



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 10:45 PM UTC

PDB ID : 6K3K / pdb_00006k3k
BMRB ID : 36193
Title : Solution structure of APOBEC3G-CD2 with ssDNA, Product B
Authors : Cao, C.; Yan, X.; Lan, W.; Wang, C.
Deposited on : 2019-05-19

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

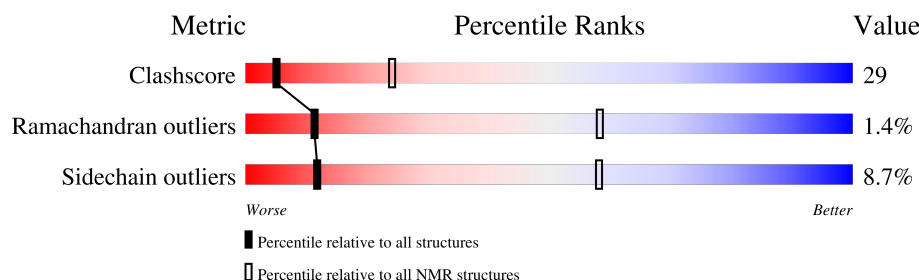
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	188	
2	B	10	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:202-A:315, A:321-A:382 (176)	0.68	3

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

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

The models can be grouped into 4 clusters and 6 single-model clusters were found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3333 atoms, of which 1577 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA dC->dU-editing enzyme APOBEC-3G.

Mol	Chain	Residues	Atoms							Trace
1	A	188	Total	C	H	N	O	S		0
			3020	985	1463	275	283	14		

- Molecule 2 is DNA/RNA hybrid called DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms								Trace
2	B	10	Total	C	H	I	N	O	P		0
			312	97	114	1	31	60	9		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

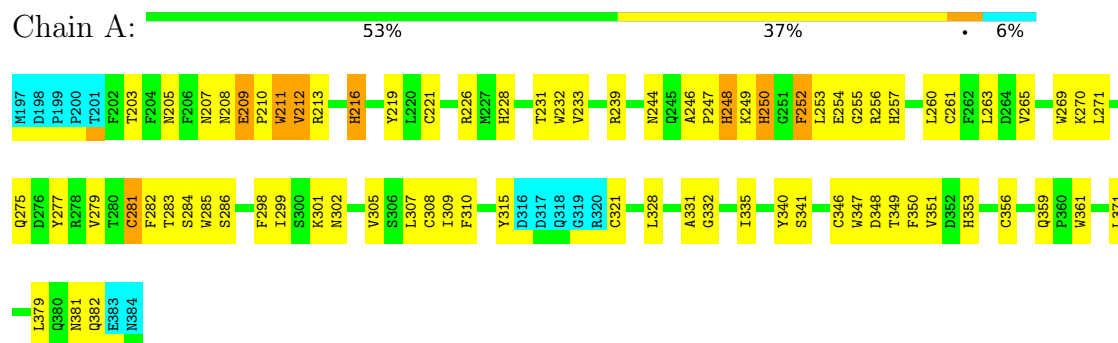
Mol	Chain	Residues	Atoms	
3	A	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')

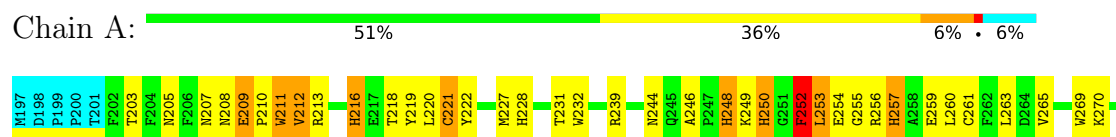


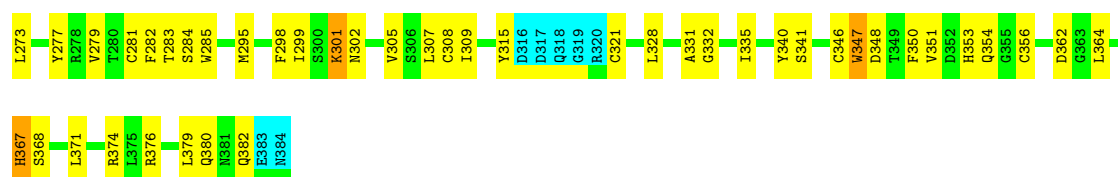
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

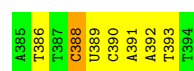
4.2.1 Score per residue for model 1

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



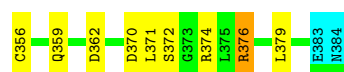
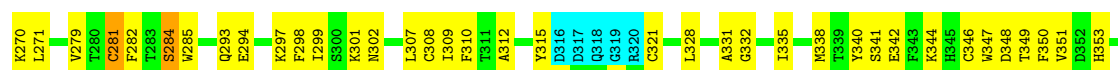
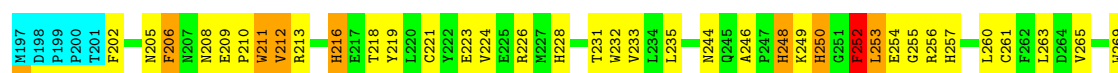


- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')



4.2.2 Score per residue for model 2

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

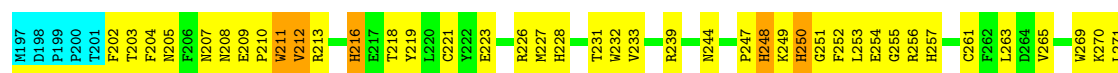


- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')



4.2.3 Score per residue for model 3 (medoid)

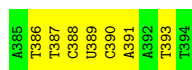
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G





- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')

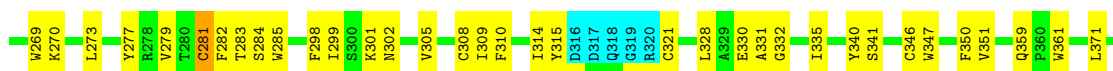
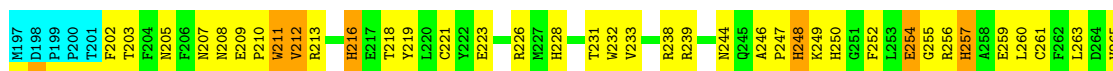
Chain B: 30% 70%



4.2.4 Score per residue for model 4

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

Chain A: 53% 36% • 6%



- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')

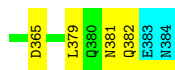
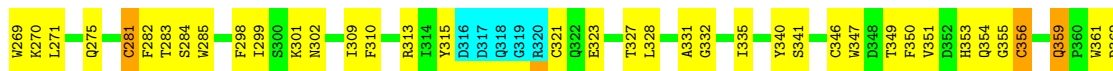
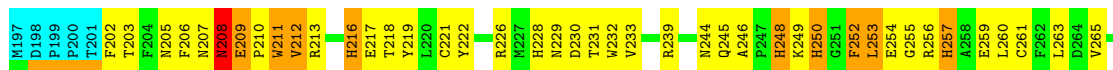
Chain B: 30% 60% 10%



4.2.5 Score per residue for model 5

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

Chain A: 49% 38% 6% • 6%

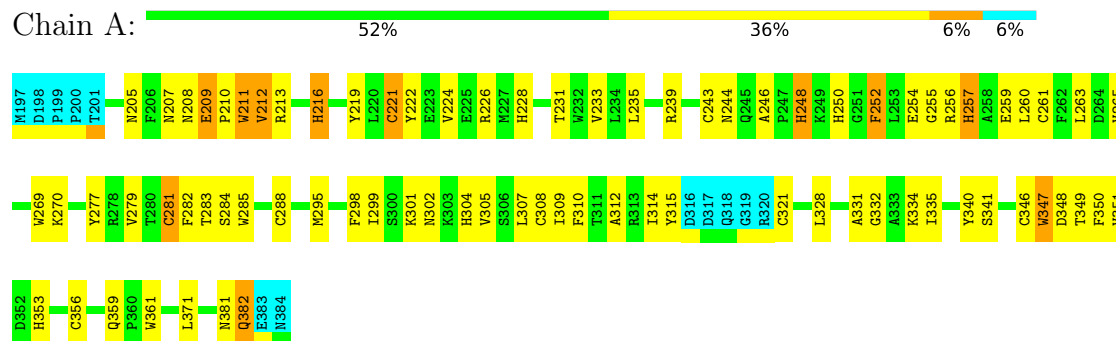


- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')



4.2.6 Score per residue for model 6

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

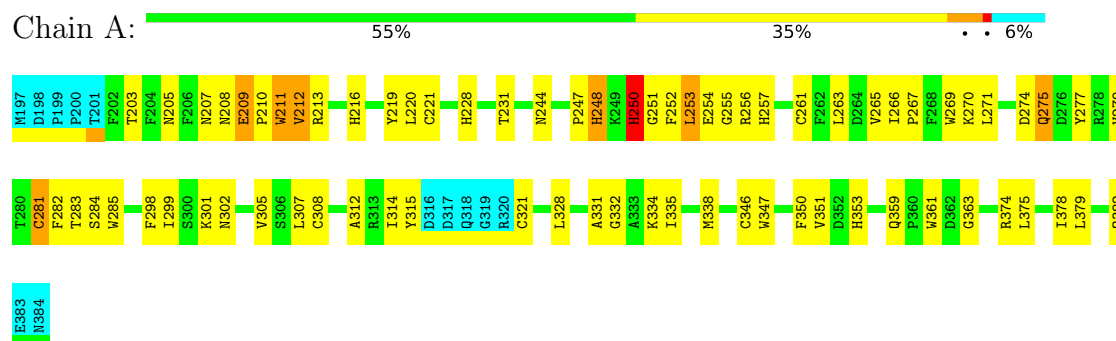


- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')



4.2.7 Score per residue for model 7

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

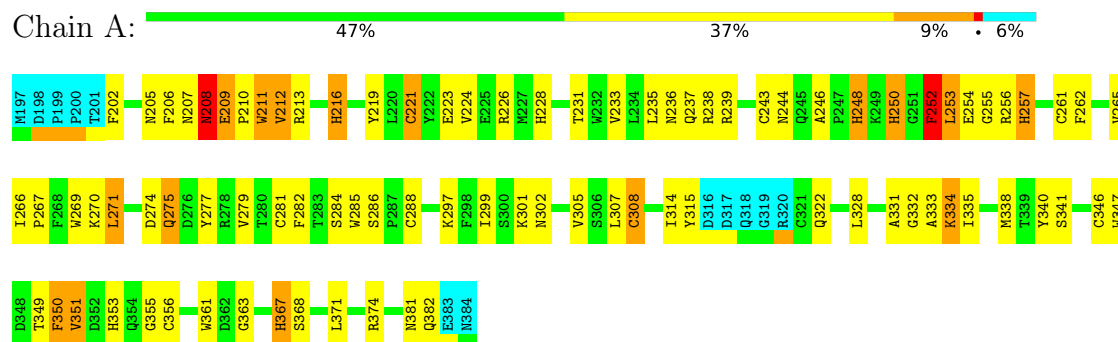


- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')



4.2.8 Score per residue for model 8

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')



4.2.9 Score per residue for model 9

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

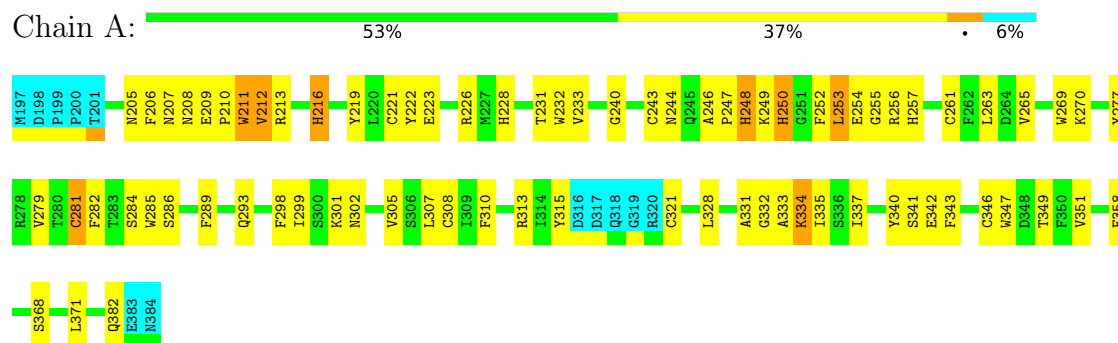


- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')



4.2.10 Score per residue for model 10

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

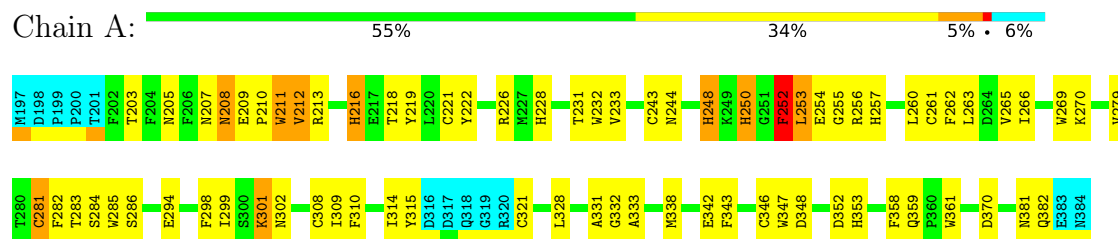


- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')



4.2.11 Score per residue for model 11

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



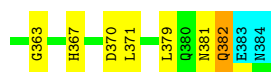
- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')



4.2.12 Score per residue for model 12

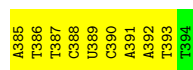
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G





- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')

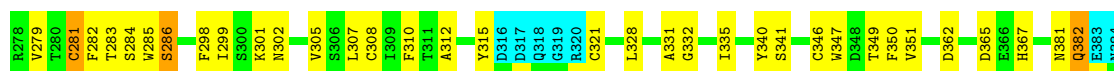
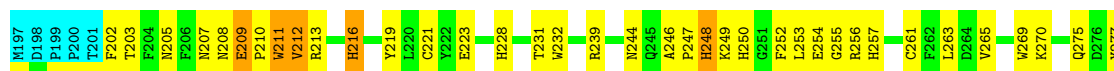
Chain B: 10% 90%



4.2.13 Score per residue for model 13

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

Chain A: 56% 34% 6%



- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')

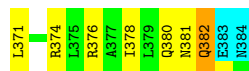
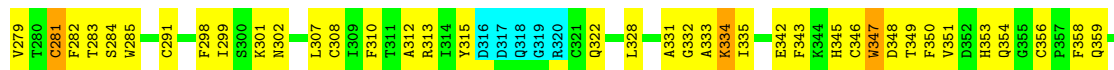
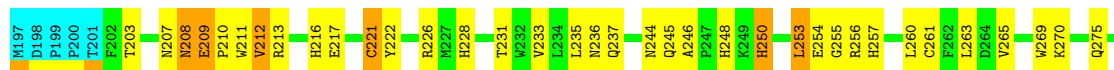
Chain B: 30% 60% 10%



4.2.14 Score per residue for model 14

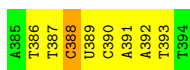
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

Chain A: 51% 38% 5% 6%



- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')

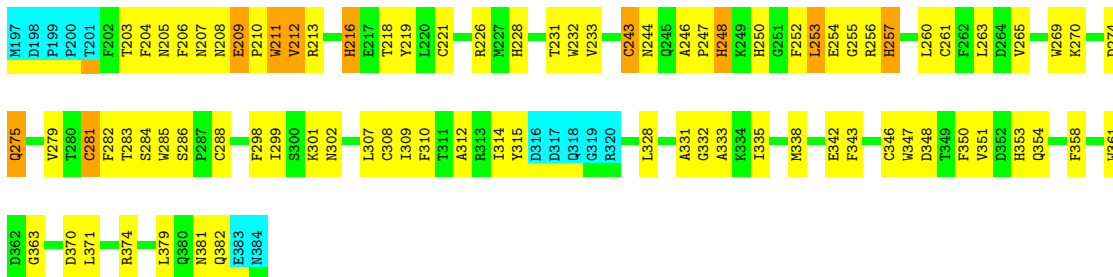
Chain B: 20% 70% 10%



4.2.15 Score per residue for model 15

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

Chain A: 49% 39% 5% 6%



- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')

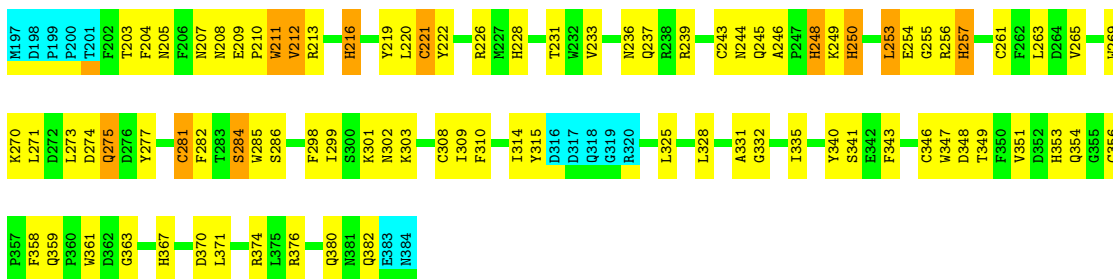
Chain B: 20% 80%



4.2.16 Score per residue for model 16

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

Chain A: 48% 40% 6% 6%



- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')

Chain B: 20% 70% 10%



4.2.17 Score per residue for model 17

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

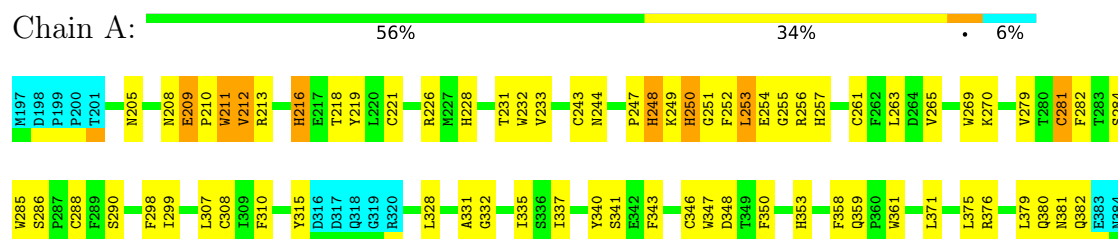


- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')



4.2.18 Score per residue for model 18

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



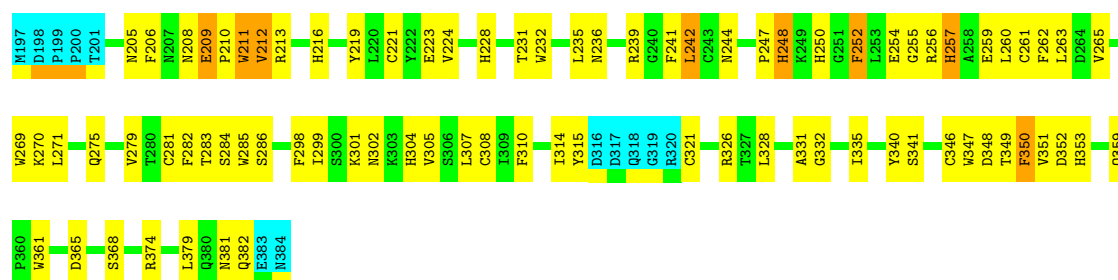
- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')



4.2.19 Score per residue for model 19

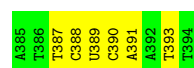
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G





- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')

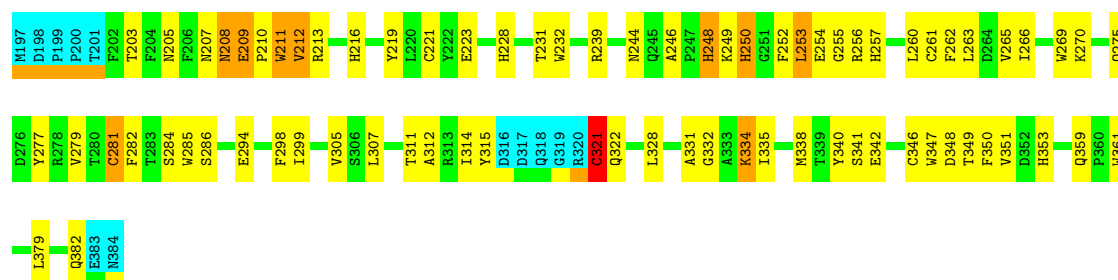
Chain B: 40% 60%



4.2.20 Score per residue for model 20

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

Chain A: 54% 35% 5% 6%



- Molecule 2: DNA/RNA (5'-D(*AP*TP*TP*CP*UP*(ICY)P*AP*AP*TP*T)-3')

Chain B: 40% 50% 10%



5 Refinement protocol and experimental data overview

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

Of the 100 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
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

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	2222
Number of shifts mapped to atoms	2222
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C38, ZN

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	1.43±0.00	0±0/1508 (0.0± 0.0%)	1.31±0.01	1±1/2043 (0.1± 0.1%)
2	B	0.72±0.01	1±0/197 (0.4± 0.2%)	0.93±0.01	0±0/299 (0.0± 0.0%)
All	All	1.37	14/34100 (0.0%)	1.27	29/46840 (0.1%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	388	DC	O3'-P	5.35	1.61	1.56	4	14

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	250	HIS	CA-CB-CG	-5.52	108.28	113.80	1	9
1	A	252	PHE	CA-CB-CG	-5.46	108.34	113.80	8	5
1	A	206	PHE	CA-CB-CG	-5.44	108.36	113.80	2	3
1	A	257	HIS	CA-CB-CG	-5.32	108.48	113.80	9	1
1	A	350	PHE	CA-CB-CG	-5.25	108.55	113.80	17	6
1	A	355	GLY	N-CA-C	-5.13	108.97	115.08	5	3
1	A	262	PHE	CA-CB-CG	-5.09	108.71	113.80	8	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1462	1383	1375	86±9
2	B	198	114	114	23±3
All	All	33220	29940	29780	1835

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:226:ARG:NH1	1:A:233:VAL:HG11	0.92	1.80	6	1
1:A:263:LEU:HD11	1:A:298:PHE:CG	0.85	2.05	1	14
1:A:271:LEU:HD13	1:A:277:TYR:CD2	0.84	2.06	16	2
2:B:393:DT:OP2	2:B:393:DT:H73	0.84	1.73	20	1
1:A:299:ILE:HD12	1:A:331:ALA:O	0.82	1.75	11	19
1:A:284:SER:OG	1:A:312:ALA:HB3	0.78	1.78	20	3
1:A:257:HIS:H	1:A:257:HIS:CD2	0.77	1.94	6	1
2:B:389:DU:H6	2:B:389:DU:O5'	0.76	1.80	7	14
1:A:307:LEU:O	1:A:333:ALA:HB1	0.76	1.81	8	3
1:A:212:VAL:O	1:A:212:VAL:HG13	0.74	1.82	17	3
1:A:212:VAL:O	1:A:212:VAL:HG23	0.73	1.82	9	1
1:A:212:VAL:HG22	1:A:212:VAL:O	0.72	1.85	11	16
1:A:203:THR:HG22	1:A:207:ASN:ND2	0.71	2.01	15	4
1:A:253:LEU:N	1:A:253:LEU:HD23	0.71	2.01	8	12
2:B:385:DA:HO5'	2:B:385:DA:H8	0.71	1.27	2	2
1:A:315:TYR:CD1	2:B:388:DC:C4	0.71	2.79	20	8
1:A:203:THR:HG22	1:A:207:ASN:HD21	0.70	1.45	15	3
1:A:315:TYR:CZ	2:B:388:DC:C4	0.70	2.79	2	3
1:A:257:HIS:N	1:A:257:HIS:CD2	0.70	2.60	15	8
1:A:343:PHE:CE1	1:A:358:PHE:CZ	0.70	2.80	15	5
1:A:312:ALA:HB2	1:A:338:MET:SD	0.70	2.25	7	2
1:A:284:SER:O	1:A:285:TRP:CG	0.70	2.44	14	20
1:A:315:TYR:CE2	2:B:388:DC:C5	0.69	2.80	13	3
1:A:315:TYR:CD2	2:B:388:DC:C4	0.69	2.79	11	2
1:A:205:ASN:ND2	1:A:219:TYR:CE1	0.69	2.61	9	4
1:A:205:ASN:ND2	1:A:219:TYR:CZ	0.69	2.61	10	9
1:A:248:HIS:N	1:A:248:HIS:ND1	0.69	2.40	13	20
1:A:205:ASN:ND2	1:A:219:TYR:CE2	0.69	2.61	13	6
1:A:205:ASN:ND2	1:A:219:TYR:CD2	0.69	2.61	8	3
1:A:205:ASN:ND2	1:A:219:TYR:CG	0.69	2.60	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:315:TYR:CE1	2:B:388:DC:C4	0.68	2.82	4	10
1:A:216:HIS:CG	1:A:216:HIS:O	0.68	2.46	6	9
2:B:389:DU:C5	2:B:390:C38:I	0.68	3.12	1	6
2:B:389:DU:C4	2:B:390:C38:I	0.68	3.12	16	7
1:A:285:TRP:CZ2	1:A:313:ARG:NH1	0.68	2.61	3	2
1:A:211:TRP:CE3	1:A:212:VAL:N	0.68	2.62	3	17
1:A:221:CYS:SG	1:A:350:PHE:CD1	0.67	2.88	19	6
1:A:282:PHE:CE1	1:A:346:CYS:SG	0.67	2.88	15	9
1:A:307:LEU:HD23	1:A:308:CYS:N	0.67	2.05	7	11
1:A:227:MET:SD	1:A:278:ARG:NE	0.67	2.68	12	1
1:A:221:CYS:SG	1:A:350:PHE:CE1	0.67	2.88	1	7
1:A:282:PHE:CZ	1:A:346:CYS:SG	0.67	2.88	2	16
1:A:282:PHE:CE2	1:A:346:CYS:SG	0.67	2.88	19	11
1:A:227:MET:SD	1:A:232:TRP:CE3	0.67	2.88	17	1
1:A:220:LEU:C	1:A:220:LEU:HD23	0.67	2.15	12	4
1:A:256:ARG:NE	1:A:261:CYS:SG	0.66	2.68	14	13
1:A:315:TYR:CE2	2:B:388:DC:C4	0.66	2.83	14	3
1:A:261:CYS:O	1:A:265:VAL:HG23	0.66	1.90	20	15
1:A:308:CYS:SG	1:A:310:PHE:CZ	0.66	2.88	2	9
1:A:208:ASN:ND2	1:A:219:TYR:CD1	0.66	2.64	4	3
1:A:216:HIS:O	1:A:216:HIS:CG	0.66	2.49	16	6
1:A:263:LEU:HD11	1:A:298:PHE:CD1	0.66	2.25	1	3
1:A:315:TYR:CE1	2:B:388:DC:N4	0.66	2.64	3	6
1:A:250:HIS:CE1	2:B:394:DT:C2	0.66	2.84	6	1
1:A:315:TYR:CE1	2:B:388:DC:N3	0.65	2.65	2	2
1:A:250:HIS:NE2	2:B:394:DT:C2	0.65	2.64	6	1
1:A:246:ALA:HB2	1:A:255:GLY:H	0.65	1.52	6	10
1:A:315:TYR:CD1	2:B:388:DC:N3	0.65	2.64	17	6
1:A:221:CYS:SG	1:A:350:PHE:CZ	0.65	2.88	20	1
1:A:209:GLU:N	1:A:210:PRO:CD	0.65	2.60	20	20
1:A:202:PHE:CE2	1:A:350:PHE:CD1	0.64	2.85	13	1
1:A:376:ARG:NH2	1:A:380:GLN:HE21	0.64	1.90	16	2
1:A:238:ARG:NH2	1:A:269:TRP:CZ3	0.64	2.66	17	1
1:A:247:PRO:O	1:A:250:HIS:ND1	0.64	2.30	15	11
1:A:226:ARG:HE	1:A:235:LEU:HD22	0.64	1.51	2	2
1:A:220:LEU:HD23	1:A:221:CYS:N	0.64	2.08	16	2
1:A:307:LEU:C	1:A:307:LEU:HD23	0.64	2.18	8	2
1:A:216:HIS:CD2	1:A:244:ASN:HD21	0.64	2.11	3	10
1:A:285:TRP:CH2	1:A:313:ARG:NH1	0.64	2.66	3	1
1:A:315:TYR:CD2	2:B:388:DC:C6	0.63	2.86	13	2
1:A:250:HIS:NE2	2:B:394:DT:N3	0.63	2.46	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:221:CYS:SG	1:A:350:PHE:CE2	0.63	2.88	6	2
1:A:299:ILE:HD13	1:A:331:ALA:O	0.63	1.94	8	1
1:A:250:HIS:CE1	1:A:252:PHE:O	0.63	2.51	10	11
1:A:348:ASP:OD1	1:A:349:THR:N	0.63	2.32	14	1
1:A:226:ARG:NE	1:A:235:LEU:HD22	0.63	2.09	14	3
2:B:386:DT:H72	2:B:387:DT:O4	0.62	1.94	18	1
1:A:281:CYS:SG	1:A:309:ILE:HG23	0.62	2.34	5	11
1:A:307:LEU:HD23	1:A:307:LEU:C	0.62	2.19	14	9
1:A:247:PRO:O	1:A:250:HIS:CE1	0.62	2.52	10	6
1:A:250:HIS:ND1	1:A:251:GLY:N	0.61	2.48	7	3
1:A:203:THR:HG22	1:A:207:ASN:OD1	0.61	1.94	7	2
1:A:299:ILE:HD11	1:A:333:ALA:HB2	0.61	1.71	9	2
1:A:293:GLN:HE21	1:A:297:LYS:NZ	0.61	1.92	2	1
1:A:347:TRP:CD1	1:A:353:HIS:HD1	0.61	2.13	7	1
1:A:315:TYR:C	1:A:315:TYR:CD1	0.61	2.79	2	3
1:A:343:PHE:CE1	1:A:358:PHE:CE2	0.61	2.89	15	2
1:A:265:VAL:CG1	1:A:269:TRP:HE1	0.61	2.09	10	17
1:A:285:TRP:CZ3	2:B:388:DC:O4'	0.61	2.53	9	20
1:A:347:TRP:CE3	1:A:348:ASP:OD2	0.61	2.54	18	5
1:A:221:CYS:SG	1:A:350:PHE:CD2	0.61	2.94	7	1
1:A:275:GLN:N	1:A:275:GLN:CD	0.60	2.59	7	4
1:A:239:ARG:NH2	1:A:350:PHE:CE2	0.60	2.69	8	1
1:A:273:LEU:CD2	1:A:273:LEU:N	0.60	2.65	1	2
1:A:328:LEU:O	1:A:332:GLY:N	0.60	2.34	12	20
1:A:250:HIS:CD2	1:A:254:GLU:OE1	0.60	2.54	8	1
1:A:315:TYR:CD1	2:B:388:DC:C2	0.60	2.89	17	4
1:A:250:HIS:NE2	1:A:252:PHE:O	0.60	2.35	19	10
1:A:256:ARG:CZ	1:A:261:CYS:SG	0.60	2.89	4	3
1:A:257:HIS:NE2	1:A:260:LEU:HD22	0.60	2.11	6	1
1:A:299:ILE:H	1:A:299:ILE:HD12	0.60	1.56	8	1
1:A:239:ARG:NE	1:A:349:THR:O	0.60	2.34	13	4
1:A:347:TRP:CD2	1:A:348:ASP:OD2	0.60	2.55	6	4
1:A:236:ASN:O	1:A:238:ARG:N	0.60	2.34	9	1
2:B:388:DC:H6	2:B:388:DC:O5'	0.60	1.79	15	7
1:A:205:ASN:CG	1:A:219:TYR:CD2	0.60	2.80	1	3
1:A:315:TYR:CD2	2:B:388:DC:C2	0.60	2.90	14	1
1:A:216:HIS:O	1:A:216:HIS:ND1	0.59	2.35	4	11
1:A:315:TYR:CD1	1:A:315:TYR:C	0.59	2.80	9	9
1:A:257:HIS:CD2	1:A:257:HIS:N	0.59	2.70	6	1
1:A:347:TRP:CE3	1:A:348:ASP:OD1	0.59	2.55	15	3
1:A:359:GLN:O	1:A:361:TRP:CE3	0.59	2.56	20	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:GLU:OE2	1:A:245:GLN:NE2	0.59	2.36	14	2
1:A:310:PHE:CE1	1:A:342:GLU:OE1	0.59	2.55	2	2
1:A:205:ASN:OD1	1:A:219:TYR:CE1	0.59	2.56	3	2
1:A:347:TRP:CD2	1:A:348:ASP:OD1	0.59	2.56	11	3
1:A:315:TYR:CE2	2:B:388:DC:N3	0.59	2.71	14	1
1:A:315:TYR:CD2	2:B:388:DC:N3	0.59	2.70	14	2
1:A:211:TRP:O	1:A:213:ARG:N	0.59	2.36	14	20
1:A:379:LEU:HD12	1:A:379:LEU:N	0.59	2.12	4	9
1:A:229:ASN:OD1	1:A:230:ASP:N	0.59	2.35	5	1
1:A:250:HIS:CG	1:A:250:HIS:O	0.59	2.55	5	8
1:A:257:HIS:CD2	2:B:390:C38:O3'	0.59	2.56	8	8
1:A:298:PHE:C	1:A:298:PHE:CD1	0.59	2.80	11	2
1:A:367:HIS:CE1	1:A:371:LEU:HD11	0.59	2.32	8	1
1:A:310:PHE:CE2	1:A:342:GLU:OE2	0.59	2.56	14	1
1:A:205:ASN:OD1	1:A:219:TYR:CD1	0.59	2.56	5	1
1:A:273:LEU:HD12	1:A:273:LEU:N	0.59	2.12	16	1
1:A:208:ASN:C	1:A:208:ASN:ND2	0.59	2.60	5	2
1:A:254:GLU:OE2	2:B:392:DA:C4	0.59	2.56	7	4
1:A:315:TYR:C	1:A:315:TYR:CD2	0.59	2.79	12	4
1:A:271:LEU:HD22	1:A:277:TYR:CE2	0.59	2.33	16	2
1:A:367:HIS:CD2	1:A:368:SER:N	0.59	2.71	8	1
1:A:315:TYR:CD2	1:A:315:TYR:C	0.59	2.80	14	3
1:A:326:ARG:NH1	1:A:381:ASN:O	0.59	2.36	17	1
1:A:376:ARG:NH2	1:A:380:GLN:OE1	0.59	2.36	18	1
1:A:205:ASN:OD1	1:A:219:TYR:CD2	0.58	2.56	1	1
1:A:256:ARG:N	2:B:391:DA:OP2	0.58	2.36	11	11
1:A:359:GLN:O	1:A:361:TRP:CZ3	0.58	2.56	18	9
1:A:205:ASN:O	1:A:208:ASN:ND2	0.58	2.36	18	6
1:A:246:ALA:CB	1:A:254:GLU:H	0.58	2.11	10	11
1:A:263:LEU:HD11	1:A:298:PHE:CB	0.58	2.29	3	17
2:B:385:DA:O5'	2:B:385:DA:C8	0.58	2.56	7	2
1:A:257:HIS:NE2	2:B:390:C38:O3'	0.58	2.37	16	8
1:A:228:HIS:ND1	1:A:275:GLN:OE1	0.58	2.36	19	4
1:A:250:HIS:NE2	1:A:254:GLU:OE1	0.58	2.36	15	3
1:A:204:PHE:O	1:A:208:ASN:ND2	0.58	2.37	3	3
1:A:254:GLU:OE1	2:B:393:DT:C6	0.58	2.57	3	2
1:A:243:CYS:O	1:A:256:ARG:NH1	0.58	2.36	15	1
1:A:260:LEU:HD11	1:A:294:GLU:OE2	0.58	1.98	12	2
1:A:339:THR:N	1:A:342:GLU:OE1	0.58	2.37	12	1
1:A:216:HIS:NE2	1:A:244:ASN:ND2	0.58	2.50	3	7
1:A:218:THR:OG1	1:A:244:ASN:ND2	0.58	2.36	3	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:293:GLN:HE21	1:A:297:LYS:HZ1	0.58	1.39	2	1
1:A:348:ASP:OD1	1:A:353:HIS:CE1	0.58	2.57	2	1
1:A:353:HIS:C	1:A:353:HIS:CD2	0.58	2.81	19	3
1:A:252:PHE:CD1	1:A:252:PHE:N	0.58	2.72	6	2
1:A:348:ASP:OD2	1:A:353:HIS:ND1	0.58	2.36	19	1
1:A:347:TRP:CE2	1:A:348:ASP:OD2	0.58	2.57	6	3
1:A:205:ASN:CG	1:A:219:TYR:CG	0.58	2.81	5	2
1:A:334:LYS:CD	1:A:334:LYS:N	0.57	2.66	10	5
1:A:216:HIS:CD2	2:B:389:DU:OP2	0.57	2.57	19	5
1:A:257:HIS:NE2	2:B:391:DA:OP1	0.57	2.37	17	8
1:A:330:GLU:OE2	1:A:382:GLN:NE2	0.57	2.36	4	1
1:A:254:GLU:OE1	2:B:392:DA:N7	0.57	2.37	6	2
1:A:284:SER:O	1:A:285:TRP:CD1	0.57	2.57	2	20
1:A:250:HIS:CG	2:B:393:DT:O2	0.57	2.58	20	13
1:A:301:LYS:O	1:A:302:ASN:ND2	0.57	2.37	10	3
1:A:255:GLY:CA	2:B:391:DA:OP2	0.57	2.52	19	15
1:A:379:LEU:CD2	1:A:379:LEU:N	0.57	2.67	1	1
1:A:348:ASP:OD1	1:A:353:HIS:ND1	0.57	2.37	2	1
1:A:315:TYR:CD2	2:B:388:DC:C5	0.57	2.93	3	3
1:A:347:TRP:CZ3	1:A:348:ASP:OD2	0.57	2.57	18	4
1:A:254:GLU:OE1	2:B:392:DA:C8	0.57	2.58	5	2
1:A:271:LEU:HD12	1:A:271:LEU:O	0.57	2.00	8	1
2:B:385:DA:H8	2:B:385:DA:O5'	0.57	1.83	12	2
1:A:241:PHE:O	1:A:242:LEU:HD12	0.57	2.00	19	1
1:A:239:ARG:HE	1:A:349:THR:CG2	0.57	2.13	5	5
1:A:315:TYR:CE2	2:B:388:DC:N4	0.57	2.73	15	2
1:A:325:LEU:CD2	1:A:325:LEU:N	0.57	2.68	16	2
2:B:393:DT:H71	2:B:393:DT:OP2	0.56	2.00	3	13
1:A:321:CYS:SG	1:A:321:CYS:O	0.56	2.63	5	2
1:A:223:GLU:OE1	1:A:349:THR:HG21	0.56	2.00	8	2
1:A:254:GLU:OE2	2:B:392:DA:C8	0.56	2.59	7	2
1:A:232:TRP:N	1:A:232:TRP:CD1	0.56	2.73	13	6
1:A:205:ASN:CG	1:A:219:TYR:CD1	0.56	2.84	5	2
1:A:254:GLU:OE2	2:B:392:DA:C5	0.56	2.58	16	3
1:A:254:GLU:OE1	2:B:392:DA:C5	0.56	2.59	14	2
1:A:250:HIS:CD2	2:B:393:DT:O2	0.56	2.59	13	2
1:A:254:GLU:OE2	2:B:393:DT:C6	0.56	2.58	8	1
1:A:299:ILE:HD12	1:A:299:ILE:N	0.56	2.16	8	1
1:A:367:HIS:ND1	1:A:367:HIS:C	0.55	2.61	1	1
1:A:223:GLU:CB	1:A:238:ARG:O	0.55	2.55	4	1
1:A:239:ARG:HE	1:A:349:THR:HG22	0.55	1.61	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:250:HIS:CE1	2:B:394:DT:O2	0.55	2.59	6	1
1:A:274:ASP:C	1:A:275:GLN:NE2	0.55	2.65	15	4
1:A:283:THR:O	1:A:338:MET:HE3	0.55	2.02	15	2
1:A:312:ALA:O	1:A:371:LEU:CD1	0.55	2.55	17	5
1:A:257:HIS:CE1	1:A:260:LEU:HD22	0.55	2.37	17	6
1:A:265:VAL:CG1	1:A:269:TRP:NE1	0.55	2.70	4	13
1:A:328:LEU:O	1:A:332:GLY:CA	0.55	2.54	2	20
1:A:340:TYR:CG	1:A:341:SER:N	0.55	2.75	16	16
1:A:212:VAL:O	1:A:212:VAL:CG1	0.55	2.55	2	2
1:A:313:ARG:NH1	2:B:386:DT:O2	0.55	2.40	5	2
2:B:394:DT:H71	2:B:394:DT:OP2	0.55	2.01	10	1
1:A:370:ASP:OD1	2:B:385:DA:N6	0.55	2.40	12	2
1:A:202:PHE:CE2	1:A:350:PHE:CG	0.54	2.96	12	4
1:A:239:ARG:NH2	1:A:349:THR:O	0.54	2.38	9	1
1:A:226:ARG:NE	1:A:228:HIS:CE1	0.54	2.74	10	1
1:A:252:PHE:N	2:B:393:DT:O4	0.54	2.40	10	1
1:A:244:ASN:O	1:A:256:ARG:O	0.54	2.25	8	20
1:A:239:ARG:NH2	1:A:350:PHE:CZ	0.54	2.75	8	2
1:A:371:LEU:N	1:A:371:LEU:CD2	0.54	2.70	4	3
1:A:370:ASP:CG	2:B:385:DA:N6	0.54	2.64	11	2
1:A:243:CYS:O	1:A:256:ARG:CZ	0.54	2.56	15	1
1:A:315:TYR:CE1	2:B:388:DC:C5	0.54	2.96	20	1
1:A:259:GLU:OE1	1:A:283:THR:HG21	0.54	2.02	19	2
1:A:370:ASP:OD2	2:B:385:DA:N6	0.54	2.40	2	1
1:A:376:ARG:NH2	1:A:380:GLN:NE2	0.54	2.54	16	2
2:B:385:DA:C8	2:B:385:DA:O5'	0.54	2.55	2	1
1:A:250:HIS:ND1	1:A:250:HIS:C	0.54	2.64	7	4
1:A:212:VAL:O	1:A:212:VAL:CG2	0.54	2.55	9	14
1:A:260:LEU:CD1	1:A:294:GLU:OE1	0.54	2.56	9	3
1:A:285:TRP:CE3	2:B:388:DC:O4'	0.54	2.61	19	14
1:A:263:LEU:HD11	1:A:298:PHE:HB2	0.54	1.80	14	2
1:A:250:HIS:CB	2:B:393:DT:O2	0.53	2.56	17	13
1:A:367:HIS:CD2	1:A:367:HIS:C	0.53	2.85	8	1
1:A:288:CYS:SG	1:A:290:SER:OG	0.53	2.62	12	2
1:A:205:ASN:ND2	1:A:219:TYR:CD1	0.53	2.76	9	2
1:A:339:THR:CB	1:A:342:GLU:OE1	0.53	2.56	12	1
1:A:315:TYR:CD1	2:B:388:DC:C5	0.53	2.97	20	1
1:A:356:CYS:SG	1:A:356:CYS:O	0.53	2.67	1	1
1:A:379:LEU:N	1:A:379:LEU:CD1	0.53	2.72	19	5
1:A:304:HIS:CE1	1:A:305:VAL:HG23	0.53	2.39	6	1
1:A:254:GLU:OE2	1:A:255:GLY:N	0.53	2.41	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:286:SER:CB	1:A:315:TYR:H	0.53	2.16	13	1
1:A:254:GLU:CD	1:A:254:GLU:C	0.53	2.77	4	3
1:A:235:LEU:HD21	1:A:238:ARG:HH11	0.53	1.62	8	1
1:A:371:LEU:CD1	1:A:374:ARG:HH11	0.53	2.17	1	1
1:A:315:TYR:CG	2:B:388:DC:C2	0.53	2.97	14	3
1:A:361:TRP:CD1	1:A:363:GLY:H	0.53	2.21	15	3
1:A:207:ASN:C	1:A:209:GLU:H	0.52	2.12	17	11
1:A:367:HIS:O	2:B:385:DA:N6	0.52	2.43	13	1
1:A:298:PHE:CD2	1:A:298:PHE:C	0.52	2.83	16	1
1:A:228:HIS:O	1:A:231:THR:O	0.52	2.27	13	20
1:A:209:GLU:OE2	1:A:313:ARG:NH2	0.52	2.42	14	1
1:A:348:ASP:CG	1:A:353:HIS:HD1	0.52	2.11	19	2
2:B:388:DC:N4	2:B:389:DU:O4	0.52	2.43	2	1
2:B:385:DA:O5'	2:B:385:DA:H8	0.52	1.87	7	1
1:A:379:LEU:N	1:A:379:LEU:HD22	0.52	2.18	1	1
1:A:216:HIS:CD2	2:B:389:DU:P	0.52	3.02	7	3
1:A:347:TRP:CE2	1:A:348:ASP:OD1	0.52	2.63	9	1
1:A:223:GLU:CD	1:A:349:THR:HG21	0.52	2.30	2	2
1:A:260:LEU:CD2	1:A:291:CYS:SG	0.52	2.98	14	1
1:A:228:HIS:CD2	1:A:275:GLN:OE1	0.51	2.63	13	2
1:A:255:GLY:O	2:B:391:DA:OP2	0.51	2.28	6	1
1:A:339:THR:CA	1:A:342:GLU:OE1	0.51	2.58	12	1
1:A:226:ARG:O	1:A:233:VAL:O	0.51	2.29	15	12
1:A:375:LEU:HD12	1:A:378:ILE:HD12	0.51	1.82	7	1
1:A:269:TRP:O	1:A:270:LYS:C	0.51	2.54	3	20
1:A:257:HIS:CD2	2:B:391:DA:P	0.51	3.03	5	8
1:A:253:LEU:N	1:A:253:LEU:CD2	0.51	2.69	2	8
1:A:376:ARG:HH22	1:A:380:GLN:HE21	0.51	1.49	16	2
1:A:223:GLU:OE2	1:A:349:THR:HG21	0.51	2.06	2	7
1:A:352:ASP:OD1	1:A:352:ASP:O	0.51	2.29	11	1
1:A:257:HIS:CD2	2:B:391:DA:OP1	0.51	2.64	17	8
1:A:205:ASN:O	1:A:208:ASN:CG	0.51	2.54	19	9
1:A:277:TYR:HB2	1:A:305:VAL:HG22	0.51	1.82	20	10
1:A:211:TRP:CZ2	1:A:217:GLU:CB	0.51	2.93	14	1
1:A:239:ARG:NH2	1:A:350:PHE:CE1	0.50	2.79	19	1
1:A:252:PHE:O	1:A:254:GLU:OE2	0.50	2.29	6	3
1:A:207:ASN:O	1:A:209:GLU:N	0.50	2.45	20	4
1:A:245:GLN:CD	1:A:248:HIS:CE1	0.50	2.89	16	1
1:A:325:LEU:N	1:A:325:LEU:HD22	0.50	2.21	17	2
1:A:301:LYS:O	1:A:302:ASN:OD1	0.50	2.30	3	15
1:A:314:ILE:O	2:B:387:DT:O4	0.50	2.30	15	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:347:TRP:O	1:A:351:VAL:O	0.50	2.28	5	5
1:A:250:HIS:O	2:B:393:DT:O2	0.50	2.29	6	1
1:A:244:ASN:OD1	1:A:244:ASN:C	0.50	2.54	2	14
1:A:297:LYS:HB3	1:A:301:LYS:HZ2	0.50	1.66	8	1
1:A:211:TRP:CD2	1:A:211:TRP:C	0.50	2.90	16	14
1:A:371:LEU:N	1:A:371:LEU:HD22	0.50	2.21	4	3
1:A:297:LYS:C	1:A:301:LYS:NZ	0.50	2.69	8	1
1:A:220:LEU:C	1:A:220:LEU:CD2	0.50	2.85	12	2
1:A:281:CYS:SG	1:A:307:LEU:HD21	0.50	2.46	13	2
1:A:239:ARG:NE	1:A:349:THR:HG22	0.50	2.22	5	1
1:A:313:ARG:NH1	2:B:386:DT:C2	0.50	2.79	10	2
1:A:314:ILE:O	1:A:374:ARG:NH1	0.50	2.43	8	1
1:A:370:ASP:CB	2:B:385:DA:H62	0.50	2.20	15	1
1:A:246:ALA:H	1:A:253:LEU:HD11	0.50	1.66	17	1
1:A:255:GLY:C	2:B:391:DA:OP2	0.49	2.55	9	20
1:A:362:ASP:C	1:A:362:ASP:OD2	0.49	2.54	2	4
1:A:310:PHE:CE2	1:A:342:GLU:OE1	0.49	2.65	11	2
1:A:255:GLY:C	2:B:391:DA:P	0.49	2.95	9	7
2:B:390:C38:H3'	2:B:390:C38:O2	0.49	2.08	13	3
1:A:246:ALA:HB3	1:A:253:LEU:HA	0.49	1.84	8	3
1:A:345:HIS:O	1:A:348:ASP:OD1	0.49	2.30	14	1
2:B:386:DT:C5	2:B:387:DT:O4	0.49	2.65	18	3
1:A:218:THR:OG1	1:A:244:ASN:CG	0.49	2.55	5	2
1:A:231:THR:HG22	1:A:232:TRP:N	0.49	2.22	9	8
1:A:223:GLU:OE2	1:A:349:THR:CG2	0.49	2.60	2	2
1:A:282:PHE:CD2	1:A:346:CYS:SG	0.49	3.05	6	6
1:A:254:GLU:OE1	1:A:254:GLU:C	0.49	2.56	19	1
1:A:252:PHE:O	1:A:254:GLU:OE1	0.49	2.31	11	2
1:A:273:LEU:N	1:A:273:LEU:HD22	0.49	2.23	4	2
1:A:362:ASP:OD1	1:A:362:ASP:C	0.49	2.55	3	2
1:A:347:TRP:NE1	1:A:353:HIS:HD1	0.49	2.06	7	1
1:A:310:PHE:CG	1:A:342:GLU:OE1	0.49	2.66	10	1
1:A:326:ARG:HH22	1:A:379:LEU:HD23	0.49	1.67	12	1
1:A:254:GLU:OE1	2:B:392:DA:C4	0.49	2.66	14	1
1:A:343:PHE:CZ	1:A:358:PHE:CZ	0.49	3.01	15	1
1:A:208:ASN:C	1:A:208:ASN:HD22	0.48	2.14	8	2
1:A:381:ASN:O	1:A:382:GLN:C	0.48	2.56	14	5
1:A:203:THR:O	1:A:207:ASN:CG	0.48	2.56	17	2
1:A:206:PHE:CZ	1:A:338:MET:HE1	0.48	2.43	2	1
1:A:262:PHE:CZ	1:A:266:ILE:HD11	0.48	2.43	11	1
1:A:347:TRP:CD1	1:A:347:TRP:C	0.48	2.88	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:298:PHE:CD1	1:A:298:PHE:C	0.48	2.88	18	3
1:A:222:TYR:CE1	1:A:262:PHE:CE2	0.48	3.02	11	1
1:A:257:HIS:O	1:A:261:CYS:SG	0.48	2.72	13	1
1:A:203:THR:O	1:A:207:ASN:N	0.48	2.45	13	4
1:A:376:ARG:O	1:A:380:GLN:N	0.48	2.44	14	3
1:A:216:HIS:CD2	1:A:216:HIS:C	0.48	2.90	3	1
1:A:216:HIS:HE2	1:A:244:ASN:CG	0.48	2.16	6	1
1:A:236:ASN:OD1	1:A:237:GLN:N	0.48	2.46	8	3
1:A:254:GLU:OE2	1:A:254:GLU:C	0.48	2.56	9	1
1:A:211:TRP:C	1:A:211:TRP:CD2	0.48	2.89	15	2
1:A:347:TRP:CE3	1:A:348:ASP:CG	0.48	2.91	18	1
1:A:263:LEU:HD11	1:A:298:PHE:CD2	0.48	2.44	15	3
1:A:209:GLU:O	1:A:209:GLU:OE2	0.48	2.31	19	1
1:A:304:HIS:NE2	1:A:305:VAL:HG23	0.48	2.24	19	1
2:B:387:DT:C7	2:B:387:DT:OP2	0.48	2.61	17	4
1:A:315:TYR:CZ	2:B:388:DC:C5	0.48	3.02	13	2
1:A:283:THR:O	1:A:310:PHE:O	0.48	2.30	6	8
1:A:340:TYR:CD1	1:A:365:ASP:OD1	0.48	2.67	5	1
1:A:307:LEU:C	1:A:307:LEU:CD2	0.48	2.87	8	11
1:A:256:ARG:CG	1:A:261:CYS:SG	0.48	3.01	11	2
1:A:205:ASN:CG	1:A:219:TYR:CE2	0.48	2.92	17	1
2:B:392:DA:H3'	2:B:393:DT:H71	0.48	1.85	2	2
1:A:203:THR:CG2	1:A:207:ASN:ND2	0.48	2.77	20	2
1:A:347:TRP:C	1:A:347:TRP:CD1	0.48	2.86	9	1
1:A:371:LEU:HD21	2:B:386:DT:O4	0.48	2.09	3	2
2:B:386:DT:H73	2:B:387:DT:O4	0.48	2.08	5	1
1:A:254:GLU:OE1	2:B:393:DT:OP2	0.48	2.32	10	1
1:A:347:TRP:CZ2	1:A:353:HIS:CG	0.48	3.02	18	1
2:B:394:DT:H6	2:B:394:DT:O5'	0.48	1.92	10	2
1:A:208:ASN:OD1	1:A:208:ASN:C	0.47	2.57	14	9
1:A:326:ARG:NH1	1:A:381:ASN:CB	0.47	2.77	19	1
1:A:212:VAL:O	1:A:212:VAL:HG22	0.47	2.09	6	1
2:B:386:DT:C7	2:B:387:DT:O4	0.47	2.62	17	7
1:A:379:LEU:O	1:A:382:GLN:OE1	0.47	2.32	17	1
1:A:308:CYS:SG	1:A:310:PHE:CE2	0.47	3.03	2	1
1:A:254:GLU:OE2	2:B:392:DA:OP2	0.47	2.32	4	3
1:A:256:ARG:NH1	2:B:394:DT:O4	0.47	2.48	10	1
2:B:393:DT:OP2	2:B:393:DT:C7	0.47	2.62	9	9
1:A:254:GLU:OE2	2:B:392:DA:N9	0.47	2.47	7	1
1:A:347:TRP:NE1	1:A:353:HIS:CB	0.47	2.78	18	6
1:A:285:TRP:CZ3	2:B:388:DC:C4'	0.47	2.97	1	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:256:ARG:O	2:B:390:C38:O1P	0.47	2.32	6	1
1:A:371:LEU:HD13	2:B:386:DT:O4	0.47	2.10	9	1
1:A:363:GLY:O	1:A:367:HIS:CD2	0.47	2.67	16	2
1:A:343:PHE:CE1	1:A:358:PHE:CE1	0.47	3.03	14	2
1:A:239:ARG:CZ	1:A:349:THR:O	0.47	2.63	16	1
1:A:367:HIS:CG	1:A:368:SER:N	0.47	2.81	1	1
2:B:393:DT:O5'	2:B:393:DT:H6	0.47	1.93	14	13
1:A:315:TYR:CD1	2:B:387:DT:C2'	0.46	2.98	12	1
1:A:253:LEU:HD12	1:A:253:LEU:N	0.46	2.25	3	2
2:B:390:C38:O2	2:B:390:C38:C3'	0.46	2.63	13	3
1:A:281:CYS:SG	1:A:307:LEU:HD11	0.46	2.51	10	3
1:A:227:MET:SD	1:A:232:TRP:CZ3	0.46	3.09	17	1
1:A:253:LEU:CD2	1:A:253:LEU:H	0.46	2.24	14	9
1:A:236:ASN:OD1	1:A:236:ASN:C	0.46	2.59	14	3
1:A:202:PHE:CE1	1:A:350:PHE:CG	0.46	3.04	5	2
1:A:226:ARG:NE	1:A:228:HIS:NE2	0.46	2.62	10	2
1:A:216:HIS:NE2	2:B:390:C38:I	0.46	3.19	19	1
1:A:223:GLU:OE1	1:A:349:THR:CG2	0.46	2.63	8	2
2:B:394:DT:OP2	2:B:394:DT:C7	0.46	2.64	10	1
1:A:347:TRP:CE2	1:A:353:HIS:CB	0.46	2.99	18	1
1:A:216:HIS:CD2	2:B:390:C38:I	0.46	3.39	19	1
2:B:394:DT:C7	2:B:394:DT:OP2	0.46	2.63	6	1
1:A:326:ARG:NH2	1:A:379:LEU:HD23	0.46	2.26	12	1
1:A:239:ARG:NE	1:A:349:THR:CG2	0.46	2.79	5	1
1:A:315:TYR:CZ	2:B:388:DC:N4	0.46	2.84	9	1
1:A:374:ARG:CZ	2:B:385:DA:O5'	0.46	2.64	9	1
1:A:347:TRP:O	1:A:351:VAL:HG13	0.45	2.11	10	4
1:A:239:ARG:NH2	1:A:350:PHE:CD1	0.45	2.85	19	1
1:A:259:GLU:OE2	1:A:283:THR:HG21	0.45	2.11	6	3
1:A:315:TYR:CD2	2:B:387:DT:C2'	0.45	2.98	8	1
1:A:337:ILE:HD11	1:A:375:LEU:HD22	0.45	1.89	18	1
1:A:353:HIS:O	1:A:356:CYS:N	0.45	2.47	14	6
1:A:253:LEU:H	1:A:253:LEU:CD2	0.45	2.21	10	1
1:A:337:ILE:CG2	1:A:368:SER:OG	0.45	2.64	10	1
2:B:390:C38:O2	2:B:390:C38:C2'	0.45	2.64	13	2
1:A:246:ALA:N	1:A:253:LEU:HD11	0.45	2.26	17	1
1:A:364:LEU:O	1:A:367:HIS:CD2	0.45	2.70	1	1
1:A:263:LEU:CD1	1:A:298:PHE:CD1	0.45	2.99	4	2
1:A:347:TRP:CZ2	1:A:348:ASP:OD2	0.45	2.70	6	1
1:A:343:PHE:CE2	1:A:358:PHE:CZ	0.45	3.05	16	2
1:A:286:SER:OG	1:A:315:TYR:N	0.45	2.46	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:299:ILE:CD1	1:A:331:ALA:O	0.45	2.64	8	1
1:A:315:TYR:CB	2:B:388:DC:C2	0.45	3.00	13	1
1:A:361:TRP:CD1	1:A:363:GLY:N	0.45	2.85	15	1
1:A:224:VAL:HG13	1:A:235:LEU:HD23	0.45	1.88	19	4
1:A:257:HIS:CD2	2:B:390:C38:H5'1	0.45	2.47	7	10
1:A:370:ASP:CG	2:B:385:DA:H62	0.45	2.20	12	2
1:A:371:LEU:CD2	2:B:385:DA:H62	0.45	2.25	18	1
1:A:216:HIS:HE2	1:A:244:ASN:ND2	0.44	2.10	6	1
1:A:273:LEU:N	1:A:273:LEU:CD1	0.44	2.81	16	1
1:A:236:ASN:HD21	1:A:349:THR:HG23	0.44	1.71	19	1
1:A:207:ASN:C	1:A:209:GLU:N	0.44	2.75	17	6
1:A:289:PHE:CE1	1:A:293:GLN:NE2	0.44	2.85	10	1
1:A:365:ASP:O	1:A:368:SER:OG	0.44	2.32	19	1
2:B:388:DC:C4	2:B:389:DU:C4	0.44	3.00	2	2
1:A:323:GLU:O	1:A:327:THR:CB	0.44	2.65	9	1
1:A:260:LEU:HD11	1:A:294:GLU:OE1	0.44	2.12	20	3
1:A:310:PHE:CD2	1:A:342:GLU:OE2	0.44	2.70	11	1
1:A:274:ASP:O	1:A:275:GLN:NE2	0.44	2.50	15	1
1:A:284:SER:HB3	1:A:312:ALA:HB3	0.44	1.90	15	1
1:A:353:HIS:O	1:A:354:GLN:C	0.44	2.60	1	5
1:A:315:TYR:CD1	2:B:387:DT:H2'	0.44	2.48	12	2
1:A:313:ARG:NH1	2:B:387:DT:O2	0.44	2.51	10	1
1:A:322:GLN:OE1	1:A:378:ILE:HD12	0.44	2.13	14	1
2:B:387:DT:OP2	2:B:387:DT:H73	0.44	2.12	17	4
1:A:281:CYS:O	1:A:281:CYS:SG	0.44	2.74	7	1
1:A:210:PRO:C	1:A:212:VAL:N	0.44	2.74	9	2
1:A:222:TYR:CE1	1:A:240:GLY:C	0.44	2.96	10	1
1:A:315:TYR:CD2	2:B:387:DT:H2'	0.43	2.48	8	1
1:A:202:PHE:CE1	1:A:346:CYS:CB	0.43	3.01	3	1
1:A:244:ASN:CA	1:A:256:ARG:O	0.43	2.67	6	1
1:A:271:LEU:CB	1:A:277:TYR:CE2	0.43	3.01	9	1
1:A:206:PHE:CE1	1:A:284:SER:OG	0.43	2.71	15	1
1:A:271:LEU:HD13	1:A:277:TYR:CE2	0.43	2.46	16	1
1:A:209:GLU:OE2	1:A:209:GLU:CA	0.43	2.67	19	1
1:A:323:GLU:O	1:A:327:THR:OG1	0.43	2.31	5	2
1:A:202:PHE:CZ	1:A:221:CYS:SG	0.43	3.12	8	1
1:A:262:PHE:CE2	1:A:266:ILE:HD11	0.43	2.48	11	1
1:A:307:LEU:HD23	1:A:333:ALA:HB2	0.43	1.91	15	1
1:A:293:GLN:NE2	1:A:297:LYS:NZ	0.43	2.64	2	1
1:A:371:LEU:CD2	1:A:371:LEU:N	0.43	2.81	18	1
1:A:222:TYR:CD1	1:A:222:TYR:C	0.43	2.97	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:211:TRP:CZ3	1:A:212:VAL:CG1	0.43	3.02	9	1
1:A:374:ARG:HH11	2:B:386:DT:H71	0.43	1.73	1	1
2:B:387:DT:H6	2:B:387:DT:O5'	0.43	1.97	17	2
1:A:222:TYR:CD2	1:A:222:TYR:C	0.43	2.97	14	2
1:A:206:PHE:CZ	1:A:338:MET:SD	0.43	3.11	8	2
1:A:202:PHE:CE2	1:A:350:PHE:CD2	0.43	3.07	12	1
1:A:340:TYR:CD2	1:A:365:ASP:OD2	0.43	2.72	13	1
1:A:205:ASN:ND2	1:A:219:TYR:CB	0.43	2.82	20	1
1:A:257:HIS:NE2	2:B:391:DA:P	0.42	2.92	17	5
1:A:265:VAL:HG12	1:A:269:TRP:CD1	0.42	2.48	4	1
1:A:233:VAL:HG12	1:A:235:LEU:H	0.42	1.74	9	1
1:A:205:ASN:OD1	1:A:219:TYR:CE2	0.42	2.72	1	2
1:A:232:TRP:CD1	1:A:232:TRP:N	0.42	2.87	18	4
1:A:242:LEU:CD2	1:A:262:PHE:N	0.42	2.82	19	1
1:A:211:TRP:CZ3	1:A:212:VAL:HG12	0.42	2.50	9	1
1:A:339:THR:O	1:A:342:GLU:OE1	0.42	2.38	12	1
2:B:386:DT:C6	2:B:387:DT:H72	0.42	2.49	15	1
1:A:347:TRP:CZ3	1:A:351:VAL:HG11	0.42	2.49	20	2
1:A:220:LEU:HD23	1:A:242:LEU:HB2	0.42	1.89	9	1
1:A:273:LEU:HD12	1:A:273:LEU:H	0.42	1.74	16	1
1:A:252:PHE:CD2	2:B:392:DA:N6	0.42	2.88	8	2
1:A:339:THR:C	1:A:342:GLU:OE1	0.42	2.63	12	1
1:A:374:ARG:NH1	2:B:386:DT:H71	0.42	2.30	1	1
1:A:282:PHE:CD1	1:A:346:CYS:SG	0.42	3.13	3	1
1:A:340:TYR:CD1	1:A:365:ASP:OD2	0.42	2.73	3	2
1:A:257:HIS:CD2	1:A:257:HIS:H	0.42	2.32	4	1
1:A:295:MET:HE3	1:A:309:ILE:CD1	0.42	2.45	6	2
1:A:371:LEU:CD1	1:A:374:ARG:NH1	0.42	2.82	1	1
1:A:208:ASN:O	1:A:211:TRP:CE3	0.42	2.73	3	1
2:B:394:DT:OP2	2:B:394:DT:H71	0.42	2.15	6	1
1:A:348:ASP:CG	1:A:353:HIS:CE1	0.41	2.98	2	1
1:A:331:ALA:C	1:A:333:ALA:H	0.41	2.21	9	1
1:A:338:MET:CB	1:A:342:GLU:OE2	0.41	2.67	20	1
2:B:386:DT:C5	2:B:387:DT:C4	0.41	3.08	18	1
1:A:203:THR:OG1	1:A:347:TRP:CZ3	0.41	2.71	20	1
1:A:347:TRP:CZ2	1:A:353:HIS:CD2	0.41	3.08	18	1
1:A:227:MET:HE1	1:A:232:TRP:HB3	0.41	1.92	3	1
1:A:347:TRP:CE3	1:A:351:VAL:HG11	0.41	2.51	5	1
1:A:353:HIS:CD2	1:A:354:GLN:N	0.41	2.89	5	1
1:A:347:TRP:CZ3	1:A:348:ASP:CG	0.41	2.98	18	1
1:A:372:SER:O	1:A:376:ARG:CG	0.41	2.69	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:226:ARG:HH11	1:A:233:VAL:HG11	0.41	1.69	6	1
1:A:283:THR:O	1:A:338:MET:CE	0.41	2.69	15	2
1:A:266:ILE:N	1:A:267:PRO:HD2	0.41	2.31	8	2
1:A:371:LEU:HD11	2:B:386:DT:O4	0.41	2.15	10	1
1:A:372:SER:O	1:A:376:ARG:N	0.41	2.50	3	1
1:A:281:CYS:SG	1:A:281:CYS:O	0.41	2.78	4	1
1:A:239:ARG:HD3	1:A:349:THR:HG22	0.41	1.92	6	1
2:B:393:DT:OP2	2:B:393:DT:H71	0.40	2.15	1	1
1:A:206:PHE:C	1:A:208:ASN:H	0.40	2.23	2	1
1:A:252:PHE:CD2	1:A:253:LEU:O	0.40	2.75	3	1
2:B:393:DT:H6	2:B:393:DT:O5'	0.40	1.99	4	1
1:A:313:ARG:NE	2:B:387:DT:O2	0.40	2.54	10	1
1:A:254:GLU:OE1	2:B:393:DT:N1	0.40	2.54	18	1
1:A:254:GLU:HB2	2:B:393:DT:H72	0.40	1.92	10	1
1:A:359:GLN:N	1:A:359:GLN:OE1	0.40	2.55	4	1
2:B:387:DT:O5'	2:B:387:DT:H6	0.40	2.00	9	1
1:A:288:CYS:SG	1:A:291:CYS:N	0.40	2.91	12	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	176/188 (94%)	165±2 (94±1%)	9±2 (5±1%)	2±1 (1±0%)	11	58
All	All	3520/3760 (94%)	3294 (94%)	176 (5%)	50 (1%)	11	58

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	212	VAL	20
1	A	382	GLN	19
1	A	208	ASN	7
1	A	321	CYS	3
1	A	237	GLN	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	158/169 (93%)	144±3 (91±2%)	14±3 (9±2%)	12	58
All	All	3160/3380 (93%)	2885 (91%)	275 (9%)	12	58

All 43 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	281	CYS	20
1	A	211	TRP	19
1	A	248	HIS	19
1	A	335	ILE	18
1	A	279	VAL	17
1	A	216	HIS	15
1	A	221	CYS	15
1	A	351	VAL	14
1	A	253	LEU	12
1	A	209	GLU	11
1	A	249	LYS	11
1	A	286	SER	10
1	A	257	HIS	9
1	A	252	PHE	8
1	A	243	CYS	8
1	A	271	LEU	7
1	A	356	CYS	5
1	A	359	GLN	5
1	A	334	LYS	5
1	A	347	TRP	4
1	A	250	HIS	4
1	A	288	CYS	4
1	A	275	GLN	4
1	A	301	LYS	3
1	A	367	HIS	3
1	A	284	SER	3
1	A	254	GLU	3
1	A	208	ASN	2
1	A	321	CYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	206	PHE	2
1	A	227	MET	1
1	A	344	LYS	1
1	A	376	ARG	1
1	A	308	CYS	1
1	A	202	PHE	1
1	A	295	MET	1
1	A	339	THR	1
1	A	261	CYS	1
1	A	303	LYS	1
1	A	220	LEU	1
1	A	242	LEU	1
1	A	266	ILE	1
1	A	311	THR	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	C38	B	390	2	18,21,22	0.45±0.01	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	C38	B	390	2	25,30,33	0.45±0.02	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C38	B	390	2	-	0±0,7,21,22	0±0,2,2,2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 80% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *data_A3G_PrB.str*

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	2222
Number of shifts mapped to atoms	2222
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	17

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	175	-0.27 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	165	0.69 ± 0.10	Should be checked
$^{13}\text{C}'$	160	-0.10 ± 0.16	None needed (< 0.5 ppm)
^{15}N	171	-0.19 ± 0.44	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 2106 atoms were assigned a chemical shift out of a possible 2639. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	828/877 (94%)	344/355 (97%)	321/352 (91%)	163/170 (96%)
Sidechain	1013/1264 (80%)	716/815 (88%)	286/391 (73%)	11/58 (19%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	205/328 (62%)	115/162 (71%)	84/143 (59%)	6/23 (26%)
Sugar	50/108 (46%)	50/63 (79%)	0/45 (0%)	0/0 (—%)
Base	10/62 (16%)	10/35 (29%)	0/18 (0%)	0/9 (0%)
Overall	2106/2639 (80%)	1235/1430 (86%)	691/949 (73%)	180/260 (69%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 2178 atoms were assigned a chemical shift out of a possible 2784. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	864/934 (93%)	358/378 (95%)	335/376 (89%)	171/180 (95%)
Sidechain	1049/1352 (78%)	743/869 (86%)	295/420 (70%)	11/63 (17%)
Aromatic	205/328 (62%)	115/162 (71%)	84/143 (59%)	6/23 (26%)
Sugar	50/108 (46%)	50/63 (79%)	0/45 (0%)	0/0 (—%)
Base	10/62 (16%)	10/35 (29%)	0/18 (0%)	0/9 (0%)
Overall	2178/2784 (78%)	1276/1507 (85%)	714/1002 (71%)	188/275 (68%)

7.1.4 Statistically unusual chemical shifts ⓘ

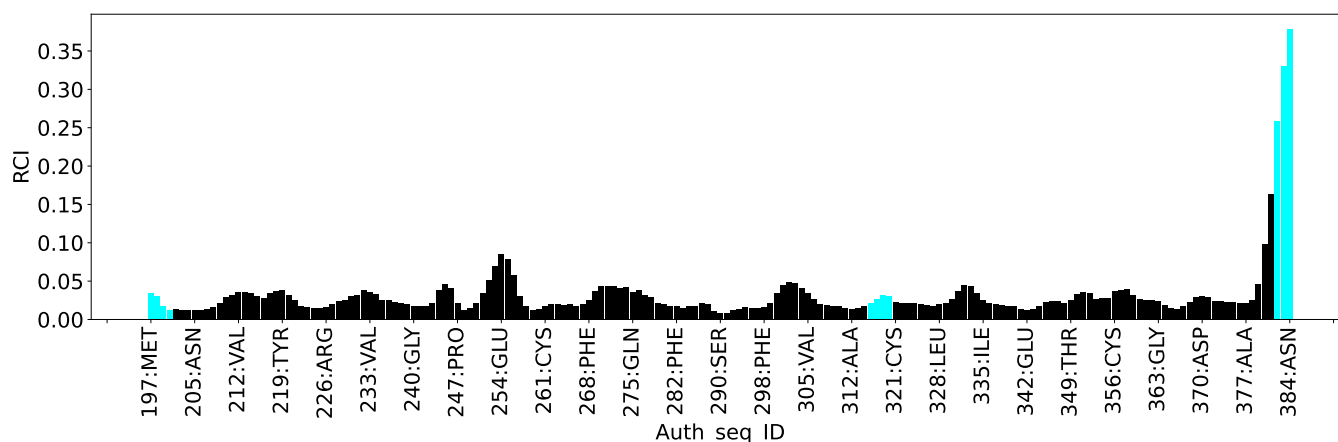
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	206	PHE	CD2	122.14	125.53 – 137.61	-7.8
1	A	340	TYR	CE2	127.67	111.68 – 124.17	7.8
1	A	206	PHE	CD1	122.14	125.33 – 137.83	-7.5
1	A	310	PHE	CD2	122.67	125.53 – 137.61	-7.4
1	A	340	TYR	CE1	127.67	111.24 – 124.66	7.2
1	A	310	PHE	CD1	122.67	125.33 – 137.83	-7.1
1	A	314	ILE	CG2	26.07	10.93 – 24.12	6.5
1	A	247	PRO	CD	43.58	45.11 – 55.58	-6.5
1	A	249	LYS	CD	22.29	23.50 – 34.42	-6.1
1	A	325	LEU	CG	33.09	21.37 – 32.19	5.8
1	A	222	TYR	CE2	125.05	111.68 – 124.17	5.7
1	A	355	GLY	H	11.65	5.23 – 11.42	5.4
1	A	219	TYR	CD1	125.40	125.84 – 139.60	-5.3
1	A	222	TYR	CE1	125.05	111.24 – 124.66	5.3
1	A	358	PHE	CD2	125.21	125.53 – 137.61	-5.3
1	A	358	PHE	CD1	125.21	125.33 – 137.83	-5.1
1	A	294	GLU	CG	30.13	30.20 – 42.01	-5.1

7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



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	2699
Intra-residue ($ i-j =0$)	1290
Sequential ($ i-j =1$)	569
Medium range ($ i-j >1$ and $ i-j <5$)	358
Long range ($ i-j \geq 5$)	432
Inter-chain	50
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	13.6
Number of long range restraints per residue ¹	2.2

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	44.2	0.2
0.2-0.5 (Medium)	10.3	0.5
>0.5 (Large)	6.6	5.18

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

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

9 Distance violation analysis ⓘ

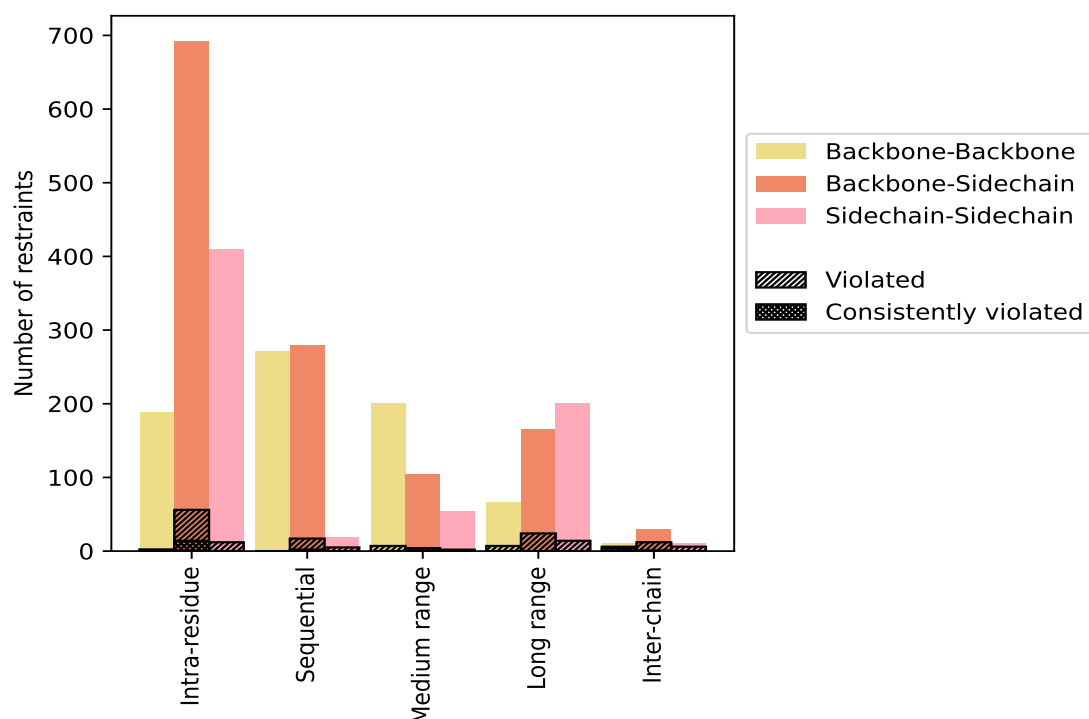
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1290	47.8	70	5.4	2.6	16	1.2	0.6
Backbone-Backbone	188	7.0	2	1.1	0.1	2	1.1	0.1
Backbone-Sidechain	692	25.6	56	8.1	2.1	14	2.0	0.5
Sidechain-Sidechain	410	15.2	12	2.9	0.4	0	0.0	0.0
Sequential ($i-j =1$)	569	21.1	22	3.9	0.8	2	0.4	0.1
Backbone-Backbone	271	10.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	279	10.3	17	6.1	0.6	2	0.7	0.1
Sidechain-Sidechain	19	0.7	5	26.3	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	358	13.3	13	3.6	0.5	1	0.3	0.0
Backbone-Backbone	200	7.4	7	3.5	0.3	0	0.0	0.0
Backbone-Sidechain	104	3.9	4	3.8	0.1	1	1.0	0.0
Sidechain-Sidechain	54	2.0	2	3.7	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	432	16.0	45	10.4	1.7	0	0.0	0.0
Backbone-Backbone	66	2.4	7	10.6	0.3	0	0.0	0.0
Backbone-Sidechain	165	6.1	24	14.5	0.9	0	0.0	0.0
Sidechain-Sidechain	201	7.4	14	7.0	0.5	0	0.0	0.0
Inter-chain	50	1.9	24	48.0	0.9	5	10.0	0.2
Backbone-Backbone	10	0.4	6	60.0	0.2	4	40.0	0.1
Backbone-Sidechain	30	1.1	12	40.0	0.4	1	3.3	0.0
Sidechain-Sidechain	10	0.4	6	60.0	0.2	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2699	100.0	174	6.4	6.4	24	0.9	0.9
Backbone-Backbone	735	27.2	22	3.0	0.8	6	0.8	0.2
Backbone-Sidechain	1270	47.1	113	8.9	4.2	18	1.4	0.7
Sidechain-Sidechain	694	25.7	39	5.6	1.4	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 [i](#)



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	36	6	2	9	11	64	0.34	4.35	0.69	0.13
2	39	7	3	9	13	71	0.32	4.22	0.64	0.13
3	35	10	4	6	13	68	0.32	3.68	0.59	0.14
4	35	8	2	10	13	68	0.31	3.77	0.6	0.13
5	35	8	5	10	13	71	0.3	4.11	0.61	0.13
6	37	5	2	7	14	65	0.43	5.18	0.95	0.15
7	31	7	4	12	12	66	0.27	3.53	0.52	0.14
8	31	6	3	5	13	58	0.39	4.07	0.71	0.15
9	37	6	3	10	13	69	0.31	3.8	0.6	0.13
10	33	8	2	3	12	58	0.37	4.46	0.74	0.13

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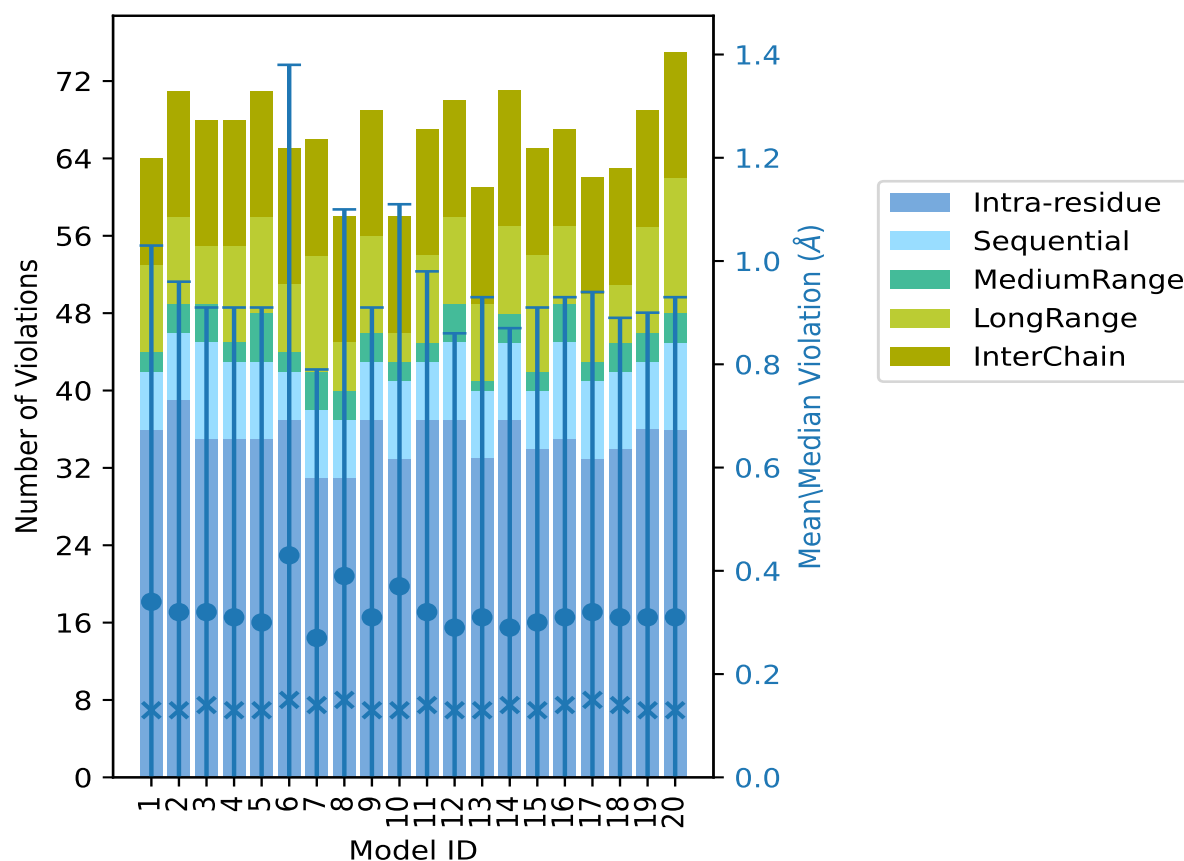
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	37	6	2	9	13	67	0.32	4.25	0.66	0.14
12	37	8	4	9	12	70	0.29	3.71	0.57	0.13
13	33	7	1	8	12	61	0.31	4.02	0.62	0.13
14	37	8	3	9	14	71	0.29	3.98	0.58	0.14
15	34	6	2	12	11	65	0.3	4.05	0.61	0.13
16	35	10	4	8	10	67	0.31	4.08	0.62	0.14
17	33	8	2	7	12	62	0.32	3.8	0.62	0.15
18	34	8	3	6	12	63	0.31	3.64	0.58	0.14
19	36	7	3	11	12	69	0.31	3.69	0.59	0.13
20	36	9	3	14	13	75	0.31	4.17	0.62	0.13

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

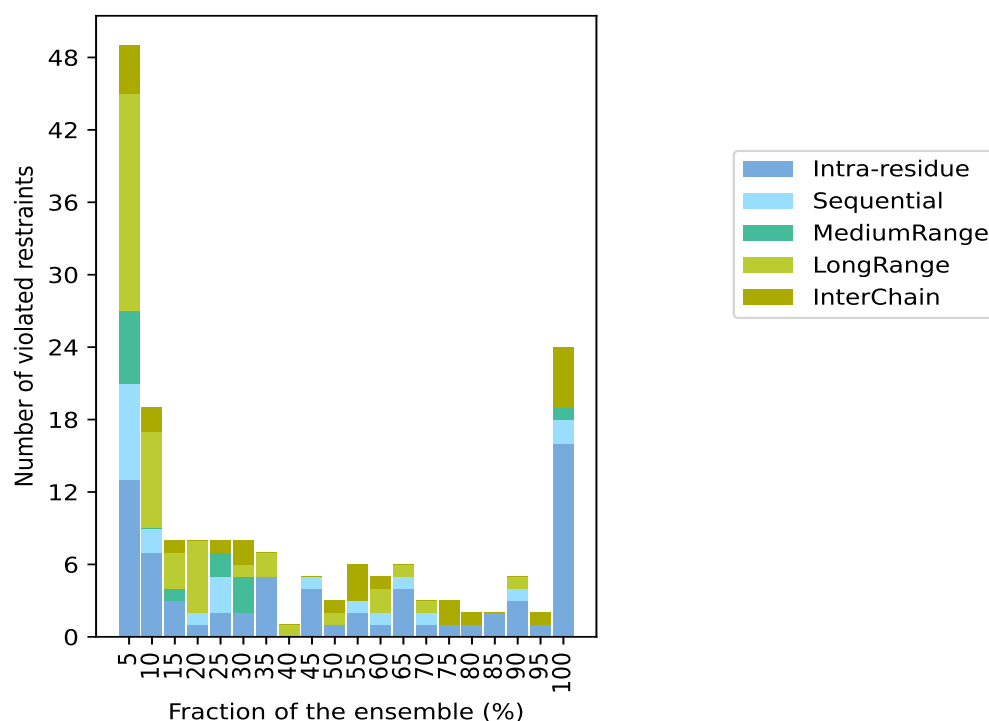
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2525(IR:1220, SQ:547, MR:345, LR:387, IC:26) restraints are 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	%
13	8	6	18	4	49	1	5.0
7	2	0	8	2	19	2	10.0
3	0	1	3	1	8	3	15.0
1	1	0	6	0	8	4	20.0
2	3	2	0	1	8	5	25.0
2	0	3	1	2	8	6	30.0
5	0	0	2	0	7	7	35.0
0	0	0	1	0	1	8	40.0
4	1	0	0	0	5	9	45.0
1	0	0	1	1	3	10	50.0
2	1	0	0	3	6	11	55.0
1	1	0	2	1	5	12	60.0
4	1	0	1	0	6	13	65.0
1	1	0	1	0	3	14	70.0
1	0	0	0	2	3	15	75.0
1	0	0	0	1	2	16	80.0
2	0	0	0	0	2	17	85.0
3	1	0	1	0	5	18	90.0
1	0	0	0	1	2	19	95.0
16	2	1	0	5	24	20	100.0

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

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

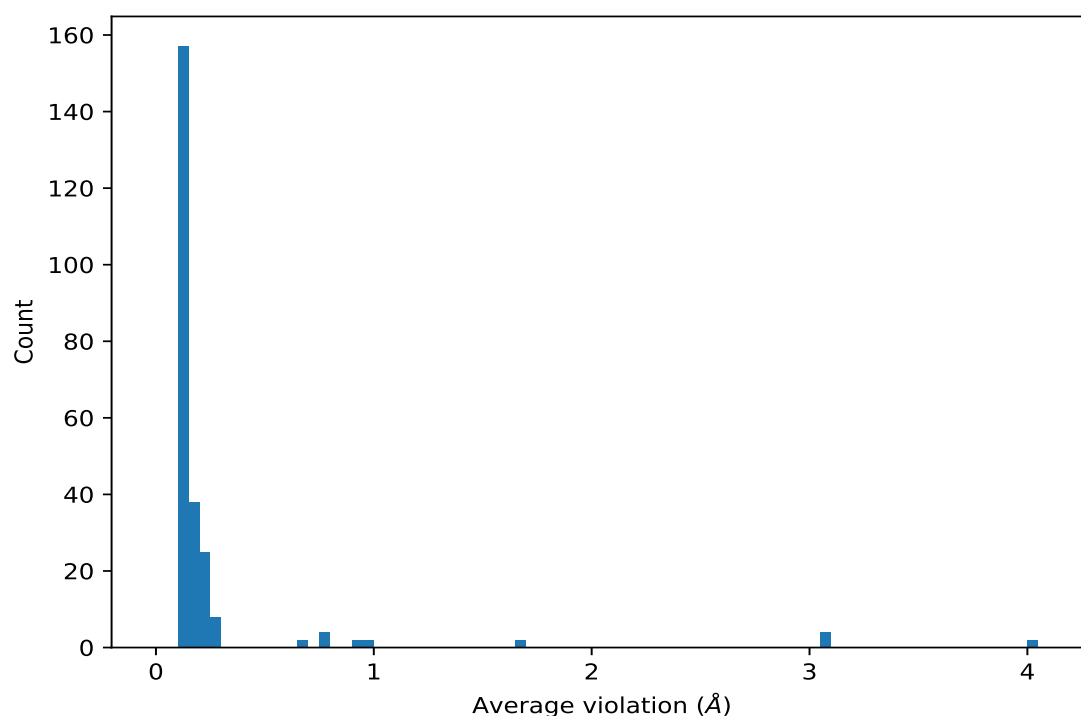
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	20	4.03	0.36	4.04
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	20	4.03	0.36	4.04
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	20	3.06	0.43	3.0
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	20	3.06	0.43	3.0
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	20	3.06	0.43	3.0
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	20	3.06	0.43	3.0
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	20	1.65	0.44	1.56
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	20	1.65	0.44	1.56
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	20	0.99	0.24	0.98
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	20	0.99	0.24	0.98
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	20	0.79	0.39	0.77
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	20	0.79	0.39	0.77
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	20	0.25	0.0	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	20	0.25	0.0	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	20	0.25	0.0	0.25
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	20	0.25	0.0	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	20	0.25	0.0	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	20	0.25	0.0	0.25
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	20	0.24	0.01	0.24
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	20	0.24	0.01	0.24
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	20	0.24	0.01	0.24
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	20	0.24	0.01	0.24
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	20	0.23	0.01	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	20	0.23	0.01	0.23
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	20	0.23	0.01	0.23
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	20	0.22	0.01	0.22
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	20	0.22	0.01	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	20	0.22	0.01	0.22
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	20	0.19	0.0	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	20	0.19	0.0	0.19
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	20	0.18	0.01	0.18
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	20	0.18	0.01	0.18
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	20	0.18	0.01	0.18
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	20	0.16	0.02	0.17
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	20	0.15	0.01	0.15
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	20	0.15	0.01	0.15
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	20	0.15	0.01	0.15
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	20	0.15	0.01	0.15
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	20	0.15	0.01	0.15
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	20	0.15	0.01	0.15
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	20	0.15	0.01	0.15
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	20	0.14	0.02	0.14
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	20	0.14	0.02	0.14
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	20	0.13	0.01	0.13
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	20	0.13	0.01	0.13
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	20	0.13	0.01	0.13
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	20	0.13	0.01	0.13
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	20	0.13	0.01	0.13
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	20	0.13	0.01	0.13
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	20	0.12	0.0	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	20	0.12	0.0	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	20	0.12	0.0	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	20	0.12	0.0	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	20	0.12	0.0	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	20	0.12	0.0	0.12
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	19	0.78	0.36	0.76
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	19	0.78	0.36	0.76
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	19	0.23	0.0	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	19	0.23	0.0	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	19	0.23	0.0	0.23
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	18	0.14	0.01	0.14
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	18	0.13	0.02	0.13
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	18	0.13	0.02	0.13
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	18	0.13	0.02	0.13
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	18	0.12	0.0	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	18	0.12	0.0	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	18	0.12	0.0	0.12
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	17	0.13	0.0	0.13
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	17	0.12	0.02	0.11
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	17	0.12	0.02	0.11
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	16	0.93	0.4	0.89
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	16	0.93	0.4	0.89
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	16	0.12	0.0	0.12
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	15	0.18	0.04	0.2
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	15	0.13	0.03	0.12
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	15	0.13	0.01	0.13
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	15	0.13	0.01	0.13
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	14	0.2	0.09	0.16
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	14	0.11	0.01	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	14	0.11	0.01	0.11
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	14	0.1	0.0	0.1
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	13	0.19	0.03	0.2
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	13	0.18	0.02	0.18
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	13	0.15	0.05	0.13
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	13	0.15	0.05	0.13
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	13	0.15	0.03	0.16
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	13	0.15	0.03	0.16
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	13	0.15	0.03	0.16
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	13	0.12	0.0	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	13	0.12	0.0	0.12
(1,90)	2:394:B:DT:H5'	1:254:A:GLU:HG2	12	0.65	0.51	0.42
(1,90)	2:394:B:DT:H5''	1:254:A:GLU:HG2	12	0.65	0.51	0.42
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG2	12	0.2	0.01	0.2
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG3	12	0.2	0.01	0.2
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD1	12	0.16	0.02	0.16
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD2	12	0.16	0.02	0.16
(1,766)	1:252:A:PHE:HA	1:252:A:PHE:HB3	12	0.13	0.0	0.13
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD2	12	0.12	0.01	0.12
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD3	12	0.12	0.01	0.12
(1,49)	2:387:B:DT:H2''	1:315:A:TYR:HA	11	0.19	0.04	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,74)	2:390:B:C38:H2'1	1:257:A:HIS:HD2	11	0.17	0.03	0.17
(1,2143)	1:347:A:TRP:HB2	1:347:A:TRP:HE1	11	0.16	0.01	0.16
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG2	11	0.15	0.02	0.15
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG3	11	0.15	0.02	0.15
(1,41)	2:385:B:DA:H8	1:374:A:ARG:H	11	0.14	0.02	0.14
(1,2645)	1:380:A:GLN:HB2	1:380:A:GLN:HE22	11	0.11	0.01	0.11
(1,2645)	1:380:A:GLN:HB3	1:380:A:GLN:HE22	11	0.11	0.01	0.11
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD1	10	0.13	0.03	0.12
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD2	10	0.13	0.03	0.12
(1,67)	2:389:B:DU:H2''	1:244:A:ASN:HB2	10	0.12	0.02	0.12
(1,1993)	1:336:A:SER:HA	1:336:A:SER:HB2	10	0.12	0.0	0.12
(1,2142)	1:347:A:TRP:HB3	1:347:A:TRP:HE1	9	0.24	0.0	0.24
(1,1609)	1:307:A:LEU:HD11	1:308:A:CYS:HA	9	0.15	0.03	0.16
(1,1609)	1:307:A:LEU:HD12	1:308:A:CYS:HA	9	0.15	0.03	0.16
(1,1609)	1:307:A:LEU:HD13	1:308:A:CYS:HA	9	0.15	0.03	0.16
(1,1609)	1:307:A:LEU:HD21	1:308:A:CYS:HA	9	0.15	0.03	0.16
(1,1609)	1:307:A:LEU:HD22	1:308:A:CYS:HA	9	0.15	0.03	0.16
(1,1609)	1:307:A:LEU:HD23	1:308:A:CYS:HA	9	0.15	0.03	0.16
(1,581)	1:235:A:LEU:HD11	1:235:A:LEU:H	9	0.12	0.02	0.12
(1,581)	1:235:A:LEU:HD12	1:235:A:LEU:H	9	0.12	0.02	0.12
(1,581)	1:235:A:LEU:HD13	1:235:A:LEU:H	9	0.12	0.02	0.12
(1,581)	1:235:A:LEU:HD21	1:235:A:LEU:H	9	0.12	0.02	0.12
(1,581)	1:235:A:LEU:HD22	1:235:A:LEU:H	9	0.12	0.02	0.12
(1,581)	1:235:A:LEU:HD23	1:235:A:LEU:H	9	0.12	0.02	0.12
(1,1849)	1:326:A:ARG:HB3	1:326:A:ARG:H	9	0.1	0.0	0.1
(1,2221)	1:352:A:ASP:HB3	1:352:A:ASP:H	9	0.1	0.0	0.1
(1,1168)	1:277:A:TYR:HA	1:306:A:SER:H	8	0.11	0.01	0.11
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG21	7	0.12	0.01	0.12
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG22	7	0.12	0.01	0.12
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG23	7	0.12	0.01	0.12
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG21	7	0.12	0.01	0.12
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG22	7	0.12	0.01	0.12
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG23	7	0.12	0.01	0.12
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB2	7	0.12	0.01	0.13
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB3	7	0.12	0.01	0.13
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB2	7	0.12	0.01	0.13
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB3	7	0.12	0.01	0.13
(1,1795)	1:323:A:GLU:HA	1:323:A:GLU:HB2	7	0.12	0.0	0.12
(1,2397)	1:366:A:GLU:HA	1:366:A:GLU:HB2	7	0.12	0.0	0.12
(1,1754)	1:314:A:ILE:HD11	1:314:A:ILE:H	7	0.11	0.01	0.11
(1,1754)	1:314:A:ILE:HD12	1:314:A:ILE:H	7	0.11	0.01	0.11
(1,1754)	1:314:A:ILE:HD13	1:314:A:ILE:H	7	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,30)	2:391:B:DA:H2'	2:391:B:DA:H8	7	0.1	0.01	0.1
(1,2406)	1:366:A:GLU:HB3	1:366:A:GLU:H	7	0.1	0.0	0.1
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE1	6	0.27	0.07	0.29
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE2	6	0.27	0.07	0.29
(1,128)	1:201:A:THR:HG21	1:201:A:THR:H	6	0.21	0.0	0.21
(1,128)	1:201:A:THR:HG22	1:201:A:THR:H	6	0.21	0.0	0.21
(1,128)	1:201:A:THR:HG23	1:201:A:THR:H	6	0.21	0.0	0.21
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG21	6	0.14	0.01	0.14
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG22	6	0.14	0.01	0.14
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG23	6	0.14	0.01	0.14
(1,77)	2:392:B:DA:H8	1:252:A:PHE:HD2	6	0.13	0.03	0.12
(1,446)	1:225:A:GLU:H	1:278:A:ARG:H	6	0.12	0.02	0.12
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB1	6	0.12	0.01	0.12
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB2	6	0.12	0.01	0.12
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB3	6	0.12	0.01	0.12
(1,2122)	1:345:A:HIS:HA	1:348:A:ASP:H	6	0.12	0.02	0.12
(1,2669)	1:381:A:ASN:HA	1:384:A:ASN:H	6	0.11	0.01	0.11
(1,718)	1:247:A:PRO:HG2	1:248:A:HIS:HD1	5	0.14	0.03	0.13
(1,718)	1:247:A:PRO:HG3	1:248:A:HIS:HD1	5	0.14	0.03	0.13
(1,1859)	1:326:A:ARG:HB2	1:327:A:THR:H	5	0.14	0.02	0.13
(1,536)	1:231:A:THR:H	1:232:A:TRP:HE1	5	0.14	0.02	0.13
(1,54)	2:388:B:DC:H2''	1:285:A:TRP:HE1	5	0.13	0.02	0.14
(1,2215)	1:351:A:VAL:HG11	1:353:A:HIS:HD2	5	0.13	0.03	0.13
(1,2215)	1:351:A:VAL:HG12	1:353:A:HIS:HD2	5	0.13	0.03	0.13
(1,2215)	1:351:A:VAL:HG13	1:353:A:HIS:HD2	5	0.13	0.03	0.13
(1,2215)	1:351:A:VAL:HG21	1:353:A:HIS:HD2	5	0.13	0.03	0.13
(1,2215)	1:351:A:VAL:HG22	1:353:A:HIS:HD2	5	0.13	0.03	0.13
(1,2215)	1:351:A:VAL:HG23	1:353:A:HIS:HD2	5	0.13	0.03	0.13
(1,109)	1:198:A:ASP:H	1:202:A:PHE:HD1	5	0.13	0.02	0.13
(1,109)	1:198:A:ASP:H	1:202:A:PHE:HD2	5	0.13	0.02	0.13
(1,1842)	1:326:A:ARG:HA	1:326:A:ARG:HB3	5	0.11	0.0	0.11
(1,2470)	1:370:A:ASP:HB3	1:370:A:ASP:H	5	0.1	0.0	0.1
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG21	4	0.2	0.02	0.2
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG22	4	0.2	0.02	0.2
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG23	4	0.2	0.02	0.2
(1,2051)	1:339:A:THR:HB	1:340:A:TYR:H	4	0.18	0.05	0.19
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB1	4	0.14	0.02	0.14
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB2	4	0.14	0.02	0.14
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB3	4	0.14	0.02	0.14
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB1	4	0.14	0.02	0.14
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB2	4	0.14	0.02	0.14
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB3	4	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB1	4	0.14	0.02	0.14
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB2	4	0.14	0.02	0.14
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB3	4	0.14	0.02	0.14
(1,489)	1:227:A:MET:HA	1:235:A:LEU:H	4	0.13	0.02	0.12
(1,97)	1:197:A:MET:HA	1:352:A:ASP:H	4	0.12	0.01	0.12
(1,122)	1:200:A:PRO:HA	1:353:A:HIS:H	4	0.12	0.01	0.12
(1,1153)	1:276:A:ASP:HA	1:276:A:ASP:HB3	4	0.12	0.0	0.12
(1,1209)	1:279:A:VAL:HB	1:307:A:LEU:HA	4	0.11	0.01	0.11
(1,13)	2:387:B:DT:H6	2:387:B:DT:H5'	3	0.2	0.06	0.22
(1,13)	2:387:B:DT:H6	2:387:B:DT:H5''	3	0.2	0.06	0.22
(1,2428)	1:367:A:HIS:HD2	1:367:A:HIS:H	3	0.15	0.04	0.13
(1,1247)	1:280:A:THR:HG21	1:308:A:CYS:H	3	0.13	0.01	0.13
(1,1247)	1:280:A:THR:HG22	1:308:A:CYS:H	3	0.13	0.01	0.13
(1,1247)	1:280:A:THR:HG23	1:308:A:CYS:H	3	0.13	0.01	0.13
(1,1554)	1:303:A:LYS:HB2	1:303:A:LYS:HE2	3	0.13	0.02	0.13
(1,1554)	1:303:A:LYS:HB2	1:303:A:LYS:HE3	3	0.13	0.02	0.13
(1,1554)	1:303:A:LYS:HB3	1:303:A:LYS:HE2	3	0.13	0.02	0.13
(1,1554)	1:303:A:LYS:HB3	1:303:A:LYS:HE3	3	0.13	0.02	0.13
(1,1379)	1:292:A:ALA:HA	1:324:A:GLY:HA2	3	0.12	0.0	0.12
(1,1379)	1:292:A:ALA:HA	1:324:A:GLY:HA3	3	0.12	0.0	0.12
(1,78)	2:392:B:DA:H1'	1:254:A:GLU:HG2	3	0.11	0.0	0.11
(1,78)	2:392:B:DA:H1'	1:254:A:GLU:HG3	3	0.11	0.0	0.11
(1,96)	1:197:A:MET:HA	1:201:A:THR:H	3	0.11	0.01	0.1
(1,2587)	1:376:A:ARG:HH21	1:382:A:GLN:H	3	0.1	0.0	0.1
(1,2587)	1:376:A:ARG:HH22	1:382:A:GLN:H	3	0.1	0.0	0.1
(1,724)	1:248:A:HIS:HB3	1:248:A:HIS:HD1	2	0.16	0.01	0.16
(1,76)	2:392:B:DA:H4'	1:250:A:HIS:HD2	2	0.16	0.01	0.16
(1,73)	2:389:B:DU:H5	1:315:A:TYR:HD1	2	0.14	0.04	0.14
(1,73)	2:389:B:DU:H5	1:315:A:TYR:HD2	2	0.14	0.04	0.14
(1,490)	1:227:A:MET:HA	1:278:A:ARG:H	2	0.14	0.03	0.14
(1,1315)	1:283:A:THR:H	1:311:A:THR:HB	2	0.14	0.03	0.14
(1,169)	1:203:A:THR:HB	1:204:A:PHE:H	2	0.14	0.01	0.14
(1,436)	1:225:A:GLU:HB2	1:278:A:ARG:HG2	2	0.12	0.01	0.12
(1,436)	1:225:A:GLU:HB2	1:278:A:ARG:HG3	2	0.12	0.01	0.12
(1,436)	1:225:A:GLU:HB3	1:278:A:ARG:HG2	2	0.12	0.01	0.12
(1,436)	1:225:A:GLU:HB3	1:278:A:ARG:HG3	2	0.12	0.01	0.12
(1,1715)	1:311:A:THR:H	1:335:A:ILE:HG12	2	0.12	0.01	0.12
(1,1715)	1:311:A:THR:H	1:335:A:ILE:HG13	2	0.12	0.01	0.12
(1,796)	1:256:A:ARG:HA	1:256:A:ARG:HB2	2	0.12	0.0	0.12
(1,1510)	1:301:A:LYS:HB3	1:301:A:LYS:HG2	2	0.12	0.0	0.12
(1,2696)	1:384:A:ASN:HA	1:384:A:ASN:HB2	2	0.12	0.0	0.12
(1,947)	1:263:A:LEU:HD11	1:298:A:PHE:H	2	0.12	0.0	0.12

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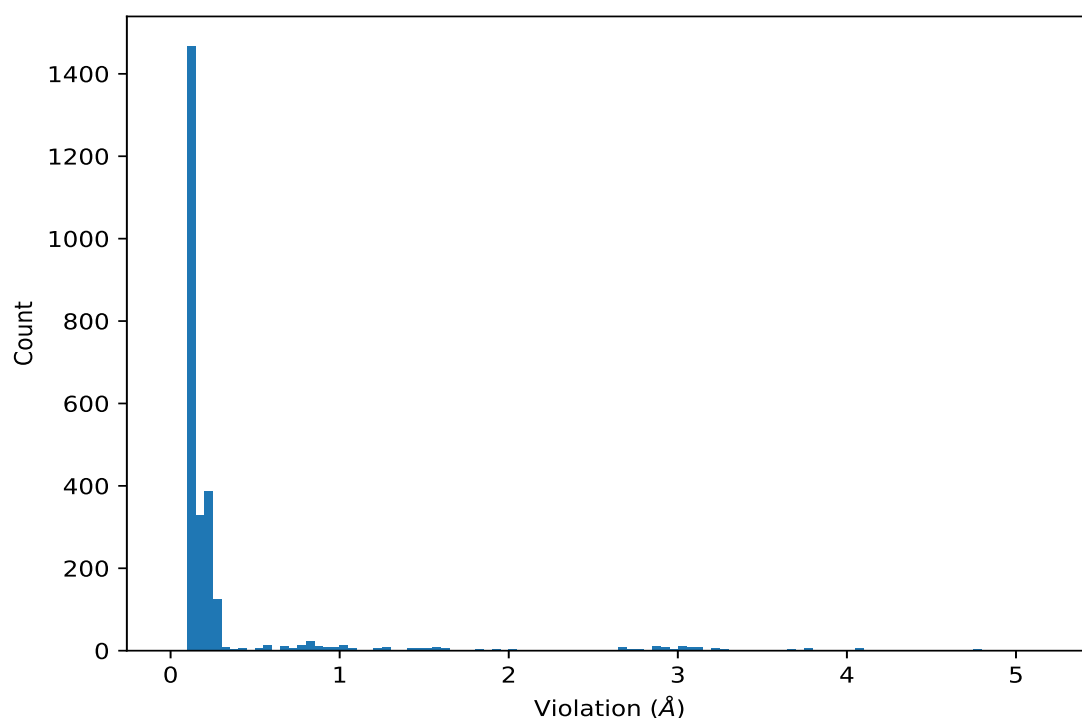
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,947)	1:263:A:LEU:HD12	1:298:A:PHE:H	2	0.12	0.0	0.12
(1,947)	1:263:A:LEU:HD13	1:298:A:PHE:H	2	0.12	0.0	0.12
(1,947)	1:263:A:LEU:HD21	1:298:A:PHE:H	2	0.12	0.0	0.12
(1,947)	1:263:A:LEU:HD22	1:298:A:PHE:H	2	0.12	0.0	0.12
(1,947)	1:263:A:LEU:HD23	1:298:A:PHE:H	2	0.12	0.0	0.12
(1,1283)	1:282:A:PHE:HA	1:346:A:CYS:HG	2	0.12	0.0	0.12
(1,2679)	1:382:A:GLN:HB2	1:382:A:GLN:H	2	0.12	0.0	0.12
(1,150)	1:202:A:PHE:HA	1:351:A:VAL:HG11	2	0.11	0.01	0.11
(1,150)	1:202:A:PHE:HA	1:351:A:VAL:HG12	2	0.11	0.01	0.11
(1,150)	1:202:A:PHE:HA	1:351:A:VAL:HG13	2	0.11	0.01	0.11
(1,1478)	1:299:A:ILE:HD11	1:300:A:SER:HB2	2	0.11	0.0	0.11
(1,1478)	1:299:A:ILE:HD11	1:300:A:SER:HB3	2	0.11	0.0	0.11
(1,1478)	1:299:A:ILE:HD12	1:300:A:SER:HB2	2	0.11	0.0	0.11
(1,1478)	1:299:A:ILE:HD12	1:300:A:SER:HB3	2	0.11	0.0	0.11
(1,1478)	1:299:A:ILE:HD13	1:300:A:SER:HB2	2	0.11	0.0	0.11
(1,1478)	1:299:A:ILE:HD13	1:300:A:SER:HB3	2	0.11	0.0	0.11
(1,2479)	1:371:A:LEU:HA	1:371:A:LEU:HG	2	0.11	0.01	0.11
(1,1960)	1:334:A:LYS:HB3	1:334:A:LYS:H	2	0.11	0.0	0.11
(1,1313)	1:283:A:THR:H	1:310:A:PHE:HE1	2	0.1	0.0	0.1
(1,1313)	1:283:A:THR:H	1:310:A:PHE:HE2	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	6	5.18
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	6	5.18
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	6	4.79
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	6	4.79
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	6	4.79
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	6	4.79
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	10	4.46
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	10	4.46
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	1	4.35
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	1	4.35
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	11	4.25
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	11	4.25
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	2	4.22
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	2	4.22
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	20	4.17
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	20	4.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	5	4.11
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	5	4.11
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	16	4.08
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	16	4.08
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	8	4.07
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	8	4.07
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	15	4.05
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	15	4.05
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	13	4.02
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	13	4.02
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	14	3.98
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	14	3.98
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	9	3.8
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	9	3.8
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	17	3.8
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	17	3.8
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	4	3.77
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	4	3.77
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	12	3.71
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	12	3.71
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	19	3.69
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	19	3.69
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	3	3.68
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	3	3.68
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	18	3.64
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	18	3.64
(1,83)	2:393:B:DT:H5'	1:255:A:GLY:H	7	3.53
(1,83)	2:393:B:DT:H5''	1:255:A:GLY:H	7	3.53
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	10	3.29
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	10	3.29
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	10	3.29
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	10	3.29
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	6	3.22
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	6	3.22
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	1	3.2
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	1	3.2
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	1	3.2
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	1	3.2
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	8	3.15
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	8	3.15
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	8	3.15
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	8	3.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	11	3.1
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	11	3.1
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	11	3.1
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	11	3.1
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	20	3.08
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	20	3.08
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	20	3.08
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	20	3.08
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	2	3.07
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	2	3.07
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	2	3.07
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	2	3.07
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	5	3.05
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	5	3.05
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	5	3.05
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	5	3.05
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	16	3.05
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	16	3.05
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	16	3.05
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	16	3.05
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	9	3.03
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	9	3.03
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	9	3.03
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	9	3.03
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	19	2.97
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	19	2.97
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	19	2.97
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	19	2.97
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	14	2.94
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	14	2.94
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	14	2.94
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	14	2.94
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	15	2.93
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	15	2.93
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	15	2.93
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	15	2.93
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	4	2.9
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	4	2.9
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	4	2.9
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	4	2.9
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	13	2.89
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	13	2.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	13	2.89
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	13	2.89
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	17	2.89
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	17	2.89
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	17	2.89
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	17	2.89
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	3	2.8
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	3	2.8
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	3	2.8
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	3	2.8
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	12	2.73
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	12	2.73
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	12	2.73
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	12	2.73
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	18	2.68
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	18	2.68
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	18	2.68
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	18	2.68
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA2	7	2.66
(1,82)	2:393:B:DT:H5'	1:255:A:GLY:HA3	7	2.66
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA2	7	2.66
(1,82)	2:393:B:DT:H5''	1:255:A:GLY:HA3	7	2.66
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	6	2.05
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	6	2.05
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	8	2.05
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	8	2.05
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	1	1.98
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	1	1.98
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	11	1.93
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	11	1.93
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	2	1.92
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	2	1.92
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	20	1.83
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	20	1.83
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	6	1.81
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	6	1.81
(1,90)	2:394:B:DT:H5'	1:254:A:GLU:HG2	10	1.76
(1,90)	2:394:B:DT:H5''	1:254:A:GLU:HG2	10	1.76
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	4	1.64
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	4	1.64
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	17	1.61
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	17	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	9	1.6
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	9	1.6
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	12	1.59
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	12	1.59
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	3	1.59
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	3	1.59
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	18	1.58
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	18	1.58
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	5	1.57
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	5	1.57
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	17	1.54
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	17	1.54
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	12	1.52
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	12	1.52
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	4	1.51
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	4	1.51
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	3	1.48
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	3	1.48
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	16	1.47
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	16	1.47
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	20	1.47
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	20	1.47
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	19	1.45
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	19	1.45
(1,90)	2:394:B:DT:H5'	1:254:A:GLU:HG2	8	1.43
(1,90)	2:394:B:DT:H5''	1:254:A:GLU:HG2	8	1.43
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	14	1.41
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	14	1.41
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	19	1.31
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	19	1.31
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	15	1.28
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	15	1.28
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	9	1.26
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	9	1.26
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	10	1.26
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	10	1.26
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	8	1.25
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	8	1.25
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	6	1.24
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	6	1.24
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	13	1.22
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	13	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	19	1.21
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	19	1.21
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	10	1.18
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	10	1.18
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	2	1.09
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	2	1.09
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	8	1.09
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	8	1.09
(1,81)	2:393:B:DT:H5'	1:254:A:GLU:HA	7	1.08
(1,81)	2:393:B:DT:H5''	1:254:A:GLU:HA	7	1.08
(1,90)	2:394:B:DT:H5'	1:254:A:GLU:HG2	3	1.04
(1,90)	2:394:B:DT:H5''	1:254:A:GLU:HG2	3	1.04
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	11	1.03
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	11	1.03
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	9	1.03
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	9	1.03
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	1	1.02
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	1	1.02
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	15	1.02
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	15	1.02
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	13	1.01
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	13	1.01
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	3	1.0
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	3	1.0
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	14	0.99
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	14	0.99
(1,90)	2:394:B:DT:H5'	1:254:A:GLU:HG2	18	0.98
(1,90)	2:394:B:DT:H5''	1:254:A:GLU:HG2	18	0.98
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	4	0.98
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	4	0.98
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	1	0.97
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	1	0.97
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	2	0.95
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	2	0.95
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	16	0.94
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	16	0.94
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	10	0.91
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	10	0.91
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	11	0.9
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	11	0.9
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	9	0.89
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	9	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	15	0.89
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	15	0.89
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	8	0.87
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	8	0.87
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	18	0.87
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	18	0.87
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	11	0.86
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	11	0.86
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	2	0.85
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	2	0.85
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	13	0.85
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	13	0.85
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	5	0.85
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	5	0.85
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	20	0.84
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	20	0.84
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	1	0.84
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	1	0.84
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	8	0.84
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	8	0.84
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	1	0.83
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	1	0.83
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	20	0.82
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	20	0.82
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	20	0.82
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	20	0.82
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	2	0.81
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	2	0.81
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	18	0.81
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	18	0.81
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	19	0.79
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	19	0.79
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	5	0.79
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	5	0.79
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	13	0.78
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	13	0.78
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	16	0.76
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	16	0.76
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	17	0.76
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	17	0.76
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	17	0.76
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	17	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	4	0.75
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	4	0.75
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	15	0.73
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	15	0.73
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	11	0.73
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	11	0.73
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	14	0.72
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	14	0.72
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	5	0.7
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	5	0.7
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	9	0.7
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	9	0.7
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	12	0.68
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	12	0.68
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	16	0.67
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	16	0.67
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	12	0.66
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	12	0.66
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	14	0.6
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	14	0.6
(1,42)	2:386:B:DT:H5'	1:370:A:ASP:HA	7	0.6
(1,42)	2:386:B:DT:H5''	1:370:A:ASP:HA	7	0.6
(1,90)	2:394:B:DT:H5'	1:254:A:GLU:HG2	6	0.59
(1,90)	2:394:B:DT:H5''	1:254:A:GLU:HG2	6	0.59
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	10	0.59
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	10	0.59
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	3	0.59
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	3	0.59
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	7	0.56
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	7	0.56
(1,37)	2:393:B:DT:H6	2:393:B:DT:H5'	10	0.55
(1,37)	2:393:B:DT:H6	2:393:B:DT:H5''	10	0.55
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	19	0.54
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	19	0.54
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	18	0.51
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	18	0.51
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	18	0.5
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	18	0.5
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	3	0.49
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	3	0.49
(1,90)	2:394:B:DT:H5'	1:254:A:GLU:HG2	5	0.43
(1,90)	2:394:B:DT:H5''	1:254:A:GLU:HG2	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	2:394:B:DT:H5'	1:254:A:GLU:HG2	14	0.42
(1,90)	2:394:B:DT:H5''	1:254:A:GLU:HG2	14	0.42
(1,90)	2:394:B:DT:H5'	1:254:A:GLU:HG2	16	0.42
(1,90)	2:394:B:DT:H5''	1:254:A:GLU:HG2	16	0.42
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	7	0.39
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	7	0.39
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	17	0.36
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	17	0.36
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	9	0.35
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE1	8	0.34
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE2	8	0.34
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	19	0.33
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE1	2	0.32
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE2	2	0.32
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	6	0.31
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	12	0.31
(1,75)	2:390:B:C38:H5'1	1:257:A:HIS:HD2	6	0.31
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	7	0.3
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	7	0.3
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE1	1	0.29
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE2	1	0.29
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE1	11	0.28
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE2	11	0.28
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE1	5	0.27
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE2	5	0.27
(1,49)	2:387:B:DT:H2''	1:315:A:TYR:HA	4	0.27
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	4	0.26
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	4	0.26
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	4	0.26
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	1	0.26
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	9	0.26
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	17	0.26
(1,2142)	1:347:A:TRP:HB3	1:347:A:TRP:HE1	1	0.25
(1,2142)	1:347:A:TRP:HB3	1:347:A:TRP:HE1	6	0.25
(1,2142)	1:347:A:TRP:HB3	1:347:A:TRP:HE1	9	0.25
(1,2142)	1:347:A:TRP:HB3	1:347:A:TRP:HE1	14	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	1	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	1	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	1	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	2	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	2	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	3	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	3	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	3	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	4	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	4	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	4	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	5	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	5	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	5	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	6	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	6	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	6	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	7	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	7	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	7	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	8	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	8	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	8	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	9	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	9	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	9	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	10	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	10	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	10	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	11	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	11	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	11	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	13	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	13	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	13	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	14	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	14	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	14	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	15	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	15	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	15	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	17	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	17	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	17	0.25
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	18	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	18	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	19	0.25
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	19	0.25
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	19	0.25
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	7	0.25
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	7	0.25
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	7	0.25
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	10	0.25
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	10	0.25
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	10	0.25
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	13	0.25
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	13	0.25
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	13	0.25
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	2	0.25
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	2	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	2	0.25
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	3	0.25
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	3	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	3	0.25
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	5	0.25
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	5	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	5	0.25
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	7	0.25
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	7	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	7	0.25
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	8	0.25
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	8	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	8	0.25
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	10	0.25
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	10	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	10	0.25
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	12	0.25
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	12	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	12	0.25
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	13	0.25
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	13	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	13	0.25
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	14	0.25
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	14	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	14	0.25
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	16	0.25
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	16	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	17	0.25
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	17	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	17	0.25
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	18	0.25
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	18	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	18	0.25
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	19	0.25
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	19	0.25
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	19	0.25
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	6	0.25
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	6	0.25
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	6	0.25
(1,13)	2:387:B:DT:H6	2:387:B:DT:H5'	7	0.25
(1,13)	2:387:B:DT:H6	2:387:B:DT:H5''	7	0.25
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	4	0.25
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	5	0.25
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	10	0.25
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	1	0.24
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	1	0.24
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	1	0.24
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	5	0.24
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	5	0.24
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	5	0.24
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	7	0.24
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	7	0.24
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	7	0.24
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	8	0.24
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	8	0.24
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	8	0.24
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	16	0.24
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	16	0.24
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	16	0.24
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	17	0.24
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	17	0.24
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	17	0.24
(1,2142)	1:347:A:TRP:HB3	1:347:A:TRP:HE1	3	0.24
(1,2142)	1:347:A:TRP:HB3	1:347:A:TRP:HE1	11	0.24
(1,2142)	1:347:A:TRP:HB3	1:347:A:TRP:HE1	15	0.24
(1,2142)	1:347:A:TRP:HB3	1:347:A:TRP:HE1	16	0.24
(1,2142)	1:347:A:TRP:HB3	1:347:A:TRP:HE1	18	0.24
(1,2051)	1:339:A:THR:HB	1:340:A:TYR:H	10	0.24
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	12	0.24
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	12	0.24
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	16	0.24
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	16	0.24
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	16	0.24
(1,1871)	1:327:A:THR:HG21	1:327:A:THR:H	20	0.24
(1,1871)	1:327:A:THR:HG22	1:327:A:THR:H	20	0.24
(1,1871)	1:327:A:THR:HG23	1:327:A:THR:H	20	0.24
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	1	0.24
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	1	0.24
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	1	0.24
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	2	0.24
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	2	0.24
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	2	0.24
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	3	0.24
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	3	0.24
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	3	0.24
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	6	0.24
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	6	0.24
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	6	0.24
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	11	0.24
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	11	0.24
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	11	0.24
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	14	0.24
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	14	0.24
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	14	0.24
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	15	0.24
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	15	0.24
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	15	0.24
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	17	0.24
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	17	0.24
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	17	0.24
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	18	0.24
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	18	0.24
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	18	0.24
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	20	0.24
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	20	0.24
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	20	0.24
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	1	0.24
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	1	0.24
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	1	0.24
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	4	0.24
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	4	0.24
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	6	0.24
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	6	0.24
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	6	0.24
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	9	0.24
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	9	0.24
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	9	0.24
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	11	0.24
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	11	0.24
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	11	0.24
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	15	0.24
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	15	0.24
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	15	0.24
(1,1466)	1:299:A:ILE:HG21	1:299:A:ILE:H	20	0.24
(1,1466)	1:299:A:ILE:HG22	1:299:A:ILE:H	20	0.24
(1,1466)	1:299:A:ILE:HG23	1:299:A:ILE:H	20	0.24
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	2	0.24
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	2	0.24
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	2	0.24
(1,90)	2:394:B:DT:H5'	1:254:A:GLU:HG2	7	0.24
(1,90)	2:394:B:DT:H5''	1:254:A:GLU:HG2	7	0.24
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	13	0.24
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	13	0.24
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	2	0.24
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	3	0.24
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	6	0.24
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	12	0.24
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	14	0.24
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	15	0.24
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	18	0.24
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	2	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	2	0.23
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	2	0.23
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	3	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	3	0.23
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	3	0.23
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	4	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	4	0.23
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	4	0.23
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	6	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	6	0.23
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	9	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	9	0.23
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	9	0.23
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	10	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	10	0.23
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	10	0.23
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	11	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	11	0.23
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	11	0.23
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	12	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	12	0.23
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	12	0.23
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	13	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	13	0.23
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	13	0.23
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	14	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	14	0.23
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	14	0.23
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	15	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	15	0.23
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	15	0.23
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	18	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	18	0.23
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	18	0.23
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	19	0.23
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	19	0.23
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	19	0.23
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	4	0.23
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	4	0.23
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	4	0.23
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	5	0.23
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	5	0.23
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	5	0.23
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	8	0.23
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	8	0.23
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	8	0.23
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	9	0.23
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	9	0.23
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	9	0.23
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	12	0.23
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	12	0.23
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	16	0.23
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	16	0.23
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	16	0.23
(1,1575)	1:305:A:VAL:HG11	1:305:A:VAL:H	19	0.23
(1,1575)	1:305:A:VAL:HG12	1:305:A:VAL:H	19	0.23
(1,1575)	1:305:A:VAL:HG13	1:305:A:VAL:H	19	0.23
(1,988)	1:266:A:ILE:HB	1:266:A:ILE:HD11	20	0.23
(1,988)	1:266:A:ILE:HB	1:266:A:ILE:HD12	20	0.23
(1,988)	1:266:A:ILE:HB	1:266:A:ILE:HD13	20	0.23
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	2	0.23
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	2	0.23
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	2	0.23
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	5	0.23
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	5	0.23
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	5	0.23
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	11	0.23
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	11	0.23
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	11	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	1	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	1	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	1	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	3	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	3	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	3	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	4	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	4	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	4	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	5	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	5	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	5	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	7	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	7	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	7	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	8	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	8	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	8	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	10	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	10	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	10	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	11	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	11	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	12	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	12	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	12	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	13	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	13	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	13	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	14	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	14	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	14	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	15	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	15	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	15	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	16	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	16	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	16	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	17	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	17	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	17	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	18	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	18	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	18	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	19	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	19	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	19	0.23
(1,283)	1:212:A:VAL:HG21	1:212:A:VAL:H	20	0.23
(1,283)	1:212:A:VAL:HG22	1:212:A:VAL:H	20	0.23
(1,283)	1:212:A:VAL:HG23	1:212:A:VAL:H	20	0.23
(1,87)	2:394:B:DT:H5'	1:254:A:GLU:HB3	12	0.23
(1,87)	2:394:B:DT:H5''	1:254:A:GLU:HB3	12	0.23
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	17	0.23
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	8	0.23
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	13	0.23
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	16	0.23
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	19	0.23
(1,2610)	1:378:A:ILE:HG21	1:378:A:ILE:H	20	0.22
(1,2610)	1:378:A:ILE:HG22	1:378:A:ILE:H	20	0.22
(1,2610)	1:378:A:ILE:HG23	1:378:A:ILE:H	20	0.22
(1,2051)	1:339:A:THR:HB	1:340:A:TYR:H	16	0.22
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG2	2	0.22
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG3	2	0.22
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	1	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	1	0.22
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	3	0.22
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	3	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	3	0.22
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	4	0.22
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	4	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	4	0.22
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	6	0.22
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	6	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	6	0.22
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	7	0.22
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	7	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	7	0.22
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	8	0.22
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	8	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	8	0.22
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	9	0.22
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	9	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	9	0.22
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	10	0.22
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	10	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	10	0.22
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	12	0.22
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	12	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	12	0.22
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	14	0.22
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	14	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	14	0.22
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	16	0.22
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	16	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	16	0.22
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	17	0.22
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	17	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	17	0.22
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	19	0.22
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	19	0.22
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	19	0.22
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	3	0.22
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	1	0.22
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	2	0.22
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	14	0.22
(1,128)	1:201:A:THR:HG21	1:201:A:THR:H	2	0.22
(1,128)	1:201:A:THR:HG22	1:201:A:THR:H	2	0.22
(1,128)	1:201:A:THR:HG23	1:201:A:THR:H	2	0.22
(1,128)	1:201:A:THR:HG21	1:201:A:THR:H	3	0.22
(1,128)	1:201:A:THR:HG22	1:201:A:THR:H	3	0.22
(1,128)	1:201:A:THR:HG23	1:201:A:THR:H	3	0.22
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG21	5	0.22
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG22	5	0.22
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG23	5	0.22
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	14	0.22
(1,49)	2:387:B:DT:H2''	1:315:A:TYR:HA	19	0.22
(1,13)	2:387:B:DT:H6	2:387:B:DT:H5'	16	0.22
(1,13)	2:387:B:DT:H6	2:387:B:DT:H5''	16	0.22
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	11	0.22
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	20	0.22
(1,2428)	1:367:A:HIS:HD2	1:367:A:HIS:H	8	0.21
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG2	3	0.21
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG3	3	0.21
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG2	14	0.21
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG3	14	0.21
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	13	0.21
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	13	0.21
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	13	0.21
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	15	0.21
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	15	0.21
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	15	0.21
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	18	0.21
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	18	0.21
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	18	0.21
(1,969)	1:265:A:VAL:HG11	1:265:A:VAL:H	20	0.21
(1,969)	1:265:A:VAL:HG12	1:265:A:VAL:H	20	0.21
(1,969)	1:265:A:VAL:HG13	1:265:A:VAL:H	20	0.21
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	5	0.21
(1,439)	1:225:A:GLU:HG2	1:232:A:TRP:HB2	1	0.21
(1,439)	1:225:A:GLU:HG2	1:232:A:TRP:HB3	1	0.21
(1,439)	1:225:A:GLU:HG3	1:232:A:TRP:HB2	1	0.21
(1,439)	1:225:A:GLU:HG3	1:232:A:TRP:HB3	1	0.21
(1,128)	1:201:A:THR:HG21	1:201:A:THR:H	1	0.21
(1,128)	1:201:A:THR:HG22	1:201:A:THR:H	1	0.21
(1,128)	1:201:A:THR:HG23	1:201:A:THR:H	1	0.21
(1,128)	1:201:A:THR:HG21	1:201:A:THR:H	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,128)	1:201:A:THR:HG22	1:201:A:THR:H	4	0.21
(1,128)	1:201:A:THR:HG23	1:201:A:THR:H	4	0.21
(1,128)	1:201:A:THR:HG21	1:201:A:THR:H	9	0.21
(1,128)	1:201:A:THR:HG22	1:201:A:THR:H	9	0.21
(1,128)	1:201:A:THR:HG23	1:201:A:THR:H	9	0.21
(1,128)	1:201:A:THR:HG21	1:201:A:THR:H	12	0.21
(1,128)	1:201:A:THR:HG22	1:201:A:THR:H	12	0.21
(1,128)	1:201:A:THR:HG23	1:201:A:THR:H	12	0.21
(1,77)	2:392:B:DA:H8	1:252:A:PHE:HD2	6	0.21
(1,74)	2:390:B:C38:H2'1	1:257:A:HIS:HD2	10	0.21
(1,74)	2:390:B:C38:H2'1	1:257:A:HIS:HD2	18	0.21
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	1	0.21
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	10	0.21
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	12	0.21
(1,49)	2:387:B:DT:H2''	1:315:A:TYR:HA	11	0.21
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	6	0.21
(1,7)	2:386:B:DT:H2'	2:386:B:DT:H5'	7	0.21
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG2	5	0.2
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG3	5	0.2
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG2	7	0.2
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG3	7	0.2
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG2	8	0.2
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG3	8	0.2
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG2	10	0.2
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG3	10	0.2
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG2	17	0.2
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG3	17	0.2
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD1	16	0.2
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD2	16	0.2
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD1	5	0.2
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD2	5	0.2
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD1	17	0.2
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD2	17	0.2
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	1	0.2
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	1	0.2
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	4	0.2
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	4	0.2
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	12	0.2
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	12	0.2
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	16	0.2
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	16	0.2
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	11	0.2
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	11	0.2
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	8	0.2
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	8	0.2
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	8	0.2
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	4	0.2
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	15	0.2
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG21	19	0.2
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG22	19	0.2
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG23	19	0.2
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG21	20	0.2
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG22	20	0.2
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG23	20	0.2
(1,74)	2:390:B:C38:H2'1	1:257:A:HIS:HD2	7	0.2
(1,74)	2:390:B:C38:H2'1	1:257:A:HIS:HD2	13	0.2
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	9	0.2
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	13	0.2
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	14	0.2
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	18	0.2
(1,49)	2:387:B:DT:H2''	1:315:A:TYR:HA	6	0.2
(1,49)	2:387:B:DT:H2''	1:315:A:TYR:HA	20	0.2
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	3	0.2
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	4	0.2
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	15	0.2
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	19	0.2
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	5	0.19
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	5	0.19
(1,1609)	1:307:A:LEU:HD11	1:308:A:CYS:HA	15	0.19
(1,1609)	1:307:A:LEU:HD12	1:308:A:CYS:HA	15	0.19
(1,1609)	1:307:A:LEU:HD13	1:308:A:CYS:HA	15	0.19
(1,1609)	1:307:A:LEU:HD21	1:308:A:CYS:HA	15	0.19
(1,1609)	1:307:A:LEU:HD22	1:308:A:CYS:HA	15	0.19
(1,1609)	1:307:A:LEU:HD23	1:308:A:CYS:HA	15	0.19
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG2	16	0.19
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG3	16	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	2	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	2	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	3	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	3	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	5	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	5	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	6	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	7	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	7	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	8	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	8	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	9	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	9	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	10	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	10	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	11	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	11	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	13	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	13	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	14	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	14	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	15	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	15	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	17	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	17	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	18	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	18	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	19	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	19	0.19
(1,1129)	1:274:A:ASP:HB2	1:275:A:GLN:H	20	0.19
(1,1129)	1:274:A:ASP:HB3	1:275:A:GLN:H	20	0.19
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	5	0.19
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	5	0.19
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	5	0.19
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	18	0.19
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	18	0.19
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	18	0.19
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	4	0.19
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	4	0.19
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	4	0.19
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	13	0.19
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	17	0.19
(1,718)	1:247:A:PRO:HG2	1:248:A:HIS:HD1	20	0.19
(1,718)	1:247:A:PRO:HG3	1:248:A:HIS:HD1	20	0.19
(1,367)	1:221:A:CYS:H	1:222:A:TYR:HE1	11	0.19
(1,367)	1:221:A:CYS:H	1:222:A:TYR:HE2	11	0.19
(1,90)	2:394:B:DT:H5'	1:254:A:GLU:HG2	4	0.19
(1,90)	2:394:B:DT:H5''	1:254:A:GLU:HG2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	2:394:B:DT:H5'	1:254:A:GLU:HB2	15	0.19
(1,88)	2:394:B:DT:H5''	1:254:A:GLU:HB2	15	0.19
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	2	0.19
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	5	0.19
(1,41)	2:385:B:DA:H8	1:374:A:ARG:H	15	0.19
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	9	0.19
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	13	0.19
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	13	0.19
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	7	0.18
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	7	0.18
(1,2215)	1:351:A:VAL:HG11	1:353:A:HIS:HD2	19	0.18
(1,2215)	1:351:A:VAL:HG12	1:353:A:HIS:HD2	19	0.18
(1,2215)	1:351:A:VAL:HG13	1:353:A:HIS:HD2	19	0.18
(1,2215)	1:351:A:VAL:HG21	1:353:A:HIS:HD2	19	0.18
(1,2215)	1:351:A:VAL:HG22	1:353:A:HIS:HD2	19	0.18
(1,2215)	1:351:A:VAL:HG23	1:353:A:HIS:HD2	19	0.18
(1,2143)	1:347:A:TRP:HB2	1:347:A:TRP:HE1	13	0.18
(1,2000)	1:336:A:SER:HB2	1:337:A:ILE:HD11	20	0.18
(1,2000)	1:336:A:SER:HB2	1:337:A:ILE:HD12	20	0.18
(1,2000)	1:336:A:SER:HB2	1:337:A:ILE:HD13	20	0.18
(1,2000)	1:336:A:SER:HB3	1:337:A:ILE:HD11	20	0.18
(1,2000)	1:336:A:SER:HB3	1:337:A:ILE:HD12	20	0.18
(1,2000)	1:336:A:SER:HB3	1:337:A:ILE:HD13	20	0.18
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG2	13	0.18
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG3	13	0.18
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG2	18	0.18
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG3	18	0.18
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD1	4	0.18
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD2	4	0.18
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	1	0.18
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	1	0.18
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	1	0.18
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	2	0.18
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	2	0.18
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	2	0.18
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	3	0.18
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	3	0.18
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	3	0.18
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	4	0.18
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	4	0.18
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	4	0.18
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	6	0.18
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	6	0.18
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	10	0.18
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	10	0.18
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	10	0.18
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	14	0.18
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	14	0.18
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	14	0.18
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	15	0.18
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	15	0.18
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	15	0.18
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	17	0.18
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	17	0.18
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	17	0.18
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	19	0.18
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	19	0.18
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	19	0.18
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	20	0.18
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	20	0.18
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	20	0.18
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	5	0.18
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	5	0.18
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	5	0.18
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	7	0.18
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	9	0.18
(1,718)	1:247:A:PRO:HG2	1:248:A:HIS:HD1	16	0.18
(1,718)	1:247:A:PRO:HG3	1:248:A:HIS:HD1	16	0.18
(1,74)	2:390:B:C38:H2'1	1:257:A:HIS:HD2	2	0.18
(1,73)	2:389:B:DU:H5	1:315:A:TYR:HD1	2	0.18
(1,73)	2:389:B:DU:H5	1:315:A:TYR:HD2	2	0.18
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	9	0.18
(1,49)	2:387:B:DT:H2''	1:315:A:TYR:HA	15	0.18
(1,49)	2:387:B:DT:H2''	1:315:A:TYR:HA	16	0.18
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	2	0.18
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	5	0.18
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	17	0.18
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	11	0.18
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	11	0.18
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	20	0.18
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	20	0.18
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	8	0.17
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	16	0.17
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	16	0.17
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	17	0.17
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	17	0.17
(1,2250)	1:354:A:GLN:HB2	1:354:A:GLN:HE22	2	0.17
(1,2250)	1:354:A:GLN:HB3	1:354:A:GLN:HE22	2	0.17
(1,2143)	1:347:A:TRP:HB2	1:347:A:TRP:HE1	2	0.17
(1,2143)	1:347:A:TRP:HB2	1:347:A:TRP:HE1	17	0.17
(1,1859)	1:326:A:ARG:HB2	1:327:A:THR:H	7	0.17
(1,1609)	1:307:A:LEU:HD11	1:308:A:CYS:HA	11	0.17
(1,1609)	1:307:A:LEU:HD12	1:308:A:CYS:HA	11	0.17
(1,1609)	1:307:A:LEU:HD13	1:308:A:CYS:HA	11	0.17
(1,1609)	1:307:A:LEU:HD21	1:308:A:CYS:HA	11	0.17
(1,1609)	1:307:A:LEU:HD22	1:308:A:CYS:HA	11	0.17
(1,1609)	1:307:A:LEU:HD23	1:308:A:CYS:HA	11	0.17
(1,1609)	1:307:A:LEU:HD11	1:308:A:CYS:HA	16	0.17
(1,1609)	1:307:A:LEU:HD12	1:308:A:CYS:HA	16	0.17
(1,1609)	1:307:A:LEU:HD13	1:308:A:CYS:HA	16	0.17
(1,1609)	1:307:A:LEU:HD21	1:308:A:CYS:HA	16	0.17
(1,1609)	1:307:A:LEU:HD22	1:308:A:CYS:HA	16	0.17
(1,1609)	1:307:A:LEU:HD23	1:308:A:CYS:HA	16	0.17
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG2	14	0.17
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG3	14	0.17
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB1	9	0.17
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB2	9	0.17
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB3	9	0.17
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB1	9	0.17
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB2	9	0.17
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB3	9	0.17
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB1	9	0.17
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB2	9	0.17
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB3	9	0.17
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG2	12	0.17
(1,1404)	1:294:A:GLU:H	1:295:A:MET:HG3	12	0.17
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD1	13	0.17
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD2	13	0.17
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD1	2	0.17
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD2	2	0.17
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD1	6	0.17
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD2	6	0.17
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD1	11	0.17
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD2	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1315)	1:283:A:THR:H	1:311:A:THR:HB	20	0.17
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	7	0.17
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	7	0.17
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	7	0.17
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	8	0.17
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	8	0.17
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	8	0.17
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	9	0.17
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	9	0.17
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	9	0.17
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	12	0.17
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	12	0.17
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	12	0.17
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	13	0.17
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	13	0.17
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	13	0.17
(1,994)	1:266:A:ILE:HG21	1:266:A:ILE:H	16	0.17
(1,994)	1:266:A:ILE:HG22	1:266:A:ILE:H	16	0.17
(1,994)	1:266:A:ILE:HG23	1:266:A:ILE:H	16	0.17
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	17	0.17
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	17	0.17
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	17	0.17
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	18	0.17
(1,724)	1:248:A:HIS:HB3	1:248:A:HIS:HD1	16	0.17
(1,536)	1:231:A:THR:H	1:232:A:TRP:HE1	19	0.17
(1,491)	1:227:A:MET:HB2	1:228:A:HIS:H	17	0.17
(1,491)	1:227:A:MET:HB3	1:228:A:HIS:H	17	0.17
(1,490)	1:227:A:MET:HA	1:278:A:ARG:H	18	0.17
(1,76)	2:392:B:DA:H4'	1:250:A:HIS:HD2	6	0.17
(1,74)	2:390:B:C38:H2'1	1:257:A:HIS:HD2	12	0.17
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	12	0.17
(1,67)	2:389:B:DU:H2''	1:244:A:ASN:HB2	19	0.17
(1,49)	2:387:B:DT:H2''	1:315:A:TYR:HA	1	0.17
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	14	0.17
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	8	0.17
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	8	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	1	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	3	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	4	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	6	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	8	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	10	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	11	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	13	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	14	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	15	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	16	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	17	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	18	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	19	0.17
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	20	0.17
(1,2143)	1:347:A:TRP:HB2	1:347:A:TRP:HE1	4	0.16
(1,2143)	1:347:A:TRP:HB2	1:347:A:TRP:HE1	12	0.16
(1,2143)	1:347:A:TRP:HB2	1:347:A:TRP:HE1	20	0.16
(1,2051)	1:339:A:THR:HB	1:340:A:TYR:H	20	0.16
(1,1961)	1:334:A:LYS:HB2	1:334:A:LYS:H	2	0.16
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	20	0.16
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	20	0.16
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	20	0.16
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	20	0.16
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	20	0.16
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	20	0.16
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	2	0.16
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	2	0.16
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	2	0.16
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	2	0.16
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	2	0.16
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	2	0.16
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	3	0.16
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	3	0.16
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	3	0.16
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	3	0.16
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	3	0.16
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	3	0.16
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	9	0.16
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	9	0.16
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	9	0.16
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	9	0.16
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	9	0.16
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	9	0.16
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	13	0.16
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	13	0.16
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	13	0.16
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	13	0.16
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	13	0.16
(1,1859)	1:326:A:ARG:HB2	1:327:A:THR:H	3	0.16
(1,1609)	1:307:A:LEU:HD11	1:308:A:CYS:HA	4	0.16
(1,1609)	1:307:A:LEU:HD12	1:308:A:CYS:HA	4	0.16
(1,1609)	1:307:A:LEU:HD13	1:308:A:CYS:HA	4	0.16
(1,1609)	1:307:A:LEU:HD21	1:308:A:CYS:HA	4	0.16
(1,1609)	1:307:A:LEU:HD22	1:308:A:CYS:HA	4	0.16
(1,1609)	1:307:A:LEU:HD23	1:308:A:CYS:HA	4	0.16
(1,1609)	1:307:A:LEU:HD11	1:308:A:CYS:HA	5	0.16
(1,1609)	1:307:A:LEU:HD12	1:308:A:CYS:HA	5	0.16
(1,1609)	1:307:A:LEU:HD13	1:308:A:CYS:HA	5	0.16
(1,1609)	1:307:A:LEU:HD21	1:308:A:CYS:HA	5	0.16
(1,1609)	1:307:A:LEU:HD22	1:308:A:CYS:HA	5	0.16
(1,1609)	1:307:A:LEU:HD23	1:308:A:CYS:HA	5	0.16
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG2	3	0.16
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG3	3	0.16
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD1	9	0.16
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD2	9	0.16
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD1	19	0.16
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD2	19	0.16
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD1	20	0.16
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD2	20	0.16
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	15	0.16
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	15	0.16
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	15	0.16
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	16	0.16
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	16	0.16
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	16	0.16
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	19	0.16
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	19	0.16
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	19	0.16
(1,724)	1:248:A:HIS:HB3	1:248:A:HIS:HD1	20	0.16
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	6	0.16
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	6	0.16
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	6	0.16
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	8	0.16
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	10	0.16
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	12	0.16
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	14	0.16
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,489)	1:227:A:MET:HA	1:235:A:LEU:H	1	0.16
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	6	0.16
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	11	0.16
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	16	0.16
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG21	8	0.16
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG22	8	0.16
(1,110)	1:198:A:ASP:H	1:203:A:THR:HG23	8	0.16
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG21	2	0.16
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG22	2	0.16
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG23	2	0.16
(1,89)	2:394:B:DT:H5'	1:254:A:GLU:HG3	6	0.16
(1,89)	2:394:B:DT:H5''	1:254:A:GLU:HG3	6	0.16
(1,74)	2:390:B:C38:H2'1	1:257:A:HIS:HD2	20	0.16
(1,48)	2:387:B:DT:H1'	1:315:A:TYR:HA	18	0.16
(1,41)	2:385:B:DA:H8	1:374:A:ARG:H	3	0.16
(1,41)	2:385:B:DA:H8	1:374:A:ARG:H	16	0.16
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	11	0.16
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	3	0.16
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	3	0.16
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	1	0.15
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	1	0.15
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	3	0.15
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	3	0.15
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	19	0.15
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	19	0.15
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	6	0.15
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	6	0.15
(1,2143)	1:347:A:TRP:HB2	1:347:A:TRP:HE1	5	0.15
(1,2143)	1:347:A:TRP:HB2	1:347:A:TRP:HE1	7	0.15
(1,2143)	1:347:A:TRP:HB2	1:347:A:TRP:HE1	8	0.15
(1,2143)	1:347:A:TRP:HB2	1:347:A:TRP:HE1	10	0.15
(1,2122)	1:345:A:HIS:HA	1:348:A:ASP:H	14	0.15
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	6	0.15
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	6	0.15
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	6	0.15
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	6	0.15
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	6	0.15
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	6	0.15
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	1	0.15
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	1	0.15
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	1	0.15
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	1	0.15
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	1	0.15
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	6	0.15
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	6	0.15
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	6	0.15
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	6	0.15
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	6	0.15
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	6	0.15
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	7	0.15
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	7	0.15
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	7	0.15
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	7	0.15
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	7	0.15
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	7	0.15
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	12	0.15
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	12	0.15
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	12	0.15
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	12	0.15
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	12	0.15
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	12	0.15
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	15	0.15
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	15	0.15
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	15	0.15
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	15	0.15
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	15	0.15
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	15	0.15
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	16	0.15
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	16	0.15
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	16	0.15
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	16	0.15
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	16	0.15
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	16	0.15
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	17	0.15
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	17	0.15
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	17	0.15
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	17	0.15
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	17	0.15
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	17	0.15
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG21	2	0.15
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG22	2	0.15
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG23	2	0.15
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG21	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG22	2	0.15
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG23	2	0.15
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	6	0.15
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	6	0.15
(1,1609)	1:307:A:LEU:HD11	1:308:A:CYS:HA	3	0.15
(1,1609)	1:307:A:LEU:HD12	1:308:A:CYS:HA	3	0.15
(1,1609)	1:307:A:LEU:HD13	1:308:A:CYS:HA	3	0.15
(1,1609)	1:307:A:LEU:HD21	1:308:A:CYS:HA	3	0.15
(1,1609)	1:307:A:LEU:HD22	1:308:A:CYS:HA	3	0.15
(1,1609)	1:307:A:LEU:HD23	1:308:A:CYS:HA	3	0.15
(1,1554)	1:303:A:LYS:HB2	1:303:A:LYS:HE2	14	0.15
(1,1554)	1:303:A:LYS:HB2	1:303:A:LYS:HE3	14	0.15
(1,1554)	1:303:A:LYS:HB3	1:303:A:LYS:HE2	14	0.15
(1,1554)	1:303:A:LYS:HB3	1:303:A:LYS:HE3	14	0.15
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG2	2	0.15
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG3	2	0.15
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG2	5	0.15
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG3	5	0.15
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG2	7	0.15
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG3	7	0.15
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG2	15	0.15
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG3	15	0.15
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG2	17	0.15
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG3	17	0.15
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG2	19	0.15
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG3	19	0.15
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB1	11	0.15
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB2	11	0.15
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB3	11	0.15
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB1	11	0.15
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB2	11	0.15
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB3	11	0.15
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB1	11	0.15
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB2	11	0.15
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB3	11	0.15
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD1	14	0.15
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD2	14	0.15
(1,817)	1:257:A:HIS:HD2	1:257:A:HIS:H	6	0.15
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	5	0.15
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	5	0.15
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	5	0.15
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	15	0.15
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	15	0.15
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	17	0.15
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	17	0.15
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	17	0.15
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	1	0.15
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	3	0.15
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	4	0.15
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	6	0.15
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	7	0.15
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	9	0.15
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	11	0.15
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	15	0.15
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	16	0.15
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	17	0.15
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	18	0.15
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	20	0.15
(1,581)	1:235:A:LEU:HD11	1:235:A:LEU:H	4	0.15
(1,581)	1:235:A:LEU:HD12	1:235:A:LEU:H	4	0.15
(1,581)	1:235:A:LEU:HD13	1:235:A:LEU:H	4	0.15
(1,581)	1:235:A:LEU:HD21	1:235:A:LEU:H	4	0.15
(1,581)	1:235:A:LEU:HD22	1:235:A:LEU:H	4	0.15
(1,581)	1:235:A:LEU:HD23	1:235:A:LEU:H	4	0.15
(1,581)	1:235:A:LEU:HD11	1:235:A:LEU:H	17	0.15
(1,581)	1:235:A:LEU:HD12	1:235:A:LEU:H	17	0.15
(1,581)	1:235:A:LEU:HD13	1:235:A:LEU:H	17	0.15
(1,581)	1:235:A:LEU:HD21	1:235:A:LEU:H	17	0.15
(1,581)	1:235:A:LEU:HD22	1:235:A:LEU:H	17	0.15
(1,581)	1:235:A:LEU:HD23	1:235:A:LEU:H	17	0.15
(1,536)	1:231:A:THR:H	1:232:A:TRP:HE1	17	0.15
(1,446)	1:225:A:GLU:H	1:278:A:ARG:H	11	0.15
(1,272)	1:211:A:TRP:HE1	1:284:A:SER:HB2	14	0.15
(1,272)	1:211:A:TRP:HE1	1:284:A:SER:HB3	14	0.15
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	3	0.15
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	7	0.15
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	10	0.15
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	13	0.15
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	20	0.15
(1,109)	1:198:A:ASP:H	1:202:A:PHE:HD1	17	0.15
(1,109)	1:198:A:ASP:H	1:202:A:PHE:HD2	17	0.15
(1,90)	2:394:B:DT:H5'	1:254:A:GLU:HG2	17	0.15
(1,90)	2:394:B:DT:H5''	1:254:A:GLU:HG2	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	2:392:B:DA:H4'	1:250:A:HIS:HD2	7	0.15
(1,74)	2:390:B:C38:H2'1	1:257:A:HIS:HD2	3	0.15
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	8	0.15
(1,67)	2:389:B:DU:H2''	1:244:A:ASN:HB2	13	0.15
(1,67)	2:389:B:DU:H2''	1:244:A:ASN:HB2	14	0.15
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	8	0.15
(1,54)	2:388:B:DC:H2''	1:285:A:TRP:HE1	5	0.15
(1,54)	2:388:B:DC:H2''	1:285:A:TRP:HE1	17	0.15
(1,49)	2:387:B:DT:H2''	1:315:A:TYR:HA	10	0.15
(1,41)	2:385:B:DA:H8	1:374:A:ARG:H	5	0.15
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	20	0.15
(1,2645)	1:380:A:GLN:HB2	1:380:A:GLN:HE22	16	0.14
(1,2645)	1:380:A:GLN:HB3	1:380:A:GLN:HE22	16	0.14
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	11	0.14
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	11	0.14
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	18	0.14
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	18	0.14
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	20	0.14
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	20	0.14
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	3	0.14
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	3	0.14
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	7	0.14
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	7	0.14
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	8	0.14
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	8	0.14
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	11	0.14
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	11	0.14
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	15	0.14
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	15	0.14
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	16	0.14
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	16	0.14
(1,2215)	1:351:A:VAL:HG11	1:353:A:HIS:HD2	8	0.14
(1,2215)	1:351:A:VAL:HG12	1:353:A:HIS:HD2	8	0.14
(1,2215)	1:351:A:VAL:HG13	1:353:A:HIS:HD2	8	0.14
(1,2215)	1:351:A:VAL:HG21	1:353:A:HIS:HD2	8	0.14
(1,2215)	1:351:A:VAL:HG22	1:353:A:HIS:HD2	8	0.14
(1,2215)	1:351:A:VAL:HG23	1:353:A:HIS:HD2	8	0.14
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	2	0.14
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	2	0.14
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	2	0.14
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	2	0.14
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	2	0.14
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	8	0.14
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	8	0.14
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	8	0.14
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	8	0.14
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	8	0.14
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	8	0.14
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	11	0.14
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	11	0.14
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	11	0.14
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	11	0.14
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	11	0.14
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	11	0.14
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	4	0.14
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	4	0.14
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	4	0.14
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	4	0.14
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	4	0.14
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	4	0.14
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	5	0.14
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	5	0.14
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	5	0.14
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	5	0.14
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	5	0.14
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	5	0.14
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	10	0.14
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	10	0.14
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	10	0.14
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	10	0.14
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	10	0.14
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	10	0.14
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	11	0.14
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	11	0.14
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	11	0.14
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	11	0.14
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	11	0.14
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	11	0.14
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	14	0.14
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	14	0.14
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	14	0.14
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	14	0.14
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	14	0.14
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	18	0.14
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	18	0.14
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	18	0.14
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	18	0.14
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	18	0.14
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	18	0.14
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	19	0.14
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	19	0.14
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	19	0.14
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	19	0.14
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	19	0.14
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	19	0.14
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	20	0.14
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	20	0.14
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	20	0.14
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	20	0.14
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	20	0.14
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	20	0.14
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG2	18	0.14
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG3	18	0.14
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD1	7	0.14
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD2	7	0.14
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD1	14	0.14
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD2	14	0.14
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD1	15	0.14
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD2	15	0.14
(1,1247)	1:280:A:THR:HG21	1:308:A:CYS:H	20	0.14
(1,1247)	1:280:A:THR:HG22	1:308:A:CYS:H	20	0.14
(1,1247)	1:280:A:THR:HG23	1:308:A:CYS:H	20	0.14
(1,1168)	1:277:A:TYR:HA	1:306:A:SER:H	12	0.14
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	3	0.14
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	3	0.14
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	4	0.14
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	4	0.14
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	5	0.14
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	5	0.14
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	11	0.14
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	11	0.14
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	12	0.14
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	12	0.14
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	14	0.14
(1,877)	1:260:A:LEU:HD11	1:294:A:GLU:H	14	0.14
(1,877)	1:260:A:LEU:HD12	1:294:A:GLU:H	14	0.14
(1,877)	1:260:A:LEU:HD13	1:294:A:GLU:H	14	0.14
(1,877)	1:260:A:LEU:HD21	1:294:A:GLU:H	14	0.14
(1,877)	1:260:A:LEU:HD22	1:294:A:GLU:H	14	0.14
(1,877)	1:260:A:LEU:HD23	1:294:A:GLU:H	14	0.14
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	1	0.14
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	1	0.14
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	1	0.14
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	1	0.14
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	1	0.14
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	1	0.14
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	8	0.14
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	8	0.14
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	8	0.14
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	12	0.14
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	12	0.14
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	12	0.14
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	18	0.14
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	18	0.14
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	18	0.14
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	2	0.14
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	5	0.14
(1,685)	1:244:A:ASN:HB2	1:244:A:ASN:H	13	0.14
(1,581)	1:235:A:LEU:HD11	1:235:A:LEU:H	19	0.14
(1,581)	1:235:A:LEU:HD12	1:235:A:LEU:H	19	0.14
(1,581)	1:235:A:LEU:HD13	1:235:A:LEU:H	19	0.14
(1,581)	1:235:A:LEU:HD21	1:235:A:LEU:H	19	0.14
(1,581)	1:235:A:LEU:HD22	1:235:A:LEU:H	19	0.14
(1,581)	1:235:A:LEU:HD23	1:235:A:LEU:H	19	0.14
(1,560)	1:234:A:LEU:HA	1:234:A:LEU:HG	9	0.14
(1,446)	1:225:A:GLU:H	1:278:A:ARG:H	14	0.14
(1,445)	1:225:A:GLU:H	1:277:A:TYR:HE1	18	0.14
(1,445)	1:225:A:GLU:H	1:277:A:TYR:HE2	18	0.14
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB2	5	0.14
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB3	5	0.14
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB2	5	0.14
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB3	5	0.14
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	2	0.14
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	4	0.14
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	9	0.14
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	14	0.14
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	18	0.14
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	19	0.14
(1,169)	1:203:A:THR:HB	1:204:A:PHE:H	16	0.14
(1,122)	1:200:A:PRO:HA	1:353:A:HIS:H	7	0.14
(1,109)	1:198:A:ASP:H	1:202:A:PHE:HD1	16	0.14
(1,109)	1:198:A:ASP:H	1:202:A:PHE:HD2	16	0.14
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG21	3	0.14
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG22	3	0.14
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG23	3	0.14
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG21	9	0.14
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG22	9	0.14
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG23	9	0.14
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG21	12	0.14
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG22	12	0.14
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG23	12	0.14
(1,97)	1:197:A:MET:HA	1:352:A:ASP:H	7	0.14
(1,74)	2:390:B:C38:H2'1	1:257:A:HIS:HD2	11	0.14
(1,74)	2:390:B:C38:H2'1	1:257:A:HIS:HD2	14	0.14
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	13	0.14
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	18	0.14
(1,54)	2:388:B:DC:H2''	1:285:A:TRP:HE1	9	0.14
(1,49)	2:387:B:DT:H2''	1:315:A:TYR:HA	7	0.14
(1,41)	2:385:B:DA:H8	1:374:A:ARG:H	7	0.14
(1,41)	2:385:B:DA:H8	1:374:A:ARG:H	19	0.14
(1,20)	2:388:B:DC:H2'	2:388:B:DC:H6	1	0.14
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	1	0.13
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	2	0.13
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	4	0.13
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	6	0.13
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	7	0.13
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	10	0.13
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	11	0.13
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	12	0.13
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	15	0.13
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	16	0.13
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	18	0.13
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	19	0.13
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	20	0.13
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	8	0.13
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2645)	1:380:A:GLN:HB2	1:380:A:GLN:HE22	1	0.13
(1,2645)	1:380:A:GLN:HB3	1:380:A:GLN:HE22	1	0.13
(1,2626)	1:379:A:LEU:HA	1:379:A:LEU:HG	1	0.13
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	4	0.13
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	4	0.13
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	9	0.13
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	9	0.13
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	10	0.13
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	10	0.13
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	15	0.13
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	15	0.13
(1,2428)	1:367:A:HIS:HD2	1:367:A:HIS:H	9	0.13
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	17	0.13
(1,2215)	1:351:A:VAL:HG11	1:353:A:HIS:HD2	10	0.13
(1,2215)	1:351:A:VAL:HG12	1:353:A:HIS:HD2	10	0.13
(1,2215)	1:351:A:VAL:HG13	1:353:A:HIS:HD2	10	0.13
(1,2215)	1:351:A:VAL:HG21	1:353:A:HIS:HD2	10	0.13
(1,2215)	1:351:A:VAL:HG22	1:353:A:HIS:HD2	10	0.13
(1,2215)	1:351:A:VAL:HG23	1:353:A:HIS:HD2	10	0.13
(1,2143)	1:347:A:TRP:HB2	1:347:A:TRP:HE1	19	0.13
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	1	0.13
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	1	0.13
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	1	0.13
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	1	0.13
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	1	0.13
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	1	0.13
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	5	0.13
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	5	0.13
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	5	0.13
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	5	0.13
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	5	0.13
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	5	0.13
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	10	0.13
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	10	0.13
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	10	0.13
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	10	0.13
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	10	0.13
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	10	0.13
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	12	0.13
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	12	0.13
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	12	0.13
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	12	0.13
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	12	0.13
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	14	0.13
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	14	0.13
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	14	0.13
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	14	0.13
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	14	0.13
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	14	0.13
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	15	0.13
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	15	0.13
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	15	0.13
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	15	0.13
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	15	0.13
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	15	0.13
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	18	0.13
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	18	0.13
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	18	0.13
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	18	0.13
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	18	0.13
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	18	0.13
(1,1888)	1:328:A:LEU:HD11	1:328:A:LEU:H	8	0.13
(1,1888)	1:328:A:LEU:HD12	1:328:A:LEU:H	8	0.13
(1,1888)	1:328:A:LEU:HD13	1:328:A:LEU:H	8	0.13
(1,1888)	1:328:A:LEU:HD21	1:328:A:LEU:H	8	0.13
(1,1888)	1:328:A:LEU:HD22	1:328:A:LEU:H	8	0.13
(1,1888)	1:328:A:LEU:HD23	1:328:A:LEU:H	8	0.13
(1,1859)	1:326:A:ARG:HB2	1:327:A:THR:H	1	0.13
(1,1859)	1:326:A:ARG:HB2	1:327:A:THR:H	4	0.13
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG21	6	0.13
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG22	6	0.13
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG23	6	0.13
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG21	6	0.13
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG22	6	0.13
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG23	6	0.13
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG21	11	0.13
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG22	11	0.13
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG23	11	0.13
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG21	11	0.13
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG22	11	0.13
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG23	11	0.13
(1,1715)	1:311:A:THR:H	1:335:A:ILE:HG12	15	0.13
(1,1715)	1:311:A:THR:H	1:335:A:ILE:HG13	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	12	0.13
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	12	0.13
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD2	3	0.13
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD3	3	0.13
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD2	11	0.13
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD3	11	0.13
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD2	16	0.13
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD3	16	0.13
(1,1554)	1:303:A:LYS:HB2	1:303:A:LYS:HE2	8	0.13
(1,1554)	1:303:A:LYS:HB2	1:303:A:LYS:HE3	8	0.13
(1,1554)	1:303:A:LYS:HB3	1:303:A:LYS:HE2	8	0.13
(1,1554)	1:303:A:LYS:HB3	1:303:A:LYS:HE3	8	0.13
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB1	6	0.13
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB2	6	0.13
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB3	6	0.13
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB1	6	0.13
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB2	6	0.13
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB3	6	0.13
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB1	6	0.13
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB2	6	0.13
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB3	6	0.13
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD1	2	0.13
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD2	2	0.13
(1,1340)	1:285:A:TRP:HZ3	1:316:A:ASP:H	10	0.13
(1,1247)	1:280:A:THR:HG21	1:308:A:CYS:H	10	0.13
(1,1247)	1:280:A:THR:HG22	1:308:A:CYS:H	10	0.13
(1,1247)	1:280:A:THR:HG23	1:308:A:CYS:H	10	0.13
(1,1209)	1:279:A:VAL:HB	1:307:A:LEU:HA	18	0.13
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	6	0.13
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	6	0.13
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	9	0.13
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	9	0.13
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	18	0.13
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	18	0.13
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	19	0.13
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	19	0.13
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	4	0.13
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	5	0.13
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	8	0.13
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	9	0.13
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	20	0.13
(1,766)	1:252:A:PHE:HA	1:252:A:PHE:HB3	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,766)	1:252:A:PHE:HA	1:252:A:PHE:HB3	4	0.13
(1,766)	1:252:A:PHE:HA	1:252:A:PHE:HB3	12	0.13
(1,766)	1:252:A:PHE:HA	1:252:A:PHE:HB3	14	0.13
(1,766)	1:252:A:PHE:HA	1:252:A:PHE:HB3	16	0.13
(1,766)	1:252:A:PHE:HA	1:252:A:PHE:HB3	18	0.13
(1,766)	1:252:A:PHE:HA	1:252:A:PHE:HB3	20	0.13
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	6	0.13
(1,733)	1:248:A:HIS:HB2	1:249:A:LYS:H	10	0.13
(1,718)	1:247:A:PRO:HG2	1:248:A:HIS:HD1	3	0.13
(1,718)	1:247:A:PRO:HG3	1:248:A:HIS:HD1	3	0.13
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	4	0.13
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	4	0.13
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	4	0.13
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	16	0.13
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	16	0.13
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	16	0.13
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	19	0.13
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	19	0.13
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	19	0.13
(1,536)	1:231:A:THR:H	1:232:A:TRP:HE1	13	0.13
(1,489)	1:227:A:MET:HA	1:235:A:LEU:H	13	0.13
(1,436)	1:225:A:GLU:HB2	1:278:A:ARG:HG2	12	0.13
(1,436)	1:225:A:GLU:HB2	1:278:A:ARG:HG3	12	0.13
(1,436)	1:225:A:GLU:HB3	1:278:A:ARG:HG2	12	0.13
(1,436)	1:225:A:GLU:HB3	1:278:A:ARG:HG3	12	0.13
(1,434)	1:225:A:GLU:HB2	1:232:A:TRP:HB2	13	0.13
(1,434)	1:225:A:GLU:HB2	1:232:A:TRP:HB3	13	0.13
(1,434)	1:225:A:GLU:HB3	1:232:A:TRP:HB2	13	0.13
(1,434)	1:225:A:GLU:HB3	1:232:A:TRP:HB3	13	0.13
(1,259)	1:210:A:PRO:HB2	1:211:A:TRP:HZ3	14	0.13
(1,259)	1:210:A:PRO:HB3	1:211:A:TRP:HZ3	14	0.13
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB2	12	0.13
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB3	12	0.13
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB2	12	0.13
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB3	12	0.13
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB2	19	0.13
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB3	19	0.13
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB2	19	0.13
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB3	19	0.13
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB2	20	0.13
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB3	20	0.13
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB2	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB3	20	0.13
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	1	0.13
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	5	0.13
(1,169)	1:203:A:THR:HB	1:204:A:PHE:H	1	0.13
(1,109)	1:198:A:ASP:H	1:202:A:PHE:HD1	7	0.13
(1,109)	1:198:A:ASP:H	1:202:A:PHE:HD2	7	0.13
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG21	1	0.13
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG22	1	0.13
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG23	1	0.13
(1,96)	1:197:A:MET:HA	1:201:A:THR:H	20	0.13
(1,77)	2:392:B:DA:H8	1:252:A:PHE:HD2	2	0.13
(1,74)	2:390:B:C38:H2'1	1:257:A:HIS:HD2	9	0.13
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	3	0.13
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB1	9	0.13
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB2	9	0.13
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB3	9	0.13
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB1	13	0.13
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB2	13	0.13
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB3	13	0.13
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB1	14	0.13
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB2	14	0.13
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB3	14	0.13
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	11	0.13
(1,49)	2:387:B:DT:H2''	1:315:A:TYR:HA	3	0.13
(1,41)	2:385:B:DA:H8	1:374:A:ARG:H	11	0.13
(1,41)	2:385:B:DA:H8	1:374:A:ARG:H	20	0.13
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	14	0.13
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	14	0.13
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	19	0.13
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	19	0.13
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	2	0.13
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	5	0.13
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	12	0.13
(1,2696)	1:384:A:ASN:HA	1:384:A:ASN:HB2	2	0.12
(1,2696)	1:384:A:ASN:HA	1:384:A:ASN:HB2	14	0.12
(1,2679)	1:382:A:GLN:HB2	1:382:A:GLN:H	14	0.12
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	3	0.12
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	8	0.12
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	9	0.12
(1,2674)	1:382:A:GLN:HA	1:382:A:GLN:HB3	13	0.12
(1,2669)	1:381:A:ASN:HA	1:384:A:ASN:H	2	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	2	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	3	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	4	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	5	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	6	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	7	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	9	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	10	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	12	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	13	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	15	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	16	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	17	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	19	0.12
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	20	0.12
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	2	0.12
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	2	0.12
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	6	0.12
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	6	0.12
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	12	0.12
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	12	0.12
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	13	0.12
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	13	0.12
(1,2479)	1:371:A:LEU:HA	1:371:A:LEU:HG	4	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	1	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	2	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	3	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	4	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	5	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	6	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	7	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	8	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	9	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	10	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	11	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	12	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	13	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	14	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	15	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	16	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	17	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	19	0.12
(1,2467)	1:370:A:ASP:HA	1:370:A:ASP:HB2	20	0.12
(1,2397)	1:366:A:GLU:HA	1:366:A:GLU:HB2	2	0.12
(1,2397)	1:366:A:GLU:HA	1:366:A:GLU:HB2	4	0.12
(1,2397)	1:366:A:GLU:HA	1:366:A:GLU:HB2	5	0.12
(1,2397)	1:366:A:GLU:HA	1:366:A:GLU:HB2	9	0.12
(1,2397)	1:366:A:GLU:HA	1:366:A:GLU:HB2	11	0.12
(1,2397)	1:366:A:GLU:HA	1:366:A:GLU:HB2	14	0.12
(1,2397)	1:366:A:GLU:HA	1:366:A:GLU:HB2	16	0.12
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	1	0.12
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	3	0.12
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	6	0.12
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	7	0.12
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	8	0.12
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	10	0.12
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	12	0.12
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	13	0.12
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	15	0.12
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	18	0.12
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	19	0.12
(1,2396)	1:366:A:GLU:HA	1:366:A:GLU:HB3	20	0.12
(1,2160)	1:347:A:TRP:HE1	1:357:A:PRO:HA	7	0.12
(1,2122)	1:345:A:HIS:HA	1:348:A:ASP:H	16	0.12
(1,2122)	1:345:A:HIS:HA	1:348:A:ASP:H	18	0.12
(1,1993)	1:336:A:SER:HA	1:336:A:SER:HB2	4	0.12
(1,1993)	1:336:A:SER:HA	1:336:A:SER:HB2	10	0.12
(1,1993)	1:336:A:SER:HA	1:336:A:SER:HB2	11	0.12
(1,1993)	1:336:A:SER:HA	1:336:A:SER:HB2	12	0.12
(1,1993)	1:336:A:SER:HA	1:336:A:SER:HB2	13	0.12
(1,1993)	1:336:A:SER:HA	1:336:A:SER:HB2	15	0.12
(1,1993)	1:336:A:SER:HA	1:336:A:SER:HB2	17	0.12
(1,1993)	1:336:A:SER:HA	1:336:A:SER:HB2	18	0.12
(1,1993)	1:336:A:SER:HA	1:336:A:SER:HB2	19	0.12
(1,1993)	1:336:A:SER:HA	1:336:A:SER:HB2	20	0.12
(1,1991)	1:335:A:ILE:H	1:379:A:LEU:HD11	16	0.12
(1,1991)	1:335:A:ILE:H	1:379:A:LEU:HD12	16	0.12
(1,1991)	1:335:A:ILE:H	1:379:A:LEU:HD13	16	0.12
(1,1991)	1:335:A:ILE:H	1:379:A:LEU:HD21	16	0.12
(1,1991)	1:335:A:ILE:H	1:379:A:LEU:HD22	16	0.12
(1,1991)	1:335:A:ILE:H	1:379:A:LEU:HD23	16	0.12
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	3	0.12
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	3	0.12
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	3	0.12
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	3	0.12
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	3	0.12
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	4	0.12
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	4	0.12
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	4	0.12
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	4	0.12
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	4	0.12
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	4	0.12
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	7	0.12
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	7	0.12
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	7	0.12
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	7	0.12
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	7	0.12
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	7	0.12
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	9	0.12
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	9	0.12
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	9	0.12
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	9	0.12
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	9	0.12
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	9	0.12
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	16	0.12
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	16	0.12
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	16	0.12
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	16	0.12
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	16	0.12
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	16	0.12
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	17	0.12
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	17	0.12
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	17	0.12
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	17	0.12
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	17	0.12
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	17	0.12
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	19	0.12
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	19	0.12
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	19	0.12
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	19	0.12
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	19	0.12
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	19	0.12
(1,1842)	1:326:A:ARG:HA	1:326:A:ARG:HB3	3	0.12
(1,1842)	1:326:A:ARG:HA	1:326:A:ARG:HB3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1795)	1:323:A:GLU:HA	1:323:A:GLU:HB2	1	0.12
(1,1795)	1:323:A:GLU:HA	1:323:A:GLU:HB2	5	0.12
(1,1795)	1:323:A:GLU:HA	1:323:A:GLU:HB2	6	0.12
(1,1795)	1:323:A:GLU:HA	1:323:A:GLU:HB2	12	0.12
(1,1795)	1:323:A:GLU:HA	1:323:A:GLU:HB2	13	0.12
(1,1795)	1:323:A:GLU:HA	1:323:A:GLU:HB2	16	0.12
(1,1795)	1:323:A:GLU:HA	1:323:A:GLU:HB2	18	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	2	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	3	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	4	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	7	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	8	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	9	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	10	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	11	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	14	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	15	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	17	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	19	0.12
(1,1794)	1:323:A:GLU:HA	1:323:A:GLU:HB3	20	0.12
(1,1754)	1:314:A:ILE:HD11	1:314:A:ILE:H	1	0.12
(1,1754)	1:314:A:ILE:HD12	1:314:A:ILE:H	1	0.12
(1,1754)	1:314:A:ILE:HD13	1:314:A:ILE:H	1	0.12
(1,1754)	1:314:A:ILE:HD11	1:314:A:ILE:H	6	0.12
(1,1754)	1:314:A:ILE:HD12	1:314:A:ILE:H	6	0.12
(1,1754)	1:314:A:ILE:HD13	1:314:A:ILE:H	6	0.12
(1,1754)	1:314:A:ILE:HD11	1:314:A:ILE:H	9	0.12
(1,1754)	1:314:A:ILE:HD12	1:314:A:ILE:H	9	0.12
(1,1754)	1:314:A:ILE:HD13	1:314:A:ILE:H	9	0.12
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG21	5	0.12
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG22	5	0.12
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG23	5	0.12
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG21	5	0.12
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG22	5	0.12
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG23	5	0.12
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG21	8	0.12
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG22	8	0.12
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG23	8	0.12
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG21	8	0.12
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG22	8	0.12
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG23	8	0.12
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG21	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG22	13	0.12
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG23	13	0.12
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG21	13	0.12
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG22	13	0.12
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG23	13	0.12
(1,1715)	1:311:A:THR:H	1:335:A:ILE:HG12	7	0.12
(1,1715)	1:311:A:THR:H	1:335:A:ILE:HG13	7	0.12
(1,1706)	1:311:A:THR:HB	1:337:A:ILE:HD11	20	0.12
(1,1706)	1:311:A:THR:HB	1:337:A:ILE:HD12	20	0.12
(1,1706)	1:311:A:THR:HB	1:337:A:ILE:HD13	20	0.12
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	5	0.12
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	5	0.12
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	20	0.12
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	20	0.12
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD2	5	0.12
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD3	5	0.12
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD2	13	0.12
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD3	13	0.12
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD2	15	0.12
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD3	15	0.12
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD2	19	0.12
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD3	19	0.12
(1,1609)	1:307:A:LEU:HD11	1:308:A:CYS:HA	18	0.12
(1,1609)	1:307:A:LEU:HD12	1:308:A:CYS:HA	18	0.12
(1,1609)	1:307:A:LEU:HD13	1:308:A:CYS:HA	18	0.12
(1,1609)	1:307:A:LEU:HD21	1:308:A:CYS:HA	18	0.12
(1,1609)	1:307:A:LEU:HD22	1:308:A:CYS:HA	18	0.12
(1,1609)	1:307:A:LEU:HD23	1:308:A:CYS:HA	18	0.12
(1,1609)	1:307:A:LEU:HD11	1:308:A:CYS:HA	20	0.12
(1,1609)	1:307:A:LEU:HD12	1:308:A:CYS:HA	20	0.12
(1,1609)	1:307:A:LEU:HD13	1:308:A:CYS:HA	20	0.12
(1,1609)	1:307:A:LEU:HD21	1:308:A:CYS:HA	20	0.12
(1,1609)	1:307:A:LEU:HD22	1:308:A:CYS:HA	20	0.12
(1,1609)	1:307:A:LEU:HD23	1:308:A:CYS:HA	20	0.12
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG2	20	0.12
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG3	20	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	2	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	3	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	4	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	5	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	6	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	9	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	10	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	11	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	12	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	15	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	16	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	17	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	18	0.12
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	20	0.12
(1,1510)	1:301:A:LYS:HB3	1:301:A:LYS:HG2	14	0.12
(1,1510)	1:301:A:LYS:HB3	1:301:A:LYS:HG2	19	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	2	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	3	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	4	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	5	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	6	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	7	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	8	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	9	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	10	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	12	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	15	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	16	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	17	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	18	0.12
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	20	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	1	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	2	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	3	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	4	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	5	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	6	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	7	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	8	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	9	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	10	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	11	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	12	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	13	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	14	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	15	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	17	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	18	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	19	0.12
(1,1503)	1:301:A:LYS:HA	1:301:A:LYS:HB2	20	0.12
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB1	20	0.12
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB2	20	0.12
(1,1483)	1:299:A:ILE:HD11	1:331:A:ALA:HB3	20	0.12
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB1	20	0.12
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB2	20	0.12
(1,1483)	1:299:A:ILE:HD12	1:331:A:ALA:HB3	20	0.12
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB1	20	0.12
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB2	20	0.12
(1,1483)	1:299:A:ILE:HD13	1:331:A:ALA:HB3	20	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	1	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	2	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	3	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	4	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	5	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	6	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	7	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	8	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	9	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	10	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	11	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	12	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	13	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	14	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	15	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	16	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	17	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	18	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	19	0.12
(1,1453)	1:299:A:ILE:HA	1:299:A:ILE:HB	20	0.12
(1,1431)	1:296:A:ALA:HB1	1:328:A:LEU:HA	1	0.12
(1,1431)	1:296:A:ALA:HB2	1:328:A:LEU:HA	1	0.12
(1,1431)	1:296:A:ALA:HB3	1:328:A:LEU:HA	1	0.12
(1,1379)	1:292:A:ALA:HA	1:324:A:GLY:HA2	7	0.12
(1,1379)	1:292:A:ALA:HA	1:324:A:GLY:HA3	7	0.12
(1,1379)	1:292:A:ALA:HA	1:324:A:GLY:HA2	9	0.12
(1,1379)	1:292:A:ALA:HA	1:324:A:GLY:HA3	9	0.12
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD1	1	0.12
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1283)	1:282:A:PHE:HA	1:346:A:CYS:HG	9	0.12
(1,1214)	1:279:A:VAL:HG21	1:280:A:THR:H	5	0.12
(1,1214)	1:279:A:VAL:HG22	1:280:A:THR:H	5	0.12
(1,1214)	1:279:A:VAL:HG23	1:280:A:THR:H	5	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	1	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	3	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	5	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	6	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	8	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	9	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	10	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	11	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	12	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	13	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	14	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	15	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	16	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	17	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	18	0.12
(1,1154)	1:276:A:ASP:HA	1:276:A:ASP:HB2	19	0.12
(1,1153)	1:276:A:ASP:HA	1:276:A:ASP:HB3	2	0.12
(1,1153)	1:276:A:ASP:HA	1:276:A:ASP:HB3	4	0.12
(1,1153)	1:276:A:ASP:HA	1:276:A:ASP:HB3	7	0.12
(1,1153)	1:276:A:ASP:HA	1:276:A:ASP:HB3	20	0.12
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	1	0.12
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	1	0.12
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	2	0.12
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	2	0.12
(1,1112)	1:273:A:LEU:HB2	1:273:A:LEU:HG	16	0.12
(1,947)	1:263:A:LEU:HD11	1:298:A:PHE:H	12	0.12
(1,947)	1:263:A:LEU:HD12	1:298:A:PHE:H	12	0.12
(1,947)	1:263:A:LEU:HD13	1:298:A:PHE:H	12	0.12
(1,947)	1:263:A:LEU:HD21	1:298:A:PHE:H	12	0.12
(1,947)	1:263:A:LEU:HD22	1:298:A:PHE:H	12	0.12
(1,947)	1:263:A:LEU:HD23	1:298:A:PHE:H	12	0.12
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	10	0.12
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	10	0.12
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	10	0.12
(1,796)	1:256:A:ARG:HA	1:256:A:ARG:HB2	10	0.12
(1,796)	1:256:A:ARG:HA	1:256:A:ARG:HB2	13	0.12
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	1	0.12
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	3	0.12
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	6	0.12
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	7	0.12
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	11	0.12
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	12	0.12
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	14	0.12
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	15	0.12
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	16	0.12
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	17	0.12
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	18	0.12
(1,795)	1:256:A:ARG:HA	1:256:A:ARG:HB3	19	0.12
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	10	0.12
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	14	0.12
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	16	0.12
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	20	0.12
(1,766)	1:252:A:PHE:HA	1:252:A:PHE:HB3	7	0.12
(1,766)	1:252:A:PHE:HA	1:252:A:PHE:HB3	10	0.12
(1,766)	1:252:A:PHE:HA	1:252:A:PHE:HB3	13	0.12
(1,766)	1:252:A:PHE:HA	1:252:A:PHE:HB3	15	0.12
(1,766)	1:252:A:PHE:HA	1:252:A:PHE:HB3	17	0.12
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	9	0.12
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	9	0.12
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	9	0.12
(1,581)	1:235:A:LEU:HD11	1:235:A:LEU:H	6	0.12
(1,581)	1:235:A:LEU:HD12	1:235:A:LEU:H	6	0.12
(1,581)	1:235:A:LEU:HD13	1:235:A:LEU:H	6	0.12
(1,581)	1:235:A:LEU:HD21	1:235:A:LEU:H	6	0.12
(1,581)	1:235:A:LEU:HD22	1:235:A:LEU:H	6	0.12
(1,581)	1:235:A:LEU:HD23	1:235:A:LEU:H	6	0.12
(1,581)	1:235:A:LEU:HD11	1:235:A:LEU:H	12	0.12
(1,581)	1:235:A:LEU:HD12	1:235:A:LEU:H	12	0.12
(1,581)	1:235:A:LEU:HD13	1:235:A:LEU:H	12	0.12
(1,581)	1:235:A:LEU:HD21	1:235:A:LEU:H	12	0.12
(1,581)	1:235:A:LEU:HD22	1:235:A:LEU:H	12	0.12
(1,581)	1:235:A:LEU:HD23	1:235:A:LEU:H	12	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	1	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	2	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	3	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	5	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	6	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	8	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	10	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	12	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	14	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	15	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	16	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	18	0.12
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	20	0.12
(1,536)	1:231:A:THR:H	1:232:A:TRP:HE1	9	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	1	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	2	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	4	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	5	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	7	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	9	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	10	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	11	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	12	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	13	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	16	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	17	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	18	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	19	0.12
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	20	0.12
(1,489)	1:227:A:MET:HA	1:235:A:LEU:H	7	0.12
(1,446)	1:225:A:GLU:H	1:278:A:ARG:H	3	0.12
(1,436)	1:225:A:GLU:HB2	1:278:A:ARG:HG2	18	0.12
(1,436)	1:225:A:GLU:HB2	1:278:A:ARG:HG3	18	0.12
(1,436)	1:225:A:GLU:HB3	1:278:A:ARG:HG2	18	0.12
(1,436)	1:225:A:GLU:HB3	1:278:A:ARG:HG3	18	0.12
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB2	15	0.12
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB3	15	0.12
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB2	15	0.12
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB3	15	0.12
(1,194)	1:204:A:PHE:HB2	1:205:A:ASN:H	12	0.12
(1,150)	1:202:A:PHE:HA	1:351:A:VAL:HG11	19	0.12
(1,150)	1:202:A:PHE:HA	1:351:A:VAL:HG12	19	0.12
(1,150)	1:202:A:PHE:HA	1:351:A:VAL:HG13	19	0.12
(1,122)	1:200:A:PRO:HA	1:353:A:HIS:H	17	0.12
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG21	4	0.12
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG22	4	0.12
(1,104)	1:198:A:ASP:HA	1:201:A:THR:HG23	4	0.12
(1,97)	1:197:A:MET:HA	1:352:A:ASP:H	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:197:A:MET:HA	1:352:A:ASP:H	17	0.12
(1,78)	2:392:B:DA:H1'	1:254:A:GLU:HG2	17	0.12
(1,78)	2:392:B:DA:H1'	1:254:A:GLU:HG3	17	0.12
(1,77)	2:392:B:DA:H8	1:252:A:PHE:HD2	1	0.12
(1,77)	2:392:B:DA:H8	1:252:A:PHE:HD2	5	0.12
(1,77)	2:392:B:DA:H8	1:252:A:PHE:HD2	11	0.12
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	2	0.12
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	7	0.12
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	15	0.12
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	19	0.12
(1,67)	2:389:B:DU:H2''	1:244:A:ASN:HB2	9	0.12
(1,67)	2:389:B:DU:H2''	1:244:A:ASN:HB2	20	0.12
(1,60)	2:388:B:DC:H3'	1:285:A:TRP:HZ3	15	0.12
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	4	0.12
(1,54)	2:388:B:DC:H2''	1:285:A:TRP:HE1	14	0.12
(1,41)	2:385:B:DA:H8	1:374:A:ARG:H	4	0.12
(1,41)	2:385:B:DA:H8	1:374:A:ARG:H	6	0.12
(1,30)	2:391:B:DA:H2'	2:391:B:DA:H8	11	0.12
(1,13)	2:387:B:DT:H6	2:387:B:DT:H5'	15	0.12
(1,13)	2:387:B:DT:H6	2:387:B:DT:H5''	15	0.12
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	2	0.12
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	2	0.12
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	5	0.12
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	5	0.12
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	12	0.12
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	12	0.12
(1,2)	2:385:B:DA:H3'	2:385:B:DA:H5'	7	0.12
(1,2679)	1:382:A:GLN:HB2	1:382:A:GLN:H	17	0.11
(1,2675)	1:382:A:GLN:HA	1:382:A:GLN:HB2	5	0.11
(1,2673)	1:381:A:ASN:H	1:383:A:GLU:H	5	0.11
(1,2669)	1:381:A:ASN:HA	1:384:A:ASN:H	7	0.11
(1,2669)	1:381:A:ASN:HA	1:384:A:ASN:H	19	0.11
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	14	0.11
(1,2664)	1:381:A:ASN:HB3	1:381:A:ASN:H	18	0.11
(1,2645)	1:380:A:GLN:HB2	1:380:A:GLN:HE22	5	0.11
(1,2645)	1:380:A:GLN:HB3	1:380:A:GLN:HE22	5	0.11
(1,2645)	1:380:A:GLN:HB2	1:380:A:GLN:HE22	6	0.11
(1,2645)	1:380:A:GLN:HB3	1:380:A:GLN:HE22	6	0.11
(1,2645)	1:380:A:GLN:HB2	1:380:A:GLN:HE22	10	0.11
(1,2645)	1:380:A:GLN:HB3	1:380:A:GLN:HE22	10	0.11
(1,2645)	1:380:A:GLN:HB2	1:380:A:GLN:HE22	11	0.11
(1,2645)	1:380:A:GLN:HB3	1:380:A:GLN:HE22	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2645)	1:380:A:GLN:HB2	1:380:A:GLN:HE22	12	0.11
(1,2645)	1:380:A:GLN:HB3	1:380:A:GLN:HE22	12	0.11
(1,2645)	1:380:A:GLN:HB2	1:380:A:GLN:HE22	15	0.11
(1,2645)	1:380:A:GLN:HB3	1:380:A:GLN:HE22	15	0.11
(1,2645)	1:380:A:GLN:HB2	1:380:A:GLN:HE22	19	0.11
(1,2645)	1:380:A:GLN:HB3	1:380:A:GLN:HE22	19	0.11
(1,2645)	1:380:A:GLN:HB2	1:380:A:GLN:HE22	20	0.11
(1,2645)	1:380:A:GLN:HB3	1:380:A:GLN:HE22	20	0.11
(1,2619)	1:378:A:ILE:HG12	1:379:A:LEU:H	14	0.11
(1,2619)	1:378:A:ILE:HG13	1:379:A:LEU:H	14	0.11
(1,2587)	1:376:A:ARG:HH21	1:382:A:GLN:H	16	0.11
(1,2587)	1:376:A:ARG:HH22	1:382:A:GLN:H	16	0.11
(1,2470)	1:370:A:ASP:HB3	1:370:A:ASP:H	3	0.11
(1,2428)	1:367:A:HIS:HD2	1:367:A:HIS:H	1	0.11
(1,2406)	1:366:A:GLU:HB3	1:366:A:GLU:H	5	0.11
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	5	0.11
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	5	0.11
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	9	0.11
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	9	0.11
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	12	0.11
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	12	0.11
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	13	0.11
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	13	0.11
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	17	0.11
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	17	0.11
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	20	0.11
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	20	0.11
(1,2221)	1:352:A:ASP:HB3	1:352:A:ASP:H	6	0.11
(1,2221)	1:352:A:ASP:HB3	1:352:A:ASP:H	14	0.11
(1,2221)	1:352:A:ASP:HB3	1:352:A:ASP:H	16	0.11
(1,2215)	1:351:A:VAL:HG11	1:353:A:HIS:HD2	18	0.11
(1,2215)	1:351:A:VAL:HG12	1:353:A:HIS:HD2	18	0.11
(1,2215)	1:351:A:VAL:HG13	1:353:A:HIS:HD2	18	0.11
(1,2215)	1:351:A:VAL:HG21	1:353:A:HIS:HD2	18	0.11
(1,2215)	1:351:A:VAL:HG22	1:353:A:HIS:HD2	18	0.11
(1,2215)	1:351:A:VAL:HG23	1:353:A:HIS:HD2	18	0.11
(1,2215)	1:351:A:VAL:HG11	1:353:A:HIS:HD2	20	0.11
(1,2215)	1:351:A:VAL:HG12	1:353:A:HIS:HD2	20	0.11
(1,2215)	1:351:A:VAL:HG13	1:353:A:HIS:HD2	20	0.11
(1,2215)	1:351:A:VAL:HG21	1:353:A:HIS:HD2	20	0.11
(1,2215)	1:351:A:VAL:HG22	1:353:A:HIS:HD2	20	0.11
(1,2215)	1:351:A:VAL:HG23	1:353:A:HIS:HD2	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2183)	1:349:A:THR:HG21	1:350:A:PHE:HE1	8	0.11
(1,2183)	1:349:A:THR:HG21	1:350:A:PHE:HE2	8	0.11
(1,2183)	1:349:A:THR:HG22	1:350:A:PHE:HE1	8	0.11
(1,2183)	1:349:A:THR:HG22	1:350:A:PHE:HE2	8	0.11
(1,2183)	1:349:A:THR:HG23	1:350:A:PHE:HE1	8	0.11
(1,2183)	1:349:A:THR:HG23	1:350:A:PHE:HE2	8	0.11
(1,2122)	1:345:A:HIS:HA	1:348:A:ASP:H	3	0.11
(1,2122)	1:345:A:HIS:HA	1:348:A:ASP:H	11	0.11
(1,1960)	1:334:A:LYS:HB3	1:334:A:LYS:H	6	0.11
(1,1902)	1:328:A:LEU:HD11	1:332:A:GLY:H	13	0.11
(1,1902)	1:328:A:LEU:HD12	1:332:A:GLY:H	13	0.11
(1,1902)	1:328:A:LEU:HD13	1:332:A:GLY:H	13	0.11
(1,1902)	1:328:A:LEU:HD21	1:332:A:GLY:H	13	0.11
(1,1902)	1:328:A:LEU:HD22	1:332:A:GLY:H	13	0.11
(1,1902)	1:328:A:LEU:HD23	1:332:A:GLY:H	13	0.11
(1,1861)	1:326:A:ARG:HD2	1:378:A:ILE:HD11	5	0.11
(1,1861)	1:326:A:ARG:HD2	1:378:A:ILE:HD12	5	0.11
(1,1861)	1:326:A:ARG:HD2	1:378:A:ILE:HD13	5	0.11
(1,1861)	1:326:A:ARG:HD3	1:378:A:ILE:HD11	5	0.11
(1,1861)	1:326:A:ARG:HD3	1:378:A:ILE:HD12	5	0.11
(1,1861)	1:326:A:ARG:HD3	1:378:A:ILE:HD13	5	0.11
(1,1849)	1:326:A:ARG:HB3	1:326:A:ARG:H	6	0.11
(1,1849)	1:326:A:ARG:HB3	1:326:A:ARG:H	12	0.11
(1,1849)	1:326:A:ARG:HB3	1:326:A:ARG:H	13	0.11
(1,1842)	1:326:A:ARG:HA	1:326:A:ARG:HB3	1	0.11
(1,1842)	1:326:A:ARG:HA	1:326:A:ARG:HB3	4	0.11
(1,1842)	1:326:A:ARG:HA	1:326:A:ARG:HB3	17	0.11
(1,1806)	1:323:A:GLU:HB3	1:324:A:GLY:H	18	0.11
(1,1770)	1:314:A:ILE:HD11	1:375:A:LEU:H	2	0.11
(1,1770)	1:314:A:ILE:HD12	1:375:A:LEU:H	2	0.11
(1,1770)	1:314:A:ILE:HD13	1:375:A:LEU:H	2	0.11
(1,1754)	1:314:A:ILE:HD11	1:314:A:ILE:H	12	0.11
(1,1754)	1:314:A:ILE:HD12	1:314:A:ILE:H	12	0.11
(1,1754)	1:314:A:ILE:HD13	1:314:A:ILE:H	12	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	3	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	3	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	4	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	4	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	7	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	7	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	11	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	13	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	13	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	16	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	16	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	19	0.11
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	19	0.11
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD2	4	0.11
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD3	4	0.11
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD2	9	0.11
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD3	9	0.11
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD2	12	0.11
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD3	12	0.11
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD2	17	0.11
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD3	17	0.11
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG2	12	0.11
(1,1542)	1:302:A:ASN:H	1:303:A:LYS:HG3	12	0.11
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	1	0.11
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	8	0.11
(1,1511)	1:301:A:LYS:HB2	1:301:A:LYS:HG2	13	0.11
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	1	0.11
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	11	0.11
(1,1508)	1:301:A:LYS:HB3	1:301:A:LYS:HG3	13	0.11
(1,1478)	1:299:A:ILE:HD11	1:300:A:SER:HB2	12	0.11
(1,1478)	1:299:A:ILE:HD11	1:300:A:SER:HB3	12	0.11
(1,1478)	1:299:A:ILE:HD12	1:300:A:SER:HB2	12	0.11
(1,1478)	1:299:A:ILE:HD12	1:300:A:SER:HB3	12	0.11
(1,1478)	1:299:A:ILE:HD13	1:300:A:SER:HB2	12	0.11
(1,1478)	1:299:A:ILE:HD13	1:300:A:SER:HB3	12	0.11
(1,1478)	1:299:A:ILE:HD11	1:300:A:SER:HB2	19	0.11
(1,1478)	1:299:A:ILE:HD11	1:300:A:SER:HB3	19	0.11
(1,1478)	1:299:A:ILE:HD12	1:300:A:SER:HB2	19	0.11
(1,1478)	1:299:A:ILE:HD12	1:300:A:SER:HB3	19	0.11
(1,1478)	1:299:A:ILE:HD13	1:300:A:SER:HB2	19	0.11
(1,1478)	1:299:A:ILE:HD13	1:300:A:SER:HB3	19	0.11
(1,1379)	1:292:A:ALA:HA	1:324:A:GLY:HA2	20	0.11
(1,1379)	1:292:A:ALA:HA	1:324:A:GLY:HA3	20	0.11
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD1	3	0.11
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD2	3	0.11
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD1	5	0.11
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD2	5	0.11
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD1	9	0.11
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD2	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD1	13	0.11
(1,1338)	1:285:A:TRP:HZ2	1:315:A:TYR:HD2	13	0.11
(1,1315)	1:283:A:THR:H	1:311:A:THR:HB	9	0.11
(1,1283)	1:282:A:PHE:HA	1:346:A:CYS:HG	14	0.11
(1,1264)	1:281:A:CYS:HB2	1:283:A:THR:HG21	12	0.11
(1,1264)	1:281:A:CYS:HB2	1:283:A:THR:HG22	12	0.11
(1,1264)	1:281:A:CYS:HB2	1:283:A:THR:HG23	12	0.11
(1,1247)	1:280:A:THR:HG21	1:308:A:CYS:H	15	0.11
(1,1247)	1:280:A:THR:HG22	1:308:A:CYS:H	15	0.11
(1,1247)	1:280:A:THR:HG23	1:308:A:CYS:H	15	0.11
(1,1209)	1:279:A:VAL:HB	1:307:A:LEU:HA	7	0.11
(1,1209)	1:279:A:VAL:HB	1:307:A:LEU:HA	20	0.11
(1,1168)	1:277:A:TYR:HA	1:306:A:SER:H	2	0.11
(1,1168)	1:277:A:TYR:HA	1:306:A:SER:H	3	0.11
(1,1168)	1:277:A:TYR:HA	1:306:A:SER:H	4	0.11
(1,1168)	1:277:A:TYR:HA	1:306:A:SER:H	11	0.11
(1,1168)	1:277:A:TYR:HA	1:306:A:SER:H	15	0.11
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	10	0.11
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	10	0.11
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	13	0.11
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	13	0.11
(1,947)	1:263:A:LEU:HD11	1:298:A:PHE:H	8	0.11
(1,947)	1:263:A:LEU:HD12	1:298:A:PHE:H	8	0.11
(1,947)	1:263:A:LEU:HD13	1:298:A:PHE:H	8	0.11
(1,947)	1:263:A:LEU:HD21	1:298:A:PHE:H	8	0.11
(1,947)	1:263:A:LEU:HD22	1:298:A:PHE:H	8	0.11
(1,947)	1:263:A:LEU:HD23	1:298:A:PHE:H	8	0.11
(1,942)	1:263:A:LEU:HD11	1:281:A:CYS:HB2	20	0.11
(1,942)	1:263:A:LEU:HD11	1:281:A:CYS:HB3	20	0.11
(1,942)	1:263:A:LEU:HD12	1:281:A:CYS:HB2	20	0.11
(1,942)	1:263:A:LEU:HD12	1:281:A:CYS:HB3	20	0.11
(1,942)	1:263:A:LEU:HD13	1:281:A:CYS:HB2	20	0.11
(1,942)	1:263:A:LEU:HD13	1:281:A:CYS:HB3	20	0.11
(1,942)	1:263:A:LEU:HD21	1:281:A:CYS:HB2	20	0.11
(1,942)	1:263:A:LEU:HD21	1:281:A:CYS:HB3	20	0.11
(1,942)	1:263:A:LEU:HD22	1:281:A:CYS:HB2	20	0.11
(1,942)	1:263:A:LEU:HD22	1:281:A:CYS:HB3	20	0.11
(1,942)	1:263:A:LEU:HD23	1:281:A:CYS:HB2	20	0.11
(1,942)	1:263:A:LEU:HD23	1:281:A:CYS:HB3	20	0.11
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	12	0.11
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	12	0.11
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	15	0.11
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE1	6	0.11
(1,769)	1:252:A:PHE:HA	1:252:A:PHE:HE2	6	0.11
(1,718)	1:247:A:PRO:HG2	1:248:A:HIS:HD1	12	0.11
(1,718)	1:247:A:PRO:HG3	1:248:A:HIS:HD1	12	0.11
(1,718)	1:247:A:PRO:HG2	1:248:A:HIS:HD1	13	0.11
(1,718)	1:247:A:PRO:HG3	1:248:A:HIS:HD1	13	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	3	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	3	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	3	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	7	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	7	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	7	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	11	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	11	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	11	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	14	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	14	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	14	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	20	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	20	0.11
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	20	0.11
(1,581)	1:235:A:LEU:HD11	1:235:A:LEU:H	3	0.11
(1,581)	1:235:A:LEU:HD12	1:235:A:LEU:H	3	0.11
(1,581)	1:235:A:LEU:HD13	1:235:A:LEU:H	3	0.11
(1,581)	1:235:A:LEU:HD21	1:235:A:LEU:H	3	0.11
(1,581)	1:235:A:LEU:HD22	1:235:A:LEU:H	3	0.11
(1,581)	1:235:A:LEU:HD23	1:235:A:LEU:H	3	0.11
(1,581)	1:235:A:LEU:HD11	1:235:A:LEU:H	9	0.11
(1,581)	1:235:A:LEU:HD12	1:235:A:LEU:H	9	0.11
(1,581)	1:235:A:LEU:HD13	1:235:A:LEU:H	9	0.11
(1,581)	1:235:A:LEU:HD21	1:235:A:LEU:H	9	0.11
(1,581)	1:235:A:LEU:HD22	1:235:A:LEU:H	9	0.11
(1,581)	1:235:A:LEU:HD23	1:235:A:LEU:H	9	0.11
(1,581)	1:235:A:LEU:HD11	1:235:A:LEU:H	18	0.11
(1,581)	1:235:A:LEU:HD12	1:235:A:LEU:H	18	0.11
(1,581)	1:235:A:LEU:HD13	1:235:A:LEU:H	18	0.11
(1,581)	1:235:A:LEU:HD21	1:235:A:LEU:H	18	0.11
(1,581)	1:235:A:LEU:HD22	1:235:A:LEU:H	18	0.11
(1,581)	1:235:A:LEU:HD23	1:235:A:LEU:H	18	0.11
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	4	0.11
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	11	0.11
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	13	0.11
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	17	0.11
(1,546)	1:233:A:VAL:HA	1:233:A:VAL:HB	19	0.11
(1,536)	1:231:A:THR:H	1:232:A:TRP:HE1	4	0.11
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	3	0.11
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	6	0.11
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	8	0.11
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	14	0.11
(1,523)	1:231:A:THR:HA	1:231:A:THR:HB	15	0.11
(1,499)	1:227:A:MET:H	1:233:A:VAL:HG11	19	0.11
(1,499)	1:227:A:MET:H	1:233:A:VAL:HG12	19	0.11
(1,499)	1:227:A:MET:H	1:233:A:VAL:HG13	19	0.11
(1,499)	1:227:A:MET:H	1:233:A:VAL:HG21	19	0.11
(1,499)	1:227:A:MET:H	1:233:A:VAL:HG22	19	0.11
(1,499)	1:227:A:MET:H	1:233:A:VAL:HG23	19	0.11
(1,490)	1:227:A:MET:HA	1:278:A:ARG:H	12	0.11
(1,472)	1:226:A:ARG:HD2	1:235:A:LEU:HA	9	0.11
(1,472)	1:226:A:ARG:HD3	1:235:A:LEU:HA	9	0.11
(1,446)	1:225:A:GLU:H	1:278:A:ARG:H	2	0.11
(1,446)	1:225:A:GLU:H	1:278:A:ARG:H	16	0.11
(1,224)	1:206:A:PHE:HZ	1:312:A:ALA:H	2	0.11
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB2	4	0.11
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB3	4	0.11
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB2	4	0.11
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB3	4	0.11
(1,167)	1:203:A:THR:HA	1:206:A:PHE:H	5	0.11
(1,155)	1:202:A:PHE:H	1:203:A:THR:HB	16	0.11
(1,137)	1:201:A:THR:HG21	1:205:A:ASN:H	14	0.11
(1,137)	1:201:A:THR:HG22	1:205:A:ASN:H	14	0.11
(1,137)	1:201:A:THR:HG23	1:205:A:ASN:H	14	0.11
(1,127)	1:201:A:THR:HB	1:201:A:THR:H	19	0.11
(1,122)	1:200:A:PRO:HA	1:353:A:HIS:H	4	0.11
(1,122)	1:200:A:PRO:HA	1:353:A:HIS:H	6	0.11
(1,109)	1:198:A:ASP:H	1:202:A:PHE:HD1	3	0.11
(1,109)	1:198:A:ASP:H	1:202:A:PHE:HD2	3	0.11
(1,98)	1:197:A:MET:HB2	1:241:A:PHE:HB2	19	0.11
(1,98)	1:197:A:MET:HB2	1:241:A:PHE:HB3	19	0.11
(1,98)	1:197:A:MET:HB3	1:241:A:PHE:HB2	19	0.11
(1,98)	1:197:A:MET:HB3	1:241:A:PHE:HB3	19	0.11
(1,90)	2:394:B:DT:H5'	1:254:A:GLU:HG2	12	0.11
(1,90)	2:394:B:DT:H5''	1:254:A:GLU:HG2	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	2:392:B:DA:H1'	1:254:A:GLU:HG2	4	0.11
(1,78)	2:392:B:DA:H1'	1:254:A:GLU:HG3	4	0.11
(1,78)	2:392:B:DA:H1'	1:254:A:GLU:HG2	19	0.11
(1,78)	2:392:B:DA:H1'	1:254:A:GLU:HG3	19	0.11
(1,77)	2:392:B:DA:H8	1:252:A:PHE:HD2	8	0.11
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	6	0.11
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB1	2	0.11
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB2	2	0.11
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB3	2	0.11
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB1	12	0.11
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB2	12	0.11
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB3	12	0.11
(1,67)	2:389:B:DU:H2''	1:244:A:ASN:HB2	4	0.11
(1,67)	2:389:B:DU:H2''	1:244:A:ASN:HB2	8	0.11
(1,66)	2:389:B:DU:H2''	1:244:A:ASN:HB3	5	0.11
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	20	0.11
(1,54)	2:388:B:DC:H2''	1:285:A:TRP:HE1	1	0.11
(1,30)	2:391:B:DA:H2'	2:391:B:DA:H8	19	0.11
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	15	0.11
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	15	0.11
(1,2698)	1:384:A:ASN:HB3	1:384:A:ASN:H	2	0.1
(1,2678)	1:382:A:GLN:HB3	1:382:A:GLN:H	5	0.1
(1,2669)	1:381:A:ASN:HA	1:384:A:ASN:H	5	0.1
(1,2669)	1:381:A:ASN:HA	1:384:A:ASN:H	9	0.1
(1,2669)	1:381:A:ASN:HA	1:384:A:ASN:H	16	0.1
(1,2645)	1:380:A:GLN:HB2	1:380:A:GLN:HE22	7	0.1
(1,2645)	1:380:A:GLN:HB3	1:380:A:GLN:HE22	7	0.1
(1,2587)	1:376:A:ARG:HH21	1:382:A:GLN:H	14	0.1
(1,2587)	1:376:A:ARG:HH22	1:382:A:GLN:H	14	0.1
(1,2587)	1:376:A:ARG:HH21	1:382:A:GLN:H	18	0.1
(1,2587)	1:376:A:ARG:HH22	1:382:A:GLN:H	18	0.1
(1,2479)	1:371:A:LEU:HA	1:371:A:LEU:HG	16	0.1
(1,2470)	1:370:A:ASP:HB3	1:370:A:ASP:H	1	0.1
(1,2470)	1:370:A:ASP:HB3	1:370:A:ASP:H	8	0.1
(1,2470)	1:370:A:ASP:HB3	1:370:A:ASP:H	9	0.1
(1,2470)	1:370:A:ASP:HB3	1:370:A:ASP:H	18	0.1
(1,2406)	1:366:A:GLU:HB3	1:366:A:GLU:H	2	0.1
(1,2406)	1:366:A:GLU:HB3	1:366:A:GLU:H	4	0.1
(1,2406)	1:366:A:GLU:HB3	1:366:A:GLU:H	9	0.1
(1,2406)	1:366:A:GLU:HB3	1:366:A:GLU:H	11	0.1
(1,2406)	1:366:A:GLU:HB3	1:366:A:GLU:H	14	0.1
(1,2406)	1:366:A:GLU:HB3	1:366:A:GLU:H	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	10	0.1
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	10	0.1
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	14	0.1
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	14	0.1
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	18	0.1
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	18	0.1
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE21	19	0.1
(1,2246)	1:354:A:GLN:HA	1:354:A:GLN:HE22	19	0.1
(1,2222)	1:352:A:ASP:HB2	1:352:A:ASP:H	11	0.1
(1,2221)	1:352:A:ASP:HB3	1:352:A:ASP:H	2	0.1
(1,2221)	1:352:A:ASP:HB3	1:352:A:ASP:H	4	0.1
(1,2221)	1:352:A:ASP:HB3	1:352:A:ASP:H	9	0.1
(1,2221)	1:352:A:ASP:HB3	1:352:A:ASP:H	15	0.1
(1,2221)	1:352:A:ASP:HB3	1:352:A:ASP:H	18	0.1
(1,2221)	1:352:A:ASP:HB3	1:352:A:ASP:H	19	0.1
(1,2179)	1:349:A:THR:HA	1:352:A:ASP:H	7	0.1
(1,2122)	1:345:A:HIS:HA	1:348:A:ASP:H	15	0.1
(1,2051)	1:339:A:THR:HB	1:340:A:TYR:H	3	0.1
(1,1960)	1:334:A:LYS:HB3	1:334:A:LYS:H	18	0.1
(1,1859)	1:326:A:ARG:HB2	1:327:A:THR:H	17	0.1
(1,1849)	1:326:A:ARG:HB3	1:326:A:ARG:H	2	0.1
(1,1849)	1:326:A:ARG:HB3	1:326:A:ARG:H	10	0.1
(1,1849)	1:326:A:ARG:HB3	1:326:A:ARG:H	11	0.1
(1,1849)	1:326:A:ARG:HB3	1:326:A:ARG:H	14	0.1
(1,1849)	1:326:A:ARG:HB3	1:326:A:ARG:H	19	0.1
(1,1849)	1:326:A:ARG:HB3	1:326:A:ARG:H	20	0.1
(1,1754)	1:314:A:ILE:HD11	1:314:A:ILE:H	5	0.1
(1,1754)	1:314:A:ILE:HD12	1:314:A:ILE:H	5	0.1
(1,1754)	1:314:A:ILE:HD13	1:314:A:ILE:H	5	0.1
(1,1754)	1:314:A:ILE:HD11	1:314:A:ILE:H	14	0.1
(1,1754)	1:314:A:ILE:HD12	1:314:A:ILE:H	14	0.1
(1,1754)	1:314:A:ILE:HD13	1:314:A:ILE:H	14	0.1
(1,1754)	1:314:A:ILE:HD11	1:314:A:ILE:H	20	0.1
(1,1754)	1:314:A:ILE:HD12	1:314:A:ILE:H	20	0.1
(1,1754)	1:314:A:ILE:HD13	1:314:A:ILE:H	20	0.1
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG21	15	0.1
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG22	15	0.1
(1,1737)	1:313:A:ARG:HD2	1:337:A:ILE:HG23	15	0.1
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG21	15	0.1
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG22	15	0.1
(1,1737)	1:313:A:ARG:HD3	1:337:A:ILE:HG23	15	0.1
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	1	0.1
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	9	0.1
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	9	0.1
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG12	17	0.1
(1,1656)	1:309:A:ILE:HA	1:335:A:ILE:HG13	17	0.1
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD2	1	0.1
(1,1623)	1:307:A:LEU:H	1:334:A:LYS:HD3	1	0.1
(1,1609)	1:307:A:LEU:HD11	1:308:A:CYS:HA	10	0.1
(1,1609)	1:307:A:LEU:HD12	1:308:A:CYS:HA	10	0.1
(1,1609)	1:307:A:LEU:HD13	1:308:A:CYS:HA	10	0.1
(1,1609)	1:307:A:LEU:HD21	1:308:A:CYS:HA	10	0.1
(1,1609)	1:307:A:LEU:HD22	1:308:A:CYS:HA	10	0.1
(1,1609)	1:307:A:LEU:HD23	1:308:A:CYS:HA	10	0.1
(1,1554)	1:303:A:LYS:HB2	1:303:A:LYS:HE2	1	0.1
(1,1554)	1:303:A:LYS:HB2	1:303:A:LYS:HE3	1	0.1
(1,1554)	1:303:A:LYS:HB3	1:303:A:LYS:HE2	1	0.1
(1,1554)	1:303:A:LYS:HB3	1:303:A:LYS:HE3	1	0.1
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD1	4	0.1
(1,1341)	1:285:A:TRP:HH2	1:315:A:TYR:HD2	4	0.1
(1,1313)	1:283:A:THR:H	1:310:A:PHE:HE1	11	0.1
(1,1313)	1:283:A:THR:H	1:310:A:PHE:HE2	11	0.1
(1,1313)	1:283:A:THR:H	1:310:A:PHE:HE1	15	0.1
(1,1313)	1:283:A:THR:H	1:310:A:PHE:HE2	15	0.1
(1,1209)	1:279:A:VAL:HB	1:307:A:LEU:HA	15	0.1
(1,1168)	1:277:A:TYR:HA	1:306:A:SER:H	1	0.1
(1,1168)	1:277:A:TYR:HA	1:306:A:SER:H	19	0.1
(1,1138)	1:275:A:GLN:HB2	1:275:A:GLN:HE21	17	0.1
(1,1138)	1:275:A:GLN:HB3	1:275:A:GLN:HE21	17	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	2	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	3	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	5	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	6	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	9	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	10	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	11	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	12	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	13	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	14	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	17	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	18	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	19	0.1
(1,1115)	1:273:A:LEU:HB3	1:273:A:LEU:H	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	2	0.1
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	2	0.1
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	2	0.1
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	7	0.1
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	7	0.1
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	7	0.1
(1,873)	1:260:A:LEU:HD21	1:291:A:CYS:HA	20	0.1
(1,873)	1:260:A:LEU:HD22	1:291:A:CYS:HA	20	0.1
(1,873)	1:260:A:LEU:HD23	1:291:A:CYS:HA	20	0.1
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	2	0.1
(1,782)	1:253:A:LEU:HG	1:254:A:GLU:HA	11	0.1
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB1	2	0.1
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB2	2	0.1
(1,689)	1:244:A:ASN:HD22	1:258:A:ALA:HB3	2	0.1
(1,640)	1:240:A:GLY:H	1:350:A:PHE:HD1	13	0.1
(1,640)	1:240:A:GLY:H	1:350:A:PHE:HD2	13	0.1
(1,581)	1:235:A:LEU:HD11	1:235:A:LEU:H	2	0.1
(1,581)	1:235:A:LEU:HD12	1:235:A:LEU:H	2	0.1
(1,581)	1:235:A:LEU:HD13	1:235:A:LEU:H	2	0.1
(1,581)	1:235:A:LEU:HD21	1:235:A:LEU:H	2	0.1
(1,581)	1:235:A:LEU:HD22	1:235:A:LEU:H	2	0.1
(1,581)	1:235:A:LEU:HD23	1:235:A:LEU:H	2	0.1
(1,489)	1:227:A:MET:HA	1:235:A:LEU:H	4	0.1
(1,446)	1:225:A:GLU:H	1:278:A:ARG:H	15	0.1
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB2	7	0.1
(1,219)	1:206:A:PHE:HE1	1:282:A:PHE:HB3	7	0.1
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB2	7	0.1
(1,219)	1:206:A:PHE:HE2	1:282:A:PHE:HB3	7	0.1
(1,150)	1:202:A:PHE:HA	1:351:A:VAL:HG11	20	0.1
(1,150)	1:202:A:PHE:HA	1:351:A:VAL:HG12	20	0.1
(1,150)	1:202:A:PHE:HA	1:351:A:VAL:HG13	20	0.1
(1,109)	1:198:A:ASP:H	1:202:A:PHE:HD1	6	0.1
(1,109)	1:198:A:ASP:H	1:202:A:PHE:HD2	6	0.1
(1,105)	1:198:A:ASP:H	1:200:A:PRO:HA	12	0.1
(1,97)	1:197:A:MET:HA	1:352:A:ASP:H	14	0.1
(1,96)	1:197:A:MET:HA	1:201:A:THR:H	5	0.1
(1,96)	1:197:A:MET:HA	1:201:A:THR:H	8	0.1
(1,73)	2:389:B:DU:H5	1:315:A:TYR:HD1	14	0.1
(1,73)	2:389:B:DU:H5	1:315:A:TYR:HD2	14	0.1
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	10	0.1
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	11	0.1
(1,70)	2:389:B:DU:H5'	1:259:A:GLU:HG3	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB1	10	0.1
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB2	10	0.1
(1,69)	2:389:B:DU:H6	1:258:A:ALA:HB3	10	0.1
(1,67)	2:389:B:DU:H2''	1:244:A:ASN:HB2	5	0.1
(1,67)	2:389:B:DU:H2''	1:244:A:ASN:HB2	16	0.1
(1,67)	2:389:B:DU:H2''	1:244:A:ASN:HB2	17	0.1
(1,56)	2:388:B:DC:H5	1:285:A:TRP:HE3	3	0.1
(1,41)	2:385:B:DA:H8	1:374:A:ARG:H	8	0.1
(1,30)	2:391:B:DA:H2'	2:391:B:DA:H8	9	0.1
(1,30)	2:391:B:DA:H2'	2:391:B:DA:H8	12	0.1
(1,30)	2:391:B:DA:H2'	2:391:B:DA:H8	13	0.1
(1,30)	2:391:B:DA:H2'	2:391:B:DA:H8	14	0.1
(1,30)	2:391:B:DA:H2'	2:391:B:DA:H8	15	0.1
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5'	16	0.1
(1,10)	2:386:B:DT:H6	2:386:B:DT:H5''	16	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found