Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 06:51 pm BST

PDB ID	:	4BS2
BMRB ID	:	19290
Title	:	NMR structure of human TDP-43 tandem RRMs in complex with UG-rich RNA
Authors	:	Lukavsky, P.J.; Daujotyte, D.; Tollervey, J.R.; Ule, J.; Stuani, C.; Buratti, E.; Baralle, F.E.; Damberger, F.F.; Allain, F.H.T.
Deposited on	:	2013-06-06

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:

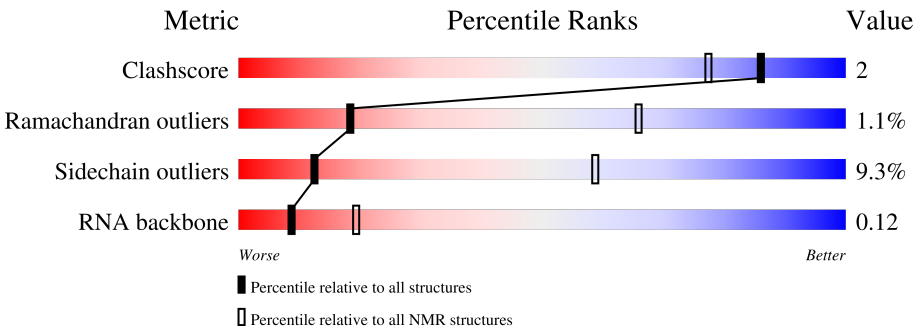
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 92%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	174	79% 10% 11%
2	B	12	17% 42% 33% 8%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:101-A:138, A:145-A:261 (155)	0.44	4

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

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

The models can be grouped into 4 clusters and 7 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3143 atoms, of which 1485 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TAR DNA-BINDING PROTEIN 43.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	174	2774	885	1373	241	265	10	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	GLY	-	expression tag	UNP Q13148
A	97	SER	-	expression tag	UNP Q13148
A	98	HIS	-	expression tag	UNP Q13148
A	99	MET	-	expression tag	UNP Q13148
A	100	ALA	-	expression tag	UNP Q13148
A	101	SER	-	expression tag	UNP Q13148

- Molecule 2 is a RNA chain called 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	12	369	116	112	48	82	11	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 79% 10% 11%

• Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B: 17% 42% 33% 8%

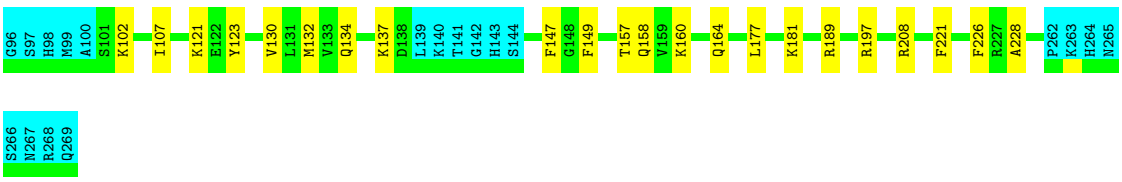
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 76% 13% 11%



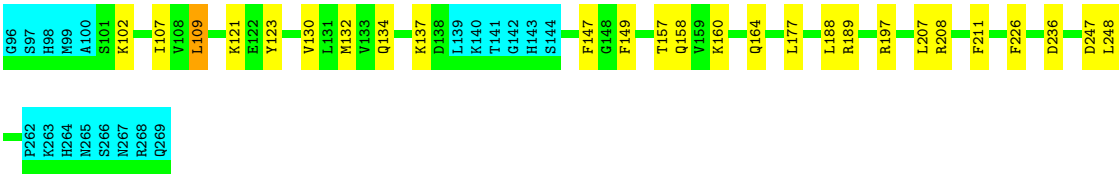
• Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B: 25% 50% 17% 8%

4.2.2 Score per residue for model 2

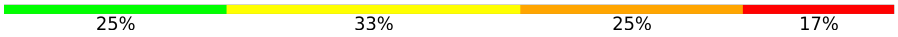
• Molecule 1: TAR DNA-BINDING PROTEIN 43

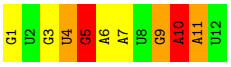
Chain A:



• Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B:

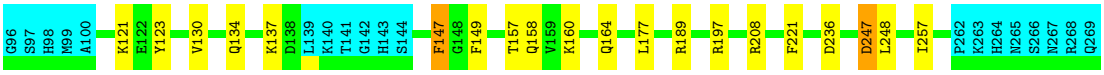




4.2.3 Score per residue for model 3

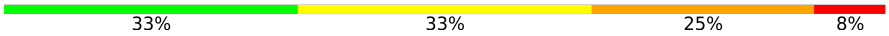
• Molecule 1: TAR DNA-BINDING PROTEIN 43

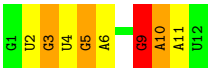
Chain A:



• Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B:

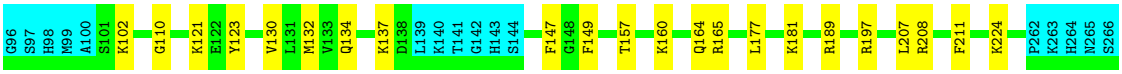




4.2.4 Score per residue for model 4 (medoid)

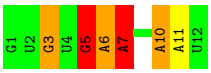
• Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A:



• Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B:



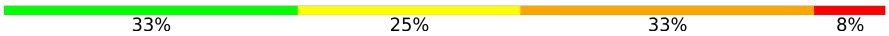
4.2.5 Score per residue for model 5

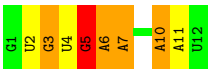
• Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A:

• Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B:

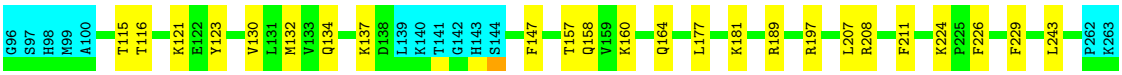


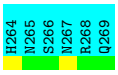


4.2.6 Score per residue for model 6

• Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A:





• Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B:

4.2.7 Score per residue for model 7

- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 79% 10% 11%

G96 S97 H98 M99 A100 K121 E122 Y123 V130 L131 M132 V133 Q134 K137 D138 L139 K140 T141 G142 H143 S144 F147 T157 Q158 V159 K160 Q164 L177 R189 R197 R208 F211 V232 P262 K263 H264 N265 S266 N267 R268 Q269

- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B: 17% 67% 8% 8%

G1 U2 G3 U4 G5 A6 A7 U8 G9 A10 A11 U12

4.2.8 Score per residue for model 8

- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 74% 14% • 11%

G96 S97 H98 M99 A100 I107 T115 T116 K121 E122 Y123 V130 L131 M132 V133 Q134 K137 D138 L139 K140 T141 G142 H143 S144 F147 G148 F149 T157 Q158 V159 K160 L177 R189 S190 V193 R197 L207 R208 F211 F221 K224 P225 A228

A240 P262 K263 H264 N265 S266 N267 R268 Q269

- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B: 8% 50% 17% 25%

G1 U2 G3 U4 G5 A6 A7 U8 G9 A10 A11 U12

4.2.9 Score per residue for model 9

- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 79% 10% 11%

G96 S97 H98 M99 A100 S101 K102 K121 E122 Y123 V130 L131 M132 V133 Q134 K137 D138 L139 K140 T141 G142 H143 S144 F147 G148 F149 T157 Q158 V159 K160 L177 K181 R189 R197 R208 D247 P262 K263 H264 N265 S266 N267 R268 Q269

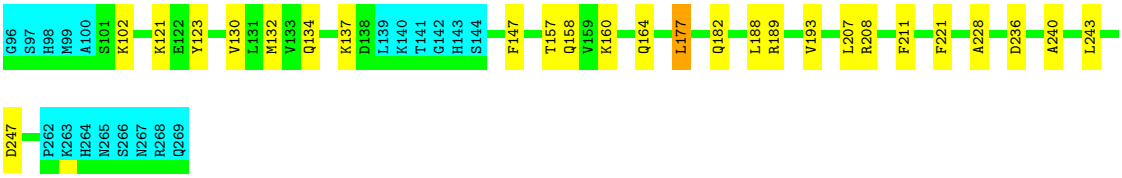
- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B: 58% 33% 8%

4.2.10 Score per residue for model 10

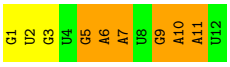
- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A:



- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

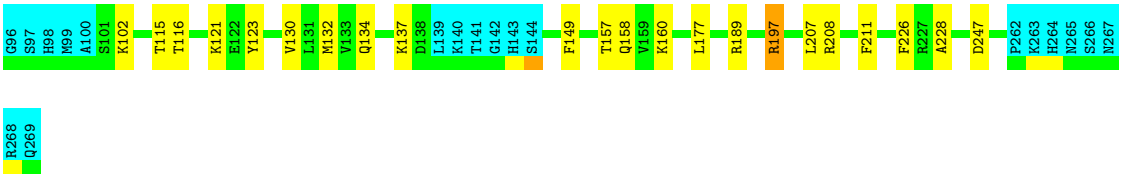
Chain B:



4.2.11 Score per residue for model 11

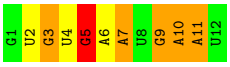
- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A:



- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

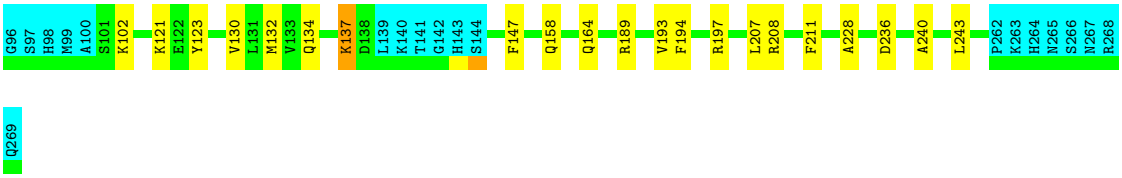
Chain B:



4.2.12 Score per residue for model 12

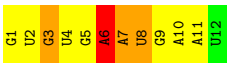
- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A:



• Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B: 8% 58% 25% 8%



4.2.13 Score per residue for model 13

• Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 76% 13% • 11%

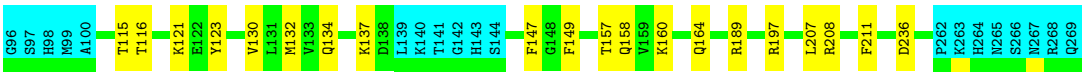
• Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B: 25% 50% 8% 17%

4.2.14 Score per residue for model 14

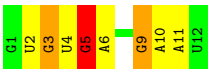
• Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 78% 11% 11%



• Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

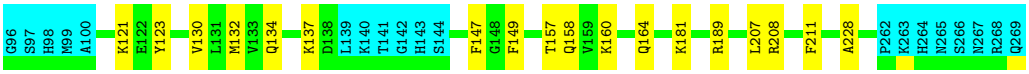
Chain B: 33% 42% 17% 8%



4.2.15 Score per residue for model 15

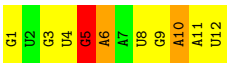
- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 79% 10% 11%



- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

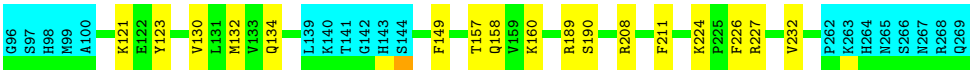
Chain B: 17% 58% 17% 8%



4.2.16 Score per residue for model 16

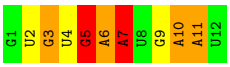
- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 79% 10% 11%



- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B: 25% 25% 33% 17%



4.2.17 Score per residue for model 17

- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 79% 10% 11%

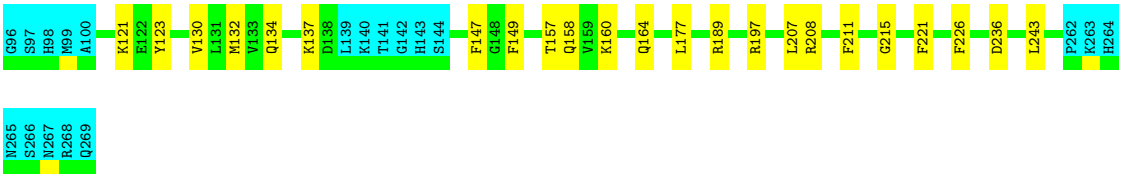
- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B: 17% 50% 25% 8%

4.2.18 Score per residue for model 18

- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 76% 13% 11%



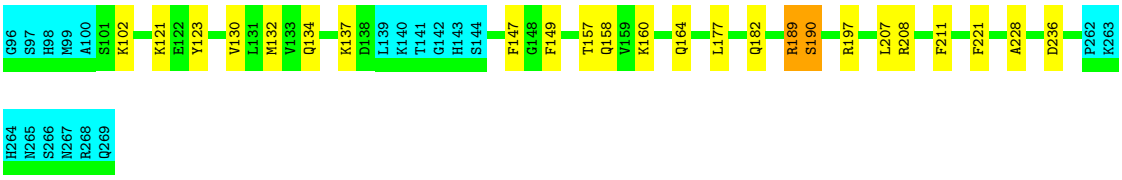
- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B: 8% 50% 33% 8%

4.2.19 Score per residue for model 19

- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 75% 13% • 11%



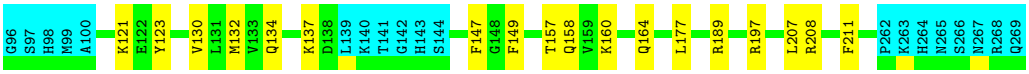
- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B: 50% 33% 17%

4.2.20 Score per residue for model 20

- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 79% 10% 11%



- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B:

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *SIMULATED ANNEALING COMBINED WITH MOLECULAR DYNAMICS IN TORSION ANGLE SPACE.*

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY AND RESTRAINT VIOLATION.*

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

Software name	**Classification**	**Version**
Amber	refinement	
CYANA	structure solution	

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	2
Total number of shifts	2382
Number of shifts mapped to atoms	2375
Number of unparsed shifts	0
Number of shifts with mapping errors	7
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.50±0.00	0±0/1283 (0.0± 0.0%)	0.74±0.01	0±0/1728 (0.0± 0.0%)
2	B	1.05±0.01	0±0/288 (0.0± 0.0%)	1.58±0.05	5±2/448 (1.0± 0.4%)
All	All	0.64	0/31420 (0.0%)	0.97	92/43520 (0.2%)

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
2	B	0.0±0.0	0.2±0.4
All	All	0	5

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	5	G	O4'-C1'-N9	7.52	114.22	108.20	11	10
2	B	5	G	C3'-C2'-C1'	-7.04	95.87	101.50	1	5
2	B	3	G	C1'-O4'-C4'	-6.95	104.34	109.90	3	12
2	B	3	G	O4'-C1'-N9	6.68	113.54	108.20	18	4
2	B	10	A	O4'-C1'-N9	6.52	113.41	108.20	8	4
2	B	9	G	O4'-C1'-N9	6.50	113.40	108.20	18	8
2	B	5	G	C1'-O4'-C4'	-6.48	104.72	109.90	11	16
2	B	6	A	O4'-C1'-N9	6.48	113.38	108.20	15	2
2	B	10	A	C5'-C4'-C3'	-6.14	106.18	116.00	19	4
2	B	7	A	O4'-C1'-N9	6.01	113.01	108.20	9	6
2	B	5	G	C5'-C4'-O4'	5.76	116.01	109.10	3	1
2	B	1	G	O4'-C1'-N9	5.70	112.76	108.20	12	9
2	B	10	A	P-O3'-C3'	5.61	126.43	119.70	15	2
2	B	4	U	P-O3'-C3'	5.42	126.20	119.70	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	9	G	C3'-C2'-C1'	5.22	105.68	101.50	14	1
2	B	7	A	C5'-C4'-C3'	-5.13	107.78	116.00	4	2
2	B	8	U	C5'-C4'-C3'	-5.11	107.82	116.00	9	2
2	B	6	A	C5'-C4'-C3'	-5.05	107.92	116.00	10	1
2	B	4	U	O4'-C1'-N1	5.04	112.23	108.20	2	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)
2	B	6	A	Sidechain	3
2	B	9	G	Sidechain	2

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1256	1232	1231	5±2
2	B	257	112	130	3±1
All	All	30260	26880	27220	120

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:ALA:HB2	2:B:6:A:C4	0.64	2.27	12	2
1:A:247:ASP:C	1:A:248:LEU:HD12	0.57	2.19	3	1
2:B:6:A:H1'	2:B:7:A:C8	0.56	2.36	12	5
1:A:149:PHE:CZ	2:B:5:G:C4	0.53	2.97	20	15
1:A:207:LEU:HD22	1:A:211:PHE:CE1	0.48	2.42	19	6
2:B:10:A:C8	2:B:10:A:H5"	0.48	2.42	1	6
1:A:221:PHE:CE2	2:B:9:G:H1'	0.47	2.43	8	4
1:A:207:LEU:HD22	1:A:211:PHE:CE2	0.46	2.44	14	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:243:LEU:HD12	1:A:243:LEU:C	0.46	2.31	5	5
2:B:6:A:H2'	2:B:7:A:C8	0.46	2.46	10	1
1:A:181:LYS:HE3	2:B:5:G:C5	0.45	2.45	6	1
2:B:10:A:C2	2:B:11:A:C4	0.45	3.04	6	2
1:A:221:PHE:CE1	2:B:9:G:H1'	0.45	2.46	19	2
1:A:157:THR:HA	1:A:160:LYS:HE2	0.45	1.89	15	19
2:B:10:A:N3	2:B:11:A:C8	0.44	2.86	2	2
2:B:9:G:C5'	2:B:9:G:N3	0.44	2.81	18	2
1:A:115:THR:HG22	1:A:116:THR:N	0.44	2.28	11	6
1:A:171:ARG:HD3	1:A:171:ARG:C	0.43	2.34	5	2
1:A:109:LEU:H	1:A:109:LEU:HD22	0.43	1.72	2	1
1:A:224:LYS:HA	1:A:225:PRO:C	0.43	2.34	8	1
1:A:228:ALA:HB2	2:B:6:A:C6	0.43	2.49	8	2
1:A:189:ARG:O	1:A:190:SER:CB	0.43	2.67	8	2
1:A:197:ARG:HD2	2:B:5:G:H1'	0.43	1.91	11	1
1:A:227:ARG:HG2	2:B:7:A:C2	0.42	2.50	16	1
1:A:107:ILE:HG22	1:A:149:PHE:CE2	0.42	2.50	1	1
1:A:147:PHE:CZ	2:B:5:G:C5'	0.42	3.02	3	1
1:A:229:PHE:CE2	2:B:8:U:H4'	0.42	2.50	6	1
1:A:211:PHE:CE1	1:A:232:VAL:HG21	0.41	2.50	7	3
1:A:193:VAL:CG1	1:A:240:ALA:HB1	0.41	2.44	8	2
2:B:10:A:C2	2:B:11:A:C8	0.41	3.08	11	2
1:A:107:ILE:CG2	1:A:149:PHE:CE2	0.41	3.04	2	1
1:A:177:LEU:CD2	1:A:182:GLN:NE2	0.41	2.84	10	1
1:A:181:LYS:HE2	1:A:181:LYS:HA	0.41	1.92	13	1
1:A:149:PHE:CE2	2:B:5:G:C5	0.41	3.09	1	2
1:A:248:LEU:HD13	1:A:257:ILE:HG12	0.41	1.93	3	1
1:A:107:ILE:HG22	1:A:149:PHE:CZ	0.41	2.50	8	1
1:A:193:VAL:HG13	1:A:240:ALA:HB1	0.41	1.92	12	1
1:A:194:PHE:CE2	2:B:8:U:C6	0.41	3.09	12	1
2:B:6:A:H2'	2:B:7:A:N7	0.41	2.30	7	1
1:A:110:GLY:HA2	2:B:3:G:C5	0.40	2.51	4	1
2:B:9:G:N3	2:B:9:G:H5"	0.40	2.32	18	1
2:B:10:A:N3	2:B:10:A:H2'	0.40	2.32	2	1
1:A:149:PHE:CZ	2:B:5:G:C5	0.40	3.09	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
1	A	155/174 (89%)	138±1 (89±1%)	15±2 (10±1%)	2±1 (1±0%)	18 66
All	All	3100/3480 (89%)	2761 (89%)	304 (10%)	35 (1%)	18 66

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

Mol	Chain	Res	Type	Models (Total)
1	A	130	VAL	20
1	A	228	ALA	5
1	A	247	ASP	5
1	A	190	SER	3
1	A	215	GLY	2

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	141/157 (90%)	128±2 (91±1%)	13±2 (9±1%)	12 59
All	All	2820/3140 (90%)	2558 (91%)	262 (9%)	12 59

All 23 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	121	LYS	20
1	A	123	TYR	20
1	A	134	GLN	20
1	A	189	ARG	20
1	A	208	ARG	20

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Mol	Chain	Res	Type	Models (Total)
1	A	132	MET	19
1	A	158	GLN	19
1	A	137	LYS	18
1	A	147	PHE	17
1	A	197	ARG	16
1	A	164	GLN	14
1	A	177	LEU	14
1	A	102	LYS	10
1	A	236	ASP	8
1	A	226	PHE	7
1	A	224	LYS	7
1	A	181	LYS	4
1	A	188	LEU	3
1	A	171	ARG	2
1	A	109	LEU	1
1	A	248	LEU	1
1	A	165	ARG	1
1	A	182	GLN	1

6.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	11/12 (92%)	8±1 (72±12%)	3±1 (27±11%)	0.12±0.07
All	All	221/240 (92%)	159 (72%)	60 (27%)	0.11

The overall RNA backbone suiteness is 0.12.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	3	G	20
2	B	10	A	19
2	B	11	A	19
2	B	6	A	18
2	B	5	G	16
2	B	9	G	16
2	B	4	U	15
2	B	7	A	12
2	B	8	U	11
2	B	2	U	9
2	B	12	U	4

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	10	A	19
2	B	3	G	14
2	B	2	U	13
2	B	6	A	5
2	B	4	U	4
2	B	7	A	2
2	B	9	G	2
2	B	1	G	1

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *YP597CN-aug12.1_withRNA2_protein2.str.csh*

7.1.1 Bookkeeping (i)

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	2197
Number of shifts mapped to atoms	2197
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	172	0.07 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	162	0.03 ± 0.06	None needed (< 0.5 ppm)
$^{13}C'$	158	0.25 ± 0.10	None needed (< 0.5 ppm)
^{15}N	159	0.25 ± 0.17	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 85%, i.e. 2002 atoms were assigned a chemical shift out of a possible 2368. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	758/774 (98%)	311/314 (99%)	300/310 (97%)	147/150 (98%)
Sidechain	1058/1178 (90%)	716/759 (94%)	324/372 (87%)	18/47 (38%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	186/196 (95%)	93/97 (96%)	91/94 (97%)	2/5 (40%)
Sugar	0/132 (0%)	0/72 (0%)	0/60 (0%)	0/0 (—%)
Base	0/88 (0%)	0/56 (0%)	0/20 (0%)	0/12 (0%)
Overall	2002/2368 (85%)	1120/1298 (86%)	715/856 (84%)	167/214 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 2197 atoms were assigned a chemical shift out of a possible 2613. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	831/869 (96%)	342/353 (97%)	330/348 (95%)	159/168 (95%)
Sidechain	1168/1306 (89%)	790/841 (94%)	357/410 (87%)	21/55 (38%)
Aromatic	198/218 (91%)	99/109 (91%)	97/100 (97%)	2/9 (22%)
Sugar	0/132 (0%)	0/72 (0%)	0/60 (0%)	0/0 (—%)
Base	0/88 (0%)	0/56 (0%)	0/20 (0%)	0/12 (0%)
Overall	2197/2613 (84%)	1231/1431 (86%)	784/938 (84%)	182/244 (75%)

7.1.4 Statistically unusual chemical shifts (i)

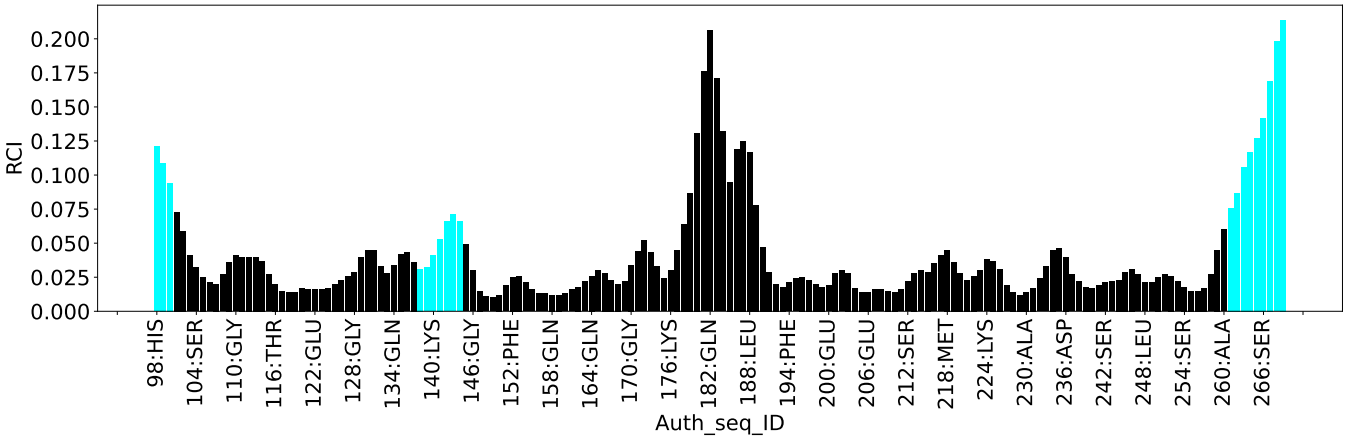
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	250	ILE	HG13	-1.28	-0.82 – 3.23	-6.1
1	A	167	MET	HB3	0.05	0.33 – 3.66	-5.8
1	A	168	ILE	HG13	-0.86	-0.82 – 3.23	-5.1
1	A	200	GLU	HB3	0.93	0.95 – 3.05	-5.1

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *YP597CN-aug12.1_withRNA2_RNA2.str.csh*

7.2.1 Bookkeeping (i)

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	185
Number of shifts mapped to atoms	178
Number of unparsed shifts	0
Number of shifts with mapping errors	7
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- No matching atom found in the structure. All 7 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	5	G	H1	12.173	0.020	1
2	B	5	G	H22	5.568	0.020	1
2	B	6	A	H2	7.805	0.020	1
2	B	7	A	H2	8.156	0.020	1
2	B	9	G	H1	10.046	0.020	1
2	B	10	A	H2	7.892	0.020	1
2	B	11	A	H2	8.104	0.020	1

7.2.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 7%, i.e. 166 atoms were assigned a chemical shift out of a possible 2368. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/774 (0%)	0/314 (0%)	0/310 (0%)	0/150 (0%)
Sidechain	0/1178 (0%)	0/759 (0%)	0/372 (0%)	0/47 (0%)
Aromatic	0/196 (0%)	0/97 (0%)	0/94 (0%)	0/5 (0%)
Sugar	131/132 (99%)	71/72 (99%)	60/60 (100%)	0/0 (—%)
Base	35/88 (40%)	19/56 (34%)	16/20 (80%)	0/12 (0%)
Overall	166/2368 (7%)	90/1298 (7%)	76/856 (9%)	0/214 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 6%, i.e. 166 atoms were assigned a chemical shift out of a possible 2613. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/869 (0%)	0/353 (0%)	0/348 (0%)	0/168 (0%)
Sidechain	0/1306 (0%)	0/841 (0%)	0/410 (0%)	0/55 (0%)
Aromatic	0/218 (0%)	0/109 (0%)	0/100 (0%)	0/9 (0%)
Sugar	131/132 (99%)	71/72 (99%)	60/60 (100%)	0/0 (—%)
Base	35/88 (40%)	19/56 (34%)	16/20 (80%)	0/12 (0%)
Overall	166/2613 (6%)	90/1431 (6%)	76/938 (8%)	0/244 (0%)

7.2.4 Statistically unusual chemical shifts (i)

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

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
2	B	4	U	H4'	3.09	3.44 – 5.28	-6.9
2	B	4	U	H5"	3.01	3.05 – 5.24	-5.2
2	B	9	G	H5'	5.42	3.12 – 5.42	5.0

7.2.5 Random Coil Index (RCI) plots (i)

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	5131
Intra-residue (|i-j|=0)	1060
Sequential (|i-j|=1)	1256
Medium range (|i-j|>1 and |i-j|<5)	791
Long range (|i-j|≥5)	1698
Inter-chain	226
Hydrogen bond restraints	100
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	42
Number of restraints per residue	27.6
Number of long range restraints per residue[1]	9.4

[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 (i)

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 (i)

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)	24.2	0.2
0.2-0.5 (Medium)	3.9	0.27
>0.5 (Large)	None	None

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)

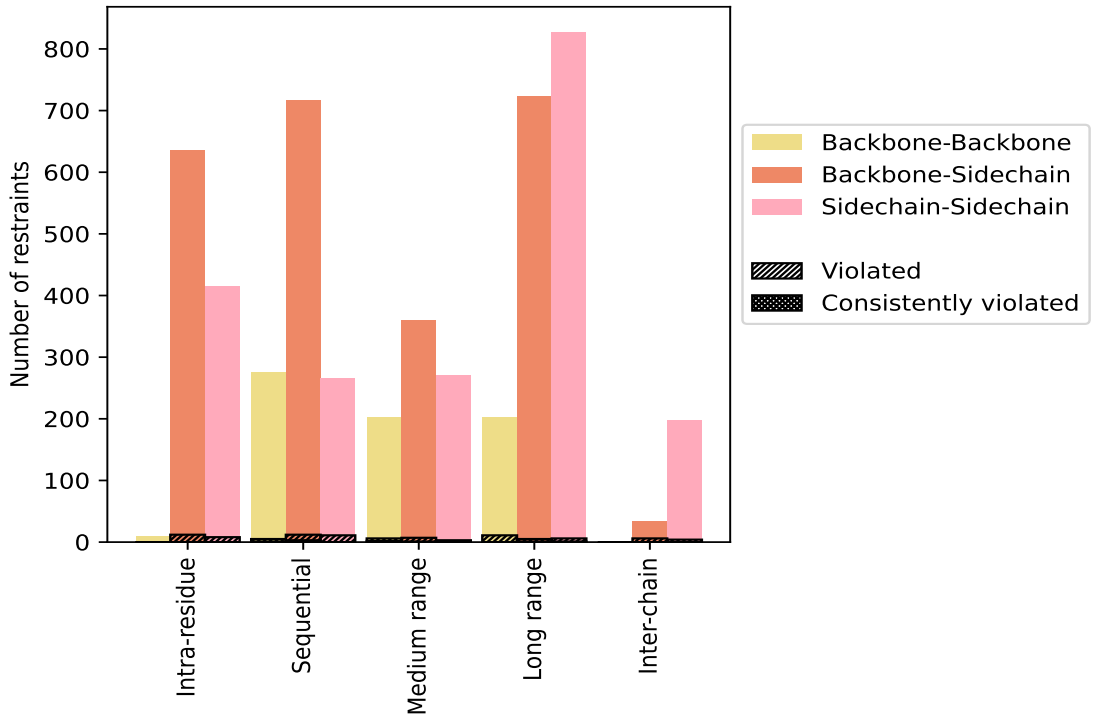
9.1 Summary of distance violations (i)

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)	1060	20.7	20	1.9	0.4	0	0.0	0.0
Backbone-Backbone	10	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	635	12.4	12	1.9	0.2	0	0.0	0.0
Sidechain-Sidechain	415	8.1	8	1.9	0.2	0	0.0	0.0
Sequential (|i-j|=1)	1256	24.5	28	2.2	0.5	4	0.3	0.1
Backbone-Backbone	275	5.4	5	1.8	0.1	1	0.4	0.0
Backbone-Sidechain	716	14.0	12	1.7	0.2	3	0.4	0.1
Sidechain-Sidechain	265	5.2	11	4.2	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	791	15.4	14	1.8	0.3	1	0.1	0.0
Backbone-Backbone	161	3.1	4	2.5	0.1	0	0.0	0.0
Backbone-Sidechain	360	7.0	7	1.9	0.1	1	0.3	0.0
Sidechain-Sidechain	270	5.3	3	1.1	0.1	0	0.0	0.0
Long range (|i-j|≥5)	1698	33.1	18	1.1	0.4	2	0.1	0.0
Backbone-Backbone	148	2.9	7	4.7	0.1	0	0.0	0.0
Backbone-Sidechain	723	14.1	5	0.7	0.1	1	0.1	0.0
Sidechain-Sidechain	827	16.1	6	0.7	0.1	1	0.1	0.0
Inter-chain	226	4.4	10	4.4	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	29	0.6	6	20.7	0.1	0	0.0	0.0
Sidechain-Sidechain	197	3.8	4	2.0	0.1	0	0.0	0.0
Hydrogen bond	100	1.9	6	6.0	0.1	2	2.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	5131	100.0	96	1.9	1.9	9	0.2	0.2
Backbone-Backbone	690	13.4	22	3.2	0.4	3	0.4	0.1
Backbone-Sidechain	2467	48.1	42	1.7	0.8	5	0.2	0.1
Sidechain-Sidechain	1974	38.5	32	1.6	0.6	1	0.1	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations (i)



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	6	7	4	9	2	28	0.16	0.25	0.04	0.15
2	5	6	4	4	4	23	0.16	0.25	0.04	0.16
3	3	6	5	7	5	26	0.15	0.24	0.04	0.14
4	1	7	6	6	6	26	0.16	0.23	0.04	0.16
5	5	9	5	8	5	32	0.15	0.23	0.03	0.14
6	5	8	5	7	3	28	0.15	0.27	0.04	0.15
7	5	8	3	6	1	23	0.16	0.26	0.04	0.14
8	5	8	5	8	3	29	0.15	0.24	0.04	0.13
9	6	7	4	6	5	28	0.15	0.24	0.04	0.13
10	3	7	6	6	2	24	0.17	0.24	0.04	0.17
11	7	8	6	9	4	34	0.14	0.24	0.04	0.13

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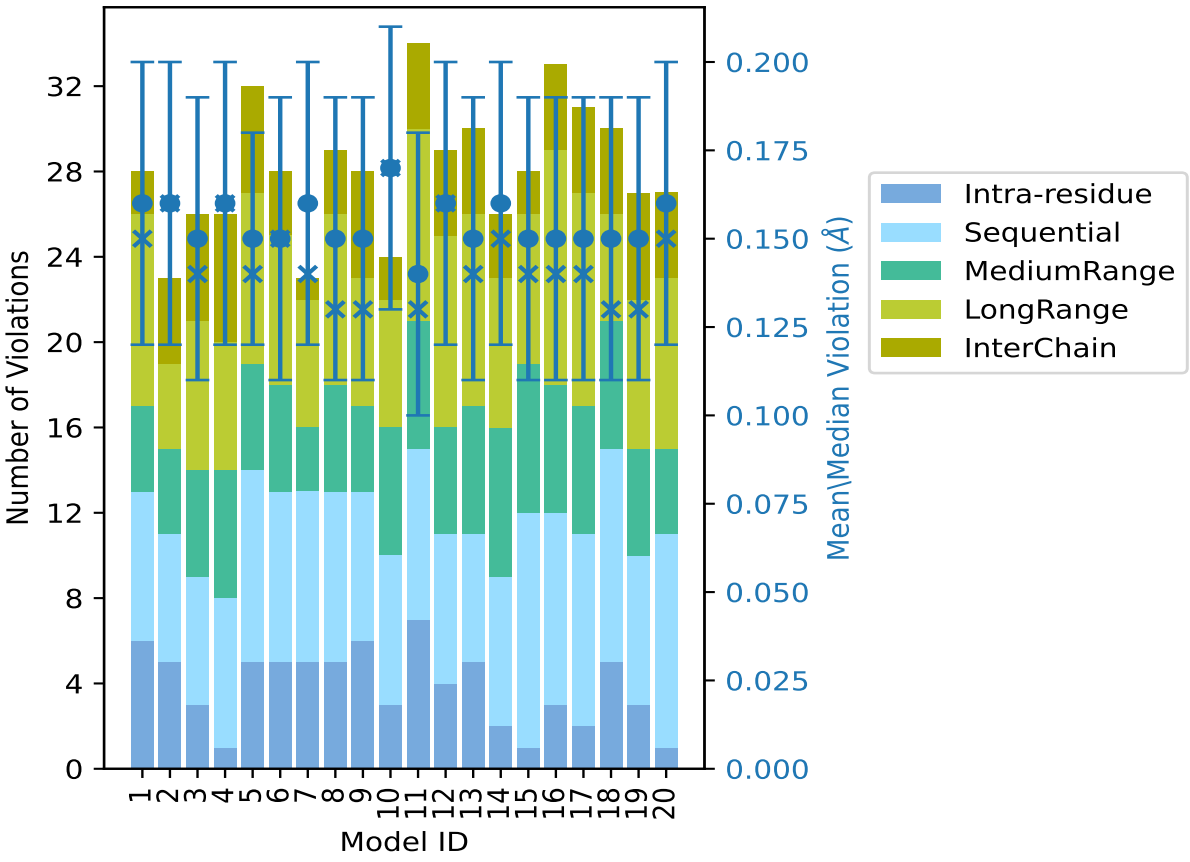
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	4	7	5	9	4	29	0.16	0.26	0.04	0.16
13	5	6	6	9	4	30	0.15	0.25	0.04	0.14
14	2	7	7	7	3	26	0.16	0.24	0.04	0.15
15	1	11	7	7	2	28	0.15	0.23	0.04	0.14
16	3	9	6	11	4	33	0.15	0.23	0.04	0.14
17	2	9	6	10	4	31	0.15	0.24	0.04	0.14
18	5	10	6	5	4	30	0.15	0.25	0.04	0.13
19	3	7	5	7	5	27	0.15	0.22	0.04	0.13
20	1	10	4	8	4	27	0.16	0.23	0.04	0.15

[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 (i)



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

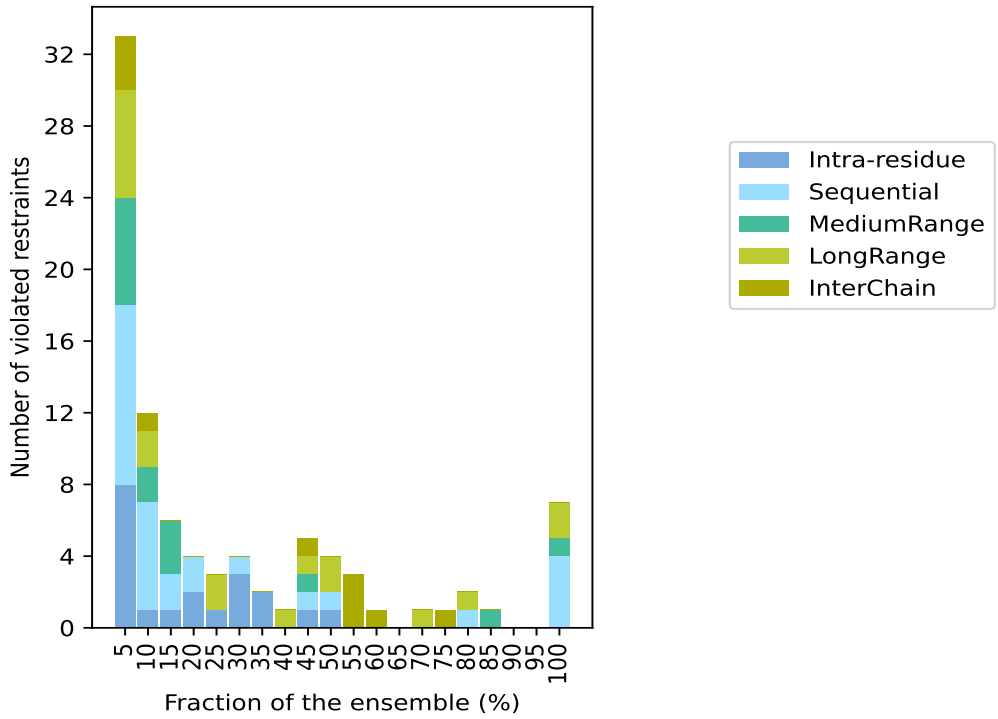
9.3 Distance violation statistics for the ensemble (i)

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, 4941(IR:1040, SQ:1228, MR:777, LR:1680, IC:216) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
8	10	6	6	3	33	1	5.0
1	6	2	2	1	12	2	10.0
1	2	3	0	0	6	3	15.0
2	2	0	0	0	4	4	20.0
1	0	0	2	0	3	5	25.0
3	1	0	0	0	4	6	30.0
2	0	0	0	0	2	7	35.0
0	0	0	1	0	1	8	40.0
1	1	1	1	1	5	9	45.0
1	1	0	2	0	4	10	50.0
0	0	0	0	3	3	11	55.0
0	0	0	0	1	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	1	0	1	14	70.0
0	0	0	0	1	1	15	75.0
0	1	0	1	0	2	16	80.0
0	0	1	0	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	4	1	2	0	7	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

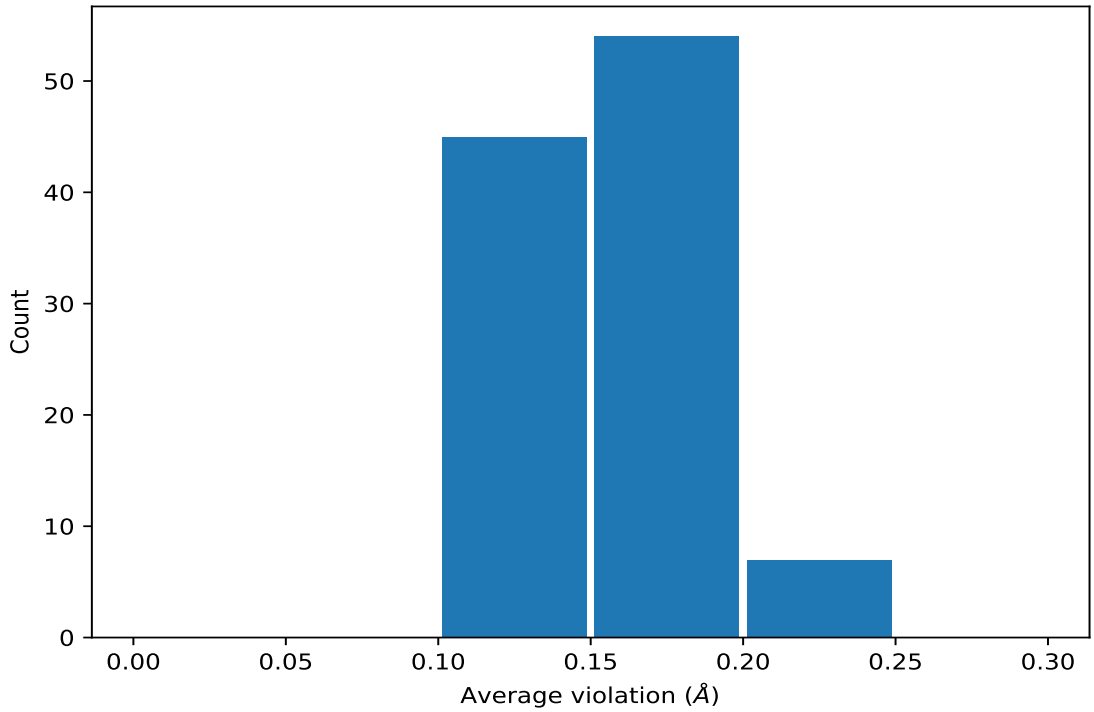
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	20	0.23	0.02	0.23
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	20	0.21	0.01	0.21
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	20	0.2	0.02	0.19
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	20	0.17	0.01	0.17
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	20	0.17	0.02	0.17
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	20	0.17	0.02	0.17
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	20	0.16	0.01	0.16
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	20	0.15	0.01	0.16
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	20	0.13	0.01	0.13
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	17	0.18	0.01	0.17
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	16	0.2	0.01	0.2
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	16	0.13	0.02	0.13
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	15	0.13	0.02	0.13
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	14	0.19	0.06	0.22
(1,4523)	2:B:8:U:H1'	1:A:263:LYS:H	12	0.15	0.03	0.14
(3,33)	1:A:147:PHE:H	1:A:136:LYS:O	11	0.18	0.07	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4520)	2:B:8:U:H4'	1:A:230:ALA:H	11	0.15	0.03	0.13
(1,4673)	2:B:9:G:H4'	1:A:231:PHE:HZ	11	0.14	0.02	0.14
(1,4567)	2:B:5:G:H5'	1:A:197:ARG:HD3	11	0.13	0.02	0.12
(1,4878)	2:B:5:G:H8	2:B:5:G:H4'	10	0.2	0.04	0.2
(1,2240)	1:A:209:GLU:HB3	1:A:210:PHE:H	10	0.13	0.01	0.12
(1,506)	1:A:208:ARG:H	1:A:219:ASP:HA	10	0.12	0.0	0.12
(1,218)	1:A:117:GLU:HG2	1:A:135:VAL:H	10	0.11	0.01	0.11
(1,749)	1:A:117:GLU:H	1:A:119:ASP:H	9	0.13	0.01	0.13
(1,4990)	2:B:11:A:H3'	2:B:12:U:H6	9	0.12	0.01	0.12
(1,4699)	2:B:4:U:H3	1:A:178:PRO:HA	9	0.12	0.01	0.11
(1,4738)	1:A:166:HIS:HD2	1:A:161:VAL:HB	9	0.12	0.01	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG12	9	0.12	0.01	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG13	9	0.12	0.01	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG21	9	0.12	0.01	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG22	9	0.12	0.01	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG23	9	0.12	0.01	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG11	9	0.12	0.01	0.11
(1,392)	1:A:221:PHE:H	1:A:233:THR:H	8	0.11	0.0	0.11
(1,4919)	2:B:8:U:H5	2:B:8:U:H3'	7	0.18	0.04	0.19
(1,496)	1:A:158:GLN:H	1:A:158:GLN:HG2	7	0.11	0.0	0.11
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD3	6	0.18	0.03	0.18
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD2	6	0.18	0.03	0.18
(3,78)	1:A:147:PHE:N	1:A:136:LYS:O	6	0.16	0.01	0.16
(1,4973)	2:B:11:A:H4'	2:B:11:A:H1'	6	0.14	0.03	0.12
(1,1679)	1:A:206:GLU:HB3	1:A:207:LEU:HB3	6	0.12	0.01	0.12
(1,4785)	2:B:2:U:H4'	2:B:2:U:H3'	6	0.11	0.0	0.11
(1,1994)	1:A:208:ARG:H	1:A:232:VAL:HB	5	0.21	0.01	0.22
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG11	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG12	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG13	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG21	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG22	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG23	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG11	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG12	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG13	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG21	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG22	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG23	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG11	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG12	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG13	5	0.19	0.01	0.19

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG21	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG22	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG23	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG11	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG12	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG13	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG21	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG22	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG23	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG11	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG12	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG13	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG21	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG22	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG23	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG11	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG12	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG13	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG21	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG22	5	0.19	0.01	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG23	5	0.19	0.01	0.19
(1,4826)	2:B:3:G:H8	2:B:3:G:H5”	5	0.12	0.01	0.11
(1,2636)	1:A:224:LYS:HG3	1:A:225:PRO:HA	4	0.16	0.03	0.16
(1,4952)	2:B:10:A:H5’	2:B:10:A:H4’	4	0.14	0.03	0.14
(1,4827)	2:B:3:G:H1’	2:B:4:U:H5	4	0.14	0.01	0.14
(1,3501)	1:A:107:ILE:H	1:A:107:ILE:HG12	4	0.12	0.01	0.12
(1,3501)	1:A:107:ILE:H	1:A:107:ILE:HG13	4	0.12	0.01	0.12
(1,674)	1:A:207:LEU:H	1:A:207:LEU:HG	3	0.24	0.02	0.24
(1,649)	1:A:239:ILE:HA	1:A:243:LEU:H	3	0.12	0.01	0.12
(1,725)	1:A:207:LEU:HB2	1:A:209:GLU:H	3	0.12	0.01	0.11
(1,1383)	1:A:164:GLN:HE22	1:A:165:ARG:H	3	0.11	0.0	0.11
(1,2461)	1:A:241:GLN:HA	1:A:244:CYS:HB3	3	0.11	0.0	0.11
(1,4899)	2:B:6:A:H8	2:B:7:A:H8	3	0.11	0.0	0.11
(3,44)	1:A:197:ARG:H	1:A:228:ALA:O	3	0.11	0.0	0.11
(1,4880)	2:B:5:G:H1’	2:B:6:A:H8	2	0.16	0.04	0.16
(1,4967)	2:B:10:A:H5’	2:B:11:A:H8	2	0.16	0.02	0.16
(1,2582)	1:A:111:LEU:HA	1:A:111:LEU:HG	2	0.15	0.0	0.15
(1,280)	1:A:137:LYS:HA	1:A:145:LYS:H	2	0.14	0.01	0.14
(1,2111)	1:A:262:PRO:HB2	1:A:263:LYS:HA	2	0.13	0.01	0.13
(1,989)	1:A:205:ASP:H	1:A:208:ARG:HD2	2	0.12	0.01	0.12
(1,1734)	1:A:168:ILE:HA	1:A:169:ASP:HB2	2	0.12	0.02	0.12
(1,4941)	2:B:9:G:H1’	2:B:10:A:H1’	2	0.12	0.02	0.12

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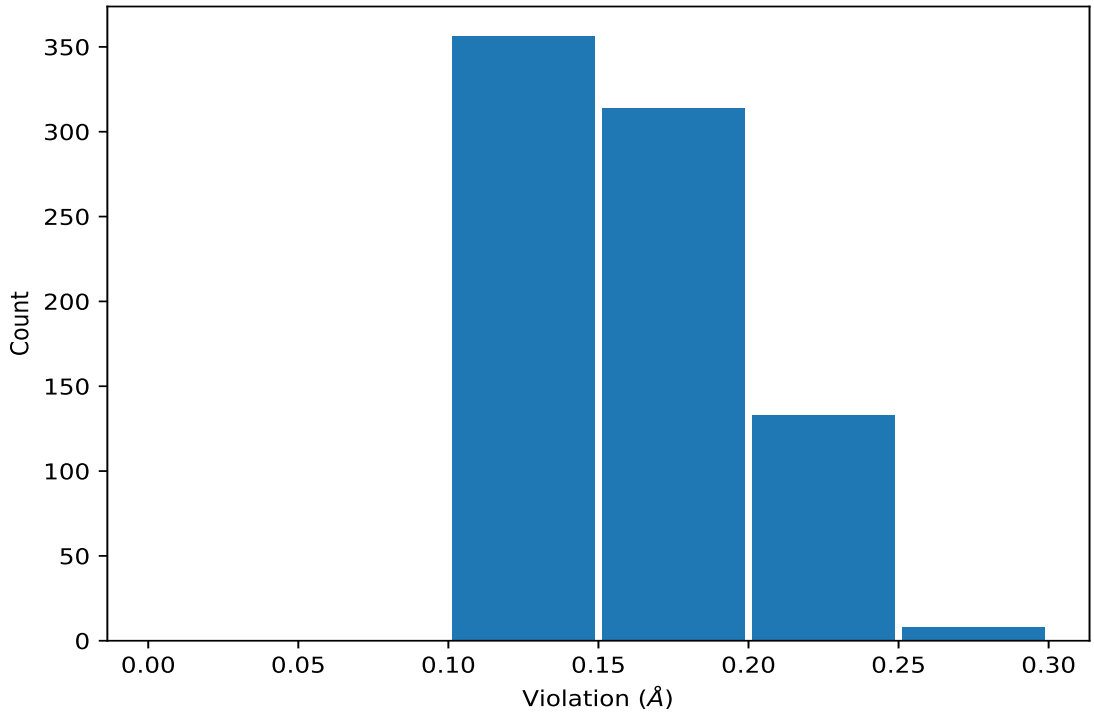
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1652)	1:A:157:THR:HA	1:A:160:LYS:HE2	2	0.12	0.0	0.12
(1,1652)	1:A:157:THR:HA	1:A:160:LYS:HE3	2	0.12	0.0	0.12
(3,22)	1:A:176:LYS:H	1:A:107:ILE:O	2	0.12	0.0	0.12
(1,48)	1:A:193:VAL:H	1:A:234:PHE:H	2	0.11	0.0	0.11
(1,1073)	1:A:243:LEU:HB3	1:A:244:CYS:H	2	0.11	0.0	0.11
(3,105)	2:B:5:G:O6	1:A:105:ASP:H	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:147:PHE:H	1:A:136:LYS:O	6	0.27
(3,33)	1:A:147:PHE:H	1:A:136:LYS:O	12	0.26
(1,674)	1:A:207:LEU:H	1:A:207:LEU:HG	7	0.26
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	1	0.25
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	2	0.25
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	7	0.25
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	18	0.25
(1,4878)	2:B:5:G:H8	2:B:5:G:H4'	13	0.25
(3,33)	1:A:147:PHE:H	1:A:136:LYS:O	8	0.24
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	9	0.24
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	10	0.24
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	17	0.24
(1,674)	1:A:207:LEU:H	1:A:207:LEU:HG	9	0.24
(1,4878)	2:B:5:G:H8	2:B:5:G:H4'	11	0.24
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	3	0.24
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	12	0.24
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	14	0.24
(3,33)	1:A:147:PHE:H	1:A:136:LYS:O	16	0.23
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	4	0.23
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	13	0.23
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	15	0.23
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	20	0.23
(1,4919)	2:B:8:U:H5	2:B:8:U:H3'	5	0.23
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	1	0.23
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	4	0.23
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	20	0.23
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	9	0.23
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	10	0.23
(1,1994)	1:A:208:ARG:H	1:A:232:VAL:HB	13	0.23
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	13	0.23
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	16	0.23
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	1	0.23
(3,33)	1:A:147:PHE:H	1:A:136:LYS:O	11	0.22
(3,33)	1:A:147:PHE:H	1:A:136:LYS:O	17	0.22
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	3	0.22
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	5	0.22
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	16	0.22
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	19	0.22
(1,4878)	2:B:5:G:H8	2:B:5:G:H4'	1	0.22
(1,4878)	2:B:5:G:H8	2:B:5:G:H4'	8	0.22
(1,4878)	2:B:5:G:H8	2:B:5:G:H4'	14	0.22
(1,4561)	2:B:5:G:H8	1:A:197:ARG:HD3	12	0.22
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	19	0.22
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	2	0.22
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	3	0.22
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	4	0.22
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	18	0.22
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	20	0.22
(1,1994)	1:A:208:ARG:H	1:A:232:VAL:HB	7	0.22
(1,1994)	1:A:208:ARG:H	1:A:232:VAL:HB	16	0.22
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	12	0.22
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	14	0.22
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	17	0.22
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	19	0.22
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	12	0.22
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	11	0.21
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	14	0.21
(1,674)	1:A:207:LEU:H	1:A:207:LEU:HG	1	0.21
(1,4919)	2:B:8:U:H5	2:B:8:U:H3'	4	0.21
(1,4523)	2:B:8:U:H1'	1:A:263:LYS:H	13	0.21
(1,4520)	2:B:8:U:H4'	1:A:230:ALA:H	9	0.21
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD3	12	0.21
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD2	12	0.21
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	16	0.21
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	17	0.21
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	15	0.21
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	11	0.21
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	1	0.21
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	2	0.21
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	3	0.21
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	6	0.21
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	7	0.21
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	10	0.21
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	11	0.21
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	15	0.21
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	4	0.21
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	8	0.21
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	8	0.2
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	12	0.2
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	1	0.2
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	2	0.2
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	18	0.2
(1,4919)	2:B:8:U:H5	2:B:8:U:H3'	9	0.2
(1,4880)	2:B:5:G:H1'	2:B:6:A:H8	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4523)	2:B:8:U:H1'	1:A:263:LYS:H	20	0.2
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG11	16	0.2
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG12	16	0.2
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG13	16	0.2
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG21	16	0.2
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG22	16	0.2
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG23	16	0.2
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG11	16	0.2
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG12	16	0.2
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG13	16	0.2
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG21	16	0.2
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG22	16	0.2
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG23	16	0.2
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG11	16	0.2
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG12	16	0.2
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG13	16	0.2
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG21	16	0.2
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG22	16	0.2
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG23	16	0.2
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG11	16	0.2
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG12	16	0.2
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG13	16	0.2
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG21	16	0.2
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG22	16	0.2
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG23	16	0.2
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG11	16	0.2
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG12	16	0.2
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG13	16	0.2
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG21	16	0.2
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG22	16	0.2
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG23	16	0.2
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG11	16	0.2
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG12	16	0.2
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG13	16	0.2
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG21	16	0.2
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG22	16	0.2
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG23	16	0.2
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD3	10	0.2
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD2	10	0.2
(1,2636)	1:A:224:LYS:HG3	1:A:225:PRO:HA	6	0.2
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	13	0.2
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1994)	1:A:208:ARG:H	1:A:232:VAL:HB	17	0.2
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	4	0.2
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	5	0.2
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	8	0.2
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	9	0.2
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	20	0.2
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	2	0.2
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	5	0.2
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	9	0.2
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	10	0.2
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	14	0.2
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	15	0.2
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	16	0.2
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	19	0.2
(3,2)	1:A:121:LYS:H	1:A:117:GLU:O	6	0.19
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	17	0.19
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	14	0.19
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	17	0.19
(1,4973)	2:B:11:A:H4'	2:B:11:A:H1'	18	0.19
(1,4919)	2:B:8:U:H5	2:B:8:U:H3'	12	0.19
(1,4919)	2:B:8:U:H5	2:B:8:U:H3'	18	0.19
(1,4881)	2:B:5:G:H2'	2:B:6:A:H8	12	0.19
(1,4878)	2:B:5:G:H8	2:B:5:G:H4'	2	0.19
(1,4523)	2:B:8:U:H1'	1:A:263:LYS:H	14	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG11	13	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG12	13	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG13	13	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG21	13	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG22	13	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG23	13	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG11	13	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG12	13	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG13	13	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG21	13	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG22	13	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG23	13	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG11	13	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG12	13	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG13	13	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG21	13	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG22	13	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG23	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG11	13	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG12	13	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG13	13	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG21	13	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG22	13	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG23	13	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG11	13	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG12	13	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG13	13	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG21	13	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG22	13	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG23	13	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG11	13	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG12	13	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG13	13	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG21	13	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG22	13	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG23	13	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG11	17	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG12	17	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG13	17	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG21	17	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG22	17	0.19
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG23	17	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG11	17	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG12	17	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG13	17	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG21	17	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG22	17	0.19
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG23	17	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG11	17	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG12	17	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG13	17	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG21	17	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG22	17	0.19
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG23	17	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG11	17	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG12	17	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG13	17	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG21	17	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG22	17	0.19
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG23	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG11	17	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG12	17	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG13	17	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG21	17	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG22	17	0.19
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG23	17	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG11	17	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG12	17	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG13	17	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG21	17	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG22	17	0.19
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG23	17	0.19
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD3	1	0.19
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD2	1	0.19
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	5	0.19
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	8	0.19
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	12	0.19
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	19	0.19
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	7	0.19
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	20	0.19
(1,1994)	1:A:208:ARG:H	1:A:232:VAL:HB	9	0.19
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	18	0.19
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	20	0.19
(3,78)	1:A:147:PHE:N	1:A:136:LYS:O	6	0.18
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	7	0.18
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	10	0.18
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	13	0.18
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	16	0.18
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	7	0.18
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	15	0.18
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	18	0.18
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	6	0.18
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	8	0.18
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	10	0.18
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	18	0.18
(1,4878)	2:B:5:G:H8	2:B:5:G:H4'	7	0.18
(1,4878)	2:B:5:G:H8	2:B:5:G:H4'	10	0.18
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	12	0.18
(1,4520)	2:B:8:U:H4'	1:A:230:ALA:H	5	0.18
(1,4520)	2:B:8:U:H4'	1:A:230:ALA:H	18	0.18
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG11	9	0.18
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG12	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG13	9	0.18
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG21	9	0.18
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG22	9	0.18
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG23	9	0.18
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG11	9	0.18
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG12	9	0.18
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG13	9	0.18
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG21	9	0.18
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG22	9	0.18
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG23	9	0.18
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG11	9	0.18
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG12	9	0.18
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG13	9	0.18
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG21	9	0.18
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG22	9	0.18
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG23	9	0.18
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG11	9	0.18
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG12	9	0.18
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG13	9	0.18
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG21	9	0.18
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG22	9	0.18
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG23	9	0.18
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG11	9	0.18
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG12	9	0.18
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG13	9	0.18
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG21	9	0.18
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG22	9	0.18
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG23	9	0.18
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG11	9	0.18
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG12	9	0.18
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG13	9	0.18
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG21	9	0.18
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG22	9	0.18
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG23	9	0.18
(1,377)	1:A:183:SER:HA	1:A:184:GLN:H	5	0.18
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD3	2	0.18
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD2	2	0.18
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD3	19	0.18
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD2	19	0.18
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	2	0.18
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	4	0.18
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	8	0.18
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	19	0.18
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	13	0.18
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	14	0.18
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	15	0.18
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	16	0.18
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	17	0.18
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	4	0.18
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	6	0.18
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	16	0.18
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	18	0.18
(1,1877)	1:A:119:ASP:H	1:A:122:GLU:HG2	18	0.18
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	3	0.18
(1,177)	1:A:260:ALA:H	1:A:261:GLU:H	17	0.18
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	3	0.17
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	4	0.17
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	9	0.17
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	15	0.17
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	1	0.17
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	2	0.17
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	3	0.17
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	4	0.17
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	5	0.17
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	8	0.17
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	9	0.17
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	10	0.17
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	11	0.17
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	12	0.17
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	16	0.17
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	19	0.17
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	20	0.17
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	4	0.17
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	13	0.17
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	16	0.17
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	20	0.17
(1,4973)	2:B:11:A:H4'	2:B:11:A:H1'	6	0.17
(1,4967)	2:B:10:A:H5'	2:B:11:A:H8	19	0.17
(1,4952)	2:B:10:A:H5'	2:B:10:A:H4'	16	0.17
(1,4878)	2:B:5:G:H8	2:B:5:G:H4'	6	0.17
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	15	0.17
(1,4673)	2:B:9:G:H4'	1:A:231:PHE:HZ	17	0.17
(1,4673)	2:B:9:G:H4'	1:A:231:PHE:HZ	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4523)	2:B:8:U:H1'	1:A:263:LYS:H	2	0.17
(1,4520)	2:B:8:U:H4'	1:A:230:ALA:H	4	0.17
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG11	7	0.17
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG12	7	0.17
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG13	7	0.17
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG21	7	0.17
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG22	7	0.17
(1,4327)	1:A:220:VAL:HG11	1:A:232:VAL:HG23	7	0.17
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG11	7	0.17
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG12	7	0.17
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG13	7	0.17
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG21	7	0.17
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG22	7	0.17
(1,4327)	1:A:220:VAL:HG12	1:A:232:VAL:HG23	7	0.17
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG11	7	0.17
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG12	7	0.17
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG13	7	0.17
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG21	7	0.17
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG22	7	0.17
(1,4327)	1:A:220:VAL:HG13	1:A:232:VAL:HG23	7	0.17
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG11	7	0.17
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG12	7	0.17
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG13	7	0.17
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG21	7	0.17
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG22	7	0.17
(1,4327)	1:A:220:VAL:HG21	1:A:232:VAL:HG23	7	0.17
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG11	7	0.17
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG12	7	0.17
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG13	7	0.17
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG21	7	0.17
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG22	7	0.17
(1,4327)	1:A:220:VAL:HG22	1:A:232:VAL:HG23	7	0.17
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG11	7	0.17
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG12	7	0.17
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG13	7	0.17
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG21	7	0.17
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG22	7	0.17
(1,4327)	1:A:220:VAL:HG23	1:A:232:VAL:HG23	7	0.17
(1,2636)	1:A:224:LYS:HG3	1:A:225:PRO:HA	5	0.17
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	3	0.17
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	10	0.17
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	12	0.17
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	14	0.17
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	18	0.17
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	20	0.17
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	5	0.17
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	11	0.17
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	17	0.17
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	1	0.17
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	10	0.17
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	11	0.17
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	14	0.17
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	17	0.17
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	19	0.17
(3,78)	1:A:147:PHE:N	1:A:136:LYS:O	8	0.16
(3,78)	1:A:147:PHE:N	1:A:136:LYS:O	16	0.16
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	19	0.16
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	20	0.16
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	6	0.16
(1,813)	1:A:153:THR:HB	1:A:154:GLU:H	13	0.16
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	1	0.16
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	5	0.16
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	11	0.16
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	12	0.16
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	17	0.16
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	19	0.16
(1,4952)	2:B:10:A:H5'	2:B:10:A:H4'	6	0.16
(1,4673)	2:B:9:G:H4'	1:A:231:PHE:HZ	4	0.16
(1,4673)	2:B:9:G:H4'	1:A:231:PHE:HZ	14	0.16
(1,4567)	2:B:5:G:H5'	1:A:197:ARG:HD3	15	0.16
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	5	0.16
(1,2566)	1:A:111:LEU:H	1:A:111:LEU:HG	2	0.16
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	5	0.16
(1,2362)	1:A:207:LEU:HG	1:A:211:PHE:HZ	15	0.16
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	3	0.16
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	4	0.16
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	10	0.16
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	12	0.16
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	13	0.16
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	14	0.16
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	15	0.16
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	19	0.16
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	2	0.16
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	5	0.16
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	8	0.16
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	12	0.16
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	13	0.16
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	15	0.16
(3,78)	1:A:147:PHE:N	1:A:136:LYS:O	11	0.15
(3,78)	1:A:147:PHE:N	1:A:136:LYS:O	12	0.15
(3,78)	1:A:147:PHE:N	1:A:136:LYS:O	17	0.15
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	6	0.15
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	2	0.15
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	3	0.15
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	14	0.15
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	15	0.15
(1,749)	1:A:117:GLU:H	1:A:119:ASP:H	5	0.15
(1,4827)	2:B:3:G:H1'	2:B:4:U:H5	20	0.15
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	1	0.15
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	11	0.15
(1,4567)	2:B:5:G:H5'	1:A:197:ARG:HD3	8	0.15
(1,4567)	2:B:5:G:H5'	1:A:197:ARG:HD3	13	0.15
(1,4567)	2:B:5:G:H5'	1:A:197:ARG:HD3	16	0.15
(1,4523)	2:B:8:U:H1'	1:A:263:LYS:H	3	0.15
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	2	0.15
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	18	0.15
(1,4520)	2:B:8:U:H4'	1:A:230:ALA:H	2	0.15
(1,280)	1:A:137:LYS:HA	1:A:145:LYS:H	16	0.15
(1,2582)	1:A:111:LEU:HA	1:A:111:LEU:HG	11	0.15
(1,2240)	1:A:209:GLU:HB3	1:A:210:PHE:H	4	0.15
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	1	0.15
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	2	0.15
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	6	0.15
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	7	0.15
(1,2077)	1:A:140:LYS:HB2	1:A:141:THR:H	6	0.15
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	1	0.15
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	5	0.14
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	11	0.14
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	12	0.14
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	14	0.14
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	7	0.14
(1,749)	1:A:117:GLU:H	1:A:119:ASP:H	14	0.14
(1,4990)	2:B:11:A:H3'	2:B:12:U:H6	2	0.14
(1,4967)	2:B:10:A:H5'	2:B:11:A:H8	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4941)	2:B:9:G:H1'	2:B:10:A:H1'	15	0.14
(1,4827)	2:B:3:G:H1'	2:B:4:U:H5	4	0.14
(1,4827)	2:B:3:G:H1'	2:B:4:U:H5	15	0.14
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	3	0.14
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	10	0.14
(1,4699)	2:B:4:U:H3	1:A:178:PRO:HA	4	0.14
(1,4673)	2:B:9:G:H4'	1:A:231:PHE:HZ	10	0.14
(1,4673)	2:B:9:G:H4'	1:A:231:PHE:HZ	13	0.14
(1,4523)	2:B:8:U:H1'	1:A:263:LYS:H	4	0.14
(1,4523)	2:B:8:U:H1'	1:A:263:LYS:H	6	0.14
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	1	0.14
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	11	0.14
(1,2636)	1:A:224:LYS:HG3	1:A:225:PRO:HA	16	0.14
(1,2582)	1:A:111:LEU:HA	1:A:111:LEU:HG	5	0.14
(1,2240)	1:A:209:GLU:HB3	1:A:210:PHE:H	5	0.14
(1,2240)	1:A:209:GLU:HB3	1:A:210:PHE:H	20	0.14
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	8	0.14
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	9	0.14
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	16	0.14
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	7	0.14
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	8	0.14
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	16	0.14
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	17	0.14
(1,2111)	1:A:262:PRO:HB2	1:A:263:LYS:HA	20	0.14
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	3	0.14
(1,1734)	1:A:168:ILE:HA	1:A:169:ASP:HB2	18	0.14
(3,12)	1:A:121:LYS:N	1:A:117:GLU:O	8	0.13
(1,989)	1:A:205:ASP:H	1:A:208:ARG:HD2	10	0.13
(1,791)	1:A:202:MET:H	1:A:253:ILE:HG13	9	0.13
(1,749)	1:A:117:GLU:H	1:A:119:ASP:H	11	0.13
(1,749)	1:A:117:GLU:H	1:A:119:ASP:H	12	0.13
(1,749)	1:A:117:GLU:H	1:A:119:ASP:H	17	0.13
(1,725)	1:A:207:LEU:HB2	1:A:209:GLU:H	3	0.13
(1,649)	1:A:239:ILE:HA	1:A:243:LEU:H	6	0.13
(1,546)	1:A:182:GLN:H	1:A:182:GLN:HB2	20	0.13
(1,4990)	2:B:11:A:H3'	2:B:12:U:H6	3	0.13
(1,4990)	2:B:11:A:H3'	2:B:12:U:H6	7	0.13
(1,4990)	2:B:11:A:H3'	2:B:12:U:H6	11	0.13
(1,4919)	2:B:8:U:H5	2:B:8:U:H3'	11	0.13
(1,4880)	2:B:5:G:H1'	2:B:6:A:H8	11	0.13
(1,4826)	2:B:3:G:H8	2:B:3:G:H5"	5	0.13
(1,4826)	2:B:3:G:H8	2:B:3:G:H5"	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	7	0.13
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	9	0.13
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	12	0.13
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	14	0.13
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	20	0.13
(1,4738)	1:A:166:HIS:HD2	1:A:161:VAL:HB	4	0.13
(1,4738)	1:A:166:HIS:HD2	1:A:161:VAL:HB	20	0.13
(1,4699)	2:B:4:U:H3	1:A:178:PRO:HA	9	0.13
(1,4699)	2:B:4:U:H3	1:A:178:PRO:HA	17	0.13
(1,4673)	2:B:9:G:H4'	1:A:231:PHE:HZ	5	0.13
(1,4673)	2:B:9:G:H4'	1:A:231:PHE:HZ	16	0.13
(1,4577)	2:B:7:A:H8	1:A:228:ALA:HA	12	0.13
(1,4567)	2:B:5:G:H5'	1:A:197:ARG:HD3	5	0.13
(1,4523)	2:B:8:U:H1'	1:A:263:LYS:H	5	0.13
(1,4523)	2:B:8:U:H1'	1:A:263:LYS:H	18	0.13
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	3	0.13
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	4	0.13
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	6	0.13
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	9	0.13
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	20	0.13
(1,4520)	2:B:8:U:H4'	1:A:230:ALA:H	16	0.13
(1,4520)	2:B:8:U:H4'	1:A:230:ALA:H	19	0.13
(1,3991)	1:A:177:LEU:HD11	1:A:182:GLN:HE22	20	0.13
(1,3991)	1:A:177:LEU:HD11	1:A:182:GLN:HE21	20	0.13
(1,3991)	1:A:177:LEU:HD12	1:A:182:GLN:HE22	20	0.13
(1,3991)	1:A:177:LEU:HD12	1:A:182:GLN:HE21	20	0.13
(1,3991)	1:A:177:LEU:HD13	1:A:182:GLN:HE22	20	0.13
(1,3991)	1:A:177:LEU:HD13	1:A:182:GLN:HE21	20	0.13
(1,3991)	1:A:177:LEU:HD21	1:A:182:GLN:HE22	20	0.13
(1,3991)	1:A:177:LEU:HD21	1:A:182:GLN:HE21	20	0.13
(1,3991)	1:A:177:LEU:HD22	1:A:182:GLN:HE22	20	0.13
(1,3991)	1:A:177:LEU:HD22	1:A:182:GLN:HE21	20	0.13
(1,3991)	1:A:177:LEU:HD23	1:A:182:GLN:HE22	20	0.13
(1,3991)	1:A:177:LEU:HD23	1:A:182:GLN:HE21	20	0.13
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG12	11	0.13
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG13	11	0.13
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG21	11	0.13
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG22	11	0.13
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG23	11	0.13
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG11	11	0.13
(1,3501)	1:A:107:ILE:H	1:A:107:ILE:HG12	3	0.13
(1,3501)	1:A:107:ILE:H	1:A:107:ILE:HG13	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2827)	1:A:116:THR:HG21	1:A:119:ASP:H	18	0.13
(1,2827)	1:A:116:THR:HG22	1:A:119:ASP:H	18	0.13
(1,2827)	1:A:116:THR:HG23	1:A:119:ASP:H	18	0.13
(1,280)	1:A:137:LYS:HA	1:A:145:LYS:H	17	0.13
(1,2240)	1:A:209:GLU:HB3	1:A:210:PHE:H	7	0.13
(1,2240)	1:A:209:GLU:HB3	1:A:210:PHE:H	19	0.13
(1,218)	1:A:117:GLU:HG2	1:A:135:VAL:H	5	0.13
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	1	0.13
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	2	0.13
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	4	0.13
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	5	0.13
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	6	0.13
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	9	0.13
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	10	0.13
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	11	0.13
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	13	0.13
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	14	0.13
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	15	0.13
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	19	0.13
(1,1679)	1:A:206:GLU:HB3	1:A:207:LEU:HB3	7	0.13
(1,1381)	1:A:108:VAL:HB	1:A:147:PHE:H	5	0.13
(1,1369)	1:A:182:GLN:HB2	1:A:182:GLN:HE22	10	0.13
(3,44)	1:A:197:ARG:H	1:A:228:ALA:O	17	0.12
(3,22)	1:A:176:LYS:H	1:A:107:ILE:O	1	0.12
(1,989)	1:A:205:ASP:H	1:A:208:ARG:HD2	11	0.12
(1,983)	1:A:265:ASN:HA	1:A:266:SER:H	8	0.12
(1,749)	1:A:117:GLU:H	1:A:119:ASP:H	8	0.12
(1,749)	1:A:117:GLU:H	1:A:119:ASP:H	13	0.12
(1,749)	1:A:117:GLU:H	1:A:119:ASP:H	19	0.12
(1,649)	1:A:239:ILE:HA	1:A:243:LEU:H	10	0.12
(1,506)	1:A:208:ARG:H	1:A:219:ASP:HA	1	0.12
(1,506)	1:A:208:ARG:H	1:A:219:ASP:HA	6	0.12
(1,506)	1:A:208:ARG:H	1:A:219:ASP:HA	10	0.12
(1,506)	1:A:208:ARG:H	1:A:219:ASP:HA	12	0.12
(1,506)	1:A:208:ARG:H	1:A:219:ASP:HA	14	0.12
(1,506)	1:A:208:ARG:H	1:A:219:ASP:HA	16	0.12
(1,4990)	2:B:11:A:H3'	2:B:12:U:H6	10	0.12
(1,4990)	2:B:11:A:H3'	2:B:12:U:H6	13	0.12
(1,4990)	2:B:11:A:H3'	2:B:12:U:H6	16	0.12
(1,4990)	2:B:11:A:H3'	2:B:12:U:H6	17	0.12
(1,4973)	2:B:11:A:H4'	2:B:11:A:H1'	1	0.12
(1,4973)	2:B:11:A:H4'	2:B:11:A:H1'	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4973)	2:B:11:A:H4'	2:B:11:A:H1'	13	0.12
(1,4973)	2:B:11:A:H4'	2:B:11:A:H1'	14	0.12
(1,496)	1:A:158:GLN:H	1:A:158:GLN:HG2	7	0.12
(1,4952)	2:B:10:A:H5'	2:B:10:A:H4'	7	0.12
(1,4919)	2:B:8:U:H5	2:B:8:U:H3'	8	0.12
(1,4899)	2:B:6:A:H8	2:B:7:A:H8	13	0.12
(1,4877)	2:B:5:G:H8	2:B:5:G:H3'	1	0.12
(1,4861)	2:B:4:U:H4'	2:B:5:G:H8	12	0.12
(1,4827)	2:B:3:G:H1'	2:B:4:U:H5	9	0.12
(1,4808)	2:B:2:U:H4'	2:B:4:U:H5	16	0.12
(1,4785)	2:B:2:U:H4'	2:B:2:U:H3'	3	0.12
(1,4785)	2:B:2:U:H4'	2:B:2:U:H3'	16	0.12
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	2	0.12
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	8	0.12
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	13	0.12
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	17	0.12
(1,4738)	1:A:166:HIS:HD2	1:A:161:VAL:HB	10	0.12
(1,4738)	1:A:166:HIS:HD2	1:A:161:VAL:HB	12	0.12
(1,4738)	1:A:166:HIS:HD2	1:A:161:VAL:HB	15	0.12
(1,4738)	1:A:166:HIS:HD2	1:A:161:VAL:HB	19	0.12
(1,472)	1:A:257:ILE:HB	1:A:258:SER:H	18	0.12
(1,4699)	2:B:4:U:H3	1:A:178:PRO:HA	11	0.12
(1,4673)	2:B:9:G:H4'	1:A:231:PHE:HZ	1	0.12
(1,4567)	2:B:5:G:H5'	1:A:197:ARG:HD3	17	0.12
(1,4567)	2:B:5:G:H5'	1:A:197:ARG:HD3	20	0.12
(1,4523)	2:B:8:U:H1'	1:A:263:LYS:H	9	0.12
(1,4523)	2:B:8:U:H1'	1:A:263:LYS:H	11	0.12
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	17	0.12
(1,4520)	2:B:8:U:H4'	1:A:230:ALA:H	11	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG12	8	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG13	8	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG21	8	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG22	8	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG23	8	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG11	8	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG12	9	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG13	9	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG21	9	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG22	9	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG23	9	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG11	9	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG12	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG13	17	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG21	17	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG22	17	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG23	17	0.12
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG11	17	0.12
(1,392)	1:A:221:PHE:H	1:A:233:THR:H	8	0.12
(1,392)	1:A:221:PHE:H	1:A:233:THR:H	13	0.12
(1,392)	1:A:221:PHE:H	1:A:233:THR:H	19	0.12
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD3	17	0.12
(1,357)	1:A:102:LYS:H	1:A:102:LYS:HD2	17	0.12
(1,3501)	1:A:107:ILE:H	1:A:107:ILE:HG12	19	0.12
(1,3501)	1:A:107:ILE:H	1:A:107:ILE:HG13	19	0.12
(1,2758)	1:A:109:LEU:H	1:A:109:LEU:HD21	2	0.12
(1,2758)	1:A:109:LEU:H	1:A:109:LEU:HD22	2	0.12
(1,2758)	1:A:109:LEU:H	1:A:109:LEU:HD23	2	0.12
(1,2641)	1:A:174:ASP:HB2	1:A:176:LYS:HG3	16	0.12
(1,2636)	1:A:224:LYS:HG3	1:A:225:PRO:HA	8	0.12
(1,256)	1:A:99:MET:HA	1:A:100:ALA:H	6	0.12
(1,2461)	1:A:241:GLN:HA	1:A:244:CYS:HB3	17	0.12
(1,2240)	1:A:209:GLU:HB3	1:A:210:PHE:H	16	0.12
(1,2240)	1:A:209:GLU:HB3	1:A:210:PHE:H	18	0.12
(1,222)	1:A:135:VAL:H	1:A:136:LYS:H	18	0.12
(1,218)	1:A:117:GLU:HG2	1:A:135:VAL:H	7	0.12
(1,218)	1:A:117:GLU:HG2	1:A:135:VAL:H	14	0.12
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	3	0.12
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	12	0.12
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	18	0.12
(1,2144)	1:A:154:GLU:HB2	1:A:155:TYR:HA	20	0.12
(1,2111)	1:A:262:PRO:HB2	1:A:263:LYS:HA	14	0.12
(1,2041)	1:A:208:ARG:HD2	1:A:217:VAL:HB	9	0.12
(1,1679)	1:A:206:GLU:HB3	1:A:207:LEU:HB3	1	0.12
(1,1679)	1:A:206:GLU:HB3	1:A:207:LEU:HB3	9	0.12
(1,1679)	1:A:206:GLU:HB3	1:A:207:LEU:HB3	17	0.12
(1,1652)	1:A:157:THR:HA	1:A:160:LYS:HE2	13	0.12
(1,1652)	1:A:157:THR:HA	1:A:160:LYS:HE3	13	0.12
(1,1383)	1:A:164:GLN:HE22	1:A:165:ARG:H	15	0.12
(1,1240)	1:A:104:SER:H	1:A:155:TYR:HA	17	0.12
(3,44)	1:A:197:ARG:H	1:A:228:ALA:O	2	0.11
(3,44)	1:A:197:ARG:H	1:A:228:ALA:O	16	0.11
(3,33)	1:A:147:PHE:H	1:A:136:LYS:O	3	0.11
(3,33)	1:A:147:PHE:H	1:A:136:LYS:O	4	0.11
(3,33)	1:A:147:PHE:H	1:A:136:LYS:O	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:147:PHE:H	1:A:136:LYS:O	19	0.11
(3,33)	1:A:147:PHE:H	1:A:136:LYS:O	20	0.11
(3,22)	1:A:176:LYS:H	1:A:107:ILE:O	13	0.11
(3,105)	2:B:5:G:O6	1:A:105:ASP:H	2	0.11
(3,105)	2:B:5:G:O6	1:A:105:ASP:H	19	0.11
(1,767)	1:A:158:GLN:HA	1:A:161:VAL:H	15	0.11
(1,749)	1:A:117:GLU:H	1:A:119:ASP:H	4	0.11
(1,725)	1:A:207:LEU:HB2	1:A:209:GLU:H	1	0.11
(1,725)	1:A:207:LEU:HB2	1:A:209:GLU:H	15	0.11
(1,67)	1:A:253:ILE:HA	1:A:255:VAL:H	14	0.11
(1,649)	1:A:239:ILE:HA	1:A:243:LEU:H	18	0.11
(1,609)	1:A:205:ASP:HB2	1:A:206:GLU:H	20	0.11
(1,54)	1:A:168:ILE:H	1:A:172:TRP:HE3	4	0.11
(1,506)	1:A:208:ARG:H	1:A:219:ASP:HA	4	0.11
(1,506)	1:A:208:ARG:H	1:A:219:ASP:HA	5	0.11
(1,506)	1:A:208:ARG:H	1:A:219:ASP:HA	8	0.11
(1,506)	1:A:208:ARG:H	1:A:219:ASP:HA	18	0.11
(1,4990)	2:B:11:A:H3'	2:B:12:U:H6	5	0.11
(1,4968)	2:B:10:A:H8	2:B:11:A:H5"	15	0.11
(1,4960)	2:B:10:A:H2'	2:B:11:A:H1'	15	0.11
(1,496)	1:A:158:GLN:H	1:A:158:GLN:HG2	6	0.11
(1,496)	1:A:158:GLN:H	1:A:158:GLN:HG2	8	0.11
(1,496)	1:A:158:GLN:H	1:A:158:GLN:HG2	9	0.11
(1,496)	1:A:158:GLN:H	1:A:158:GLN:HG2	11	0.11
(1,496)	1:A:158:GLN:H	1:A:158:GLN:HG2	13	0.11
(1,496)	1:A:158:GLN:H	1:A:158:GLN:HG2	18	0.11
(1,4952)	2:B:10:A:H5'	2:B:10:A:H4'	11	0.11
(1,4941)	2:B:9:G:H1'	2:B:10:A:H1'	17	0.11
(1,4899)	2:B:6:A:H8	2:B:7:A:H8	6	0.11
(1,4899)	2:B:6:A:H8	2:B:7:A:H8	7	0.11
(1,4878)	2:B:5:G:H8	2:B:5:G:H4'	12	0.11
(1,485)	1:A:262:PRO:HB2	1:A:263:LYS:H	20	0.11
(1,4826)	2:B:3:G:H8	2:B:3:G:H5"	8	0.11
(1,4826)	2:B:3:G:H8	2:B:3:G:H5"	18	0.11
(1,4826)	2:B:3:G:H8	2:B:3:G:H5"	19	0.11
(1,48)	1:A:193:VAL:H	1:A:234:PHE:H	1	0.11
(1,48)	1:A:193:VAL:H	1:A:234:PHE:H	11	0.11
(1,4785)	2:B:2:U:H4'	2:B:2:U:H3'	6	0.11
(1,4785)	2:B:2:U:H4'	2:B:2:U:H3'	11	0.11
(1,4785)	2:B:2:U:H4'	2:B:2:U:H3'	13	0.11
(1,4785)	2:B:2:U:H4'	2:B:2:U:H3'	18	0.11
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4740)	1:A:166:HIS:HE1	1:A:161:VAL:H	16	0.11
(1,4738)	1:A:166:HIS:HD2	1:A:161:VAL:HB	1	0.11
(1,4738)	1:A:166:HIS:HD2	1:A:161:VAL:HB	3	0.11
(1,4738)	1:A:166:HIS:HD2	1:A:161:VAL:HB	14	0.11
(1,4699)	2:B:4:U:H3	1:A:178:PRO:HA	3	0.11
(1,4699)	2:B:4:U:H3	1:A:178:PRO:HA	6	0.11
(1,4699)	2:B:4:U:H3	1:A:178:PRO:HA	13	0.11
(1,4699)	2:B:4:U:H3	1:A:178:PRO:HA	16	0.11
(1,4699)	2:B:4:U:H3	1:A:178:PRO:HA	19	0.11
(1,4673)	2:B:9:G:H4'	1:A:231:PHE:HZ	9	0.11
(1,4673)	2:B:9:G:H4'	1:A:231:PHE:HZ	12	0.11
(1,4567)	2:B:5:G:H5'	1:A:197:ARG:HD3	3	0.11
(1,4567)	2:B:5:G:H5'	1:A:197:ARG:HD3	4	0.11
(1,4567)	2:B:5:G:H5'	1:A:197:ARG:HD3	7	0.11
(1,4567)	2:B:5:G:H5'	1:A:197:ARG:HD3	19	0.11
(1,4546)	2:B:4:U:H2'	1:A:179:ASN:HB3	18	0.11
(1,4523)	2:B:8:U:H1'	1:A:263:LYS:H	8	0.11
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	10	0.11
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	15	0.11
(1,4521)	2:B:8:U:H5	1:A:259:ASN:H	19	0.11
(1,4520)	2:B:8:U:H4'	1:A:230:ALA:H	3	0.11
(1,4520)	2:B:8:U:H4'	1:A:230:ALA:H	8	0.11
(1,4520)	2:B:8:U:H4'	1:A:230:ALA:H	14	0.11
(1,420)	1:A:107:ILE:H	1:A:107:ILE:HG12	3	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG12	2	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG13	2	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG21	2	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG22	2	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG23	2	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG11	2	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG12	5	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG13	5	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG21	5	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG22	5	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG23	5	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG11	5	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG12	7	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG13	7	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG21	7	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG22	7	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG23	7	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG11	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG12	13	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG13	13	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG21	13	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG22	13	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG23	13	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG11	13	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG12	16	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG13	16	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG21	16	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG22	16	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG23	16	0.11
(1,3928)	1:A:161:VAL:H	1:A:161:VAL:HG11	16	0.11
(1,392)	1:A:221:PHE:H	1:A:233:THR:H	1	0.11
(1,392)	1:A:221:PHE:H	1:A:233:THR:H	3	0.11
(1,392)	1:A:221:PHE:H	1:A:233:THR:H	5	0.11
(1,392)	1:A:221:PHE:H	1:A:233:THR:H	12	0.11
(1,392)	1:A:221:PHE:H	1:A:233:THR:H	15	0.11
(1,3501)	1:A:107:ILE:H	1:A:107:ILE:HG12	12	0.11
(1,3501)	1:A:107:ILE:H	1:A:107:ILE:HG13	12	0.11
(1,3501)	1:A:107:ILE:H	1:A:107:ILE:HG12	15	0.11
(1,3501)	1:A:107:ILE:H	1:A:107:ILE:HG13	15	0.11
(1,289)	1:A:248:LEU:H	1:A:257:ILE:H	11	0.11
(1,2686)	1:A:177:LEU:HD21	1:A:182:GLN:HE21	20	0.11
(1,2686)	1:A:177:LEU:HD22	1:A:182:GLN:HE21	20	0.11
(1,2686)	1:A:177:LEU:HD23	1:A:182:GLN:HE21	20	0.11
(1,2461)	1:A:241:GLN:HA	1:A:244:CYS:HB3	9	0.11
(1,2461)	1:A:241:GLN:HA	1:A:244:CYS:HB3	14	0.11
(1,2240)	1:A:209:GLU:HB3	1:A:210:PHE:H	8	0.11
(1,2240)	1:A:209:GLU:HB3	1:A:210:PHE:H	11	0.11
(1,2240)	1:A:209:GLU:HB3	1:A:210:PHE:H	17	0.11
(1,218)	1:A:117:GLU:HG2	1:A:135:VAL:H	6	0.11
(1,218)	1:A:117:GLU:HG2	1:A:135:VAL:H	9	0.11
(1,218)	1:A:117:GLU:HG2	1:A:135:VAL:H	11	0.11
(1,218)	1:A:117:GLU:HG2	1:A:135:VAL:H	13	0.11
(1,218)	1:A:117:GLU:HG2	1:A:135:VAL:H	16	0.11
(1,218)	1:A:117:GLU:HG2	1:A:135:VAL:H	18	0.11
(1,218)	1:A:117:GLU:HG2	1:A:135:VAL:H	19	0.11
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	5	0.11
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	6	0.11
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	8	0.11
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	11	0.11
(1,2161)	1:A:127:PHE:HZ	1:A:161:VAL:HB	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2125)	1:A:99:MET:H	1:A:99:MET:HG3	5	0.11
(1,2065)	1:A:140:LYS:H	1:A:140:LYS:HB3	1	0.11
(1,1734)	1:A:168:ILE:HA	1:A:169:ASP:HB2	16	0.11
(1,1679)	1:A:206:GLU:HB3	1:A:207:LEU:HB3	11	0.11
(1,1679)	1:A:206:GLU:HB3	1:A:207:LEU:HB3	18	0.11
(1,1652)	1:A:157:THR:HA	1:A:160:LYS:HE2	15	0.11
(1,1652)	1:A:157:THR:HA	1:A:160:LYS:HE3	15	0.11
(1,1383)	1:A:164:GLN:HE22	1:A:165:ARG:H	1	0.11
(1,1383)	1:A:164:GLN:HE22	1:A:165:ARG:H	14	0.11
(1,1314)	1:A:103:THR:H	1:A:182:GLN:H	15	0.11
(1,1073)	1:A:243:LEU:HB3	1:A:244:CYS:H	6	0.11
(1,1073)	1:A:243:LEU:HB3	1:A:244:CYS: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