Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 05:30 AM EDT

PDB ID	:	2JP9
BMRB ID	:	15532
Title	:	Structure of the Wilms Tumor Suppressor Protein Zinc Finger Domain Bound to DNA
Authors	:	Stoll, R.; Lee, B.M.; Debler, E.W.; Laity, J.H.; Wilson, I.A.; Dyson, H.J.; Wright, P.E.
Deposited on	:	2007-04-30

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:

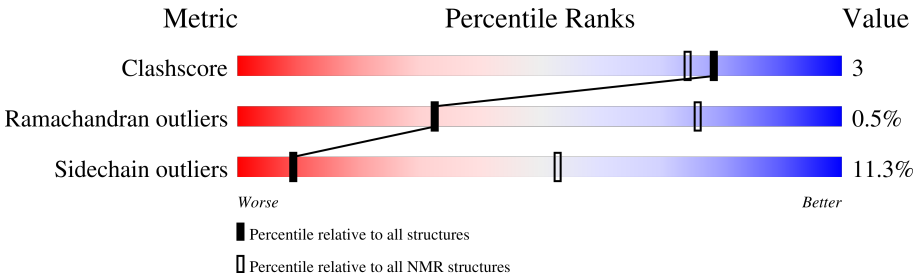
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 9%.

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



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

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

Mol	Chain	Length	Quality of chain
1	B	17	41% 53% 6%
2	C	17	59% 41%
3	A	119	66% 18% • 13%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:7-A:32 (26)	0.52	11
2	A:37-A:39, A:46-A:119 (77)	0.61	1

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

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

The models can be grouped into 3 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3069 atoms, of which 1357 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP *DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	B	17	541	164	189	67	104	17	0

- Molecule 2 is a DNA chain called DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP *DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	C	17	532	161	187	67	100	17	0

- Molecule 3 is a protein called Wilms tumor 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
3	A	119	1992	622	981	210	168	11	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP Q4VXV4

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
4	A	4	4	4

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

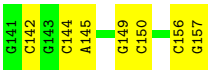
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for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

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:

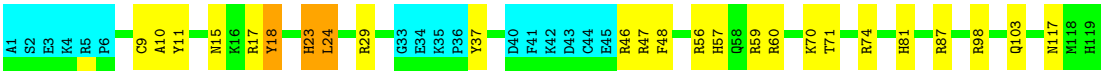
• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:



• Molecule 3: Wilms tumor 1

Chain A:



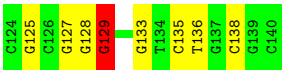
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:



• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

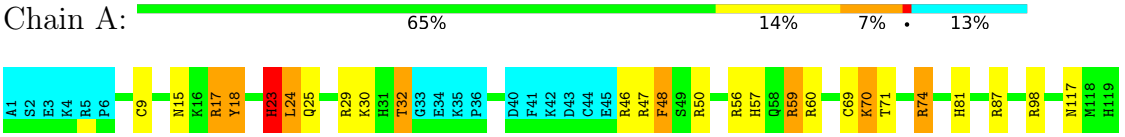
• Molecule 3: Wilms tumor 1

4.2.2 Score per residue for model 2

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

• Molecule 3: Wilms tumor 1



4.2.3 Score per residue for model 3

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

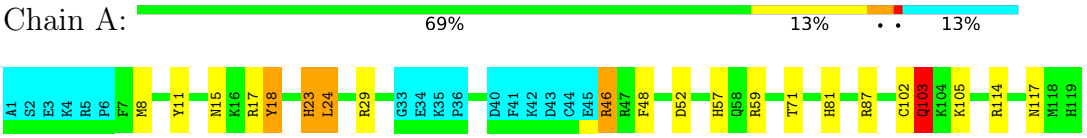
Chain B:

• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:

• Molecule 3: Wilms tumor 1

Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

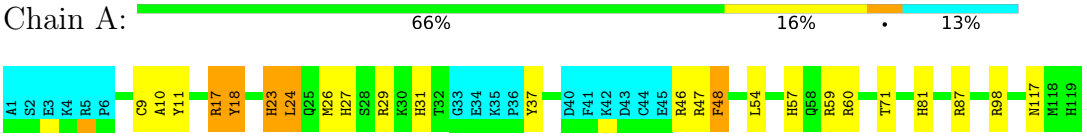
Chain B:

• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:

• Molecule 3: Wilms tumor 1

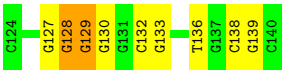
Chain A:



4.2.5 Score per residue for model 5

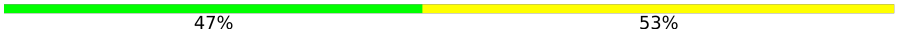
• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:



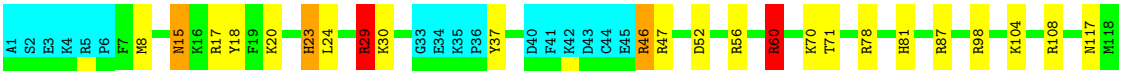
• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:



• Molecule 3: Wilms tumor 1

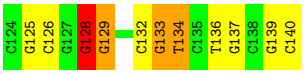
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:

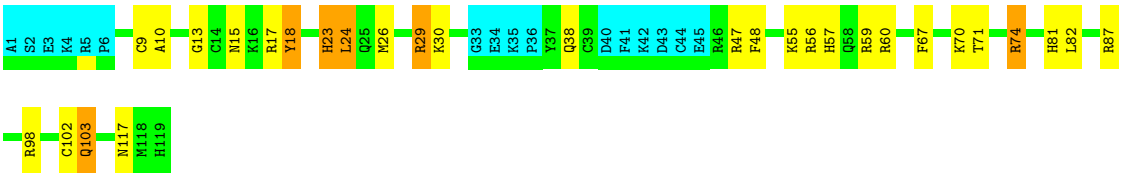


• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:

• Molecule 3: Wilms tumor 1

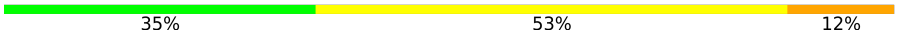
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:

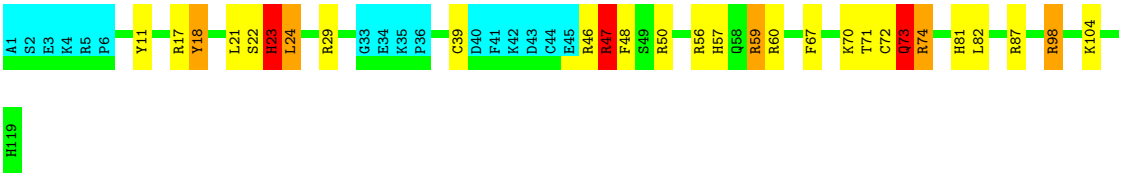


• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:

• Molecule 3: Wilms tumor 1

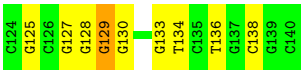
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:

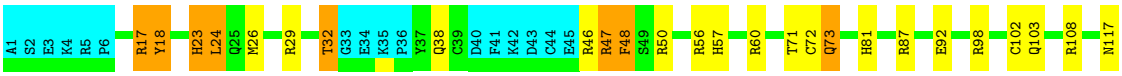


• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:

• Molecule 3: Wilms tumor 1

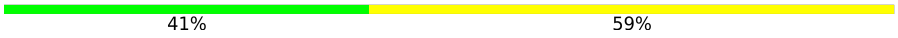
Chain A:

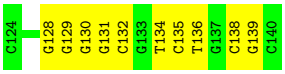


4.2.9 Score per residue for model 9

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

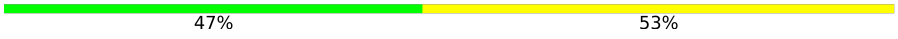
Chain B:

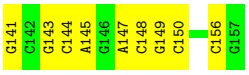




• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

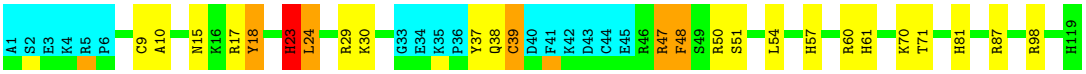
Chain C:





• Molecule 3: Wilms tumor 1

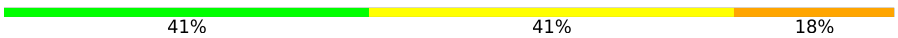
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:



• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:

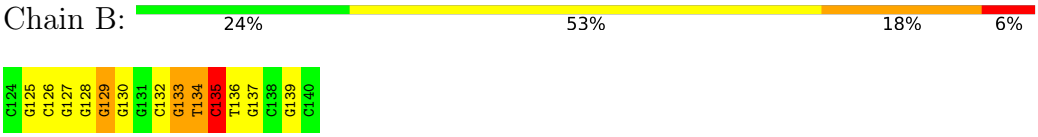
• Molecule 3: Wilms tumor 1

Chain A:

4.2.11 Score per residue for model 11

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:

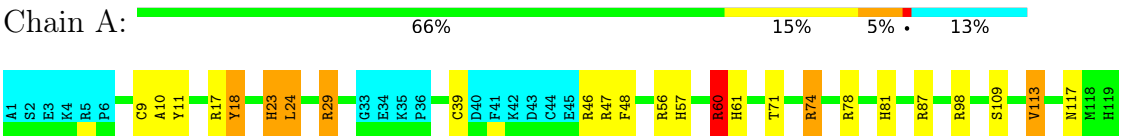


• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:

• Molecule 3: Wilms tumor 1

Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:

• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:

• Molecule 3: Wilms tumor 1

Chain A:

4.2.13 Score per residue for model 13

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

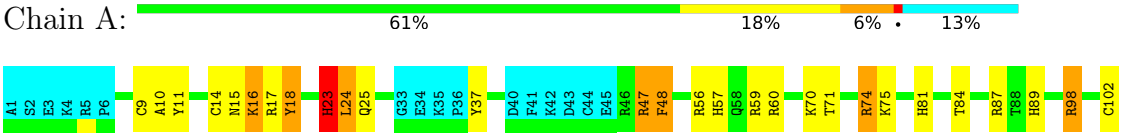
Chain B:

• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:

• Molecule 3: Wilms tumor 1

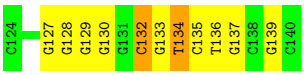
Chain A:



4.2.14 Score per residue for model 14

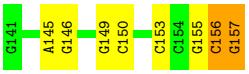
• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:



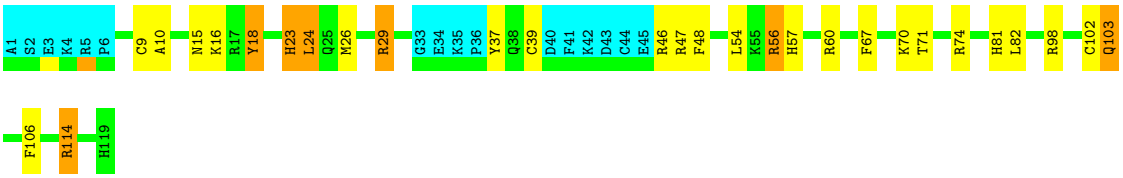
• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:



• Molecule 3: Wilms tumor 1

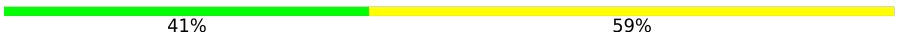
Chain A:

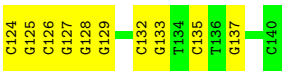


4.2.15 Score per residue for model 15

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

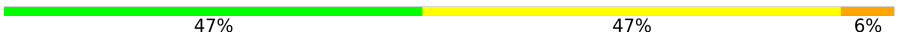
Chain B:

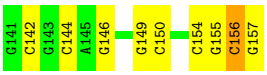




• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

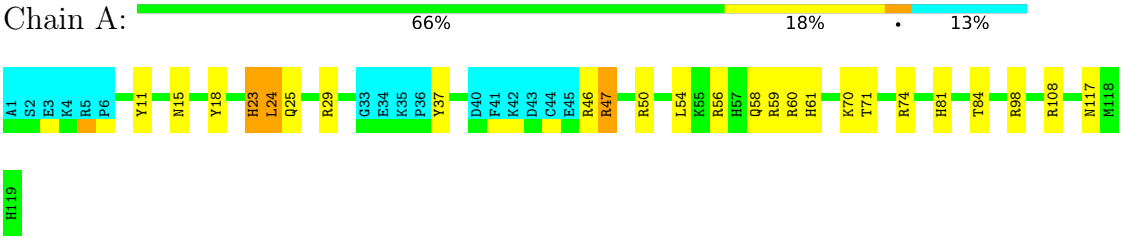
Chain C:





• Molecule 3: Wilms tumor 1

Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

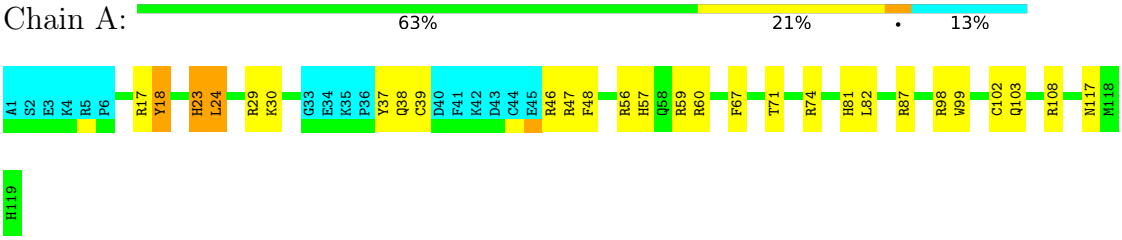
Chain B:

• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:

• Molecule 3: Wilms tumor 1

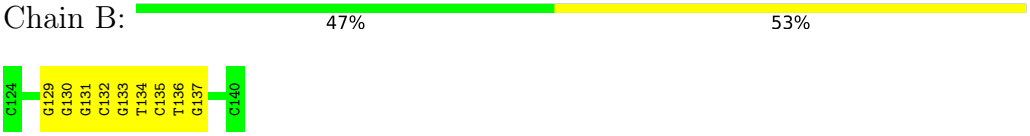
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:

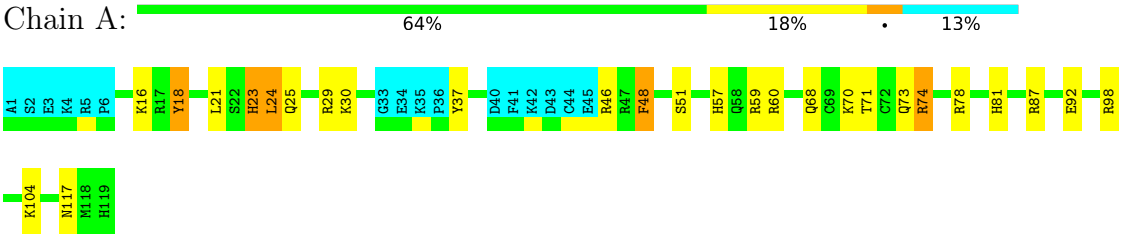


• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:

• Molecule 3: Wilms tumor 1

Chain A:



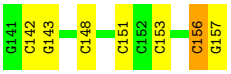
4.2.18 Score per residue for model 18

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:

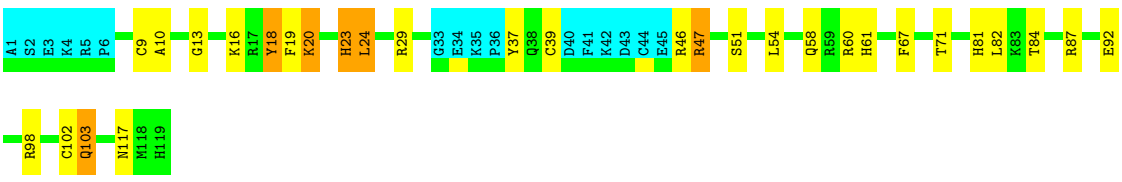
• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:



• Molecule 3: Wilms tumor 1

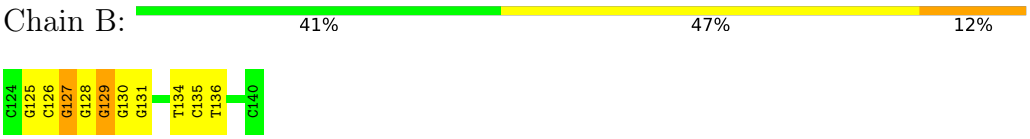
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:

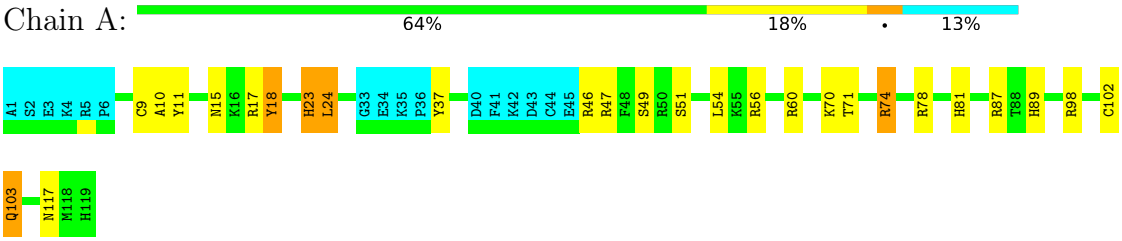


• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:

• Molecule 3: Wilms tumor 1

Chain A:



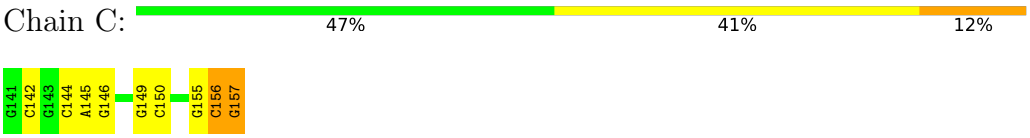
4.2.20 Score per residue for model 20

• Molecule 1: DNA (5'-D(P*DCP*DGP*DCP*DGP*DGP*DGP*DGP*DGP*DCP*DGP*DTP*DCP*DTP*DGP*DCP*DGP*DC)-3')

Chain B:

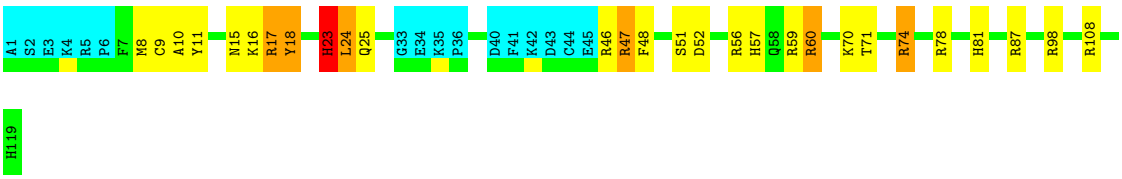
• Molecule 2: DNA (5'-D(P*DGP*DCP*DGP*DCP*DAP*DGP*DAP*DCP*DGP*DCP*DCP*DCP*DCP*DCP*DGP*DCP*DG)-3')

Chain C:



• Molecule 3: Wilms tumor 1

Chain A:


A1
S2
E3
K4
R5
P6
F7
M8
C9
A10
Y11
N15
K16
R17
Y18
H23
L24
Q25
G33
E34
K35
P36
D40
F41
K42
D43
C44
E45
R46
R47
F48
S51
D52
R56
H57
Q58
R59
R60
K70
T71
R74
R78
H81
R87
R98
R108
H119

5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
Amber	structure solution	
Amber	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	220
Number of shifts mapped to atoms	220
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	9%

6 Model quality (i)

6.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	B	1.68±0.13	4±3/394 (0.9± 0.7%)	1.64±0.08	10±3/607 (1.6± 0.5%)
2	C	1.51±0.06	1±1/386 (0.1± 0.2%)	1.57±0.05	8±2/592 (1.3± 0.4%)
3	A	0.72±0.00	0±0/910 (0.0± 0.0%)	1.06±0.05	10±2/1211 (0.8± 0.2%)
All	All	1.21	84/33800 (0.2%)	1.36	550/48200 (1.1%)

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

Mol	Chain	Chirality	Planarity
1	B	0.0±0.0	2.1±1.5
2	C	0.0±0.0	0.9±0.8
3	A	0.0±0.0	2.9±1.4
All	All	0	120

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	134	DT	C5-C7	13.61	1.58	1.50	9	9
1	B	136	DT	C5-C7	12.60	1.57	1.50	13	8
1	B	135	DC	C5'-C4'	9.39	1.61	1.51	11	3
1	B	128	DG	C4'-C3'	8.38	1.61	1.53	6	1
1	B	127	DG	C2'-C1'	8.14	1.60	1.52	19	1
1	B	134	DT	C5-C6	7.79	1.39	1.34	17	2
1	B	134	DT	C2'-C1'	7.60	1.59	1.52	11	2
1	B	136	DT	C5-C6	7.55	1.39	1.34	11	1
1	B	134	DT	C4-C5	7.46	1.51	1.45	17	2
1	B	136	DT	N3-C4	7.43	1.44	1.38	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	134	DT	O3'-P	7.35	1.70	1.61	17	1
1	B	134	DT	N1-C2	7.30	1.43	1.38	17	4
1	B	134	DT	N3-C4	6.98	1.44	1.38	13	1
1	B	134	DT	P-O5'	6.79	1.66	1.59	13	3
1	B	136	DT	C2'-C1'	6.72	1.59	1.52	14	2
1	B	135	DC	N1-C6	-6.48	1.33	1.37	13	2
2	C	147	DA	C4'-O4'	-6.42	1.38	1.45	3	1
2	C	145	DA	N9-C4	-6.32	1.34	1.37	13	1
1	B	134	DT	C4'-O4'	-6.30	1.38	1.45	14	3
1	B	135	DC	C4'-O4'	-6.15	1.38	1.45	20	1
1	B	137	DG	P-O5'	6.09	1.65	1.59	16	2
1	B	130	DG	C4'-O4'	-5.99	1.39	1.45	10	1
1	B	128	DG	C4'-O4'	-5.85	1.39	1.45	15	1
1	B	135	DC	N3-C4	-5.66	1.29	1.33	14	1
2	C	144	DC	C4-N4	-5.65	1.28	1.33	1	1
1	B	136	DT	P-O5'	5.63	1.65	1.59	9	1
1	B	135	DC	C4-N4	-5.61	1.28	1.33	9	2
1	B	136	DT	C4'-C3'	5.53	1.58	1.53	9	1
2	C	154	DC	C4'-O4'	-5.51	1.39	1.45	19	1
1	B	135	DC	O4'-C1'	5.47	1.48	1.42	11	1
1	B	136	DT	O3'-P	5.46	1.67	1.61	14	1
1	B	136	DT	C5'-C4'	5.45	1.57	1.51	16	1
1	B	135	DC	P-O5'	5.45	1.65	1.59	17	1
2	C	145	DA	C6-N6	-5.43	1.29	1.33	10	1
1	B	134	DT	N1-C6	-5.41	1.34	1.38	14	1
2	C	153	DC	C2'-C1'	5.38	1.57	1.52	6	1
1	B	136	DT	N1-C2	5.33	1.42	1.38	11	1
1	B	133	DG	P-O5'	5.31	1.65	1.59	18	1
1	B	135	DC	C2-N3	5.30	1.40	1.35	11	1
1	B	130	DG	P-O5'	5.25	1.65	1.59	14	1
1	B	134	DT	C2-N3	5.25	1.42	1.37	17	1
1	B	127	DG	C4'-O4'	-5.21	1.39	1.45	19	1
2	C	151	DC	C2'-C1'	5.20	1.57	1.52	19	1
1	B	133	DG	C4'-O4'	-5.15	1.39	1.45	17	1
2	C	144	DC	P-O5'	5.14	1.64	1.59	7	2
1	B	137	DG	C2-N2	-5.14	1.29	1.34	16	1
1	B	136	DT	C3'-C2'	5.13	1.58	1.52	13	2
1	B	127	DG	C2-N2	-5.05	1.29	1.34	19	1
2	C	146	DG	C4'-O4'	-5.05	1.40	1.45	19	1
2	C	149	DG	P-O5'	5.04	1.64	1.59	16	1
1	B	129	DG	C2-N3	5.01	1.36	1.32	12	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	134	DT	O4'-C4'-C3'	12.64	113.59	106.00	11	9
3	A	23	HIS	CA-CB-CG	11.10	132.47	113.60	15	20
2	C	150	DC	O4'-C4'-C3'	10.56	112.33	106.00	15	17
2	C	155	DG	O4'-C4'-C3'	10.14	112.08	106.00	8	8
1	B	130	DG	O4'-C4'-C3'	9.71	111.83	106.00	20	11
3	A	29	ARG	NE-CZ-NH1	9.71	125.15	120.30	16	14
3	A	60	ARG	NE-CZ-NH1	9.57	125.08	120.30	1	18
1	B	127	DG	O4'-C4'-C3'	9.52	111.72	106.00	14	6
3	A	108	ARG	NE-CZ-NH2	-9.38	115.61	120.30	8	4
3	A	98	ARG	NE-CZ-NH1	9.19	124.89	120.30	9	17
3	A	78	ARG	NE-CZ-NH2	-9.09	115.75	120.30	20	1
1	B	135	DC	O4'-C4'-C3'	9.03	111.42	106.00	7	3
3	A	108	ARG	NE-CZ-NH1	8.99	124.79	120.30	20	5
2	C	151	DC	O4'-C4'-C3'	8.87	111.32	106.00	3	7
1	B	132	DC	O4'-C4'-C3'	8.68	111.21	106.00	18	15
3	A	59	ARG	NE-CZ-NH1	8.68	124.64	120.30	2	12
2	C	149	DG	O4'-C4'-C3'	8.65	111.19	106.00	12	9
2	C	156	DC	O4'-C4'-C3'	8.63	111.18	106.00	18	13
2	C	153	DC	O4'-C4'-C3'	8.59	111.16	106.00	14	6
3	A	17	ARG	NE-CZ-NH1	8.54	124.57	120.30	9	11
1	B	138	DC	O4'-C4'-C3'	8.52	111.11	106.00	8	6
1	B	133	DG	O4'-C4'-C3'	8.48	111.09	106.00	7	7
1	B	136	DT	O4'-C4'-C3'	8.42	111.05	106.00	4	10
2	C	142	DC	O4'-C4'-C3'	8.30	110.98	106.00	5	11
3	A	114	ARG	NE-CZ-NH1	8.30	124.45	120.30	14	2
1	B	128	DG	O4'-C4'-C3'	8.29	110.98	106.00	18	3
3	A	113	VAL	CA-CB-CG2	8.26	123.29	110.90	11	1
2	C	154	DC	O4'-C4'-C3'	8.25	110.95	106.00	2	9
1	B	137	DG	O4'-C4'-C3'	8.25	110.95	106.00	7	11
3	A	56	ARG	NE-CZ-NH1	8.21	124.41	120.30	13	13
3	A	47	ARG	NE-CZ-NH1	7.90	124.25	120.30	15	15
1	B	134	DT	C1'-O4'-C4'	-7.90	102.20	110.10	17	1
2	C	144	DC	O4'-C4'-C3'	7.87	110.72	106.00	2	10
2	C	145	DA	O4'-C4'-C3'	7.82	110.69	106.00	3	9
3	A	87	ARG	NE-CZ-NH1	7.67	124.13	120.30	13	18
1	B	128	DG	C1'-O4'-C4'	-7.62	102.48	110.10	19	2
3	A	74	ARG	NE-CZ-NH1	7.57	124.09	120.30	6	12
3	A	46	ARG	NE-CZ-NH1	7.56	124.08	120.30	20	14
2	C	148	DC	O4'-C4'-C3'	7.55	110.53	106.00	11	4
2	C	141	DG	O4'-C4'-C3'	7.48	110.49	106.00	3	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	78	ARG	NE-CZ-NH1	7.45	124.03	120.30	20	3
1	B	134	DT	O4'-C1'-C2'	-7.42	99.96	105.90	4	5
1	B	133	DG	C4'-C3'-C2'	-7.42	96.43	103.10	7	3
1	B	126	DC	O4'-C1'-C2'	-7.41	99.97	105.90	19	4
3	A	74	ARG	NE-CZ-NH2	-7.40	116.60	120.30	6	1
1	B	132	DC	C4'-C3'-C2'	-7.34	96.50	103.10	13	1
1	B	139	DG	O4'-C4'-C3'	7.28	110.37	106.00	9	7
1	B	129	DG	C8-N9-C4	-7.01	103.59	106.40	12	1
3	A	60	ARG	CD-NE-CZ	7.01	133.41	123.60	1	1
2	C	143	DG	O4'-C4'-C3'	7.00	110.20	106.00	19	4
1	B	131	DG	O4'-C4'-C3'	6.98	110.19	106.00	9	3
2	C	147	DA	O4'-C4'-C3'	6.93	110.16	106.00	3	9
1	B	128	DG	C3'-C2'-C1'	-6.89	94.23	102.50	9	1
1	B	129	DG	O4'-C4'-C3'	6.88	110.13	106.00	4	2
1	B	136	DT	O3'-P-O5'	-6.86	90.97	104.00	11	3
1	B	124	DC	O4'-C4'-C3'	6.81	110.09	106.00	2	1
2	C	145	DA	P-O3'-C3'	6.79	127.85	119.70	14	3
2	C	151	DC	O4'-C1'-C2'	-6.78	100.48	105.90	19	1
1	B	133	DG	O4'-C1'-C2'	-6.76	100.49	105.90	17	2
1	B	125	DG	O4'-C4'-C3'	6.73	110.04	106.00	8	8
2	C	145	DA	O4'-C1'-C2'	-6.51	100.69	105.90	14	1
2	C	142	DC	P-O3'-C3'	6.45	127.43	119.70	10	4
1	B	128	DG	O3'-P-O5'	-6.41	91.81	104.00	6	1
1	B	136	DT	C5-C6-N1	-6.37	119.88	123.70	17	3
1	B	135	DC	C4'-C3'-C2'	-6.37	97.37	103.10	7	3
1	B	126	DC	O4'-C4'-C3'	6.36	109.81	106.00	12	4
1	B	135	DC	O4'-C1'-C2'	-6.32	100.84	105.90	1	7
3	A	50	ARG	NE-CZ-NH1	6.24	123.42	120.30	9	3
3	A	50	ARG	NE-CZ-NH2	-6.20	117.20	120.30	2	2
2	C	153	DC	O4'-C1'-C2'	-6.16	100.98	105.90	8	2
1	B	126	DC	C1'-O4'-C4'	-6.12	103.98	110.10	7	5
1	B	134	DT	C3'-C2'-C1'	-6.12	95.16	102.50	17	1
1	B	134	DT	C4'-C3'-C2'	-6.08	97.62	103.10	14	2
1	B	134	DT	C5-C6-N1	-6.05	120.07	123.70	16	4
1	B	136	DT	P-O3'-C3'	6.03	126.94	119.70	11	1
1	B	129	DG	O3'-P-O5'	-5.88	92.83	104.00	12	1
3	A	39	CYS	CA-CB-SG	-5.85	103.47	114.00	9	4
2	C	153	DC	P-O3'-C3'	5.82	126.69	119.70	18	1
1	B	133	DG	C8-N9-C4	-5.82	104.07	106.40	11	2
1	B	127	DG	C8-N9-C4	-5.82	104.07	106.40	19	1
1	B	136	DT	C4'-C3'-C2'	-5.77	97.90	103.10	17	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	128	DG	P-O3'-C3'	5.77	126.63	119.70	6	1
1	B	130	DG	C4'-C3'-C2'	-5.75	97.92	103.10	20	2
1	B	135	DC	P-O3'-C3'	5.72	126.57	119.70	13	1
2	C	154	DC	O4'-C1'-C2'	5.72	110.48	105.90	19	1
2	C	152	DC	O4'-C4'-C3'	5.71	109.42	106.00	4	2
1	B	131	DG	C4'-C3'-C2'	-5.66	98.00	103.10	9	1
3	A	84	THR	CA-CB-CG2	5.63	120.28	112.40	18	5
2	C	146	DG	O4'-C4'-C3'	5.57	109.34	106.00	7	4
2	C	153	DC	C4'-C3'-C2'	-5.57	98.09	103.10	12	1
1	B	137	DG	C4'-C3'-C2'	-5.56	98.09	103.10	11	2
1	B	136	DT	C4-C5-C6	5.49	121.29	118.00	9	2
1	B	124	DC	O4'-C1'-C2'	5.48	110.28	105.90	2	1
2	C	157	DG	O4'-C4'-C3'	5.47	109.28	106.00	7	1
1	B	131	DG	O4'-C1'-C2'	-5.46	101.53	105.90	18	2
1	B	134	DT	C5'-C4'-C3'	-5.45	104.29	114.10	8	2
1	B	133	DG	O3'-P-O5'	-5.44	93.67	104.00	17	2
2	C	145	DA	C4'-C3'-C2'	-5.42	98.22	103.10	20	1
1	B	126	DC	C4'-C3'-C2'	-5.41	98.24	103.10	12	1
1	B	127	DG	C3'-C2'-C1'	5.33	108.89	102.50	14	1
1	B	126	DC	C3'-C2'-C1'	-5.32	96.12	102.50	7	1
2	C	147	DA	C1'-O4'-C4'	-5.31	104.79	110.10	13	2
3	A	56	ARG	NE-CZ-NH2	-5.30	117.65	120.30	1	1
3	A	74	ARG	CD-NE-CZ	5.30	131.03	123.60	6	1
2	C	150	DC	C4'-C3'-C2'	-5.29	98.33	103.10	9	1
2	C	143	DG	P-O3'-C3'	5.26	126.01	119.70	8	1
1	B	128	DG	O4'-C1'-C2'	5.24	110.10	105.90	19	1
3	A	32	THR	CA-CB-CG2	5.24	119.73	112.40	8	2
2	C	150	DC	C3'-C2'-C1'	5.23	108.77	102.50	9	2
1	B	132	DC	O4'-C1'-C2'	-5.23	101.72	105.90	13	1
1	B	137	DG	O4'-C1'-C2'	5.21	110.07	105.90	13	1
2	C	149	DG	C4'-C3'-C2'	-5.20	98.42	103.10	20	1
1	B	129	DG	O4'-C1'-C2'	-5.18	101.76	105.90	5	1
2	C	144	DC	P-O3'-C3'	5.16	125.90	119.70	16	2
1	B	136	DT	O4'-C1'-C2'	5.16	110.03	105.90	8	1
1	B	134	DT	C4-C5-C6	5.15	121.09	118.00	3	2
1	B	140	DC	O4'-C4'-C3'	5.14	109.09	106.00	20	2
1	B	129	DG	P-O3'-C3'	5.12	125.84	119.70	6	1
1	B	137	DG	O3'-P-O5'	-5.10	94.31	104.00	7	1
3	A	114	ARG	NE-CZ-NH2	-5.07	117.77	120.30	14	1
3	A	98	ARG	NE-CZ-NH2	-5.04	117.78	120.30	4	2
1	B	137	DG	P-O3'-C3'	5.04	125.75	119.70	17	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
3	A	18	TYR	Sidechain	19
1	B	127	DG	Sidechain	12
1	B	129	DG	Sidechain	9
3	A	11	TYR	Sidechain	9
3	A	48	PHE	Sidechain	8
2	C	157	DG	Sidechain	7
3	A	23	HIS	Sidechain	7
1	B	134	DT	Sidechain	6
2	C	146	DG	Sidechain	5
3	A	37	TYR	Sidechain	4
1	B	124	DC	Sidechain	3
1	B	128	DG	Sidechain	3
2	C	149	DG	Sidechain	3
1	B	133	DG	Sidechain	3
3	A	47	ARG	Sidechain	3
1	B	131	DG	Sidechain	3
2	C	155	DG	Sidechain	2
1	B	130	DG	Sidechain	2
3	A	78	ARG	Sidechain	2
3	A	29	ARG	Sidechain	1
3	A	98	ARG	Sidechain	1
1	B	135	DC	Sidechain	1
2	C	145	DA	Sidechain	1
2	C	156	DC	Sidechain	1
1	B	132	DC	Sidechain	1
3	A	56	ARG	Sidechain	1
3	A	106	PHE	Sidechain	1
3	A	74	ARG	Sidechain	1
3	A	60	ARG	Sidechain	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	352	189	188	2±1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
2	C	345	187	188	1±0
3	A	884	863	863	7±2
All	All	31700	24780	24810	159

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:18:TYR:CD2	3:A:24:LEU:HD23	0.69	2.22	18	3
3:A:37:TYR:HB3	3:A:54:LEU:HD22	0.67	1.65	18	9
3:A:18:TYR:CD1	3:A:24:LEU:HD23	0.66	2.26	20	16
3:A:67:PHE:HB3	3:A:82:LEU:HD13	0.62	1.72	16	7
3:A:109:SER:O	3:A:113:VAL:HG13	0.56	2.00	11	1
1:B:128:DG:C8	3:A:81:HIS:CE1	0.52	2.98	16	9
1:B:129:DG:N7	3:A:81:HIS:CE1	0.50	2.80	11	20
2:C:144:DC:N4	3:A:29:ARG:HH22	0.50	2.04	6	1
3:A:48:PHE:CZ	3:A:57:HIS:CG	0.50	3.00	2	16
1:B:129:DG:H3'	3:A:60:ARG:NE	0.49	2.22	11	1
3:A:9:CYS:SG	3:A:10:ALA:N	0.49	2.86	14	11
2:C:156:DC:H2"	2:C:157:DG:C8	0.49	2.43	18	15
3:A:24:LEU:O	3:A:24:LEU:HD22	0.46	2.10	1	11
1:B:134:DT:H2"	1:B:135:DC:C6	0.46	2.45	16	2
3:A:102:CYS:SG	3:A:103:GLN:N	0.46	2.89	6	8
1:B:129:DG:N7	3:A:81:HIS:HE1	0.46	2.09	4	4
1:B:134:DT:H2"	1:B:135:DC:C5	0.46	2.46	7	2
3:A:60:ARG:N	3:A:60:ARG:HD3	0.45	2.27	11	1
3:A:11:TYR:CD2	3:A:31:HIS:CE1	0.45	3.05	4	2
3:A:102:CYS:SG	3:A:104:LYS:CE	0.44	3.06	13	1
1:B:129:DG:H2'	3:A:60:ARG:CZ	0.44	2.43	5	1
1:B:135:DC:H41	3:A:29:ARG:NH2	0.43	2.11	11	1
3:A:14:CYS:SG	3:A:15:ASN:N	0.43	2.91	1	1
3:A:14:CYS:SG	3:A:16:LYS:HE3	0.43	2.54	13	1
3:A:19:PHE:O	3:A:20:LYS:C	0.42	2.57	18	1
1:B:134:DT:C2	1:B:135:DC:C4	0.41	3.08	4	1
3:A:68:GLN:NE2	3:A:68:GLN:H	0.41	2.13	17	1
2:C:149:DG:C4	2:C:150:DC:C5	0.41	3.09	1	1
3:A:25:GLN:HE21	3:A:29:ARG:NH1	0.41	2.14	2	1
3:A:72:CYS:SG	3:A:73:GLN:N	0.41	2.90	7	1
3:A:19:PHE:CG	3:A:20:LYS:N	0.41	2.89	18	1
3:A:18:TYR:CE1	3:A:27:HIS:CD2	0.40	3.09	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:69:CYS:SG	3:A:70:LYS:HE2	0.40	2.56	2	1
3:A:24:LEU:HD22	3:A:24:LEU:O	0.40	2.17	16	4
3:A:72:CYS:O	3:A:73:GLN:CB	0.40	2.69	8	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	
3	A	102/119 (86%)	95±2 (93±2%)	6±2 (6±2%)	1±1 (1±1%)	32	76
All	All	2040/2380 (86%)	1904 (93%)	125 (6%)	11 (1%)	32	76

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	A	103	GLN	3
3	A	13	GLY	3
3	A	15	ASN	2
3	A	73	GLN	1
3	A	99	TRP	1
3	A	20	LYS	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	
3	A	98/112 (88%)	87±2 (89±2%)	11±2 (11±2%)	9	53
All	All	1960/2240 (88%)	1738 (89%)	222 (11%)	9	53

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

Mol	Chain	Res	Type	Models (Total)
3	A	23	HIS	20
3	A	24	LEU	20
3	A	71	THR	20
3	A	117	ASN	15
3	A	70	LYS	14
3	A	47	ARG	9
3	A	15	ASN	9
3	A	51	SER	7
3	A	74	ARG	7
3	A	17	ARG	6
3	A	30	LYS	6
3	A	29	ARG	5
3	A	38	GLN	5
3	A	103	GLN	5
3	A	26	MET	5
3	A	16	LYS	5
3	A	32	THR	4
3	A	8	MET	4
3	A	46	ARG	4
3	A	104	LYS	4
3	A	73	GLN	4
3	A	92	GLU	4
3	A	25	GLN	4
3	A	60	ARG	3
3	A	59	ARG	3
3	A	52	ASP	3
3	A	21	LEU	3
3	A	39	CYS	3
3	A	98	ARG	3
3	A	55	LYS	2
3	A	61	HIS	2
3	A	89	HIS	2
3	A	58	GLN	2
3	A	53	GLN	1
3	A	9	CYS	1
3	A	105	LYS	1
3	A	20	LYS	1
3	A	22	SER	1
3	A	87	ARG	1
3	A	37	TYR	1
3	A	75	LYS	1

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Mol	Chain	Res	Type	Models (Total)
3	A	114	ARG	1
3	A	49	SER	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 9% for the well-defined parts and 9% 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	220
Number of shifts mapped to atoms	220
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	109	-0.35 ± 0.35	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 9%, i.e. 196 atoms were assigned a chemical shift out of a possible 2207. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	194/510 (38%)	97/205 (47%)	0/206 (0%)	97/99 (98%)
Sidechain	0/820 (0%)	0/520 (0%)	0/238 (0%)	0/62 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	2/186 (1%)	1/97 (1%)	0/77 (0%)	1/12 (8%)
Sugar	0/408 (0%)	0/238 (0%)	0/170 (0%)	0/0 (—%)
Base	0/283 (0%)	0/181 (0%)	0/53 (0%)	0/49 (0%)
Overall	196/2207 (9%)	98/1241 (8%)	0/744 (0%)	98/222 (44%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 9%, i.e. 220 atoms were assigned a chemical shift out of a possible 2411. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	218/587 (37%)	109/236 (46%)	0/238 (0%)	109/113 (96%)
Sidechain	0/937 (0%)	0/592 (0%)	0/277 (0%)	0/68 (0%)
Aromatic	2/196 (1%)	1/102 (1%)	0/82 (0%)	1/12 (8%)
Sugar	0/408 (0%)	0/238 (0%)	0/170 (0%)	0/0 (—%)
Base	0/283 (0%)	0/181 (0%)	0/53 (0%)	0/49 (0%)
Overall	220/2411 (9%)	110/1349 (8%)	0/820 (0%)	110/242 (45%)

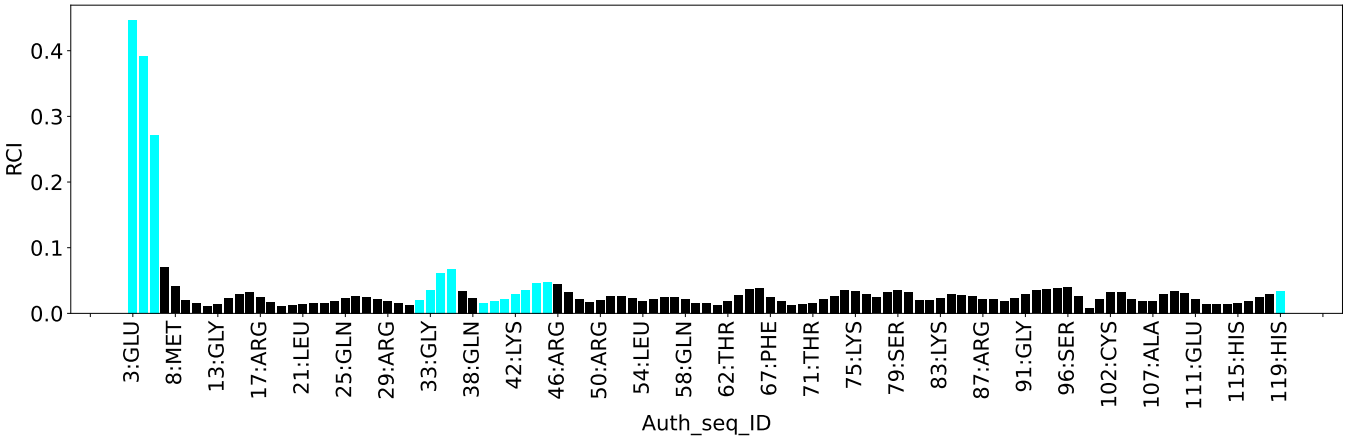
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.0
0.1
0.2
0.3
0.4
3:GLU
8:MET
13:GLY
17:ARG
21:LEU
25:GLN
29:ARG
33:GLY
38:GLN
42:LYS
46:ARG
50:ARG
54:LEU
58:GLN
62:THR
67:PHE
71:THR
75:LYS
79:SER
83:LYS
87:ARG
91:GLY
96:SER
102:CYS
107:ALA
111:GLU
115:HIS
119:HIS
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1012
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	70
Medium range (|i-j|>1 and |i-j|<5)	277
Long range (|i-j|≥5)	309
Inter-chain	180
Hydrogen bond restraints	176
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	6.6
Number of long range restraints per residue[1]	2.3

[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)	44.5	0.2
0.2-0.5 (Medium)	25.6	0.5
>0.5 (Large)	26.6	2.2

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

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

9 Distance violation analysis (i)

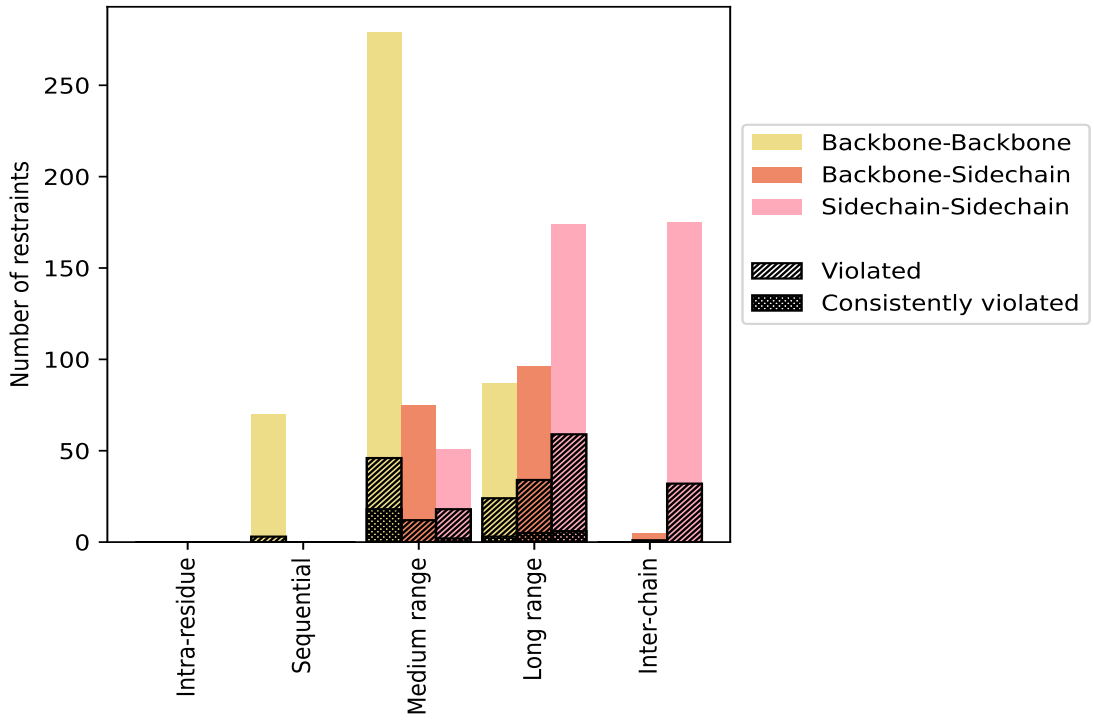
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	70	6.9	3	4.3	0.3	0	0.0	0.0
Backbone-Backbone	70	6.9	3	4.3	0.3	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	277	27.4	32	11.6	3.2	3	1.1	0.3
Backbone-Backbone	151	14.9	2	1.3	0.2	1	0.7	0.1
Backbone-Sidechain	75	7.4	12	16.0	1.2	0	0.0	0.0
Sidechain-Sidechain	51	5.0	18	35.3	1.8	2	3.9	0.2
Long range (|i-j|≥5)	309	30.5	110	35.6	10.9	14	4.5	1.4
Backbone-Backbone	39	3.9	17	43.6	1.7	3	7.7	0.3
Backbone-Sidechain	96	9.5	34	35.4	3.4	5	5.2	0.5
Sidechain-Sidechain	174	17.2	59	33.9	5.8	6	3.4	0.6
Inter-chain	180	17.8	33	18.3	3.3	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	5	0.5	1	20.0	0.1	0	0.0	0.0
Sidechain-Sidechain	175	17.3	32	18.3	3.2	0	0.0	0.0
Hydrogen bond	176	17.4	51	29.0	5.0	17	9.7	1.7
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1012	100.0	229	22.6	22.6	34	3.4	3.4
Backbone-Backbone	436	43.1	73	16.7	7.2	21	4.8	2.1
Backbone-Sidechain	176	17.4	47	26.7	4.6	5	2.8	0.5
Sidechain-Sidechain	400	39.5	109	27.3	10.8	8	2.0	0.8

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	1	41	49	12	103	0.45	2.03	0.5	0.21
2	0	0	37	50	9	96	0.52	1.98	0.51	0.24
3	0	0	39	46	4	89	0.5	1.96	0.52	0.23
4	0	0	36	50	7	93	0.52	2.02	0.55	0.22
5	0	0	36	49	13	98	0.47	2.05	0.52	0.22
6	0	0	39	39	6	84	0.42	1.92	0.48	0.2
7	0	2	38	53	7	100	0.5	2.2	0.51	0.23
8	0	0	41	45	7	93	0.51	1.88	0.54	0.22
9	0	0	42	54	5	101	0.48	2.02	0.5	0.22
10	0	0	38	51	5	94	0.48	2.02	0.53	0.21
11	0	0	38	53	11	102	0.47	1.92	0.49	0.22

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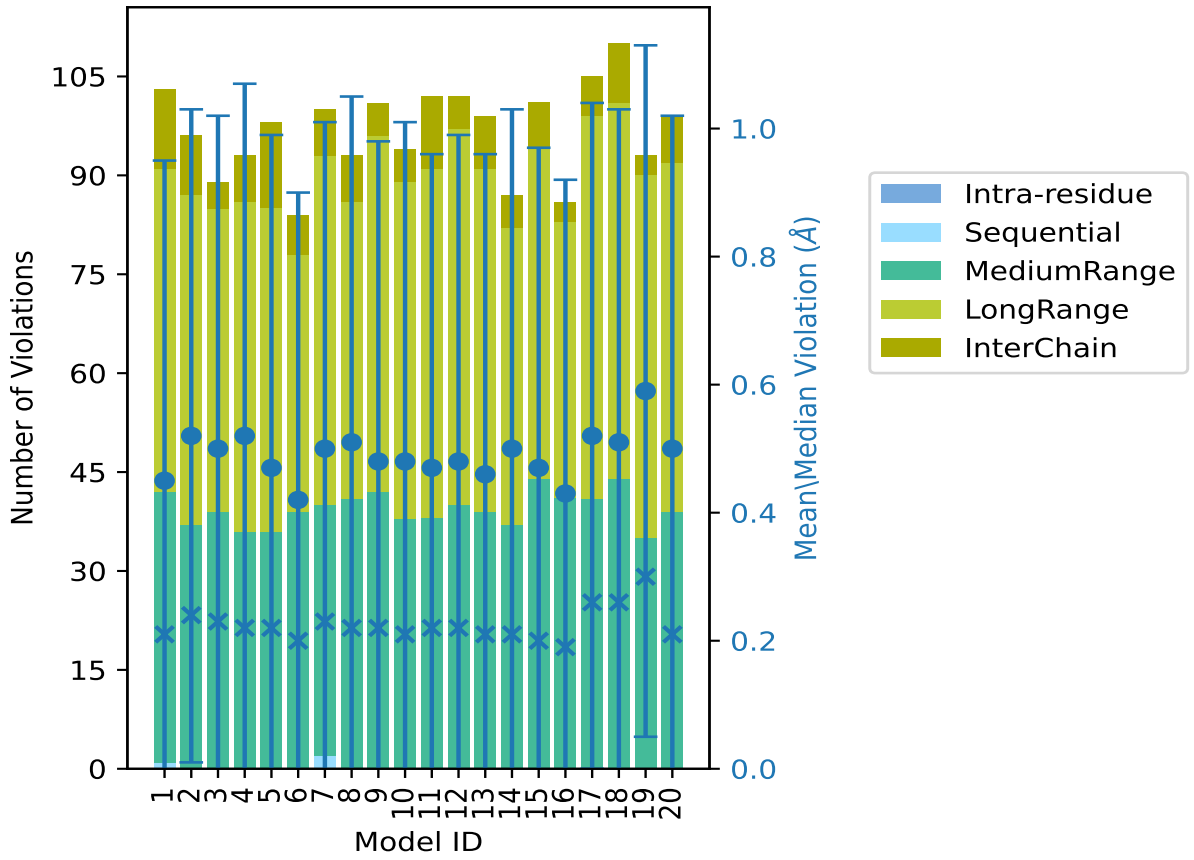
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	40	57	5	102	0.48	1.89	0.51	0.22
13	0	0	39	52	8	99	0.46	2.05	0.5	0.21
14	0	0	37	45	5	87	0.5	2.02	0.53	0.21
15	0	0	44	50	7	101	0.47	2.1	0.5	0.2
16	0	0	41	42	3	86	0.43	1.89	0.49	0.19
17	0	0	41	58	6	105	0.52	2.17	0.52	0.26
18	0	0	44	57	9	110	0.51	1.85	0.52	0.26
19	0	0	35	55	3	93	0.59	1.95	0.54	0.3
20	0	0	39	53	7	99	0.5	2.0	0.52	0.21

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

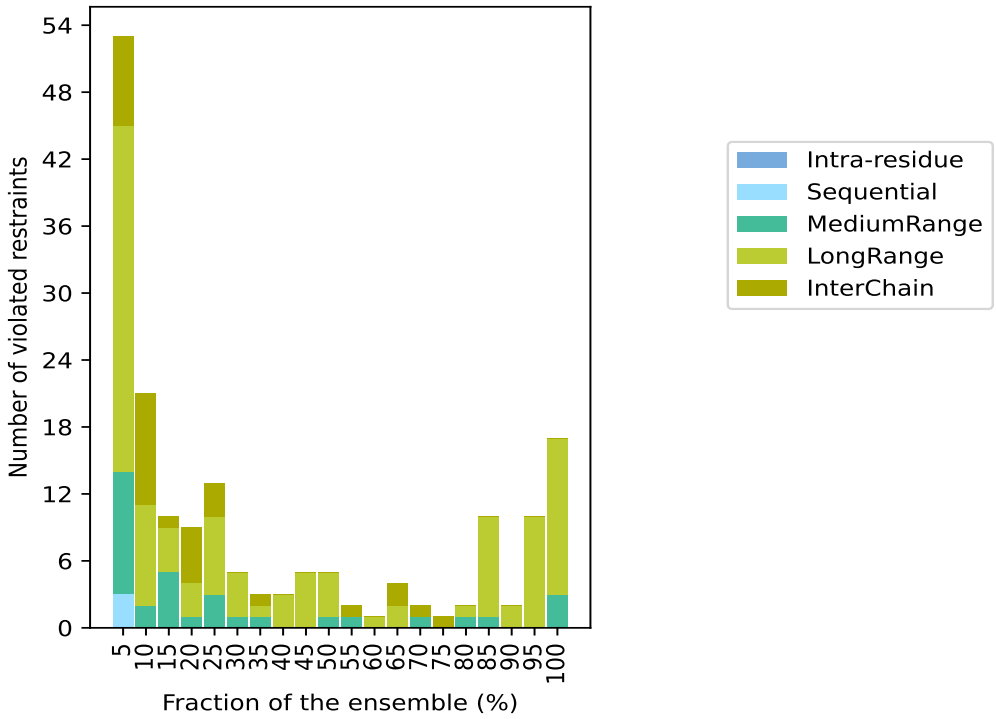
9.3 Distance violation statistics for the ensemble (i)

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, 658(IR:0, SQ:67, MR:245, LR:199, IC:147) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	3	11	31	8	53	1	5.0
0	0	2	9	10	21	2	10.0
0	0	5	4	1	10	3	15.0
0	0	1	3	5	9	4	20.0
0	0	3	7	3	13	5	25.0
0	0	1	4	0	5	6	30.0
0	0	1	1	1	3	7	35.0
0	0	0	3	0	3	8	40.0
0	0	0	5	0	5	9	45.0
0	0	1	4	0	5	10	50.0
0	0	1	0	1	2	11	55.0
0	0	0	1	0	1	12	60.0
0	0	0	2	2	4	13	65.0
0	0	1	0	1	2	14	70.0
0	0	0	0	1	1	15	75.0
0	0	1	1	0	2	16	80.0
0	0	1	9	0	10	17	85.0
0	0	0	2	0	2	18	90.0
0	0	0	10	0	10	19	95.0
0	0	3	14	0	17	20	100.0

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

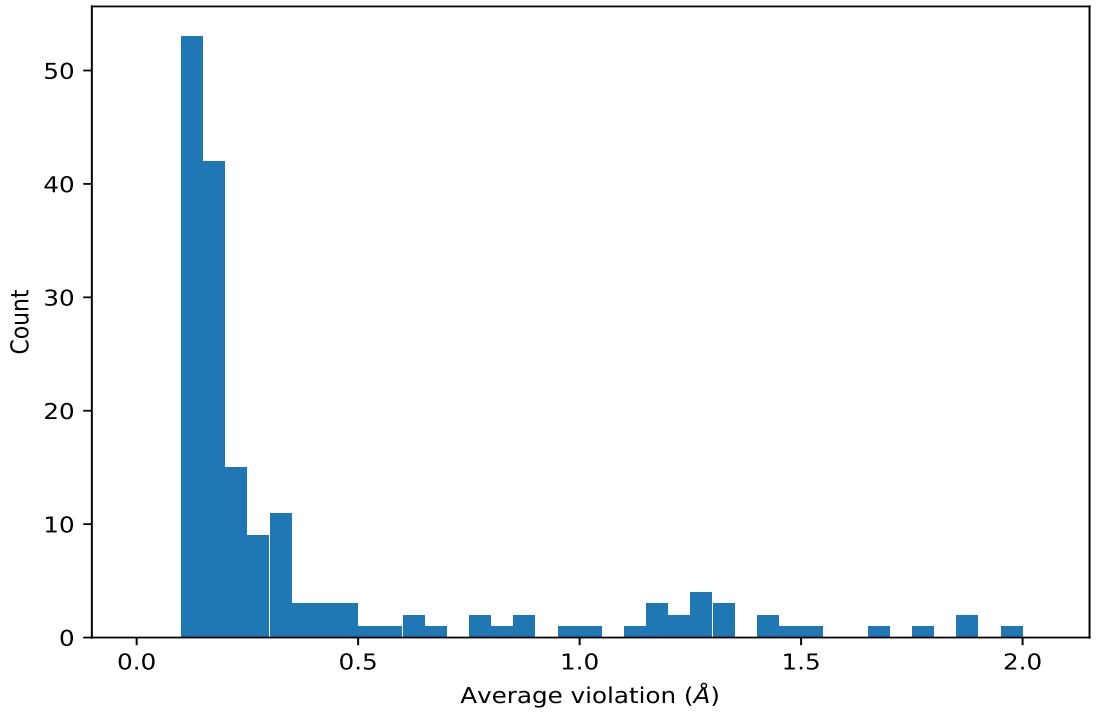
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	20	1.77	0.04	1.75
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	20	1.66	0.02	1.65
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	20	1.54	0.05	1.54
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	20	1.43	0.03	1.42
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	20	1.32	0.04	1.32
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	20	1.18	0.04	1.17
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	20	1.17	0.03	1.17
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	20	1.15	0.02	1.15
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	20	1.13	0.06	1.14
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	20	0.85	0.03	0.86
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	20	0.38	0.01	0.38
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	20	0.34	0.04	0.35
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	20	0.32	0.03	0.32
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	20	0.31	0.06	0.35
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	20	0.3	0.03	0.31
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	20	0.3	0.05	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	20	0.29	0.07	0.32
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	20	0.29	0.04	0.3
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	20	0.28	0.04	0.3
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	20	0.26	0.06	0.26
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	20	0.25	0.05	0.26
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	20	0.23	0.05	0.24
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	20	0.23	0.02	0.23
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	20	0.21	0.03	0.21
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	20	0.2	0.04	0.2
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	20	0.19	0.03	0.2
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	20	0.18	0.03	0.18
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	20	0.18	0.04	0.18
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	20	0.17	0.05	0.16
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	20	0.17	0.02	0.18
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	20	0.16	0.03	0.17
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	20	0.16	0.03	0.15
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	20	0.15	0.03	0.16
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	20	0.15	0.02	0.15
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	19	1.87	0.11	1.89
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	19	1.46	0.11	1.5
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	19	1.34	0.11	1.33
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	19	1.28	0.13	1.31
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	19	0.97	0.1	1.02
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	19	0.79	0.06	0.8
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	19	0.58	0.12	0.6
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	19	0.4	0.13	0.42
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	19	0.38	0.16	0.37
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	19	0.23	0.04	0.22
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	19	0.21	0.04	0.22
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	19	0.19	0.02	0.19
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	19	0.19	0.04	0.2
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	19	0.16	0.04	0.16
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	19	0.15	0.03	0.15
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	18	0.32	0.03	0.32
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	18	0.16	0.03	0.16
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	17	1.99	0.11	2.02
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	17	1.87	0.07	1.88
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	17	1.41	0.03	1.41
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	17	1.28	0.07	1.27
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	17	1.2	0.04	1.2
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	17	1.03	0.06	1.0
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	17	0.68	0.06	0.67

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	17	0.5	0.04	0.51
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	17	0.16	0.03	0.17
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	17	0.13	0.01	0.12
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	16	0.18	0.02	0.18
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	16	0.17	0.06	0.15
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	16	0.14	0.02	0.14
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	16	0.14	0.02	0.15
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	15	0.21	0.07	0.21
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	15	0.18	0.06	0.17
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	15	0.16	0.04	0.16
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	15	0.13	0.01	0.13
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	14	0.21	0.02	0.22
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	14	0.14	0.02	0.14
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	14	0.11	0.0	0.11
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	13	0.29	0.15	0.25
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	13	0.2	0.01	0.2
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	13	0.2	0.03	0.21
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	13	0.18	0.05	0.2
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	13	0.13	0.02	0.13
(1,143)	3:A:68:GLN:HA	3:A:74:ARG:H	12	0.19	0.06	0.17
(2,94)	3:A:26:MET:N	3:A:22:SER:O	12	0.18	0.05	0.18
(2,19)	3:A:30:LYS:H	3:A:27:HIS:O	12	0.12	0.01	0.13
(2,107)	3:A:58:GLN:N	3:A:54:LEU:O	11	0.15	0.04	0.14
(1,739)	1:B:133:DG:C6	3:A:50:ARG:CZ	11	0.14	0.03	0.14
(2,101)	3:A:39:CYS:N	3:A:46:ARG:O	11	0.14	0.02	0.14
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG21	11	0.12	0.01	0.12
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG22	11	0.12	0.01	0.12
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG23	11	0.12	0.01	0.12
(1,377)	3:A:37:TYR:CD2	3:A:50:ARG:CA	10	1.23	0.44	1.27
(1,11)	3:A:8:MET:HA	3:A:16:LYS:H	10	0.22	0.07	0.2
(1,577)	3:A:97:CYS:CB	3:A:99:TRP:CB	10	0.15	0.05	0.13
(1,308)	3:A:11:TYR:CD2	3:A:34:GLU:CB	10	0.15	0.03	0.15
(1,10)	3:A:19:PHE:HA	3:A:7:PHE:H	10	0.13	0.02	0.12
(1,374)	3:A:37:TYR:CE2	3:A:50:ARG:CA	9	1.28	0.36	1.26
(1,378)	3:A:37:TYR:CD2	3:A:51:SER:CA	9	0.87	0.29	0.82
(1,376)	3:A:37:TYR:CE2	3:A:51:SER:CB	9	0.44	0.28	0.44
(1,380)	3:A:37:TYR:CD2	3:A:54:LEU:CB	9	0.35	0.17	0.29
(1,333)	3:A:18:TYR:CE2	3:A:27:HIS:CE1	9	0.25	0.17	0.2
(1,375)	3:A:37:TYR:CE2	3:A:51:SER:CA	8	0.62	0.23	0.61
(2,96)	3:A:28:SER:N	3:A:24:LEU:O	8	0.16	0.06	0.13
(1,75)	3:A:47:ARG:HA	3:A:39:CYS:H	8	0.15	0.02	0.15
(1,502)	3:A:76:PHE:CB	3:A:82:LEU:CD1	8	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,719)	1:B:129:DG:C6	3:A:81:HIS:CE1	7	0.16	0.02	0.17
(2,21)	3:A:31:HIS:H	3:A:28:SER:O	7	0.14	0.02	0.13
(1,452)	3:A:59:ARG:CA	3:A:62:THR:CG2	7	0.14	0.02	0.13
(1,208)	3:A:96:SER:HA	3:A:106:PHE:H	7	0.13	0.01	0.13
(1,299)	3:A:11:TYR:CE1	3:A:34:GLU:CA	6	0.26	0.21	0.18
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD1	6	0.16	0.02	0.16
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD2	6	0.16	0.02	0.16
(1,288)	3:A:11:TYR:CA	3:A:31:HIS:CE1	6	0.15	0.02	0.16
(1,484)	3:A:69:CYS:CA	3:A:74:ARG:CA	6	0.15	0.03	0.14
(1,341)	3:A:19:PHE:CB	3:A:23:HIS:CD2	6	0.14	0.02	0.15
(2,49)	3:A:67:PHE:H	3:A:76:PHE:O	6	0.12	0.01	0.12
(2,123)	3:A:97:CYS:N	3:A:104:LYS:O	6	0.12	0.0	0.12
(1,274)	3:A:7:PHE:CD2	3:A:20:LYS:CA	5	1.32	0.64	1.73
(1,271)	3:A:7:PHE:CE2	3:A:20:LYS:CA	5	1.26	0.58	1.61
(1,304)	3:A:11:TYR:CD2	3:A:14:CYS:CB	5	0.77	0.81	0.12
(1,267)	3:A:7:PHE:CD1	3:A:24:LEU:CD1	5	0.62	0.29	0.63
(1,379)	3:A:37:TYR:CD2	3:A:51:SER:CB	5	0.34	0.26	0.21
(1,404)	3:A:41:PHE:CE2	3:A:44:CYS:CB	5	0.33	0.43	0.12
(1,388)	3:A:39:CYS:CB	3:A:41:PHE:CB	5	0.18	0.05	0.16
(1,262)	3:A:7:PHE:CB	3:A:18:TYR:CB	5	0.15	0.02	0.15
(1,209)	3:A:105:LYS:HA	3:A:97:CYS:H	5	0.13	0.03	0.11
(1,696)	1:B:128:DG:N7	3:A:81:HIS:CB	5	0.13	0.01	0.13
(2,5)	3:A:7:PHE:H	3:A:18:TYR:O	5	0.13	0.02	0.12
(1,659)	3:A:80:ASP:HA	2:C:150:DC:H6	5	0.12	0.01	0.12
(2,105)	3:A:56:ARG:N	3:A:52:ASP:O	5	0.12	0.02	0.11
(1,141)	3:A:75:LYS:HA	3:A:69:CYS:H	5	0.12	0.01	0.11
(1,706)	1:B:129:DG:C5'	3:A:60:ARG:CD	5	0.12	0.02	0.11
(1,338)	3:A:18:TYR:CD2	3:A:27:HIS:CD2	4	0.2	0.14	0.13
(1,535)	3:A:87:ARG:CA	3:A:90:THR:CB	4	0.18	0.02	0.18
(1,715)	1:B:129:DG:C2'	3:A:78:ARG:CZ	4	0.16	0.05	0.14
(1,301)	3:A:11:TYR:CE2	3:A:31:HIS:CB	4	0.14	0.02	0.14
(1,382)	3:A:38:GLN:CA	3:A:47:ARG:CA	4	0.14	0.02	0.13
(1,752)	2:C:147:DA:N6	3:A:52:ASP:CG	4	0.14	0.02	0.14
(1,737)	1:B:132:DC:C5	3:A:50:ARG:CZ	4	0.12	0.01	0.12
(1,762)	2:C:149:DG:N7	3:A:80:ASP:CB	4	0.12	0.01	0.12
(2,43)	3:A:61:HIS:H	3:A:58:GLN:O	4	0.12	0.01	0.12
(1,738)	1:B:132:DC:C6	3:A:50:ARG:CZ	4	0.12	0.0	0.12
(1,408)	3:A:41:PHE:CD2	3:A:44:CYS:CA	3	0.49	0.42	0.2
(1,294)	3:A:11:TYR:CD1	3:A:31:HIS:CB	3	0.48	0.27	0.58
(1,447)	3:A:58:GLN:CA	3:A:61:HIS:CD2	3	0.34	0.03	0.34
(2,90)	3:A:9:CYS:N	3:A:16:LYS:O	3	0.24	0.09	0.2
(1,537)	3:A:87:ARG:CB	3:A:90:THR:CB	3	0.2	0.03	0.21

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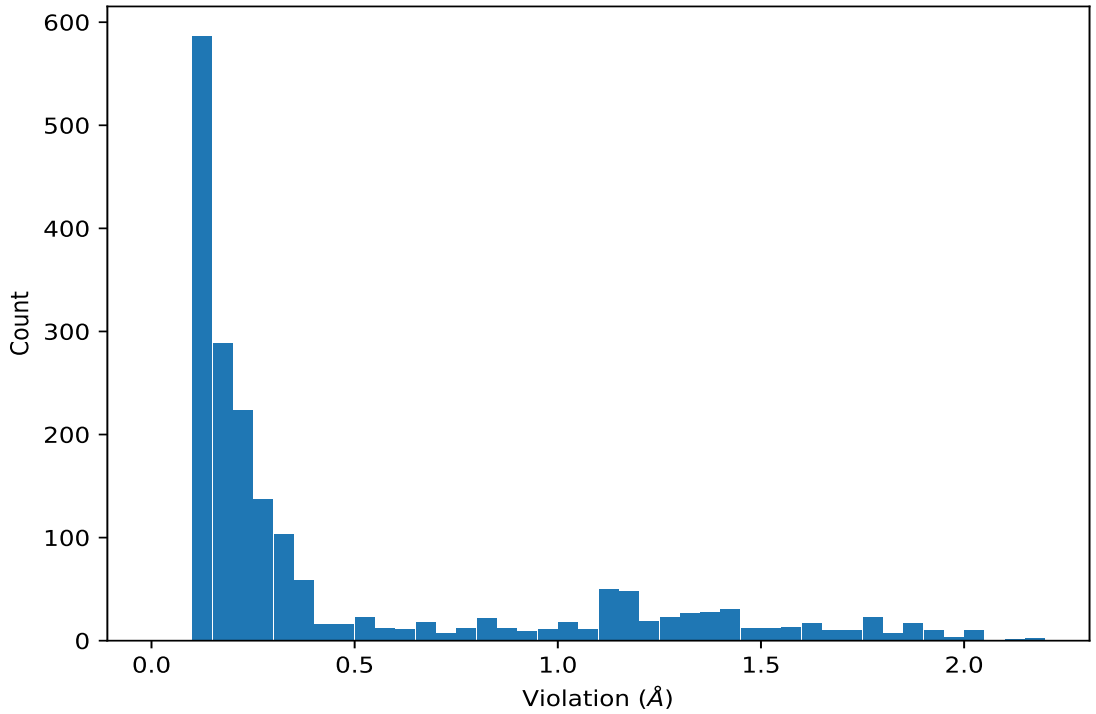
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,93)	3:A:25:GLN:N	3:A:21:LEU:O	3	0.15	0.01	0.15
(1,140)	3:A:68:GLN:HA	3:A:76:PHE:H	3	0.14	0.01	0.14
(1,670)	1:B:126:DC:N4	3:A:108:ARG:CZ	3	0.13	0.02	0.14
(1,13)	3:A:7:PHE:H	3:A:18:TYR:H	3	0.12	0.01	0.12
(1,331)	3:A:18:TYR:CE2	3:A:27:HIS:CB	3	0.12	0.01	0.12
(1,533)	3:A:85:HIS:CE1	3:A:88:THR:CG2	3	0.12	0.0	0.12
(1,442)	3:A:55:LYS:CA	3:A:58:GLN:CA	3	0.11	0.0	0.11
(1,428)	3:A:48:PHE:CE2	3:A:57:HIS:CD2	2	0.83	0.72	0.83
(1,293)	3:A:11:TYR:CD1	3:A:31:HIS:CA	2	0.48	0.08	0.48
(1,307)	3:A:11:TYR:CD2	3:A:31:HIS:CE1	2	0.44	0.05	0.44
(1,710)	1:B:129:DG:C4'	3:A:60:ARG:CZ	2	0.34	0.01	0.34
(1,270)	3:A:7:PHE:CE1	3:A:21:LEU:CD1	2	0.32	0.16	0.32
(1,707)	1:B:129:DG:C5'	3:A:60:ARG:CZ	2	0.26	0.01	0.26
(1,709)	1:B:129:DG:C4'	3:A:60:ARG:CD	2	0.24	0.02	0.24
(1,298)	3:A:11:TYR:CE1	3:A:31:HIS:CB	2	0.16	0.02	0.16
(1,498)	3:A:72:CYS:CB	3:A:89:HIS:CE1	2	0.16	0.05	0.16
(1,651)	3:A:115:HIS:CD2	3:A:119:HIS:CD2	2	0.16	0.02	0.16
(1,691)	1:B:128:DG:C6	3:A:81:HIS:CE1	2	0.15	0.01	0.15
(1,704)	1:B:129:DG:C5'	3:A:60:ARG:CB	2	0.15	0.0	0.15
(1,282)	3:A:9:CYS:CA	3:A:27:HIS:CD2	2	0.14	0.03	0.14
(1,763)	2:C:149:DG:N7	3:A:80:ASP:CG	2	0.14	0.02	0.14
(1,767)	2:C:150:DC:N4	3:A:80:ASP:CB	2	0.14	0.01	0.14
(1,583)	3:A:97:CYS:CB	3:A:116:HIS:CE1	2	0.13	0.01	0.13
(1,680)	1:B:127:DG:C4'	3:A:74:ARG:CZ	2	0.12	0.02	0.12
(1,764)	2:C:149:DG:C8	3:A:80:ASP:CB	2	0.12	0.02	0.12
(2,87)	3:A:119:HIS:H	3:A:116:HIS:O	2	0.12	0.01	0.12
(1,386)	3:A:38:GLN:CB	3:A:47:ARG:CB	2	0.12	0.01	0.12
(1,740)	1:B:133:DG:C5	3:A:50:ARG:CZ	2	0.12	0.01	0.12
(1,200)	3:A:83:LYS:HA	3:A:86:THR:HG21	2	0.12	0.0	0.12
(1,200)	3:A:83:LYS:HA	3:A:86:THR:HG22	2	0.12	0.0	0.12
(1,200)	3:A:83:LYS:HA	3:A:86:THR: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)
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	7	2.2
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	17	2.17
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	15	2.1
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	5	2.05
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	13	2.05
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	1	2.03
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	9	2.02
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	4	2.02
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	10	2.02
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	14	2.02
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	5	2.0
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	13	2.0
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	20	2.0
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	2	1.98
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	3	1.96
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	4	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	1	1.95
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	19	1.95
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	10	1.94
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	20	1.94
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	7	1.93
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	10	1.92
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	6	1.92
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	9	1.92
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	11	1.92
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	14	1.91
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	19	1.9
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	12	1.89
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	16	1.89
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	2	1.89
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	3	1.89
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	3	1.89
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	4	1.88
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	11	1.88
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	11	1.88
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	17	1.88
(1,274)	3:A:7:PHE:CD2	3:A:20:LYS:CA	8	1.88
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	5	1.87
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	12	1.87
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	20	1.87
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	15	1.86
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	18	1.85
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	1	1.85
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	10	1.84
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	17	1.84
(1,374)	3:A:37:TYR:CE2	3:A:50:ARG:CA	8	1.84
(1,374)	3:A:37:TYR:CE2	3:A:50:ARG:CA	18	1.84
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	18	1.83
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	4	1.81
(1,377)	3:A:37:TYR:CD2	3:A:50:ARG:CA	8	1.8
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	13	1.79
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	14	1.79
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	9	1.79
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	6	1.79
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	11	1.78
(1,304)	3:A:11:TYR:CD2	3:A:14:CYS:CB	18	1.78
(1,274)	3:A:7:PHE:CD2	3:A:20:LYS:CA	18	1.78
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	7	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	2	1.77
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	8	1.77
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	14	1.77
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	15	1.77
(1,377)	3:A:37:TYR:CD2	3:A:50:ARG:CA	18	1.77
(1,278)	3:A:8:MET:CA	3:A:18:TYR:CD2	12	1.77
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	2	1.76
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	3	1.75
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	8	1.75
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	9	1.75
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	15	1.75
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	16	1.75
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	19	1.75
(1,304)	3:A:11:TYR:CD2	3:A:14:CYS:CB	17	1.75
(1,271)	3:A:7:PHE:CE2	3:A:20:LYS:CA	18	1.75
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	1	1.74
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	6	1.74
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	12	1.74
(1,432)	3:A:48:PHE:CD2	3:A:54:LEU:CD1	19	1.74
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	13	1.73
(1,274)	3:A:7:PHE:CD2	3:A:20:LYS:CA	4	1.73
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	5	1.72
(1,560)	3:A:95:PHE:CE1	3:A:107:ALA:CA	20	1.71
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	5	1.71
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	17	1.71
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	16	1.7
(1,323)	3:A:18:TYR:CE1	3:A:23:HIS:CE1	7	1.7
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	8	1.68
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	17	1.68
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	3	1.67
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	9	1.67
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	11	1.67
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	13	1.67
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	1	1.66
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	19	1.66
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	6	1.65
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	12	1.65
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	14	1.65
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	15	1.65
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	20	1.65
(1,271)	3:A:7:PHE:CE2	3:A:20:LYS:CA	8	1.65
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	2	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	7	1.64
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	18	1.64
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	5	1.63
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	8	1.63
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	20	1.63
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	4	1.63
(1,554)	3:A:95:PHE:CD1	3:A:106:PHE:CA	10	1.63
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	16	1.62
(1,271)	3:A:7:PHE:CE2	3:A:20:LYS:CA	4	1.61
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	5	1.6
(1,470)	3:A:67:PHE:CE1	3:A:77:SER:CA	19	1.59
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	16	1.59
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	16	1.58
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	3	1.57
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	9	1.57
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	19	1.57
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	3	1.57
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	1	1.56
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	2	1.56
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	10	1.56
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	12	1.56
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	16	1.55
(1,428)	3:A:48:PHE:CE2	3:A:57:HIS:CD2	19	1.55
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	6	1.54
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	12	1.54
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	15	1.53
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	17	1.53
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	7	1.52
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	7	1.52
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	9	1.52
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	13	1.51
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	20	1.51
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	17	1.5
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	1	1.5
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	11	1.5
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	4	1.49
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	10	1.49
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	13	1.49
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	18	1.49
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	12	1.49
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	4	1.49
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	18	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	12	1.48
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	14	1.47
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	4	1.46
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	10	1.46
(1,378)	3:A:37:TYR:CD2	3:A:51:SER:CA	8	1.46
(1,562)	3:A:95:PHE:CE1	3:A:108:ARG:CB	11	1.45
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	13	1.45
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	14	1.45
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	7	1.45
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	19	1.45
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	11	1.44
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	8	1.44
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	5	1.44
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	3	1.43
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	8	1.43
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	17	1.43
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	18	1.43
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	2	1.43
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	11	1.43
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	12	1.43
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	17	1.43
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	2	1.42
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	9	1.42
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	16	1.42
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	19	1.42
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	10	1.42
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	1	1.41
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	5	1.41
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	7	1.41
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	12	1.41
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	15	1.41
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	2	1.41
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	14	1.41
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	4	1.41
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	1	1.41
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	4	1.41
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	6	1.4
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	5	1.4
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	18	1.4
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	6	1.4
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	10	1.4
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	13	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	20	1.4
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	10	1.39
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	17	1.39
(1,377)	3:A:37:TYR:CD2	3:A:50:ARG:CA	7	1.39
(1,377)	3:A:37:TYR:CD2	3:A:50:ARG:CA	20	1.39
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	3	1.39
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	9	1.39
(1,556)	3:A:95:PHE:CD1	3:A:107:ALA:CA	20	1.38
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	19	1.38
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	8	1.38
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	14	1.38
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	4	1.37
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	15	1.37
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	16	1.36
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	8	1.36
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	2	1.36
(1,409)	3:A:41:PHE:CD2	3:A:44:CYS:CB	18	1.36
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	19	1.36
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	1	1.35
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	15	1.35
(1,418)	3:A:48:PHE:CD1	3:A:53:GLN:CB	19	1.35
(1,316)	3:A:18:TYR:CD1	3:A:23:HIS:CD2	15	1.35
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	3	1.34
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	14	1.34
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	10	1.34
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	8	1.33
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	9	1.33
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	11	1.33
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	12	1.33
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	14	1.33
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	2	1.33
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	6	1.33
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	13	1.32
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	17	1.32
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	20	1.32
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	2	1.32
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	5	1.32
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	18	1.32
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	20	1.31
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	4	1.31
(1,374)	3:A:37:TYR:CE2	3:A:50:ARG:CA	20	1.31
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	14	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	2	1.3
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	4	1.3
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	6	1.3
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	15	1.3
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	5	1.3
(1,374)	3:A:37:TYR:CE2	3:A:50:ARG:CA	7	1.3
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	1	1.3
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	14	1.29
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	18	1.29
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	3	1.28
(1,431)	3:A:48:PHE:CD2	3:A:54:LEU:CB	19	1.28
(1,377)	3:A:37:TYR:CD2	3:A:50:ARG:CA	12	1.28
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	12	1.28
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	17	1.27
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	5	1.27
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	3	1.27
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	11	1.27
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	17	1.27
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	8	1.26
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	7	1.26
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	3	1.26
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	15	1.26
(1,377)	3:A:37:TYR:CD2	3:A:50:ARG:CA	17	1.26
(1,374)	3:A:37:TYR:CE2	3:A:50:ARG:CA	17	1.26
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	7	1.26
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	20	1.26
(1,555)	3:A:95:PHE:CD1	3:A:106:PHE:CB	10	1.25
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	1	1.25
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	19	1.25
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	5	1.25
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	3	1.24
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	5	1.24
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	11	1.24
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	15	1.24
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	20	1.23
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	9	1.23
(1,374)	3:A:37:TYR:CE2	3:A:50:ARG:CA	2	1.23
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	12	1.23
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	17	1.23
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	9	1.23
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	5	1.22
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	8	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	20	1.22
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	19	1.22
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	17	1.21
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	3	1.21
(1,420)	3:A:48:PHE:CE1	3:A:53:GLN:CB	19	1.21
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	10	1.21
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	20	1.21
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	4	1.2
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	16	1.2
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	19	1.2
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	12	1.2
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	11	1.2
(1,466)	3:A:67:PHE:CD1	3:A:77:SER:CA	19	1.2
(1,404)	3:A:41:PHE:CE2	3:A:44:CYS:CB	18	1.2
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	3	1.2
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	20	1.19
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	14	1.19
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	2	1.19
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	9	1.19
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	19	1.19
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	7	1.19
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	11	1.19
(1,471)	3:A:67:PHE:CE1	3:A:78:ARG:CA	13	1.19
(1,400)	3:A:41:PHE:CE1	3:A:61:HIS:CA	18	1.19
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	2	1.19
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	13	1.19
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	2	1.18
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	14	1.18
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	13	1.18
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	2	1.18
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	9	1.18
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	1	1.18
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	16	1.18
(1,377)	3:A:37:TYR:CD2	3:A:50:ARG:CA	2	1.18
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	1	1.18
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	15	1.17
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	4	1.17
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	11	1.17
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	15	1.17
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	17	1.17
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	1	1.17
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	6	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	12	1.17
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	15	1.17
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	17	1.17
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	6	1.17
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	6	1.17
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	8	1.16
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	2	1.16
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	6	1.16
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	7	1.16
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	1	1.16
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	20	1.16
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	15	1.16
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	9	1.16
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	1	1.15
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	10	1.15
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	1	1.15
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	9	1.15
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	10	1.15
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	12	1.15
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	18	1.15
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	7	1.15
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	10	1.15
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	10	1.15
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	15	1.15
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	7	1.15
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	19	1.15
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	13	1.15
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	13	1.14
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	18	1.14
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	19	1.14
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	4	1.14
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	18	1.14
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	13	1.14
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	14	1.14
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	14	1.14
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	7	1.13
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	16	1.13
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	19	1.13
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	7	1.13
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	8	1.13
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	16	1.13
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	20	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	13	1.13
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	4	1.13
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	11	1.13
(1,377)	3:A:37:TYR:CD2	3:A:50:ARG:CA	9	1.13
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	5	1.13
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	4	1.13
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	3	1.12
(1,566)	3:A:95:PHE:CE2	3:A:109:SER:CB	5	1.12
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	14	1.12
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	17	1.12
(1,557)	3:A:95:PHE:CD1	3:A:108:ARG:CA	18	1.12
(1,374)	3:A:37:TYR:CE2	3:A:50:ARG:CA	9	1.12
(1,317)	3:A:18:TYR:CD1	3:A:23:HIS:CE1	7	1.12
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	3	1.11
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	5	1.11
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	10	1.11
(1,322)	3:A:18:TYR:CE1	3:A:23:HIS:CD2	15	1.11
(1,561)	3:A:95:PHE:CE1	3:A:108:ARG:CA	11	1.1
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	9	1.1
(1,375)	3:A:37:TYR:CE2	3:A:51:SER:CA	8	1.1
(1,271)	3:A:7:PHE:CE2	3:A:20:LYS:CA	16	1.1
(1,467)	3:A:67:PHE:CD1	3:A:78:ARG:CA	13	1.09
(1,408)	3:A:41:PHE:CD2	3:A:44:CYS:CA	18	1.09
(1,376)	3:A:37:TYR:CE2	3:A:51:SER:CB	8	1.09
(1,378)	3:A:37:TYR:CD2	3:A:51:SER:CA	17	1.08
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	6	1.07
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	4	1.07
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	17	1.07
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	13	1.06
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	7	1.05
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	3	1.05
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	14	1.05
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	1	1.04
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	2	1.04
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	15	1.04
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	18	1.04
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	19	1.04
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	20	1.04
(1,267)	3:A:7:PHE:CD1	3:A:24:LEU:CD1	18	1.04
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	9	1.03
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	9	1.03
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	6	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	8	1.02
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	11	1.02
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	17	1.02
(1,374)	3:A:37:TYR:CE2	3:A:50:ARG:CA	12	1.02
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	11	1.01
(1,569)	3:A:95:PHE:CD2	3:A:112:LEU:CD2	12	1.0
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	7	1.0
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	9	1.0
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	14	0.99
(1,378)	3:A:37:TYR:CD2	3:A:51:SER:CA	7	0.99
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	11	0.99
(1,426)	3:A:48:PHE:CE2	3:A:54:LEU:CD1	19	0.98
(1,425)	3:A:48:PHE:CE2	3:A:54:LEU:CB	19	0.98
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	1	0.98
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	12	0.98
(1,274)	3:A:7:PHE:CD2	3:A:20:LYS:CA	16	0.98
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	13	0.97
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	19	0.97
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	20	0.96
(1,336)	3:A:18:TYR:CD2	3:A:24:LEU:CD2	2	0.93
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	19	0.92
(1,377)	3:A:37:TYR:CD2	3:A:50:ARG:CA	11	0.92
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	11	0.91
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	3	0.91
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	5	0.91
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	18	0.9
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	19	0.9
(1,378)	3:A:37:TYR:CD2	3:A:51:SER:CA	2	0.9
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	14	0.89
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	4	0.89
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	12	0.88
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	13	0.88
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	4	0.88
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	4	0.87
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	10	0.87
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	1	0.86
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	2	0.86
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	6	0.86
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	7	0.86
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	10	0.86
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	3	0.85
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	9	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	15	0.85
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	8	0.85
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	8	0.84
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	18	0.84
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	1	0.84
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	19	0.84
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	19	0.83
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	20	0.83
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	9	0.82
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	15	0.82
(1,379)	3:A:37:TYR:CD2	3:A:51:SER:CB	8	0.82
(1,378)	3:A:37:TYR:CD2	3:A:51:SER:CA	9	0.82
(1,267)	3:A:7:PHE:CD1	3:A:24:LEU:CD1	4	0.82
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	13	0.81
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	5	0.8
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	17	0.8
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	2	0.8
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	7	0.8
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	14	0.8
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	5	0.8
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	12	0.79
(1,401)	3:A:41:PHE:CE1	3:A:61:HIS:CB	18	0.79
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	10	0.79
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	20	0.78
(1,378)	3:A:37:TYR:CD2	3:A:51:SER:CA	20	0.78
(1,568)	3:A:95:PHE:CD2	3:A:109:SER:CB	16	0.77
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	10	0.77
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	17	0.77
(1,378)	3:A:37:TYR:CD2	3:A:51:SER:CA	18	0.76
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	11	0.75
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	4	0.75
(1,294)	3:A:11:TYR:CD1	3:A:31:HIS:CB	17	0.75
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	12	0.74
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	16	0.74
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	19	0.73
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	15	0.73
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	14	0.72
(1,299)	3:A:11:TYR:CE1	3:A:34:GLU:CA	18	0.72
(1,375)	3:A:37:TYR:CE2	3:A:51:SER:CA	7	0.71
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	3	0.7
(1,375)	3:A:37:TYR:CE2	3:A:51:SER:CA	2	0.7
(1,333)	3:A:18:TYR:CE2	3:A:27:HIS:CE1	15	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	17	0.7
(1,477)	3:A:67:PHE:CD2	3:A:79:SER:CB	16	0.69
(1,417)	3:A:48:PHE:CD1	3:A:53:GLN:CA	19	0.69
(1,378)	3:A:37:TYR:CD2	3:A:51:SER:CA	12	0.69
(1,375)	3:A:37:TYR:CE2	3:A:51:SER:CA	17	0.69
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	1	0.69
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	15	0.68
(1,478)	3:A:67:PHE:CD2	3:A:82:LEU:CD1	5	0.67
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	18	0.67
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	3	0.67
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	7	0.67
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	6	0.66
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	9	0.66
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	20	0.65
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	11	0.65
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	11	0.64
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	3	0.63
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	20	0.63
(1,267)	3:A:7:PHE:CD1	3:A:24:LEU:CD1	16	0.63
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	1	0.62
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	7	0.62
(1,376)	3:A:37:TYR:CE2	3:A:51:SER:CB	17	0.62
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	13	0.61
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	15	0.61
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	12	0.61
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	13	0.61
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	2	0.6
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	8	0.6
(1,380)	3:A:37:TYR:CD2	3:A:54:LEU:CB	7	0.6
(1,374)	3:A:37:TYR:CE2	3:A:50:ARG:CA	11	0.6
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	2	0.6
(1,330)	3:A:18:TYR:CE2	3:A:24:LEU:CD2	19	0.6
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	9	0.58
(1,294)	3:A:11:TYR:CD1	3:A:31:HIS:CB	18	0.58
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	13	0.56
(1,293)	3:A:11:TYR:CD1	3:A:31:HIS:CA	17	0.56
(1,434)	3:A:48:PHE:CD2	3:A:57:HIS:CD2	19	0.55
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	2	0.55
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	14	0.54
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	17	0.54
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	1	0.54
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	9	0.54
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	18	0.53
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	4	0.53
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	18	0.53
(1,380)	3:A:37:TYR:CD2	3:A:54:LEU:CB	12	0.53
(1,375)	3:A:37:TYR:CE2	3:A:51:SER:CA	18	0.53
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	4	0.53
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	17	0.52
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	20	0.52
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	15	0.51
(1,411)	3:A:41:PHE:CD2	3:A:61:HIS:CE1	18	0.51
(1,380)	3:A:37:TYR:CD2	3:A:54:LEU:CB	8	0.51
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	14	0.51
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	20	0.5
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	10	0.5
(1,376)	3:A:37:TYR:CE2	3:A:51:SER:CB	7	0.5
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	6	0.5
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	10	0.5
(1,255)	3:A:110:ASP:HA	3:A:113:VAL:HB	11	0.5
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	20	0.49
(1,376)	3:A:37:TYR:CE2	3:A:51:SER:CB	2	0.49
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	15	0.49
(1,307)	3:A:11:TYR:CD2	3:A:31:HIS:CE1	17	0.49
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	2	0.48
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	11	0.48
(1,270)	3:A:7:PHE:CE1	3:A:21:LEU:CD1	18	0.48
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	5	0.47
(1,430)	3:A:48:PHE:CD2	3:A:54:LEU:CA	19	0.47
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	13	0.46
(1,380)	3:A:37:TYR:CD2	3:A:54:LEU:CB	2	0.46
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	17	0.46
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	12	0.46
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	15	0.45
(1,375)	3:A:37:TYR:CE2	3:A:51:SER:CA	9	0.45
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	3	0.45
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	9	0.44
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	17	0.44
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	3	0.44
(1,376)	3:A:37:TYR:CE2	3:A:51:SER:CB	9	0.44
(1,338)	3:A:18:TYR:CD2	3:A:27:HIS:CD2	15	0.44
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	19	0.44
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	7	0.42
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	8	0.42
(1,318)	3:A:18:TYR:CD1	3:A:24:LEU:CA	5	0.42
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	11	0.41
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	2	0.41
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	17	0.41
(1,293)	3:A:11:TYR:CD1	3:A:31:HIS:CA	18	0.41
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	16	0.4
(1,379)	3:A:37:TYR:CD2	3:A:51:SER:CB	17	0.4
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	3	0.39
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	7	0.39
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	13	0.39
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	17	0.39
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	19	0.39
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	3	0.39
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	12	0.39
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	13	0.39
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	4	0.38
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	6	0.38
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	11	0.38
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	12	0.38
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	15	0.38
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	16	0.38
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	19	0.38
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	20	0.38
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	18	0.38
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	8	0.38
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	20	0.38
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	1	0.38
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	8	0.38
(1,447)	3:A:58:GLN:CA	3:A:61:HIS:CD2	12	0.38
(1,375)	3:A:37:TYR:CE2	3:A:51:SER:CA	12	0.38
(1,307)	3:A:11:TYR:CD2	3:A:31:HIS:CE1	18	0.38
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	15	0.37
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	3	0.37
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	5	0.37
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	7	0.37
(2,90)	3:A:9:CYS:N	3:A:16:LYS:O	1	0.37
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	5	0.37
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	8	0.37
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	10	0.37
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	14	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	3	0.37
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	12	0.37
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	14	0.37
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	14	0.37
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	9	0.37
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	11	0.37
(1,375)	3:A:37:TYR:CE2	3:A:51:SER:CA	20	0.37
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	20	0.37
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	19	0.37
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	13	0.36
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	8	0.36
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	9	0.36
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	12	0.36
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	16	0.36
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	17	0.36
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	1	0.36
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	2	0.36
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	9	0.36
(2,125)	3:A:112:LEU:N	3:A:108:ARG:O	18	0.36
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	10	0.36
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	11	0.36
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	15	0.36
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	18	0.36
(1,710)	1:B:129:DG:C4'	3:A:60:ARG:CZ	11	0.36
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	9	0.36
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	17	0.36
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	2	0.35
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	4	0.35
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	5	0.35
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	11	0.35
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	13	0.35
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	15	0.35
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	20	0.35
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	10	0.35
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	5	0.35
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	6	0.35
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	16	0.35
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	7	0.35
(1,4)	3:A:16:LYS:HA	3:A:17:ARG:H	1	0.35
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	15	0.35
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	3	0.35
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	3	0.35
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	8	0.35
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	16	0.35
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	13	0.34
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	2	0.34
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	10	0.34
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	19	0.34
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	1	0.34
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	14	0.34
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	8	0.34
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	3	0.34
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	13	0.34
(1,447)	3:A:58:GLN:CA	3:A:61:HIS:CD2	15	0.34
(1,429)	3:A:48:PHE:CE2	3:A:57:HIS:CE1	19	0.34
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	6	0.34
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	19	0.33
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	11	0.33
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	11	0.33
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	15	0.33
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	13	0.33
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	19	0.33
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	2	0.33
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	5	0.33
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	6	0.33
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	15	0.33
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	19	0.33
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	11	0.33
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	18	0.33
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	5	0.33
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	7	0.33
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	15	0.33
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	20	0.33
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	4	0.33
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	18	0.33
(1,710)	1:B:129:DG:C4'	3:A:60:ARG:CZ	5	0.33
(1,475)	3:A:67:PHE:CE2	3:A:79:SER:CB	16	0.33
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	17	0.33
(1,378)	3:A:37:TYR:CD2	3:A:51:SER:CA	11	0.33
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	4	0.33
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	7	0.33
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	11	0.33
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	19	0.32
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	12	0.32
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	17	0.32
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	1	0.32
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	8	0.32
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	13	0.32
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	16	0.32
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	17	0.32
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	20	0.32
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	1	0.32
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	5	0.32
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	15	0.32
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	16	0.32
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	20	0.32
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	10	0.32
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	12	0.32
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	1	0.32
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	9	0.32
(1,376)	3:A:37:TYR:CE2	3:A:51:SER:CB	20	0.32
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	13	0.32
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	16	0.32
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	20	0.32
(1,267)	3:A:7:PHE:CD1	3:A:24:LEU:CD1	8	0.32
(1,11)	3:A:8:MET:HA	3:A:16:LYS:H	1	0.32
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	10	0.31
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	11	0.31
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	2	0.31
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	10	0.31
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	12	0.31
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	16	0.31
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	4	0.31
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	4	0.31
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	12	0.31
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	2	0.31
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	7	0.31
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	9	0.31
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	17	0.31
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	16	0.31
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	7	0.31
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	9	0.31
(1,407)	3:A:41:PHE:CE2	3:A:61:HIS:CE1	18	0.31
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	9	0.31
(1,143)	3:A:68:GLN:HA	3:A:74:ARG:H	8	0.31
(1,11)	3:A:8:MET:HA	3:A:16:LYS:H	18	0.31
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	12	0.3
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	1	0.3
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	5	0.3
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	17	0.3
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	18	0.3
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	2	0.3
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	11	0.3
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	6	0.3
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	10	0.3
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	14	0.3
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	12	0.3
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	5	0.3
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	2	0.3
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	11	0.3
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	18	0.3
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	19	0.3
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	13	0.3
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	17	0.3
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	6	0.3
(1,577)	3:A:97:CYS:CB	3:A:99:TRP:CB	16	0.3
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	10	0.3
(1,447)	3:A:58:GLN:CA	3:A:61:HIS:CD2	18	0.3
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	18	0.3
(1,333)	3:A:18:TYR:CE2	3:A:27:HIS:CE1	3	0.3
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	5	0.3
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	12	0.3
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	14	0.3
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	15	0.3
(1,11)	3:A:8:MET:HA	3:A:16:LYS:H	3	0.3
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	16	0.29
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	20	0.29
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	3	0.29
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	7	0.29
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	20	0.29
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	9	0.29
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	16	0.29
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	17	0.29
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	18	0.29
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	19	0.29
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	14	0.29
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	10	0.29
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	10	0.29
(1,380)	3:A:37:TYR:CD2	3:A:54:LEU:CB	17	0.29
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	3	0.29
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	5	0.29
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	8	0.29
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	11	0.29
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	14	0.29
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	2	0.29
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	5	0.29
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	13	0.29
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	19	0.29
(1,267)	3:A:7:PHE:CD1	3:A:24:LEU:CD1	5	0.29
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	17	0.28
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	15	0.28
(2,96)	3:A:28:SER:N	3:A:24:LEU:O	6	0.28
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	7	0.28
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	14	0.28
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	7	0.28
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	12	0.28
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	19	0.28
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	6	0.28
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	13	0.28
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	1	0.28
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	6	0.28
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	12	0.28
(1,14)	3:A:21:LEU:H	3:A:22:SER:H	7	0.28
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	5	0.27
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	6	0.27
(2,94)	3:A:26:MET:N	3:A:22:SER:O	17	0.27
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	19	0.27
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	3	0.27
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	14	0.27
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	1	0.27
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	7	0.27
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	8	0.27
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	12	0.27
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	7	0.27
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	8	0.27
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	15	0.27
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	17	0.27
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	8	0.27
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	5	0.27
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	14	0.27
(1,376)	3:A:37:TYR:CE2	3:A:51:SER:CB	18	0.27
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	10	0.27
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	4	0.27
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	3	0.26
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	4	0.26
(2,94)	3:A:26:MET:N	3:A:22:SER:O	7	0.26
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	18	0.26
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	18	0.26
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	3	0.26
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	2	0.26
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	18	0.26
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	18	0.26
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	3	0.26
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	4	0.26
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	17	0.26
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	4	0.26
(1,707)	1:B:129:DG:C5'	3:A:60:ARG:CZ	5	0.26
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	4	0.26
(1,279)	3:A:8:MET:CB	3:A:16:LYS:CA	18	0.26
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	4	0.26
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	10	0.26
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	14	0.26
(1,143)	3:A:68:GLN:HA	3:A:74:ARG:H	4	0.26
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	14	0.25
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	18	0.25
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	9	0.25
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	13	0.25
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	9	0.25
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	10	0.25
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	2	0.25
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	3	0.25
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	10	0.25
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	14	0.25
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	2	0.25
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	18	0.25
(2,103)	3:A:54:LEU:N	3:A:50:ARG:O	2	0.25
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	12	0.25
(1,709)	1:B:129:DG:C4'	3:A:60:ARG:CD	5	0.25
(1,707)	1:B:129:DG:C5'	3:A:60:ARG:CZ	11	0.25
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	5	0.25
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	1	0.25
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	4	0.25
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	3	0.25
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	5	0.25
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	18	0.25
(1,333)	3:A:18:TYR:CE2	3:A:27:HIS:CE1	5	0.25
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	6	0.25
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	1	0.25
(1,299)	3:A:11:TYR:CE1	3:A:34:GLU:CA	19	0.25
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	17	0.25
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	6	0.24
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	13	0.24
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	7	0.24
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	2	0.24
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	6	0.24
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	20	0.24
(2,119)	3:A:87:ARG:N	3:A:84:THR:O	9	0.24
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	2	0.24
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	16	0.24
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	8	0.24
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	9	0.24
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	2	0.24
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	5	0.24
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	14	0.24
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	16	0.24
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	11	0.24
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	4	0.24
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	4	0.24
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	13	0.24
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	18	0.24
(1,388)	3:A:39:CYS:CB	3:A:41:PHE:CB	9	0.24
(1,380)	3:A:37:TYR:CD2	3:A:54:LEU:CB	11	0.24
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	12	0.24
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	17	0.24
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	20	0.24
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	12	0.24
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	4	0.24
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	18	0.24
(1,143)	3:A:68:GLN:HA	3:A:74:ARG:H	6	0.24
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	4	0.23
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	14	0.23
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	3	0.23
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	1	0.23
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	8	0.23
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	1	0.23
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	9	0.23
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	20	0.23
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	10	0.23
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	3	0.23
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	13	0.23
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	11	0.23
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	13	0.23
(1,715)	1:B:129:DG:C2'	3:A:78:ARG:CZ	11	0.23
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	6	0.23
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	5	0.23
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	12	0.23
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	15	0.23
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	20	0.23
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	5	0.23
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	7	0.23
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	7	0.23
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	14	0.23
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	2	0.23
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	8	0.23
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	9	0.23
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	13	0.23
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	15	0.23
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	19	0.23
(1,11)	3:A:8:MET:HA	3:A:16:LYS:H	10	0.23
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	7	0.22
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	8	0.22
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	17	0.22
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	4	0.22
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	18	0.22
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	4	0.22
(2,94)	3:A:26:MET:N	3:A:22:SER:O	10	0.22
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	12	0.22
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	3	0.22
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	20	0.22
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	9	0.22
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	12	0.22
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	11	0.22
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	9	0.22
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	18	0.22
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	4	0.22
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	6	0.22
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	1	0.22
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	2	0.22
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	3	0.22
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	5	0.22
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	6	0.22
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	13	0.22
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	15	0.22
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	12	0.22
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	19	0.22
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	1	0.22
(2,107)	3:A:58:GLN:N	3:A:54:LEU:O	4	0.22
(2,107)	3:A:58:GLN:N	3:A:54:LEU:O	17	0.22
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	6	0.22
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	20	0.22
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	3	0.22
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	1	0.22
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	13	0.22
(1,739)	1:B:133:DG:C6	3:A:50:ARG:CZ	15	0.22
(1,709)	1:B:129:DG:C4'	3:A:60:ARG:CD	11	0.22
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	8	0.22
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	11	0.22
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	9	0.22
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	11	0.22
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	17	0.22
(1,537)	3:A:87:ARG:CB	3:A:90:THR:CB	15	0.22
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	1	0.22
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	9	0.22
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	19	0.22
(1,388)	3:A:39:CYS:CB	3:A:41:PHE:CB	18	0.22
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	1	0.22
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	8	0.22
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	6	0.22
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	9	0.22
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	12	0.22
(1,143)	3:A:68:GLN:HA	3:A:74:ARG:H	7	0.22
(1,11)	3:A:8:MET:HA	3:A:16:LYS:H	7	0.22
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	2	0.21
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	16	0.21
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	1	0.21
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	8	0.21
(2,97)	3:A:29:ARG:N	3:A:26:MET:O	14	0.21
(2,96)	3:A:28:SER:N	3:A:24:LEU:O	17	0.21
(2,94)	3:A:26:MET:N	3:A:22:SER:O	2	0.21
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	4	0.21
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	5	0.21
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	8	0.21
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	9	0.21
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	14	0.21
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	11	0.21
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	13	0.21
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	6	0.21
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	2	0.21
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	4	0.21
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	11	0.21
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	12	0.21
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	13	0.21
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	17	0.21
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	6	0.21
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	10	0.21
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	4	0.21
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	7	0.21
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	15	0.21
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	19	0.21
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	11	0.21
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	16	0.21
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	3	0.21
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	11	0.21
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	20	0.21
(2,114)	3:A:82:LEU:N	3:A:78:ARG:O	4	0.21
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	1	0.21
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	11	0.21
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	1	0.21
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	20	0.21
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	18	0.21
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	10	0.21
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	1	0.21
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	7	0.21
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	13	0.21
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	1	0.21
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	10	0.21
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	2	0.21
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	5	0.21
(1,537)	3:A:87:ARG:CB	3:A:90:THR:CB	6	0.21
(1,498)	3:A:72:CYS:CB	3:A:89:HIS:CE1	1	0.21
(1,379)	3:A:37:TYR:CD2	3:A:51:SER:CB	9	0.21
(1,351)	3:A:22:SER:CA	3:A:24:LEU:CA	19	0.21
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	10	0.21
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	11	0.21
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	13	0.21
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	13	0.21
(1,299)	3:A:11:TYR:CE1	3:A:34:GLU:CA	17	0.21
(1,274)	3:A:7:PHE:CD2	3:A:20:LYS:CA	5	0.21
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	1	0.21
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	6	0.21
(1,143)	3:A:68:GLN:HA	3:A:74:ARG:H	13	0.21
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	1	0.2
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	8	0.2
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	14	0.2
(2,90)	3:A:9:CYS:N	3:A:16:LYS:O	15	0.2
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	2	0.2
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	11	0.2
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	13	0.2
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	15	0.2
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	16	0.2
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	17	0.2
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	8	0.2
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	9	0.2
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	1	0.2
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	10	0.2
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	14	0.2
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	15	0.2
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	12	0.2
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	6	0.2
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	14	0.2
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	1	0.2
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	14	0.2
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	15	0.2
(2,108)	3:A:59:ARG:N	3:A:56:ARG:O	3	0.2
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	7	0.2
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	12	0.2
(1,75)	3:A:47:ARG:HA	3:A:39:CYS:H	12	0.2
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	2	0.2
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	2	0.2
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	6	0.2
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	7	0.2
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	8	0.2
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	15	0.2
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	18	0.2
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	8	0.2
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	16	0.2
(1,484)	3:A:69:CYS:CA	3:A:74:ARG:CA	4	0.2
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	12	0.2
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	2	0.2
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	15	0.2
(1,408)	3:A:41:PHE:CD2	3:A:44:CYS:CA	11	0.2
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	19	0.2
(1,333)	3:A:18:TYR:CE2	3:A:27:HIS:CE1	17	0.2
(1,333)	3:A:18:TYR:CE2	3:A:27:HIS:CE1	19	0.2
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	2	0.2
(1,308)	3:A:11:TYR:CD2	3:A:34:GLU:CB	7	0.2
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	16	0.2
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	20	0.2
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	4	0.2
(2,96)	3:A:28:SER:N	3:A:24:LEU:O	14	0.19
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	6	0.19
(2,94)	3:A:26:MET:N	3:A:22:SER:O	18	0.19
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	6	0.19
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	1	0.19
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	10	0.19
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	20	0.19
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	7	0.19
(2,63)	3:A:88:THR:H	3:A:85:HIS:O	16	0.19
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	5	0.19
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	10	0.19
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	20	0.19
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	10	0.19
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	18	0.19
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	8	0.19
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	9	0.19
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	16	0.19
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	9	0.19
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	14	0.19
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	3	0.19
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	11	0.19
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	16	0.19
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	6	0.19
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	10	0.19
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	5	0.19
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	1	0.19
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	10	0.19
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	9	0.19
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	13	0.19
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	14	0.19
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	11	0.19
(2,107)	3:A:58:GLN:N	3:A:54:LEU:O	8	0.19
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	10	0.19
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	16	0.19
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	3	0.19
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	4	0.19
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	6	0.19
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	10	0.19
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	20	0.19
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	1	0.19
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	4	0.19
(1,719)	1:B:129:DG:C6	3:A:81:HIS:CE1	19	0.19
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	3	0.19
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	3	0.19
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	12	0.19
(1,687)	1:B:128:DG:C2'	3:A:81:HIS:CE1	13	0.19
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	20	0.19
(1,577)	3:A:97:CYS:CB	3:A:99:TRP:CB	9	0.19
(1,535)	3:A:87:ARG:CA	3:A:90:THR:CB	3	0.19
(1,535)	3:A:87:ARG:CA	3:A:90:THR:CB	6	0.19
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	5	0.19
(1,380)	3:A:37:TYR:CD2	3:A:54:LEU:CB	20	0.19
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD1	14	0.19
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD2	14	0.19
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	7	0.19
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	2	0.19
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	4	0.19
(1,300)	3:A:11:TYR:CE1	3:A:34:GLU:CB	18	0.19
(1,298)	3:A:11:TYR:CE1	3:A:31:HIS:CB	17	0.19
(1,271)	3:A:7:PHE:CE2	3:A:20:LYS:CA	5	0.19
(1,262)	3:A:7:PHE:CB	3:A:18:TYR:CB	19	0.19
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	5	0.19
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	1	0.19
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	3	0.19
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	5	0.19
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	9	0.19
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	12	0.19
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	13	0.19
(1,11)	3:A:8:MET:HA	3:A:16:LYS:H	13	0.19
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	7	0.18
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	8	0.18
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	9	0.18
(2,94)	3:A:26:MET:N	3:A:22:SER:O	8	0.18
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	1	0.18
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	2	0.18
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	3	0.18
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	12	0.18
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	16	0.18
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	7	0.18
(2,21)	3:A:31:HIS:H	3:A:28:SER:O	1	0.18
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	5	0.18
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	8	0.18
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	18	0.18
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	18	0.18
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	1	0.18
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	14	0.18
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	20	0.18
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	12	0.18
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	5	0.18
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	16	0.18
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	3	0.18
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	11	0.18
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	4	0.18
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	14	0.18
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	20	0.18
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	4	0.18
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	10	0.18
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	7	0.18
(2,101)	3:A:39:CYS:N	3:A:46:ARG:O	16	0.18
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	17	0.18
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	8	0.18
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	9	0.18
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	15	0.18
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	9	0.18
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	17	0.18
(1,719)	1:B:129:DG:C6	3:A:81:HIS:CE1	16	0.18
(1,715)	1:B:129:DG:C2'	3:A:78:ARG:CZ	5	0.18
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	12	0.18
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	15	0.18
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	2	0.18
(1,651)	3:A:115:HIS:CD2	3:A:119:HIS:CD2	7	0.18
(1,535)	3:A:87:ARG:CA	3:A:90:THR:CB	15	0.18
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	8	0.18
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	17	0.18
(1,452)	3:A:59:ARG:CA	3:A:62:THR:CG2	11	0.18
(1,408)	3:A:41:PHE:CD2	3:A:44:CYS:CA	9	0.18
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	11	0.18
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	13	0.18
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	14	0.18
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	19	0.18
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	20	0.18
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	2	0.18
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	9	0.18
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	9	0.18
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	17	0.18
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	20	0.18
(1,308)	3:A:11:TYR:CD2	3:A:34:GLU:CB	6	0.18
(1,308)	3:A:11:TYR:CD2	3:A:34:GLU:CB	20	0.18
(1,288)	3:A:11:TYR:CA	3:A:31:HIS:CE1	2	0.18
(1,282)	3:A:9:CYS:CA	3:A:27:HIS:CD2	1	0.18
(1,25)	3:A:32:THR:H	3:A:33:GLY:H	7	0.18
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	4	0.18
(1,209)	3:A:105:LYS:HA	3:A:97:CYS:H	10	0.18
(1,143)	3:A:68:GLN:HA	3:A:74:ARG:H	14	0.18
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	10	0.18
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	11	0.18
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	3:A:8:MET:HA	3:A:16:LYS:H	9	0.18
(1,10)	3:A:19:PHE:HA	3:A:7:PHE:H	12	0.18
(2,94)	3:A:26:MET:N	3:A:22:SER:O	9	0.17
(2,93)	3:A:25:GLN:N	3:A:21:LEU:O	6	0.17
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	6	0.17
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	6	0.17
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	15	0.17
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	19	0.17
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	12	0.17
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	11	0.17
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	20	0.17
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	13	0.17
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	18	0.17
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	13	0.17
(2,126)	3:A:113:VAL:N	3:A:109:SER:O	17	0.17
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	2	0.17
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	5	0.17
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	13	0.17
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	15	0.17
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	19	0.17
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	12	0.17
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	15	0.17
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	1	0.17
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	14	0.17
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	6	0.17
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	9	0.17
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	17	0.17
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	6	0.17
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	7	0.17
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	20	0.17
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	14	0.17
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	19	0.17
(2,101)	3:A:39:CYS:N	3:A:46:ARG:O	10	0.17
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	2	0.17
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	17	0.17
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	11	0.17
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	19	0.17
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	20	0.17
(1,75)	3:A:47:ARG:HA	3:A:39:CYS:H	15	0.17
(1,739)	1:B:133:DG:C6	3:A:50:ARG:CZ	12	0.17
(1,719)	1:B:129:DG:C6	3:A:81:HIS:CE1	14	0.17
(1,719)	1:B:129:DG:C6	3:A:81:HIS:CE1	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	10	0.17
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	13	0.17
(1,652)	3:A:115:HIS:CD2	3:A:119:HIS:CE1	14	0.17
(1,502)	3:A:76:PHE:CB	3:A:82:LEU:CD1	2	0.17
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	12	0.17
(1,474)	3:A:67:PHE:CE2	3:A:79:SER:CA	16	0.17
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	4	0.17
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	11	0.17
(1,452)	3:A:59:ARG:CA	3:A:62:THR:CG2	7	0.17
(1,382)	3:A:38:GLN:CA	3:A:47:ARG:CA	12	0.17
(1,368)	3:A:31:HIS:CB	3:A:34:GLU:CB	3	0.17
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	2	0.17
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	10	0.17
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	6	0.17
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	14	0.17
(1,333)	3:A:18:TYR:CE2	3:A:27:HIS:CE1	10	0.17
(1,333)	3:A:18:TYR:CE2	3:A:27:HIS:CE1	12	0.17
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	20	0.17
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	7	0.17
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	11	0.17
(1,288)	3:A:11:TYR:CA	3:A:31:HIS:CE1	4	0.17
(1,288)	3:A:11:TYR:CA	3:A:31:HIS:CE1	12	0.17
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	2	0.17
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	7	0.17
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	11	0.17
(1,210)	3:A:107:ALA:HA	3:A:95:PHE:H	7	0.17
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	20	0.17
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	20	0.16
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	2	0.16
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	4	0.16
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	9	0.16
(2,5)	3:A:7:PHE:H	3:A:18:TYR:O	12	0.16
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	2	0.16
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	11	0.16
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	15	0.16
(2,21)	3:A:31:HIS:H	3:A:28:SER:O	13	0.16
(2,21)	3:A:31:HIS:H	3:A:28:SER:O	18	0.16
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	3	0.16
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	7	0.16
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	13	0.16
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	20	0.16
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	7	0.16
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	15	0.16
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	2	0.16
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	14	0.16
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	20	0.16
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	17	0.16
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	18	0.16
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	18	0.16
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	4	0.16
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	10	0.16
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	11	0.16
(2,107)	3:A:58:GLN:N	3:A:54:LEU:O	1	0.16
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	9	0.16
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	15	0.16
(2,101)	3:A:39:CYS:N	3:A:46:ARG:O	7	0.16
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	10	0.16
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	11	0.16
(1,763)	2:C:149:DG:N7	3:A:80:ASP:CG	5	0.16
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	2	0.16
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	6	0.16
(1,739)	1:B:133:DG:C6	3:A:50:ARG:CZ	2	0.16
(1,739)	1:B:133:DG:C6	3:A:50:ARG:CZ	6	0.16
(1,691)	1:B:128:DG:C6	3:A:81:HIS:CE1	4	0.16
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	6	0.16
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	10	0.16
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	12	0.16
(1,537)	3:A:87:ARG:CB	3:A:90:THR:CB	3	0.16
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	5	0.16
(1,448)	3:A:58:GLN:CA	3:A:62:THR:CG2	15	0.16
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	3	0.16
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	5	0.16
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	9	0.16
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	10	0.16
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	13	0.16
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	16	0.16
(1,388)	3:A:39:CYS:CB	3:A:41:PHE:CB	12	0.16
(1,380)	3:A:37:TYR:CD2	3:A:54:LEU:CB	9	0.16
(1,379)	3:A:37:TYR:CD2	3:A:51:SER:CB	7	0.16
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD1	4	0.16
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD2	4	0.16
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD1	10	0.16
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD2	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	4	0.16
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	13	0.16
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	15	0.16
(1,347)	3:A:20:LYS:CB	3:A:23:HIS:CB	16	0.16
(1,341)	3:A:19:PHE:CB	3:A:23:HIS:CD2	7	0.16
(1,341)	3:A:19:PHE:CB	3:A:23:HIS:CD2	16	0.16
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	11	0.16
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	1	0.16
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	12	0.16
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	14	0.16
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	15	0.16
(1,308)	3:A:11:TYR:CD2	3:A:34:GLU:CB	13	0.16
(1,270)	3:A:7:PHE:CE1	3:A:21:LEU:CD1	5	0.16
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	6	0.16
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	19	0.16
(1,209)	3:A:105:LYS:HA	3:A:97:CYS:H	17	0.16
(1,208)	3:A:96:SER:HA	3:A:106:PHE:H	1	0.16
(1,143)	3:A:68:GLN:HA	3:A:74:ARG:H	9	0.16
(1,143)	3:A:68:GLN:HA	3:A:74:ARG:H	10	0.16
(1,143)	3:A:68:GLN:HA	3:A:74:ARG:H	11	0.16
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	6	0.16
(1,11)	3:A:8:MET:HA	3:A:16:LYS:H	5	0.16
(1,10)	3:A:19:PHE:HA	3:A:7:PHE:H	3	0.16
(2,94)	3:A:26:MET:N	3:A:22:SER:O	16	0.15
(2,93)	3:A:25:GLN:N	3:A:21:LEU:O	19	0.15
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	17	0.15
(2,90)	3:A:9:CYS:N	3:A:16:LYS:O	10	0.15
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	12	0.15
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	19	0.15
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	4	0.15
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	13	0.15
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	17	0.15
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	1	0.15
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	13	0.15
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	14	0.15
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	16	0.15
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	18	0.15
(2,19)	3:A:30:LYS:H	3:A:27:HIS:O	16	0.15
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	9	0.15
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	16	0.15
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	17	0.15
(2,132)	3:A:119:HIS:N	3:A:116:HIS:O	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	7	0.15
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	4	0.15
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	5	0.15
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	12	0.15
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	5	0.15
(2,129)	3:A:116:HIS:N	3:A:112:LEU:O	17	0.15
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	5	0.15
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	16	0.15
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	20	0.15
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	20	0.15
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	9	0.15
(2,107)	3:A:58:GLN:N	3:A:54:LEU:O	9	0.15
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	3	0.15
(2,105)	3:A:56:ARG:N	3:A:52:ASP:O	2	0.15
(2,101)	3:A:39:CYS:N	3:A:46:ARG:O	4	0.15
(2,101)	3:A:39:CYS:N	3:A:46:ARG:O	13	0.15
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	19	0.15
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	15	0.15
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	19	0.15
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	8	0.15
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	18	0.15
(1,758)	2:C:147:DA:C8	3:A:52:ASP:CB	1	0.15
(1,752)	2:C:147:DA:N6	3:A:52:ASP:CG	2	0.15
(1,75)	3:A:47:ARG:HA	3:A:39:CYS:H	3	0.15
(1,75)	3:A:47:ARG:HA	3:A:39:CYS:H	19	0.15
(1,739)	1:B:133:DG:C6	3:A:50:ARG:CZ	18	0.15
(1,719)	1:B:129:DG:C6	3:A:81:HIS:CE1	4	0.15
(1,719)	1:B:129:DG:C6	3:A:81:HIS:CE1	17	0.15
(1,706)	1:B:129:DG:C5'	3:A:60:ARG:CD	20	0.15
(1,704)	1:B:129:DG:C5'	3:A:60:ARG:CB	11	0.15
(1,696)	1:B:128:DG:N7	3:A:81:HIS:CB	1	0.15
(1,694)	1:B:128:DG:C5	3:A:81:HIS:CD2	18	0.15
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	1	0.15
(1,670)	1:B:126:DC:N4	3:A:108:ARG:CZ	5	0.15
(1,577)	3:A:97:CYS:CB	3:A:99:TRP:CB	3	0.15
(1,577)	3:A:97:CYS:CB	3:A:99:TRP:CB	10	0.15
(1,484)	3:A:69:CYS:CA	3:A:74:ARG:CA	18	0.15
(1,476)	3:A:67:PHE:CD2	3:A:79:SER:CA	16	0.15
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	7	0.15
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	14	0.15
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	1	0.15
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	3:A:39:CYS:CB	3:A:41:PHE:CB	15	0.15
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD1	1	0.15
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD2	1	0.15
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD1	9	0.15
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD2	9	0.15
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	1	0.15
(1,345)	3:A:20:LYS:CA	3:A:23:HIS:CE1	16	0.15
(1,341)	3:A:19:PHE:CB	3:A:23:HIS:CD2	15	0.15
(1,338)	3:A:18:TYR:CD2	3:A:27:HIS:CD2	17	0.15
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	13	0.15
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	12	0.15
(1,308)	3:A:11:TYR:CD2	3:A:34:GLU:CB	16	0.15
(1,301)	3:A:11:TYR:CE2	3:A:31:HIS:CB	2	0.15
(1,301)	3:A:11:TYR:CE2	3:A:31:HIS:CB	9	0.15
(1,288)	3:A:11:TYR:CA	3:A:31:HIS:CE1	13	0.15
(1,262)	3:A:7:PHE:CB	3:A:18:TYR:CB	8	0.15
(1,262)	3:A:7:PHE:CB	3:A:18:TYR:CB	17	0.15
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	20	0.15
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	14	0.15
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	18	0.15
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	19	0.15
(1,140)	3:A:68:GLN:HA	3:A:76:PHE:H	14	0.15
(2,96)	3:A:28:SER:N	3:A:24:LEU:O	4	0.14
(2,95)	3:A:27:HIS:N	3:A:23:HIS:O	20	0.14
(2,93)	3:A:25:GLN:N	3:A:21:LEU:O	12	0.14
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	3	0.14
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	13	0.14
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	18	0.14
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	11	0.14
(2,61)	3:A:87:ARG:H	3:A:84:THR:O	14	0.14
(2,49)	3:A:67:PHE:H	3:A:76:PHE:O	12	0.14
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	4	0.14
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	6	0.14
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	17	0.14
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	19	0.14
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	20	0.14
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	1	0.14
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	8	0.14
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	15	0.14
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	16	0.14
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	17	0.14
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	15	0.14
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	4	0.14
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	12	0.14
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	11	0.14
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	12	0.14
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	5	0.14
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	8	0.14
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	2	0.14
(2,109)	3:A:60:ARG:N	3:A:57:HIS:O	17	0.14
(2,107)	3:A:58:GLN:N	3:A:54:LEU:O	19	0.14
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	5	0.14
(2,101)	3:A:39:CYS:N	3:A:46:ARG:O	19	0.14
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	5	0.14
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	19	0.14
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	20	0.14
(1,77)	3:A:38:GLN:HA	3:A:46:ARG:H	14	0.14
(1,767)	2:C:150:DC:N4	3:A:80:ASP:CB	20	0.14
(1,764)	2:C:149:DG:C8	3:A:80:ASP:CB	5	0.14
(1,762)	2:C:149:DG:N7	3:A:80:ASP:CB	7	0.14
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	12	0.14
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	16	0.14
(1,752)	2:C:147:DA:N6	3:A:52:ASP:CG	1	0.14
(1,752)	2:C:147:DA:N6	3:A:52:ASP:CG	4	0.14
(1,75)	3:A:47:ARG:HA	3:A:39:CYS:H	8	0.14
(1,75)	3:A:47:ARG:HA	3:A:39:CYS:H	9	0.14
(1,75)	3:A:47:ARG:HA	3:A:39:CYS:H	18	0.14
(1,739)	1:B:133:DG:C6	3:A:50:ARG:CZ	14	0.14
(1,737)	1:B:132:DC:C5	3:A:50:ARG:CZ	11	0.14
(1,727)	1:B:130:DG:C6	3:A:78:ARG:CZ	20	0.14
(1,704)	1:B:129:DG:C5'	3:A:60:ARG:CB	5	0.14
(1,696)	1:B:128:DG:N7	3:A:81:HIS:CB	2	0.14
(1,691)	1:B:128:DG:C6	3:A:81:HIS:CE1	9	0.14
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	8	0.14
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	13	0.14
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	15	0.14
(1,680)	1:B:127:DG:C4'	3:A:74:ARG:CZ	15	0.14
(1,670)	1:B:126:DC:N4	3:A:108:ARG:CZ	8	0.14
(1,660)	3:A:84:THR:HG21	1:B:126:DC:H6	18	0.14
(1,660)	3:A:84:THR:HG22	1:B:126:DC:H6	18	0.14
(1,660)	3:A:84:THR:HG23	1:B:126:DC:H6	18	0.14
(1,659)	3:A:80:ASP:HA	2:C:150:DC:H6	13	0.14
(1,651)	3:A:115:HIS:CD2	3:A:119:HIS:CD2	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	15	0.14
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	17	0.14
(1,583)	3:A:97:CYS:CB	3:A:116:HIS:CE1	6	0.14
(1,535)	3:A:87:ARG:CA	3:A:90:THR:CB	18	0.14
(1,502)	3:A:76:PHE:CB	3:A:82:LEU:CD1	15	0.14
(1,497)	3:A:72:CYS:CB	3:A:74:ARG:CB	7	0.14
(1,484)	3:A:69:CYS:CA	3:A:74:ARG:CA	12	0.14
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	3	0.14
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	10	0.14
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	4	0.14
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	6	0.14
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	8	0.14
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	17	0.14
(1,382)	3:A:38:GLN:CA	3:A:47:ARG:CA	2	0.14
(1,377)	3:A:37:TYR:CD2	3:A:50:ARG:CA	13	0.14
(1,373)	3:A:37:TYR:CD1	3:A:54:LEU:CD2	13	0.14
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	7	0.14
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	16	0.14
(1,354)	3:A:22:SER:CB	3:A:25:GLN:CB	12	0.14
(1,341)	3:A:19:PHE:CB	3:A:23:HIS:CD2	14	0.14
(1,341)	3:A:19:PHE:CB	3:A:23:HIS:CD2	20	0.14
(1,333)	3:A:18:TYR:CE2	3:A:27:HIS:CE1	11	0.14
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	3	0.14
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	5	0.14
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	6	0.14
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	10	0.14
(1,308)	3:A:11:TYR:CD2	3:A:34:GLU:CB	4	0.14
(1,299)	3:A:11:TYR:CE1	3:A:34:GLU:CA	13	0.14
(1,299)	3:A:11:TYR:CE1	3:A:34:GLU:CA	15	0.14
(1,298)	3:A:11:TYR:CE1	3:A:31:HIS:CB	18	0.14
(1,288)	3:A:11:TYR:CA	3:A:31:HIS:CE1	3	0.14
(1,272)	3:A:7:PHE:CE2	3:A:21:LEU:CA	4	0.14
(1,269)	3:A:7:PHE:CE1	3:A:21:LEU:CB	5	0.14
(1,262)	3:A:7:PHE:CB	3:A:18:TYR:CB	15	0.14
(1,262)	3:A:7:PHE:CB	3:A:18:TYR:CB	18	0.14
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	1	0.14
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	9	0.14
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	15	0.14
(1,208)	3:A:96:SER:HA	3:A:106:PHE:H	4	0.14
(1,143)	3:A:68:GLN:HA	3:A:74:ARG:H	5	0.14
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	2	0.14
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	8	0.14
(1,141)	3:A:75:LYS:HA	3:A:69:CYS:H	6	0.14
(1,140)	3:A:68:GLN:HA	3:A:76:PHE:H	5	0.14
(1,13)	3:A:7:PHE:H	3:A:18:TYR:H	6	0.14
(1,11)	3:A:8:MET:HA	3:A:16:LYS:H	2	0.14
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	6	0.13
(2,94)	3:A:26:MET:N	3:A:22:SER:O	20	0.13
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	5	0.13
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	8	0.13
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	15	0.13
(2,87)	3:A:119:HIS:H	3:A:116:HIS:O	10	0.13
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	5	0.13
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	13	0.13
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	20	0.13
(2,5)	3:A:7:PHE:H	3:A:18:TYR:O	6	0.13
(2,49)	3:A:67:PHE:H	3:A:76:PHE:O	10	0.13
(2,43)	3:A:61:HIS:H	3:A:58:GLN:O	4	0.13
(2,43)	3:A:61:HIS:H	3:A:58:GLN:O	8	0.13
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	8	0.13
(2,21)	3:A:31:HIS:H	3:A:28:SER:O	4	0.13
(2,19)	3:A:30:LYS:H	3:A:27:HIS:O	1	0.13
(2,19)	3:A:30:LYS:H	3:A:27:HIS:O	2	0.13
(2,19)	3:A:30:LYS:H	3:A:27:HIS:O	5	0.13
(2,19)	3:A:30:LYS:H	3:A:27:HIS:O	6	0.13
(2,19)	3:A:30:LYS:H	3:A:27:HIS:O	11	0.13
(2,19)	3:A:30:LYS:H	3:A:27:HIS:O	15	0.13
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	2	0.13
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	19	0.13
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	1	0.13
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	4	0.13
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	9	0.13
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	19	0.13
(2,123)	3:A:97:CYS:N	3:A:104:LYS:O	2	0.13
(2,123)	3:A:97:CYS:N	3:A:104:LYS:O	14	0.13
(2,121)	3:A:89:HIS:N	3:A:86:THR:O	15	0.13
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	7	0.13
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	8	0.13
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	9	0.13
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	10	0.13
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	16	0.13
(2,107)	3:A:58:GLN:N	3:A:54:LEU:O	6	0.13
(2,107)	3:A:58:GLN:N	3:A:54:LEU:O	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	8	0.13
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	10	0.13
(2,105)	3:A:56:ARG:N	3:A:52:ASP:O	3	0.13
(2,101)	3:A:39:CYS:N	3:A:46:ARG:O	11	0.13
(2,101)	3:A:39:CYS:N	3:A:46:ARG:O	14	0.13
(2,101)	3:A:39:CYS:N	3:A:46:ARG:O	20	0.13
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	1	0.13
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	2	0.13
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	4	0.13
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	8	0.13
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	12	0.13
(1,767)	2:C:150:DC:N4	3:A:80:ASP:CB	17	0.13
(1,762)	2:C:149:DG:N7	3:A:80:ASP:CB	17	0.13
(1,740)	1:B:133:DG:C5	3:A:50:ARG:CZ	15	0.13
(1,739)	1:B:133:DG:C6	3:A:50:ARG:CZ	9	0.13
(1,737)	1:B:132:DC:C5	3:A:50:ARG:CZ	13	0.13
(1,719)	1:B:129:DG:C6	3:A:81:HIS:CE1	9	0.13
(1,696)	1:B:128:DG:N7	3:A:81:HIS:CB	7	0.13
(1,696)	1:B:128:DG:N7	3:A:81:HIS:CB	13	0.13
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	3	0.13
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	5	0.13
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	11	0.13
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	18	0.13
(1,659)	3:A:80:ASP:HA	2:C:150:DC:H6	18	0.13
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	1	0.13
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	3	0.13
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	5	0.13
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	7	0.13
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	9	0.13
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	12	0.13
(1,577)	3:A:97:CYS:CB	3:A:99:TRP:CB	18	0.13
(1,577)	3:A:97:CYS:CB	3:A:99:TRP:CB	19	0.13
(1,502)	3:A:76:PHE:CB	3:A:82:LEU:CD1	8	0.13
(1,484)	3:A:69:CYS:CA	3:A:74:ARG:CA	3	0.13
(1,484)	3:A:69:CYS:CA	3:A:74:ARG:CA	10	0.13
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	6	0.13
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	12	0.13
(1,452)	3:A:59:ARG:CA	3:A:62:THR:CG2	1	0.13
(1,452)	3:A:59:ARG:CA	3:A:62:THR:CG2	10	0.13
(1,452)	3:A:59:ARG:CA	3:A:62:THR:CG2	12	0.13
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	14	0.13
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,404)	3:A:41:PHE:CE2	3:A:44:CYS:CB	15	0.13
(1,396)	3:A:41:PHE:CB	3:A:61:HIS:CE1	12	0.13
(1,395)	3:A:41:PHE:CB	3:A:61:HIS:CD2	11	0.13
(1,386)	3:A:38:GLN:CB	3:A:47:ARG:CB	14	0.13
(1,380)	3:A:37:TYR:CD2	3:A:54:LEU:CB	15	0.13
(1,379)	3:A:37:TYR:CD2	3:A:51:SER:CB	20	0.13
(1,376)	3:A:37:TYR:CE2	3:A:51:SER:CB	12	0.13
(1,366)	3:A:29:ARG:CB	3:A:32:THR:CG2	6	0.13
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	9	0.13
(1,331)	3:A:18:TYR:CE2	3:A:27:HIS:CB	8	0.13
(1,329)	3:A:18:TYR:CE2	3:A:24:LEU:CB	1	0.13
(1,328)	3:A:18:TYR:CE2	3:A:24:LEU:CA	18	0.13
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	20	0.13
(1,311)	3:A:18:TYR:CA	3:A:24:LEU:CB	16	0.13
(1,308)	3:A:11:TYR:CD2	3:A:34:GLU:CB	14	0.13
(1,301)	3:A:11:TYR:CE2	3:A:31:HIS:CB	13	0.13
(1,268)	3:A:7:PHE:CE1	3:A:21:LEU:CA	10	0.13
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	3	0.13
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	18	0.13
(1,208)	3:A:96:SER:HA	3:A:106:PHE:H	11	0.13
(1,208)	3:A:96:SER:HA	3:A:106:PHE:H	18	0.13
(1,208)	3:A:96:SER:HA	3:A:106:PHE:H	19	0.13
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG21	1	0.13
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG22	1	0.13
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG23	1	0.13
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG21	10	0.13
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG22	10	0.13
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG23	10	0.13
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG21	13	0.13
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG22	13	0.13
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG23	13	0.13
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG21	15	0.13
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG22	15	0.13
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG23	15	0.13
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	15	0.13
(1,10)	3:A:19:PHE:HA	3:A:7:PHE:H	13	0.13
(1,10)	3:A:19:PHE:HA	3:A:7:PHE:H	20	0.13
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	11	0.12
(2,98)	3:A:30:LYS:N	3:A:27:HIS:O	18	0.12
(2,96)	3:A:28:SER:N	3:A:24:LEU:O	3	0.12
(2,96)	3:A:28:SER:N	3:A:24:LEU:O	12	0.12
(2,96)	3:A:28:SER:N	3:A:24:LEU:O	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	3:A:26:MET:N	3:A:22:SER:O	1	0.12
(2,94)	3:A:26:MET:N	3:A:22:SER:O	15	0.12
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	14	0.12
(2,87)	3:A:119:HIS:H	3:A:116:HIS:O	14	0.12
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	7	0.12
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	4	0.12
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	7	0.12
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	13	0.12
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	14	0.12
(2,7)	3:A:24:LEU:H	3:A:20:LYS:O	5	0.12
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	8	0.12
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	9	0.12
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	10	0.12
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	16	0.12
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	17	0.12
(2,5)	3:A:7:PHE:H	3:A:18:TYR:O	13	0.12
(2,49)	3:A:67:PHE:H	3:A:76:PHE:O	7	0.12
(2,49)	3:A:67:PHE:H	3:A:76:PHE:O	14	0.12
(2,49)	3:A:67:PHE:H	3:A:76:PHE:O	16	0.12
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	9	0.12
(2,3)	3:A:9:CYS:H	3:A:16:LYS:O	1	0.12
(2,21)	3:A:31:HIS:H	3:A:28:SER:O	2	0.12
(2,21)	3:A:31:HIS:H	3:A:28:SER:O	17	0.12
(2,19)	3:A:30:LYS:H	3:A:27:HIS:O	4	0.12
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	10	0.12
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	12	0.12
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	19	0.12
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	19	0.12
(2,130)	3:A:117:ASN:N	3:A:114:ARG:O	11	0.12
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	7	0.12
(2,123)	3:A:97:CYS:N	3:A:104:LYS:O	8	0.12
(2,123)	3:A:97:CYS:N	3:A:104:LYS:O	10	0.12
(2,123)	3:A:97:CYS:N	3:A:104:LYS:O	17	0.12
(2,123)	3:A:97:CYS:N	3:A:104:LYS:O	20	0.12
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	16	0.12
(2,116)	3:A:84:THR:N	3:A:80:ASP:O	17	0.12
(2,115)	3:A:83:LYS:N	3:A:79:SER:O	19	0.12
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	6	0.12
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	3	0.12
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	12	0.12
(2,101)	3:A:39:CYS:N	3:A:46:ARG:O	5	0.12
(2,101)	3:A:39:CYS:N	3:A:46:ARG:O	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	17	0.12
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	18	0.12
(1,783)	3:A:108:ARG:CD	1:B:126:DC:C2'	18	0.12
(1,762)	2:C:149:DG:N7	3:A:80:ASP:CB	2	0.12
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	13	0.12
(1,743)	1:B:134:DT:C4	3:A:50:ARG:CZ	11	0.12
(1,739)	1:B:133:DG:C6	3:A:50:ARG:CZ	16	0.12
(1,739)	1:B:133:DG:C6	3:A:50:ARG:CZ	20	0.12
(1,738)	1:B:132:DC:C6	3:A:50:ARG:CZ	4	0.12
(1,738)	1:B:132:DC:C6	3:A:50:ARG:CZ	17	0.12
(1,737)	1:B:132:DC:C5	3:A:50:ARG:CZ	1	0.12
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	7	0.12
(1,688)	1:B:128:DG:C1'	3:A:81:HIS:CE1	19	0.12
(1,659)	3:A:80:ASP:HA	2:C:150:DC:H6	10	0.12
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	2	0.12
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	4	0.12
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	6	0.12
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	8	0.12
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	10	0.12
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	13	0.12
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	16	0.12
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	18	0.12
(1,583)	3:A:97:CYS:CB	3:A:116:HIS:CE1	3	0.12
(1,577)	3:A:97:CYS:CB	3:A:99:TRP:CB	8	0.12
(1,577)	3:A:97:CYS:CB	3:A:99:TRP:CB	15	0.12
(1,577)	3:A:97:CYS:CB	3:A:99:TRP:CB	17	0.12
(1,536)	3:A:87:ARG:CA	3:A:90:THR:CG2	10	0.12
(1,533)	3:A:85:HIS:CE1	3:A:88:THR:CG2	11	0.12
(1,533)	3:A:85:HIS:CE1	3:A:88:THR:CG2	18	0.12
(1,533)	3:A:85:HIS:CE1	3:A:88:THR:CG2	20	0.12
(1,502)	3:A:76:PHE:CB	3:A:82:LEU:CD1	9	0.12
(1,502)	3:A:76:PHE:CB	3:A:82:LEU:CD1	17	0.12
(1,502)	3:A:76:PHE:CB	3:A:82:LEU:CD1	20	0.12
(1,484)	3:A:69:CYS:CA	3:A:74:ARG:CA	8	0.12
(1,452)	3:A:59:ARG:CA	3:A:62:THR:CG2	16	0.12
(1,442)	3:A:55:LYS:CA	3:A:58:GLN:CA	17	0.12
(1,404)	3:A:41:PHE:CE2	3:A:44:CYS:CB	20	0.12
(1,382)	3:A:38:GLN:CA	3:A:47:ARG:CA	11	0.12
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD1	15	0.12
(1,372)	3:A:37:TYR:CB	3:A:54:LEU:CD2	15	0.12
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	6	0.12
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,331)	3:A:18:TYR:CE2	3:A:27:HIS:CB	18	0.12
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	7	0.12
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	11	0.12
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	17	0.12
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	8	0.12
(1,308)	3:A:11:TYR:CD2	3:A:34:GLU:CB	11	0.12
(1,308)	3:A:11:TYR:CD2	3:A:34:GLU:CB	12	0.12
(1,308)	3:A:11:TYR:CD2	3:A:34:GLU:CB	15	0.12
(1,304)	3:A:11:TYR:CD2	3:A:14:CYS:CB	8	0.12
(1,273)	3:A:7:PHE:CE2	3:A:21:LEU:CB	10	0.12
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	10	0.12
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	14	0.12
(1,208)	3:A:96:SER:HA	3:A:106:PHE:H	13	0.12
(1,200)	3:A:83:LYS:HA	3:A:86:THR:HG21	13	0.12
(1,200)	3:A:83:LYS:HA	3:A:86:THR:HG22	13	0.12
(1,200)	3:A:83:LYS:HA	3:A:86:THR:HG23	13	0.12
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG21	6	0.12
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG22	6	0.12
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG23	6	0.12
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG21	18	0.12
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG22	18	0.12
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG23	18	0.12
(1,143)	3:A:68:GLN:HA	3:A:74:ARG:H	12	0.12
(1,141)	3:A:75:LYS:HA	3:A:69:CYS:H	16	0.12
(1,140)	3:A:68:GLN:HA	3:A:76:PHE:H	6	0.12
(1,13)	3:A:7:PHE:H	3:A:18:TYR:H	4	0.12
(1,10)	3:A:19:PHE:HA	3:A:7:PHE:H	17	0.12
(2,99)	3:A:31:HIS:N	3:A:28:SER:O	12	0.11
(2,96)	3:A:28:SER:N	3:A:24:LEU:O	9	0.11
(2,94)	3:A:26:MET:N	3:A:22:SER:O	13	0.11
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	1	0.11
(2,92)	3:A:24:LEU:N	3:A:20:LYS:O	12	0.11
(2,83)	3:A:117:ASN:H	3:A:114:ARG:O	19	0.11
(2,79)	3:A:115:HIS:H	3:A:111:GLU:O	3	0.11
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	3	0.11
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	6	0.11
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	8	0.11
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	11	0.11
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	12	0.11
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	15	0.11
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	16	0.11
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	19	0.11
(2,73)	3:A:112:LEU:H	3:A:108:ARG:O	20	0.11
(2,65)	3:A:89:HIS:H	3:A:86:THR:O	18	0.11
(2,5)	3:A:7:PHE:H	3:A:18:TYR:O	11	0.11
(2,5)	3:A:7:PHE:H	3:A:18:TYR:O	20	0.11
(2,49)	3:A:67:PHE:H	3:A:76:PHE:O	3	0.11
(2,43)	3:A:61:HIS:H	3:A:58:GLN:O	1	0.11
(2,43)	3:A:61:HIS:H	3:A:58:GLN:O	17	0.11
(2,39)	3:A:59:ARG:H	3:A:56:ARG:O	5	0.11
(2,21)	3:A:31:HIS:H	3:A:28:SER:O	9	0.11
(2,19)	3:A:30:LYS:H	3:A:27:HIS:O	3	0.11
(2,19)	3:A:30:LYS:H	3:A:27:HIS:O	9	0.11
(2,19)	3:A:30:LYS:H	3:A:27:HIS:O	13	0.11
(2,19)	3:A:30:LYS:H	3:A:27:HIS:O	19	0.11
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	6	0.11
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	14	0.11
(2,17)	3:A:29:ARG:H	3:A:26:MET:O	15	0.11
(2,15)	3:A:28:SER:H	3:A:24:LEU:O	16	0.11
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	3	0.11
(2,131)	3:A:118:MET:N	3:A:115:HIS:O	18	0.11
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	8	0.11
(2,128)	3:A:115:HIS:N	3:A:111:GLU:O	17	0.11
(2,127)	3:A:114:ARG:N	3:A:110:ASP:O	7	0.11
(2,120)	3:A:88:THR:N	3:A:85:HIS:O	9	0.11
(2,112)	3:A:69:CYS:N	3:A:74:ARG:O	19	0.11
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	13	0.11
(2,110)	3:A:61:HIS:N	3:A:58:GLN:O	19	0.11
(2,107)	3:A:58:GLN:N	3:A:54:LEU:O	5	0.11
(2,107)	3:A:58:GLN:N	3:A:54:LEU:O	10	0.11
(2,107)	3:A:58:GLN:N	3:A:54:LEU:O	14	0.11
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	2	0.11
(2,106)	3:A:57:HIS:N	3:A:53:GLN:O	16	0.11
(2,105)	3:A:56:ARG:N	3:A:52:ASP:O	1	0.11
(2,105)	3:A:56:ARG:N	3:A:52:ASP:O	15	0.11
(2,105)	3:A:56:ARG:N	3:A:52:ASP:O	18	0.11
(2,104)	3:A:55:LYS:N	3:A:51:SER:O	5	0.11
(1,9)	3:A:17:ARG:HA	3:A:9:CYS:H	15	0.11
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	6	0.11
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	13	0.11
(1,791)	3:A:109:SER:CB	2:C:150:DC:C3'	14	0.11
(1,781)	2:C:154:DC:N4	3:A:114:ARG:CZ	14	0.11
(1,768)	2:C:150:DC:N4	3:A:80:ASP:CG	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,764)	2:C:149:DG:C8	3:A:80:ASP:CB	1	0.11
(1,763)	2:C:149:DG:N7	3:A:80:ASP:CG	8	0.11
(1,762)	2:C:149:DG:N7	3:A:80:ASP:CB	11	0.11
(1,76)	3:A:49:SER:HA	3:A:37:TYR:H	7	0.11
(1,752)	2:C:147:DA:N6	3:A:52:ASP:CG	17	0.11
(1,75)	3:A:47:ARG:HA	3:A:39:CYS:H	13	0.11
(1,740)	1:B:133:DG:C5	3:A:50:ARG:CZ	2	0.11
(1,739)	1:B:133:DG:C6	3:A:50:ARG:CZ	5	0.11
(1,739)	1:B:133:DG:C6	3:A:50:ARG:CZ	13	0.11
(1,738)	1:B:132:DC:C6	3:A:50:ARG:CZ	1	0.11
(1,738)	1:B:132:DC:C6	3:A:50:ARG:CZ	3	0.11
(1,737)	1:B:132:DC:C5	3:A:50:ARG:CZ	16	0.11
(1,715)	1:B:129:DG:C2'	3:A:78:ARG:CZ	1	0.11
(1,715)	1:B:129:DG:C2'	3:A:78:ARG:CZ	9	0.11
(1,706)	1:B:129:DG:C5'	3:A:60:ARG:CD	1	0.11
(1,706)	1:B:129:DG:C5'	3:A:60:ARG:CD	7	0.11
(1,706)	1:B:129:DG:C5'	3:A:60:ARG:CD	14	0.11
(1,706)	1:B:129:DG:C5'	3:A:60:ARG:CD	18	0.11
(1,696)	1:B:128:DG:N7	3:A:81:HIS:CB	9	0.11
(1,683)	1:B:127:DG:C6	3:A:108:ARG:CZ	4	0.11
(1,680)	1:B:127:DG:C4'	3:A:74:ARG:CZ	6	0.11
(1,670)	1:B:126:DC:N4	3:A:108:ARG:CZ	20	0.11
(1,659)	3:A:80:ASP:HA	2:C:150:DC:H6	4	0.11
(1,659)	3:A:80:ASP:HA	2:C:150:DC:H6	7	0.11
(1,638)	3:A:110:ASP:CB	3:A:113:VAL:CG2	20	0.11
(1,585)	3:A:98:ARG:CB	3:A:116:HIS:CE1	16	0.11
(1,577)	3:A:97:CYS:CB	3:A:99:TRP:CB	1	0.11
(1,545)	3:A:93:LYS:CB	3:A:106:PHE:CA	10	0.11
(1,509)	3:A:76:PHE:CE2	3:A:85:HIS:CD2	16	0.11
(1,502)	3:A:76:PHE:CB	3:A:82:LEU:CD1	1	0.11
(1,502)	3:A:76:PHE:CB	3:A:82:LEU:CD1	18	0.11
(1,498)	3:A:72:CYS:CB	3:A:89:HIS:CE1	13	0.11
(1,487)	3:A:69:CYS:CB	3:A:72:CYS:CB	20	0.11
(1,465)	3:A:67:PHE:CB	3:A:82:LEU:CD1	16	0.11
(1,458)	3:A:65:LYS:CB	3:A:76:PHE:CA	1	0.11
(1,452)	3:A:59:ARG:CA	3:A:62:THR:CG2	6	0.11
(1,442)	3:A:55:LYS:CA	3:A:58:GLN:CA	1	0.11
(1,442)	3:A:55:LYS:CA	3:A:58:GLN:CA	14	0.11
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	15	0.11
(1,440)	3:A:54:LEU:CA	3:A:57:HIS:CB	20	0.11
(1,428)	3:A:48:PHE:CE2	3:A:57:HIS:CD2	11	0.11
(1,404)	3:A:41:PHE:CE2	3:A:44:CYS:CB	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,404)	3:A:41:PHE:CE2	3:A:44:CYS:CB	19	0.11
(1,388)	3:A:39:CYS:CB	3:A:41:PHE:CB	11	0.11
(1,386)	3:A:38:GLN:CB	3:A:47:ARG:CB	1	0.11
(1,382)	3:A:38:GLN:CA	3:A:47:ARG:CA	4	0.11
(1,376)	3:A:37:TYR:CE2	3:A:51:SER:CB	16	0.11
(1,370)	3:A:37:TYR:CB	3:A:48:PHE:CB	5	0.11
(1,365)	3:A:29:ARG:CA	3:A:32:THR:CG2	2	0.11
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	3	0.11
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	8	0.11
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	15	0.11
(1,356)	3:A:24:LEU:CD2	3:A:27:HIS:CB	17	0.11
(1,341)	3:A:19:PHE:CB	3:A:23:HIS:CD2	9	0.11
(1,338)	3:A:18:TYR:CD2	3:A:27:HIS:CD2	3	0.11
(1,338)	3:A:18:TYR:CD2	3:A:27:HIS:CD2	6	0.11
(1,333)	3:A:18:TYR:CE2	3:A:27:HIS:CE1	7	0.11
(1,332)	3:A:18:TYR:CE2	3:A:27:HIS:CD2	9	0.11
(1,331)	3:A:18:TYR:CE2	3:A:27:HIS:CB	16	0.11
(1,327)	3:A:18:TYR:CE1	3:A:27:HIS:CB	19	0.11
(1,324)	3:A:18:TYR:CE1	3:A:24:LEU:CA	1	0.11
(1,319)	3:A:18:TYR:CD1	3:A:24:LEU:CB	16	0.11
(1,304)	3:A:11:TYR:CD2	3:A:14:CYS:CB	10	0.11
(1,304)	3:A:11:TYR:CD2	3:A:14:CYS:CB	11	0.11
(1,301)	3:A:11:TYR:CE2	3:A:31:HIS:CB	16	0.11
(1,299)	3:A:11:TYR:CE1	3:A:34:GLU:CA	3	0.11
(1,294)	3:A:11:TYR:CD1	3:A:31:HIS:CB	7	0.11
(1,288)	3:A:11:TYR:CA	3:A:31:HIS:CE1	20	0.11
(1,282)	3:A:9:CYS:CA	3:A:27:HIS:CD2	10	0.11
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	5	0.11
(1,211)	3:A:96:SER:HA	3:A:104:LYS:H	12	0.11
(1,209)	3:A:105:LYS:HA	3:A:97:CYS:H	5	0.11
(1,209)	3:A:105:LYS:HA	3:A:97:CYS:H	15	0.11
(1,209)	3:A:105:LYS:HA	3:A:97:CYS:H	18	0.11
(1,208)	3:A:96:SER:HA	3:A:106:PHE:H	9	0.11
(1,200)	3:A:83:LYS:HA	3:A:86:THR:HG21	8	0.11
(1,200)	3:A:83:LYS:HA	3:A:86:THR:HG22	8	0.11
(1,200)	3:A:83:LYS:HA	3:A:86:THR:HG23	8	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG21	2	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG22	2	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG23	2	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG21	3	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG22	3	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG23	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG21	7	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG22	7	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG23	7	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG21	8	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG22	8	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG23	8	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG21	11	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG22	11	0.11
(1,197)	3:A:81:HIS:HA	3:A:84:THR:HG23	11	0.11
(1,143)	3:A:68:GLN:HA	3:A:74:ARG:H	15	0.11
(1,142)	3:A:77:SER:HA	3:A:67:PHE:H	17	0.11
(1,141)	3:A:75:LYS:HA	3:A:69:CYS:H	8	0.11
(1,141)	3:A:75:LYS:HA	3:A:69:CYS:H	9	0.11
(1,141)	3:A:75:LYS:HA	3:A:69:CYS:H	17	0.11
(1,13)	3:A:7:PHE:H	3:A:18:TYR:H	12	0.11
(1,11)	3:A:8:MET:HA	3:A:16:LYS:H	16	0.11
(1,10)	3:A:19:PHE:HA	3:A:7:PHE:H	5	0.11
(1,10)	3:A:19:PHE:HA	3:A:7:PHE:H	6	0.11
(1,10)	3:A:19:PHE:HA	3:A:7:PHE:H	11	0.11
(1,10)	3:A:19:PHE:HA	3:A:7:PHE:H	16	0.11
(1,10)	3:A:19:PHE:HA	3:A:7:PHE:H	18	0.11

10 Dihedral-angle violation analysis (i)

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