HD11	4	0.16
(1,240)	1:B:348:GLU:HB2	1:B:351:LEU:HD12	4	0.16
(1,240)	1:B:348:GLU:HB2	1:B:351:LEU:HD13	4	0.16
(1,1166)	1:B:401:LEU:HB3	1:B:390:TRP:HH2	4	0.16
(1,1166)	1:A:401:LEU:HB3	1:A:390:TRP:HH2	4	0.16
(1,352)	1:B:361:HIS:HD2	1:B:361:HIS:HA	10	0.15
(1,352)	1:A:361:HIS:HD2	1:A:361:HIS:HA	10	0.15
(1,302)	1:A:358:THR:HG21	1:A:354:SER:HB2	2	0.15
(1,302)	1:A:358:THR:HG22	1:A:354:SER:HB2	2	0.15
(1,302)	1:A:358:THR:HG23	1:A:354:SER:HB2	2	0.15
(1,302)	1:B:358:THR:HG21	1:B:354:SER:HB2	2	0.15
(1,302)	1:B:358:THR:HG22	1:B:354:SER:HB2	2	0.15
(1,302)	1:B:358:THR:HG23	1:B:354:SER:HB2	2	0.15
(1,301)	1:A:354:SER:HB2	1:A:358:THR:HG21	2	0.15
(1,301)	1:A:354:SER:HB2	1:A:358:THR:HG22	2	0.15
(1,301)	1:A:354:SER:HB2	1:A:358:THR:HG23	2	0.15
(1,301)	1:B:354:SER:HB2	1:B:358:THR:HG21	2	0.15
(1,301)	1:B:354:SER:HB2	1:B:358:THR:HG22	2	0.15
(1,301)	1:B:354:SER:HB2	1:B:358:THR:HG23	2	0.15
(1,240)	1:A:348:GLU:HB2	1:A:351:LEU:HD11	10	0.15
(1,240)	1:A:348:GLU:HB2	1:A:351:LEU:HD12	10	0.15
(1,240)	1:A:348:GLU:HB2	1:A:351:LEU:HD13	10	0.15
(1,240)	1:B:348:GLU:HB2	1:B:351:LEU:HD11	10	0.15
(1,240)	1:B:348:GLU:HB2	1:B:351:LEU:HD12	10	0.15
(1,240)	1:B:348:GLU:HB2	1:B:351:LEU:HD13	10	0.15
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE1	6	0.13
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE2	6	0.13
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE1	6	0.13
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE2	6	0.13
(1,538)	1:B:372:HIS:HD2	1:B:371:GLU:HG2	10	0.13
(1,538)	1:A:372:HIS:HD2	1:A:371:GLU:HG2	10	0.13
(1,1166)	1:B:401:LEU:HB3	1:B:390:TRP:HH2	8	0.13
(1,1166)	1:A:401:LEU:HB3	1:A:390:TRP:HH2	8	0.13
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE1	8	0.12
(1,983)	1:A:393:GLN:HE22	1:A:368:TYR:HE2	8	0.12
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE1	8	0.12
(1,983)	1:B:393:GLN:HE22	1:B:368:TYR:HE2	8	0.12
(1,1166)	1:B:401:LEU:HB3	1:B:390:TRP:HH2	1	0.12
(1,1166)	1:A:401:LEU:HB3	1:A:390:TRP:HH2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,686)	1:A:374:ASP:HB2	1:A:377:THR:HG21	8	0.11
(1,686)	1:A:374:ASP:HB2	1:A:377:THR:HG22	8	0.11
(1,686)	1:A:374:ASP:HB2	1:A:377:THR:HG23	8	0.11
(1,686)	1:B:374:ASP:HB2	1:B:377:THR:HG21	8	0.11
(1,686)	1:B:374:ASP:HB2	1:B:377:THR:HG22	8	0.11
(1,686)	1:B:374:ASP:HB2	1:B:377:THR:HG23	8	0.11
(1,685)	1:B:377:THR:HG21	1:B:374:ASP:HA	1	0.11
(1,685)	1:B:377:THR:HG22	1:B:374:ASP:HA	1	0.11
(1,685)	1:B:377:THR:HG23	1:B:374:ASP:HA	1	0.11
(1,685)	1:A:377:THR:HG21	1:A:374:ASP:HA	1	0.11
(1,685)	1:A:377:THR:HG22	1:A:374:ASP:HA	1	0.11
(1,685)	1:A:377:THR:HG23	1:A:374:ASP:HA	1	0.11
(1,538)	1:B:372:HIS:HD2	1:B:371:GLU:HG2	4	0.11
(1,538)	1:A:372:HIS:HD2	1:A:371:GLU:HG2	4	0.11
(1,352)	1:B:361:HIS:HD2	1:B:361:HIS:HA	5	0.11
(1,352)	1:A:361:HIS:HD2	1:A:361:HIS:HA	5	0.11
(1,318)	1:A:359:TRP:H	1:A:358:THR:HB	1	0.11
(1,318)	1:B:359:TRP:H	1:B:358:THR:HB	1	0.11
(1,318)	1:A:359:TRP:H	1:A:358:THR:HB	3	0.11
(1,318)	1:B:359:TRP:H	1:B:358:THR:HB	3	0.11
(1,302)	1:A:358:THR:HG21	1:A:354:SER:HB2	8	0.11
(1,302)	1:A:358:THR:HG22	1:A:354:SER:HB2	8	0.11
(1,302)	1:A:358:THR:HG23	1:A:354:SER:HB2	8	0.11
(1,302)	1:B:358:THR:HG21	1:B:354:SER:HB2	8	0.11
(1,302)	1:B:358:THR:HG22	1:B:354:SER:HB2	8	0.11
(1,302)	1:B:358:THR:HG23	1:B:354:SER:HB2	8	0.11
(1,301)	1:A:354:SER:HB2	1:A:358:THR:HG21	8	0.11
(1,301)	1:A:354:SER:HB2	1:A:358:THR:HG22	8	0.11
(1,301)	1:A:354:SER:HB2	1:A:358:THR:HG23	8	0.11
(1,301)	1:B:354:SER:HB2	1:B:358:THR:HG21	8	0.11
(1,301)	1:B:354:SER:HB2	1:B:358:THR:HG22	8	0.11
(1,301)	1:B:354:SER:HB2	1:B:358:THR:HG23	8	0.11
(1,240)	1:A:348:GLU:HB2	1:A:351:LEU:HD11	3	0.11
(1,240)	1:A:348:GLU:HB2	1:A:351:LEU:HD12	3	0.11
(1,240)	1:A:348:GLU:HB2	1:A:351:LEU:HD13	3	0.11
(1,240)	1:B:348:GLU:HB2	1:B:351:LEU:HD11	3	0.11
(1,240)	1:B:348:GLU:HB2	1:B:351:LEU:HD12	3	0.11
(1,240)	1:B:348:GLU:HB2	1:B:351:LEU:HD13	3	0.11
(1,1166)	1:B:401:LEU:HB3	1:B:390:TRP:HH2	6	0.11
(1,1166)	1:A:401:LEU:HB3	1:A:390:TRP:HH2	6	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found