Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 07:23 PM EDT

PDB ID	:	2LUP
BMRB ID	:	18534
Title	:	RDC refined solution structure of double-stranded RNA binding domain of S. cerevisiae RNase III (rnt1p) in complex with the terminal RNA hairpin of snr47 precursor
Authors	:	Wang, Z.; Feigon, J.
Deposited on	:	2012-06-19

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

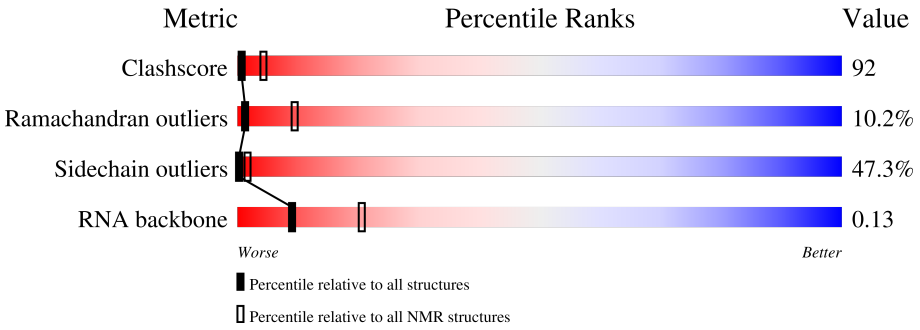
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 71%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428
RNA backbone	4643	676

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

Mol	Chain	Length	Quality of chain
1	A	32	44% 47% 9%
2	B	90	12% 43% 34% · 9%

2 Ensemble composition and analysis (i)

This entry contains 16 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	B:366-B:447 (82)	0.86	5

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 5 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2437 atoms, of which 1067 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA (32-MER).

Mol	Chain	Residues	Atoms						Trace
1	A	32	Total	C	H	N	O	P	0
			1028	306	346	124	221	31	

- Molecule 2 is a protein called Ribonuclease 3.

Mol	Chain	Residues	Atoms						Trace
2	B	90	Total	C	H	N	O	S	0
			1409	429	721	129	127	3	

There are 2 discrepancies between the modelled and reference sequences:

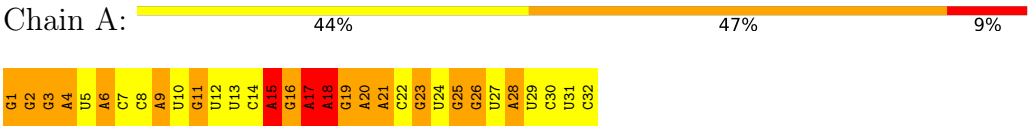
Chain	Residue	Modelled	Actual	Comment	Reference
B	364	GLY	-	expression tag	UNP Q02555
B	365	SER	-	expression tag	UNP Q02555

4 Residue-property plots

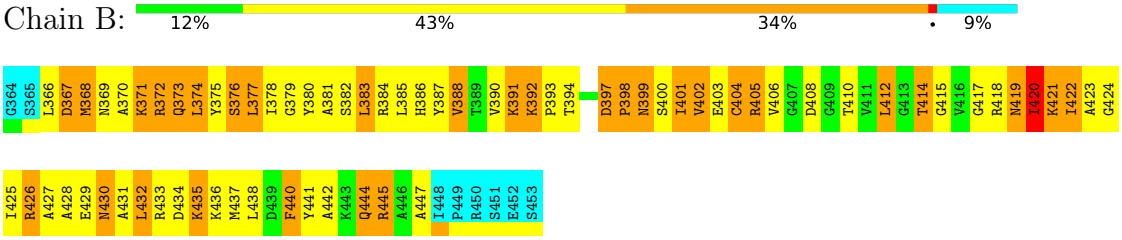
4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: RNA (32-MER)



• Molecule 2: Ribonuclease 3

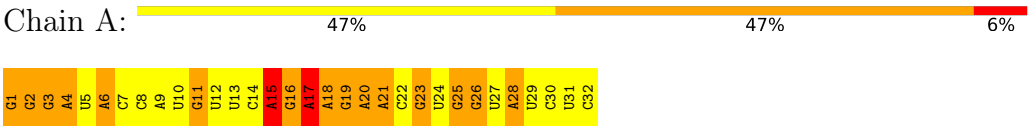


4.2 Scores per residue for each member of the ensemble

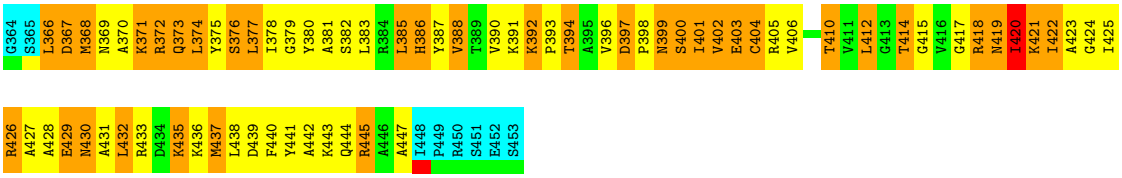
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: RNA (32-MER)



• Molecule 2: Ribonuclease 3

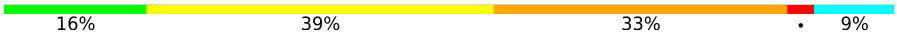


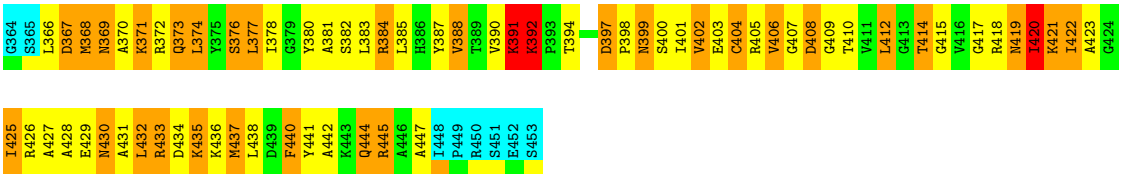
4.2.2 Score per residue for model 2

• Molecule 1: RNA (32-MER)

Chain A: 

• Molecule 2: Ribonuclease 3

Chain B: 



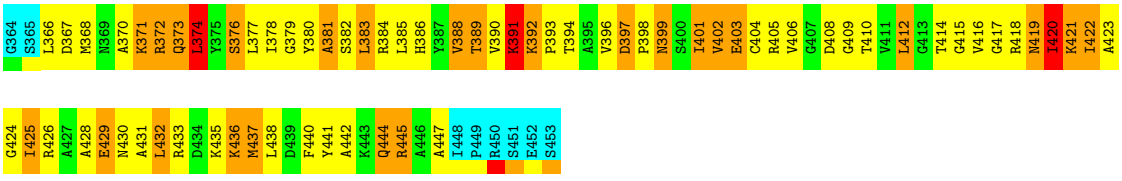
4.2.3 Score per residue for model 3

• Molecule 1: RNA (32-MER)

Chain A: 

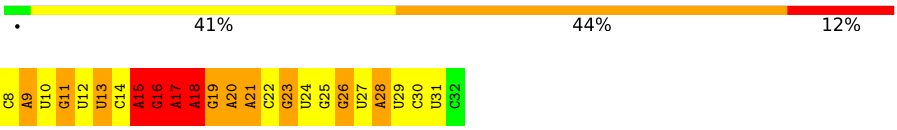
• Molecule 2: Ribonuclease 3

Chain B: 

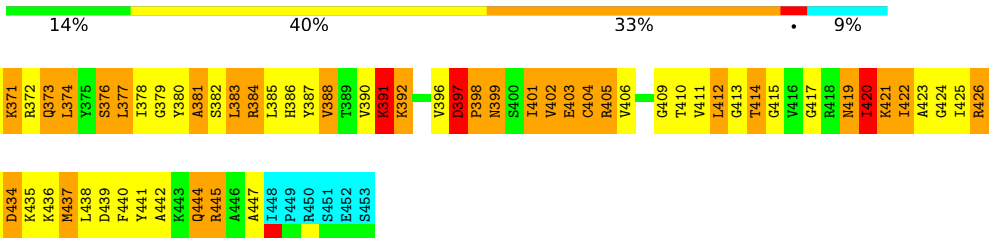


4.2.4 Score per residue for model 4

• Molecule 1: RNA (32-MER)

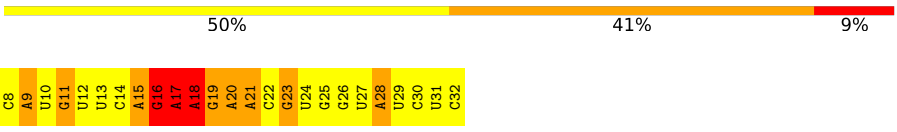
Chain A: 

• Molecule 2: Ribonuclease 3

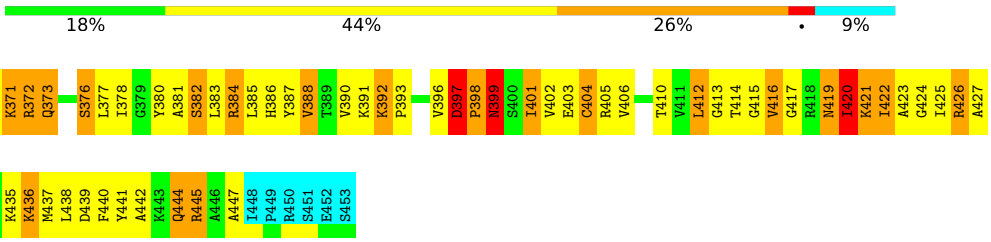
Chain B: 

4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: RNA (32-MER)

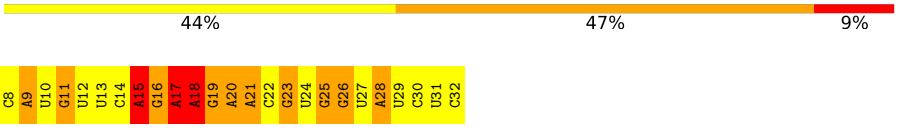
Chain A: 

• Molecule 2: Ribonuclease 3

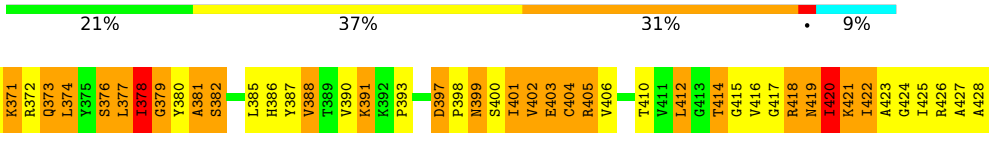
Chain B: 

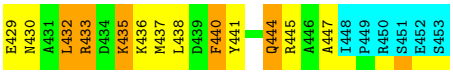
4.2.6 Score per residue for model 6

• Molecule 1: RNA (32-MER)

Chain A: 

• Molecule 2: Ribonuclease 3

Chain B: 



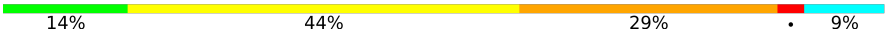
4.2.7 Score per residue for model 7

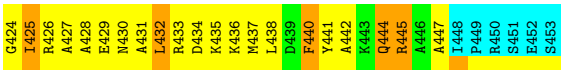
• Molecule 1: RNA (32-MER)

Chain A:

• Molecule 2: Ribonuclease 3

Chain B:





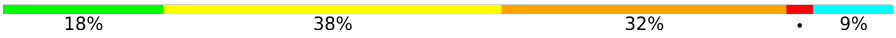
4.2.8 Score per residue for model 8

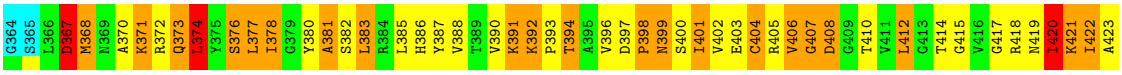
• Molecule 1: RNA (32-MER)

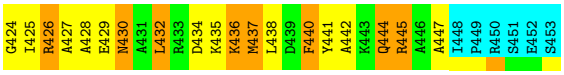
Chain A:

• Molecule 2: Ribonuclease 3

Chain B:







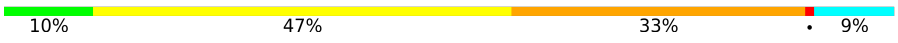
4.2.9 Score per residue for model 9

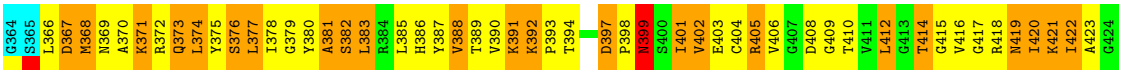
• Molecule 1: RNA (32-MER)

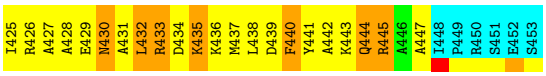
Chain A:

• Molecule 2: Ribonuclease 3

Chain B:







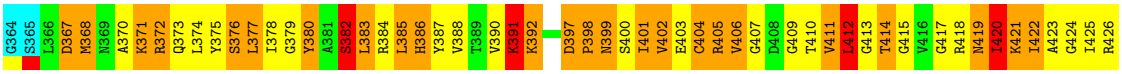
4.2.10 Score per residue for model 10

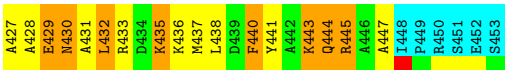
• Molecule 1: RNA (32-MER)

Chain A:

• Molecule 2: Ribonuclease 3

Chain B:





4.2.11 Score per residue for model 11

• Molecule 1: RNA (32-MER)

Chain A:

• Molecule 2: Ribonuclease 3

Chain B:

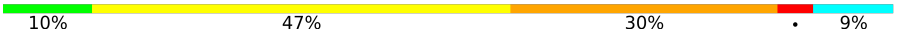
4.2.12 Score per residue for model 12

• Molecule 1: RNA (32-MER)

Chain A:

• Molecule 2: Ribonuclease 3

Chain B:



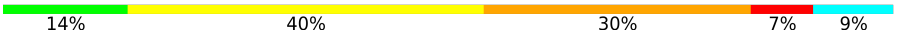
4.2.13 Score per residue for model 13

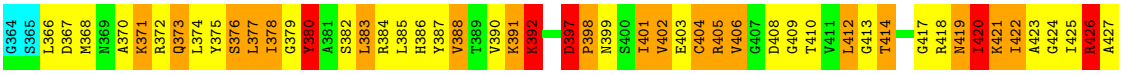
• Molecule 1: RNA (32-MER)

Chain A:

• Molecule 2: Ribonuclease 3

Chain B:





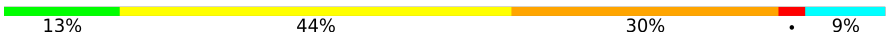
4.2.14 Score per residue for model 14

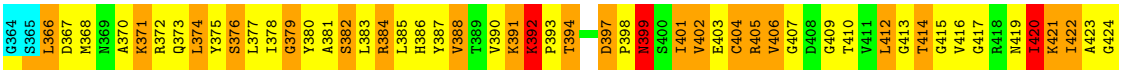
• Molecule 1: RNA (32-MER)

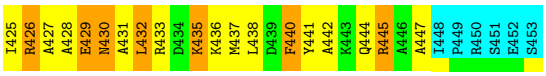
Chain A:

• Molecule 2: Ribonuclease 3

Chain B:







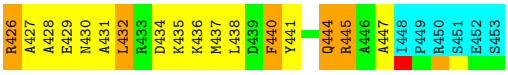
4.2.15 Score per residue for model 15

• Molecule 1: RNA (32-MER)

Chain A:

• Molecule 2: Ribonuclease 3

Chain B:



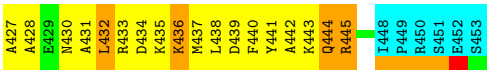
4.2.16 Score per residue for model 16

• Molecule 1: RNA (32-MER)

Chain A:

• Molecule 2: Ribonuclease 3

Chain B:


A427
A428
E429
N430
A431
L432
R433
D434
K435
K436
M437
L438
D439
F440
Y441
A442
K443
Q444
R445
T448
P449
R450
S451
E452
S453

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 16 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	structure solution	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1317
Number of shifts mapped to atoms	1317
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

6 Model quality (i)

6.1 Standard geometry (i)

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	1.13±0.01	0±0/763 (0.0± 0.0%)	1.99±0.01	43±1/1188 (3.7± 0.1%)
2	B	0.27±0.02	0±0/638 (0.0± 0.0%)	0.45±0.02	0±0/859 (0.0± 0.0%)
All	All	0.85	0/22416 (0.0%)	1.55	695/32752 (2.1%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	25	G	N7-C8-N9	9.54	117.87	113.10	10	16
1	A	11	G	N7-C8-N9	9.40	117.80	113.10	16	16
1	A	16	G	N7-C8-N9	9.33	117.77	113.10	6	16
1	A	19	G	N7-C8-N9	9.30	117.75	113.10	10	16
1	A	1	G	N7-C8-N9	9.29	117.74	113.10	16	16
1	A	2	G	N7-C8-N9	9.29	117.74	113.10	12	16
1	A	23	G	N7-C8-N9	9.24	117.72	113.10	1	16
1	A	3	G	N7-C8-N9	9.20	117.70	113.10	8	16
1	A	26	G	N7-C8-N9	9.09	117.65	113.10	7	16
1	A	4	A	N7-C8-N9	7.81	117.70	113.80	7	16
1	A	18	A	N7-C8-N9	7.79	117.70	113.80	13	16
1	A	6	A	N7-C8-N9	7.75	117.67	113.80	9	16
1	A	17	A	N7-C8-N9	7.67	117.64	113.80	12	16
1	A	20	A	N7-C8-N9	7.66	117.63	113.80	15	16
1	A	21	A	N7-C8-N9	7.59	117.60	113.80	4	16
1	A	9	A	N7-C8-N9	7.58	117.59	113.80	10	16
1	A	28	A	N7-C8-N9	7.57	117.59	113.80	9	16
1	A	15	A	N7-C8-N9	7.55	117.58	113.80	12	16
1	A	23	G	C8-N9-C4	-7.05	103.58	106.40	1	16
1	A	25	G	C8-N9-C4	-7.04	103.58	106.40	8	16
1	A	2	G	C8-N9-C4	-6.86	103.66	106.40	12	16
1	A	16	G	C8-N9-C4	-6.84	103.66	106.40	6	16
1	A	1	G	C8-N9-C4	-6.81	103.68	106.40	2	16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	26	G	C8-N9-C4	-6.81	103.68	106.40	9	16
1	A	19	G	C8-N9-C4	-6.80	103.68	106.40	10	16
1	A	11	G	C8-N9-C4	-6.76	103.70	106.40	5	16
1	A	3	G	C8-N9-C4	-6.54	103.78	106.40	13	16
1	A	18	A	C8-N9-C4	-6.11	103.36	105.80	5	16
1	A	20	A	C8-N9-C4	-5.93	103.43	105.80	15	16
1	A	17	A	C8-N9-C4	-5.76	103.49	105.80	11	16
1	A	9	A	C8-N9-C4	-5.74	103.50	105.80	10	16
1	A	15	A	C8-N9-C4	-5.71	103.51	105.80	8	16
1	A	21	A	C8-N9-C4	-5.68	103.53	105.80	7	16
1	A	6	A	C8-N9-C4	-5.66	103.54	105.80	8	16
1	A	4	A	C8-N9-C4	-5.54	103.58	105.80	8	16
1	A	28	A	C8-N9-C4	-5.53	103.59	105.80	10	15
1	A	25	G	C5-N7-C8	-5.41	101.59	104.30	10	10
1	A	11	G	C5-N7-C8	-5.30	101.65	104.30	16	14
1	A	2	G	C5-N7-C8	-5.26	101.67	104.30	8	13
1	A	19	G	C5-N7-C8	-5.25	101.67	104.30	12	15
1	A	3	G	C5-N7-C8	-5.25	101.67	104.30	5	16
1	A	23	G	C5-N7-C8	-5.25	101.67	104.30	3	14
1	A	1	G	C5-N7-C8	-5.21	101.69	104.30	16	14
1	A	16	G	C5-N7-C8	-5.20	101.70	104.30	13	12
1	A	26	G	C5-N7-C8	-5.17	101.71	104.30	1	12

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	682	346	346	94±10
2	B	630	664	663	126±9
All	All	20992	16160	16144	3434

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 92.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:370:ALA:HB3	2:B:428:ALA:HB1	1.03	1.25	15	2
2:B:374:LEU:HD11	2:B:428:ALA:HB2	1.01	1.32	16	4
2:B:370:ALA:HB1	2:B:428:ALA:HB1	1.00	1.28	14	14
2:B:380:TYR:CB	2:B:383:LEU:HD22	0.98	1.88	13	1
2:B:374:LEU:HD11	2:B:428:ALA:CB	0.97	1.88	16	5
2:B:370:ALA:HB1	2:B:428:ALA:CB	0.97	1.90	6	13
2:B:401:ILE:HD12	2:B:416:VAL:HG23	0.94	1.35	11	2
1:A:29:U:O2'	1:A:30:C:H5'	0.94	1.62	9	14
1:A:1:G:HO2'	1:A:2:G:H8	0.94	1.01	15	2
1:A:30:C:O2'	1:A:31:U:H5'	0.94	1.61	4	16
2:B:374:LEU:HD12	2:B:385:LEU:HD21	0.94	1.38	15	1
2:B:388:VAL:HG23	2:B:403:GLU:CB	0.92	1.95	9	10
1:A:12:U:O2'	1:A:13:U:H5'	0.91	1.66	8	15
1:A:2:G:O2'	1:A:3:G:H5'	0.88	1.67	8	10
2:B:370:ALA:CB	2:B:428:ALA:HB1	0.88	1.97	15	3
2:B:390:VAL:HG23	2:B:401:ILE:HG23	0.88	1.43	16	15
2:B:385:LEU:HD22	2:B:386:HIS:N	0.87	1.83	15	1
1:A:20:A:O2'	1:A:21:A:H5'	0.86	1.70	10	12
2:B:412:LEU:HD12	2:B:437:MET:SD	0.86	2.10	4	10
2:B:419:ASN:O	2:B:420:ILE:HG23	0.86	1.69	15	3
2:B:370:ALA:HB1	2:B:428:ALA:HB3	0.86	1.44	10	8
2:B:388:VAL:HG23	2:B:403:GLU:HB2	0.85	1.48	9	4
1:A:15:A:O2'	1:A:16:G:H5'	0.84	1.72	13	7
1:A:15:A:H2'	1:A:16:G:O4'	0.84	1.71	6	11
2:B:373:GLN:O	2:B:378:ILE:HG23	0.84	1.70	15	1
1:A:27:U:O2'	1:A:28:A:H5'	0.84	1.72	12	16
2:B:406:VAL:HG13	2:B:412:LEU:HD21	0.84	1.49	4	7
2:B:432:LEU:HA	2:B:438:LEU:HD11	0.84	1.49	9	15
2:B:373:GLN:NE2	2:B:438:LEU:HD22	0.84	1.87	15	3
1:A:30:C:O2'	2:B:396:VAL:HG12	0.83	1.73	4	2
2:B:417:GLY:HA3	2:B:422:ILE:HD13	0.83	1.50	5	16
1:A:1:G:HO5'	1:A:1:G:H8	0.83	0.88	5	2
2:B:383:LEU:HD11	2:B:385:LEU:HB2	0.83	1.48	7	2
2:B:429:GLU:HA	2:B:432:LEU:HD22	0.83	1.49	9	4
1:A:9:A:O2'	1:A:10:U:H5'	0.83	1.74	16	4
2:B:374:LEU:HD13	2:B:387:TYR:OH	0.82	1.74	7	7
1:A:17:A:H1'	1:A:18:A:OP1	0.82	1.73	13	2
2:B:401:ILE:HD12	2:B:416:VAL:CG2	0.82	2.04	11	2
2:B:388:VAL:HG23	2:B:403:GLU:HB3	0.81	1.52	14	8
2:B:385:LEU:HD13	2:B:385:LEU:O	0.81	1.74	15	1
1:A:1:G:O2'	1:A:2:G:H5'	0.81	1.75	9	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:G:O2'	1:A:20:A:H5'	0.81	1.75	3	3
2:B:373:GLN:OE1	2:B:377:LEU:HD23	0.81	1.76	11	3
2:B:402:VAL:HG21	2:B:423:ALA:O	0.81	1.76	15	16
2:B:380:TYR:HB3	2:B:383:LEU:HD22	0.80	1.51	13	1
2:B:432:LEU:C	2:B:432:LEU:HD23	0.80	1.96	10	7
2:B:383:LEU:HD22	2:B:383:LEU:O	0.80	1.77	7	2
1:A:29:U:H2'	1:A:30:C:O4'	0.80	1.77	8	8
2:B:377:LEU:O	2:B:378:ILE:HD13	0.80	1.76	14	9
2:B:410:THR:HG21	2:B:441:TYR:OH	0.79	1.76	11	3
1:A:20:A:H2'	1:A:21:A:O4'	0.78	1.78	5	10
1:A:22:C:O5'	1:A:22:C:H6	0.78	1.61	1	14
2:B:383:LEU:O	2:B:383:LEU:HD23	0.78	1.78	14	4
2:B:428:ALA:O	2:B:432:LEU:HD13	0.77	1.79	5	2
1:A:13:U:O2'	1:A:14:C:H5'	0.77	1.80	6	7
1:A:31:U:O2'	1:A:32:C:H5'	0.76	1.80	13	5
1:A:3:G:HO2'	1:A:4:A:C5'	0.76	1.93	1	8
2:B:420:ILE:O	2:B:423:ALA:HB3	0.76	1.81	15	16
2:B:425:ILE:HD13	2:B:425:ILE:N	0.76	1.96	3	5
1:A:12:U:H6	1:A:12:U:O5'	0.76	1.63	7	11
1:A:10:U:O5'	1:A:10:U:H6	0.76	1.63	4	2
1:A:22:C:O2'	1:A:23:G:H5'	0.76	1.81	1	14
2:B:383:LEU:HD22	2:B:384:ARG:N	0.76	1.94	10	1
2:B:380:TYR:CD1	2:B:383:LEU:HD12	0.75	2.16	1	2
1:A:17:A:O5'	1:A:17:A:H8	0.75	1.64	6	2
2:B:401:ILE:HB	2:B:416:VAL:HG22	0.75	1.59	11	1
2:B:383:LEU:HD13	2:B:383:LEU:C	0.75	2.02	11	2
2:B:380:TYR:HB2	2:B:383:LEU:HD22	0.75	1.59	13	1
1:A:14:C:C5	1:A:15:A:C8	0.74	2.75	10	9
2:B:402:VAL:CG2	2:B:423:ALA:HB1	0.74	2.13	5	8
2:B:385:LEU:HG	2:B:406:VAL:HG12	0.74	1.57	4	6
1:A:21:A:HO2'	1:A:22:C:H6	0.73	1.20	1	4
1:A:1:G:H8	1:A:1:G:O5'	0.73	1.66	14	2
2:B:373:GLN:CD	2:B:377:LEU:HD23	0.73	2.03	15	1
1:A:6:A:O2'	1:A:7:C:H5'	0.73	1.84	12	5
2:B:412:LEU:HD13	2:B:412:LEU:N	0.73	1.97	1	7
1:A:23:G:O2'	1:A:24:U:H5'	0.73	1.83	7	16
2:B:383:LEU:HD12	2:B:384:ARG:N	0.72	1.99	15	1
1:A:22:C:H6	1:A:22:C:O5'	0.72	1.66	3	2
2:B:402:VAL:HG21	2:B:423:ALA:C	0.72	2.03	5	14
2:B:366:LEU:HD23	2:B:369:ASN:ND2	0.72	2.00	6	1
1:A:17:A:H4'	1:A:18:A:OP1	0.72	1.83	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:A:O2'	1:A:18:A:P	0.71	2.48	8	5
2:B:411:VAL:HG12	2:B:411:VAL:O	0.71	1.84	11	2
1:A:5:U:H6	1:A:5:U:O5'	0.71	1.67	12	5
1:A:15:A:C6	1:A:16:G:C8	0.71	2.79	12	11
2:B:417:GLY:CA	2:B:422:ILE:HD13	0.71	2.16	8	16
1:A:24:U:H6	1:A:24:U:O5'	0.71	1.68	9	10
1:A:18:A:H2'	1:A:19:G:O4'	0.70	1.85	13	9
2:B:432:LEU:C	2:B:438:LEU:HD11	0.70	2.06	13	2
1:A:26:G:HO2'	1:A:27:U:C5'	0.70	1.98	2	9
2:B:374:LEU:HD23	2:B:374:LEU:N	0.70	2.01	14	10
2:B:366:LEU:HD23	2:B:366:LEU:O	0.70	1.86	1	1
1:A:14:C:C4	1:A:15:A:C4	0.70	2.79	15	4
1:A:8:C:N4	1:A:9:A:N6	0.69	2.39	8	12
1:A:28:A:O2'	1:A:29:U:C6	0.69	2.45	8	2
1:A:15:A:C6	1:A:16:G:N7	0.69	2.60	2	6
2:B:401:ILE:HD12	2:B:415:GLY:O	0.69	1.88	16	2
2:B:432:LEU:HD23	2:B:433:ARG:N	0.69	2.03	11	5
2:B:406:VAL:HG23	2:B:410:THR:HB	0.69	1.62	2	3
2:B:404:CYS:SG	2:B:431:ALA:HB2	0.69	2.26	3	3
2:B:385:LEU:HA	2:B:406:VAL:HG12	0.69	1.64	3	11
2:B:432:LEU:CA	2:B:438:LEU:HD11	0.69	2.17	6	13
2:B:366:LEU:HD12	2:B:367:ASP:N	0.69	2.03	15	1
1:A:15:A:C5	1:A:16:G:C8	0.69	2.81	8	14
2:B:431:ALA:O	2:B:438:LEU:HD21	0.68	1.87	4	4
2:B:391:LYS:HB2	2:B:401:ILE:HG22	0.68	1.64	8	9
2:B:432:LEU:HA	2:B:438:LEU:HD21	0.68	1.65	16	7
2:B:378:ILE:O	2:B:383:LEU:HD13	0.68	1.87	1	2
2:B:379:GLY:CA	2:B:383:LEU:HD21	0.68	2.19	15	1
1:A:17:A:O2'	1:A:18:A:N9	0.68	2.27	13	4
2:B:383:LEU:HD22	2:B:383:LEU:C	0.68	2.09	10	2
2:B:383:LEU:HD13	2:B:384:ARG:N	0.68	2.04	16	3
1:A:12:U:O2'	1:A:13:U:C5'	0.68	2.42	7	16
1:A:23:G:O2'	1:A:24:U:C5'	0.67	2.42	7	15
2:B:385:LEU:HD13	2:B:385:LEU:C	0.67	2.10	15	1
1:A:1:G:O5'	1:A:1:G:C8	0.67	2.46	14	1
1:A:4:A:C6	1:A:5:U:C4	0.67	2.82	9	1
1:A:15:A:O2'	1:A:18:A:N1	0.67	2.26	10	6
1:A:13:U:O2'	1:A:14:C:C5'	0.67	2.43	14	16
1:A:26:G:O2'	1:A:27:U:H5'	0.67	1.90	16	5
1:A:23:G:C6	1:A:24:U:C4	0.67	2.83	16	3
1:A:18:A:C2	2:B:372:ARG:CZ	0.67	2.78	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:380:TYR:CE1	2:B:383:LEU:HD12	0.67	2.25	10	2
2:B:380:TYR:CD2	2:B:383:LEU:HD12	0.67	2.25	14	2
1:A:19:G:C2	2:B:372:ARG:NH2	0.67	2.63	10	2
1:A:14:C:N4	1:A:15:A:C5	0.66	2.64	13	2
2:B:419:ASN:O	2:B:421:LYS:N	0.66	2.28	14	13
1:A:17:A:O2'	1:A:18:A:C1'	0.66	2.44	13	6
2:B:379:GLY:HA2	2:B:383:LEU:HD21	0.66	1.67	15	2
1:A:1:G:C2	1:A:2:G:C5	0.66	2.82	15	3
1:A:11:G:O2'	1:A:12:U:C5'	0.66	2.44	12	16
1:A:20:A:O5'	1:A:20:A:H8	0.66	1.72	5	11
1:A:9:A:O2'	1:A:10:U:C5'	0.66	2.43	16	5
2:B:380:TYR:O	2:B:381:ALA:HB2	0.66	1.90	3	4
2:B:406:VAL:HG22	2:B:410:THR:HB	0.66	1.66	11	1
2:B:378:ILE:HG22	2:B:383:LEU:HD11	0.66	1.67	1	2
1:A:28:A:O2'	1:A:29:U:C5'	0.66	2.44	3	14
1:A:15:A:O2'	1:A:18:A:N6	0.66	2.27	11	4
2:B:373:GLN:HE22	2:B:438:LEU:HD22	0.66	1.50	10	2
1:A:18:A:H8	1:A:18:A:O5'	0.66	1.74	15	3
2:B:367:ASP:HB3	2:B:425:ILE:HG23	0.66	1.68	9	1
1:A:21:A:O2'	1:A:22:C:C6	0.66	2.49	2	4
2:B:423:ALA:O	2:B:427:ALA:HB2	0.66	1.90	5	3
1:A:19:G:C4	2:B:372:ARG:NH2	0.65	2.63	5	2
1:A:7:C:O5'	1:A:7:C:H6	0.65	1.74	11	9
1:A:6:A:O2'	1:A:7:C:C5'	0.65	2.44	12	6
1:A:15:A:C5	1:A:16:G:N7	0.65	2.64	15	7
2:B:420:ILE:C	2:B:420:ILE:HD12	0.65	2.11	7	8
1:A:30:C:O2'	1:A:31:U:C5'	0.65	2.44	3	14
1:A:3:G:C2	1:A:4:A:C5	0.65	2.85	7	2
1:A:30:C:C4	1:A:31:U:C5	0.65	2.85	5	10
2:B:402:VAL:HG23	2:B:415:GLY:O	0.65	1.91	11	4
1:A:1:G:C8	1:A:1:G:O5'	0.65	2.48	5	3
2:B:376:SER:O	2:B:377:LEU:HD12	0.65	1.91	5	1
1:A:19:G:O2'	1:A:20:A:C5'	0.65	2.44	3	7
1:A:27:U:O2'	1:A:28:A:C5'	0.65	2.44	14	10
2:B:420:ILE:HD12	2:B:420:ILE:C	0.65	2.13	3	4
1:A:18:A:C5	2:B:372:ARG:NH2	0.65	2.65	5	1
1:A:17:A:C2	2:B:372:ARG:NH1	0.65	2.65	15	1
1:A:22:C:O2'	1:A:23:G:C5'	0.65	2.44	1	13
2:B:370:ALA:O	2:B:373:GLN:N	0.65	2.30	15	16
1:A:3:G:O2'	1:A:4:A:C5'	0.64	2.43	11	13
1:A:31:U:O2'	1:A:32:C:C5'	0.64	2.45	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:367:ASP:HA	2:B:425:ILE:HG23	0.64	1.67	5	2
1:A:1:G:C2	1:A:2:G:N7	0.64	2.65	7	2
1:A:10:U:O2'	1:A:11:G:C5'	0.64	2.46	1	12
1:A:18:A:N3	2:B:372:ARG:CG	0.64	2.60	1	4
2:B:419:ASN:O	2:B:420:ILE:CG2	0.64	2.44	15	3
2:B:373:GLN:CG	2:B:432:LEU:HD12	0.64	2.22	13	1
2:B:401:ILE:HD12	2:B:415:GLY:C	0.64	2.13	16	1
1:A:10:U:H6	1:A:10:U:O5'	0.64	1.74	11	8
2:B:374:LEU:HD13	2:B:387:TYR:CZ	0.64	2.27	16	1
1:A:20:A:O2'	1:A:21:A:C5'	0.64	2.45	8	13
2:B:370:ALA:HA	2:B:432:LEU:HD22	0.64	1.70	1	2
2:B:370:ALA:HA	2:B:432:LEU:HD13	0.64	1.68	9	1
1:A:18:A:N3	2:B:372:ARG:NE	0.64	2.46	10	2
1:A:14:C:N4	1:A:15:A:C4	0.64	2.65	8	4
2:B:380:TYR:CE1	2:B:382:SER:O	0.64	2.51	7	1
1:A:11:G:C2	1:A:23:G:C2	0.64	2.86	10	2
1:A:26:G:O2'	1:A:27:U:C5'	0.64	2.46	16	11
1:A:15:A:O2'	1:A:16:G:C5'	0.64	2.46	13	2
1:A:1:G:N3	1:A:2:G:C8	0.63	2.65	7	3
2:B:419:ASN:C	2:B:420:ILE:HG23	0.63	2.14	6	3
2:B:370:ALA:HB2	2:B:432:LEU:CD1	0.63	2.22	15	1
1:A:14:C:H2'	1:A:15:A:O4'	0.63	1.93	7	12
1:A:29:U:O2'	1:A:30:C:C5'	0.63	2.46	12	9
2:B:421:LYS:CD	2:B:422:ILE:N	0.63	2.62	8	9
1:A:24:U:C2	1:A:25:G:N7	0.63	2.67	10	1
2:B:375:TYR:CE1	2:B:385:LEU:CD1	0.63	2.81	15	1
1:A:12:U:H2'	1:A:13:U:O4'	0.63	1.94	8	3
2:B:380:TYR:O	2:B:381:ALA:HB3	0.63	1.94	8	2
2:B:421:LYS:HD3	2:B:422:ILE:N	0.63	2.09	3	9
1:A:28:A:HO2'	1:A:29:U:C5'	0.63	2.06	9	3
2:B:387:TYR:HB2	2:B:404:CYS:HA	0.63	1.71	12	1
1:A:30:C:N4	1:A:31:U:C4	0.62	2.67	1	10
2:B:420:ILE:HD12	2:B:421:LYS:N	0.62	2.08	3	8
2:B:424:GLY:O	2:B:427:ALA:HB3	0.62	1.93	7	9
2:B:370:ALA:CB	2:B:428:ALA:HB3	0.62	2.22	10	4
2:B:366:LEU:HD12	2:B:369:ASN:ND2	0.62	2.10	9	1
1:A:4:A:O2'	1:A:5:U:C5'	0.62	2.47	14	4
1:A:19:G:N3	2:B:372:ARG:CZ	0.62	2.62	5	2
2:B:366:LEU:HD23	2:B:369:ASN:HD22	0.62	1.53	6	1
2:B:366:LEU:HD12	2:B:367:ASP:H	0.62	1.52	15	1
1:A:1:G:O2'	1:A:2:G:H8	0.62	1.74	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:A:C2'	1:A:19:G:O4'	0.62	2.48	1	10
2:B:419:ASN:H	2:B:422:ILE:HD11	0.62	1.54	7	14
1:A:17:A:C8	1:A:18:A:C2	0.62	2.88	5	1
2:B:385:LEU:HD23	2:B:386:HIS:N	0.62	2.10	14	2
1:A:18:A:O2'	1:A:19:G:O4'	0.62	2.17	11	8
2:B:383:LEU:HD22	2:B:385:LEU:HB2	0.62	1.70	14	1
2:B:422:ILE:O	2:B:426:ARG:CB	0.62	2.48	9	16
1:A:18:A:O2'	1:A:19:G:OP1	0.61	2.15	11	1
2:B:374:LEU:HD12	2:B:385:LEU:HD11	0.61	1.72	12	1
2:B:374:LEU:CD1	2:B:385:LEU:HD21	0.61	2.20	15	1
1:A:7:C:H6	1:A:7:C:O5'	0.61	1.78	4	1
1:A:17:A:O5'	1:A:17:A:C8	0.61	2.53	8	3
2:B:425:ILE:N	2:B:425:ILE:HD12	0.61	2.09	4	3
2:B:432:LEU:O	2:B:438:LEU:HD11	0.61	1.96	13	1
1:A:11:G:O2'	1:A:12:U:O5'	0.61	2.19	15	16
1:A:27:U:H6	1:A:27:U:O5'	0.61	1.78	12	5
2:B:374:LEU:HD21	2:B:432:LEU:HD23	0.61	1.69	4	2
2:B:429:GLU:O	2:B:432:LEU:N	0.61	2.33	13	2
2:B:383:LEU:HD13	2:B:384:ARG:H	0.61	1.54	10	1
1:A:11:G:O2'	1:A:12:U:O4'	0.61	2.18	15	13
2:B:380:TYR:CD1	2:B:445:ARG:CD	0.61	2.83	7	2
2:B:420:ILE:O	2:B:423:ALA:N	0.61	2.34	13	16
1:A:15:A:C2	1:A:19:G:O6	0.61	2.53	13	2
1:A:3:G:O2'	1:A:4:A:O5'	0.61	2.19	7	13
2:B:402:VAL:HB	2:B:427:ALA:HB2	0.61	1.72	2	6
2:B:370:ALA:HB2	2:B:432:LEU:HD13	0.60	1.73	15	1
2:B:368:MET:CE	2:B:369:ASN:ND2	0.60	2.64	5	4
1:A:20:A:C2	1:A:21:A:C4	0.60	2.89	12	5
2:B:377:LEU:C	2:B:378:ILE:HD13	0.60	2.16	8	3
1:A:16:G:N2	1:A:16:G:OP2	0.60	2.34	9	10
1:A:17:A:O2'	1:A:18:A:O4'	0.60	2.19	5	11
1:A:2:G:O2'	1:A:3:G:C5'	0.60	2.47	8	2
1:A:28:A:O2'	1:A:29:U:O5'	0.60	2.19	12	16
2:B:405:ARG:HB2	2:B:411:VAL:HG22	0.60	1.74	12	2
1:A:2:G:C6	1:A:3:G:C5	0.60	2.89	5	4
1:A:11:G:HO2'	1:A:12:U:C5'	0.60	2.10	7	7
2:B:401:ILE:HB	2:B:416:VAL:HG23	0.60	1.74	9	3
1:A:10:U:O2'	1:A:11:G:O5'	0.60	2.19	16	5
1:A:18:A:O3'	1:A:19:G:C8	0.60	2.54	11	1
1:A:21:A:O2'	1:A:22:C:O5'	0.60	2.20	12	13
1:A:18:A:N3	2:B:372:ARG:CZ	0.60	2.65	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:421:LYS:HG2	2:B:425:ILE:HD13	0.60	1.72	10	1
2:B:374:LEU:N	2:B:374:LEU:CD2	0.60	2.64	15	5
1:A:4:A:C5	1:A:5:U:C4	0.60	2.90	9	1
2:B:401:ILE:HD12	2:B:416:VAL:HB	0.59	1.72	9	3
1:A:16:G:H1'	1:A:17:A:OP2	0.59	1.97	14	2
2:B:373:GLN:HG3	2:B:432:LEU:HD12	0.59	1.74	13	1
1:A:17:A:C1'	1:A:18:A:OP1	0.59	2.49	5	2
2:B:402:VAL:O	2:B:414:THR:HG22	0.59	1.96	10	5
1:A:17:A:O2'	1:A:18:A:O5'	0.59	2.20	5	4
2:B:444:GLN:HG3	2:B:445:ARG:N	0.59	2.11	9	3
1:A:16:G:H5"	1:A:17:A:N7	0.59	2.12	4	3
2:B:407:GLY:O	2:B:408:ASP:CB	0.59	2.49	8	1
2:B:373:GLN:CB	2:B:432:LEU:HD12	0.59	2.27	13	1
2:B:372:ARG:O	2:B:376:SER:CB	0.59	2.51	11	15
2:B:405:ARG:HA	2:B:410:THR:O	0.59	1.97	7	14
2:B:432:LEU:C	2:B:432:LEU:CD2	0.59	2.70	15	7
1:A:13:U:O2'	1:A:14:C:O4'	0.59	2.19	16	10
2:B:376:SER:C	2:B:377:LEU:HD12	0.59	2.18	5	1
2:B:429:GLU:O	2:B:432:LEU:CD2	0.59	2.50	10	5
1:A:18:A:O3'	1:A:19:G:H8	0.59	1.80	11	1
1:A:3:G:O2'	1:A:4:A:H5'	0.59	1.98	11	8
2:B:435:LYS:CG	2:B:436:LYS:N	0.59	2.65	12	14
2:B:381:ALA:O	2:B:383:LEU:N	0.59	2.35	9	1
1:A:30:C:C4	1:A:31:U:C4	0.59	2.91	6	10
1:A:31:U:O2'	1:A:32:C:O5'	0.59	2.21	1	7
1:A:13:U:O2'	1:A:14:C:O5'	0.59	2.21	4	13
1:A:20:A:O2'	1:A:21:A:O5'	0.59	2.21	14	3
1:A:16:G:OP2	1:A:16:G:N2	0.59	2.36	4	3
2:B:406:VAL:CG1	2:B:412:LEU:HD21	0.59	2.24	4	6
1:A:1:G:O2'	1:A:2:G:O5'	0.59	2.21	4	6
1:A:24:U:O2'	1:A:25:G:O5'	0.59	2.17	10	3
2:B:415:GLY:CA	2:B:426:ARG:CG	0.59	2.81	4	9
2:B:374:LEU:HD11	2:B:428:ALA:HB1	0.59	1.72	3	1
2:B:378:ILE:HG23	2:B:441:TYR:CB	0.59	2.28	3	4
1:A:18:A:C3'	1:A:19:G:C8	0.59	2.86	11	1
2:B:375:TYR:CE1	2:B:385:LEU:HD11	0.59	2.32	15	1
1:A:22:C:O5'	1:A:22:C:C6	0.58	2.53	2	11
1:A:6:A:O2'	1:A:7:C:O5'	0.58	2.21	13	4
1:A:18:A:N3	2:B:372:ARG:HG2	0.58	2.14	1	3
2:B:382:SER:O	2:B:383:LEU:CB	0.58	2.51	7	1
1:A:20:A:OP1	2:B:375:TYR:CE2	0.58	2.57	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:A:O2'	1:A:22:C:O4'	0.58	2.21	1	7
2:B:378:ILE:O	2:B:378:ILE:HG22	0.58	1.99	1	1
2:B:385:LEU:HD21	2:B:387:TYR:CE1	0.58	2.33	7	1
1:A:16:G:O2'	1:A:17:A:P	0.58	2.61	13	2
2:B:368:MET:CE	2:B:369:ASN:CB	0.58	2.81	2	1
1:A:23:G:O2'	1:A:24:U:O5'	0.58	2.21	6	13
2:B:429:GLU:CA	2:B:432:LEU:HD22	0.58	2.28	9	3
1:A:16:G:H4'	1:A:17:A:OP2	0.58	1.97	16	3
2:B:374:LEU:HD13	2:B:387:TYR:HH	0.58	1.58	2	1
2:B:387:TYR:CB	2:B:404:CYS:HA	0.58	2.29	12	1
1:A:19:G:O2'	1:A:20:A:O4'	0.57	2.20	2	10
1:A:25:G:C6	1:A:26:G:C6	0.57	2.92	1	12
1:A:26:G:O2'	1:A:27:U:O5'	0.57	2.22	11	11
2:B:380:TYR:CE2	2:B:381:ALA:O	0.57	2.57	1	1
1:A:14:C:N4	1:A:15:A:C2	0.57	2.72	15	1
2:B:420:ILE:O	2:B:423:ALA:CB	0.57	2.52	4	16
2:B:380:TYR:CD1	2:B:445:ARG:HD2	0.57	2.34	6	1
1:A:15:A:C2'	1:A:16:G:O5'	0.57	2.53	11	2
2:B:380:TYR:O	2:B:381:ALA:CB	0.57	2.51	9	5
2:B:402:VAL:HG23	2:B:423:ALA:HB1	0.57	1.74	5	2
1:A:17:A:H4'	1:A:18:A:OP2	0.57	1.99	13	1
2:B:380:TYR:CD2	2:B:381:ALA:O	0.57	2.58	1	1
2:B:381:ALA:O	2:B:382:SER:CB	0.57	2.53	1	4
1:A:18:A:C4	2:B:372:ARG:CZ	0.57	2.87	5	1
1:A:16:G:C1'	1:A:17:A:OP2	0.57	2.52	11	2
1:A:4:A:O2'	1:A:5:U:O5'	0.57	2.23	14	8
2:B:428:ALA:O	2:B:432:LEU:HD23	0.57	1.99	2	4
1:A:17:A:C4'	1:A:18:A:OP1	0.57	2.52	6	4
2:B:383:LEU:HD23	2:B:383:LEU:C	0.57	2.19	14	2
1:A:31:U:O2'	1:A:32:C:O4'	0.57	2.20	10	3
2:B:383:LEU:HD12	2:B:441:TYR:CE1	0.57	2.34	8	2
2:B:429:GLU:O	2:B:432:LEU:HD22	0.57	1.99	10	3
2:B:390:VAL:HG23	2:B:401:ILE:CG2	0.57	2.30	2	5
1:A:8:C:C4	1:A:9:A:N7	0.57	2.73	2	11
1:A:16:G:C4'	1:A:17:A:OP2	0.57	2.53	14	4
1:A:11:G:N3	1:A:23:G:C2	0.57	2.72	16	2
2:B:370:ALA:CB	2:B:428:ALA:CB	0.56	2.80	13	8
2:B:421:LYS:O	2:B:424:GLY:N	0.56	2.38	16	13
2:B:380:TYR:CD2	2:B:445:ARG:CD	0.56	2.88	10	1
2:B:401:ILE:CD1	2:B:416:VAL:CG2	0.56	2.81	11	2
1:A:21:A:O5'	1:A:21:A:H8	0.56	1.83	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:C:O2'	1:A:9:A:O5'	0.56	2.22	16	1
2:B:380:TYR:CG	2:B:445:ARG:CG	0.56	2.89	1	1
2:B:390:VAL:O	2:B:391:LYS:CB	0.56	2.53	2	16
1:A:6:A:HO2'	1:A:7:C:C5'	0.56	2.13	6	3
1:A:1:G:N2	1:A:2:G:C5	0.56	2.73	7	2
1:A:1:G:N2	1:A:2:G:C4	0.56	2.72	15	2
2:B:374:LEU:O	2:B:379:GLY:N	0.56	2.37	7	1
2:B:405:ARG:CG	2:B:410:THR:O	0.56	2.53	10	1
2:B:387:TYR:OH	2:B:431:ALA:CB	0.56	2.54	15	1
2:B:399:ASN:HA	2:B:417:GLY:O	0.56	2.01	2	15
2:B:412:LEU:N	2:B:412:LEU:HD13	0.56	2.16	3	5
1:A:20:A:O2'	1:A:21:A:O4'	0.56	2.22	6	2
1:A:7:C:N4	1:A:8:C:N4	0.56	2.53	11	2
1:A:18:A:N1	2:B:368:MET:SD	0.56	2.79	16	1
1:A:1:G:O2'	1:A:2:G:C5'	0.56	2.53	4	2
1:A:24:U:O5'	1:A:24:U:H6	0.56	1.84	8	3
2:B:380:TYR:CD2	2:B:382:SER:OG	0.56	2.57	10	1
1:A:9:A:O2'	1:A:10:U:O5'	0.56	2.24	8	3
2:B:385:LEU:C	2:B:385:LEU:HD23	0.56	2.21	16	5
2:B:387:TYR:CZ	2:B:404:CYS:SG	0.56	2.98	16	3
2:B:380:TYR:CD2	2:B:445:ARG:HD2	0.56	2.36	10	1
2:B:367:ASP:O	2:B:370:ALA:N	0.56	2.39	2	13
2:B:370:ALA:HB3	2:B:428:ALA:CB	0.56	2.31	9	1
2:B:419:ASN:OD1	2:B:422:ILE:HD11	0.56	2.00	9	3
2:B:385:LEU:HD22	2:B:385:LEU:C	0.56	2.22	15	1
2:B:383:LEU:O	2:B:383:LEU:HD13	0.55	2.01	11	1
1:A:30:C:O2'	2:B:395:ALA:O	0.55	2.24	12	1
1:A:3:G:N3	1:A:4:A:C8	0.55	2.74	7	1
2:B:425:ILE:O	2:B:428:ALA:N	0.55	2.40	12	8
2:B:374:LEU:N	2:B:374:LEU:HD23	0.55	2.16	15	1
2:B:380:TYR:CD1	2:B:445:ARG:HG2	0.55	2.37	1	3
1:A:4:A:HO2'	1:A:5:U:C5'	0.55	2.15	6	4
1:A:21:A:O2'	1:A:22:C:C5'	0.55	2.54	3	6
1:A:8:C:N4	1:A:9:A:C6	0.55	2.74	10	1
2:B:383:LEU:HD23	2:B:384:ARG:H	0.55	1.62	13	1
1:A:7:C:C4	1:A:8:C:N4	0.55	2.74	1	3
2:B:422:ILE:O	2:B:426:ARG:HB3	0.55	2.02	6	14
2:B:419:ASN:O	2:B:420:ILE:CG1	0.55	2.54	9	3
2:B:440:PHE:CE2	2:B:441:TYR:CE1	0.55	2.94	6	1
2:B:368:MET:CE	2:B:369:ASN:N	0.55	2.70	11	1
2:B:373:GLN:NE2	2:B:378:ILE:CG2	0.55	2.70	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:A:N7	1:A:16:G:N7	0.55	2.54	8	3
2:B:404:CYS:O	2:B:412:LEU:N	0.55	2.40	4	9
2:B:391:LYS:O	2:B:392:LYS:C	0.55	2.46	1	15
2:B:425:ILE:N	2:B:425:ILE:CD1	0.55	2.67	9	9
2:B:380:TYR:CD1	2:B:445:ARG:HD3	0.55	2.36	7	3
2:B:401:ILE:CG1	2:B:415:GLY:O	0.55	2.55	7	2
2:B:399:ASN:O	2:B:399:ASN:ND2	0.54	2.40	2	6
2:B:415:GLY:HA3	2:B:426:ARG:CG	0.54	2.33	4	5
2:B:386:HIS:O	2:B:405:ARG:O	0.54	2.25	4	10
2:B:380:TYR:CZ	2:B:383:LEU:HG	0.54	2.38	11	1
2:B:411:VAL:O	2:B:413:GLY:N	0.54	2.40	11	1
2:B:429:GLU:O	2:B:431:ALA:N	0.54	2.40	13	2
2:B:422:ILE:N	2:B:422:ILE:HD12	0.54	2.17	15	15
1:A:27:U:O5'	1:A:27:U:H6	0.54	1.86	2	5
2:B:405:ARG:CB	2:B:410:THR:O	0.54	2.56	4	6
1:A:17:A:N3	2:B:372:ARG:NH1	0.54	2.56	15	1
2:B:380:TYR:CE1	2:B:445:ARG:HD3	0.54	2.37	7	1
2:B:383:LEU:C	2:B:383:LEU:CD1	0.54	2.75	16	2
2:B:404:CYS:O	2:B:404:CYS:SG	0.54	2.66	12	1
1:A:27:U:C2'	1:A:28:A:O5'	0.54	2.56	14	13
1:A:28:A:O2'	1:A:29:U:H5'	0.54	2.02	4	8
2:B:412:LEU:N	2:B:412:LEU:CD1	0.54	2.70	5	5
2:B:428:ALA:O	2:B:432:LEU:CD2	0.54	2.56	8	3
2:B:380:TYR:CE1	2:B:445:ARG:NE	0.54	2.76	6	1
2:B:411:VAL:HG12	2:B:412:LEU:N	0.54	2.17	10	1
1:A:17:A:O2'	1:A:18:A:C8	0.54	2.60	13	5
2:B:404:CYS:O	2:B:412:LEU:HD22	0.54	2.02	1	1
1:A:17:A:N7	1:A:18:A:C2	0.54	2.76	5	1
2:B:422:ILE:O	2:B:426:ARG:CG	0.54	2.55	15	2
2:B:370:ALA:HB2	2:B:429:GLU:OE2	0.54	2.01	14	1
2:B:386:HIS:CB	2:B:405:ARG:O	0.54	2.56	10	3
1:A:16:G:N3	1:A:16:G:H2'	0.54	2.18	2	5
2:B:429:GLU:O	2:B:433:ARG:CG	0.54	2.56	10	1
1:A:10:U:O2'	1:A:11:G:H5'	0.54	2.03	5	9
2:B:368:MET:HE1	2:B:369:ASN:HB3	0.54	1.80	2	1
2:B:380:TYR:OH	2:B:382:SER:CB	0.54	2.55	6	1
2:B:411:VAL:O	2:B:412:LEU:CB	0.54	2.55	10	1
2:B:404:CYS:HG	2:B:413:GLY:C	0.54	2.05	13	2
2:B:418:ARG:CG	2:B:419:ASN:OD1	0.54	2.56	2	3
1:A:3:G:C4	1:A:4:A:N7	0.54	2.76	7	1
2:B:398:PRO:CB	2:B:418:ARG:O	0.54	2.56	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:378:ILE:O	2:B:383:LEU:CD1	0.53	2.56	1	2
1:A:8:C:N4	1:A:9:A:H62	0.53	1.99	3	10
2:B:440:PHE:CE2	2:B:441:TYR:CZ	0.53	2.96	15	2
1:A:8:C:O2'	1:A:9:A:C8	0.53	2.61	16	1
2:B:419:ASN:OD1	2:B:419:ASN:N	0.53	2.41	16	1
2:B:391:LYS:O	2:B:392:LYS:O	0.53	2.27	2	12
1:A:15:A:C2'	1:A:18:A:H61	0.53	2.14	11	4
2:B:367:ASP:HB3	2:B:425:ILE:HD12	0.53	1.79	8	1
2:B:405:ARG:CA	2:B:410:THR:O	0.53	2.56	4	12
1:A:4:A:C5	1:A:5:U:C5	0.53	2.96	9	1
1:A:18:A:N3	2:B:372:ARG:HG3	0.53	2.18	5	5
2:B:428:ALA:O	2:B:432:LEU:CD1	0.53	2.56	5	1
1:A:1:G:N3	1:A:2:G:N7	0.53	2.57	15	2
2:B:440:PHE:CD1	2:B:440:PHE:C	0.53	2.80	9	7
2:B:383:LEU:HB2	2:B:441:TYR:CE2	0.53	2.38	10	1
2:B:373:GLN:HB2	2:B:432:LEU:HD12	0.53	1.78	13	1
1:A:21:A:O2'	1:A:22:C:H5'	0.53	2.03	14	1
1:A:20:A:N3	2:B:371:LYS:HE2	0.53	2.18	15	1
2:B:368:MET:HE2	2:B:369:ASN:ND2	0.53	2.18	1	1
2:B:398:PRO:O	2:B:399:ASN:C	0.53	2.47	1	16
2:B:444:GLN:O	2:B:447:ALA:N	0.53	2.42	2	2
2:B:397:ASP:O	2:B:399:ASN:N	0.53	2.42	11	5
2:B:387:TYR:CE2	2:B:427:ALA:HB1	0.53	2.38	8	6
2:B:373:GLN:OE1	2:B:378:ILE:CG1	0.53	2.57	11	2
1:A:5:U:O2'	1:A:6:A:H5'	0.53	2.04	16	3
1:A:18:A:O5'	1:A:18:A:C8	0.53	2.60	15	2
2:B:441:TYR:O	2:B:444:GLN:CG	0.53	2.57	16	3
2:B:415:GLY:CA	2:B:426:ARG:HG3	0.53	2.34	12	3
2:B:380:TYR:CZ	2:B:382:SER:HB2	0.53	2.39	6	1
1:A:6:A:OP1	2:B:420:ILE:HG21	0.53	2.04	14	2
1:A:18:A:C2	2:B:372:ARG:HG3	0.53	2.39	1	2
2:B:419:ASN:O	2:B:420:ILE:HG13	0.53	2.04	6	16
2:B:439:ASP:O	2:B:442:ALA:N	0.53	2.42	16	8
2:B:426:ARG:O	2:B:430:ASN:ND2	0.53	2.42	14	6
1:A:30:C:C2'	1:A:31:U:O5'	0.52	2.58	3	12
2:B:429:GLU:HA	2:B:432:LEU:HD21	0.52	1.81	3	4
1:A:18:A:C4	2:B:372:ARG:NE	0.52	2.77	5	1
1:A:18:A:C4	2:B:372:ARG:NH2	0.52	2.77	5	1
1:A:12:U:O5'	1:A:12:U:H6	0.52	1.87	9	2
1:A:20:A:O2'	2:B:371:LYS:CB	0.52	2.57	8	1
2:B:429:GLU:O	2:B:430:ASN:C	0.52	2.46	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:401:ILE:CB	2:B:416:VAL:HG22	0.52	2.32	11	1
2:B:375:TYR:O	2:B:379:GLY:N	0.52	2.42	1	1
2:B:394:THR:CG2	2:B:397:ASP:OD1	0.52	2.57	1	2
2:B:402:VAL:CG2	2:B:423:ALA:O	0.52	2.57	2	13
2:B:412:LEU:HD13	2:B:412:LEU:H	0.52	1.64	11	4
2:B:411:VAL:O	2:B:412:LEU:HB2	0.52	2.03	10	1
2:B:444:GLN:O	2:B:444:GLN:NE2	0.52	2.42	12	1
2:B:394:THR:OG1	2:B:396:VAL:HG22	0.52	2.05	1	1
2:B:435:LYS:HG3	2:B:436:LYS:N	0.52	2.20	16	13
1:A:17:A:O2'	1:A:18:A:OP1	0.52	2.27	2	3
2:B:389:THR:CG2	2:B:389:THR:O	0.52	2.57	3	1
2:B:378:ILE:O	2:B:380:TYR:N	0.52	2.42	7	2
2:B:416:VAL:O	2:B:416:VAL:HG13	0.52	2.03	6	1
2:B:379:GLY:O	2:B:380:TYR:O	0.52	2.27	13	2
2:B:370:ALA:HB1	2:B:428:ALA:C	0.52	2.24	9	1
2:B:380:TYR:CE2	2:B:382:SER:HB2	0.52	2.39	10	1
1:A:6:A:OP1	2:B:393:PRO:CG	0.52	2.57	15	1
2:B:441:TYR:O	2:B:444:GLN:N	0.52	2.43	12	3
2:B:435:LYS:HG2	2:B:436:LYS:N	0.52	2.19	9	2
1:A:20:A:O2'	2:B:371:LYS:HB3	0.52	2.05	8	2
2:B:374:LEU:CD1	2:B:387:TYR:OH	0.52	2.56	2	5
2:B:418:ARG:NH1	2:B:419:ASN:OD1	0.52	2.43	6	1
1:A:29:U:C2'	1:A:30:C:C5'	0.52	2.87	12	3
2:B:380:TYR:CZ	2:B:383:LEU:HB3	0.52	2.40	8	1
1:A:28:A:O2'	1:A:29:U:H6	0.52	1.83	8	2
2:B:373:GLN:O	2:B:377:LEU:CB	0.52	2.58	13	5
1:A:16:G:C5'	1:A:17:A:N7	0.52	2.73	11	1
2:B:414:THR:O	2:B:430:ASN:ND2	0.52	2.42	10	6
2:B:401:ILE:HD11	2:B:414:THR:OG1	0.52	2.04	3	4
2:B:368:MET:HE2	2:B:369:ASN:N	0.52	2.19	11	1
2:B:385:LEU:HA	2:B:406:VAL:CG1	0.52	2.35	8	9
2:B:373:GLN:OE1	2:B:438:LEU:HD22	0.52	2.05	11	1
2:B:380:TYR:CD2	2:B:383:LEU:HB3	0.52	2.40	16	2
2:B:372:ARG:O	2:B:376:SER:HB2	0.51	2.06	5	3
1:A:17:A:O2'	1:A:18:A:H1'	0.51	2.05	6	2
2:B:390:VAL:O	2:B:401:ILE:CG2	0.51	2.59	11	1
2:B:402:VAL:CG2	2:B:423:ALA:C	0.51	2.78	16	11
2:B:380:TYR:CE2	2:B:383:LEU:N	0.51	2.78	5	1
1:A:3:G:C2	1:A:4:A:N7	0.51	2.79	7	1
1:A:24:U:O4	1:A:25:G:O6	0.51	2.29	3	3
1:A:19:G:O2'	1:A:20:A:O5'	0.51	2.28	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:373:GLN:OE1	2:B:432:LEU:CB	0.51	2.58	10	1
1:A:29:U:O2	2:B:395:ALA:CB	0.51	2.58	16	2
2:B:385:LEU:HD22	2:B:387:TYR:HE1	0.51	1.64	11	1
2:B:385:LEU:HD21	2:B:387:TYR:HE1	0.51	1.65	7	4
2:B:425:ILE:HG22	2:B:425:ILE:O	0.51	2.04	4	1
2:B:374:LEU:HD11	2:B:431:ALA:CB	0.51	2.34	12	2
2:B:383:LEU:O	2:B:383:LEU:CD2	0.51	2.54	11	1
1:A:13:U:HO2'	1:A:14:C:C5'	0.51	2.19	15	2
2:B:380:TYR:C	2:B:380:TYR:CD1	0.51	2.84	9	1
2:B:390:VAL:CG2	2:B:401:ILE:HG23	0.51	2.31	1	4
2:B:398:PRO:HB2	2:B:418:ARG:O	0.51	2.05	16	4
2:B:427:ALA:O	2:B:430:ASN:HB2	0.51	2.06	11	11
1:A:17:A:O3'	1:A:18:A:O4'	0.51	2.28	6	1
2:B:432:LEU:CD2	2:B:432:LEU:C	0.51	2.79	7	1
1:A:16:G:O4'	1:A:18:A:N6	0.51	2.44	12	1
2:B:383:LEU:HD23	2:B:384:ARG:N	0.51	2.21	13	1
1:A:17:A:O3'	1:A:18:A:C8	0.51	2.63	6	1
2:B:417:GLY:C	2:B:422:ILE:HD13	0.51	2.26	13	4
2:B:383:LEU:HD22	2:B:384:ARG:C	0.51	2.26	10	1
2:B:421:LYS:HG2	2:B:425:ILE:HD11	0.51	1.81	3	1
1:A:4:A:O2'	1:A:5:U:H5'	0.51	2.06	6	2
2:B:368:MET:CE	2:B:369:ASN:CG	0.51	2.79	9	1
1:A:9:A:C2'	1:A:10:U:O5'	0.51	2.59	16	2
1:A:18:A:O2'	2:B:376:SER:HB2	0.51	2.04	12	1
2:B:387:TYR:HB2	2:B:403:GLU:O	0.51	2.06	12	1
1:A:30:C:HO2'	1:A:31:U:H5'	0.51	1.65	4	1
1:A:22:C:H2'	1:A:23:G:O4'	0.51	2.05	5	1
1:A:8:C:C4	1:A:9:A:C5	0.51	2.99	10	1
2:B:386:HIS:CA	2:B:405:ARG:O	0.50	2.59	10	2
2:B:374:LEU:HD22	2:B:431:ALA:HB3	0.50	1.83	7	2
2:B:380:TYR:CE2	2:B:383:LEU:HD12	0.50	2.41	2	2
2:B:380:TYR:CE1	2:B:381:ALA:O	0.50	2.64	9	1
2:B:374:LEU:HD21	2:B:428:ALA:HB1	0.50	1.82	11	1
1:A:12:U:C2'	1:A:13:U:O5'	0.50	2.59	4	12
1:A:14:C:C5	1:A:15:A:N7	0.50	2.79	12	4
2:B:378:ILE:HG22	2:B:383:LEU:CD1	0.50	2.35	1	2
2:B:391:LYS:CB	2:B:401:ILE:HG22	0.50	2.36	6	3
2:B:374:LEU:HD11	2:B:431:ALA:HB3	0.50	1.82	10	1
1:A:25:G:O6	1:A:26:G:O6	0.50	2.29	1	5
2:B:387:TYR:CZ	2:B:404:CYS:HB3	0.50	2.41	2	6
2:B:415:GLY:CA	2:B:426:ARG:HG2	0.50	2.36	3	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:414:THR:N	2:B:430:ASN:OD1	0.50	2.44	10	6
1:A:12:U:C2'	1:A:13:U:O4'	0.50	2.59	3	1
2:B:419:ASN:O	2:B:419:ASN:CG	0.50	2.48	8	4
1:A:24:U:HO2'	1:A:25:G:C5'	0.50	2.19	10	2
2:B:380:TYR:CD2	2:B:381:ALA:N	0.50	2.80	1	1
2:B:369:ASN:ND2	2:B:370:ALA:N	0.50	2.60	2	1
1:A:20:A:O5'	1:A:20:A:C8	0.50	2.63	10	5
2:B:373:GLN:O	2:B:377:LEU:HB2	0.50	2.06	12	6
2:B:422:ILE:O	2:B:426:ARG:HG2	0.50	2.06	5	3
2:B:404:CYS:SG	2:B:430:ASN:HB2	0.50	2.47	12	1
1:A:21:A:H2'	1:A:22:C:C6	0.50	2.42	9	15
2:B:416:VAL:O	2:B:416:VAL:CG1	0.50	2.59	6	2
2:B:385:LEU:HG	2:B:406:VAL:HG11	0.50	1.82	14	1
2:B:366:LEU:HD23	2:B:366:LEU:C	0.50	2.25	1	1
2:B:429:GLU:O	2:B:433:ARG:N	0.50	2.44	9	1
2:B:383:LEU:HD13	2:B:385:LEU:N	0.50	2.21	7	1
2:B:367:ASP:N	2:B:367:ASP:OD1	0.50	2.44	12	2
2:B:431:ALA:O	2:B:437:MET:CE	0.50	2.59	16	1
1:A:19:G:HO2'	1:A:20:A:C5'	0.50	2.20	5	1
1:A:14:C:N4	1:A:15:A:N3	0.50	2.59	15	1
1:A:22:C:C2'	1:A:23:G:O5'	0.49	2.60	16	5
2:B:372:ARG:O	2:B:376:SER:HB3	0.49	2.07	10	10
2:B:422:ILE:O	2:B:426:ARG:HB2	0.49	2.07	14	10
2:B:419:ASN:N	2:B:422:ILE:HD11	0.49	2.21	7	6
1:A:20:A:HO2'	1:A:21:A:H5'	0.49	1.66	8	2
1:A:17:A:HO2'	1:A:18:A:P	0.49	2.27	8	1
2:B:384:ARG:CG	2:B:384:ARG:O	0.49	2.60	11	1
2:B:387:TYR:CE2	2:B:404:CYS:SG	0.49	2.98	11	1
2:B:402:VAL:CB	2:B:427:ALA:HB2	0.49	2.37	2	1
1:A:19:G:C4	2:B:372:ARG:CZ	0.49	2.94	5	1
1:A:9:A:N1	1:A:25:G:C6	0.49	2.80	10	1
2:B:380:TYR:CG	2:B:445:ARG:HD3	0.49	2.43	4	6
1:A:11:G:HO2'	1:A:12:U:C4'	0.49	2.20	7	3
1:A:21:A:C2'	1:A:22:C:C6	0.49	2.96	2	4
2:B:390:VAL:O	2:B:391:LYS:HB2	0.49	2.07	2	5
2:B:378:ILE:HB	2:B:441:TYR:CB	0.49	2.38	15	1
2:B:368:MET:HE3	2:B:369:ASN:CG	0.49	2.27	9	1
1:A:15:A:C2	1:A:18:A:N6	0.49	2.81	10	2
2:B:394:THR:HG23	2:B:397:ASP:OD1	0.49	2.07	1	1
2:B:403:GLU:OE1	2:B:411:VAL:HG13	0.49	2.06	4	1
2:B:387:TYR:CE2	2:B:404:CYS:HB3	0.49	2.43	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:373:GLN:O	2:B:373:GLN:NE2	0.49	2.46	7	2
2:B:421:LYS:C	2:B:423:ALA:N	0.49	2.66	13	9
2:B:380:TYR:CE1	2:B:445:ARG:CZ	0.49	2.96	6	1
1:A:5:U:OP1	2:B:419:ASN:OD1	0.49	2.30	8	3
1:A:18:A:C2	2:B:372:ARG:NH1	0.49	2.81	12	1
2:B:401:ILE:HG13	2:B:402:VAL:N	0.49	2.23	5	11
2:B:380:TYR:CE2	2:B:383:LEU:HG	0.49	2.43	14	2
1:A:3:G:HO2'	1:A:4:A:H8	0.49	1.50	11	1
2:B:371:LYS:HG2	2:B:372:ARG:N	0.49	2.23	14	1
2:B:431:ALA:O	2:B:437:MET:HE3	0.49	2.06	16	1
1:A:10:U:O2'	1:A:11:G:O4'	0.49	2.30	1	5
2:B:383:LEU:HD11	2:B:385:LEU:CB	0.49	2.30	7	1
1:A:5:U:OP1	2:B:419:ASN:O	0.49	2.31	9	1
2:B:378:ILE:HG23	2:B:441:TYR:HB3	0.49	1.83	13	1
2:B:394:THR:O	2:B:398:PRO:CD	0.49	2.60	12	2
2:B:380:TYR:CE1	2:B:444:GLN:CD	0.49	2.86	16	1
2:B:383:LEU:C	2:B:383:LEU:CD2	0.48	2.82	10	3
2:B:380:TYR:CD2	2:B:445:ARG:HD3	0.48	2.43	1	1
2:B:380:TYR:CE1	2:B:383:LEU:HB2	0.48	2.44	5	2
2:B:389:THR:HG23	2:B:400:SER:OG	0.48	2.08	11	1
1:A:14:C:N4	1:A:15:A:C6	0.48	2.82	13	1
2:B:385:LEU:C	2:B:385:LEU:CD1	0.48	2.80	15	1
2:B:373:GLN:NE2	2:B:373:GLN:C	0.48	2.66	2	1
2:B:419:ASN:O	2:B:419:ASN:OD1	0.48	2.31	4	2
1:A:17:A:C2	2:B:372:ARG:NH2	0.48	2.82	7	1
2:B:372:ARG:NH1	2:B:377:LEU:CD2	0.48	2.77	7	1
2:B:434:ASP:OD2	2:B:437:MET:CB	0.48	2.62	9	1
2:B:380:TYR:CD1	2:B:380:TYR:N	0.48	2.81	11	2
1:A:17:A:C2'	1:A:18:A:C1'	0.48	2.90	16	1
2:B:380:TYR:CE1	2:B:383:LEU:CB	0.48	2.96	1	1
2:B:387:TYR:CD2	2:B:427:ALA:HB1	0.48	2.44	4	2
2:B:426:ARG:O	2:B:430:ASN:CG	0.48	2.52	7	4
2:B:368:MET:O	2:B:371:LYS:HD2	0.48	2.08	14	1
2:B:379:GLY:C	2:B:380:TYR:CD1	0.48	2.87	15	1
2:B:404:CYS:HB3	2:B:413:GLY:HA3	0.48	1.83	16	1
2:B:368:MET:HE1	2:B:369:ASN:CB	0.48	2.38	2	1
2:B:426:ARG:O	2:B:430:ASN:OD1	0.48	2.31	9	2
2:B:368:MET:HA	2:B:371:LYS:CD	0.48	2.39	15	3
1:A:8:C:C5	1:A:9:A:N7	0.48	2.82	14	1
1:A:9:A:H2'	1:A:10:U:O4'	0.48	2.08	16	1
2:B:380:TYR:CZ	2:B:382:SER:CB	0.48	2.96	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:G:OP2	1:A:16:G:C2	0.48	2.66	14	1
2:B:385:LEU:HG	2:B:406:VAL:CG1	0.48	2.39	14	5
2:B:423:ALA:O	2:B:427:ALA:CB	0.48	2.62	5	2
2:B:383:LEU:O	2:B:384:ARG:C	0.48	2.52	11	1
2:B:383:LEU:HB2	2:B:441:TYR:CE1	0.48	2.44	11	1
1:A:19:G:H21	2:B:371:LYS:NZ	0.48	2.06	15	1
2:B:404:CYS:CB	2:B:413:GLY:HA3	0.48	2.39	16	1
1:A:2:G:C2'	1:A:3:G:O5'	0.48	2.61	4	3
1:A:15:A:H2'	1:A:16:G:O5'	0.48	2.08	11	2
1:A:9:A:C6	1:A:10:U:C4	0.48	3.01	16	1
2:B:410:THR:CG2	2:B:441:TYR:OH	0.48	2.61	1	1
2:B:384:ARG:O	2:B:406:VAL:HG12	0.48	2.08	16	2
2:B:420:ILE:CD1	2:B:421:LYS:N	0.48	2.77	3	2
1:A:18:A:C6	2:B:372:ARG:NH2	0.48	2.81	5	1
1:A:20:A:C2'	1:A:21:A:O4'	0.48	2.59	5	3
2:B:385:LEU:HD22	2:B:387:TYR:CE1	0.48	2.44	11	1
1:A:14:C:C4	1:A:15:A:C5	0.48	3.02	13	1
2:B:378:ILE:HD12	2:B:378:ILE:C	0.48	2.29	15	1
2:B:436:LYS:O	2:B:440:PHE:CB	0.47	2.62	13	3
2:B:397:ASP:N	2:B:398:PRO:CD	0.47	2.77	11	5
2:B:374:LEU:O	2:B:378:ILE:C	0.47	2.52	10	6
1:A:1:G:C2	1:A:2:G:C8	0.47	3.02	7	3
1:A:4:A:N6	1:A:5:U:O4	0.47	2.46	9	1
2:B:378:ILE:HD12	2:B:379:GLY:N	0.47	2.23	15	1
2:B:401:ILE:HD12	2:B:416:VAL:HG22	0.47	1.84	15	1
2:B:396:VAL:HG23	2:B:397:ASP:OD2	0.47	2.09	16	1
2:B:390:VAL:O	2:B:391:LYS:HB3	0.47	2.08	12	6
1:A:19:G:C5	2:B:372:ARG:NH2	0.47	2.82	5	1
1:A:12:U:HO2'	1:A:13:U:H5'	0.47	1.65	8	2
1:A:14:C:C2'	1:A:15:A:O5'	0.47	2.62	15	1
2:B:402:VAL:O	2:B:414:THR:CG2	0.47	2.62	1	2
2:B:374:LEU:HD21	2:B:432:LEU:CD2	0.47	2.39	2	2
2:B:414:THR:O	2:B:430:ASN:OD1	0.47	2.32	6	5
1:A:12:U:O5'	1:A:12:U:C6	0.47	2.56	7	2
1:A:18:A:N3	2:B:372:ARG:HD2	0.47	2.25	16	1
2:B:380:TYR:CD1	2:B:445:ARG:CG	0.47	2.97	1	1
2:B:440:PHE:CE2	2:B:441:TYR:CE2	0.47	3.02	14	1
2:B:366:LEU:O	2:B:367:ASP:C	0.47	2.53	11	4
2:B:370:ALA:HA	2:B:432:LEU:CD2	0.47	2.39	1	2
2:B:383:LEU:HD12	2:B:383:LEU:C	0.47	2.30	15	1
2:B:412:LEU:CD1	2:B:437:MET:SD	0.47	3.03	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:C:HO2'	2:B:396:VAL:HG12	0.47	1.67	4	1
2:B:404:CYS:SG	2:B:413:GLY:O	0.47	2.72	10	5
1:A:5:U:OP1	2:B:419:ASN:CB	0.47	2.62	9	1
2:B:376:SER:O	2:B:377:LEU:CD2	0.47	2.62	12	1
2:B:393:PRO:CG	2:B:420:ILE:HG21	0.47	2.38	16	1
2:B:380:TYR:CZ	2:B:383:LEU:HA	0.47	2.44	1	1
2:B:412:LEU:HD22	2:B:412:LEU:H	0.47	1.70	2	3
1:A:14:C:O2'	2:B:368:MET:HB3	0.47	2.10	2	1
1:A:29:U:HO2'	1:A:30:C:H5'	0.47	1.66	7	3
2:B:411:VAL:O	2:B:412:LEU:C	0.47	2.52	11	1
2:B:375:TYR:O	2:B:378:ILE:O	0.47	2.32	13	1
1:A:2:G:C5	1:A:3:G:N7	0.47	2.83	1	2
2:B:405:ARG:HB2	2:B:410:THR:O	0.47	2.10	5	9
2:B:368:MET:HE2	2:B:369:ASN:CB	0.47	2.40	2	1
2:B:434:ASP:CB	2:B:437:MET:HB3	0.47	2.39	15	5
2:B:419:ASN:O	2:B:420:ILE:CB	0.47	2.63	9	3
2:B:440:PHE:CE1	2:B:444:GLN:HG3	0.47	2.44	6	1
1:A:30:C:N4	1:A:31:U:O4	0.47	2.48	6	3
2:B:373:GLN:OE1	2:B:432:LEU:HB3	0.47	2.10	10	2
2:B:437:MET:SD	2:B:441:TYR:CE1	0.47	3.08	10	1
2:B:390:VAL:O	2:B:401:ILE:HG23	0.47	2.10	11	2
2:B:373:GLN:HG3	2:B:432:LEU:CG	0.47	2.40	13	1
2:B:415:GLY:HA2	2:B:426:ARG:HG2	0.47	1.87	6	8
1:A:13:U:C2'	1:A:14:C:O5'	0.47	2.63	3	2
2:B:380:TYR:CE1	2:B:383:LEU:HD23	0.47	2.44	3	1
2:B:433:ARG:O	2:B:433:ARG:HG2	0.47	2.10	6	1
2:B:399:ASN:OD1	2:B:399:ASN:O	0.47	2.33	11	1
2:B:373:GLN:HG3	2:B:432:LEU:CD1	0.47	2.39	13	1
2:B:418:ARG:HG2	2:B:419:ASN:OD1	0.47	2.10	13	1
1:A:4:A:H2'	1:A:5:U:C6	0.46	2.45	12	12
2:B:421:LYS:O	2:B:423:ALA:N	0.46	2.48	13	5
2:B:378:ILE:O	2:B:379:GLY:C	0.46	2.53	6	2
2:B:380:TYR:CE2	2:B:382:SER:CB	0.46	2.97	10	1
1:A:20:A:OP1	2:B:375:TYR:CD2	0.46	2.68	13	1
1:A:24:U:O2'	1:A:25:G:C5'	0.46	2.63	10	2
2:B:425:ILE:O	2:B:427:ALA:N	0.46	2.48	1	7
2:B:380:TYR:CE2	2:B:383:LEU:CG	0.46	2.99	2	1
2:B:373:GLN:HG3	2:B:432:LEU:CB	0.46	2.40	5	4
1:A:5:U:O4'	2:B:398:PRO:HB3	0.46	2.09	11	1
2:B:405:ARG:HG3	2:B:406:VAL:N	0.46	2.25	12	1
2:B:421:LYS:CD	2:B:421:LYS:C	0.46	2.83	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:366:LEU:O	2:B:369:ASN:HB2	0.46	2.11	11	4
1:A:20:A:O2'	2:B:371:LYS:HG2	0.46	2.10	7	2
2:B:404:CYS:O	2:B:411:VAL:C	0.46	2.54	10	1
2:B:387:TYR:OH	2:B:431:ALA:HB2	0.46	2.10	15	2
2:B:420:ILE:HG13	2:B:421:LYS:N	0.46	2.24	2	4
1:A:30:C:O2'	2:B:396:VAL:CG1	0.46	2.56	4	1
1:A:3:G:N3	1:A:4:A:N7	0.46	2.64	7	1
1:A:24:U:O2'	1:A:25:G:H8	0.46	1.94	10	2
2:B:405:ARG:HG2	2:B:406:VAL:N	0.46	2.24	10	1
2:B:372:ARG:CD	2:B:376:SER:HB3	0.46	2.41	11	1
2:B:385:LEU:HD23	2:B:406:VAL:CG1	0.46	2.40	15	1
2:B:398:PRO:O	2:B:399:ASN:O	0.46	2.32	1	3
2:B:441:TYR:O	2:B:444:GLN:HG3	0.46	2.10	16	2
2:B:414:THR:C	2:B:430:ASN:OD1	0.46	2.54	7	4
2:B:368:MET:N	2:B:371:LYS:HE2	0.46	2.26	4	2
2:B:408:ASP:OD1	2:B:408:ASP:O	0.46	2.33	8	1
2:B:373:GLN:CD	2:B:438:LEU:HD22	0.46	2.30	11	1
2:B:367:ASP:OD1	2:B:367:ASP:N	0.46	2.49	7	3
2:B:367:ASP:OD2	2:B:425:ILE:CD1	0.46	2.64	6	1
1:A:19:G:H2'	1:A:20:A:C8	0.46	2.46	13	3
2:B:375:TYR:O	2:B:379:GLY:CA	0.46	2.64	1	2
2:B:441:TYR:O	2:B:442:ALA:C	0.46	2.54	2	7
2:B:372:ARG:O	2:B:376:SER:OG	0.46	2.32	3	1
2:B:442:ALA:O	2:B:445:ARG:N	0.46	2.43	5	4
2:B:411:VAL:O	2:B:412:LEU:HD22	0.46	2.11	10	1
2:B:370:ALA:O	2:B:371:LYS:C	0.46	2.55	3	16
2:B:383:LEU:CD1	2:B:385:LEU:HB2	0.46	2.34	7	1
2:B:411:VAL:O	2:B:411:VAL:CG1	0.46	2.56	11	1
1:A:22:C:O3'	2:B:421:LYS:HE2	0.46	2.11	12	1
2:B:410:THR:HG22	2:B:412:LEU:HD13	0.46	1.86	12	1
1:A:23:G:C5	1:A:24:U:C5	0.45	3.03	16	3
2:B:373:GLN:O	2:B:377:LEU:HB3	0.45	2.12	11	3
2:B:367:ASP:CG	2:B:425:ILE:HD12	0.45	2.32	6	1
2:B:368:MET:HG3	2:B:369:ASN:N	0.45	2.26	15	1
2:B:403:GLU:OE1	2:B:411:VAL:HG11	0.45	2.11	16	1
2:B:404:CYS:SG	2:B:412:LEU:HD23	0.45	2.51	3	1
2:B:380:TYR:CG	2:B:381:ALA:N	0.45	2.83	6	1
2:B:383:LEU:CD1	2:B:385:LEU:N	0.45	2.80	7	1
1:A:18:A:C8	1:A:18:A:O5'	0.45	2.70	9	1
2:B:404:CYS:SG	2:B:430:ASN:CB	0.45	3.04	12	1
2:B:375:TYR:O	2:B:379:GLY:HA3	0.45	2.11	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:430:ASN:O	2:B:433:ARG:HG2	0.45	2.12	12	1
2:B:383:LEU:O	2:B:384:ARG:HB3	0.45	2.11	16	3
2:B:374:LEU:HD21	2:B:428:ALA:O	0.45	2.12	13	2
2:B:380:TYR:CE1	2:B:444:GLN:OE1	0.45	2.69	16	1
2:B:396:VAL:O	2:B:397:ASP:CB	0.45	2.64	5	3
2:B:440:PHE:CZ	2:B:444:GLN:OE1	0.45	2.70	13	1
1:A:1:G:HO2'	1:A:2:G:C5'	0.45	2.24	1	4
1:A:11:G:H2'	1:A:12:U:C6	0.45	2.47	16	8
2:B:412:LEU:O	2:B:434:ASP:OD2	0.45	2.35	2	1
2:B:429:GLU:O	2:B:433:ARG:HB2	0.45	2.12	2	1
2:B:422:ILE:HD12	2:B:422:ILE:N	0.45	2.27	4	1
2:B:425:ILE:O	2:B:425:ILE:CG2	0.45	2.65	4	1
1:A:20:A:HO2'	1:A:21:A:C5'	0.45	2.24	6	1
2:B:373:GLN:HA	2:B:377:LEU:HB2	0.45	1.88	12	1
2:B:380:TYR:CB	2:B:383:LEU:CD2	0.45	2.81	13	1
2:B:434:ASP:HB3	2:B:437:MET:HB3	0.45	1.89	15	1
1:A:18:A:C2	2:B:368:MET:SD	0.45	3.10	16	1
1:A:27:U:H2'	1:A:28:A:O5'	0.45	2.12	14	5
2:B:393:PRO:HB3	2:B:398:PRO:O	0.45	2.12	1	10
2:B:414:THR:O	2:B:430:ASN:CG	0.45	2.55	4	4
1:A:5:U:O2'	2:B:393:PRO:HB2	0.45	2.12	3	2
2:B:367:ASP:O	2:B:368:MET:C	0.45	2.55	10	13
2:B:415:GLY:HA3	2:B:426:ARG:HG3	0.45	1.88	4	2
1:A:29:U:C2'	1:A:30:C:O5'	0.45	2.65	16	5
2:B:368:MET:HG2	2:B:369:ASN:N	0.45	2.26	5	1
2:B:433:ARG:O	2:B:433:ARG:CG	0.45	2.65	6	1
2:B:380:TYR:CB	2:B:445:ARG:HD3	0.45	2.42	14	2
2:B:385:LEU:HD23	2:B:387:TYR:CD1	0.45	2.46	10	1
1:A:29:U:H2'	1:A:30:C:C5'	0.45	2.42	12	1
2:B:412:LEU:CB	2:B:431:ALA:HA	0.45	2.41	12	1
2:B:380:TYR:CZ	2:B:383:LEU:HB2	0.45	2.46	5	1
2:B:402:VAL:CG2	2:B:423:ALA:CB	0.45	2.92	5	1
1:A:12:U:C2'	1:A:13:U:C5'	0.45	2.95	8	1
2:B:380:TYR:CE2	2:B:382:SER:OG	0.45	2.70	10	1
2:B:367:ASP:HB3	2:B:425:ILE:HG13	0.45	1.88	11	1
2:B:415:GLY:N	2:B:430:ASN:OD1	0.45	2.50	12	1
2:B:426:ARG:CZ	2:B:426:ARG:HA	0.45	2.42	13	1
2:B:403:GLU:OE2	2:B:405:ARG:CZ	0.45	2.65	14	1
2:B:419:ASN:CG	2:B:422:ILE:HD11	0.45	2.33	9	2
2:B:436:LYS:O	2:B:440:PHE:HB2	0.45	2.11	1	1
1:A:23:G:C2'	1:A:24:U:O5'	0.45	2.65	14	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:367:ASP:CA	2:B:425:ILE:HG23	0.45	2.42	3	1
2:B:367:ASP:HB3	2:B:425:ILE:CG1	0.45	2.41	11	3
2:B:384:ARG:O	2:B:406:VAL:HB	0.45	2.11	13	5
2:B:385:LEU:HA	2:B:406:VAL:CB	0.45	2.42	5	1
2:B:436:LYS:O	2:B:440:PHE:HB3	0.45	2.12	13	1
2:B:377:LEU:HG	2:B:377:LEU:O	0.45	2.12	15	1
2:B:383:LEU:C	2:B:383:LEU:HD13	0.44	2.32	7	1
2:B:441:TYR:O	2:B:444:GLN:HG2	0.44	2.12	9	1
1:A:9:A:H2'	1:A:10:U:O5'	0.44	2.13	16	1
2:B:367:ASP:OD2	2:B:425:ILE:HD11	0.44	2.12	2	1
1:A:30:C:H2'	1:A:31:U:O5'	0.44	2.12	9	2
2:B:378:ILE:HG22	2:B:383:LEU:HD13	0.44	1.87	4	1
2:B:440:PHE:CD1	2:B:440:PHE:O	0.44	2.70	6	2
1:A:17:A:C2'	1:A:18:A:O4'	0.44	2.64	16	2
2:B:381:ALA:O	2:B:382:SER:C	0.44	2.55	9	1
1:A:19:G:H21	2:B:372:ARG:NH2	0.44	2.10	16	1
2:B:380:TYR:CG	2:B:445:ARG:HG2	0.44	2.48	1	1
2:B:404:CYS:C	2:B:412:LEU:HD22	0.44	2.33	1	1
2:B:406:VAL:HG21	2:B:441:TYR:OH	0.44	2.12	3	1
1:A:19:G:HO2'	1:A:20:A:C4'	0.44	2.26	5	1
2:B:380:TYR:O	2:B:381:ALA:C	0.44	2.55	7	1
2:B:434:ASP:OD2	2:B:437:MET:HB2	0.44	2.12	9	1
2:B:399:ASN:C	2:B:399:ASN:OD1	0.44	2.56	11	1
1:A:12:U:O2'	1:A:13:U:O4'	0.44	2.36	3	1
2:B:399:ASN:OD1	2:B:417:GLY:O	0.44	2.36	6	1
2:B:386:HIS:C	2:B:405:ARG:O	0.44	2.55	10	1
2:B:401:ILE:HB	2:B:416:VAL:CG2	0.44	2.38	11	1
2:B:387:TYR:HA	2:B:403:GLU:O	0.44	2.12	12	1
1:A:17:A:C3'	1:A:18:A:O4'	0.44	2.65	16	1
1:A:30:C:C5	1:A:31:U:C5	0.44	3.05	1	1
1:A:20:A:C2'	1:A:21:A:O5'	0.44	2.66	8	2
2:B:368:MET:N	2:B:371:LYS:HE3	0.44	2.28	2	1
2:B:401:ILE:HG13	2:B:415:GLY:O	0.44	2.13	7	1
1:A:10:U:HO2'	1:A:11:G:P	0.44	2.36	16	1
1:A:6:A:H2'	1:A:7:C:C6	0.44	2.47	10	10
2:B:422:ILE:HD12	2:B:422:ILE:H	0.44	1.72	9	11
2:B:374:LEU:HD23	2:B:374:LEU:H	0.44	1.69	14	4
2:B:434:ASP:N	2:B:434:ASP:OD1	0.44	2.51	4	1
1:A:11:G:N2	1:A:23:G:C4	0.44	2.86	16	2
1:A:9:A:C2	1:A:25:G:C6	0.44	3.06	10	1
1:A:11:G:N3	1:A:23:G:N2	0.44	2.65	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:415:GLY:CA	2:B:426:ARG:HD2	0.44	2.42	5	1
2:B:405:ARG:CG	2:B:406:VAL:N	0.44	2.81	7	1
2:B:407:GLY:O	2:B:408:ASP:HB2	0.44	2.10	8	1
2:B:404:CYS:HB3	2:B:413:GLY:O	0.44	2.13	11	1
2:B:402:VAL:HG21	2:B:427:ALA:HB2	0.44	1.89	15	1
2:B:401:ILE:HA	2:B:415:GLY:O	0.44	2.13	15	4
2:B:420:ILE:C	2:B:420:ILE:CD1	0.44	2.82	3	2
2:B:385:LEU:CG	2:B:406:VAL:HG12	0.44	2.37	4	1
2:B:388:VAL:CG2	2:B:405:ARG:HD3	0.44	2.43	9	1
1:A:22:C:O3'	2:B:421:LYS:HE3	0.44	2.13	2	1
2:B:401:ILE:HD13	2:B:402:VAL:N	0.44	2.27	4	1
2:B:367:ASP:CB	2:B:425:ILE:HG23	0.44	2.40	9	1
1:A:18:A:O2'	2:B:376:SER:CB	0.44	2.66	12	1
1:A:11:G:C2	1:A:23:G:C4	0.43	3.06	2	2
2:B:399:ASN:HB2	2:B:417:GLY:O	0.43	2.12	11	2
2:B:391:LYS:HB2	2:B:401:ILE:CG2	0.43	2.43	6	2
2:B:408:ASP:CG	2:B:408:ASP:O	0.43	2.56	12	1
2:B:383:LEU:HD11	2:B:385:LEU:HB3	0.43	1.88	15	1
2:B:380:TYR:OH	2:B:445:ARG:HA	0.43	2.13	16	1
2:B:394:THR:O	2:B:398:PRO:HD3	0.43	2.13	12	4
2:B:406:VAL:HG23	2:B:407:GLY:N	0.43	2.27	14	1
2:B:380:TYR:CZ	2:B:444:GLN:CD	0.43	2.92	16	1
2:B:368:MET:HE2	2:B:369:ASN:CA	0.43	2.42	2	1
2:B:412:LEU:HG	2:B:437:MET:CE	0.43	2.44	13	4
1:A:19:G:C2	2:B:372:ARG:CZ	0.43	3.00	10	2
2:B:385:LEU:CA	2:B:406:VAL:HG12	0.43	2.42	2	2
2:B:397:ASP:O	2:B:397:ASP:CG	0.43	2.57	7	1
1:A:20:A:C5'	2:B:375:TYR:HB2	0.43	2.43	11	1
2:B:401:ILE:CD1	2:B:416:VAL:HG22	0.43	2.43	15	1
2:B:420:ILE:O	2:B:421:LYS:C	0.43	2.56	11	10
2:B:380:TYR:OH	2:B:382:SER:HB2	0.43	2.13	6	1
2:B:397:ASP:O	2:B:397:ASP:OD1	0.43	2.36	7	1
1:A:15:A:O5'	2:B:368:MET:SD	0.43	2.76	10	1
2:B:374:LEU:HD21	2:B:431:ALA:HB3	0.43	1.91	12	1
1:A:16:G:HO2'	1:A:17:A:P	0.43	2.36	16	2
2:B:368:MET:HA	2:B:371:LYS:CE	0.43	2.43	2	2
2:B:399:ASN:CB	2:B:418:ARG:HA	0.43	2.43	12	2
1:A:23:G:H2'	1:A:24:U:C6	0.43	2.49	15	5
1:A:10:U:O5'	1:A:10:U:C6	0.43	2.56	4	1
2:B:441:TYR:O	2:B:444:GLN:HB2	0.43	2.13	4	4
1:A:11:G:C2	1:A:23:G:N3	0.43	2.86	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:380:TYR:HB2	2:B:383:LEU:CD2	0.43	2.39	13	1
2:B:368:MET:O	2:B:371:LYS:CD	0.43	2.66	14	1
2:B:374:LEU:O	2:B:378:ILE:HG13	0.43	2.13	15	1
2:B:425:ILE:O	2:B:426:ARG:C	0.43	2.57	16	5
1:A:5:U:C4'	2:B:398:PRO:HB3	0.43	2.44	5	1
1:A:17:A:HO2'	1:A:18:A:C1'	0.43	2.24	6	1
2:B:382:SER:O	2:B:382:SER:OG	0.43	2.36	8	1
2:B:372:ARG:NH1	2:B:372:ARG:HB3	0.43	2.29	13	1
1:A:21:A:C2'	1:A:22:C:O5'	0.43	2.66	14	1
2:B:374:LEU:HA	2:B:378:ILE:CG1	0.43	2.44	15	1
1:A:22:C:H2'	1:A:23:G:O5'	0.43	2.14	16	1
2:B:399:ASN:CA	2:B:417:GLY:O	0.43	2.66	12	2
2:B:406:VAL:N	2:B:410:THR:O	0.43	2.50	10	2
2:B:437:MET:SD	2:B:437:MET:C	0.43	2.97	16	5
2:B:393:PRO:C	2:B:394:THR:CG2	0.43	2.87	14	2
2:B:432:LEU:HA	2:B:438:LEU:CD1	0.43	2.40	11	2
1:A:21:A:HO2'	1:A:22:C:C5'	0.43	2.25	4	2
2:B:367:ASP:CB	2:B:425:ILE:HG13	0.43	2.43	7	1
2:B:396:VAL:O	2:B:397:ASP:HB3	0.43	2.14	7	2
1:A:18:A:H4'	1:A:19:G:OP1	0.43	2.13	11	1
2:B:425:ILE:HG22	2:B:426:ARG:N	0.43	2.28	11	1
1:A:24:U:O2'	1:A:25:G:C8	0.43	2.72	16	1
2:B:368:MET:HE3	2:B:369:ASN:N	0.43	2.29	16	1
1:A:11:G:N2	1:A:23:G:N3	0.42	2.67	10	1
2:B:435:LYS:HB2	2:B:435:LYS:NZ	0.42	2.29	10	1
1:A:15:A:O2'	2:B:368:MET:SD	0.42	2.65	12	1
2:B:368:MET:O	2:B:372:ARG:HB2	0.42	2.14	13	1
1:A:26:G:H2'	1:A:27:U:C6	0.42	2.49	12	7
2:B:373:GLN:HG2	2:B:377:LEU:HD22	0.42	1.91	5	1
2:B:396:VAL:O	2:B:397:ASP:OD1	0.42	2.37	5	1
2:B:380:TYR:O	2:B:382:SER:N	0.42	2.52	7	1
2:B:383:LEU:HD13	2:B:384:ARG:C	0.42	2.35	7	1
2:B:401:ILE:CD1	2:B:415:GLY:O	0.42	2.67	8	1
2:B:443:LYS:CD	2:B:443:LYS:C	0.42	2.87	10	1
2:B:442:ALA:O	2:B:445:ARG:CB	0.42	2.68	14	1
2:B:373:GLN:OE1	2:B:377:LEU:HG	0.42	2.15	13	2
2:B:368:MET:HE3	2:B:369:ASN:ND2	0.42	2.29	9	1
2:B:411:VAL:C	2:B:413:GLY:N	0.42	2.72	11	1
1:A:14:C:C4	1:A:15:A:C8	0.42	3.08	1	1
2:B:369:ASN:ND2	2:B:429:GLU:OE2	0.42	2.53	2	1
1:A:16:G:O2'	1:A:17:A:OP1	0.42	2.32	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:U:H2'	1:A:30:C:O5'	0.42	2.14	11	1
2:B:440:PHE:CD2	2:B:441:TYR:CE1	0.42	3.08	1	1
2:B:367:ASP:OD2	2:B:425:ILE:CG1	0.42	2.68	2	1
2:B:368:MET:CE	2:B:369:ASN:HB3	0.42	2.42	2	1
2:B:404:CYS:SG	2:B:413:GLY:C	0.42	2.98	4	4
1:A:17:A:H2'	1:A:18:A:C4	0.42	2.50	7	1
1:A:7:C:O2'	1:A:8:C:H5'	0.42	2.15	8	1
2:B:380:TYR:CE2	2:B:445:ARG:HG2	0.42	2.48	11	1
2:B:367:ASP:O	2:B:371:LYS:CG	0.42	2.67	13	1
1:A:14:C:C5	1:A:15:A:C5	0.42	3.07	15	1
1:A:8:C:C2'	1:A:9:A:C8	0.42	3.02	16	1
2:B:366:LEU:O	2:B:369:ASN:N	0.42	2.53	11	2
2:B:415:GLY:HA2	2:B:426:ARG:CG	0.42	2.45	6	4
1:A:19:G:N3	2:B:372:ARG:NH2	0.42	2.66	5	2
2:B:396:VAL:O	2:B:397:ASP:HB2	0.42	2.15	3	2
2:B:428:ALA:O	2:B:431:ALA:N	0.42	2.52	7	1
1:A:6:A:OP1	2:B:393:PRO:HG3	0.42	2.13	15	1
1:A:24:U:HO2'	1:A:25:G:H8	0.42	1.57	16	1
1:A:18:A:O5'	1:A:18:A:H8	0.42	1.97	9	1
2:B:376:SER:O	2:B:377:LEU:HD22	0.42	2.15	12	1
2:B:373:GLN:CG	2:B:432:LEU:HB2	0.42	2.45	13	1
1:A:13:U:HO2'	1:A:14:C:C4'	0.42	2.28	15	2
1:A:10:U:O2'	1:A:11:G:H8	0.42	1.98	10	1
2:B:374:LEU:N	2:B:374:LEU:HD22	0.42	2.30	10	1
2:B:378:ILE:CG2	2:B:441:TYR:CG	0.42	3.03	3	1
2:B:367:ASP:O	2:B:371:LYS:HD3	0.42	2.15	7	1
1:A:12:U:O2'	1:A:13:U:O5'	0.42	2.38	11	1
2:B:439:ASP:O	2:B:440:PHE:C	0.42	2.58	12	2
2:B:441:TYR:HA	2:B:444:GLN:HG2	0.42	1.92	12	1
1:A:16:G:OP2	1:A:16:G:N3	0.42	2.53	14	1
2:B:384:ARG:O	2:B:406:VAL:HA	0.42	2.15	16	1
2:B:380:TYR:CG	2:B:445:ARG:CD	0.41	3.03	1	1
2:B:380:TYR:CB	2:B:445:ARG:CD	0.41	2.98	1	1
2:B:399:ASN:OD1	2:B:418:ARG:HA	0.41	2.15	6	1
2:B:388:VAL:HG21	2:B:405:ARG:HD3	0.41	1.92	9	1
2:B:429:GLU:O	2:B:429:GLU:OE1	0.41	2.38	10	1
2:B:422:ILE:N	2:B:422:ILE:CD1	0.41	2.82	15	1
2:B:372:ARG:HA	2:B:376:SER:HB2	0.41	1.92	16	1
2:B:432:LEU:HA	2:B:438:LEU:CD2	0.41	2.41	16	1
1:A:17:A:C2'	1:A:18:A:C8	0.41	3.03	1	1
2:B:400:SER:O	2:B:423:ALA:HB2	0.41	2.15	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:A:H2'	1:A:22:C:C5	0.41	2.50	15	2
1:A:20:A:H8	1:A:20:A:O5'	0.41	1.97	4	1
2:B:383:LEU:CD1	2:B:441:TYR:CE1	0.41	3.03	8	1
2:B:422:ILE:H	2:B:422:ILE:CD1	0.41	2.28	8	2
1:A:28:A:H2'	1:A:29:U:C6	0.41	2.50	12	2
2:B:432:LEU:O	2:B:438:LEU:CD1	0.41	2.68	13	1
2:B:400:SER:O	2:B:423:ALA:CB	0.41	2.68	2	2
1:A:3:G:C2'	1:A:4:A:O5'	0.41	2.68	14	2
2:B:406:VAL:HG23	2:B:410:THR:CB	0.41	2.38	2	1
2:B:378:ILE:HD12	2:B:441:TYR:HB2	0.41	1.92	3	1
2:B:386:HIS:NE2	2:B:405:ARG:HG3	0.41	2.30	3	1
2:B:421:LYS:HD3	2:B:421:LYS:C	0.41	2.36	7	2
1:A:29:U:C4	1:A:30:C:C5	0.41	3.08	10	1
2:B:412:LEU:CG	2:B:437:MET:SD	0.41	3.09	12	1
2:B:429:GLU:HA	2:B:432:LEU:HD11	0.41	1.91	14	1
2:B:367:ASP:CG	2:B:425:ILE:HG13	0.41	2.36	7	1
1:A:20:A:C2'	1:A:21:A:C5'	0.41	2.98	10	1
2:B:411:VAL:CG1	2:B:412:LEU:N	0.41	2.82	10	1
2:B:429:GLU:C	2:B:432:LEU:HD22	0.41	2.35	10	1
1:A:15:A:N1	1:A:16:G:C8	0.41	2.89	12	1
1:A:20:A:H2'	1:A:21:A:C8	0.41	2.51	14	1
2:B:368:MET:HA	2:B:371:LYS:HD2	0.41	1.92	14	1
2:B:378:ILE:O	2:B:383:LEU:HD12	0.41	2.15	5	1
2:B:385:LEU:CD2	2:B:387:TYR:CD1	0.41	3.03	10	1
2:B:367:ASP:CG	2:B:425:ILE:HG12	0.41	2.36	12	1
2:B:430:ASN:O	2:B:433:ARG:CG	0.41	2.69	12	1
2:B:391:LYS:CE	2:B:391:LYS:HA	0.41	2.44	15	1
1:A:20:A:O2'	2:B:371:LYS:HD3	0.41	2.15	4	1
1:A:19:G:O4'	2:B:376:SER:OG	0.41	2.39	6	1
2:B:367:ASP:C	2:B:371:LYS:CD	0.41	2.88	7	1
2:B:407:GLY:O	2:B:408:ASP:HB3	0.41	2.16	12	1
2:B:391:LYS:O	2:B:391:LYS:CD	0.41	2.69	2	2
2:B:429:GLU:O	2:B:433:ARG:HB3	0.41	2.16	12	1
1:A:21:A:O2'	1:A:22:C:H6	0.41	1.94	2	1
2:B:421:LYS:HG2	2:B:425:ILE:CG1	0.41	2.46	5	1
2:B:421:LYS:HG2	2:B:425:ILE:HG12	0.41	1.91	5	1
2:B:378:ILE:HG13	2:B:438:LEU:CD2	0.41	2.46	7	1
2:B:366:LEU:HA	2:B:369:ASN:ND2	0.41	2.31	9	1
2:B:396:VAL:O	2:B:397:ASP:CG	0.41	2.59	12	1
2:B:441:TYR:CD1	2:B:444:GLN:HG2	0.41	2.51	12	1
1:A:17:A:C1'	1:A:18:A:P	0.41	3.09	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:434:ASP:CG	2:B:437:MET:CB	0.41	2.89	13	1
2:B:380:TYR:CE1	2:B:383:LEU:HA	0.41	2.50	14	1
1:A:5:U:O5'	1:A:5:U:H6	0.41	1.97	15	1
1:A:13:U:O2'	1:A:14:C:C4'	0.41	2.68	1	1
2:B:418:ARG:HG3	2:B:419:ASN:OD1	0.41	2.16	2	1
1:A:2:G:H2'	1:A:3:G:O5'	0.41	2.14	4	1
2:B:417:GLY:HA3	2:B:422:ILE:CD1	0.41	2.39	13	1
2:B:380:TYR:CZ	2:B:383:LEU:CA	0.40	3.04	1	1
2:B:381:ALA:O	2:B:382:SER:OG	0.40	2.39	1	1
2:B:404:CYS:SG	2:B:427:ALA:HA	0.40	2.56	1	1
2:B:429:GLU:HA	2:B:432:LEU:CD2	0.40	2.46	3	2
2:B:367:ASP:HA	2:B:425:ILE:CG2	0.40	2.41	5	1
2:B:397:ASP:HB2	2:B:399:ASN:OD1	0.40	2.16	7	1
1:A:31:U:HO2'	1:A:32:C:C5'	0.40	2.29	9	1
2:B:437:MET:O	2:B:440:PHE:HB3	0.40	2.17	14	2
1:A:5:U:O2'	1:A:6:A:C5'	0.40	2.69	14	1
2:B:434:ASP:HB3	2:B:437:MET:CB	0.40	2.46	15	1
2:B:380:TYR:HB2	2:B:383:LEU:HG	0.40	1.93	16	1
2:B:437:MET:HG2	2:B:441:TYR:CE2	0.40	2.51	4	1
2:B:380:TYR:CE1	2:B:383:LEU:HB3	0.40	2.51	8	1
2:B:380:TYR:CE2	2:B:382:SER:C	0.40	2.94	8	1
2:B:366:LEU:HG	2:B:369:ASN:CB	0.40	2.46	11	1
2:B:414:THR:OG1	2:B:415:GLY:N	0.40	2.54	11	1
2:B:366:LEU:CD1	2:B:367:ASP:N	0.40	2.79	15	1
1:A:18:A:N3	2:B:372:ARG:CD	0.40	2.85	16	1
2:B:387:TYR:CE1	2:B:404:CYS:SG	0.40	2.97	16	1
1:A:11:G:N2	1:A:12:U:O2	0.40	2.55	1	1
2:B:404:CYS:SG	2:B:427:ALA:O	0.40	2.74	2	1
1:A:24:U:O5'	1:A:24:U:C6	0.40	2.61	9	1
2:B:371:LYS:HB2	2:B:371:LYS:NZ	0.40	2.31	11	1
2:B:386:HIS:O	2:B:405:ARG:HG2	0.40	2.16	12	1
1:A:6:A:HO2'	1:A:7:C:H5'	0.40	1.77	13	1
1:A:8:C:H2'	1:A:9:A:C8	0.40	2.50	16	1
2:B:381:ALA:O	2:B:382:SER:HB2	0.40	2.16	2	1
1:A:19:G:O4'	2:B:376:SER:HB2	0.40	2.17	3	1
1:A:22:C:HO2'	1:A:23:G:H5'	0.40	1.73	5	1
2:B:420:ILE:CG1	2:B:421:LYS:N	0.40	2.84	7	1
2:B:380:TYR:CZ	2:B:445:ARG:HG2	0.40	2.52	11	1
2:B:391:LYS:O	2:B:391:LYS:HD2	0.40	2.15	16	1
2:B:394:THR:OG1	2:B:397:ASP:OD1	0.40	2.40	16	1
2:B:367:ASP:O	2:B:371:LYS:HG2	0.40	2.17	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:366:LEU:O	2:B:369:ASN:ND2	0.40	2.50	2	1
2:B:405:ARG:HG3	2:B:410:THR:O	0.40	2.17	7	1
2:B:368:MET:HE1	2:B:369:ASN:ND2	0.40	2.32	11	1
2:B:412:LEU:HB3	2:B:437:MET:SD	0.40	2.57	12	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	82/90 (91%)	56±2 (68±3%)	18±3 (22±3%)	8±2 (10±2%)	1	9
All	All	1312/1440 (91%)	889 (68%)	289 (22%)	134 (10%)	1	9

All 23 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	397	ASP	16
2	B	420	ILE	16
2	B	392	LYS	15
2	B	399	ASN	13
2	B	391	LYS	10
2	B	409	GLY	8
2	B	381	ALA	8
2	B	398	PRO	6
2	B	367	ASP	5
2	B	374	LEU	5
2	B	382	SER	5
2	B	426	ARG	4
2	B	379	GLY	4
2	B	378	ILE	4
2	B	407	GLY	3
2	B	408	ASP	2
2	B	430	ASN	2
2	B	412	LEU	2

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Mol	Chain	Res	Type	Models (Total)
2	B	380	TYR	2
2	B	383	LEU	1
2	B	411	VAL	1
2	B	384	ARG	1
2	B	425	ILE	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	65/72 (90%)	34±3 (53±4%)	31±3 (47±4%)	0 2
All	All	1040/1152 (90%)	548 (53%)	492 (47%)	0 2

All 58 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	376	SER	16
2	B	388	VAL	16
2	B	412	LEU	16
2	B	421	LYS	16
2	B	422	ILE	16
2	B	432	LEU	16
2	B	371	LYS	15
2	B	444	GLN	15
2	B	445	ARG	15
2	B	440	PHE	15
2	B	373	GLN	14
2	B	420	ILE	14
2	B	402	VAL	13
2	B	419	ASN	13
2	B	433	ARG	13
2	B	401	ILE	12
2	B	391	LYS	11
2	B	374	LEU	10
2	B	377	LEU	10
2	B	404	CYS	10

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Mol	Chain	Res	Type	Models (Total)
2	B	367	ASP	10
2	B	414	THR	9
2	B	429	GLU	9
2	B	383	LEU	9
2	B	366	LEU	8
2	B	368	MET	8
2	B	372	ARG	8
2	B	418	ARG	8
2	B	430	ASN	8
2	B	435	LYS	8
2	B	392	LYS	8
2	B	382	SER	8
2	B	405	ARG	8
2	B	403	GLU	7
2	B	443	LYS	7
2	B	406	VAL	7
2	B	397	ASP	7
2	B	400	SER	6
2	B	437	MET	6
2	B	384	ARG	6
2	B	408	ASP	6
2	B	426	ARG	6
2	B	385	LEU	5
2	B	394	THR	5
2	B	399	ASN	5
2	B	425	ILE	5
2	B	436	LYS	5
2	B	380	TYR	5
2	B	386	HIS	4
2	B	378	ILE	3
2	B	410	THR	2
2	B	389	THR	2
2	B	434	ASP	2
2	B	398	PRO	2
2	B	369	ASN	1
2	B	416	VAL	1
2	B	375	TYR	1
2	B	387	TYR	1

6.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	31/32 (97%)	4±2 (14±5%)	2±1 (5±3%)	0.13±0.02
All	All	497/512 (97%)	67 (13%)	24 (5%)	0.13

The overall RNA backbone suiteness is 0.13.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	17	A	16
1	A	18	A	15
1	A	15	A	13
1	A	13	U	6
1	A	16	G	5
1	A	3	G	3
1	A	21	A	2
1	A	4	A	2
1	A	22	C	1
1	A	28	A	1
1	A	19	G	1
1	A	8	C	1
1	A	10	U	1

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	17	A	13
1	A	16	G	5
1	A	3	G	2
1	A	1	G	1
1	A	28	A	1
1	A	18	A	1
1	A	7	C	1

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

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

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1317
Number of shifts mapped to atoms	1317
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	89	2.18 ± 0.24	Should be applied
$^{13}C_{\beta}$	82	2.66 ± 0.21	Should be applied
$^{13}C'$	0	—	None (insufficient data)
^{15}N	84	0.51 ± 0.38	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 71%, i.e. 1241 atoms were assigned a chemical shift out of a possible 1738. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	327/413 (79%)	166/169 (98%)	82/164 (50%)	79/80 (99%)
Sidechain	444/670 (66%)	270/437 (62%)	168/199 (84%)	6/34 (18%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	8/54 (15%)	8/25 (32%)	0/27 (0%)	0/2 (0%)
Sugar	352/352 (100%)	192/192 (100%)	160/160 (100%)	0/0 (—%)
Base	110/249 (44%)	63/153 (41%)	47/55 (85%)	0/41 (0%)
Overall	1241/1738 (71%)	699/976 (72%)	457/605 (76%)	85/157 (54%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 1301 atoms were assigned a chemical shift out of a possible 1833. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	353/452 (78%)	180/185 (97%)	89/180 (49%)	84/87 (97%)
Sidechain	478/726 (66%)	289/473 (61%)	183/216 (85%)	6/37 (16%)
Aromatic	8/54 (15%)	8/25 (32%)	0/27 (0%)	0/2 (0%)
Sugar	352/352 (100%)	192/192 (100%)	160/160 (100%)	0/0 (—%)
Base	110/249 (44%)	63/153 (41%)	47/55 (85%)	0/41 (0%)
Overall	1301/1833 (71%)	732/1028 (71%)	479/638 (75%)	90/167 (54%)

7.1.4 Statistically unusual chemical shifts (i)

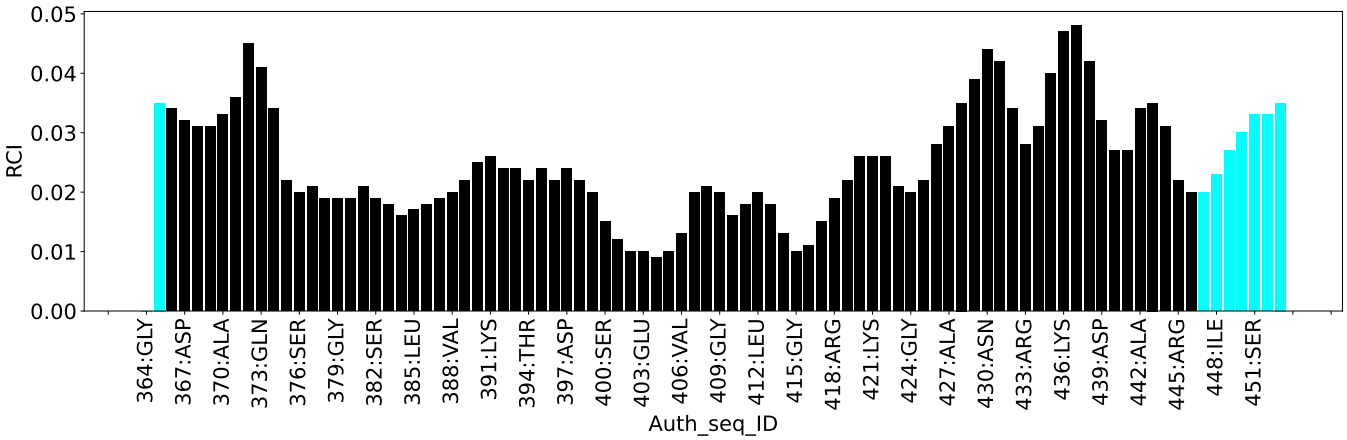
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	B	391	LYS	CG	33.40	19.35 – 30.45	7.7
1	B	444	GLN	CG	26.40	28.36 – 39.21	-6.8
1	B	421	LYS	CD	22.42	23.50 – 34.42	-6.0
1	B	392	LYS	CD	22.50	23.50 – 34.42	-5.9
1	B	420	ILE	CD1	22.46	5.18 – 21.60	5.5
1	B	451	SER	CB	55.96	56.28 – 71.32	-5.2
1	B	401	ILE	CG2	10.80	10.93 – 24.12	-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 B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2360
Intra-residue (|i-j|=0)	832
Sequential (|i-j|=1)	756
Medium range (|i-j|>1 and |i-j|<5)	329
Long range (|i-j|≥5)	397
Inter-chain	46
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	227
Number of unmapped restraints	0
Number of restraints per residue	21.2
Number of long range restraints per residue[1]	3.3

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	25.1	0.2
0.2-0.5 (Medium)	4.0	0.48
>0.5 (Large)	2.9	3.2

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.9	2.1
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

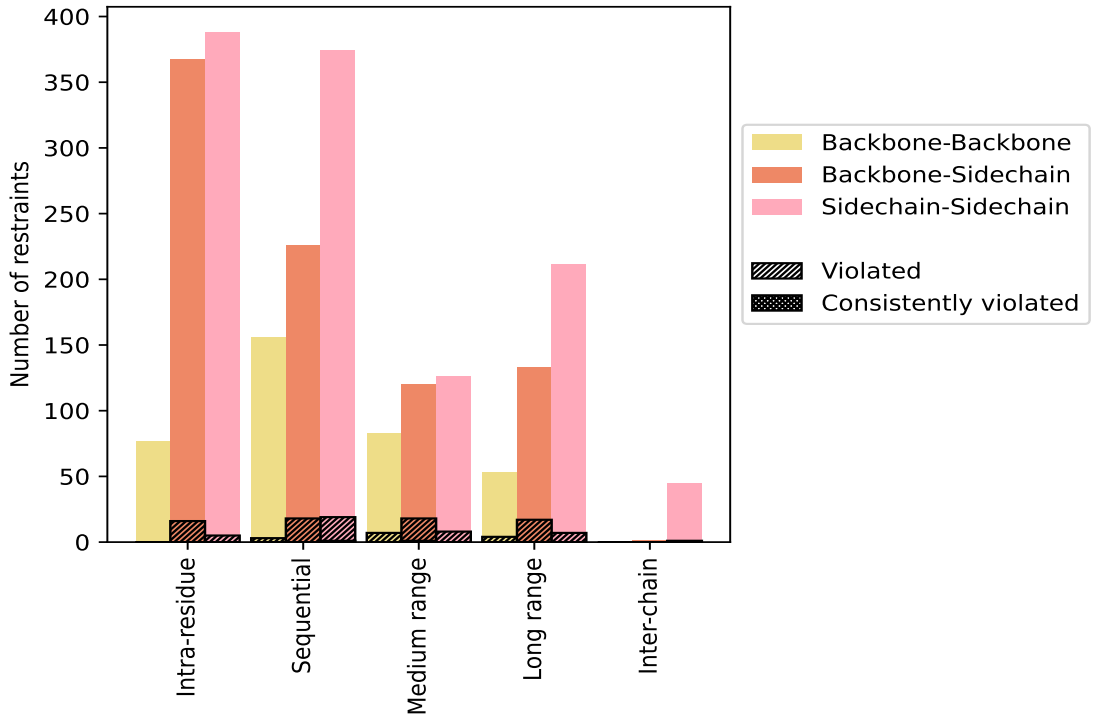
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	832	35.3	21	2.5	0.9	0	0.0	0.0
Backbone-Backbone	77	3.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	367	15.6	16	4.4	0.7	0	0.0	0.0
Sidechain-Sidechain	388	16.4	5	1.3	0.2	0	0.0	0.0
Sequential (|i-j|=1)	756	32.0	40	5.3	1.7	1	0.1	0.0
Backbone-Backbone	156	6.6	3	1.9	0.1	0	0.0	0.0
Backbone-Sidechain	226	9.6	18	8.0	0.8	0	0.0	0.0
Sidechain-Sidechain	374	15.8	19	5.1	0.8	1	0.3	0.0
Medium range (|i-j|>1 & |i-j|<5)	329	13.9	33	10.0	1.4	1	0.3	0.0
Backbone-Backbone	83	3.5	7	8.4	0.3	0	0.0	0.0
Backbone-Sidechain	120	5.1	18	15.0	0.8	1	0.8	0.0
Sidechain-Sidechain	126	5.3	8	6.3	0.3	0	0.0	0.0
Long range (|i-j|≥5)	397	16.8	28	7.1	1.2	0	0.0	0.0
Backbone-Backbone	53	2.2	4	7.5	0.2	0	0.0	0.0
Backbone-Sidechain	133	5.6	17	12.8	0.7	0	0.0	0.0
Sidechain-Sidechain	211	8.9	7	3.3	0.3	0	0.0	0.0
Inter-chain	46	1.9	1	2.2	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	45	1.9	1	2.2	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2360	100.0	123	5.2	5.2	2	0.1	0.1
Backbone-Backbone	369	15.6	14	3.8	0.6	0	0.0	0.0
Backbone-Sidechain	847	35.9	69	8.1	2.9	1	0.1	0.0
Sidechain-Sidechain	1144	48.5	40	3.5	1.7	1	0.1	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	4	9	9	7	1	30	0.2	1.01	0.17	0.16
2	3	12	10	5	1	31	0.25	1.39	0.31	0.14
3	7	11	10	5	0	33	0.29	2.27	0.46	0.13
4	2	13	8	7	1	31	0.28	1.66	0.39	0.13
5	3	11	7	9	0	30	0.2	1.16	0.19	0.14
6	5	13	9	8	0	35	0.24	1.81	0.35	0.15
7	6	13	11	9	0	39	0.28	2.06	0.44	0.14
8	5	10	8	7	0	30	0.27	1.57	0.34	0.15
9	6	11	6	7	1	31	0.32	1.78	0.42	0.14
10	3	10	14	6	1	34	0.22	1.52	0.29	0.13
11	5	13	6	10	1	35	0.35	2.17	0.5	0.17

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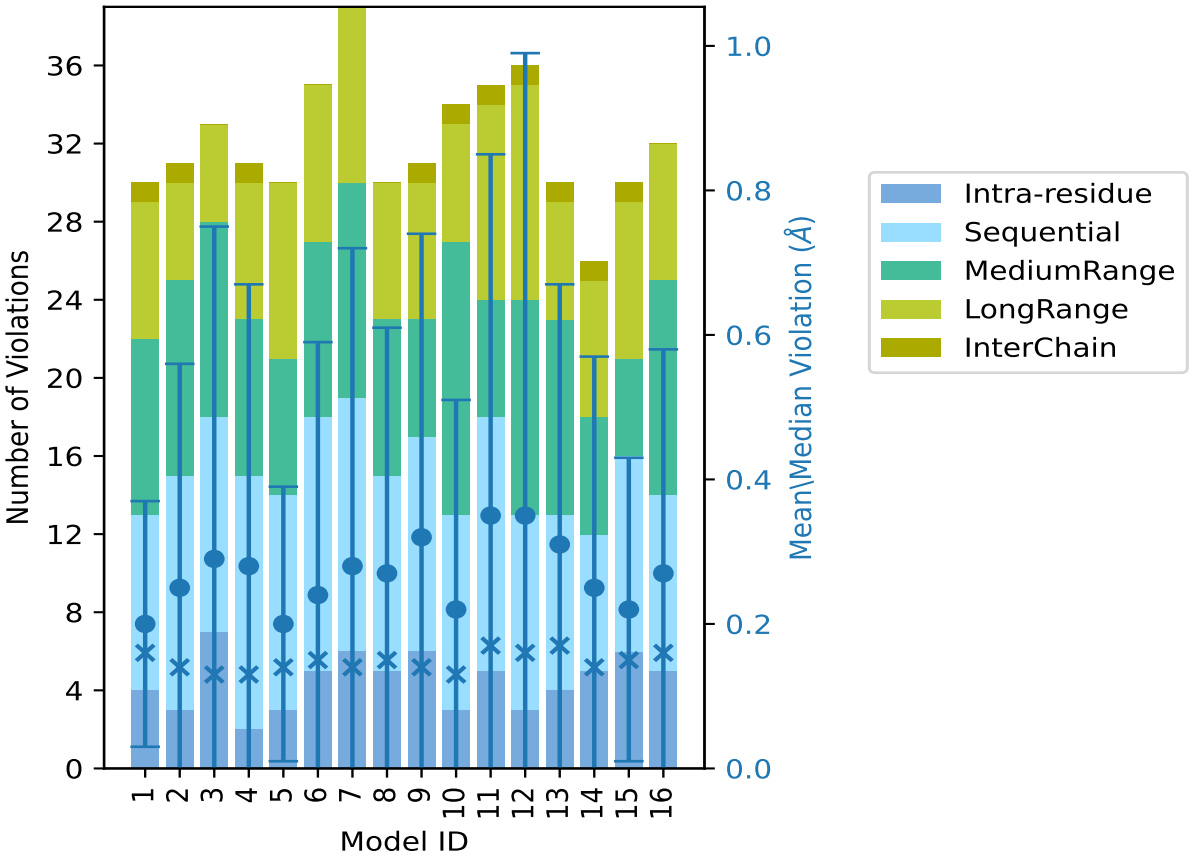
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	3	10	11	11	1	36	0.35	3.2	0.64	0.16
13	4	9	10	6	1	30	0.31	1.58	0.36	0.17
14	5	7	6	7	1	26	0.25	1.58	0.32	0.14
15	6	10	5	8	1	30	0.22	1.1	0.21	0.15
16	5	9	11	7	0	32	0.27	1.51	0.31	0.16

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

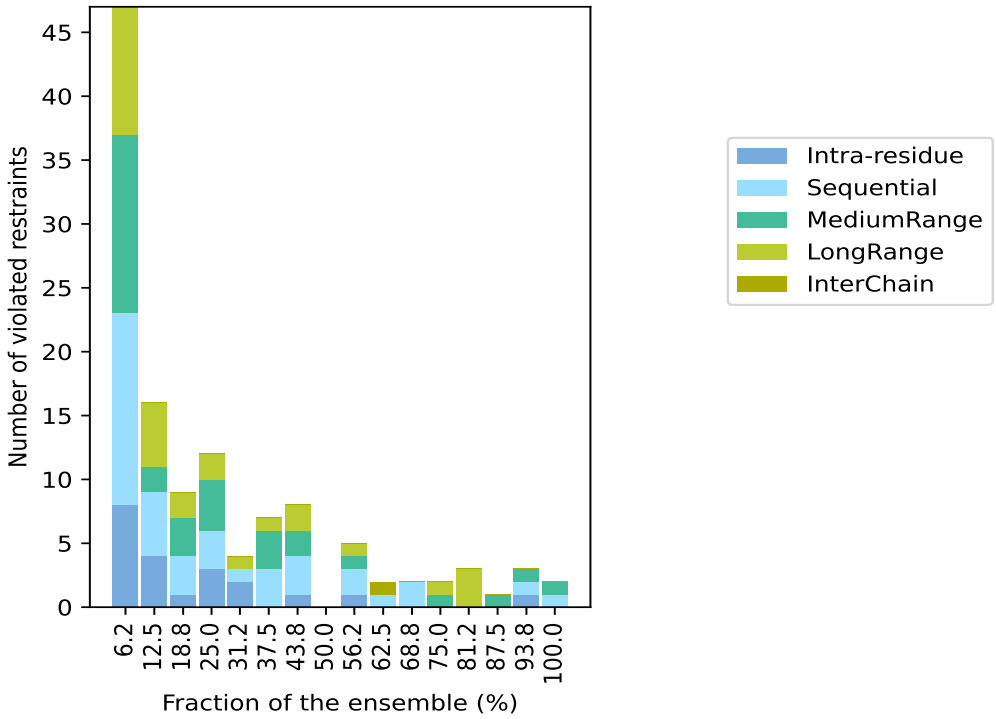
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2237(IR:811, SQ:716, MR:296, LR:369, IC:45) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
8	15	14	10	0	47	1	6.2
4	5	2	5	0	16	2	12.5
1	3	3	2	0	9	3	18.8
3	3	4	2	0	12	4	25.0
2	1	0	1	0	4	5	31.2
0	3	3	1	0	7	6	37.5
1	3	2	2	0	8	7	43.8
0	0	0	0	0	0	8	50.0
1	2	1	1	0	5	9	56.2
0	1	0	0	1	2	10	62.5
0	2	0	0	0	2	11	68.8
0	0	1	1	0	2	12	75.0
0	0	0	3	0	3	13	81.2
0	0	1	0	0	1	14	87.5
1	1	1	0	0	3	15	93.8
0	1	1	0	0	2	16	100.0

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

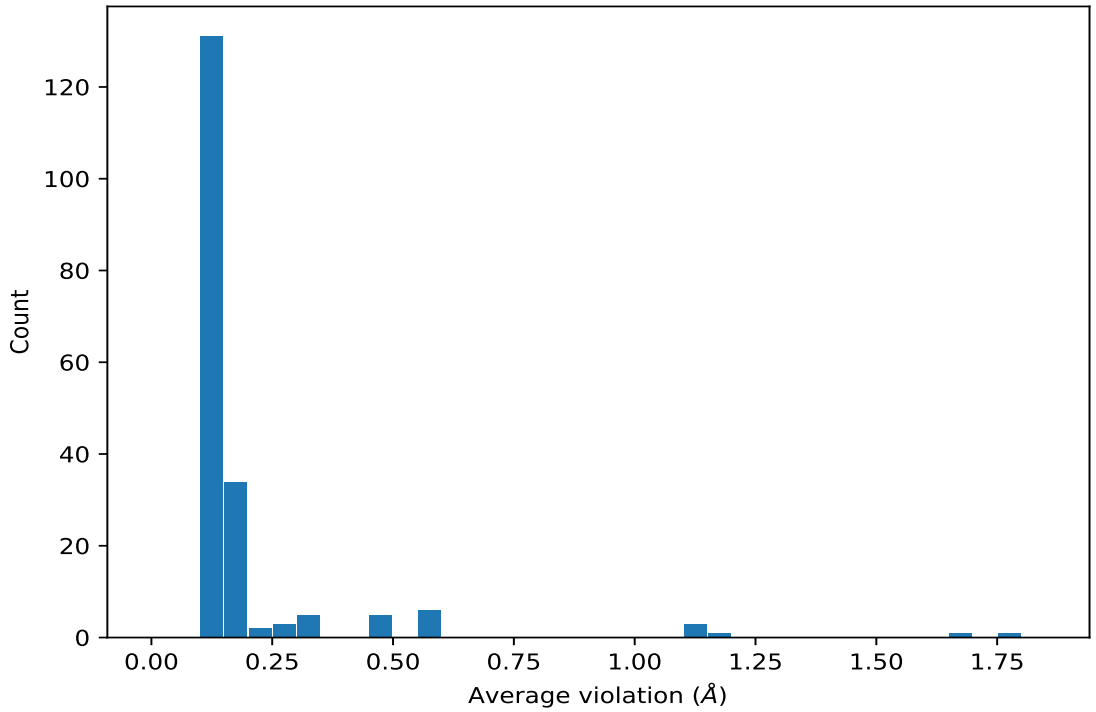
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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)
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	16	1.16	0.15	1.12
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	16	1.15	0.52	1.5
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	16	1.15	0.52	1.5
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	16	1.15	0.52	1.5
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	15	0.23	0.05	0.22
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	15	0.23	0.05	0.22
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	15	0.16	0.03	0.16
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	15	0.16	0.03	0.16
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	15	0.16	0.03	0.16
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	15	0.16	0.03	0.16
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	15	0.15	0.02	0.15
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	15	0.15	0.02	0.15
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	14	0.16	0.02	0.17
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	13	0.19	0.03	0.19
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	13	0.19	0.03	0.19
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	13	0.17	0.03	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	13	0.17	0.03	0.16
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	13	0.17	0.03	0.16
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	13	0.14	0.02	0.15
(1,1249)	2:B:394:THR:H	2:B:399:ASN:H	12	0.17	0.03	0.16
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB2	12	0.13	0.01	0.13
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB3	12	0.13	0.01	0.13
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB2	12	0.13	0.01	0.13
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB3	12	0.13	0.01	0.13
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB2	12	0.13	0.01	0.13
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB3	12	0.13	0.01	0.13
(1,1240)	2:B:394:THR:H	2:B:393:PRO:HB2	11	0.15	0.02	0.14
(1,615)	1:A:29:U:H5	1:A:28:A:H1'	11	0.13	0.02	0.13
(1,727)	2:B:377:LEU:HD11	1:A:18:A:H2	10	0.56	0.27	0.52
(1,727)	2:B:377:LEU:HD12	1:A:18:A:H2	10	0.56	0.27	0.52
(1,727)	2:B:377:LEU:HD13	1:A:18:A:H2	10	0.56	0.27	0.52
(1,727)	2:B:377:LEU:HD21	1:A:18:A:H2	10	0.56	0.27	0.52
(1,727)	2:B:377:LEU:HD22	1:A:18:A:H2	10	0.56	0.27	0.52
(1,727)	2:B:377:LEU:HD23	1:A:18:A:H2	10	0.56	0.27	0.52
(1,143)	1:A:8:C:H6	1:A:7:C:H1'	10	0.13	0.02	0.12
(1,1705)	2:B:421:LYS:H	2:B:421:LYS:HD3	9	0.19	0.01	0.19
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB2	9	0.16	0.04	0.15
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB3	9	0.16	0.04	0.15
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG11	9	0.15	0.05	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG12	9	0.15	0.05	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG13	9	0.15	0.05	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG21	9	0.15	0.05	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG22	9	0.15	0.05	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG23	9	0.15	0.05	0.13
(1,2240)	2:B:447:ALA:H	2:B:448:ILE:HB	9	0.14	0.01	0.14
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB2	9	0.14	0.02	0.13
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB3	9	0.14	0.02	0.13
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HG	9	0.14	0.02	0.13
(1,1129)	2:B:387:TYR:HE1	2:B:404:CYS:HB3	7	1.77	0.94	2.06
(1,1130)	2:B:387:TYR:HE1	2:B:404:CYS:HB2	7	1.67	0.42	1.66
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG2	7	0.16	0.02	0.16
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG3	7	0.16	0.02	0.16
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG21	7	0.15	0.04	0.15
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG22	7	0.15	0.04	0.15
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG23	7	0.15	0.04	0.15
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG21	7	0.15	0.04	0.15
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG22	7	0.15	0.04	0.15
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG23	7	0.15	0.04	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD11	7	0.14	0.02	0.14
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD12	7	0.14	0.02	0.14
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD13	7	0.14	0.02	0.14
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD11	7	0.14	0.02	0.14
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD12	7	0.14	0.02	0.14
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD13	7	0.14	0.02	0.14
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD11	7	0.14	0.02	0.14
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD12	7	0.14	0.02	0.14
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD13	7	0.14	0.02	0.14
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG2	7	0.14	0.02	0.13
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG3	7	0.14	0.02	0.13
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG2	7	0.14	0.02	0.13
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG3	7	0.14	0.02	0.13
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG2	7	0.14	0.02	0.13
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG3	7	0.14	0.02	0.13
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB2	7	0.13	0.01	0.13
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB3	7	0.13	0.01	0.13
(1,672)	1:A:31:U:H6	1:A:30:C:H1'	7	0.12	0.02	0.11
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA2	6	0.18	0.04	0.18
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA3	6	0.18	0.04	0.18
(1,2347)	2:B:406:VAL:HG11	2:B:410:THR:HA	6	0.18	0.04	0.18
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA2	6	0.18	0.04	0.18
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA3	6	0.18	0.04	0.18
(1,2347)	2:B:406:VAL:HG12	2:B:410:THR:HA	6	0.18	0.04	0.18
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA2	6	0.18	0.04	0.18
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA3	6	0.18	0.04	0.18
(1,2347)	2:B:406:VAL:HG13	2:B:410:THR:HA	6	0.18	0.04	0.18
(1,1284)	2:B:397:ASP:H	2:B:396:VAL:HA	6	0.18	0.04	0.18
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD11	6	0.14	0.02	0.14
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD12	6	0.14	0.02	0.14
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD13	6	0.14	0.02	0.14
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD11	6	0.14	0.02	0.14
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD12	6	0.14	0.02	0.14
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD13	6	0.14	0.02	0.14
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD11	6	0.14	0.02	0.14
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD12	6	0.14	0.02	0.14
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD13	6	0.14	0.02	0.14
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD11	6	0.14	0.02	0.14
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD12	6	0.14	0.02	0.14
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD13	6	0.14	0.02	0.14
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD11	6	0.13	0.03	0.12
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD12	6	0.13	0.03	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD13	6	0.13	0.03	0.12
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB1	6	0.13	0.01	0.12
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB2	6	0.13	0.01	0.12
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB3	6	0.13	0.01	0.12
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG21	6	0.13	0.02	0.12
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG22	6	0.13	0.02	0.12
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG23	6	0.13	0.02	0.12
(1,534)	1:A:26:G:H8	1:A:25:G:H1'	6	0.12	0.01	0.12
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD11	5	0.29	0.09	0.24
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD12	5	0.29	0.09	0.24
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD13	5	0.29	0.09	0.24
(1,52)	1:A:3:G:H8	1:A:3:G:H5"	5	0.14	0.01	0.14
(1,1377)	2:B:401:ILE:H	2:B:401:ILE:HB	5	0.13	0.01	0.13
(1,1122)	2:B:387:TYR:HE1	2:B:402:VAL:HB	5	0.12	0.0	0.12
(1,1122)	2:B:387:TYR:HE2	2:B:402:VAL:HB	5	0.12	0.0	0.12
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG21	4	0.48	0.23	0.44
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG22	4	0.48	0.23	0.44
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG23	4	0.48	0.23	0.44
(1,1589)	2:B:414:THR:H	2:B:430:ASN:HA	4	0.17	0.05	0.16
(1,924)	2:B:377:LEU:H	2:B:377:LEU:HG	4	0.16	0.04	0.16
(1,2184)	2:B:444:GLN:H	2:B:444:GLN:HE21	4	0.16	0.04	0.16
(1,2184)	2:B:444:GLN:H	2:B:444:GLN:HE22	4	0.16	0.04	0.16
(1,281)	1:A:13:U:H6	1:A:12:U:H1'	4	0.16	0.04	0.16
(1,1760)	2:B:424:GLY:H	2:B:421:LYS:HD2	4	0.15	0.03	0.14
(1,1760)	2:B:424:GLY:H	2:B:421:LYS:HD3	4	0.15	0.03	0.14
(1,1948)	2:B:434:ASP:H	2:B:438:LEU:HG	4	0.14	0.02	0.14
(1,1374)	2:B:401:ILE:HG21	2:B:416:VAL:HA	4	0.14	0.02	0.13
(1,1374)	2:B:401:ILE:HG22	2:B:416:VAL:HA	4	0.14	0.02	0.13
(1,1374)	2:B:401:ILE:HG23	2:B:416:VAL:HA	4	0.14	0.02	0.13
(1,504)	1:A:25:G:H8	1:A:24:U:H1'	4	0.13	0.01	0.14
(1,1073)	2:B:385:LEU:H	2:B:386:HIS:H	4	0.13	0.01	0.13
(1,1615)	2:B:416:VAL:H	2:B:416:VAL:HB	4	0.13	0.01	0.13
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG21	4	0.12	0.0	0.12
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG22	4	0.12	0.0	0.12
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG23	4	0.12	0.0	0.12
(1,2327)	2:B:367:ASP:H	2:B:366:LEU:HB2	3	0.34	0.05	0.33
(1,2327)	2:B:367:ASP:H	2:B:366:LEU:HB3	3	0.34	0.05	0.33
(1,2327)	2:B:367:ASP:H	2:B:366:LEU:HG	3	0.34	0.05	0.33
(1,1767)	2:B:424:GLY:H	2:B:426:ARG:H	3	0.17	0.03	0.16
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG11	3	0.13	0.01	0.13
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG12	3	0.13	0.01	0.13
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG13	3	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG21	3	0.13	0.01	0.13
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG22	3	0.13	0.01	0.13
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG23	3	0.13	0.01	0.13
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG11	3	0.13	0.01	0.13
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG12	3	0.13	0.01	0.13
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG13	3	0.13	0.01	0.13
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG21	3	0.13	0.01	0.13
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG22	3	0.13	0.01	0.13
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG23	3	0.13	0.01	0.13
(1,1671)	2:B:419:ASN:H	2:B:421:LYS:H	3	0.13	0.01	0.12
(1,1239)	2:B:394:THR:H	2:B:393:PRO:HB3	3	0.12	0.01	0.12
(1,439)	1:A:23:G:H1	1:A:10:U:H5	3	0.11	0.0	0.11
(1,456)	1:A:23:G:H8	1:A:23:G:H5"	3	0.11	0.0	0.11
(1,477)	1:A:24:U:H6	1:A:23:G:H1'	3	0.11	0.0	0.11
(1,1672)	2:B:419:ASN:H	2:B:422:ILE:HD11	3	0.11	0.0	0.11
(1,1672)	2:B:419:ASN:H	2:B:422:ILE:HD12	3	0.11	0.0	0.11
(1,1672)	2:B:419:ASN:H	2:B:422:ILE:HD13	3	0.11	0.0	0.11
(1,983)	2:B:380:TYR:H	2:B:380:TYR:HE1	2	0.46	0.02	0.46
(1,983)	2:B:380:TYR:H	2:B:380:TYR:HE2	2	0.46	0.02	0.46
(1,977)	2:B:380:TYR:HE1	2:B:381:ALA:HA	2	0.35	0.04	0.35
(1,977)	2:B:380:TYR:HE2	2:B:381:ALA:HA	2	0.35	0.04	0.35
(1,2174)	2:B:444:GLN:HE22	2:B:444:GLN:HB2	2	0.18	0.06	0.18
(1,2174)	2:B:444:GLN:HE22	2:B:444:GLN:HB3	2	0.18	0.06	0.18
(1,1003)	2:B:383:LEU:H	2:B:380:TYR:H	2	0.15	0.03	0.15
(1,1404)	2:B:403:GLU:H	2:B:389:THR:HB	2	0.14	0.02	0.14
(1,1071)	2:B:385:LEU:H	2:B:385:LEU:HG	2	0.14	0.02	0.14
(1,2356)	2:B:430:ASN:HD21	2:B:414:THR:HA	2	0.13	0.02	0.13
(1,2356)	2:B:430:ASN:HD21	2:B:427:ALA:HA	2	0.13	0.02	0.13
(1,642)	1:A:30:C:H6	1:A:29:U:H1'	2	0.12	0.01	0.12
(1,1414)	2:B:404:CYS:H	2:B:405:ARG:HB2	2	0.12	0.02	0.12
(1,1414)	2:B:404:CYS:H	2:B:405:ARG:HB3	2	0.12	0.02	0.12
(1,1806)	2:B:427:ALA:H	2:B:402:VAL:HG11	2	0.12	0.02	0.12
(1,1806)	2:B:427:ALA:H	2:B:402:VAL:HG12	2	0.12	0.02	0.12
(1,1806)	2:B:427:ALA:H	2:B:402:VAL:HG13	2	0.12	0.02	0.12
(1,2185)	2:B:444:GLN:H	2:B:444:GLN:HG2	2	0.12	0.02	0.12
(1,2185)	2:B:444:GLN:H	2:B:444:GLN:HG3	2	0.12	0.02	0.12
(1,2300)	2:B:450:ARG:H	2:B:449:PRO:HG2	2	0.12	0.02	0.12
(1,2300)	2:B:450:ARG:H	2:B:449:PRO:HG3	2	0.12	0.02	0.12
(1,1400)	2:B:403:GLU:HA	2:B:414:THR:HG21	2	0.12	0.01	0.12
(1,1400)	2:B:403:GLU:HA	2:B:414:THR:HG22	2	0.12	0.01	0.12
(1,1400)	2:B:403:GLU:HA	2:B:414:THR:HG23	2	0.12	0.01	0.12
(1,2168)	2:B:444:GLN:HE21	2:B:441:TYR:HA	2	0.12	0.01	0.12

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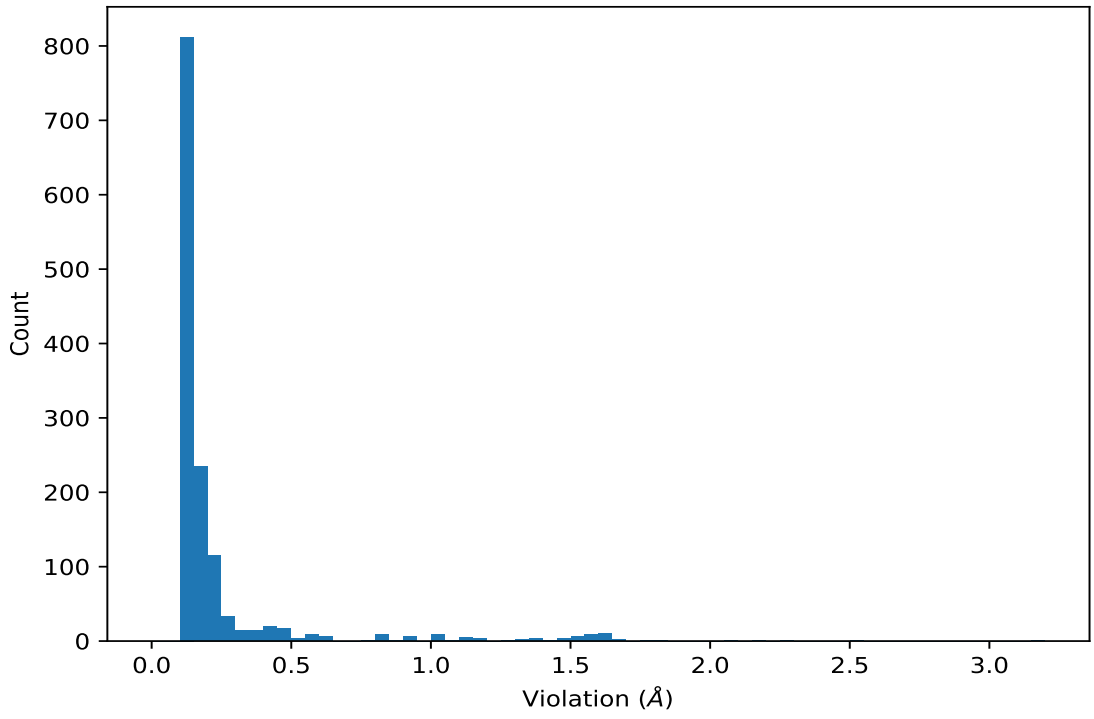
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2168)	2:B:444:GLN:HE22	2:B:441:TYR:HA	2	0.12	0.01	0.12
(1,390)	1:A:20:A:H8	1:A:19:G:H1'	2	0.12	0.0	0.12
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG11	2	0.12	0.0	0.12
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG12	2	0.12	0.0	0.12
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG13	2	0.12	0.0	0.12
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG21	2	0.12	0.0	0.12
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG22	2	0.12	0.0	0.12
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG23	2	0.12	0.0	0.12

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1129)	2:B:387:TYR:HE1	2:B:404:CYS:HB3	12	3.2
(1,1130)	2:B:387:TYR:HE1	2:B:404:CYS:HB2	12	2.51
(1,1129)	2:B:387:TYR:HE1	2:B:404:CYS:HB3	3	2.27
(1,1129)	2:B:387:TYR:HE1	2:B:404:CYS:HB3	11	2.17
(1,1129)	2:B:387:TYR:HE1	2:B:404:CYS:HB3	7	2.06
(1,1130)	2:B:387:TYR:HE1	2:B:404:CYS:HB2	6	1.81
(1,1129)	2:B:387:TYR:HE1	2:B:404:CYS:HB3	9	1.78
(1,1130)	2:B:387:TYR:HE1	2:B:404:CYS:HB2	11	1.7
(1,1130)	2:B:387:TYR:HE1	2:B:404:CYS:HB2	4	1.66
(1,1130)	2:B:387:TYR:HE1	2:B:404:CYS:HB2	3	1.62
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	7	1.61
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	7	1.61
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	7	1.61
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	9	1.61
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	9	1.61
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	9	1.61
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	11	1.6
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	11	1.6
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	11	1.6
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	13	1.58
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	13	1.58
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	13	1.58
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	14	1.58
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	14	1.58
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	14	1.58
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	8	1.57
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	8	1.57
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	8	1.57
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	10	1.52
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	10	1.52
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	10	1.52
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	16	1.51
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	16	1.51
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	16	1.51
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	4	1.48
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	4	1.48
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	4	1.48
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	13	1.47
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	6	1.43
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	2	1.39
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	2	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	2	1.39
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	8	1.31
(1,1130)	2:B:387:TYR:HE1	2:B:404:CYS:HB2	7	1.31
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	11	1.29
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	4	1.2
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	10	1.17
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	5	1.16
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	7	1.13
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	2	1.12
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	12	1.11
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	16	1.11
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	15	1.1
(1,1130)	2:B:387:TYR:HE1	2:B:404:CYS:HB2	9	1.05
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	14	1.03
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	3	1.02
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	1	1.01
(1,727)	2:B:377:LEU:HD11	1:A:18:A:H2	2	1.0
(1,727)	2:B:377:LEU:HD12	1:A:18:A:H2	2	1.0
(1,727)	2:B:377:LEU:HD13	1:A:18:A:H2	2	1.0
(1,727)	2:B:377:LEU:HD21	1:A:18:A:H2	2	1.0
(1,727)	2:B:377:LEU:HD22	1:A:18:A:H2	2	1.0
(1,727)	2:B:377:LEU:HD23	1:A:18:A:H2	2	1.0
(1,727)	2:B:377:LEU:HD11	1:A:18:A:H2	13	0.94
(1,727)	2:B:377:LEU:HD12	1:A:18:A:H2	13	0.94
(1,727)	2:B:377:LEU:HD13	1:A:18:A:H2	13	0.94
(1,727)	2:B:377:LEU:HD21	1:A:18:A:H2	13	0.94
(1,727)	2:B:377:LEU:HD22	1:A:18:A:H2	13	0.94
(1,727)	2:B:377:LEU:HD23	1:A:18:A:H2	13	0.94
(1,614)	1:A:29:U:H4'	1:A:30:C:H5"	9	0.88
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG21	8	0.84
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG22	8	0.84
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG23	8	0.84
(1,727)	2:B:377:LEU:HD11	1:A:18:A:H2	15	0.81
(1,727)	2:B:377:LEU:HD12	1:A:18:A:H2	15	0.81
(1,727)	2:B:377:LEU:HD13	1:A:18:A:H2	15	0.81
(1,727)	2:B:377:LEU:HD21	1:A:18:A:H2	15	0.81
(1,727)	2:B:377:LEU:HD22	1:A:18:A:H2	15	0.81
(1,727)	2:B:377:LEU:HD23	1:A:18:A:H2	15	0.81
(1,1129)	2:B:387:TYR:HE1	2:B:404:CYS:HB3	16	0.77
(1,727)	2:B:377:LEU:HD11	1:A:18:A:H2	11	0.62
(1,727)	2:B:377:LEU:HD12	1:A:18:A:H2	11	0.62
(1,727)	2:B:377:LEU:HD13	1:A:18:A:H2	11	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,727)	2:B:377:LEU:HD21	1:A:18:A:H2	11	0.62
(1,727)	2:B:377:LEU:HD22	1:A:18:A:H2	11	0.62
(1,727)	2:B:377:LEU:HD23	1:A:18:A:H2	11	0.62
(1,727)	2:B:377:LEU:HD11	1:A:18:A:H2	4	0.58
(1,727)	2:B:377:LEU:HD12	1:A:18:A:H2	4	0.58
(1,727)	2:B:377:LEU:HD13	1:A:18:A:H2	4	0.58
(1,727)	2:B:377:LEU:HD21	1:A:18:A:H2	4	0.58
(1,727)	2:B:377:LEU:HD22	1:A:18:A:H2	4	0.58
(1,727)	2:B:377:LEU:HD23	1:A:18:A:H2	4	0.58
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	12	0.55
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	12	0.55
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	12	0.55
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	5	0.51
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	5	0.51
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	5	0.51
(1,983)	2:B:380:TYR:H	2:B:380:TYR:HE1	13	0.48
(1,983)	2:B:380:TYR:H	2:B:380:TYR:HE2	13	0.48
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	1	0.48
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	1	0.48
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	1	0.48
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	6	0.47
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	6	0.47
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	6	0.47
(1,727)	2:B:377:LEU:HD11	1:A:18:A:H2	9	0.45
(1,727)	2:B:377:LEU:HD12	1:A:18:A:H2	9	0.45
(1,727)	2:B:377:LEU:HD13	1:A:18:A:H2	9	0.45
(1,727)	2:B:377:LEU:HD21	1:A:18:A:H2	9	0.45
(1,727)	2:B:377:LEU:HD22	1:A:18:A:H2	9	0.45
(1,727)	2:B:377:LEU:HD23	1:A:18:A:H2	9	0.45
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG21	16	0.45
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG22	16	0.45
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG23	16	0.45
(1,983)	2:B:380:TYR:H	2:B:380:TYR:HE1	16	0.44
(1,983)	2:B:380:TYR:H	2:B:380:TYR:HE2	16	0.44
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	15	0.44
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	15	0.44
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	15	0.44
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG11	3	0.43
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG12	3	0.43
(1,1484)	2:B:408:ASP:H	2:B:406:VAL:HG13	3	0.43
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG21	2	0.42
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG22	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG23	2	0.42
(1,2327)	2:B:367:ASP:H	2:B:366:LEU:HB2	8	0.41
(1,2327)	2:B:367:ASP:H	2:B:366:LEU:HB3	8	0.41
(1,2327)	2:B:367:ASP:H	2:B:366:LEU:HG	8	0.41
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD11	13	0.41
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD12	13	0.41
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD13	13	0.41
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD11	9	0.4
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD12	9	0.4
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD13	9	0.4
(1,977)	2:B:380:TYR:HE1	2:B:381:ALA:HA	16	0.39
(1,977)	2:B:380:TYR:HE2	2:B:381:ALA:HA	16	0.39
(1,727)	2:B:377:LEU:HD11	1:A:18:A:H2	14	0.38
(1,727)	2:B:377:LEU:HD12	1:A:18:A:H2	14	0.38
(1,727)	2:B:377:LEU:HD13	1:A:18:A:H2	14	0.38
(1,727)	2:B:377:LEU:HD21	1:A:18:A:H2	14	0.38
(1,727)	2:B:377:LEU:HD22	1:A:18:A:H2	14	0.38
(1,727)	2:B:377:LEU:HD23	1:A:18:A:H2	14	0.38
(1,727)	2:B:377:LEU:HD11	1:A:18:A:H2	10	0.37
(1,727)	2:B:377:LEU:HD12	1:A:18:A:H2	10	0.37
(1,727)	2:B:377:LEU:HD13	1:A:18:A:H2	10	0.37
(1,727)	2:B:377:LEU:HD21	1:A:18:A:H2	10	0.37
(1,727)	2:B:377:LEU:HD22	1:A:18:A:H2	10	0.37
(1,727)	2:B:377:LEU:HD23	1:A:18:A:H2	10	0.37
(1,999)	2:B:383:LEU:HD21	2:B:380:TYR:HE1	13	0.35
(1,999)	2:B:383:LEU:HD21	2:B:380:TYR:HE2	13	0.35
(1,999)	2:B:383:LEU:HD22	2:B:380:TYR:HE1	13	0.35
(1,999)	2:B:383:LEU:HD22	2:B:380:TYR:HE2	13	0.35
(1,999)	2:B:383:LEU:HD23	2:B:380:TYR:HE1	13	0.35
(1,999)	2:B:383:LEU:HD23	2:B:380:TYR:HE2	13	0.35
(1,928)	2:B:377:LEU:H	2:B:379:GLY:H	13	0.34
(1,2327)	2:B:367:ASP:H	2:B:366:LEU:HB2	9	0.33
(1,2327)	2:B:367:ASP:H	2:B:366:LEU:HB3	9	0.33
(1,2327)	2:B:367:ASP:H	2:B:366:LEU:HG	9	0.33
(1,977)	2:B:380:TYR:HE1	2:B:381:ALA:HA	13	0.31
(1,977)	2:B:380:TYR:HE2	2:B:381:ALA:HA	13	0.31
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	14	0.31
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	14	0.31
(1,1552)	2:B:412:LEU:HD21	2:B:411:VAL:HA	16	0.3
(1,1552)	2:B:412:LEU:HD22	2:B:411:VAL:HA	16	0.3
(1,1552)	2:B:412:LEU:HD23	2:B:411:VAL:HA	16	0.3
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	5	0.3
(1,2327)	2:B:367:ASP:H	2:B:366:LEU:HB2	11	0.29
(1,2327)	2:B:367:ASP:H	2:B:366:LEU:HB3	11	0.29
(1,2327)	2:B:367:ASP:H	2:B:366:LEU:HG	11	0.29
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	10	0.28
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	10	0.28
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG11	15	0.27
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG12	15	0.27
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG13	15	0.27
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG21	15	0.27
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG22	15	0.27
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG23	15	0.27
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	13	0.27
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	13	0.27
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	15	0.27
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	15	0.27
(1,797)	2:B:369:ASN:HD22	2:B:369:ASN:HA	2	0.26
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	1	0.26
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	1	0.26
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	15	0.25
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	15	0.25
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB2	6	0.25
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB3	6	0.25
(1,1589)	2:B:414:THR:H	2:B:430:ASN:HA	12	0.25
(1,1284)	2:B:397:ASP:H	2:B:396:VAL:HA	12	0.25
(1,1109)	2:B:387:TYR:HA	2:B:404:CYS:HA	12	0.25
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	4	0.25
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	4	0.25
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	4	0.25
(1,898)	2:B:375:TYR:H	2:B:376:SER:HB2	5	0.24
(1,898)	2:B:375:TYR:H	2:B:376:SER:HB3	5	0.24
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA2	3	0.24
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA3	3	0.24
(1,2347)	2:B:406:VAL:HG11	2:B:410:THR:HA	3	0.24
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA2	3	0.24
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA3	3	0.24
(1,2347)	2:B:406:VAL:HG12	2:B:410:THR:HA	3	0.24
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA2	3	0.24
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA3	3	0.24
(1,2347)	2:B:406:VAL:HG13	2:B:410:THR:HA	3	0.24
(1,2174)	2:B:444:GLN:HE22	2:B:444:GLN:HB2	14	0.24
(1,2174)	2:B:444:GLN:HE22	2:B:444:GLN:HB3	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD11	12	0.24
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD12	12	0.24
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD13	12	0.24
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	10	0.24
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	10	0.24
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG21	11	0.24
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG22	11	0.24
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG23	11	0.24
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG21	11	0.24
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG22	11	0.24
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG23	11	0.24
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	8	0.24
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	8	0.24
(1,800)	2:B:369:ASN:H	2:B:366:LEU:HA	1	0.23
(1,727)	2:B:377:LEU:HD11	1:A:18:A:H2	1	0.23
(1,727)	2:B:377:LEU:HD12	1:A:18:A:H2	1	0.23
(1,727)	2:B:377:LEU:HD13	1:A:18:A:H2	1	0.23
(1,727)	2:B:377:LEU:HD21	1:A:18:A:H2	1	0.23
(1,727)	2:B:377:LEU:HD22	1:A:18:A:H2	1	0.23
(1,727)	2:B:377:LEU:HD23	1:A:18:A:H2	1	0.23
(1,1125)	2:B:387:TYR:HE1	2:B:404:CYS:HA	12	0.23
(1,1125)	2:B:387:TYR:HE2	2:B:404:CYS:HA	12	0.23
(1,924)	2:B:377:LEU:H	2:B:377:LEU:HG	12	0.22
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	3	0.22
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	3	0.22
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	3	0.22
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	3	0.22
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	14	0.22
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	14	0.22
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	16	0.22
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	16	0.22
(1,281)	1:A:13:U:H6	1:A:12:U:H1'	3	0.21
(1,2184)	2:B:444:GLN:H	2:B:444:GLN:HE21	7	0.21
(1,2184)	2:B:444:GLN:H	2:B:444:GLN:HE22	7	0.21
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	1	0.21
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	1	0.21
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	1	0.21
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	1	0.21
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	13	0.21
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	13	0.21
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	13	0.21
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD11	10	0.21
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD12	10	0.21
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD13	10	0.21
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	9	0.21
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	9	0.21
(1,1767)	2:B:424:GLY:H	2:B:426:ARG:H	15	0.21
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG2	2	0.21
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG3	2	0.21
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG21	12	0.21
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG22	12	0.21
(1,1485)	2:B:408:ASP:H	2:B:406:VAL:HG23	12	0.21
(1,1284)	2:B:397:ASP:H	2:B:396:VAL:HA	2	0.21
(1,1284)	2:B:397:ASP:H	2:B:396:VAL:HA	11	0.21
(1,1249)	2:B:394:THR:H	2:B:399:ASN:H	5	0.21
(1,1249)	2:B:394:THR:H	2:B:399:ASN:H	9	0.21
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	2	0.21
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	2	0.21
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	4	0.21
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	4	0.21
(1,87)	1:A:5:U:H6	1:A:4:A:H1'	11	0.2
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA2	1	0.2
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA3	1	0.2
(1,2347)	2:B:406:VAL:HG11	2:B:410:THR:HA	1	0.2
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA2	1	0.2
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA3	1	0.2
(1,2347)	2:B:406:VAL:HG12	2:B:410:THR:HA	1	0.2
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA2	1	0.2
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA3	1	0.2
(1,2347)	2:B:406:VAL:HG13	2:B:410:THR:HA	1	0.2
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA2	15	0.2
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA3	15	0.2
(1,2347)	2:B:406:VAL:HG11	2:B:410:THR:HA	15	0.2
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA2	15	0.2
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA3	15	0.2
(1,2347)	2:B:406:VAL:HG12	2:B:410:THR:HA	15	0.2
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA2	15	0.2
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA3	15	0.2
(1,2347)	2:B:406:VAL:HG13	2:B:410:THR:HA	15	0.2
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	11	0.2
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	11	0.2
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	11	0.2
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD11	11	0.2
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD12	11	0.2
(1,1921)	2:B:433:ARG:H	2:B:432:LEU:HD13	11	0.2
(1,1705)	2:B:421:LYS:H	2:B:421:LYS:HD3	5	0.2
(1,1705)	2:B:421:LYS:H	2:B:421:LYS:HD3	7	0.2
(1,1249)	2:B:394:THR:H	2:B:399:ASN:H	3	0.2
(1,1249)	2:B:394:THR:H	2:B:399:ASN:H	14	0.2
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	6	0.2
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	6	0.2
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	3	0.2
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	3	0.2
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	3	0.2
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	5	0.2
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	5	0.2
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	5	0.2
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	14	0.2
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	14	0.2
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	14	0.2
(1,2275)	2:B:449:PRO:HB2	2:B:448:ILE:HA	10	0.19
(1,2275)	2:B:449:PRO:HB3	2:B:448:ILE:HA	10	0.19
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	4	0.19
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	4	0.19
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	8	0.19
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	8	0.19
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	11	0.19
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	11	0.19
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	13	0.19
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	13	0.19
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	11	0.19
(1,1705)	2:B:421:LYS:H	2:B:421:LYS:HD3	1	0.19
(1,1705)	2:B:421:LYS:H	2:B:421:LYS:HD3	3	0.19
(1,1705)	2:B:421:LYS:H	2:B:421:LYS:HD3	8	0.19
(1,1705)	2:B:421:LYS:H	2:B:421:LYS:HD3	10	0.19
(1,1705)	2:B:421:LYS:H	2:B:421:LYS:HD3	16	0.19
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	11	0.19
(1,1489)	2:B:408:ASP:H	2:B:408:ASP:HB2	8	0.19
(1,1489)	2:B:408:ASP:H	2:B:408:ASP:HB3	8	0.19
(1,1249)	2:B:394:THR:H	2:B:399:ASN:H	8	0.19
(1,1240)	2:B:394:THR:H	2:B:393:PRO:HB2	12	0.19
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	15	0.19
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	15	0.19
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	2:B:369:ASN:HD22	2:B:368:MET:HE1	2	0.18
(1,796)	2:B:369:ASN:HD22	2:B:368:MET:HE2	2	0.18
(1,796)	2:B:369:ASN:HD22	2:B:368:MET:HE3	2	0.18
(1,727)	2:B:377:LEU:HD11	1:A:18:A:H2	12	0.18
(1,727)	2:B:377:LEU:HD12	1:A:18:A:H2	12	0.18
(1,727)	2:B:377:LEU:HD13	1:A:18:A:H2	12	0.18
(1,727)	2:B:377:LEU:HD21	1:A:18:A:H2	12	0.18
(1,727)	2:B:377:LEU:HD22	1:A:18:A:H2	12	0.18
(1,727)	2:B:377:LEU:HD23	1:A:18:A:H2	12	0.18
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB2	9	0.18
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB3	9	0.18
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HG	9	0.18
(1,2184)	2:B:444:GLN:H	2:B:444:GLN:HE21	9	0.18
(1,2184)	2:B:444:GLN:H	2:B:444:GLN:HE22	9	0.18
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	12	0.18
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	12	0.18
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	12	0.18
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	12	0.18
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	7	0.18
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	7	0.18
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	11	0.18
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	11	0.18
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	13	0.18
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	13	0.18
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD11	12	0.18
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD12	12	0.18
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD13	12	0.18
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB2	7	0.18
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB3	7	0.18
(1,1760)	2:B:424:GLY:H	2:B:421:LYS:HD2	16	0.18
(1,1760)	2:B:424:GLY:H	2:B:421:LYS:HD3	16	0.18
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	4	0.18
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	10	0.18
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG2	6	0.18
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG3	6	0.18
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG2	6	0.18
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG3	6	0.18
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG2	6	0.18
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG3	6	0.18
(1,1589)	2:B:414:THR:H	2:B:430:ASN:HA	11	0.18
(1,1432)	2:B:405:ARG:H	2:B:388:VAL:HG11	12	0.18
(1,1432)	2:B:405:ARG:H	2:B:388:VAL:HG12	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1432)	2:B:405:ARG:H	2:B:388:VAL:HG13	12	0.18
(1,1432)	2:B:405:ARG:H	2:B:388:VAL:HG21	12	0.18
(1,1432)	2:B:405:ARG:H	2:B:388:VAL:HG22	12	0.18
(1,1432)	2:B:405:ARG:H	2:B:388:VAL:HG23	12	0.18
(1,1240)	2:B:394:THR:H	2:B:393:PRO:HB2	5	0.18
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	7	0.18
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	7	0.18
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	11	0.18
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	11	0.18
(1,1003)	2:B:383:LEU:H	2:B:380:TYR:H	13	0.18
(1,615)	1:A:29:U:H5	1:A:28:A:H1'	4	0.17
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD11	13	0.17
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD12	13	0.17
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD13	13	0.17
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD11	13	0.17
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD12	13	0.17
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD13	13	0.17
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD11	13	0.17
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD12	13	0.17
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD13	13	0.17
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD11	13	0.17
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD12	13	0.17
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD13	13	0.17
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA2	6	0.17
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA3	6	0.17
(1,2347)	2:B:406:VAL:HG11	2:B:410:THR:HA	6	0.17
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA2	6	0.17
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA3	6	0.17
(1,2347)	2:B:406:VAL:HG12	2:B:410:THR:HA	6	0.17
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA2	6	0.17
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA3	6	0.17
(1,2347)	2:B:406:VAL:HG13	2:B:410:THR:HA	6	0.17
(1,2240)	2:B:447:ALA:H	2:B:448:ILE:HB	16	0.17
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	4	0.17
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	4	0.17
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG2	15	0.17
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG3	15	0.17
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	1	0.17
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	2	0.17
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	7	0.17
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	12	0.17
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD11	6	0.17
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD12	6	0.17
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD13	6	0.17
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD11	6	0.17
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD12	6	0.17
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD13	6	0.17
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD11	6	0.17
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD12	6	0.17
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD13	6	0.17
(1,1705)	2:B:421:LYS:H	2:B:421:LYS:HD3	11	0.17
(1,1374)	2:B:401:ILE:HG21	2:B:416:VAL:HA	11	0.17
(1,1374)	2:B:401:ILE:HG22	2:B:416:VAL:HA	11	0.17
(1,1374)	2:B:401:ILE:HG23	2:B:416:VAL:HA	11	0.17
(1,1249)	2:B:394:THR:H	2:B:399:ASN:H	1	0.17
(1,1240)	2:B:394:THR:H	2:B:393:PRO:HB2	8	0.17
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	3	0.17
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	3	0.17
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	13	0.17
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	13	0.17
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	13	0.17
(1,936)	2:B:378:ILE:HD11	2:B:378:ILE:HG21	15	0.16
(1,936)	2:B:378:ILE:HD11	2:B:378:ILE:HG22	15	0.16
(1,936)	2:B:378:ILE:HD11	2:B:378:ILE:HG23	15	0.16
(1,936)	2:B:378:ILE:HD12	2:B:378:ILE:HG21	15	0.16
(1,936)	2:B:378:ILE:HD12	2:B:378:ILE:HG22	15	0.16
(1,936)	2:B:378:ILE:HD12	2:B:378:ILE:HG23	15	0.16
(1,936)	2:B:378:ILE:HD13	2:B:378:ILE:HG21	15	0.16
(1,936)	2:B:378:ILE:HD13	2:B:378:ILE:HG22	15	0.16
(1,936)	2:B:378:ILE:HD13	2:B:378:ILE:HG23	15	0.16
(1,924)	2:B:377:LEU:H	2:B:377:LEU:HG	6	0.16
(1,924)	2:B:377:LEU:H	2:B:377:LEU:HG	8	0.16
(1,281)	1:A:13:U:H6	1:A:12:U:H1'	14	0.16
(1,2359)	2:B:442:ALA:H	2:B:380:TYR:HE1	6	0.16
(1,2359)	2:B:442:ALA:H	2:B:380:TYR:HE2	6	0.16
(1,2359)	2:B:442:ALA:H	2:B:441:TYR:HE1	6	0.16
(1,2359)	2:B:442:ALA:H	2:B:441:TYR:HE2	6	0.16
(1,2240)	2:B:447:ALA:H	2:B:448:ILE:HB	5	0.16
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	4	0.16
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	4	0.16
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	4	0.16
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	4	0.16
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	6	0.16
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	6	0.16
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	6	0.16
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	7	0.16
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	7	0.16
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	7	0.16
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	7	0.16
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	1	0.16
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	1	0.16
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	10	0.16
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	10	0.16
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	15	0.16
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	15	0.16
(1,1948)	2:B:434:ASP:H	2:B:438:LEU:HG	1	0.16
(1,1948)	2:B:434:ASP:H	2:B:438:LEU:HG	16	0.16
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	1	0.16
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	1	0.16
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	7	0.16
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	7	0.16
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	12	0.16
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	12	0.16
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB2	8	0.16
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB3	8	0.16
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB2	10	0.16
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB3	10	0.16
(1,1767)	2:B:424:GLY:H	2:B:426:ARG:H	11	0.16
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG2	4	0.16
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG3	4	0.16
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG2	12	0.16
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG3	12	0.16
(1,1760)	2:B:424:GLY:H	2:B:421:LYS:HD2	10	0.16
(1,1760)	2:B:424:GLY:H	2:B:421:LYS:HD3	10	0.16
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	16	0.16
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD11	2	0.16
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD12	2	0.16
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD13	2	0.16
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD11	2	0.16
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD12	2	0.16
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD13	2	0.16
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD11	2	0.16
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD12	2	0.16
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD13	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG21	6	0.16
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG22	6	0.16
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG23	6	0.16
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG21	6	0.16
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG22	6	0.16
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG23	6	0.16
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	1	0.16
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	2	0.16
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	7	0.16
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	14	0.16
(1,143)	1:A:8:C:H6	1:A:7:C:H1'	1	0.16
(1,1404)	2:B:403:GLU:H	2:B:389:THR:HB	16	0.16
(1,1377)	2:B:401:ILE:H	2:B:401:ILE:HB	6	0.16
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG21	16	0.16
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG22	16	0.16
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG23	16	0.16
(1,1249)	2:B:394:THR:H	2:B:399:ASN:H	15	0.16
(1,1240)	2:B:394:THR:H	2:B:393:PRO:HB2	7	0.16
(1,1240)	2:B:394:THR:H	2:B:393:PRO:HB2	9	0.16
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG11	2	0.16
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG12	2	0.16
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG13	2	0.16
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG21	2	0.16
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG22	2	0.16
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG23	2	0.16
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG11	6	0.16
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG12	6	0.16
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG13	6	0.16
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG21	6	0.16
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG22	6	0.16
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG23	6	0.16
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE1	9	0.16
(1,1136)	2:B:387:TYR:H	2:B:387:TYR:HE2	9	0.16
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	8	0.16
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	8	0.16
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	8	0.16
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	9	0.16
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	9	0.16
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	9	0.16
(1,1079)	2:B:386:HIS:HA	2:B:388:VAL:HG11	15	0.16
(1,1079)	2:B:386:HIS:HA	2:B:388:VAL:HG12	15	0.16
(1,1079)	2:B:386:HIS:HA	2:B:388:VAL:HG13	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1071)	2:B:385:LEU:H	2:B:385:LEU:HG	16	0.16
(1,672)	1:A:31:U:H6	1:A:30:C:H1'	10	0.15
(1,52)	1:A:3:G:H8	1:A:3:G:H5"	7	0.15
(1,52)	1:A:3:G:H8	1:A:3:G:H5"	11	0.15
(1,281)	1:A:13:U:H6	1:A:12:U:H1'	6	0.15
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB2	2	0.15
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB3	2	0.15
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HG	2	0.15
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB2	7	0.15
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB3	7	0.15
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HG	7	0.15
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB2	10	0.15
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB3	10	0.15
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HG	10	0.15
(1,2356)	2:B:430:ASN:HD21	2:B:414:THR:HA	15	0.15
(1,2356)	2:B:430:ASN:HD21	2:B:427:ALA:HA	15	0.15
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD11	7	0.15
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD12	7	0.15
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD13	7	0.15
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD11	7	0.15
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD12	7	0.15
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD13	7	0.15
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD11	7	0.15
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD12	7	0.15
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD13	7	0.15
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD11	7	0.15
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD12	7	0.15
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD13	7	0.15
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA2	5	0.15
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA3	5	0.15
(1,2347)	2:B:406:VAL:HG11	2:B:410:THR:HA	5	0.15
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA2	5	0.15
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA3	5	0.15
(1,2347)	2:B:406:VAL:HG12	2:B:410:THR:HA	5	0.15
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA2	5	0.15
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA3	5	0.15
(1,2347)	2:B:406:VAL:HG13	2:B:410:THR:HA	5	0.15
(1,2240)	2:B:447:ALA:H	2:B:448:ILE:HB	7	0.15
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	8	0.15
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	8	0.15
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	8	0.15
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	3	0.15
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	3	0.15
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	6	0.15
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	6	0.15
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB2	1	0.15
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB3	1	0.15
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB2	3	0.15
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB3	3	0.15
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB2	16	0.15
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB3	16	0.15
(1,1767)	2:B:424:GLY:H	2:B:426:ARG:H	5	0.15
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG2	14	0.15
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG3	14	0.15
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	3	0.15
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	8	0.15
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG2	12	0.15
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG3	12	0.15
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG2	12	0.15
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG3	12	0.15
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG2	12	0.15
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG3	12	0.15
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD11	8	0.15
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD12	8	0.15
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD13	8	0.15
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD11	8	0.15
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD12	8	0.15
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD13	8	0.15
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD11	8	0.15
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD12	8	0.15
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD13	8	0.15
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB2	1	0.15
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB3	1	0.15
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB2	1	0.15
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB3	1	0.15
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB2	1	0.15
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB3	1	0.15
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB2	8	0.15
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB3	8	0.15
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB2	8	0.15
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB3	8	0.15
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB2	8	0.15
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB3	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB2	14	0.15
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB3	14	0.15
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB2	14	0.15
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB3	14	0.15
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB2	14	0.15
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB3	14	0.15
(1,1705)	2:B:421:LYS:H	2:B:421:LYS:HD3	6	0.15
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG21	3	0.15
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG22	3	0.15
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG23	3	0.15
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG21	3	0.15
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG22	3	0.15
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG23	3	0.15
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG21	7	0.15
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG22	7	0.15
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG23	7	0.15
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG21	7	0.15
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG22	7	0.15
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG23	7	0.15
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	3	0.15
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	5	0.15
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	13	0.15
(1,143)	1:A:8:C:H6	1:A:7:C:H1'	5	0.15
(1,143)	1:A:8:C:H6	1:A:7:C:H1'	15	0.15
(1,1284)	2:B:397:ASP:H	2:B:396:VAL:HA	13	0.15
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB1	6	0.15
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB2	6	0.15
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB3	6	0.15
(1,1249)	2:B:394:THR:H	2:B:399:ASN:H	6	0.15
(1,1249)	2:B:394:THR:H	2:B:399:ASN:H	16	0.15
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB2	12	0.15
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB3	12	0.15
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG11	8	0.15
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG12	8	0.15
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG13	8	0.15
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG21	8	0.15
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG22	8	0.15
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG23	8	0.15
(1,1129)	2:B:387:TYR:HE1	2:B:404:CYS:HB3	6	0.15
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	11	0.15
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	11	0.15
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1088)	2:B:386:HIS:HE1	2:B:384:ARG:HB2	12	0.15
(1,1088)	2:B:386:HIS:HE1	2:B:384:ARG:HB3	12	0.15
(1,672)	1:A:31:U:H6	1:A:30:C:H1'	7	0.14
(1,615)	1:A:29:U:H5	1:A:28:A:H1'	6	0.14
(1,615)	1:A:29:U:H5	1:A:28:A:H1'	12	0.14
(1,534)	1:A:26:G:H8	1:A:25:G:H1'	4	0.14
(1,534)	1:A:26:G:H8	1:A:25:G:H1'	15	0.14
(1,52)	1:A:3:G:H8	1:A:3:G:H5"	1	0.14
(1,504)	1:A:25:G:H8	1:A:24:U:H1'	6	0.14
(1,504)	1:A:25:G:H8	1:A:24:U:H1'	14	0.14
(1,294)	1:A:14:C:H6	1:A:13:U:H1'	5	0.14
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD11	14	0.14
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD12	14	0.14
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD13	14	0.14
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD11	14	0.14
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD12	14	0.14
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD13	14	0.14
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD11	14	0.14
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD12	14	0.14
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD13	14	0.14
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD11	14	0.14
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD12	14	0.14
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD13	14	0.14
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG11	10	0.14
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG12	10	0.14
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG13	10	0.14
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG21	10	0.14
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG22	10	0.14
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG23	10	0.14
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG11	10	0.14
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG12	10	0.14
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG13	10	0.14
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG21	10	0.14
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG22	10	0.14
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG23	10	0.14
(1,2300)	2:B:450:ARG:H	2:B:449:PRO:HG2	13	0.14
(1,2300)	2:B:450:ARG:H	2:B:449:PRO:HG3	13	0.14
(1,2240)	2:B:447:ALA:H	2:B:448:ILE:HB	4	0.14
(1,2240)	2:B:447:ALA:H	2:B:448:ILE:HB	6	0.14
(1,2240)	2:B:447:ALA:H	2:B:448:ILE:HB	8	0.14
(1,2240)	2:B:447:ALA:H	2:B:448:ILE:HB	14	0.14
(1,2185)	2:B:444:GLN:H	2:B:444:GLN:HG2	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2185)	2:B:444:GLN:H	2:B:444:GLN:HG3	7	0.14
(1,2184)	2:B:444:GLN:H	2:B:444:GLN:HE21	14	0.14
(1,2184)	2:B:444:GLN:H	2:B:444:GLN:HE22	14	0.14
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	2	0.14
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	2	0.14
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	2	0.14
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	2	0.14
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	10	0.14
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	10	0.14
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	10	0.14
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	10	0.14
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	16	0.14
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	16	0.14
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	16	0.14
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	16	0.14
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	2	0.14
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	2	0.14
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	16	0.14
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	16	0.14
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD11	5	0.14
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD12	5	0.14
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD13	5	0.14
(1,1806)	2:B:427:ALA:H	2:B:402:VAL:HG11	5	0.14
(1,1806)	2:B:427:ALA:H	2:B:402:VAL:HG12	5	0.14
(1,1806)	2:B:427:ALA:H	2:B:402:VAL:HG13	5	0.14
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG2	9	0.14
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG3	9	0.14
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG2	13	0.14
(1,1761)	2:B:424:GLY:H	2:B:421:LYS:HG3	13	0.14
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	5	0.14
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	6	0.14
(1,1748)	2:B:423:ALA:H	2:B:420:ILE:HB	14	0.14
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG2	9	0.14
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG3	9	0.14
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG2	9	0.14
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG3	9	0.14
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG2	9	0.14
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG3	9	0.14
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD11	13	0.14
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD12	13	0.14
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD13	13	0.14
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD11	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD12	13	0.14
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD13	13	0.14
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD11	13	0.14
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD12	13	0.14
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD13	13	0.14
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB2	7	0.14
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB3	7	0.14
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB2	7	0.14
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB3	7	0.14
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB2	7	0.14
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB3	7	0.14
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB2	13	0.14
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB3	13	0.14
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB2	13	0.14
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB3	13	0.14
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB2	13	0.14
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB3	13	0.14
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG21	1	0.14
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG22	1	0.14
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG23	1	0.14
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG21	1	0.14
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG22	1	0.14
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG23	1	0.14
(1,1671)	2:B:419:ASN:H	2:B:421:LYS:H	14	0.14
(1,1615)	2:B:416:VAL:H	2:B:416:VAL:HB	6	0.14
(1,1615)	2:B:416:VAL:H	2:B:416:VAL:HB	9	0.14
(1,1569)	2:B:413:GLY:H	2:B:411:VAL:HG21	16	0.14
(1,1569)	2:B:413:GLY:H	2:B:411:VAL:HG22	16	0.14
(1,1569)	2:B:413:GLY:H	2:B:411:VAL:HG23	16	0.14
(1,1414)	2:B:404:CYS:H	2:B:405:ARG:HB2	12	0.14
(1,1414)	2:B:404:CYS:H	2:B:405:ARG:HB3	12	0.14
(1,1377)	2:B:401:ILE:H	2:B:401:ILE:HB	15	0.14
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG21	13	0.14
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG22	13	0.14
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG23	13	0.14
(1,1321)	2:B:399:ASN:HD22	2:B:399:ASN:H	9	0.14
(1,1284)	2:B:397:ASP:H	2:B:396:VAL:HA	7	0.14
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB1	2	0.14
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB2	2	0.14
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB3	2	0.14
(1,1249)	2:B:394:THR:H	2:B:399:ASN:H	11	0.14
(1,1240)	2:B:394:THR:H	2:B:393:PRO:HB2	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1240)	2:B:394:THR:H	2:B:393:PRO:HB2	2	0.14
(1,1240)	2:B:394:THR:H	2:B:393:PRO:HB2	11	0.14
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB2	7	0.14
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB3	7	0.14
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	1	0.14
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	1	0.14
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	1	0.14
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	6	0.14
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	6	0.14
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	6	0.14
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	7	0.14
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	7	0.14
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	7	0.14
(1,1073)	2:B:385:LEU:H	2:B:386:HIS:H	1	0.14
(1,1073)	2:B:385:LEU:H	2:B:386:HIS:H	12	0.14
(1,775)	2:B:368:MET:HE1	2:B:366:LEU:HD11	9	0.13
(1,775)	2:B:368:MET:HE1	2:B:366:LEU:HD12	9	0.13
(1,775)	2:B:368:MET:HE1	2:B:366:LEU:HD13	9	0.13
(1,775)	2:B:368:MET:HE1	2:B:366:LEU:HD21	9	0.13
(1,775)	2:B:368:MET:HE1	2:B:366:LEU:HD22	9	0.13
(1,775)	2:B:368:MET:HE1	2:B:366:LEU:HD23	9	0.13
(1,775)	2:B:368:MET:HE2	2:B:366:LEU:HD11	9	0.13
(1,775)	2:B:368:MET:HE2	2:B:366:LEU:HD12	9	0.13
(1,775)	2:B:368:MET:HE2	2:B:366:LEU:HD13	9	0.13
(1,775)	2:B:368:MET:HE2	2:B:366:LEU:HD21	9	0.13
(1,775)	2:B:368:MET:HE2	2:B:366:LEU:HD22	9	0.13
(1,775)	2:B:368:MET:HE2	2:B:366:LEU:HD23	9	0.13
(1,775)	2:B:368:MET:HE3	2:B:366:LEU:HD11	9	0.13
(1,775)	2:B:368:MET:HE3	2:B:366:LEU:HD12	9	0.13
(1,775)	2:B:368:MET:HE3	2:B:366:LEU:HD13	9	0.13
(1,775)	2:B:368:MET:HE3	2:B:366:LEU:HD21	9	0.13
(1,775)	2:B:368:MET:HE3	2:B:366:LEU:HD22	9	0.13
(1,775)	2:B:368:MET:HE3	2:B:366:LEU:HD23	9	0.13
(1,746)	2:B:366:LEU:HA	2:B:366:LEU:HD11	1	0.13
(1,746)	2:B:366:LEU:HA	2:B:366:LEU:HD12	1	0.13
(1,746)	2:B:366:LEU:HA	2:B:366:LEU:HD13	1	0.13
(1,746)	2:B:366:LEU:HA	2:B:366:LEU:HD21	1	0.13
(1,746)	2:B:366:LEU:HA	2:B:366:LEU:HD22	1	0.13
(1,746)	2:B:366:LEU:HA	2:B:366:LEU:HD23	1	0.13
(1,672)	1:A:31:U:H6	1:A:30:C:H1'	8	0.13
(1,642)	1:A:30:C:H6	1:A:29:U:H1'	9	0.13
(1,615)	1:A:29:U:H5	1:A:28:A:H1'	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:A:29:U:H5	1:A:28:A:H1'	7	0.13
(1,615)	1:A:29:U:H5	1:A:28:A:H1'	13	0.13
(1,534)	1:A:26:G:H8	1:A:25:G:H1'	9	0.13
(1,52)	1:A:3:G:H8	1:A:3:G:H5"	3	0.13
(1,504)	1:A:25:G:H8	1:A:24:U:H1'	11	0.13
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB2	4	0.13
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB3	4	0.13
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HG	4	0.13
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB2	13	0.13
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB3	13	0.13
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HG	13	0.13
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD11	8	0.13
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD12	8	0.13
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD13	8	0.13
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD11	8	0.13
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD12	8	0.13
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD13	8	0.13
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD11	8	0.13
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD12	8	0.13
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD13	8	0.13
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD11	8	0.13
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD12	8	0.13
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD13	8	0.13
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA2	4	0.13
(1,2347)	2:B:406:VAL:HG11	2:B:407:GLY:HA3	4	0.13
(1,2347)	2:B:406:VAL:HG11	2:B:410:THR:HA	4	0.13
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA2	4	0.13
(1,2347)	2:B:406:VAL:HG12	2:B:407:GLY:HA3	4	0.13
(1,2347)	2:B:406:VAL:HG12	2:B:410:THR:HA	4	0.13
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA2	4	0.13
(1,2347)	2:B:406:VAL:HG13	2:B:407:GLY:HA3	4	0.13
(1,2347)	2:B:406:VAL:HG13	2:B:410:THR:HA	4	0.13
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG11	11	0.13
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG12	11	0.13
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG13	11	0.13
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG21	11	0.13
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG22	11	0.13
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG23	11	0.13
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG11	11	0.13
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG12	11	0.13
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG13	11	0.13
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG21	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG22	11	0.13
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG23	11	0.13
(1,2240)	2:B:447:ALA:H	2:B:448:ILE:HB	3	0.13
(1,2240)	2:B:447:ALA:H	2:B:448:ILE:HB	13	0.13
(1,2168)	2:B:444:GLN:HE21	2:B:441:TYR:HA	10	0.13
(1,2168)	2:B:444:GLN:HE22	2:B:441:TYR:HA	10	0.13
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	9	0.13
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	9	0.13
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	9	0.13
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	9	0.13
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	5	0.13
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	5	0.13
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	9	0.13
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	9	0.13
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	12	0.13
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	12	0.13
(1,2061)	2:B:439:ASP:H	2:B:440:PHE:HD1	1	0.13
(1,2061)	2:B:439:ASP:H	2:B:440:PHE:HD2	1	0.13
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB2	5	0.13
(1,1883)	2:B:431:ALA:H	2:B:373:GLN:HB3	5	0.13
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB2	5	0.13
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB3	5	0.13
(1,1758)	2:B:424:GLY:H	2:B:420:ILE:HD11	6	0.13
(1,1758)	2:B:424:GLY:H	2:B:420:ILE:HD12	6	0.13
(1,1758)	2:B:424:GLY:H	2:B:420:ILE:HD13	6	0.13
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG2	10	0.13
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG3	10	0.13
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG2	10	0.13
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG3	10	0.13
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG2	10	0.13
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG3	10	0.13
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD11	3	0.13
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD12	3	0.13
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD13	3	0.13
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD11	3	0.13
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD12	3	0.13
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD13	3	0.13
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD11	3	0.13
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD12	3	0.13
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD13	3	0.13
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD11	10	0.13
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD12	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD13	10	0.13
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD11	10	0.13
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD12	10	0.13
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD13	10	0.13
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD11	10	0.13
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD12	10	0.13
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD13	10	0.13
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB2	4	0.13
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB3	4	0.13
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB2	4	0.13
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB3	4	0.13
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB2	4	0.13
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB3	4	0.13
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB2	10	0.13
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB3	10	0.13
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB2	10	0.13
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB3	10	0.13
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB2	10	0.13
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB3	10	0.13
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB2	16	0.13
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB3	16	0.13
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB2	16	0.13
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB3	16	0.13
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB2	16	0.13
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB3	16	0.13
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG21	5	0.13
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG22	5	0.13
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG23	5	0.13
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG21	5	0.13
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG22	5	0.13
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG23	5	0.13
(1,1589)	2:B:414:THR:H	2:B:430:ASN:HA	10	0.13
(1,143)	1:A:8:C:H6	1:A:7:C:H1'	11	0.13
(1,1400)	2:B:403:GLU:HA	2:B:414:THR:HG21	5	0.13
(1,1400)	2:B:403:GLU:HA	2:B:414:THR:HG22	5	0.13
(1,1400)	2:B:403:GLU:HA	2:B:414:THR:HG23	5	0.13
(1,1377)	2:B:401:ILE:H	2:B:401:ILE:HB	9	0.13
(1,1374)	2:B:401:ILE:HG21	2:B:416:VAL:HA	7	0.13
(1,1374)	2:B:401:ILE:HG22	2:B:416:VAL:HA	7	0.13
(1,1374)	2:B:401:ILE:HG23	2:B:416:VAL:HA	7	0.13
(1,1374)	2:B:401:ILE:HG21	2:B:416:VAL:HA	10	0.13
(1,1374)	2:B:401:ILE:HG22	2:B:416:VAL:HA	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1374)	2:B:401:ILE:HG23	2:B:416:VAL:HA	10	0.13
(1,1365)	2:B:401:ILE:HD11	2:B:416:VAL:HA	4	0.13
(1,1365)	2:B:401:ILE:HD12	2:B:416:VAL:HA	4	0.13
(1,1365)	2:B:401:ILE:HD13	2:B:416:VAL:HA	4	0.13
(1,1284)	2:B:397:ASP:H	2:B:396:VAL:HA	10	0.13
(1,1240)	2:B:394:THR:H	2:B:393:PRO:HB2	10	0.13
(1,1240)	2:B:394:THR:H	2:B:393:PRO:HB2	14	0.13
(1,1239)	2:B:394:THR:H	2:B:393:PRO:HB3	3	0.13
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB2	2	0.13
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB3	2	0.13
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB2	3	0.13
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB3	3	0.13
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB2	11	0.13
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB3	11	0.13
(1,1178)	2:B:390:VAL:HG21	2:B:403:GLU:HA	16	0.13
(1,1178)	2:B:390:VAL:HG22	2:B:403:GLU:HA	16	0.13
(1,1178)	2:B:390:VAL:HG23	2:B:403:GLU:HA	16	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG11	4	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG12	4	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG13	4	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG21	4	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG22	4	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG23	4	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG11	11	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG12	11	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG13	11	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG21	11	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG22	11	0.13
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG23	11	0.13
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG21	2	0.13
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG22	2	0.13
(1,1105)	2:B:386:HIS:H	2:B:406:VAL:HG23	2	0.13
(1,1037)	2:B:384:ARG:H	2:B:385:LEU:HD11	7	0.13
(1,1037)	2:B:384:ARG:H	2:B:385:LEU:HD12	7	0.13
(1,1037)	2:B:384:ARG:H	2:B:385:LEU:HD13	7	0.13
(1,923)	2:B:377:LEU:H	2:B:377:LEU:HD21	15	0.12
(1,923)	2:B:377:LEU:H	2:B:377:LEU:HD22	15	0.12
(1,923)	2:B:377:LEU:H	2:B:377:LEU:HD23	15	0.12
(1,789)	2:B:369:ASN:HB2	2:B:372:ARG:HB2	10	0.12
(1,789)	2:B:369:ASN:HB2	2:B:372:ARG:HB3	10	0.12
(1,789)	2:B:369:ASN:HB3	2:B:372:ARG:HB2	10	0.12
(1,789)	2:B:369:ASN:HB3	2:B:372:ARG:HB3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,642)	1:A:30:C:H6	1:A:29:U:H1'	3	0.12
(1,615)	1:A:29:U:H5	1:A:28:A:H1'	3	0.12
(1,615)	1:A:29:U:H5	1:A:28:A:H1'	14	0.12
(1,615)	1:A:29:U:H5	1:A:28:A:H1'	15	0.12
(1,534)	1:A:26:G:H8	1:A:25:G:H1'	2	0.12
(1,504)	1:A:25:G:H8	1:A:24:U:H1'	9	0.12
(1,423)	1:A:22:C:H6	1:A:21:A:H1'	14	0.12
(1,390)	1:A:20:A:H8	1:A:19:G:H1'	3	0.12
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB2	5	0.12
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB3	5	0.12
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HG	5	0.12
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG11	1	0.12
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG12	1	0.12
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG13	1	0.12
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG21	1	0.12
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG22	1	0.12
(1,2345)	2:B:403:GLU:H	2:B:388:VAL:HG23	1	0.12
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG11	1	0.12
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG12	1	0.12
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG13	1	0.12
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG21	1	0.12
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG22	1	0.12
(1,2345)	2:B:403:GLU:H	2:B:390:VAL:HG23	1	0.12
(1,2344)	2:B:402:VAL:H	2:B:401:ILE:HD11	2	0.12
(1,2344)	2:B:402:VAL:H	2:B:401:ILE:HD12	2	0.12
(1,2344)	2:B:402:VAL:H	2:B:401:ILE:HD13	2	0.12
(1,2344)	2:B:402:VAL:H	2:B:401:ILE:HG21	2	0.12
(1,2344)	2:B:402:VAL:H	2:B:401:ILE:HG22	2	0.12
(1,2344)	2:B:402:VAL:H	2:B:401:ILE:HG23	2	0.12
(1,2255)	2:B:448:ILE:HD11	2:B:449:PRO:HD3	10	0.12
(1,2255)	2:B:448:ILE:HD12	2:B:449:PRO:HD3	10	0.12
(1,2255)	2:B:448:ILE:HD13	2:B:449:PRO:HD3	10	0.12
(1,2174)	2:B:444:GLN:HE22	2:B:444:GLN:HB2	12	0.12
(1,2174)	2:B:444:GLN:HE22	2:B:444:GLN:HB3	12	0.12
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	15	0.12
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	15	0.12
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	15	0.12
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	15	0.12
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	6	0.12
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	6	0.12
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE1	8	0.12
(1,2086)	2:B:440:PHE:H	2:B:441:TYR:HE2	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD11	4	0.12
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD12	4	0.12
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD13	4	0.12
(1,1948)	2:B:434:ASP:H	2:B:438:LEU:HG	4	0.12
(1,1948)	2:B:434:ASP:H	2:B:438:LEU:HG	11	0.12
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB2	9	0.12
(1,1780)	2:B:425:ILE:H	2:B:421:LYS:HB3	9	0.12
(1,1760)	2:B:424:GLY:H	2:B:421:LYS:HD2	3	0.12
(1,1760)	2:B:424:GLY:H	2:B:421:LYS:HD3	3	0.12
(1,1760)	2:B:424:GLY:H	2:B:421:LYS:HD2	6	0.12
(1,1760)	2:B:424:GLY:H	2:B:421:LYS:HD3	6	0.12
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG2	3	0.12
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG3	3	0.12
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG2	3	0.12
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG3	3	0.12
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG2	3	0.12
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG3	3	0.12
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG2	7	0.12
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG3	7	0.12
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG2	7	0.12
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG3	7	0.12
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG2	7	0.12
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG3	7	0.12
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB2	3	0.12
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB3	3	0.12
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB2	3	0.12
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB3	3	0.12
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB2	3	0.12
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB3	3	0.12
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB2	6	0.12
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB3	6	0.12
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB2	6	0.12
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB3	6	0.12
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB2	6	0.12
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB3	6	0.12
(1,1671)	2:B:419:ASN:H	2:B:421:LYS:H	3	0.12
(1,1671)	2:B:419:ASN:H	2:B:421:LYS:H	7	0.12
(1,1615)	2:B:416:VAL:H	2:B:416:VAL:HB	14	0.12
(1,1589)	2:B:414:THR:H	2:B:430:ASN:HA	4	0.12
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	4	0.12
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	6	0.12
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1494)	2:B:409:GLY:H	2:B:406:VAL:HG21	10	0.12
(1,1494)	2:B:409:GLY:H	2:B:406:VAL:HG22	10	0.12
(1,1494)	2:B:409:GLY:H	2:B:406:VAL:HG23	10	0.12
(1,1455)	2:B:406:VAL:HG11	2:B:441:TYR:HE1	11	0.12
(1,1455)	2:B:406:VAL:HG11	2:B:441:TYR:HE2	11	0.12
(1,1455)	2:B:406:VAL:HG12	2:B:441:TYR:HE1	11	0.12
(1,1455)	2:B:406:VAL:HG12	2:B:441:TYR:HE2	11	0.12
(1,1455)	2:B:406:VAL:HG13	2:B:441:TYR:HE1	11	0.12
(1,1455)	2:B:406:VAL:HG13	2:B:441:TYR:HE2	11	0.12
(1,143)	1:A:8:C:H6	1:A:7:C:H1'	2	0.12
(1,143)	1:A:8:C:H6	1:A:7:C:H1'	4	0.12
(1,143)	1:A:8:C:H6	1:A:7:C:H1'	6	0.12
(1,143)	1:A:8:C:H6	1:A:7:C:H1'	9	0.12
(1,1404)	2:B:403:GLU:H	2:B:389:THR:HB	6	0.12
(1,1377)	2:B:401:ILE:H	2:B:401:ILE:HB	3	0.12
(1,1377)	2:B:401:ILE:H	2:B:401:ILE:HB	14	0.12
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG21	8	0.12
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG22	8	0.12
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG23	8	0.12
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG11	2	0.12
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG12	2	0.12
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG13	2	0.12
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG21	2	0.12
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG22	2	0.12
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG23	2	0.12
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB1	7	0.12
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB2	7	0.12
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB3	7	0.12
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB1	10	0.12
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB2	10	0.12
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB3	10	0.12
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB1	13	0.12
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB2	13	0.12
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB3	13	0.12
(1,1249)	2:B:394:THR:H	2:B:399:ASN:H	2	0.12
(1,1240)	2:B:394:THR:H	2:B:393:PRO:HB2	16	0.12
(1,1239)	2:B:394:THR:H	2:B:393:PRO:HB3	4	0.12
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG21	2	0.12
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG22	2	0.12
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG23	2	0.12
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG21	10	0.12
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG22	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG23	10	0.12
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG11	5	0.12
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG12	5	0.12
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG13	5	0.12
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG21	5	0.12
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG22	5	0.12
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG23	5	0.12
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG11	7	0.12
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG12	7	0.12
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG13	7	0.12
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG21	7	0.12
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG22	7	0.12
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG23	7	0.12
(1,1122)	2:B:387:TYR:HE1	2:B:402:VAL:HB	1	0.12
(1,1122)	2:B:387:TYR:HE2	2:B:402:VAL:HB	1	0.12
(1,1122)	2:B:387:TYR:HE1	2:B:402:VAL:HB	5	0.12
(1,1122)	2:B:387:TYR:HE2	2:B:402:VAL:HB	5	0.12
(1,1122)	2:B:387:TYR:HE1	2:B:402:VAL:HB	8	0.12
(1,1122)	2:B:387:TYR:HE2	2:B:402:VAL:HB	8	0.12
(1,1122)	2:B:387:TYR:HE1	2:B:402:VAL:HB	15	0.12
(1,1122)	2:B:387:TYR:HE2	2:B:402:VAL:HB	15	0.12
(1,1073)	2:B:385:LEU:H	2:B:386:HIS:H	10	0.12
(1,106)	1:A:6:A:H8	1:A:5:U:H1'	9	0.12
(1,1058)	2:B:385:LEU:HD21	2:B:404:CYS:HA	15	0.12
(1,1058)	2:B:385:LEU:HD22	2:B:404:CYS:HA	15	0.12
(1,1058)	2:B:385:LEU:HD23	2:B:404:CYS:HA	15	0.12
(1,1003)	2:B:383:LEU:H	2:B:380:TYR:H	16	0.12
(1,958)	2:B:379:GLY:H	2:B:375:TYR:HA	8	0.11
(1,924)	2:B:377:LEU:H	2:B:377:LEU:HG	3	0.11
(1,881)	2:B:375:TYR:HA	2:B:378:ILE:HG12	1	0.11
(1,881)	2:B:375:TYR:HA	2:B:378:ILE:HG13	1	0.11
(1,807)	2:B:369:ASN:H	2:B:369:ASN:HD22	5	0.11
(1,801)	2:B:369:ASN:H	2:B:366:LEU:HD11	5	0.11
(1,801)	2:B:369:ASN:H	2:B:366:LEU:HD12	5	0.11
(1,801)	2:B:369:ASN:H	2:B:366:LEU:HD13	5	0.11
(1,801)	2:B:369:ASN:H	2:B:366:LEU:HD21	5	0.11
(1,801)	2:B:369:ASN:H	2:B:366:LEU:HD22	5	0.11
(1,801)	2:B:369:ASN:H	2:B:366:LEU:HD23	5	0.11
(1,760)	2:B:366:LEU:H	2:B:367:ASP:H	16	0.11
(1,672)	1:A:31:U:H6	1:A:30:C:H1'	4	0.11
(1,672)	1:A:31:U:H6	1:A:30:C:H1'	6	0.11
(1,672)	1:A:31:U:H6	1:A:30:C:H1'	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,672)	1:A:31:U:H6	1:A:30:C:H1'	15	0.11
(1,615)	1:A:29:U:H5	1:A:28:A:H1'	1	0.11
(1,615)	1:A:29:U:H5	1:A:28:A:H1'	2	0.11
(1,596)	1:A:28:A:H8	1:A:28:A:H5"	16	0.11
(1,534)	1:A:26:G:H8	1:A:25:G:H1'	8	0.11
(1,534)	1:A:26:G:H8	1:A:25:G:H1'	11	0.11
(1,52)	1:A:3:G:H8	1:A:3:G:H5"	10	0.11
(1,477)	1:A:24:U:H6	1:A:23:G:H1'	4	0.11
(1,477)	1:A:24:U:H6	1:A:23:G:H1'	7	0.11
(1,477)	1:A:24:U:H6	1:A:23:G:H1'	15	0.11
(1,456)	1:A:23:G:H8	1:A:23:G:H5"	11	0.11
(1,456)	1:A:23:G:H8	1:A:23:G:H5"	13	0.11
(1,456)	1:A:23:G:H8	1:A:23:G:H5"	15	0.11
(1,439)	1:A:23:G:H1	1:A:10:U:H5	10	0.11
(1,439)	1:A:23:G:H1	1:A:10:U:H5	14	0.11
(1,439)	1:A:23:G:H1	1:A:10:U:H5	16	0.11
(1,405)	1:A:21:A:H8	1:A:20:A:H1'	4	0.11
(1,390)	1:A:20:A:H8	1:A:19:G:H1'	6	0.11
(1,281)	1:A:13:U:H6	1:A:12:U:H1'	4	0.11
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB2	8	0.11
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB3	8	0.11
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HG	8	0.11
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB2	14	0.11
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HB3	14	0.11
(1,2358)	2:B:433:ARG:H	2:B:412:LEU:HG	14	0.11
(1,2356)	2:B:430:ASN:HD21	2:B:414:THR:HA	7	0.11
(1,2356)	2:B:430:ASN:HD21	2:B:427:ALA:HA	7	0.11
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD11	1	0.11
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD12	1	0.11
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD13	1	0.11
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD11	1	0.11
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD12	1	0.11
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD13	1	0.11
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD11	1	0.11
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD12	1	0.11
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD13	1	0.11
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD11	1	0.11
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD12	1	0.11
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD13	1	0.11
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD11	10	0.11
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD12	10	0.11
(1,2354)	2:B:426:ARG:HD2	2:B:422:ILE:HD13	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD11	10	0.11
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD12	10	0.11
(1,2354)	2:B:426:ARG:HD2	2:B:425:ILE:HD13	10	0.11
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD11	10	0.11
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD12	10	0.11
(1,2354)	2:B:426:ARG:HD3	2:B:422:ILE:HD13	10	0.11
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD11	10	0.11
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD12	10	0.11
(1,2354)	2:B:426:ARG:HD3	2:B:425:ILE:HD13	10	0.11
(1,2300)	2:B:450:ARG:H	2:B:449:PRO:HG2	2	0.11
(1,2300)	2:B:450:ARG:H	2:B:449:PRO:HG3	2	0.11
(1,2185)	2:B:444:GLN:H	2:B:444:GLN:HG2	9	0.11
(1,2185)	2:B:444:GLN:H	2:B:444:GLN:HG3	9	0.11
(1,2184)	2:B:444:GLN:H	2:B:444:GLN:HE21	8	0.11
(1,2184)	2:B:444:GLN:H	2:B:444:GLN:HE22	8	0.11
(1,2168)	2:B:444:GLN:HE21	2:B:441:TYR:HA	3	0.11
(1,2168)	2:B:444:GLN:HE22	2:B:441:TYR:HA	3	0.11
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB2	5	0.11
(1,2114)	2:B:441:TYR:HE1	2:B:444:GLN:HB3	5	0.11
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB2	5	0.11
(1,2114)	2:B:441:TYR:HE2	2:B:444:GLN:HB3	5	0.11
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD11	3	0.11
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD12	3	0.11
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD13	3	0.11
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD11	7	0.11
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD12	7	0.11
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD13	7	0.11
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD11	10	0.11
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD12	10	0.11
(1,2078)	2:B:440:PHE:H	2:B:438:LEU:HD13	10	0.11
(1,1896)	2:B:431:ALA:H	2:B:434:ASP:H	2	0.11
(1,1806)	2:B:427:ALA:H	2:B:402:VAL:HG11	12	0.11
(1,1806)	2:B:427:ALA:H	2:B:402:VAL:HG12	12	0.11
(1,1806)	2:B:427:ALA:H	2:B:402:VAL:HG13	12	0.11
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG2	2	0.11
(1,1745)	2:B:423:ALA:HB1	2:B:426:ARG:HG3	2	0.11
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG2	2	0.11
(1,1745)	2:B:423:ALA:HB2	2:B:426:ARG:HG3	2	0.11
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG2	2	0.11
(1,1745)	2:B:423:ALA:HB3	2:B:426:ARG:HG3	2	0.11
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD11	7	0.11
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD12	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1743)	2:B:423:ALA:HB1	2:B:422:ILE:HD13	7	0.11
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD11	7	0.11
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD12	7	0.11
(1,1743)	2:B:423:ALA:HB2	2:B:422:ILE:HD13	7	0.11
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD11	7	0.11
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD12	7	0.11
(1,1743)	2:B:423:ALA:HB3	2:B:422:ILE:HD13	7	0.11
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB2	2	0.11
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB3	2	0.11
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB2	2	0.11
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB3	2	0.11
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB2	2	0.11
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB3	2	0.11
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB2	12	0.11
(1,1721)	2:B:422:ILE:HG21	2:B:426:ARG:HB3	12	0.11
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB2	12	0.11
(1,1721)	2:B:422:ILE:HG22	2:B:426:ARG:HB3	12	0.11
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB2	12	0.11
(1,1721)	2:B:422:ILE:HG23	2:B:426:ARG:HB3	12	0.11
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG21	8	0.11
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG22	8	0.11
(1,1691)	2:B:421:LYS:HD2	2:B:420:ILE:HG23	8	0.11
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG21	8	0.11
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG22	8	0.11
(1,1691)	2:B:421:LYS:HD3	2:B:420:ILE:HG23	8	0.11
(1,1672)	2:B:419:ASN:H	2:B:422:ILE:HD11	4	0.11
(1,1672)	2:B:419:ASN:H	2:B:422:ILE:HD12	4	0.11
(1,1672)	2:B:419:ASN:H	2:B:422:ILE:HD13	4	0.11
(1,1672)	2:B:419:ASN:H	2:B:422:ILE:HD11	7	0.11
(1,1672)	2:B:419:ASN:H	2:B:422:ILE:HD12	7	0.11
(1,1672)	2:B:419:ASN:H	2:B:422:ILE:HD13	7	0.11
(1,1672)	2:B:419:ASN:H	2:B:422:ILE:HD11	16	0.11
(1,1672)	2:B:419:ASN:H	2:B:422:ILE:HD12	16	0.11
(1,1672)	2:B:419:ASN:H	2:B:422:ILE:HD13	16	0.11
(1,1615)	2:B:416:VAL:H	2:B:416:VAL:HB	3	0.11
(1,1612)	2:B:416:VAL:H	2:B:402:VAL:HG21	16	0.11
(1,1612)	2:B:416:VAL:H	2:B:402:VAL:HG22	16	0.11
(1,1612)	2:B:416:VAL:H	2:B:402:VAL:HG23	16	0.11
(1,1541)	2:B:411:VAL:H	2:B:412:LEU:HD11	16	0.11
(1,1541)	2:B:411:VAL:H	2:B:412:LEU:HD12	16	0.11
(1,1541)	2:B:411:VAL:H	2:B:412:LEU:HD13	16	0.11
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1520)	2:B:411:VAL:HA	2:B:403:GLU:HA	15	0.11
(1,143)	1:A:8:C:H6	1:A:7:C:H1'	7	0.11
(1,143)	1:A:8:C:H6	1:A:7:C:H1'	12	0.11
(1,1414)	2:B:404:CYS:H	2:B:405:ARG:HB2	16	0.11
(1,1414)	2:B:404:CYS:H	2:B:405:ARG:HB3	16	0.11
(1,1400)	2:B:403:GLU:HA	2:B:414:THR:HG21	15	0.11
(1,1400)	2:B:403:GLU:HA	2:B:414:THR:HG22	15	0.11
(1,1400)	2:B:403:GLU:HA	2:B:414:THR:HG23	15	0.11
(1,1374)	2:B:401:ILE:HG21	2:B:416:VAL:HA	13	0.11
(1,1374)	2:B:401:ILE:HG22	2:B:416:VAL:HA	13	0.11
(1,1374)	2:B:401:ILE:HG23	2:B:416:VAL:HA	13	0.11
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG21	1	0.11
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG22	1	0.11
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG23	1	0.11
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG21	5	0.11
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG22	5	0.11
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG23	5	0.11
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG21	7	0.11
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG22	7	0.11
(1,1331)	2:B:399:ASN:H	2:B:420:ILE:HG23	7	0.11
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG11	12	0.11
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG12	12	0.11
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG13	12	0.11
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG21	12	0.11
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG22	12	0.11
(1,1318)	2:B:399:ASN:HD21	2:B:416:VAL:HG23	12	0.11
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB1	12	0.11
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB2	12	0.11
(1,1283)	2:B:397:ASP:H	2:B:395:ALA:HB3	12	0.11
(1,1249)	2:B:394:THR:H	2:B:399:ASN:H	12	0.11
(1,1239)	2:B:394:THR:H	2:B:393:PRO:HB3	15	0.11
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB2	4	0.11
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB3	4	0.11
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB2	13	0.11
(1,1201)	2:B:391:LYS:H	2:B:391:LYS:HB3	13	0.11
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG21	11	0.11
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG22	11	0.11
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG23	11	0.11
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG21	12	0.11
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG22	12	0.11
(1,1196)	2:B:391:LYS:H	2:B:389:THR:HG23	12	0.11
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG11	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG12	9	0.11
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG13	9	0.11
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG21	9	0.11
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG22	9	0.11
(1,1164)	2:B:389:THR:H	2:B:388:VAL:HG23	9	0.11
(1,1122)	2:B:387:TYR:HE1	2:B:402:VAL:HB	14	0.11
(1,1122)	2:B:387:TYR:HE2	2:B:402:VAL:HB	14	0.11
(1,1115)	2:B:387:TYR:HD1	2:B:402:VAL:HG21	12	0.11
(1,1115)	2:B:387:TYR:HD1	2:B:402:VAL:HG22	12	0.11
(1,1115)	2:B:387:TYR:HD1	2:B:402:VAL:HG23	12	0.11
(1,1115)	2:B:387:TYR:HD2	2:B:402:VAL:HG21	12	0.11
(1,1115)	2:B:387:TYR:HD2	2:B:402:VAL:HG22	12	0.11
(1,1115)	2:B:387:TYR:HD2	2:B:402:VAL:HG23	12	0.11
(1,1073)	2:B:385:LEU:H	2:B:386:HIS:H	11	0.11
(1,1071)	2:B:385:LEU:H	2:B:385:LEU:HG	15	0.11

10 Dihedral-angle violation analysis

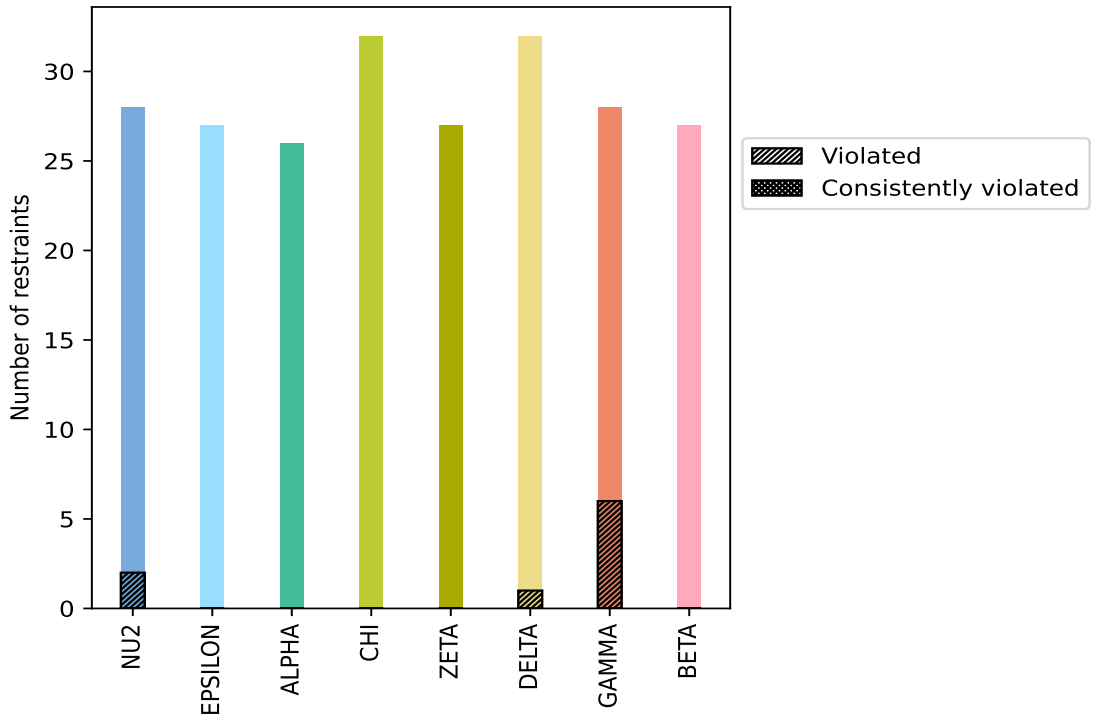
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
NU2	28	12.3	2	7.1	0.9	0	0.0	0.0
EPSILON	27	11.9	0	0.0	0.0	0	0.0	0.0
ALPHA	26	11.5	0	0.0	0.0	0	0.0	0.0
CHI	32	14.1	0	0.0	0.0	0	0.0	0.0
ZETA	27	11.9	0	0.0	0.0	0	0.0	0.0
DELTA	32	14.1	1	3.1	0.4	0	0.0	0.0
GAMMA	28	12.3	6	21.4	2.6	0	0.0	0.0
BETA	27	11.9	0	0.0	0.0	0	0.0	0.0
Total	227	100.0	9	4.0	4.0	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



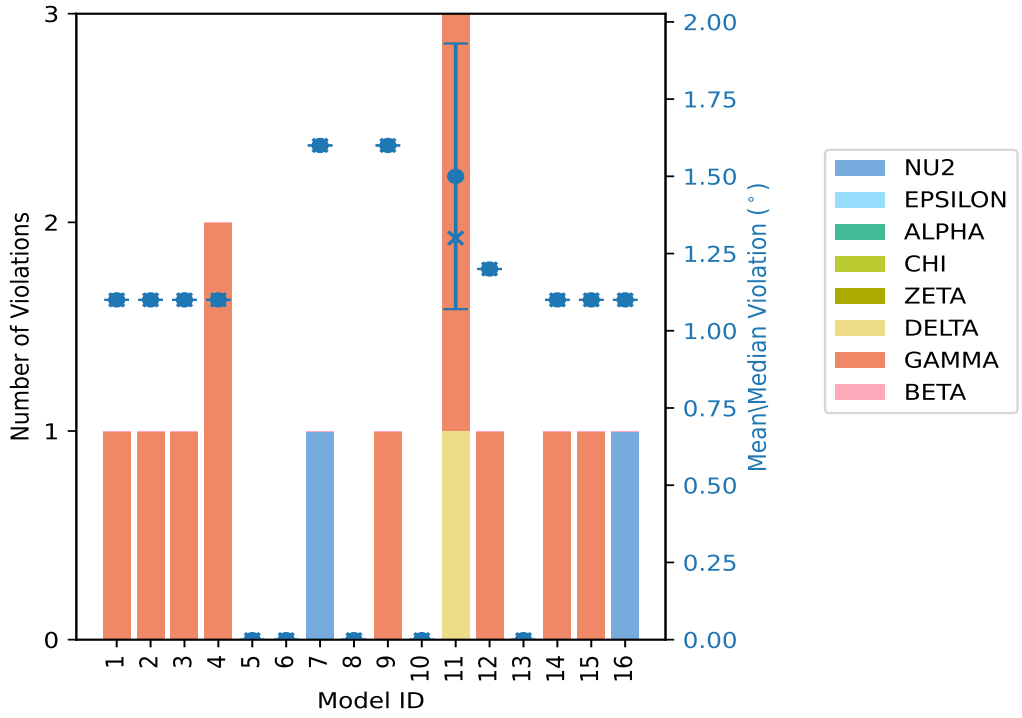
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations									Mean (°)	Max (°)	SD (°)	Median (°)
	NU2	EPSILON	ALPHA	CHI	ZETA	DELTA	GAMMA	BETA	Total				
1	0	0	0	0	0	0	1	0	1	1.1	1.1	0.0	1.1
2	0	0	0	0	0	0	1	0	1	1.1	1.1	0.0	1.1
3	0	0	0	0	0	0	1	0	1	1.1	1.1	0.0	1.1
4	0	0	0	0	0	0	2	0	2	1.1	1.1	0.0	1.1
5	0	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	1	0	0	0	0	0	0	0	1	1.6	1.6	0.0	1.6
8	0	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0	0	1	0	1	1.6	1.6	0.0	1.6
10	0	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0	0	1	2	0	3	1.5	2.1	0.43	1.3
12	0	0	0	0	0	0	1	0	1	1.2	1.2	0.0	1.2
13	0	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0	0	1	0	1	1.1	1.1	0.0	1.1
15	0	0	0	0	0	0	1	0	1	1.1	1.1	0.0	1.1
16	1	0	0	0	0	0	0	0	1	1.1	1.1	0.0	1.1

10.2.1 Bar graph : Dihedral violation statistics for each model



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

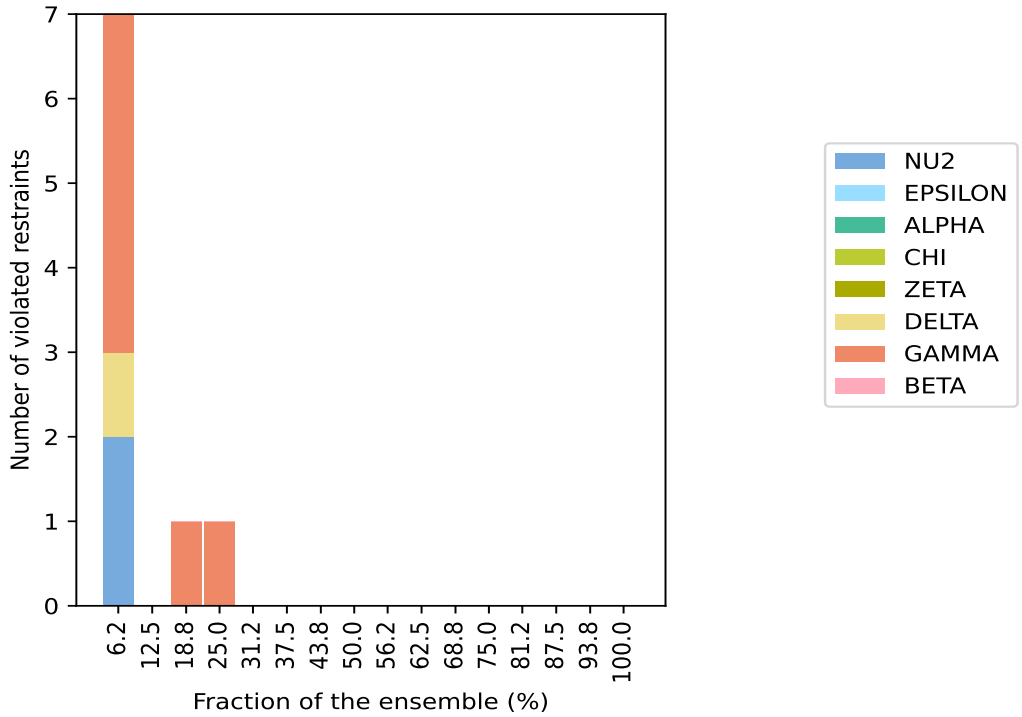
10.3 Dihedral-angle violation statistics for the ensemble (i)

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

Number of violated restraints									Fraction of the ensemble	
NU2	EPSILON	ALPHA	CHI	ZETA	DELTA	GAMMA	BETA	Total	Count[1]	%
2	0	0	0	0	1	4	0	7	1	6.2
0	0	0	0	0	0	0	0	0	2	12.5
0	0	0	0	0	0	1	0	1	3	18.8
0	0	0	0	0	0	1	0	1	4	25.0
0	0	0	0	0	0	0	0	0	5	31.2
0	0	0	0	0	0	0	0	0	6	37.5
0	0	0	0	0	0	0	0	0	7	43.8
0	0	0	0	0	0	0	0	0	8	50.0
0	0	0	0	0	0	0	0	0	9	56.2
0	0	0	0	0	0	0	0	0	10	62.5
0	0	0	0	0	0	0	0	0	11	68.8
0	0	0	0	0	0	0	0	0	12	75.0
0	0	0	0	0	0	0	0	0	13	81.2
0	0	0	0	0	0	0	0	0	14	87.5
0	0	0	0	0	0	0	0	0	15	93.8
0	0	0	0	0	0	0	0	0	16	100.0

[1] Number of models with violations

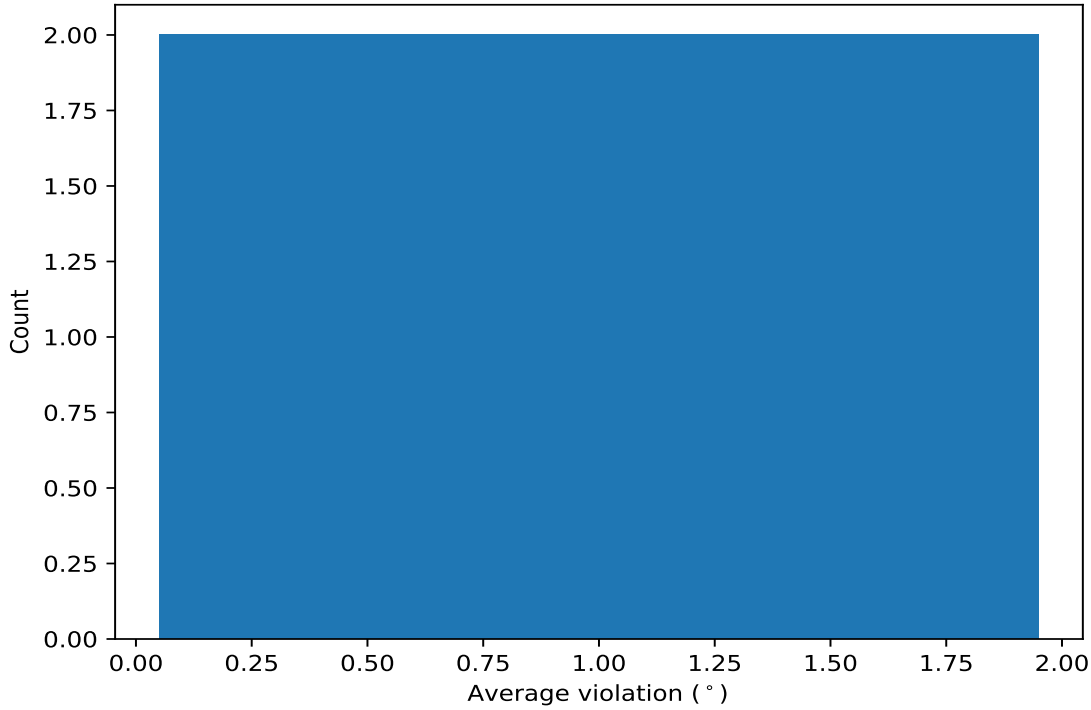
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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



10.4.2 Table: Most violated dihedral-angle restraints

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

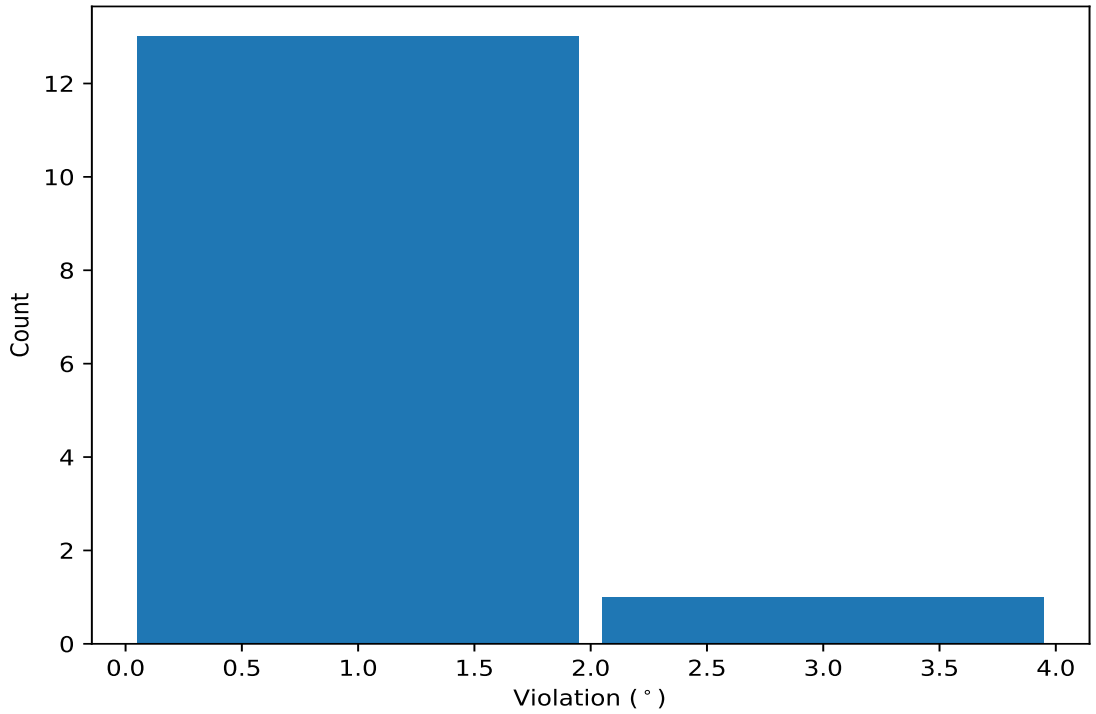
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,131)	1:A:23:G:O5’	1:A:23:G:C5’	1:A:23:G:C4’	1:A:23:G:C3’	4	1.23	0.22	1.1
(1,123)	1:A:11:G:O5’	1:A:11:G:C5’	1:A:11:G:C4’	1:A:11:G:C3’	3	1.17	0.09	1.1

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,212)	1:A:17:A:C5’	1:A:17:A:C4’	1:A:17:A:C3’	1:A:17:A:O3’	11	2.1
(1,170)	1:A:3:G:C1’	1:A:3:G:C2’	1:A:3:G:C3’	1:A:3:G:C4’	7	1.6
(1,131)	1:A:23:G:O5’	1:A:23:G:C5’	1:A:23:G:C4’	1:A:23:G:C3’	9	1.6
(1,123)	1:A:11:G:O5’	1:A:11:G:C5’	1:A:11:G:C4’	1:A:11:G:C3’	11	1.3
(1,124)	1:A:12:U:O5’	1:A:12:U:C5’	1:A:12:U:C4’	1:A:12:U:C3’	12	1.2
(1,187)	1:A:24:U:C1’	1:A:24:U:C2’	1:A:24:U:C3’	1:A:24:U:C4’	16	1.1
(1,131)	1:A:23:G:O5’	1:A:23:G:C5’	1:A:23:G:C4’	1:A:23:G:C3’	3	1.1
(1,131)	1:A:23:G:O5’	1:A:23:G:C5’	1:A:23:G:C4’	1:A:23:G:C3’	11	1.1
(1,131)	1:A:23:G:O5’	1:A:23:G:C5’	1:A:23:G:C4’	1:A:23:G:C3’	14	1.1
(1,130)	1:A:22:C:O5’	1:A:22:C:C5’	1:A:22:C:C4’	1:A:22:C:C3’	2	1.1
(1,127)	1:A:19:G:O5’	1:A:19:G:C5’	1:A:19:G:C4’	1:A:19:G:C3’	1	1.1
(1,123)	1:A:11:G:O5’	1:A:11:G:C5’	1:A:11:G:C4’	1:A:11:G:C3’	4	1.1
(1,123)	1:A:11:G:O5’	1:A:11:G:C5’	1:A:11:G:C4’	1:A:11:G:C3’	15	1.1
(1,121)	1:A:9:A:O5’	1:A:9:A:C5’	1:A:9:A:C4’	1:A:9:A:C3’	4	1.1