Full wwPDB NMR Structure Validation Report (i)

Dec 25, 2024 – 11:24 AM EST

PDB ID	:	6GVU
BMRB ID	:	34291
Title	:	NMR structure of the DNA-bound helix bundle domain from the functional pRN1 primase
Authors	:	Boudet, J.; Lipps, G.; Allain, F.H.-T.
Deposited on	:	2018-06-21

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:

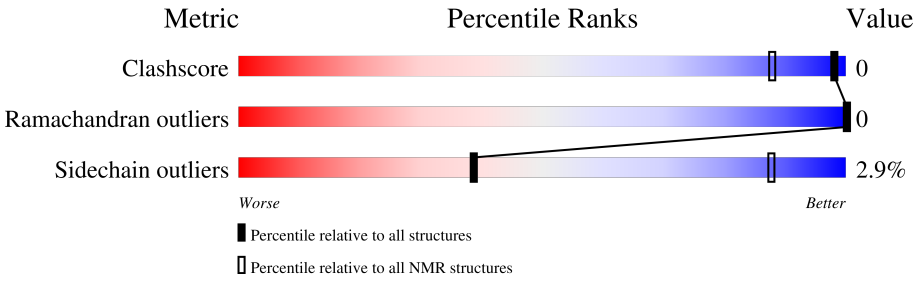
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 65%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	9	56% 44%
2	B	115	95% . .

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	B:257-B:342, B:347-B:370 (110)	0.67	8

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2224 atoms, of which 1094 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	9	283	87	104	30	54	8	0

- Molecule 2 is a protein called functional pRN1 primase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	115	1941	611	990	160	177	3	0

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

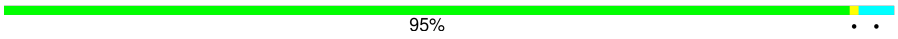
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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.

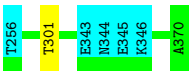
• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:





4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

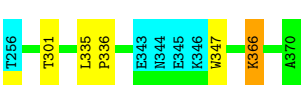
4.2.1 Score per residue for model 1

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:



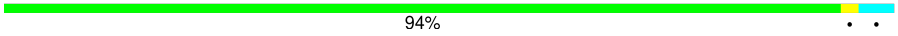
4.2.2 Score per residue for model 2

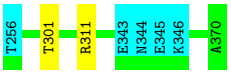
• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:





4.2.3 Score per residue for model 3

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:

4.2.4 Score per residue for model 4

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:

4.2.5 Score per residue for model 5

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

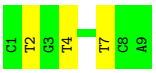
• Molecule 2: functional pRN1 primase

Chain B:

4.2.6 Score per residue for model 6

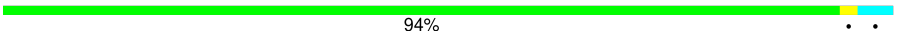
• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

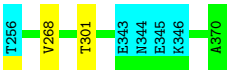
Chain A:



• Molecule 2: functional pRN1 primase

Chain B:

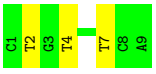




4.2.7 Score per residue for model 7

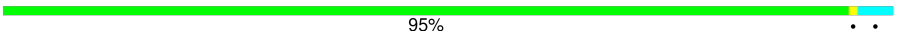
• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

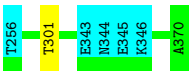
Chain A:



• Molecule 2: functional pRN1 primase

Chain B:





4.2.8 Score per residue for model 8 (medoid)

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A: 

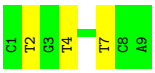
• Molecule 2: functional pRN1 primase

Chain B: 

4.2.9 Score per residue for model 9

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A: 



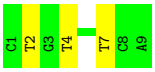
• Molecule 2: functional pRN1 primase

Chain B: 

4.2.10 Score per residue for model 10

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A: 



• Molecule 2: functional pRN1 primase

Chain B: 

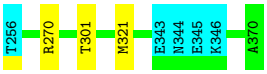
4.2.11 Score per residue for model 11

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:



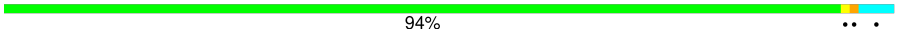
4.2.12 Score per residue for model 12

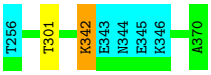
• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:





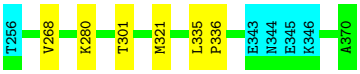
4.2.13 Score per residue for model 13

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:



4.2.14 Score per residue for model 14

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:

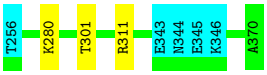
4.2.15 Score per residue for model 15

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:



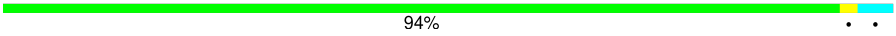
4.2.16 Score per residue for model 16

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:



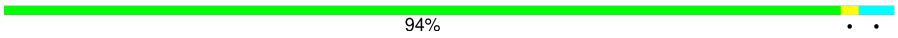
4.2.17 Score per residue for model 17

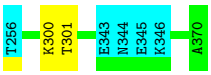
• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:

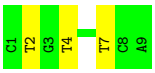




4.2.18 Score per residue for model 18

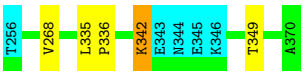
• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:



• Molecule 2: functional pRN1 primase

Chain B:



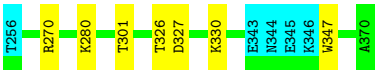
4.2.19 Score per residue for model 19

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:



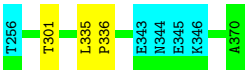
4.2.20 Score per residue for model 20

• Molecule 1: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*CP*A)-3')

Chain A:

• Molecule 2: functional pRN1 primase

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 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 calculation	
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	1186
Number of shifts mapped to atoms	1186
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	65%

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	1.06±0.01	0±0/199 (0.0± 0.0%)	1.65±0.02	5±1/305 (1.8± 0.3%)
2	B	0.49±0.00	0±0/927 (0.0± 0.0%)	0.70±0.01	0±0/1247 (0.0± 0.0%)
All	All	0.63	0/22520 (0.0%)	0.97	109/31040 (0.4%)

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	A	4	DT	O4'-C1'-N1	7.39	113.17	108.00	7	20
1	A	4	DT	C6-C5-C7	-6.41	119.06	122.90	13	20
1	A	2	DT	C6-C5-C7	-6.08	119.25	122.90	13	20
1	A	7	DT	C6-C5-C7	-5.89	119.37	122.90	19	20
1	A	6	DC	O4'-C1'-N1	5.63	111.94	108.00	8	13
1	A	2	DT	C4-C5-C6	5.31	121.19	118.00	19	2
1	A	4	DT	C4-C5-C6	5.29	121.17	118.00	8	8
1	A	5	DG	O4'-C1'-N9	5.15	111.61	108.00	17	1
1	A	7	DT	C4-C5-C6	5.15	121.09	118.00	10	5

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
2	B	909	950	949	1±1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	21760	21080	21060	12

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:342:LYS:HE2	2:B:342:LYS:HA	0.49	1.84	5	2
2:B:342:LYS:HE3	2:B:342:LYS:HA	0.48	1.85	18	1
2:B:366:LYS:HE2	2:B:366:LYS:HA	0.47	1.86	1	1
2:B:335:LEU:N	2:B:336:PRO:CD	0.43	2.81	20	4
2:B:335:LEU:N	2:B:336:PRO:HD3	0.43	2.28	4	2
2:B:291:LEU:HD22	2:B:291:LEU:C	0.40	2.36	9	1
2:B:327:ASP:HB3	2:B:330:LYS:HE2	0.40	1.93	19	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	109/115 (95%)	107±1 (98±1%)	2±1 (2±1%)	0±0 (0±0%)	100	100
All	All	2180/2300 (95%)	2145 (98%)	35 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	103/108 (95%)	100±1 (97±1%)	3±1 (3±1%)	39	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2060/2160 (95%)	2001 (97%)	59 (3%)	39 88

All 17 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	301	THR	19
2	B	270	ARG	6
2	B	311	ARG	4
2	B	326	THR	4
2	B	268	VAL	4
2	B	280	LYS	4
2	B	347	TRP	3
2	B	342	LYS	3
2	B	321	MET	3
2	B	349	THR	2
2	B	366	LYS	1
2	B	334	LEU	1
2	B	291	LEU	1
2	B	276	VAL	1
2	B	263	LEU	1
2	B	309	ARG	1
2	B	300	LYS	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 oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 65% for the well-defined parts and 64% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

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	1186
Number of shifts mapped to atoms	1186
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	66	-0.97 ± 0.29	Should be checked
$^{13}C_{\beta}$	90	0.27 ± 0.18	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	101	1.32 ± 0.52	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 65%, i.e. 1151 atoms were assigned a chemical shift out of a possible 1778. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	353/543 (65%)	191/218 (88%)	64/220 (29%)	98/105 (93%)
Sidechain	657/952 (69%)	452/615 (73%)	205/301 (68%)	0/36 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	68/107 (64%)	38/52 (73%)	27/49 (55%)	3/6 (50%)
Sugar	61/108 (56%)	61/63 (97%)	0/45 (0%)	0/0 (—%)
Base	12/68 (18%)	12/41 (29%)	0/16 (0%)	0/11 (0%)
Overall	1151/1778 (65%)	754/989 (76%)	296/631 (47%)	101/158 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 64%, i.e. 1177 atoms were assigned a chemical shift out of a possible 1843. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	364/568 (64%)	197/228 (86%)	66/230 (29%)	101/110 (92%)
Sidechain	672/992 (68%)	462/639 (72%)	210/315 (67%)	0/38 (0%)
Aromatic	68/107 (64%)	38/52 (73%)	27/49 (55%)	3/6 (50%)
Sugar	61/108 (56%)	61/63 (97%)	0/45 (0%)	0/0 (—%)
Base	12/68 (18%)	12/41 (29%)	0/16 (0%)	0/11 (0%)
Overall	1177/1843 (64%)	770/1023 (75%)	303/655 (46%)	104/165 (63%)

7.1.4 Statistically unusual chemical shifts (i)

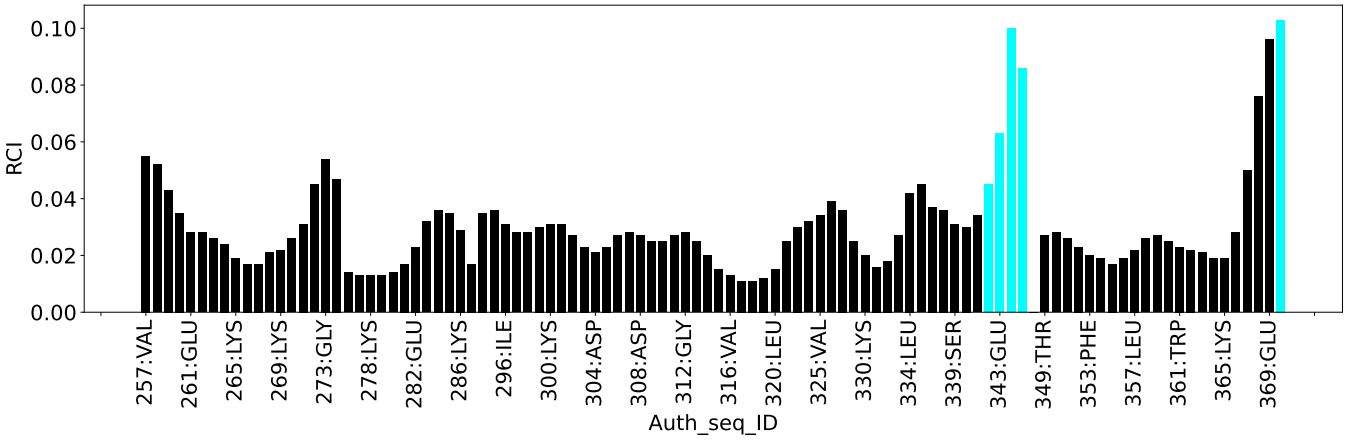
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	B	320	LEU	CD2	11.15	15.73 – 32.47	-7.7
1	B	320	LEU	HD11	2.35	-0.61 – 2.12	5.8
1	B	320	LEU	HD12	2.35	-0.61 – 2.12	5.8
1	B	320	LEU	HD13	2.35	-0.61 – 2.12	5.8

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 B:


RCI
0.10
0.08
0.06
0.04
0.02
0.00
257:VAL
261:GLU
265:LYS
269:LYS
273:GLY
278:LYS
282:GLU
286:LYS
296:ILE
300:LYS
304:ASP
308:ASP
312:GLY
316:VAL
320:LEU
325:VAL
330:LYS
334:LEU
339:SER
343:GLU
349:THR
353:PHE
357:LEU
361:TRP
365:LYS
369:GLU
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	1808
Intra-residue (|i-j|=0)	468
Sequential (|i-j|=1)	440
Medium range (|i-j|>1 and |i-j|<5)	403
Long range (|i-j|≥5)	256
Inter-chain	79
Hydrogen bond restraints	162
Disulfide bond restraints	0
Total dihedral-angle restraints	192
Number of unmapped restraints	0
Number of restraints per residue	16.1
Number of long range restraints per residue[1]	2.1

[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)	21.8	0.2
0.2-0.5 (Medium)	9.8	0.5
>0.5 (Large)	51.2	2.46

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.3	4.73
10.0-20.0 (Medium)	0.1	10.21
>20.0 (Large)	None	None

9 Distance violation analysis (i)

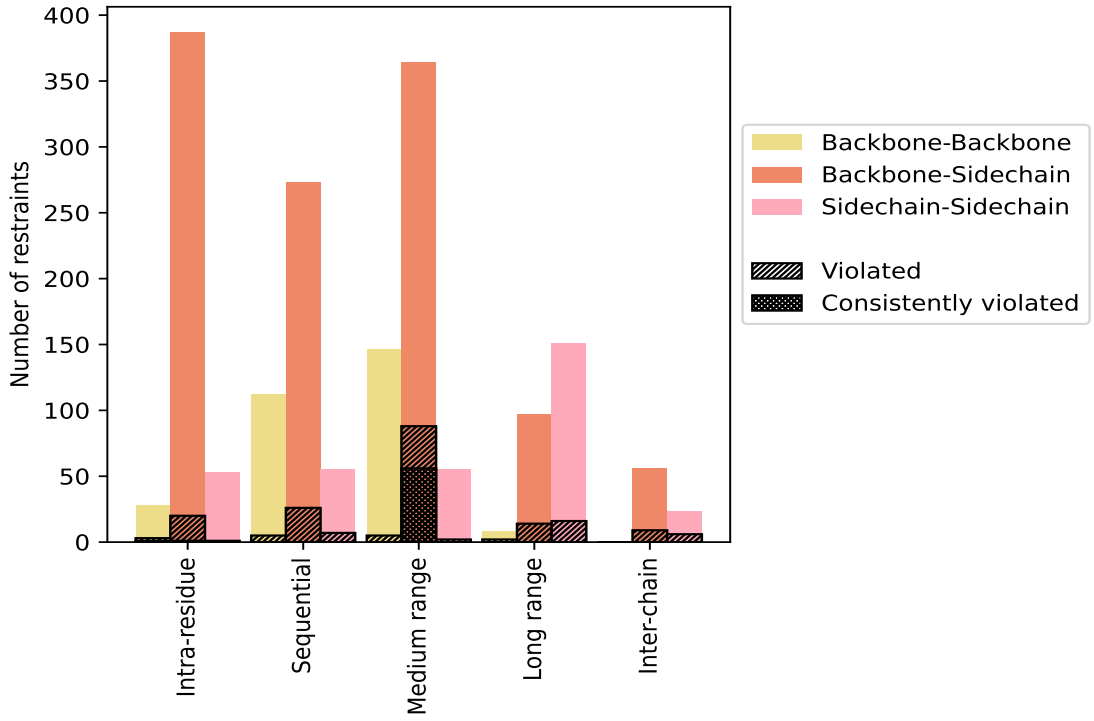
9.1 Summary of distance violations (i)

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)	468	25.9	24	5.1	1.3	2	0.4	0.1
Backbone-Backbone	28	1.5	3	10.7	0.2	1	3.6	0.1
Backbone-Sidechain	387	21.4	20	5.2	1.1	1	0.3	0.1
Sidechain-Sidechain	53	2.9	1	1.9	0.1	0	0.0	0.0
Sequential (|i-j|=1)	440	24.3	38	8.6	2.1	0	0.0	0.0
Backbone-Backbone	112	6.2	5	4.5	0.3	0	0.0	0.0
Backbone-Sidechain	273	15.1	26	9.5	1.4	0	0.0	0.0
Sidechain-Sidechain	55	3.0	7	12.7	0.4	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	403	22.3	19	4.7	1.1	0	0.0	0.0
Backbone-Backbone	146	8.1	5	3.4	0.3	0	0.0	0.0
Backbone-Sidechain	202	11.2	12	5.9	0.7	0	0.0	0.0
Sidechain-Sidechain	55	3.0	2	3.6	0.1	0	0.0	0.0
Long range (|i-j|≥5)	256	14.2	32	12.5	1.8	0	0.0	0.0
Backbone-Backbone	8	0.4	2	25.0	0.1	0	0.0	0.0
Backbone-Sidechain	97	5.4	14	14.4	0.8	0	0.0	0.0
Sidechain-Sidechain	151	8.4	16	10.6	0.9	0	0.0	0.0
Inter-chain	79	4.4	15	19.0	0.8	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	56	3.1	9	16.1	0.5	0	0.0	0.0
Sidechain-Sidechain	23	1.3	6	26.1	0.3	0	0.0	0.0
Hydrogen bond	162	9.0	76	46.9	4.2	56	34.6	3.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1808	100.0	204	11.3	11.3	58	3.2	3.2
Backbone-Backbone	294	16.3	15	5.1	0.8	1	0.3	0.1
Backbone-Sidechain	1177	65.1	157	13.3	8.7	57	4.8	3.2
Sidechain-Sidechain	337	18.6	32	9.5	1.8	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	7	9	66	2	4	88	0.58	2.46	0.41	0.59
2	5	6	66	5	3	85	0.57	2.02	0.36	0.6
3	6	8	63	7	3	87	0.54	1.11	0.34	0.59
4	5	8	67	5	4	89	0.56	1.92	0.37	0.58
5	8	8	70	3	2	91	0.54	1.52	0.35	0.56
6	7	7	66	2	4	86	0.6	2.34	0.39	0.66
7	6	6	68	5	4	89	0.58	2.4	0.41	0.57
8	2	5	65	3	4	79	0.6	1.55	0.33	0.62
9	5	7	66	3	3	84	0.57	1.31	0.34	0.64
10	6	4	66	6	3	85	0.57	1.49	0.34	0.63

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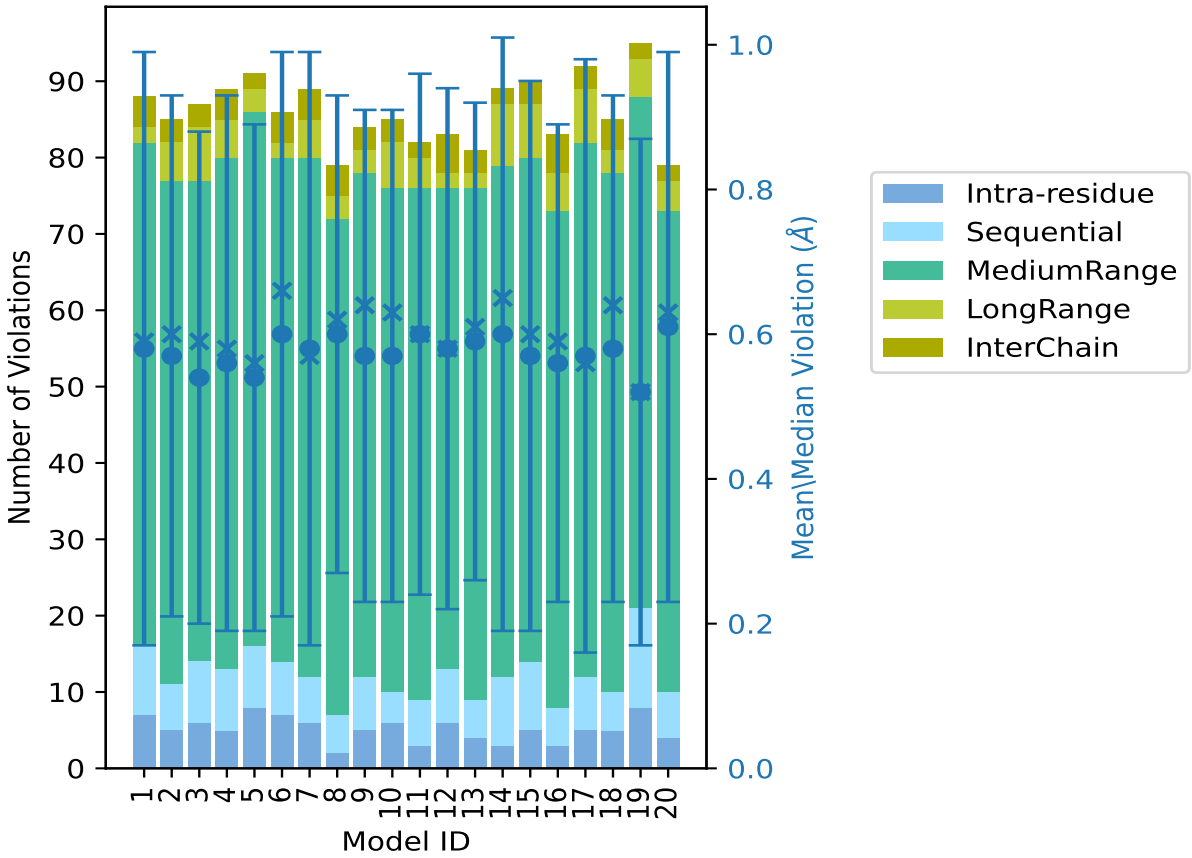
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	3	6	67	4	2	82	0.6	1.94	0.36	0.6
12	6	7	63	2	5	83	0.58	2.02	0.36	0.58
13	4	5	67	2	3	81	0.59	1.61	0.33	0.61
14	3	9	67	8	2	89	0.6	2.13	0.41	0.65
15	5	9	66	7	3	90	0.57	1.9	0.38	0.6
16	3	5	65	5	5	83	0.56	1.32	0.33	0.59
17	5	7	70	7	3	92	0.57	2.45	0.41	0.56
18	5	5	68	3	4	85	0.58	1.65	0.35	0.64
19	8	13	67	5	2	95	0.52	1.55	0.35	0.52
20	4	6	63	4	2	79	0.61	2.16	0.38	0.63

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

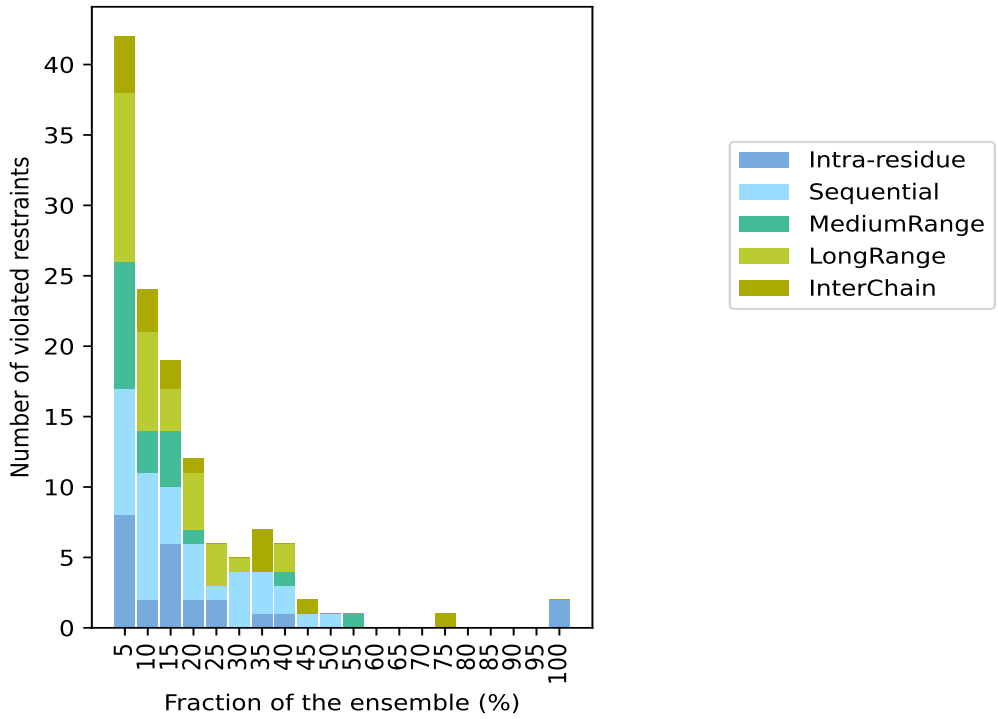
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1518(IR:444, SQ:402, MR:384, LR:224, IC:64) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
8	9	9	12	4	42	1	5.0
2	9	3	7	3	24	2	10.0
6	4	4	3	2	19	3	15.0
2	4	1	4	1	12	4	20.0
2	1	0	3	0	6	5	25.0
0	4	0	1	0	5	6	30.0
1	3	0	0	3	7	7	35.0
1	2	1	2	0	6	8	40.0
0	1	0	0	1	2	9	45.0
0	1	0	0	0	1	10	50.0
0	0	1	0	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	1	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
2	0	0	0	0	2	20	100.0

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

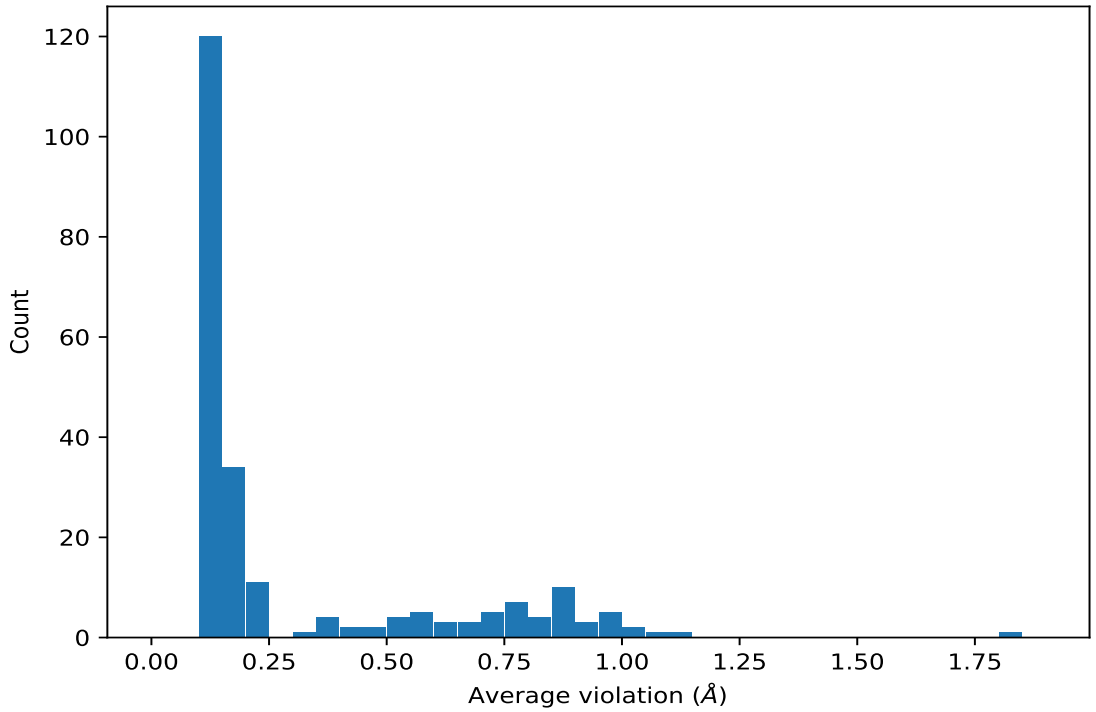
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of theviolation 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)
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	20	1.83	0.4	1.82
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	20	1.1	0.31	1.03
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	20	1.06	0.02	1.06
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	20	1.01	0.04	1.0
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	20	1.0	0.1	1.02
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	20	0.98	0.41	0.96
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	20	0.97	0.04	0.98
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	20	0.97	0.06	0.99
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	20	0.97	0.06	0.95
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	20	0.97	0.06	0.98
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	20	0.94	0.04	0.94
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	20	0.93	0.07	0.93
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	20	0.91	0.07	0.92
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	20	0.89	0.07	0.92
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	20	0.89	0.07	0.9
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	20	0.89	0.1	0.9

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	20	0.88	0.03	0.88
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	20	0.87	0.04	0.88
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	20	0.87	0.08	0.88
(6,150)	2:362:B:SER:N	2:358:B:SER:O	20	0.86	0.02	0.86
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	20	0.86	0.07	0.88
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	20	0.86	0.08	0.87
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	20	0.85	0.2	0.96
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	20	0.83	0.4	0.82
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	20	0.83	0.16	0.84
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	20	0.82	0.07	0.82
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	20	0.81	0.06	0.82
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	20	0.79	0.13	0.8
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	20	0.78	0.09	0.76
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	20	0.77	0.05	0.77
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	20	0.76	0.14	0.8
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	20	0.75	0.08	0.74
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	20	0.75	0.18	0.7
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	20	0.75	0.05	0.74
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	20	0.73	0.15	0.74
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	20	0.73	0.13	0.74
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	20	0.72	0.07	0.73
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	20	0.7	0.11	0.64
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	20	0.7	0.03	0.7
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	20	0.67	0.15	0.64
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	20	0.65	0.11	0.62
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	20	0.65	0.13	0.64
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	20	0.64	0.16	0.58
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	20	0.63	0.08	0.66
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	20	0.61	0.03	0.61
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	20	0.59	0.08	0.58
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	20	0.57	0.15	0.54
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	20	0.56	0.06	0.55
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	20	0.55	0.04	0.57
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	20	0.55	0.05	0.54
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	20	0.54	0.06	0.52
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	20	0.53	0.06	0.5
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	20	0.53	0.09	0.52
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	20	0.53	0.03	0.52
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	20	0.49	0.07	0.48
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	20	0.47	0.07	0.48
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	20	0.42	0.02	0.42
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	20	0.38	0.04	0.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	19	0.3	0.07	0.31
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	18	0.14	0.01	0.14
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	16	0.13	0.01	0.12
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	15	0.15	0.03	0.15
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	15	0.13	0.02	0.13
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	14	0.14	0.03	0.14
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	14	0.13	0.02	0.13
(6,24)	2:285:B:THR:H	2:281:B:GLU:O	12	0.4	0.34	0.3
(6,14)	2:270:B:ARG:H	2:266:B:GLU:O	12	0.14	0.03	0.14
(1,687)	2:263:B:LEU:HG	2:266:B:GLU:H	11	0.14	0.02	0.14
(1,1435)	1:5:A:DG:H3'	1:6:A:DC:H5	10	0.12	0.01	0.12
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB2	9	0.37	0.23	0.35
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB3	9	0.37	0.23	0.35
(6,68)	2:332:B:LEU:H	2:328:B:PRO:O	9	0.14	0.03	0.14
(1,1466)	1:7:A:DT:H1'	1:8:A:DC:H3'	9	0.13	0.01	0.13
(6,23)	2:285:B:THR:N	2:281:B:GLU:O	8	0.37	0.33	0.18
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB2	8	0.14	0.03	0.14
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB3	8	0.14	0.03	0.14
(1,1473)	1:8:A:DC:H3'	1:9:A:DA:H8	8	0.14	0.04	0.13
(1,586)	2:298:B:GLU:H	2:298:B:GLU:HG3	8	0.13	0.01	0.13
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG21	8	0.13	0.02	0.12
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG22	8	0.13	0.02	0.12
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG23	8	0.13	0.02	0.12
(1,994)	2:341:B:ALA:HA	2:353:B:PHE:HD2	8	0.12	0.02	0.12
(1,619)	2:301:B:THR:HB	2:302:B:TYR:HA	8	0.12	0.01	0.12
(4,64)	1:4:A:DT:H3	2:341:B:ALA:HA	7	0.17	0.03	0.15
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD2	7	0.15	0.03	0.16
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD3	7	0.15	0.03	0.16
(1,1002)	2:346:B:LYS:HB2	2:347:B:TRP:HD1	7	0.14	0.02	0.14
(1,1002)	2:346:B:LYS:HB3	2:347:B:TRP:HD1	7	0.14	0.02	0.14
(1,1445)	1:6:A:DC:H1'	1:7:A:DT:H6	7	0.14	0.04	0.12
(4,32)	1:4:A:DT:H3'	2:352:B:TYR:HD2	7	0.14	0.04	0.11
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5'	7	0.12	0.01	0.11
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5"	7	0.12	0.01	0.11
(1,1477)	1:9:A:DA:H1'	1:9:A:DA:H8	7	0.11	0.01	0.11
(1,618)	2:301:B:THR:HB	2:302:B:TYR:HE2	6	0.14	0.03	0.13
(1,1474)	1:8:A:DC:H5'	1:9:A:DA:H8	6	0.14	0.05	0.12
(1,1474)	1:8:A:DC:H5"	1:9:A:DA:H8	6	0.14	0.05	0.12
(1,1406)	1:3:A:DG:H3'	1:4:A:DT:H6	6	0.13	0.02	0.12
(1,1004)	2:266:B:GLU:HB3	2:361:B:TRP:HD1	6	0.12	0.01	0.12
(1,1462)	1:7:A:DT:H3'	1:8:A:DC:H6	6	0.11	0.01	0.12
(1,1369)	1:1:A:DC:H4'	1:1:A:DC:H6	5	0.15	0.03	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1219)	2:302:B:TYR:H	2:337:B:ARG:HB2	5	0.13	0.02	0.13
(1,1219)	2:302:B:TYR:H	2:337:B:ARG:HB3	5	0.13	0.02	0.13
(1,1470)	1:8:A:DC:H1'	1:8:A:DC:H3'	5	0.13	0.05	0.11
(1,513)	2:270:B:ARG:HD2	2:325:B:VAL:HA	5	0.13	0.02	0.13
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD21	5	0.12	0.02	0.12
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD22	5	0.12	0.02	0.12
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD23	5	0.12	0.02	0.12
(6,98)	2:355:B:ILE:H	2:351:B:LYS:O	5	0.11	0.01	0.11
(1,22)	2:359:B:LYS:HB3	2:360:B:ALA:H	5	0.11	0.0	0.11
(1,1461)	1:7:A:DT:H2'	1:8:A:DC:H6	4	0.18	0.03	0.19
(1,1461)	1:7:A:DT:H2"	1:8:A:DC:H6	4	0.18	0.03	0.19
(4,65)	1:4:A:DT:H3	2:340:B:LYS:H	4	0.16	0.06	0.16
(1,1324)	2:343:B:GLU:HA	2:344:B:ASN:HB2	4	0.16	0.02	0.17
(1,1324)	2:343:B:GLU:HA	2:344:B:ASN:HB3	4	0.16	0.02	0.17
(1,58)	2:276:B:VAL:H	2:330:B:LYS:HA	4	0.15	0.05	0.13
(1,1145)	2:280:B:LYS:HB2	2:281:B:GLU:H	4	0.14	0.02	0.15
(1,1145)	2:280:B:LYS:HB3	2:281:B:GLU:H	4	0.14	0.02	0.15
(1,1377)	1:1:A:DC:H4'	1:2:A:DT:H6	4	0.14	0.05	0.12
(1,351)	2:331:B:ILE:H	2:331:B:ILE:HG13	4	0.14	0.03	0.13
(1,523)	2:270:B:ARG:HD3	2:361:B:TRP:HZ2	4	0.13	0.01	0.13
(1,515)	2:270:B:ARG:HD3	2:325:B:VAL:HA	4	0.12	0.01	0.12
(1,886)	2:331:B:ILE:HG21	2:353:B:PHE:HA	4	0.12	0.01	0.12
(1,886)	2:331:B:ILE:HG22	2:353:B:PHE:HA	4	0.12	0.01	0.12
(1,886)	2:331:B:ILE:HG23	2:353:B:PHE:HA	4	0.12	0.01	0.12
(1,1413)	1:4:A:DT:H3'	1:4:A:DT:H6	4	0.11	0.0	0.11
(1,702)	2:363:B:VAL:HA	2:367:B:TYR:HB2	4	0.1	0.0	0.11
(1,1287)	2:330:B:LYS:HA	2:330:B:LYS:HG2	3	0.22	0.0	0.22
(1,1287)	2:330:B:LYS:HA	2:330:B:LYS:HG3	3	0.22	0.0	0.22
(1,1468)	1:8:A:DC:H5'	1:8:A:DC:H6	3	0.22	0.01	0.22
(1,1468)	1:8:A:DC:H5"	1:8:A:DC:H6	3	0.22	0.01	0.22
(4,28)	1:7:A:DT:H71	2:322:B:LYS:HD2	3	0.22	0.06	0.26
(4,28)	1:7:A:DT:H71	2:322:B:LYS:HD3	3	0.22	0.06	0.26
(4,28)	1:7:A:DT:H72	2:322:B:LYS:HD2	3	0.22	0.06	0.26
(4,28)	1:7:A:DT:H72	2:322:B:LYS:HD3	3	0.22	0.06	0.26
(4,28)	1:7:A:DT:H73	2:322:B:LYS:HD2	3	0.22	0.06	0.26
(4,28)	1:7:A:DT:H73	2:322:B:LYS:HD3	3	0.22	0.06	0.26
(1,1404)	1:3:A:DG:H1'	1:4:A:DT:H6	3	0.2	0.02	0.2
(1,638)	2:269:B:LYS:H	2:269:B:LYS:HD2	3	0.18	0.06	0.16
(1,638)	2:269:B:LYS:H	2:269:B:LYS:HD3	3	0.18	0.06	0.16
(1,1045)	2:311:B:ARG:HG2	2:315:B:HIS:HD2	3	0.17	0.0	0.17
(1,1045)	2:311:B:ARG:HG3	2:315:B:HIS:HD2	3	0.17	0.0	0.17
(4,62)	1:4:A:DT:H3	2:352:B:TYR:HD1	3	0.15	0.03	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,62)	1:4:A:DT:H3	2:352:B:TYR:HD2	3	0.15	0.03	0.16
(1,1396)	1:3:A:DG:H2'	1:3:A:DG:H8	3	0.14	0.02	0.13
(1,448)	2:332:B:LEU:HD11	2:342:B:LYS:H	3	0.13	0.03	0.12
(1,448)	2:332:B:LEU:HD12	2:342:B:LYS:H	3	0.13	0.03	0.12
(1,448)	2:332:B:LEU:HD13	2:342:B:LYS:H	3	0.13	0.03	0.12
(1,1155)	2:280:B:LYS:HG2	2:296:B:ILE:HD11	3	0.13	0.02	0.12
(1,1155)	2:280:B:LYS:HG2	2:296:B:ILE:HD12	3	0.13	0.02	0.12
(1,1155)	2:280:B:LYS:HG2	2:296:B:ILE:HD13	3	0.13	0.02	0.12
(1,1155)	2:280:B:LYS:HG3	2:296:B:ILE:HD11	3	0.13	0.02	0.12
(1,1155)	2:280:B:LYS:HG3	2:296:B:ILE:HD12	3	0.13	0.02	0.12
(1,1155)	2:280:B:LYS:HG3	2:296:B:ILE:HD13	3	0.13	0.02	0.12
(1,662)	2:276:B:VAL:HA	2:279:B:ILE:HG12	3	0.13	0.04	0.1
(6,34)	2:297:B:CYS:H	2:293:B:LYS:O	3	0.12	0.01	0.13
(1,1388)	1:2:A:DT:H1'	1:3:A:DG:H8	3	0.12	0.01	0.13
(1,1397)	1:3:A:DG:H3'	1:3:A:DG:H8	3	0.12	0.02	0.11
(6,8)	2:262:B:GLU:H	2:258:B:VAL:O	3	0.12	0.01	0.11
(1,1059)	2:266:B:GLU:HB3	2:361:B:TRP:HZ2	3	0.11	0.01	0.12
(1,1368)	1:1:A:DC:H3'	1:1:A:DC:H6	3	0.11	0.01	0.12
(1,1)	2:369:B:GLU:H	2:370:B:ALA:H	3	0.11	0.01	0.1
(1,720)	2:257:B:VAL:HA	2:261:B:GLU:HG2	3	0.11	0.01	0.1
(1,720)	2:257:B:VAL:HA	2:261:B:GLU:HG3	3	0.11	0.01	0.1
(1,1389)	1:2:A:DT:H3'	1:3:A:DG:H8	3	0.11	0.01	0.1
(1,614)	2:265:B:LYS:H	2:268:B:VAL:HB	3	0.1	0.0	0.1
(1,690)	2:368:B:LEU:H	2:368:B:LEU:HG	2	0.19	0.02	0.19
(1,1176)	2:292:B:ILE:HG12	2:296:B:ILE:HD11	2	0.18	0.02	0.18
(1,1176)	2:292:B:ILE:HG12	2:296:B:ILE:HD12	2	0.18	0.02	0.18
(1,1176)	2:292:B:ILE:HG12	2:296:B:ILE:HD13	2	0.18	0.02	0.18
(1,1176)	2:292:B:ILE:HG13	2:296:B:ILE:HD11	2	0.18	0.02	0.18
(1,1176)	2:292:B:ILE:HG13	2:296:B:ILE:HD12	2	0.18	0.02	0.18
(1,1176)	2:292:B:ILE:HG13	2:296:B:ILE:HD13	2	0.18	0.02	0.18
(4,60)	1:4:A:DT:H3	2:340:B:LYS:HA	2	0.18	0.01	0.18
(4,55)	1:4:A:DT:H3	2:340:B:LYS:HG2	2	0.18	0.06	0.18
(4,55)	1:4:A:DT:H3	2:340:B:LYS:HG3	2	0.18	0.06	0.18
(1,666)	2:276:B:VAL:HA	2:279:B:ILE:HG13	2	0.15	0.03	0.15
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG11	2	0.15	0.0	0.15
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG12	2	0.15	0.0	0.15
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG13	2	0.15	0.0	0.15
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG21	2	0.15	0.0	0.15
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG22	2	0.15	0.0	0.15
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG23	2	0.15	0.0	0.15
(1,495)	2:295:B:ILE:HG21	2:301:B:THR:H	2	0.14	0.02	0.14
(1,495)	2:295:B:ILE:HG22	2:301:B:THR:H	2	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,495)	2:295:B:ILE:HG23	2:301:B:THR:H	2	0.14	0.02	0.14
(1,1110)	2:273:B:GLY:HA2	2:274:B:LYS:HE2	2	0.14	0.02	0.14
(1,1110)	2:273:B:GLY:HA2	2:274:B:LYS:HE3	2	0.14	0.02	0.14
(1,1110)	2:273:B:GLY:HA3	2:274:B:LYS:HE2	2	0.14	0.02	0.14
(1,1110)	2:273:B:GLY:HA3	2:274:B:LYS:HE3	2	0.14	0.02	0.14
(1,1335)	2:351:B:LYS:HA	2:351:B:LYS:HD2	2	0.13	0.01	0.13
(1,1335)	2:351:B:LYS:HA	2:351:B:LYS:HD3	2	0.13	0.01	0.13
(1,669)	2:295:B:ILE:HG12	2:302:B:TYR:HD1	2	0.12	0.02	0.12
(1,919)	2:283:B:ILE:HG21	2:323:B:HIS:HB2	2	0.12	0.01	0.12
(1,919)	2:283:B:ILE:HG22	2:323:B:HIS:HB2	2	0.12	0.01	0.12
(1,919)	2:283:B:ILE:HG23	2:323:B:HIS:HB2	2	0.12	0.01	0.12
(6,100)	2:354:B:VAL:H	2:350:B:GLN:O	2	0.12	0.0	0.12
(1,367)	2:365:B:LYS:HB2	2:366:B:LYS:H	2	0.12	0.02	0.12
(1,727)	2:366:B:LYS:HG2	2:367:B:TYR:HB2	2	0.12	0.0	0.12
(1,727)	2:366:B:LYS:HG3	2:367:B:TYR:HB2	2	0.12	0.0	0.12
(1,881)	2:326:B:THR:HG21	2:360:B:ALA:HB1	2	0.12	0.0	0.12
(1,881)	2:326:B:THR:HG21	2:360:B:ALA:HB2	2	0.12	0.0	0.12
(1,881)	2:326:B:THR:HG21	2:360:B:ALA:HB3	2	0.12	0.0	0.12
(1,881)	2:326:B:THR:HG22	2:360:B:ALA:HB1	2	0.12	0.0	0.12
(1,881)	2:326:B:THR:HG22	2:360:B:ALA:HB2	2	0.12	0.0	0.12
(1,881)	2:326:B:THR:HG22	2:360:B:ALA:HB3	2	0.12	0.0	0.12
(1,881)	2:326:B:THR:HG23	2:360:B:ALA:HB1	2	0.12	0.0	0.12
(1,881)	2:326:B:THR:HG23	2:360:B:ALA:HB2	2	0.12	0.0	0.12
(1,881)	2:326:B:THR:HG23	2:360:B:ALA:HB3	2	0.12	0.0	0.12
(1,1449)	1:6:A:DC:H3'	1:7:A:DT:H4'	2	0.12	0.0	0.12
(1,850)	2:341:B:ALA:HB1	2:352:B:TYR:HB3	2	0.11	0.0	0.11
(1,850)	2:341:B:ALA:HB2	2:352:B:TYR:HB3	2	0.11	0.0	0.11
(1,850)	2:341:B:ALA:HB3	2:352:B:TYR:HB3	2	0.11	0.0	0.11
(1,1010)	2:314:B:TRP:HD1	2:315:B:HIS:HD2	2	0.11	0.01	0.11
(1,1288)	2:330:B:LYS:HB2	2:331:B:ILE:HA	2	0.11	0.0	0.11
(1,1288)	2:330:B:LYS:HB3	2:331:B:ILE:HA	2	0.11	0.0	0.11
(4,41)	1:4:A:DT:H5'	2:355:B:ILE:HG12	2	0.11	0.01	0.11
(4,41)	1:4:A:DT:H5'	2:355:B:ILE:HG13	2	0.11	0.01	0.11
(4,41)	1:4:A:DT:H5"	2:355:B:ILE:HG12	2	0.11	0.01	0.11
(4,41)	1:4:A:DT:H5"	2:355:B:ILE:HG13	2	0.11	0.01	0.11
(1,581)	2:261:B:GLU:HG2	2:262:B:GLU:H	2	0.11	0.0	0.11
(1,581)	2:261:B:GLU:HG3	2:262:B:GLU:H	2	0.11	0.0	0.11
(1,642)	2:300:B:LYS:HD2	2:301:B:THR:H	2	0.11	0.0	0.11
(1,642)	2:300:B:LYS:HD3	2:301:B:THR:H	2	0.11	0.0	0.11
(1,893)	2:295:B:ILE:HG21	2:302:B:TYR:HB3	2	0.11	0.0	0.11
(1,893)	2:295:B:ILE:HG22	2:302:B:TYR:HB3	2	0.11	0.0	0.11
(1,893)	2:295:B:ILE:HG23	2:302:B:TYR:HB3	2	0.11	0.0	0.11

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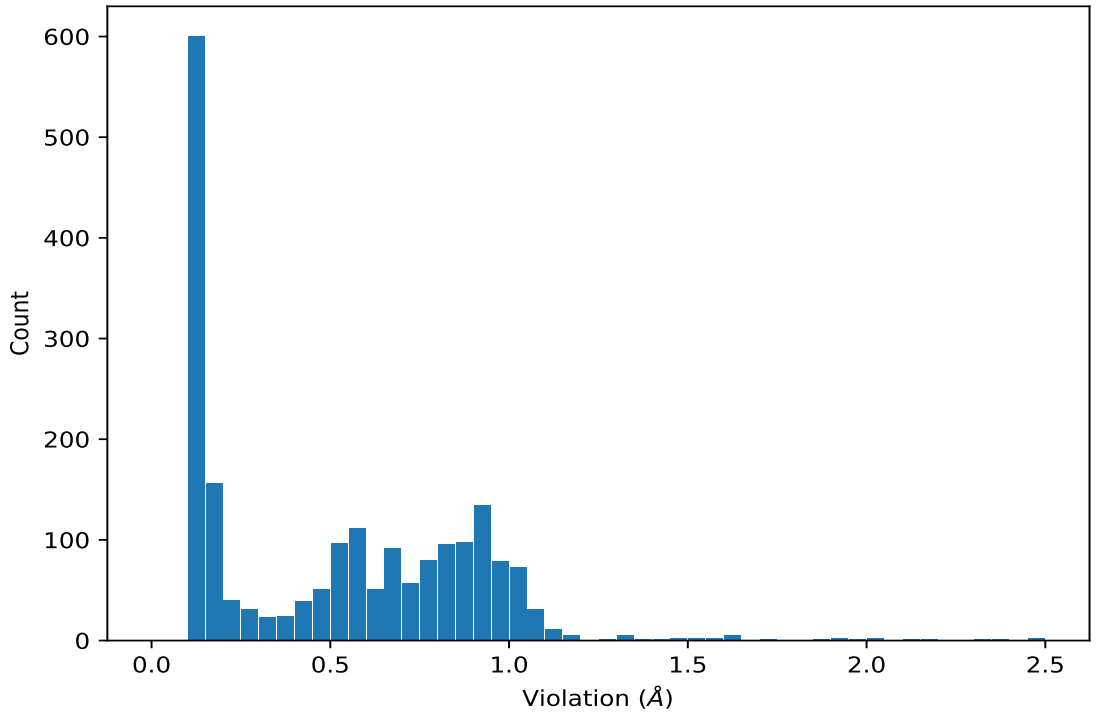
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1424)	1:5:A:DG:H8	1:4:A:DT:H4'	2	0.11	0.0	0.11
(1,1056)	2:266:B:GLU:HA	2:361:B:TRP:HZ2	2	0.1	0.0	0.1

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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



9.5.2 Table : All distance violations

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)
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	1	2.46
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	17	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	7	2.4
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	6	2.34
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	20	2.16
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	14	2.13
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	2	2.02
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	12	2.02
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	14	1.97
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	11	1.94
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	4	1.92
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	15	1.9
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	15	1.73
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	18	1.65
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	1	1.64
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	13	1.61
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	7	1.6
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	17	1.6
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	8	1.55
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	19	1.55
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	6	1.53
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	5	1.52
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	10	1.49
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	1	1.46
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	17	1.45
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	7	1.4
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	20	1.34
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	6	1.34
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	16	1.32
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	14	1.32
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	9	1.31
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	16	1.26
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	17	1.19
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	12	1.19
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	8	1.17
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	20	1.16
(6,24)	2:285:B:THR:H	2:281:B:GLU:O	14	1.16
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	11	1.15
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	13	1.15
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	19	1.15
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	14	1.13
(6,24)	2:285:B:THR:H	2:281:B:GLU:O	15	1.13
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	20	1.12
(6,162)	2:350:B:GLN:N	2:346:B:LYS:O	3	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	2	1.11
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	4	1.1
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	7	1.1
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	14	1.1
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	1	1.09
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	3	1.09
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	5	1.08
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	6	1.08
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	10	1.08
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	4	1.07
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	12	1.07
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	14	1.07
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	15	1.07
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	20	1.07
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	11	1.07
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	1	1.07
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	7	1.07
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	4	1.07
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	4	1.06
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	19	1.06
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	11	1.06
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	1	1.06
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	8	1.06
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	10	1.06
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	7	1.06
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	5	1.05
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	10	1.05
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	2	1.05
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	16	1.05
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	14	1.05
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	16	1.05
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	19	1.05
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	20	1.05
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	3	1.05
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	11	1.05
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	6	1.04
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	11	1.04
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	9	1.04
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	18	1.04
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	19	1.04
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	9	1.04
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	17	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	4	1.04
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	6	1.04
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	5	1.04
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	12	1.04
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	7	1.03
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	7	1.03
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	8	1.03
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	3	1.03
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	13	1.03
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	13	1.03
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	15	1.03
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	2	1.03
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	10	1.03
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	18	1.03
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	3	1.02
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	9	1.02
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	13	1.02
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	16	1.02
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	17	1.02
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	18	1.02
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	11	1.02
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	11	1.02
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	17	1.02
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	5	1.02
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	9	1.02
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	4	1.02
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	2	1.02
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	12	1.02
(6,155)	2:357:B:LEU:N	2:353:B:PHE:O	17	1.01
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	18	1.01
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	5	1.01
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	1	1.01
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	3	1.01
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	12	1.01
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	1	1.01
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	11	1.01
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	17	1.01
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	14	1.01
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	18	1.01
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	9	1.01
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	2	1.01
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	4	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	10	1.01
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	1	1.0
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	8	1.0
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	10	1.0
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	18	1.0
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	2	1.0
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	11	1.0
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	20	1.0
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	4	1.0
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	6	1.0
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	9	1.0
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	10	1.0
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	13	1.0
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	11	1.0
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	9	1.0
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	10	1.0
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	20	1.0
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	19	1.0
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	3	1.0
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	5	1.0
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	9	1.0
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	13	1.0
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	13	1.0
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	13	1.0
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	20	0.99
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	9	0.99
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	4	0.99
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	16	0.99
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	4	0.99
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	7	0.99
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	19	0.99
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	3	0.99
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	7	0.99
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	12	0.99
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	8	0.99
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	18	0.99
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	4	0.99
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	2	0.99
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	10	0.99
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	15	0.99
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	16	0.99
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	5	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	18	0.98
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	18	0.98
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	7	0.98
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	12	0.98
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	17	0.98
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	20	0.98
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	9	0.98
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	7	0.98
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	4	0.98
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	6	0.98
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	14	0.98
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	19	0.98
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	20	0.98
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	20	0.98
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	6	0.98
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	6	0.98
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	19	0.98
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	20	0.98
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	12	0.98
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	16	0.98
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	19	0.98
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	1	0.97
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	8	0.97
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	2	0.97
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	5	0.97
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	5	0.97
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	8	0.97
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	10	0.97
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	5	0.97
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	8	0.97
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	3	0.97
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	15	0.97
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	5	0.97
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	7	0.97
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	12	0.97
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	15	0.97
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	18	0.97
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	15	0.97
(6,23)	2:285:B:THR:N	2:281:B:GLU:O	14	0.97
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	14	0.96
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	13	0.96
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	6	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	11	0.96
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	8	0.96
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	13	0.96
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	15	0.96
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	16	0.96
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	7	0.96
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	18	0.96
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	18	0.96
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	2	0.96
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	16	0.96
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	17	0.96
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	11	0.96
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	10	0.96
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	11	0.96
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	8	0.96
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	5	0.96
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	14	0.96
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	1	0.96
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	20	0.96
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	6	0.95
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	3	0.95
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	4	0.95
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	3	0.95
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	10	0.95
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	11	0.95
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	14	0.95
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	2	0.95
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	19	0.95
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	12	0.95
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	7	0.95
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	1	0.95
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	2	0.95
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	4	0.95
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	11	0.95
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	15	0.95
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	17	0.95
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	19	0.95
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	19	0.95
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	3	0.95
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	8	0.95
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	16	0.95
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	17	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	17	0.95
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	15	0.94
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	11	0.94
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	14	0.94
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	1	0.94
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	6	0.94
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	14	0.94
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	18	0.94
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	17	0.94
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	9	0.94
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	6	0.94
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	15	0.94
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	9	0.94
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	8	0.94
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	3	0.94
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	9	0.94
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	12	0.94
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	16	0.94
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	16	0.94
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	11	0.94
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	14	0.93
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	20	0.93
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	17	0.93
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	19	0.93
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	13	0.93
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	19	0.93
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	20	0.93
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	9	0.93
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	3	0.93
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	9	0.93
(6,138)	2:314:B:TRP:N	2:310:B:SER:O	16	0.93
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	10	0.93
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	5	0.93
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	6	0.93
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	4	0.93
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	19	0.93
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	20	0.93
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	1	0.93
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	6	0.93
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	12	0.93
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	13	0.93
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	6	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	12	0.92
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	9	0.92
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	15	0.92
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	19	0.92
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	5	0.92
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	2	0.92
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	15	0.92
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	14	0.92
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	7	0.92
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	12	0.92
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	15	0.92
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	15	0.92
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	6	0.92
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	19	0.92
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	14	0.92
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	2	0.92
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	5	0.92
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	6	0.92
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	1	0.92
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	10	0.92
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	13	0.92
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	18	0.92
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	3	0.92
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	4	0.92
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	7	0.92
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	8	0.92
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	18	0.92
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	4	0.92
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	8	0.91
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	16	0.91
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	12	0.91
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	1	0.91
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	16	0.91
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	20	0.91
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	4	0.91
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	18	0.91
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	19	0.91
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	4	0.91
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	14	0.91
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	7	0.91
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	14	0.91
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	17	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	18	0.91
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	8	0.91
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	11	0.91
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	17	0.91
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	17	0.9
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	18	0.9
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	2	0.9
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	7	0.9
(6,150)	2:362:B:SER:N	2:358:B:SER:O	8	0.9
(6,150)	2:362:B:SER:N	2:358:B:SER:O	17	0.9
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	3	0.9
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	12	0.9
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	18	0.9
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	11	0.9
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	15	0.9
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	2	0.9
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	16	0.9
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	2	0.9
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	8	0.9
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	9	0.9
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	11	0.9
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	14	0.9
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	15	0.9
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	13	0.9
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	3	0.9
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	14	0.9
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	15	0.9
(6,23)	2:285:B:THR:N	2:281:B:GLU:O	15	0.9
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	12	0.89
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	17	0.89
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	7	0.89
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	8	0.89
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	16	0.89
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	18	0.89
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	10	0.89
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	1	0.89
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	11	0.89
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	5	0.89
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	17	0.89
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	3	0.89
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	13	0.89
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	15	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	10	0.89
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	7	0.88
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	10	0.88
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	17	0.88
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	1	0.88
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	8	0.88
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	16	0.88
(6,150)	2:362:B:SER:N	2:358:B:SER:O	2	0.88
(6,150)	2:362:B:SER:N	2:358:B:SER:O	4	0.88
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	4	0.88
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	11	0.88
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	19	0.88
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	19	0.88
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	10	0.88
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	12	0.88
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	20	0.88
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	8	0.88
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	13	0.88
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	3	0.88
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	4	0.88
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	7	0.88
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	6	0.88
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	12	0.88
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	5	0.88
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	9	0.88
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	18	0.88
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	19	0.87
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	3	0.87
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	5	0.87
(6,150)	2:362:B:SER:N	2:358:B:SER:O	1	0.87
(6,150)	2:362:B:SER:N	2:358:B:SER:O	11	0.87
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	1	0.87
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	10	0.87
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	20	0.87
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	6	0.87
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	10	0.87
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	2	0.87
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	13	0.87
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	17	0.87
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	7	0.87
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	9	0.87
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	13	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	20	0.87
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	5	0.87
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	17	0.87
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	17	0.87
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	9	0.87
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	20	0.87
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	5	0.86
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	12	0.86
(6,150)	2:362:B:SER:N	2:358:B:SER:O	6	0.86
(6,150)	2:362:B:SER:N	2:358:B:SER:O	9	0.86
(6,150)	2:362:B:SER:N	2:358:B:SER:O	12	0.86
(6,150)	2:362:B:SER:N	2:358:B:SER:O	13	0.86
(6,150)	2:362:B:SER:N	2:358:B:SER:O	14	0.86
(6,150)	2:362:B:SER:N	2:358:B:SER:O	16	0.86
(6,150)	2:362:B:SER:N	2:358:B:SER:O	18	0.86
(6,150)	2:362:B:SER:N	2:358:B:SER:O	19	0.86
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	2	0.86
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	5	0.86
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	6	0.86
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	13	0.86
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	15	0.86
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	19	0.86
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	10	0.86
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	12	0.86
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	2	0.86
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	14	0.86
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	7	0.86
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	20	0.86
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	1	0.86
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	6	0.86
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	8	0.86
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	13	0.86
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	14	0.86
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	18	0.86
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	2	0.86
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	8	0.86
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	17	0.86
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	18	0.86
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	3	0.86
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	20	0.86
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	2	0.86
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	7	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	1	0.85
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	14	0.85
(6,150)	2:362:B:SER:N	2:358:B:SER:O	7	0.85
(6,150)	2:362:B:SER:N	2:358:B:SER:O	10	0.85
(6,150)	2:362:B:SER:N	2:358:B:SER:O	15	0.85
(6,136)	2:316:B:VAL:N	2:312:B:GLY:O	14	0.85
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	4	0.85
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	6	0.85
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	13	0.85
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	4	0.85
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	16	0.85
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	17	0.85
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	10	0.85
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	14	0.85
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	7	0.85
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	7	0.84
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	9	0.84
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	18	0.84
(6,150)	2:362:B:SER:N	2:358:B:SER:O	3	0.84
(6,150)	2:362:B:SER:N	2:358:B:SER:O	20	0.84
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	3	0.84
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	14	0.84
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	14	0.84
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	8	0.84
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	1	0.84
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	16	0.84
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	13	0.84
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	5	0.84
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	9	0.84
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	10	0.84
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	19	0.84
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	6	0.84
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	8	0.84
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	5	0.84
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	9	0.84
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	4	0.84
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	13	0.83
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	3	0.83
(6,150)	2:362:B:SER:N	2:358:B:SER:O	5	0.83
(6,146)	2:366:B:LYS:N	2:362:B:SER:O	7	0.83
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	2	0.83
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	12	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	5	0.83
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	12	0.83
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	14	0.83
(6,116)	2:269:B:LYS:N	2:265:B:LYS:O	1	0.83
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	15	0.83
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	12	0.83
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	11	0.83
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	9	0.83
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	10	0.83
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	6	0.83
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	10	0.83
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	18	0.83
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	4	0.82
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	5	0.82
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	10	0.82
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	8	0.82
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	12	0.82
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	4	0.82
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	4	0.82
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	13	0.82
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	18	0.82
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	12	0.82
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	20	0.82
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	4	0.82
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	1	0.82
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	6	0.82
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	19	0.82
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB2	6	0.82
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB3	6	0.82
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	17	0.81
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	19	0.81
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	17	0.81
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	16	0.81
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	18	0.81
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	14	0.81
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	18	0.81
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	20	0.81
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	4	0.81
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	2	0.81
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	2	0.81
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	15	0.8
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	15	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	11	0.8
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	18	0.8
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	6	0.8
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	1	0.8
(6,127)	2:295:B:ILE:N	2:291:B:LEU:O	16	0.8
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	9	0.8
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	1	0.8
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	2	0.8
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	15	0.8
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	16	0.8
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	5	0.8
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	15	0.8
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	2	0.79
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	11	0.79
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	14	0.79
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	10	0.79
(6,149)	2:363:B:VAL:N	2:359:B:LYS:O	9	0.79
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	12	0.79
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	15	0.79
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	15	0.79
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	16	0.79
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	15	0.79
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	3	0.79
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	5	0.79
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	10	0.79
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	11	0.79
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	5	0.79
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	16	0.79
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	17	0.78
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	18	0.78
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	6	0.78
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	17	0.78
(6,133)	2:319:B:TYR:N	2:315:B:HIS:O	15	0.78
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	18	0.78
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	1	0.78
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	3	0.78
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	12	0.78
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	14	0.78
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	19	0.78
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	6	0.78
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	12	0.78
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	19	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	6	0.77
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	2	0.77
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	17	0.77
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	19	0.77
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	4	0.77
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	11	0.77
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	13	0.77
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	3	0.77
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	9	0.77
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	14	0.77
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	2	0.77
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	7	0.77
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	2	0.77
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	3	0.77
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	13	0.77
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	17	0.77
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	1	0.77
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	8	0.77
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	9	0.76
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	20	0.76
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	6	0.76
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	15	0.76
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	16	0.76
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	16	0.76
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	20	0.76
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	16	0.76
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	4	0.76
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	17	0.76
(6,120)	2:285:B:THR:N	2:281:B:GLU:O	7	0.76
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	7	0.76
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	8	0.76
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	18	0.76
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	14	0.75
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	3	0.75
(6,151)	2:361:B:TRP:N	2:357:B:LEU:O	2	0.75
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	7	0.75
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	6	0.75
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	14	0.75
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	1	0.75
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	2	0.75
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	10	0.75
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	5	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	12	0.75
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	20	0.75
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	3	0.75
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	15	0.75
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	14	0.75
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	15	0.75
(6,112)	2:262:B:GLU:N	2:258:B:VAL:O	3	0.75
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	3	0.75
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	13	0.74
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	11	0.74
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	20	0.74
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	9	0.74
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	10	0.74
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	13	0.74
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	1	0.74
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	10	0.74
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	1	0.74
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	6	0.74
(6,117)	2:268:B:VAL:N	2:264:B:ARG:O	1	0.74
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	20	0.74
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	6	0.74
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	13	0.74
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	7	0.73
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	9	0.73
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	13	0.73
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	4	0.73
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	15	0.73
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	5	0.73
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	6	0.73
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	4	0.73
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	7	0.73
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	2	0.73
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	8	0.73
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	15	0.73
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	9	0.72
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	10	0.72
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	10	0.72
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	13	0.72
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	11	0.72
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	6	0.72
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	13	0.72
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	14	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	17	0.72
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	8	0.72
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	16	0.72
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	11	0.72
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	9	0.72
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	3	0.71
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	4	0.71
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	3	0.71
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	9	0.71
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	4	0.71
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	5	0.71
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	13	0.71
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	18	0.71
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	4	0.71
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	16	0.71
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	3	0.71
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	9	0.71
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	9	0.71
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	10	0.71
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	1	0.71
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	4	0.71
(6,109)	2:265:B:LYS:N	2:261:B:GLU:O	20	0.71
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	8	0.71
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	15	0.7
(6,157)	2:355:B:ILE:N	2:351:B:LYS:O	13	0.7
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	5	0.7
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	8	0.7
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	12	0.7
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	15	0.7
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	17	0.7
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	18	0.7
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	16	0.7
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	20	0.7
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	9	0.7
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	2	0.7
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	19	0.7
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	9	0.69
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	2	0.69
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	13	0.69
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	1	0.69
(6,142)	2:332:B:LEU:N	2:328:B:PRO:O	2	0.69
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	18	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	15	0.69
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	2	0.69
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	7	0.69
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	6	0.69
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	3	0.69
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	14	0.69
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	10	0.69
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	11	0.69
(6,111)	2:263:B:LEU:N	2:259:B:GLU:O	15	0.69
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	3	0.69
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	8	0.68
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	16	0.68
(6,158)	2:354:B:VAL:N	2:350:B:GLN:O	18	0.68
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	18	0.68
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	20	0.68
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	6	0.68
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	10	0.68
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	8	0.68
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	9	0.68
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	7	0.68
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	11	0.68
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	8	0.68
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	11	0.68
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	19	0.68
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	20	0.68
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	11	0.68
(6,114)	2:260:B:PHE:N	2:256:B:THR:O	12	0.68
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB2	1	0.68
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB3	1	0.68
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	16	0.67
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	20	0.67
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	1	0.67
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	5	0.67
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	5	0.67
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	13	0.67
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	16	0.67
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	7	0.67
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	8	0.67
(6,134)	2:318:B:LEU:N	2:314:B:TRP:O	18	0.67
(6,129)	2:323:B:HIS:N	2:319:B:TYR:O	15	0.67
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	6	0.67
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	19	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,113)	2:261:B:GLU:N	2:257:B:VAL:O	19	0.67
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	5	0.67
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	19	0.67
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	9	0.67
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	19	0.66
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	6	0.66
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	14	0.66
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	20	0.66
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	5	0.66
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	8	0.66
(6,145)	2:367:B:TYR:N	2:363:B:VAL:O	20	0.66
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	5	0.66
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	1	0.66
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	10	0.66
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	6	0.66
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	14	0.66
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	2	0.66
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	10	0.65
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	14	0.65
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	18	0.65
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	14	0.65
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	15	0.65
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	12	0.65
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	16	0.65
(6,131)	2:321:B:MET:N	2:317:B:ILE:O	19	0.65
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	8	0.65
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	7	0.65
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	12	0.65
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	11	0.65
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	18	0.65
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	10	0.65
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	11	0.64
(6,156)	2:356:B:THR:N	2:352:B:TYR:O	16	0.64
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	19	0.64
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	3	0.64
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	9	0.64
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	3	0.64
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	11	0.64
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	18	0.64
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	18	0.64
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	17	0.64
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	1	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	7	0.64
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	2	0.63
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	2	0.63
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	13	0.63
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	16	0.63
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	20	0.63
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	10	0.63
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	9	0.63
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	8	0.63
(6,115)	2:270:B:ARG:N	2:266:B:GLU:O	7	0.63
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	17	0.63
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	10	0.63
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	12	0.63
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	20	0.63
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	8	0.62
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	19	0.62
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	6	0.62
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	17	0.62
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	4	0.62
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	9	0.62
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	4	0.62
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	9	0.62
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	3	0.62
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	1	0.62
(6,119)	2:266:B:GLU:N	2:262:B:GLU:O	3	0.62
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	4	0.62
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	6	0.62
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	8	0.62
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	12	0.61
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	12	0.61
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	1	0.61
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	1	0.61
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	11	0.61
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	4	0.61
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	19	0.61
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	15	0.61
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	8	0.61
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	13	0.61
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	11	0.61
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	13	0.61
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	15	0.6
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	2	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	4	0.6
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	14	0.6
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	19	0.6
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	10	0.6
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	5	0.6
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	3	0.6
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	2	0.6
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	15	0.6
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	1	0.6
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	5	0.6
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	12	0.6
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	7	0.6
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	3	0.6
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	13	0.6
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	13	0.6
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	13	0.6
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	15	0.6
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	13	0.59
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	1	0.59
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	2	0.59
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	5	0.59
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	9	0.59
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	16	0.59
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	18	0.59
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	3	0.59
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	8	0.59
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	11	0.59
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	7	0.59
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	5	0.59
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	13	0.59
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	1	0.59
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	9	0.59
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	14	0.59
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	16	0.59
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	3	0.59
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	5	0.59
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	14	0.59
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	16	0.59
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	5	0.58
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	11	0.58
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	15	0.58
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	17	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	1	0.58
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	6	0.58
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	4	0.58
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	17	0.58
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	14	0.58
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	17	0.58
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	17	0.58
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	19	0.58
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	13	0.58
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	17	0.58
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	12	0.58
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	12	0.58
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	3	0.58
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	8	0.58
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	10	0.58
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	18	0.58
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	7	0.57
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	3	0.57
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	7	0.57
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	11	0.57
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	20	0.57
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	15	0.57
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	18	0.57
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	8	0.57
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	20	0.57
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	4	0.57
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	6	0.57
(6,123)	2:282:B:GLU:N	2:278:B:LYS:O	8	0.57
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	18	0.57
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	17	0.57
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	8	0.56
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	17	0.56
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	13	0.56
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	8	0.56
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	12	0.56
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	16	0.56
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	20	0.56
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	12	0.56
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	1	0.56
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	5	0.56
(6,122)	2:283:B:ILE:N	2:279:B:ILE:O	11	0.56
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	10	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	6	0.56
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	1	0.56
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	11	0.56
(1,1456)	1:7:A:DT:H4'	1:7:A:DT:H6	19	0.56
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	11	0.55
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	16	0.55
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	19	0.55
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	3	0.55
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	6	0.55
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	16	0.55
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	8	0.55
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	17	0.55
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	1	0.55
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	3	0.55
(6,140)	2:334:B:LEU:N	2:330:B:LYS:O	5	0.55
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	6	0.55
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	1	0.55
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	13	0.55
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	6	0.55
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	7	0.55
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	14	0.55
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	11	0.55
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	5	0.55
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	18	0.55
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	8	0.55
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	19	0.55
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	19	0.54
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	11	0.54
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	2	0.54
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	8	0.54
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	9	0.54
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	11	0.54
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	14	0.54
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	15	0.54
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	17	0.54
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	10	0.54
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	1	0.54
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	11	0.54
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	11	0.54
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	17	0.54
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	2	0.54
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	9	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	10	0.54
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	4	0.53
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	12	0.53
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	4	0.53
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	1	0.53
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	4	0.53
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	13	0.53
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	14	0.53
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	10	0.53
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	15	0.53
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	2	0.53
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	7	0.53
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	19	0.53
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	6	0.53
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	3	0.53
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	10	0.53
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	16	0.53
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	9	0.53
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	12	0.53
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	16	0.53
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	20	0.53
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	7	0.53
(6,160)	2:352:B:TYR:N	2:348:B:ASN:O	20	0.52
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	13	0.52
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	17	0.52
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	20	0.52
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	12	0.52
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	16	0.52
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	16	0.52
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	15	0.52
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	13	0.52
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	2	0.52
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	14	0.52
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	19	0.52
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	12	0.52
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	14	0.52
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	7	0.52
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	2	0.52
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	20	0.52
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	5	0.52
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	7	0.51
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	4	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	9	0.51
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	18	0.51
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	4	0.51
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	7	0.51
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	13	0.51
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	18	0.51
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	19	0.51
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	13	0.51
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	2	0.51
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	13	0.51
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	18	0.51
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	15	0.51
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	19	0.51
(6,125)	2:297:B:CYS:N	2:293:B:LYS:O	2	0.51
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	19	0.51
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	13	0.51
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	10	0.5
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	2	0.5
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	9	0.5
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	20	0.5
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	14	0.5
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	8	0.5
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	3	0.5
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	10	0.5
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	5	0.5
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	6	0.5
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	19	0.5
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	7	0.5
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	17	0.5
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	19	0.5
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	10	0.5
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	1	0.5
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	4	0.5
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	4	0.5
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	12	0.5
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	15	0.5
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	17	0.5
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	20	0.5
(6,110)	2:264:B:ARG:N	2:260:B:PHE:O	12	0.5
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	3	0.49
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	11	0.49
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	18	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	12	0.49
(6,152)	2:360:B:ALA:N	2:356:B:THR:O	11	0.49
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	5	0.49
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	12	0.49
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	11	0.49
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	4	0.49
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	19	0.49
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	12	0.49
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	11	0.49
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	10	0.49
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	5	0.48
(6,153)	2:359:B:LYS:N	2:355:B:ILE:O	19	0.48
(6,148)	2:364:B:VAL:N	2:360:B:ALA:O	17	0.48
(6,144)	2:368:B:LEU:N	2:364:B:VAL:O	12	0.48
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	1	0.48
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	15	0.48
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	17	0.48
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	20	0.48
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	7	0.48
(6,132)	2:320:B:LEU:N	2:316:B:VAL:O	8	0.48
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	3	0.48
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	10	0.48
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	14	0.48
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	18	0.48
(6,128)	2:294:B:GLU:N	2:290:B:LYS:O	12	0.48
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	2	0.48
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	20	0.48
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	19	0.48
(6,154)	2:358:B:SER:N	2:354:B:VAL:O	10	0.47
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	17	0.47
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	5	0.47
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	3	0.47
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	15	0.47
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	5	0.47
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	7	0.47
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	16	0.47
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	8	0.46
(6,139)	2:313:B:ASP:N	2:309:B:ARG:O	8	0.46
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	9	0.46
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	12	0.46
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	6	0.46
(6,118)	2:267:B:LEU:N	2:263:B:LEU:O	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	4	0.46
(6,161)	2:351:B:LYS:N	2:347:B:TRP:O	2	0.45
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	8	0.45
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	10	0.45
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	14	0.45
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	16	0.45
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	4	0.44
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	12	0.44
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	17	0.44
(6,143)	2:369:B:GLU:N	2:365:B:LYS:O	1	0.44
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	20	0.44
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	8	0.44
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	9	0.44
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	9	0.44
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	11	0.44
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB2	13	0.44
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB3	13	0.44
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	6	0.43
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	11	0.43
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	19	0.43
(6,135)	2:317:B:ILE:N	2:313:B:ASP:O	20	0.43
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	20	0.43
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	14	0.43
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	16	0.43
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	5	0.43
(6,159)	2:353:B:PHE:N	2:349:B:THR:O	6	0.42
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	18	0.42
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	20	0.42
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	5	0.42
(6,121)	2:284:B:CYS:N	2:280:B:LYS:O	5	0.42
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	16	0.42
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	6	0.42
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	7	0.42
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	20	0.42
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	1	0.41
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	2	0.41
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	5	0.41
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	13	0.41
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	15	0.41
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	7	0.41
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	2	0.41
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	4	0.41
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	15	0.4
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	8	0.4
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	3	0.39
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	16	0.39
(6,124)	2:280:B:LYS:N	2:276:B:VAL:O	20	0.39
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	1	0.39
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	17	0.39
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	9	0.38
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	14	0.38
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	1	0.38
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	16	0.38
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	3	0.38
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	2	0.38
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	11	0.38
(1,1027)	2:323:B:HIS:HA	2:323:B:HIS:HD2	19	0.38
(6,130)	2:322:B:LYS:N	2:318:B:LEU:O	16	0.37
(6,126)	2:296:B:ILE:N	2:292:B:ILE:O	18	0.37
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB2	17	0.37
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB3	17	0.37
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	13	0.37
(6,147)	2:365:B:LYS:N	2:361:B:TRP:O	7	0.36
(6,24)	2:285:B:THR:H	2:281:B:GLU:O	16	0.36
(6,24)	2:285:B:THR:H	2:281:B:GLU:O	17	0.36
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	8	0.36
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	10	0.36
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	15	0.36
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	2	0.35
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	4	0.35
(6,137)	2:315:B:HIS:N	2:311:B:ARG:O	18	0.35
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	9	0.35
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB2	4	0.35
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB3	4	0.35
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	9	0.35
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	14	0.35
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	16	0.35
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	18	0.35
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	19	0.35
(6,141)	2:333:B:GLU:N	2:329:B:ASP:O	7	0.34
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	6	0.34
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	3	0.34
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	16	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	7	0.32
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	17	0.32
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	19	0.32
(6,24)	2:285:B:THR:H	2:281:B:GLU:O	19	0.32
(1,1431)	1:5:A:DG:H2'	1:5:A:DG:H5"	12	0.32
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	9	0.31
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	2	0.31
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	12	0.31
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	16	0.3
(6,24)	2:285:B:THR:H	2:281:B:GLU:O	11	0.3
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	10	0.29
(6,24)	2:285:B:THR:H	2:281:B:GLU:O	8	0.29
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	5	0.28
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	13	0.27
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	20	0.27
(1,809)	2:330:B:LYS:HA	2:330:B:LYS:HE3	2	0.27
(1,638)	2:269:B:LYS:H	2:269:B:LYS:HD2	7	0.27
(1,638)	2:269:B:LYS:H	2:269:B:LYS:HD3	7	0.27
(6,108)	2:350:B:GLN:H	2:346:B:LYS:O	3	0.26
(6,23)	2:285:B:THR:N	2:281:B:GLU:O	16	0.26
(4,28)	1:7:A:DT:H71	2:322:B:LYS:HD2	5	0.26
(4,28)	1:7:A:DT:H71	2:322:B:LYS:HD3	5	0.26
(4,28)	1:7:A:DT:H72	2:322:B:LYS:HD2	5	0.26
(4,28)	1:7:A:DT:H72	2:322:B:LYS:HD3	5	0.26
(4,28)	1:7:A:DT:H73	2:322:B:LYS:HD2	5	0.26
(4,28)	1:7:A:DT:H73	2:322:B:LYS:HD3	5	0.26
(4,28)	1:7:A:DT:H71	2:322:B:LYS:HD2	7	0.26
(4,28)	1:7:A:DT:H71	2:322:B:LYS:HD3	7	0.26
(4,28)	1:7:A:DT:H72	2:322:B:LYS:HD2	7	0.26
(4,28)	1:7:A:DT:H72	2:322:B:LYS:HD3	7	0.26
(4,28)	1:7:A:DT:H73	2:322:B:LYS:HD2	7	0.26
(4,28)	1:7:A:DT:H73	2:322:B:LYS:HD3	7	0.26
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	1	0.25
(6,24)	2:285:B:THR:H	2:281:B:GLU:O	4	0.25
(6,24)	2:285:B:THR:H	2:281:B:GLU:O	13	0.25
(1,1474)	1:8:A:DC:H5'	1:9:A:DA:H8	15	0.25
(1,1474)	1:8:A:DC:H5"	1:9:A:DA:H8	15	0.25
(1,1237)	2:309:B:ARG:HA	2:309:B:ARG:HD2	17	0.25
(1,1237)	2:309:B:ARG:HA	2:309:B:ARG:HD3	17	0.25
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	18	0.24
(4,65)	1:4:A:DT:H3	2:340:B:LYS:H	11	0.24
(4,55)	1:4:A:DT:H3	2:340:B:LYS:HG2	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,55)	1:4:A:DT:H3	2:340:B:LYS:HG3	12	0.24
(1,1470)	1:8:A:DC:H1'	1:8:A:DC:H3'	9	0.24
(1,1468)	1:8:A:DC:H5'	1:8:A:DC:H6	19	0.24
(1,1468)	1:8:A:DC:H5"	1:8:A:DC:H6	19	0.24
(1,58)	2:276:B:VAL:H	2:330:B:LYS:HA	7	0.24
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	4	0.23
(4,64)	1:4:A:DT:H3	2:341:B:ALA:HA	3	0.23
(1,1473)	1:8:A:DC:H3'	1:9:A:DA:H8	14	0.23
(1,1404)	1:3:A:DG:H1'	1:4:A:DT:H6	12	0.23
(1,1287)	2:330:B:LYS:HA	2:330:B:LYS:HG2	7	0.23
(1,1287)	2:330:B:LYS:HA	2:330:B:LYS:HG3	7	0.23
(1,1028)	2:323:B:HIS:HB2	2:323:B:HIS:HD2	19	0.23
(1,1468)	1:8:A:DC:H5'	1:8:A:DC:H6	5	0.22
(1,1468)	1:8:A:DC:H5"	1:8:A:DC:H6	5	0.22
(1,1377)	1:1:A:DC:H4'	1:2:A:DT:H6	19	0.22
(1,1287)	2:330:B:LYS:HA	2:330:B:LYS:HG2	12	0.22
(1,1287)	2:330:B:LYS:HA	2:330:B:LYS:HG3	12	0.22
(1,1287)	2:330:B:LYS:HA	2:330:B:LYS:HG2	15	0.22
(1,1287)	2:330:B:LYS:HA	2:330:B:LYS:HG3	15	0.22
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	12	0.21
(1,1468)	1:8:A:DC:H5'	1:8:A:DC:H6	18	0.21
(1,1468)	1:8:A:DC:H5"	1:8:A:DC:H6	18	0.21
(1,690)	2:368:B:LEU:H	2:368:B:LEU:HG	5	0.21
(1,618)	2:301:B:THR:HB	2:302:B:TYR:HE2	6	0.21
(6,14)	2:270:B:ARG:H	2:266:B:GLU:O	11	0.2
(4,65)	1:4:A:DT:H3	2:340:B:LYS:H	4	0.2
(4,32)	1:4:A:DT:H3'	2:352:B:TYR:HD2	9	0.2
(1,1461)	1:7:A:DT:H2'	1:8:A:DC:H6	18	0.2
(1,1461)	1:7:A:DT:H2"	1:8:A:DC:H6	18	0.2
(1,1445)	1:6:A:DC:H1'	1:7:A:DT:H6	9	0.2
(1,1404)	1:3:A:DG:H1'	1:4:A:DT:H6	14	0.2
(1,1176)	2:292:B:ILE:HG12	2:296:B:ILE:HD11	18	0.2
(1,1176)	2:292:B:ILE:HG12	2:296:B:ILE:HD12	18	0.2
(1,1176)	2:292:B:ILE:HG12	2:296:B:ILE:HD13	18	0.2
(1,1176)	2:292:B:ILE:HG13	2:296:B:ILE:HD11	18	0.2
(1,1176)	2:292:B:ILE:HG13	2:296:B:ILE:HD12	18	0.2
(1,1176)	2:292:B:ILE:HG13	2:296:B:ILE:HD13	18	0.2
(6,68)	2:332:B:LEU:H	2:328:B:PRO:O	7	0.19
(6,68)	2:332:B:LEU:H	2:328:B:PRO:O	20	0.19
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	14	0.19
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	2	0.19
(6,23)	2:285:B:THR:N	2:281:B:GLU:O	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,64)	1:4:A:DT:H3	2:341:B:ALA:HA	19	0.19
(4,62)	1:4:A:DT:H3	2:352:B:TYR:HD1	10	0.19
(4,60)	1:4:A:DT:H3	2:340:B:LYS:HA	6	0.19
(1,1461)	1:7:A:DT:H2'	1:8:A:DC:H6	5	0.19
(1,1461)	1:7:A:DT:H2"	1:8:A:DC:H6	5	0.19
(1,1461)	1:7:A:DT:H2'	1:8:A:DC:H6	19	0.19
(1,1461)	1:7:A:DT:H2"	1:8:A:DC:H6	19	0.19
(1,1369)	1:1:A:DC:H4'	1:1:A:DC:H6	15	0.19
(1,1074)	2:263:B:LEU:HB2	2:264:B:ARG:H	6	0.19
(1,1074)	2:263:B:LEU:HB3	2:264:B:ARG:H	6	0.19
(1,562)	2:258:B:VAL:HG11	2:259:B:GLU:HG2	15	0.19
(1,562)	2:258:B:VAL:HG11	2:259:B:GLU:HG3	15	0.19
(1,562)	2:258:B:VAL:HG12	2:259:B:GLU:HG2	15	0.19
(1,562)	2:258:B:VAL:HG12	2:259:B:GLU:HG3	15	0.19
(1,562)	2:258:B:VAL:HG13	2:259:B:GLU:HG2	15	0.19
(1,562)	2:258:B:VAL:HG13	2:259:B:GLU:HG3	15	0.19
(1,562)	2:258:B:VAL:HG21	2:259:B:GLU:HG2	15	0.19
(1,562)	2:258:B:VAL:HG21	2:259:B:GLU:HG3	15	0.19
(1,562)	2:258:B:VAL:HG22	2:259:B:GLU:HG2	15	0.19
(1,562)	2:258:B:VAL:HG22	2:259:B:GLU:HG3	15	0.19
(1,562)	2:258:B:VAL:HG23	2:259:B:GLU:HG2	15	0.19
(1,562)	2:258:B:VAL:HG23	2:259:B:GLU:HG3	15	0.19
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	7	0.18
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	9	0.18
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	16	0.18
(6,24)	2:285:B:THR:H	2:281:B:GLU:O	10	0.18
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB2	18	0.18
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB3	18	0.18
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD2	1	0.18
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD3	1	0.18
(4,32)	1:4:A:DT:H3'	2:352:B:TYR:HD2	13	0.18
(1,1445)	1:6:A:DC:H1'	1:7:A:DT:H6	14	0.18
(1,1404)	1:3:A:DG:H1'	1:4:A:DT:H6	10	0.18
(1,1369)	1:1:A:DC:H4'	1:1:A:DC:H6	2	0.18
(1,1324)	2:343:B:GLU:HA	2:344:B:ASN:HB2	11	0.18
(1,1324)	2:343:B:GLU:HA	2:344:B:ASN:HB3	11	0.18
(1,662)	2:276:B:VAL:HA	2:279:B:ILE:HG12	6	0.18
(1,609)	2:276:B:VAL:HB	2:277:B:GLU:H	4	0.18
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	18	0.17
(6,23)	2:285:B:THR:N	2:281:B:GLU:O	8	0.17
(4,64)	1:4:A:DT:H3	2:341:B:ALA:HA	8	0.17
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB2	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB3	2	0.17
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB2	10	0.17
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB3	10	0.17
(4,60)	1:4:A:DT:H3	2:340:B:LYS:HA	12	0.17
(4,56)	1:4:A:DT:H3	2:340:B:LYS:HE2	8	0.17
(4,56)	1:4:A:DT:H3	2:340:B:LYS:HE3	8	0.17
(4,32)	1:4:A:DT:H3'	2:352:B:TYR:HD2	18	0.17
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	12	0.17
(1,1406)	1:3:A:DG:H3'	1:4:A:DT:H6	6	0.17
(1,1324)	2:343:B:GLU:HA	2:344:B:ASN:HB2	4	0.17
(1,1324)	2:343:B:GLU:HA	2:344:B:ASN:HB3	4	0.17
(1,1324)	2:343:B:GLU:HA	2:344:B:ASN:HB2	13	0.17
(1,1324)	2:343:B:GLU:HA	2:344:B:ASN:HB3	13	0.17
(1,1145)	2:280:B:LYS:HB2	2:281:B:GLU:H	14	0.17
(1,1145)	2:280:B:LYS:HB3	2:281:B:GLU:H	14	0.17
(1,1122)	2:276:B:VAL:HG11	2:330:B:LYS:HE2	17	0.17
(1,1122)	2:276:B:VAL:HG11	2:330:B:LYS:HE3	17	0.17
(1,1122)	2:276:B:VAL:HG12	2:330:B:LYS:HE2	17	0.17
(1,1122)	2:276:B:VAL:HG12	2:330:B:LYS:HE3	17	0.17
(1,1122)	2:276:B:VAL:HG13	2:330:B:LYS:HE2	17	0.17
(1,1122)	2:276:B:VAL:HG13	2:330:B:LYS:HE3	17	0.17
(1,1122)	2:276:B:VAL:HG21	2:330:B:LYS:HE2	17	0.17
(1,1122)	2:276:B:VAL:HG21	2:330:B:LYS:HE3	17	0.17
(1,1122)	2:276:B:VAL:HG22	2:330:B:LYS:HE2	17	0.17
(1,1122)	2:276:B:VAL:HG22	2:330:B:LYS:HE3	17	0.17
(1,1122)	2:276:B:VAL:HG23	2:330:B:LYS:HE2	17	0.17
(1,1122)	2:276:B:VAL:HG23	2:330:B:LYS:HE3	17	0.17
(1,1045)	2:311:B:ARG:HG2	2:315:B:HIS:HD2	1	0.17
(1,1045)	2:311:B:ARG:HG3	2:315:B:HIS:HD2	1	0.17
(1,1045)	2:311:B:ARG:HG2	2:315:B:HIS:HD2	18	0.17
(1,1045)	2:311:B:ARG:HG3	2:315:B:HIS:HD2	18	0.17
(1,1002)	2:346:B:LYS:HB2	2:347:B:TRP:HD1	6	0.17
(1,1002)	2:346:B:LYS:HB3	2:347:B:TRP:HD1	6	0.17
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB2	6	0.17
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB3	6	0.17
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB2	8	0.17
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB3	8	0.17
(1,690)	2:368:B:LEU:H	2:368:B:LEU:HG	3	0.17
(1,687)	2:263:B:LEU:HG	2:266:B:GLU:H	7	0.17
(1,666)	2:276:B:VAL:HA	2:279:B:ILE:HG13	5	0.17
(1,448)	2:332:B:LEU:HD11	2:342:B:LYS:H	11	0.17
(1,448)	2:332:B:LEU:HD12	2:342:B:LYS:H	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	2:332:B:LEU:HD13	2:342:B:LYS:H	11	0.17
(1,351)	2:331:B:ILE:H	2:331:B:ILE:HG13	1	0.17
(6,68)	2:332:B:LEU:H	2:328:B:PRO:O	4	0.16
(6,68)	2:332:B:LEU:H	2:328:B:PRO:O	14	0.16
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	12	0.16
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	1	0.16
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	5	0.16
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	7	0.16
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	19	0.16
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	5	0.16
(6,14)	2:270:B:ARG:H	2:266:B:GLU:O	8	0.16
(6,14)	2:270:B:ARG:H	2:266:B:GLU:O	14	0.16
(4,62)	1:4:A:DT:H3	2:352:B:TYR:HD2	11	0.16
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB2	16	0.16
(4,61)	1:4:A:DT:H3	2:310:B:SER:HB3	16	0.16
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD2	2	0.16
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD3	2	0.16
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD2	7	0.16
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD3	7	0.16
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD2	17	0.16
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD3	17	0.16
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	14	0.16
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	19	0.16
(1,1396)	1:3:A:DG:H2'	1:3:A:DG:H8	10	0.16
(1,1219)	2:302:B:TYR:H	2:337:B:ARG:HB2	6	0.16
(1,1219)	2:302:B:TYR:H	2:337:B:ARG:HB3	6	0.16
(1,1219)	2:302:B:TYR:H	2:337:B:ARG:HB2	17	0.16
(1,1219)	2:302:B:TYR:H	2:337:B:ARG:HB3	17	0.16
(1,1176)	2:292:B:ILE:HG12	2:296:B:ILE:HD11	4	0.16
(1,1176)	2:292:B:ILE:HG12	2:296:B:ILE:HD12	4	0.16
(1,1176)	2:292:B:ILE:HG12	2:296:B:ILE:HD13	4	0.16
(1,1176)	2:292:B:ILE:HG13	2:296:B:ILE:HD11	4	0.16
(1,1176)	2:292:B:ILE:HG13	2:296:B:ILE:HD12	4	0.16
(1,1176)	2:292:B:ILE:HG13	2:296:B:ILE:HD13	4	0.16
(1,1155)	2:280:B:LYS:HG2	2:296:B:ILE:HD11	14	0.16
(1,1155)	2:280:B:LYS:HG2	2:296:B:ILE:HD12	14	0.16
(1,1155)	2:280:B:LYS:HG2	2:296:B:ILE:HD13	14	0.16
(1,1155)	2:280:B:LYS:HG3	2:296:B:ILE:HD11	14	0.16
(1,1155)	2:280:B:LYS:HG3	2:296:B:ILE:HD12	14	0.16
(1,1155)	2:280:B:LYS:HG3	2:296:B:ILE:HD13	14	0.16
(1,1110)	2:273:B:GLY:HA2	2:274:B:LYS:HE2	7	0.16
(1,1110)	2:273:B:GLY:HA2	2:274:B:LYS:HE3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1110)	2:273:B:GLY:HA3	2:274:B:LYS:HE2	7	0.16
(1,1110)	2:273:B:GLY:HA3	2:274:B:LYS:HE3	7	0.16
(1,1045)	2:311:B:ARG:HG2	2:315:B:HIS:HD2	7	0.16
(1,1045)	2:311:B:ARG:HG3	2:315:B:HIS:HD2	7	0.16
(1,1002)	2:346:B:LYS:HB2	2:347:B:TRP:HD1	4	0.16
(1,1002)	2:346:B:LYS:HB3	2:347:B:TRP:HD1	4	0.16
(1,1002)	2:346:B:LYS:HB2	2:347:B:TRP:HD1	11	0.16
(1,1002)	2:346:B:LYS:HB3	2:347:B:TRP:HD1	11	0.16
(1,994)	2:341:B:ALA:HA	2:353:B:PHE:HD2	14	0.16
(1,994)	2:341:B:ALA:HA	2:353:B:PHE:HD2	17	0.16
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB2	9	0.16
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB3	9	0.16
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG21	12	0.16
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG22	12	0.16
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG23	12	0.16
(1,687)	2:263:B:LEU:HG	2:266:B:GLU:H	11	0.16
(1,638)	2:269:B:LYS:H	2:269:B:LYS:HD2	16	0.16
(1,638)	2:269:B:LYS:H	2:269:B:LYS:HD3	16	0.16
(1,593)	2:274:B:LYS:HB2	2:279:B:ILE:HD11	11	0.16
(1,593)	2:274:B:LYS:HB2	2:279:B:ILE:HD12	11	0.16
(1,593)	2:274:B:LYS:HB2	2:279:B:ILE:HD13	11	0.16
(1,593)	2:274:B:LYS:HB3	2:279:B:ILE:HD11	11	0.16
(1,593)	2:274:B:LYS:HB3	2:279:B:ILE:HD12	11	0.16
(1,593)	2:274:B:LYS:HB3	2:279:B:ILE:HD13	11	0.16
(1,513)	2:270:B:ARG:HD2	2:325:B:VAL:HA	1	0.16
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	5	0.15
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	5	0.15
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	10	0.15
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	13	0.15
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	1	0.15
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	10	0.15
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	15	0.15
(6,23)	2:285:B:THR:N	2:281:B:GLU:O	11	0.15
(6,23)	2:285:B:THR:N	2:281:B:GLU:O	13	0.15
(6,23)	2:285:B:THR:N	2:281:B:GLU:O	19	0.15
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	11	0.15
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	13	0.15
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	15	0.15
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	18	0.15
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	20	0.15
(6,14)	2:270:B:ARG:H	2:266:B:GLU:O	18	0.15
(6,14)	2:270:B:ARG:H	2:266:B:GLU:O	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,64)	1:4:A:DT:H3	2:341:B:ALA:HA	6	0.15
(4,64)	1:4:A:DT:H3	2:341:B:ALA:HA	15	0.15
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	3	0.15
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	8	0.15
(1,1473)	1:8:A:DC:H3'	1:9:A:DA:H8	20	0.15
(1,1466)	1:7:A:DT:H1'	1:8:A:DC:H3'	12	0.15
(1,1445)	1:6:A:DC:H1'	1:7:A:DT:H6	12	0.15
(1,1435)	1:5:A:DG:H3'	1:6:A:DC:H5	14	0.15
(1,1406)	1:3:A:DG:H3'	1:4:A:DT:H6	4	0.15
(1,1305)	2:337:B:ARG:H	2:338:B:ASP:HB2	5	0.15
(1,1305)	2:337:B:ARG:H	2:338:B:ASP:HB3	5	0.15
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG11	2	0.15
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG12	2	0.15
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG13	2	0.15
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG21	2	0.15
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG22	2	0.15
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG23	2	0.15
(1,1145)	2:280:B:LYS:HB2	2:281:B:GLU:H	15	0.15
(1,1145)	2:280:B:LYS:HB3	2:281:B:GLU:H	15	0.15
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB2	5	0.15
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB3	5	0.15
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG21	20	0.15
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG22	20	0.15
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG23	20	0.15
(1,687)	2:263:B:LEU:HG	2:266:B:GLU:H	3	0.15
(1,687)	2:263:B:LEU:HG	2:266:B:GLU:H	18	0.15
(1,586)	2:298:B:GLU:H	2:298:B:GLU:HG3	6	0.15
(1,586)	2:298:B:GLU:H	2:298:B:GLU:HG3	17	0.15
(1,495)	2:295:B:ILE:HG21	2:301:B:THR:H	3	0.15
(1,495)	2:295:B:ILE:HG22	2:301:B:THR:H	3	0.15
(1,495)	2:295:B:ILE:HG23	2:301:B:THR:H	3	0.15
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD21	10	0.15
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD22	10	0.15
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD23	10	0.15
(1,351)	2:331:B:ILE:H	2:331:B:ILE:HG13	6	0.15
(6,98)	2:355:B:ILE:H	2:351:B:LYS:O	18	0.14
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	6	0.14
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	10	0.14
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	14	0.14
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	15	0.14
(6,68)	2:332:B:LEU:H	2:328:B:PRO:O	1	0.14
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	4	0.14
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	8	0.14
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	15	0.14
(6,50)	2:319:B:TYR:H	2:315:B:HIS:O	7	0.14
(6,30)	2:282:B:GLU:H	2:278:B:LYS:O	19	0.14
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	2	0.14
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	10	0.14
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	14	0.14
(6,14)	2:270:B:ARG:H	2:266:B:GLU:O	2	0.14
(6,14)	2:270:B:ARG:H	2:266:B:GLU:O	10	0.14
(4,64)	1:4:A:DT:H3	2:341:B:ALA:HA	20	0.14
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD2	15	0.14
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD3	15	0.14
(4,28)	1:7:A:DT:H71	2:322:B:LYS:HD2	1	0.14
(4,28)	1:7:A:DT:H71	2:322:B:LYS:HD3	1	0.14
(4,28)	1:7:A:DT:H72	2:322:B:LYS:HD2	1	0.14
(4,28)	1:7:A:DT:H72	2:322:B:LYS:HD3	1	0.14
(4,28)	1:7:A:DT:H73	2:322:B:LYS:HD2	1	0.14
(4,28)	1:7:A:DT:H73	2:322:B:LYS:HD3	1	0.14
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	15	0.14
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	16	0.14
(1,1473)	1:8:A:DC:H3'	1:9:A:DA:H8	19	0.14
(1,1466)	1:7:A:DT:H1'	1:8:A:DC:H3'	7	0.14
(1,1466)	1:7:A:DT:H1'	1:8:A:DC:H3'	14	0.14
(1,1397)	1:3:A:DG:H3'	1:3:A:DG:H8	10	0.14
(1,1335)	2:351:B:LYS:HA	2:351:B:LYS:HD2	1	0.14
(1,1335)	2:351:B:LYS:HA	2:351:B:LYS:HD3	1	0.14
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG11	5	0.14
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG12	5	0.14
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG13	5	0.14
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG21	5	0.14
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG22	5	0.14
(1,1278)	2:323:B:HIS:H	2:325:B:VAL:HG23	5	0.14
(1,1145)	2:280:B:LYS:HB2	2:281:B:GLU:H	13	0.14
(1,1145)	2:280:B:LYS:HB3	2:281:B:GLU:H	13	0.14
(1,1004)	2:266:B:GLU:HB3	2:361:B:TRP:HD1	4	0.14
(1,1002)	2:346:B:LYS:HB2	2:347:B:TRP:HD1	19	0.14
(1,1002)	2:346:B:LYS:HB3	2:347:B:TRP:HD1	19	0.14
(1,784)	2:276:B:VAL:HG21	2:330:B:LYS:HA	2	0.14
(1,784)	2:276:B:VAL:HG22	2:330:B:LYS:HA	2	0.14
(1,784)	2:276:B:VAL:HG23	2:330:B:LYS:HA	2	0.14
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG21	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG22	2	0.14
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG23	2	0.14
(1,687)	2:263:B:LEU:HG	2:266:B:GLU:H	12	0.14
(1,687)	2:263:B:LEU:HG	2:266:B:GLU:H	13	0.14
(1,687)	2:263:B:LEU:HG	2:266:B:GLU:H	17	0.14
(1,671)	2:295:B:ILE:HG13	2:302:B:TYR:HD1	9	0.14
(1,669)	2:295:B:ILE:HG12	2:302:B:TYR:HD1	3	0.14
(1,619)	2:301:B:THR:HB	2:302:B:TYR:HA	14	0.14
(1,618)	2:301:B:THR:HB	2:302:B:TYR:HE2	17	0.14
(1,586)	2:298:B:GLU:H	2:298:B:GLU:HG3	10	0.14
(1,523)	2:270:B:ARG:HD3	2:361:B:TRP:HZ2	18	0.14
(1,515)	2:270:B:ARG:HD3	2:325:B:VAL:HA	17	0.14
(1,513)	2:270:B:ARG:HD2	2:325:B:VAL:HA	14	0.14
(1,58)	2:276:B:VAL:H	2:330:B:LYS:HA	8	0.14
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	1	0.13
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	3	0.13
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	12	0.13
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	8	0.13
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	19	0.13
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	3	0.13
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	9	0.13
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	17	0.13
(6,34)	2:297:B:CYS:H	2:293:B:LYS:O	6	0.13
(6,34)	2:297:B:CYS:H	2:293:B:LYS:O	16	0.13
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	3	0.13
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	6	0.13
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	7	0.13
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	16	0.13
(6,14)	2:270:B:ARG:H	2:266:B:GLU:O	1	0.13
(6,14)	2:270:B:ARG:H	2:266:B:GLU:O	6	0.13
(6,8)	2:262:B:GLU:H	2:258:B:VAL:O	9	0.13
(4,64)	1:4:A:DT:H3	2:341:B:ALA:HA	1	0.13
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	6	0.13
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	9	0.13
(1,1473)	1:8:A:DC:H3'	1:9:A:DA:H8	5	0.13
(1,1473)	1:8:A:DC:H3'	1:9:A:DA:H8	18	0.13
(1,1466)	1:7:A:DT:H1'	1:8:A:DC:H3'	1	0.13
(1,1466)	1:7:A:DT:H1'	1:8:A:DC:H3'	8	0.13
(1,1435)	1:5:A:DG:H3'	1:6:A:DC:H5	5	0.13
(1,1435)	1:5:A:DG:H3'	1:6:A:DC:H5	9	0.13
(1,1435)	1:5:A:DG:H3'	1:6:A:DC:H5	19	0.13
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5'	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5"	4	0.13
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5'	20	0.13
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5"	20	0.13
(1,1406)	1:3:A:DG:H3'	1:4:A:DT:H6	3	0.13
(1,1396)	1:3:A:DG:H2'	1:3:A:DG:H8	14	0.13
(1,1388)	1:2:A:DT:H1'	1:3:A:DG:H8	1	0.13
(1,1388)	1:2:A:DT:H1'	1:3:A:DG:H8	6	0.13
(1,1369)	1:1:A:DC:H4'	1:1:A:DC:H6	5	0.13
(1,1219)	2:302:B:TYR:H	2:337:B:ARG:HB2	3	0.13
(1,1219)	2:302:B:TYR:H	2:337:B:ARG:HB3	3	0.13
(1,1004)	2:266:B:GLU:HB3	2:361:B:TRP:HD1	14	0.13
(1,1002)	2:346:B:LYS:HB2	2:347:B:TRP:HD1	15	0.13
(1,1002)	2:346:B:LYS:HB3	2:347:B:TRP:HD1	15	0.13
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB2	1	0.13
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB3	1	0.13
(1,919)	2:283:B:ILE:HG21	2:323:B:HIS:HB2	15	0.13
(1,919)	2:283:B:ILE:HG22	2:323:B:HIS:HB2	15	0.13
(1,919)	2:283:B:ILE:HG23	2:323:B:HIS:HB2	15	0.13
(1,886)	2:331:B:ILE:HG21	2:353:B:PHE:HA	19	0.13
(1,886)	2:331:B:ILE:HG22	2:353:B:PHE:HA	19	0.13
(1,886)	2:331:B:ILE:HG23	2:353:B:PHE:HA	19	0.13
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG21	16	0.13
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG22	16	0.13
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG23	16	0.13
(1,687)	2:263:B:LEU:HG	2:266:B:GLU:H	4	0.13
(1,646)	2:283:B:ILE:HG13	2:319:B:TYR:HE1	11	0.13
(1,646)	2:283:B:ILE:HG13	2:319:B:TYR:HE2	11	0.13
(1,618)	2:301:B:THR:HB	2:302:B:TYR:HE2	3	0.13
(1,618)	2:301:B:THR:HB	2:302:B:TYR:HE2	19	0.13
(1,586)	2:298:B:GLU:H	2:298:B:GLU:HG3	3	0.13
(1,586)	2:298:B:GLU:H	2:298:B:GLU:HG3	5	0.13
(1,586)	2:298:B:GLU:H	2:298:B:GLU:HG3	12	0.13
(1,570)	2:277:B:GLU:HG2	2:278:B:LYS:HE2	15	0.13
(1,570)	2:277:B:GLU:HG2	2:278:B:LYS:HE3	15	0.13
(1,570)	2:277:B:GLU:HG3	2:278:B:LYS:HE2	15	0.13
(1,570)	2:277:B:GLU:HG3	2:278:B:LYS:HE3	15	0.13
(1,523)	2:270:B:ARG:HD3	2:361:B:TRP:HZ2	2	0.13
(1,523)	2:270:B:ARG:HD3	2:361:B:TRP:HZ2	16	0.13
(1,513)	2:270:B:ARG:HD2	2:325:B:VAL:HA	9	0.13
(1,367)	2:365:B:LYS:HB2	2:366:B:LYS:H	14	0.13
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD21	17	0.13
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD22	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD23	17	0.13
(1,272)	2:302:B:TYR:HA	2:306:B:ASN:H	17	0.13
(6,100)	2:354:B:VAL:H	2:350:B:GLN:O	1	0.12
(6,100)	2:354:B:VAL:H	2:350:B:GLN:O	13	0.12
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	11	0.12
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	16	0.12
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	19	0.12
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	20	0.12
(6,68)	2:332:B:LEU:H	2:328:B:PRO:O	9	0.12
(6,67)	2:332:B:LEU:N	2:328:B:PRO:O	20	0.12
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	6	0.12
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	20	0.12
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	2	0.12
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	6	0.12
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	9	0.12
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	17	0.12
(6,42)	2:323:B:HIS:H	2:319:B:TYR:O	14	0.12
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	11	0.12
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	20	0.12
(6,24)	2:285:B:THR:H	2:281:B:GLU:O	18	0.12
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	9	0.12
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	12	0.12
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	17	0.12
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	19	0.12
(6,14)	2:270:B:ARG:H	2:266:B:GLU:O	3	0.12
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD2	9	0.12
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD3	9	0.12
(4,41)	1:4:A:DT:H5'	2:355:B:ILE:HG12	13	0.12
(4,41)	1:4:A:DT:H5'	2:355:B:ILE:HG13	13	0.12
(4,41)	1:4:A:DT:H5"	2:355:B:ILE:HG12	13	0.12
(4,41)	1:4:A:DT:H5"	2:355:B:ILE:HG13	13	0.12
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	5	0.12
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	20	0.12
(1,1477)	1:9:A:DA:H1'	1:9:A:DA:H8	4	0.12
(1,1474)	1:8:A:DC:H5'	1:9:A:DA:H8	11	0.12
(1,1474)	1:8:A:DC:H5"	1:9:A:DA:H8	11	0.12
(1,1474)	1:8:A:DC:H5'	1:9:A:DA:H8	13	0.12
(1,1474)	1:8:A:DC:H5"	1:9:A:DA:H8	13	0.12
(1,1466)	1:7:A:DT:H1'	1:8:A:DC:H3'	4	0.12
(1,1466)	1:7:A:DT:H1'	1:8:A:DC:H3'	10	0.12
(1,1462)	1:7:A:DT:H3'	1:8:A:DC:H6	7	0.12
(1,1462)	1:7:A:DT:H3'	1:8:A:DC:H6	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1462)	1:7:A:DT:H3'	1:8:A:DC:H6	10	0.12
(1,1461)	1:7:A:DT:H2'	1:8:A:DC:H6	9	0.12
(1,1461)	1:7:A:DT:H2"	1:8:A:DC:H6	9	0.12
(1,1449)	1:6:A:DC:H3'	1:7:A:DT:H4'	11	0.12
(1,1445)	1:6:A:DC:H1'	1:7:A:DT:H6	3	0.12
(1,1435)	1:5:A:DG:H3'	1:6:A:DC:H5	2	0.12
(1,1435)	1:5:A:DG:H3'	1:6:A:DC:H5	12	0.12
(1,1435)	1:5:A:DG:H3'	1:6:A:DC:H5	16	0.12
(1,1413)	1:4:A:DT:H3'	1:4:A:DT:H6	4	0.12
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5'	3	0.12
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5"	3	0.12
(1,1396)	1:3:A:DG:H2'	1:3:A:DG:H8	12	0.12
(1,1389)	1:2:A:DT:H3'	1:3:A:DG:H8	16	0.12
(1,1377)	1:1:A:DC:H4'	1:2:A:DT:H6	1	0.12
(1,1369)	1:1:A:DC:H4'	1:1:A:DC:H6	9	0.12
(1,1368)	1:1:A:DC:H3'	1:1:A:DC:H6	1	0.12
(1,1368)	1:1:A:DC:H3'	1:1:A:DC:H6	19	0.12
(1,1335)	2:351:B:LYS:HA	2:351:B:LYS:HD2	3	0.12
(1,1335)	2:351:B:LYS:HA	2:351:B:LYS:HD3	3	0.12
(1,1324)	2:343:B:GLU:HA	2:344:B:ASN:HB2	16	0.12
(1,1324)	2:343:B:GLU:HA	2:344:B:ASN:HB3	16	0.12
(1,1155)	2:280:B:LYS:HG2	2:296:B:ILE:HD11	4	0.12
(1,1155)	2:280:B:LYS:HG2	2:296:B:ILE:HD12	4	0.12
(1,1155)	2:280:B:LYS:HG2	2:296:B:ILE:HD13	4	0.12
(1,1155)	2:280:B:LYS:HG3	2:296:B:ILE:HD11	4	0.12
(1,1155)	2:280:B:LYS:HG3	2:296:B:ILE:HD12	4	0.12
(1,1155)	2:280:B:LYS:HG3	2:296:B:ILE:HD13	4	0.12
(1,1059)	2:266:B:GLU:HB3	2:361:B:TRP:HZ2	4	0.12
(1,1059)	2:266:B:GLU:HB3	2:361:B:TRP:HZ2	7	0.12
(1,1054)	2:295:B:ILE:HG21	2:302:B:TYR:HE2	7	0.12
(1,1054)	2:295:B:ILE:HG22	2:302:B:TYR:HE2	7	0.12
(1,1054)	2:295:B:ILE:HG23	2:302:B:TYR:HE2	7	0.12
(1,1041)	2:311:B:ARG:HA	2:315:B:HIS:HD2	11	0.12
(1,1010)	2:314:B:TRP:HD1	2:315:B:HIS:HD2	19	0.12
(1,1004)	2:266:B:GLU:HB3	2:361:B:TRP:HD1	3	0.12
(1,1004)	2:266:B:GLU:HB3	2:361:B:TRP:HD1	17	0.12
(1,994)	2:341:B:ALA:HA	2:353:B:PHE:HD2	3	0.12
(1,994)	2:341:B:ALA:HA	2:353:B:PHE:HD2	20	0.12
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB2	7	0.12
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB3	7	0.12
(1,919)	2:283:B:ILE:HG21	2:323:B:HIS:HB2	14	0.12
(1,919)	2:283:B:ILE:HG22	2:323:B:HIS:HB2	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,919)	2:283:B:ILE:HG23	2:323:B:HIS:HB2	14	0.12
(1,886)	2:331:B:ILE:HG21	2:353:B:PHE:HA	2	0.12
(1,886)	2:331:B:ILE:HG22	2:353:B:PHE:HA	2	0.12
(1,886)	2:331:B:ILE:HG23	2:353:B:PHE:HA	2	0.12
(1,886)	2:331:B:ILE:HG21	2:353:B:PHE:HA	12	0.12
(1,886)	2:331:B:ILE:HG22	2:353:B:PHE:HA	12	0.12
(1,886)	2:331:B:ILE:HG23	2:353:B:PHE:HA	12	0.12
(1,881)	2:326:B:THR:HG21	2:360:B:ALA:HB1	10	0.12
(1,881)	2:326:B:THR:HG21	2:360:B:ALA:HB2	10	0.12
(1,881)	2:326:B:THR:HG21	2:360:B:ALA:HB3	10	0.12
(1,881)	2:326:B:THR:HG22	2:360:B:ALA:HB1	10	0.12
(1,881)	2:326:B:THR:HG22	2:360:B:ALA:HB2	10	0.12
(1,881)	2:326:B:THR:HG22	2:360:B:ALA:HB3	10	0.12
(1,881)	2:326:B:THR:HG23	2:360:B:ALA:HB1	10	0.12
(1,881)	2:326:B:THR:HG23	2:360:B:ALA:HB2	10	0.12
(1,881)	2:326:B:THR:HG23	2:360:B:ALA:HB3	10	0.12
(1,749)	2:295:B:ILE:HG21	2:301:B:THR:HG21	10	0.12
(1,749)	2:295:B:ILE:HG21	2:301:B:THR:HG22	10	0.12
(1,749)	2:295:B:ILE:HG21	2:301:B:THR:HG23	10	0.12
(1,749)	2:295:B:ILE:HG22	2:301:B:THR:HG21	10	0.12
(1,749)	2:295:B:ILE:HG22	2:301:B:THR:HG22	10	0.12
(1,749)	2:295:B:ILE:HG22	2:301:B:THR:HG23	10	0.12
(1,749)	2:295:B:ILE:HG23	2:301:B:THR:HG21	10	0.12
(1,749)	2:295:B:ILE:HG23	2:301:B:THR:HG22	10	0.12
(1,749)	2:295:B:ILE:HG23	2:301:B:THR:HG23	10	0.12
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG21	3	0.12
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG22	3	0.12
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG23	3	0.12
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG21	10	0.12
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG22	10	0.12
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG23	10	0.12
(1,727)	2:366:B:LYS:HG2	2:367:B:TYR:HB2	1	0.12
(1,727)	2:366:B:LYS:HG3	2:367:B:TYR:HB2	1	0.12
(1,720)	2:257:B:VAL:HA	2:261:B:GLU:HG2	5	0.12
(1,720)	2:257:B:VAL:HA	2:261:B:GLU:HG3	5	0.12
(1,706)	2:322:B:LYS:HA	2:364:B:VAL:HA	15	0.12
(1,693)	2:329:B:ASP:HA	2:332:B:LEU:HG	7	0.12
(1,687)	2:263:B:LEU:HG	2:266:B:GLU:H	1	0.12
(1,687)	2:263:B:LEU:HG	2:266:B:GLU:H	8	0.12
(1,666)	2:276:B:VAL:HA	2:279:B:ILE:HG13	13	0.12
(1,638)	2:269:B:LYS:H	2:269:B:LYS:HD2	1	0.12
(1,638)	2:269:B:LYS:H	2:269:B:LYS:HD3	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	2:301:B:THR:HB	2:302:B:TYR:HA	5	0.12
(1,619)	2:301:B:THR:HB	2:302:B:TYR:HA	6	0.12
(1,619)	2:301:B:THR:HB	2:302:B:TYR:HA	15	0.12
(1,619)	2:301:B:THR:HB	2:302:B:TYR:HA	17	0.12
(1,619)	2:301:B:THR:HB	2:302:B:TYR:HA	19	0.12
(1,618)	2:301:B:THR:HB	2:302:B:TYR:HE2	14	0.12
(1,618)	2:301:B:THR:HB	2:302:B:TYR:HE2	15	0.12
(1,586)	2:298:B:GLU:H	2:298:B:GLU:HG3	19	0.12
(1,523)	2:270:B:ARG:HD3	2:361:B:TRP:HZ2	20	0.12
(1,515)	2:270:B:ARG:HD3	2:325:B:VAL:HA	20	0.12
(1,495)	2:295:B:ILE:HG21	2:301:B:THR:H	5	0.12
(1,495)	2:295:B:ILE:HG22	2:301:B:THR:H	5	0.12
(1,495)	2:295:B:ILE:HG23	2:301:B:THR:H	5	0.12
(1,448)	2:332:B:LEU:HD11	2:342:B:LYS:H	3	0.12
(1,448)	2:332:B:LEU:HD12	2:342:B:LYS:H	3	0.12
(1,448)	2:332:B:LEU:HD13	2:342:B:LYS:H	3	0.12
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD21	16	0.12
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD22	16	0.12
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD23	16	0.12
(1,189)	2:356:B:THR:HB	2:357:B:LEU:H	9	0.12
(1,58)	2:276:B:VAL:H	2:330:B:LYS:HA	18	0.12
(1,1)	2:369:B:GLU:H	2:370:B:ALA:H	20	0.12
(6,107)	2:350:B:GLN:N	2:346:B:LYS:O	3	0.11
(6,104)	2:352:B:TYR:H	2:348:B:ASN:O	19	0.11
(6,98)	2:355:B:ILE:H	2:351:B:LYS:O	4	0.11
(6,98)	2:355:B:ILE:H	2:351:B:LYS:O	6	0.11
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	4	0.11
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	8	0.11
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	9	0.11
(6,68)	2:332:B:LEU:H	2:328:B:PRO:O	13	0.11
(6,68)	2:332:B:LEU:H	2:328:B:PRO:O	17	0.11
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	10	0.11
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	17	0.11
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	11	0.11
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	14	0.11
(6,60)	2:314:B:TRP:H	2:310:B:SER:O	18	0.11
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	5	0.11
(6,38)	2:295:B:ILE:H	2:291:B:LEU:O	14	0.11
(6,34)	2:297:B:CYS:H	2:293:B:LYS:O	17	0.11
(6,24)	2:285:B:THR:H	2:281:B:GLU:O	5	0.11
(6,16)	2:269:B:LYS:H	2:265:B:LYS:O	4	0.11
(6,14)	2:270:B:ARG:H	2:266:B:GLU:O	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,12)	2:260:B:PHE:H	2:256:B:THR:O	17	0.11
(6,8)	2:262:B:GLU:H	2:258:B:VAL:O	5	0.11
(6,8)	2:262:B:GLU:H	2:258:B:VAL:O	13	0.11
(4,65)	1:4:A:DT:H3	2:340:B:LYS:H	16	0.11
(4,62)	1:4:A:DT:H3	2:352:B:TYR:HD2	4	0.11
(4,55)	1:4:A:DT:H3	2:340:B:LYS:HG2	8	0.11
(4,55)	1:4:A:DT:H3	2:340:B:LYS:HG3	8	0.11
(4,32)	1:4:A:DT:H3'	2:352:B:TYR:HD2	2	0.11
(4,32)	1:4:A:DT:H3'	2:352:B:TYR:HD2	14	0.11
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	4	0.11
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	7	0.11
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	18	0.11
(1,1477)	1:9:A:DA:H1'	1:9:A:DA:H8	3	0.11
(1,1477)	1:9:A:DA:H1'	1:9:A:DA:H8	6	0.11
(1,1477)	1:9:A:DA:H1'	1:9:A:DA:H8	11	0.11
(1,1477)	1:9:A:DA:H1'	1:9:A:DA:H8	13	0.11
(1,1477)	1:9:A:DA:H1'	1:9:A:DA:H8	17	0.11
(1,1474)	1:8:A:DC:H5'	1:9:A:DA:H8	6	0.11
(1,1474)	1:8:A:DC:H5"	1:9:A:DA:H8	6	0.11
(1,1474)	1:8:A:DC:H5'	1:9:A:DA:H8	9	0.11
(1,1474)	1:8:A:DC:H5"	1:9:A:DA:H8	9	0.11
(1,1473)	1:8:A:DC:H3'	1:9:A:DA:H8	1	0.11
(1,1473)	1:8:A:DC:H3'	1:9:A:DA:H8	12	0.11
(1,1471)	1:8:A:DC:H1'	1:8:A:DC:H4'	9	0.11
(1,1470)	1:8:A:DC:H1'	1:8:A:DC:H3'	5	0.11
(1,1470)	1:8:A:DC:H1'	1:8:A:DC:H3'	18	0.11
(1,1470)	1:8:A:DC:H1'	1:8:A:DC:H3'	19	0.11
(1,1466)	1:7:A:DT:H1'	1:8:A:DC:H3'	2	0.11
(1,1466)	1:7:A:DT:H1'	1:8:A:DC:H3'	16	0.11
(1,1462)	1:7:A:DT:H3'	1:8:A:DC:H6	2	0.11
(1,1449)	1:6:A:DC:H3'	1:7:A:DT:H4'	8	0.11
(1,1445)	1:6:A:DC:H1'	1:7:A:DT:H6	18	0.11
(1,1445)	1:6:A:DC:H1'	1:7:A:DT:H6	20	0.11
(1,1435)	1:5:A:DG:H3'	1:6:A:DC:H5	13	0.11
(1,1435)	1:5:A:DG:H3'	1:6:A:DC:H5	15	0.11
(1,1424)	1:5:A:DG:H8	1:4:A:DT:H4'	3	0.11
(1,1413)	1:4:A:DT:H3'	1:4:A:DT:H6	5	0.11
(1,1413)	1:4:A:DT:H3'	1:4:A:DT:H6	6	0.11
(1,1413)	1:4:A:DT:H3'	1:4:A:DT:H6	10	0.11
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5'	1	0.11
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5"	1	0.11
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5'	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5"	8	0.11
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5'	17	0.11
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5"	17	0.11
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5'	19	0.11
(1,1409)	1:3:A:DG:H1'	1:4:A:DT:H5"	19	0.11
(1,1406)	1:3:A:DG:H3'	1:4:A:DT:H6	1	0.11
(1,1406)	1:3:A:DG:H3'	1:4:A:DT:H6	5	0.11
(1,1406)	1:3:A:DG:H3'	1:4:A:DT:H6	13	0.11
(1,1397)	1:3:A:DG:H3'	1:3:A:DG:H8	12	0.11
(1,1377)	1:1:A:DC:H4'	1:2:A:DT:H6	3	0.11
(1,1369)	1:1:A:DC:H4'	1:1:A:DC:H6	7	0.11
(1,1297)	2:333:B:GLU:HA	2:342:B:LYS:HE2	10	0.11
(1,1297)	2:333:B:GLU:HA	2:342:B:LYS:HE3	10	0.11
(1,1288)	2:330:B:LYS:HB2	2:331:B:ILE:HA	7	0.11
(1,1288)	2:330:B:LYS:HB3	2:331:B:ILE:HA	7	0.11
(1,1288)	2:330:B:LYS:HB2	2:331:B:ILE:HA	15	0.11
(1,1288)	2:330:B:LYS:HB3	2:331:B:ILE:HA	15	0.11
(1,1219)	2:302:B:TYR:H	2:337:B:ARG:HB2	9	0.11
(1,1219)	2:302:B:TYR:H	2:337:B:ARG:HB3	9	0.11
(1,1219)	2:302:B:TYR:H	2:337:B:ARG:HB2	14	0.11
(1,1219)	2:302:B:TYR:H	2:337:B:ARG:HB3	14	0.11
(1,1155)	2:280:B:LYS:HG2	2:296:B:ILE:HD11	15	0.11
(1,1155)	2:280:B:LYS:HG2	2:296:B:ILE:HD12	15	0.11
(1,1155)	2:280:B:LYS:HG2	2:296:B:ILE:HD13	15	0.11
(1,1155)	2:280:B:LYS:HG3	2:296:B:ILE:HD11	15	0.11
(1,1155)	2:280:B:LYS:HG3	2:296:B:ILE:HD12	15	0.11
(1,1155)	2:280:B:LYS:HG3	2:296:B:ILE:HD13	15	0.11
(1,1145)	2:280:B:LYS:HB2	2:281:B:GLU:H	19	0.11
(1,1145)	2:280:B:LYS:HB3	2:281:B:GLU:H	19	0.11
(1,1110)	2:273:B:GLY:HA2	2:274:B:LYS:HE2	18	0.11
(1,1110)	2:273:B:GLY:HA2	2:274:B:LYS:HE3	18	0.11
(1,1110)	2:273:B:GLY:HA3	2:274:B:LYS:HE2	18	0.11
(1,1110)	2:273:B:GLY:HA3	2:274:B:LYS:HE3	18	0.11
(1,1026)	2:346:B:LYS:HB2	2:347:B:TRP:HE3	5	0.11
(1,1026)	2:346:B:LYS:HB3	2:347:B:TRP:HE3	5	0.11
(1,1004)	2:266:B:GLU:HB3	2:361:B:TRP:HD1	5	0.11
(1,1002)	2:346:B:LYS:HB2	2:347:B:TRP:HD1	17	0.11
(1,1002)	2:346:B:LYS:HB3	2:347:B:TRP:HD1	17	0.11
(1,994)	2:341:B:ALA:HA	2:353:B:PHE:HD2	4	0.11
(1,994)	2:341:B:ALA:HA	2:353:B:PHE:HD2	10	0.11
(1,994)	2:341:B:ALA:HA	2:353:B:PHE:HD2	15	0.11
(1,994)	2:341:B:ALA:HA	2:353:B:PHE:HD2	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB2	14	0.11
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB3	14	0.11
(1,893)	2:295:B:ILE:HG21	2:302:B:TYR:HB3	18	0.11
(1,893)	2:295:B:ILE:HG22	2:302:B:TYR:HB3	18	0.11
(1,893)	2:295:B:ILE:HG23	2:302:B:TYR:HB3	18	0.11
(1,881)	2:326:B:THR:HG21	2:360:B:ALA:HB1	16	0.11
(1,881)	2:326:B:THR:HG21	2:360:B:ALA:HB2	16	0.11
(1,881)	2:326:B:THR:HG21	2:360:B:ALA:HB3	16	0.11
(1,881)	2:326:B:THR:HG22	2:360:B:ALA:HB1	16	0.11
(1,881)	2:326:B:THR:HG22	2:360:B:ALA:HB2	16	0.11
(1,881)	2:326:B:THR:HG22	2:360:B:ALA:HB3	16	0.11
(1,881)	2:326:B:THR:HG23	2:360:B:ALA:HB1	16	0.11
(1,881)	2:326:B:THR:HG23	2:360:B:ALA:HB2	16	0.11
(1,881)	2:326:B:THR:HG23	2:360:B:ALA:HB3	16	0.11
(1,859)	2:263:B:LEU:HA	2:263:B:LEU:HD11	6	0.11
(1,859)	2:263:B:LEU:HA	2:263:B:LEU:HD12	6	0.11
(1,859)	2:263:B:LEU:HA	2:263:B:LEU:HD13	6	0.11
(1,859)	2:263:B:LEU:HA	2:263:B:LEU:HD21	6	0.11
(1,859)	2:263:B:LEU:HA	2:263:B:LEU:HD22	6	0.11
(1,859)	2:263:B:LEU:HA	2:263:B:LEU:HD23	6	0.11
(1,850)	2:341:B:ALA:HB1	2:352:B:TYR:HB3	13	0.11
(1,850)	2:341:B:ALA:HB2	2:352:B:TYR:HB3	13	0.11
(1,850)	2:341:B:ALA:HB3	2:352:B:TYR:HB3	13	0.11
(1,850)	2:341:B:ALA:HB1	2:352:B:TYR:HB3	14	0.11
(1,850)	2:341:B:ALA:HB2	2:352:B:TYR:HB3	14	0.11
(1,850)	2:341:B:ALA:HB3	2:352:B:TYR:HB3	14	0.11
(1,763)	2:280:B:LYS:HA	2:320:B:LEU:HD21	15	0.11
(1,763)	2:280:B:LYS:HA	2:320:B:LEU:HD22	15	0.11
(1,763)	2:280:B:LYS:HA	2:320:B:LEU:HD23	15	0.11
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG21	17	0.11
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG22	17	0.11
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG23	17	0.11
(1,727)	2:366:B:LYS:HG2	2:367:B:TYR:HB2	20	0.11
(1,727)	2:366:B:LYS:HG3	2:367:B:TYR:HB2	20	0.11
(1,704)	2:355:B:ILE:HA	2:358:B:SER:HA	17	0.11
(1,702)	2:363:B:VAL:HA	2:367:B:TYR:HB2	15	0.11
(1,702)	2:363:B:VAL:HA	2:367:B:TYR:HB2	19	0.11
(1,687)	2:263:B:LEU:HG	2:266:B:GLU:H	10	0.11
(1,669)	2:295:B:ILE:HG12	2:302:B:TYR:HD1	19	0.11
(1,642)	2:300:B:LYS:HD2	2:301:B:THR:H	17	0.11
(1,642)	2:300:B:LYS:HD3	2:301:B:THR:H	17	0.11
(1,619)	2:301:B:THR:HB	2:302:B:TYR:HA	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	2:298:B:GLU:H	2:298:B:GLU:HG3	13	0.11
(1,581)	2:261:B:GLU:HG2	2:262:B:GLU:H	10	0.11
(1,581)	2:261:B:GLU:HG3	2:262:B:GLU:H	10	0.11
(1,515)	2:270:B:ARG:HD3	2:325:B:VAL:HA	7	0.11
(1,515)	2:270:B:ARG:HD3	2:325:B:VAL:HA	13	0.11
(1,513)	2:270:B:ARG:HD2	2:325:B:VAL:HA	8	0.11
(1,513)	2:270:B:ARG:HD2	2:325:B:VAL:HA	11	0.11
(1,484)	2:271:B:ASP:HB2	2:326:B:THR:H	6	0.11
(1,449)	2:339:B:SER:H	2:342:B:LYS:H	2	0.11
(1,448)	2:332:B:LEU:HD11	2:342:B:LYS:H	4	0.11
(1,448)	2:332:B:LEU:HD12	2:342:B:LYS:H	4	0.11
(1,448)	2:332:B:LEU:HD13	2:342:B:LYS:H	4	0.11
(1,387)	2:330:B:LYS:HA	2:333:B:GLU:H	10	0.11
(1,382)	2:294:B:GLU:HA	2:298:B:GLU:H	18	0.11
(1,379)	2:292:B:ILE:HD11	2:296:B:ILE:H	7	0.11
(1,379)	2:292:B:ILE:HD12	2:296:B:ILE:H	7	0.11
(1,379)	2:292:B:ILE:HD13	2:296:B:ILE:H	7	0.11
(1,351)	2:331:B:ILE:H	2:331:B:ILE:HG13	4	0.11
(1,351)	2:331:B:ILE:H	2:331:B:ILE:HG13	20	0.11
(1,22)	2:359:B:LYS:HB3	2:360:B:ALA:H	2	0.11
(1,22)	2:359:B:LYS:HB3	2:360:B:ALA:H	9	0.11
(1,22)	2:359:B:LYS:HB3	2:360:B:ALA:H	19	0.11
(6,98)	2:355:B:ILE:H	2:351:B:LYS:O	2	0.1
(6,98)	2:355:B:ILE:H	2:351:B:LYS:O	15	0.1
(6,94)	2:357:B:LEU:H	2:353:B:PHE:O	18	0.1
(6,68)	2:332:B:LEU:H	2:328:B:PRO:O	11	0.1
(6,64)	2:334:B:LEU:H	2:330:B:LYS:O	3	0.1
(6,14)	2:270:B:ARG:H	2:266:B:GLU:O	12	0.1
(6,2)	2:265:B:LYS:H	2:261:B:GLU:O	2	0.1
(4,65)	1:4:A:DT:H3	2:340:B:LYS:H	18	0.1
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD2	3	0.1
(4,57)	1:4:A:DT:H3	2:340:B:LYS:HD3	3	0.1
(4,46)	1:2:A:DT:H4'	2:351:B:LYS:HE2	7	0.1
(4,46)	1:2:A:DT:H4'	2:351:B:LYS:HE3	7	0.1
(4,41)	1:4:A:DT:H5'	2:355:B:ILE:HG12	16	0.1
(4,41)	1:4:A:DT:H5'	2:355:B:ILE:HG13	16	0.1
(4,41)	1:4:A:DT:H5"	2:355:B:ILE:HG12	16	0.1
(4,41)	1:4:A:DT:H5"	2:355:B:ILE:HG13	16	0.1
(4,32)	1:4:A:DT:H3'	2:352:B:TYR:HD2	16	0.1
(4,32)	1:4:A:DT:H3'	2:352:B:TYR:HD2	17	0.1
(4,15)	1:6:A:DC:H1'	2:314:B:TRP:HE1	10	0.1
(4,14)	1:5:A:DG:H1'	2:314:B:TRP:HE1	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,11)	1:5:A:DG:H3'	2:314:B:TRP:HD1	12	0.1
(1,1477)	1:9:A:DA:H1'	1:9:A:DA:H8	20	0.1
(1,1474)	1:8:A:DC:H5'	1:9:A:DA:H8	3	0.1
(1,1474)	1:8:A:DC:H5"	1:9:A:DA:H8	3	0.1
(1,1473)	1:8:A:DC:H3'	1:9:A:DA:H8	7	0.1
(1,1470)	1:8:A:DC:H1'	1:8:A:DC:H3'	15	0.1
(1,1464)	1:7:A:DT:H1'	1:8:A:DC:H5'	19	0.1
(1,1464)	1:7:A:DT:H1'	1:8:A:DC:H5"	19	0.1
(1,1462)	1:7:A:DT:H3'	1:8:A:DC:H6	1	0.1
(1,1462)	1:7:A:DT:H3'	1:8:A:DC:H6	4	0.1
(1,1447)	1:6:A:DC:H4'	1:7:A:DT:H6	2	0.1
(1,1445)	1:6:A:DC:H1'	1:7:A:DT:H6	2	0.1
(1,1435)	1:5:A:DG:H3'	1:6:A:DC:H5	17	0.1
(1,1424)	1:5:A:DG:H8	1:4:A:DT:H4'	8	0.1
(1,1397)	1:3:A:DG:H3'	1:3:A:DG:H8	7	0.1
(1,1389)	1:2:A:DT:H3'	1:3:A:DG:H8	3	0.1
(1,1389)	1:2:A:DT:H3'	1:3:A:DG:H8	18	0.1
(1,1388)	1:2:A:DT:H1'	1:3:A:DG:H8	19	0.1
(1,1377)	1:1:A:DC:H4'	1:2:A:DT:H6	12	0.1
(1,1368)	1:1:A:DC:H3'	1:1:A:DC:H6	2	0.1
(1,1316)	2:342:B:LYS:H	2:342:B:LYS:HE2	1	0.1
(1,1316)	2:342:B:LYS:H	2:342:B:LYS:HE3	1	0.1
(1,1282)	2:325:B:VAL:HG11	2:327:B:ASP:H	5	0.1
(1,1282)	2:325:B:VAL:HG12	2:327:B:ASP:H	5	0.1
(1,1282)	2:325:B:VAL:HG13	2:327:B:ASP:H	5	0.1
(1,1282)	2:325:B:VAL:HG21	2:327:B:ASP:H	5	0.1
(1,1282)	2:325:B:VAL:HG22	2:327:B:ASP:H	5	0.1
(1,1282)	2:325:B:VAL:HG23	2:327:B:ASP:H	5	0.1
(1,1059)	2:266:B:GLU:HB3	2:361:B:TRP:HZ2	5	0.1
(1,1056)	2:266:B:GLU:HA	2:361:B:TRP:HZ2	14	0.1
(1,1056)	2:266:B:GLU:HA	2:361:B:TRP:HZ2	19	0.1
(1,1010)	2:314:B:TRP:HD1	2:315:B:HIS:HD2	12	0.1
(1,1004)	2:266:B:GLU:HB3	2:361:B:TRP:HD1	2	0.1
(1,1002)	2:346:B:LYS:HB2	2:347:B:TRP:HD1	1	0.1
(1,1002)	2:346:B:LYS:HB3	2:347:B:TRP:HD1	1	0.1
(1,999)	2:341:B:ALA:HB1	2:353:B:PHE:HE2	19	0.1
(1,999)	2:341:B:ALA:HB2	2:353:B:PHE:HE2	19	0.1
(1,999)	2:341:B:ALA:HB3	2:353:B:PHE:HE2	19	0.1
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB2	16	0.1
(1,933)	2:308:B:ASP:HA	2:311:B:ARG:HB3	16	0.1
(1,893)	2:295:B:ILE:HG21	2:302:B:TYR:HB3	7	0.1
(1,893)	2:295:B:ILE:HG22	2:302:B:TYR:HB3	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	2:295:B:ILE:HG23	2:302:B:TYR:HB3	7	0.1
(1,886)	2:331:B:ILE:HG21	2:353:B:PHE:HA	15	0.1
(1,886)	2:331:B:ILE:HG22	2:353:B:PHE:HA	15	0.1
(1,886)	2:331:B:ILE:HG23	2:353:B:PHE:HA	15	0.1
(1,822)	2:269:B:LYS:HA	2:269:B:LYS:HE2	18	0.1
(1,822)	2:269:B:LYS:HA	2:269:B:LYS:HE3	18	0.1
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG21	15	0.1
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG22	15	0.1
(1,744)	2:341:B:ALA:H	2:349:B:THR:HG23	15	0.1
(1,720)	2:257:B:VAL:HA	2:261:B:GLU:HG2	4	0.1
(1,720)	2:257:B:VAL:HA	2:261:B:GLU:HG3	4	0.1
(1,720)	2:257:B:VAL:HA	2:261:B:GLU:HG2	16	0.1
(1,720)	2:257:B:VAL:HA	2:261:B:GLU:HG3	16	0.1
(1,702)	2:363:B:VAL:HA	2:367:B:TYR:HB2	2	0.1
(1,702)	2:363:B:VAL:HA	2:367:B:TYR:HB2	4	0.1
(1,662)	2:276:B:VAL:HA	2:279:B:ILE:HG12	15	0.1
(1,662)	2:276:B:VAL:HA	2:279:B:ILE:HG12	17	0.1
(1,642)	2:300:B:LYS:HD2	2:301:B:THR:H	4	0.1
(1,642)	2:300:B:LYS:HD3	2:301:B:THR:H	4	0.1
(1,619)	2:301:B:THR:HB	2:302:B:TYR:HA	7	0.1
(1,614)	2:265:B:LYS:H	2:268:B:VAL:HB	5	0.1
(1,614)	2:265:B:LYS:H	2:268:B:VAL:HB	7	0.1
(1,614)	2:265:B:LYS:H	2:268:B:VAL:HB	15	0.1
(1,581)	2:261:B:GLU:HG2	2:262:B:GLU:H	11	0.1
(1,581)	2:261:B:GLU:HG3	2:262:B:GLU:H	11	0.1
(1,367)	2:365:B:LYS:HB2	2:366:B:LYS:H	11	0.1
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD21	1	0.1
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD22	1	0.1
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD23	1	0.1
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD21	8	0.1
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD22	8	0.1
(1,360)	2:280:B:LYS:H	2:320:B:LEU:HD23	8	0.1
(1,58)	2:276:B:VAL:H	2:330:B:LYS:HA	19	0.1
(1,22)	2:359:B:LYS:HB3	2:360:B:ALA:H	16	0.1
(1,22)	2:359:B:LYS:HB3	2:360:B:ALA:H	17	0.1
(1,1)	2:369:B:GLU:H	2:370:B:ALA:H	5	0.1
(1,1)	2:369:B:GLU:H	2:370:B:ALA:H	9	0.1

10 Dihedral-angle violation analysis

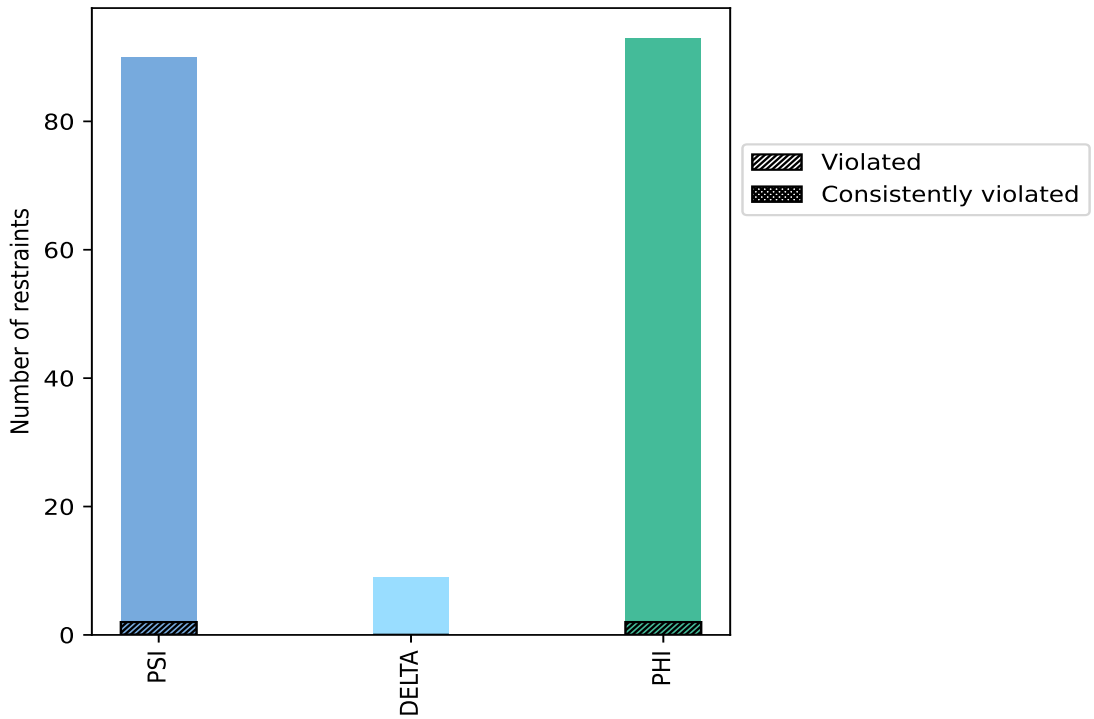
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	90	46.9	2	2.2	1.0	0	0.0	0.0
DELTA	9	4.7	0	0.0	0.0	0	0.0	0.0
PHI	93	48.4	2	2.2	1.0	0	0.0	0.0
Total	192	100.0	4	2.1	2.1	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



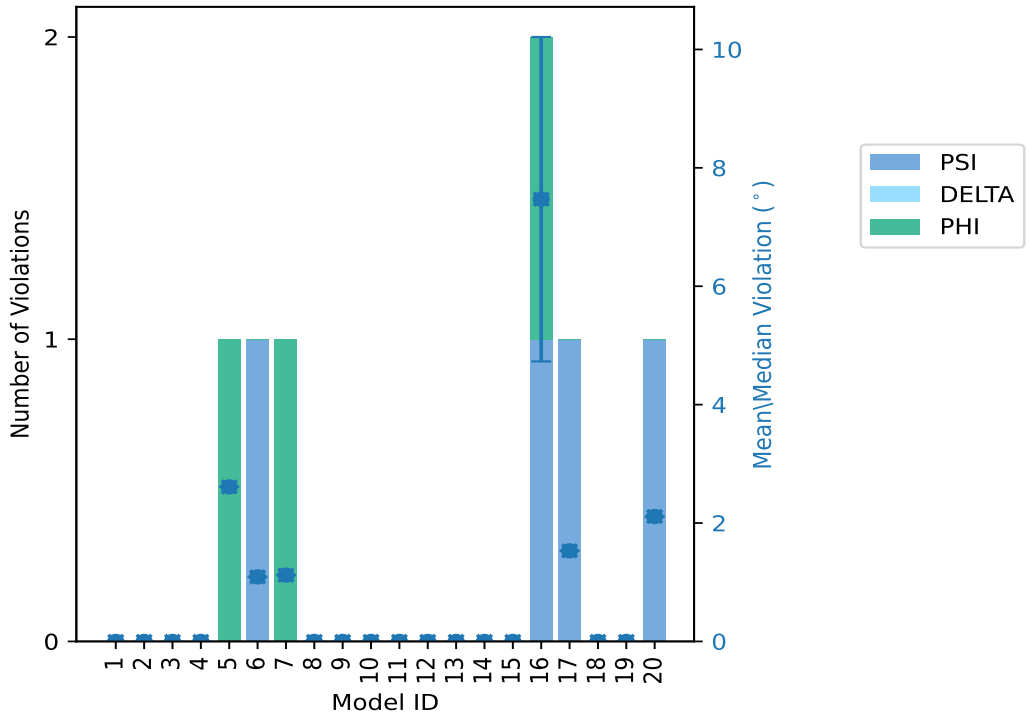
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

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

Model ID	Number of violations				Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	DELTA	PHI	Total				
1	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	1	1	2.61	2.61	0.0	2.61
6	1	0	0	1	1.09	1.09	0.0	1.09
7	0	0	1	1	1.12	1.12	0.0	1.12
8	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0.0	0.0	0.0	0.0
16	1	0	1	2	7.47	10.21	2.74	7.47
17	1	0	0	1	1.53	1.53	0.0	1.53
18	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0	0.0	0.0	0.0	0.0
20	1	0	0	1	2.11	2.11	0.0	2.11

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble

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

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

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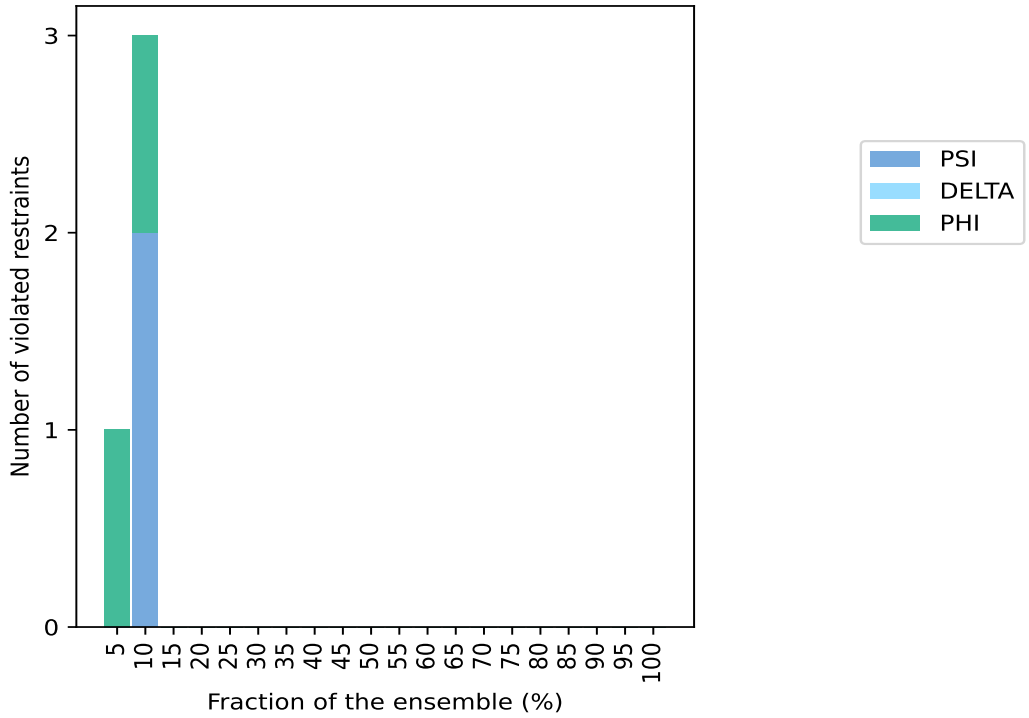
Number of violated restraints				Fraction of the ensemble	
PSI	DELTA	PHI	Total	Count[1]	%
0	0	0	0	12	60.0
0	0	0	0	13	65.0
0	0	0	0	14	70.0
0	0	0	0	15	75.0
0	0	0	0	16	80.0
0	0	0	0	17	85.0
0	0	0	0	18	90.0
0	0	0	0	19	95.0
0	0	0	0	20	100.0

[1] Number of models with violations

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

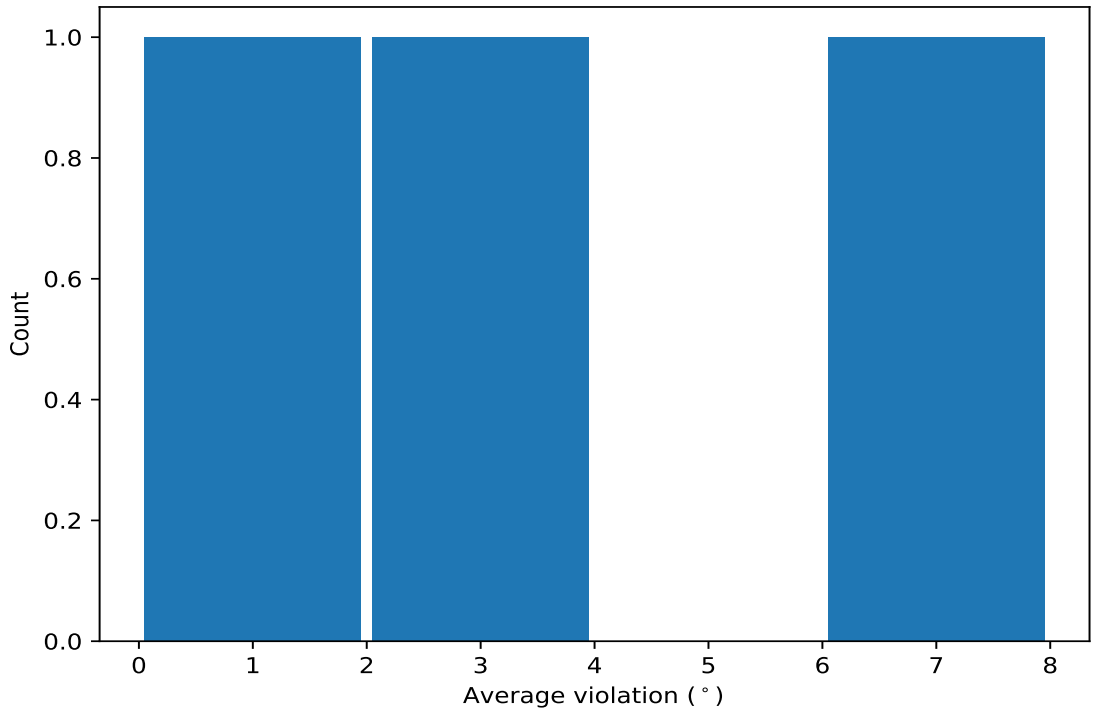


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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

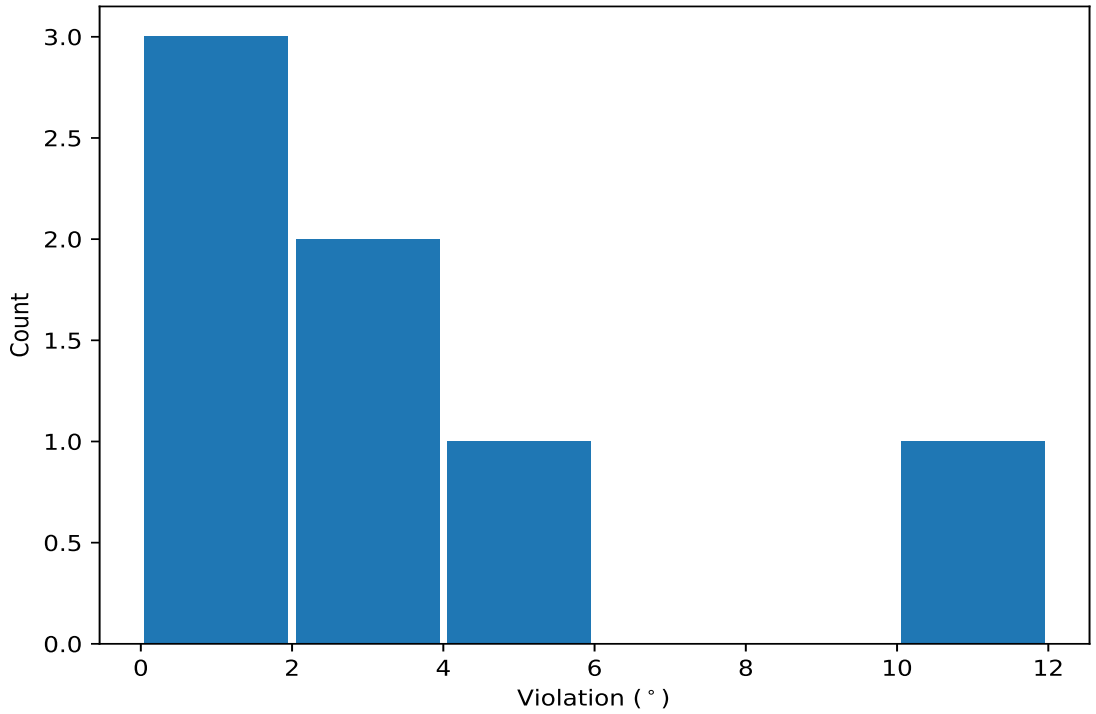
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,137)	2:337:B:ARG:C	2:338:B:ASP:N	2:338:B:ASP:CA	2:338:B:ASP:C	2	6.41	3.8	6.41
(1,55)	2:282:B:GLU:N	2:282:B:GLU:CA	2:282:B:GLU:C	2:283:B:ILE:N	2	3.42	1.31	3.42
(1,76)	2:301:B:THR:N	2:301:B:THR:CA	2:301:B:THR:C	2:302:B:TYR:N	2	1.31	0.22	1.31

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,137)	2:337:B:ARG:C	2:338:B:ASP:N	2:338:B:ASP:CA	2:338:B:ASP:C	16	10.21
(1,55)	2:282:B:GLU:N	2:282:B:GLU:CA	2:282:B:GLU:C	2:283:B:ILE:N	16	4.73
(1,137)	2:337:B:ARG:C	2:338:B:ASP:N	2:338:B:ASP:CA	2:338:B:ASP:C	5	2.61
(1,55)	2:282:B:GLU:N	2:282:B:GLU:CA	2:282:B:GLU:C	2:283:B:ILE:N	20	2.11
(1,76)	2:301:B:THR:N	2:301:B:THR:CA	2:301:B:THR:C	2:302:B:TYR:N	17	1.53
(1,115)	2:320:B:LEU:C	2:321:B:MET:N	2:321:B:MET:CA	2:321:B:MET:C	7	1.12
(1,76)	2:301:B:THR:N	2:301:B:THR:CA	2:301:B:THR:C	2:302:B:TYR:N	6	1.09