Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 08:36 PM EDT

PDB ID	:	2N40
BMRB ID	:	25663
Title	:	Solution structure of the link module of human tsg-6 in presence of a chondroitin 4-sulfate hexasaccharide
Authors	:	Park, Y.; Prestegard, J.H.
Deposited on	:	2015-06-16

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:

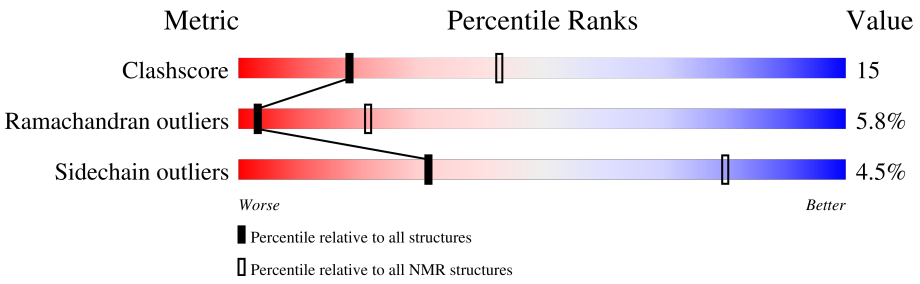
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 84%.

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	A	98	72% 24% .

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:1-A:95 (95)	1.25	19

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

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

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

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1529 atoms, of which 758 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tumor necrosis factor-inducible gene 6 protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	98	1529	492	758	142	132	5	0

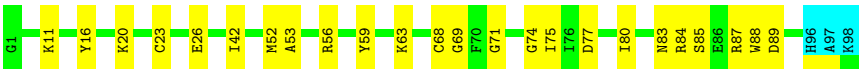
4 Residue-property plots (i)

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: Tumor necrosis factor-inducible gene 6 protein

Chain A: 72% 24%



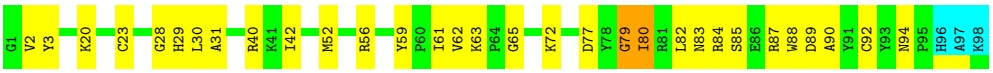
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Tumor necrosis factor-inducible gene 6 protein

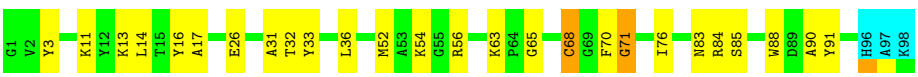
Chain A: 65% 30%



4.2.2 Score per residue for model 2

• Molecule 1: Tumor necrosis factor-inducible gene 6 protein

Chain A: 70% 24%



4.2.3 Score per residue for model 3

• Molecule 1: Tumor necrosis factor-inducible gene 6 protein

Chain A: 63% 31%

G1 V2 Y3 H4 R5 R8 K11 Y12 T15 Y16 A17 E18 G28 H29 L30 A31 T32 Y33 I42 G50 W51 M52 A53 R56 V57 G58 Y59 K72 T73 G74 I75 I76 D77 Y78 R81 L82 N83 R84 S85 E86 R87 W88 H96 A97 K98

4.2.4 Score per residue for model 4

• Molecule 1: Tumor necrosis factor-inducible gene 6 protein

Chain A: 66% 30%

G1 R8 T15 Y16 K20 C23 E24 F25 H29 L30 A31 T32 Y33 L36 E37 R40 K41 I42 M52 A53 K54 G55 G58 Y59 P60 I61 V62 C68 G69 F70 G71 N83 R84 S85 E86 R87 W88 H96 A97 K98

4.2.5 Score per residue for model 5

• Molecule 1: Tumor necrosis factor-inducible gene 6 protein

Chain A: 65% 26% 5%

G1 Y12 K20 C23 E24 F25 E26 G27 G28 L36 A39 R40 K41 I42 M52 A53 K54 G55 R56 Y59 P60 I61 V62 K63 P64 G65 P66 N67 C68 G74 I75 I76 D77 Y78 G79 I80 R81 L82 N83 R87 W88 D89 H96 A97 K98

4.2.6 Score per residue for model 6

• Molecule 1: Tumor necrosis factor-inducible gene 6 protein

Chain A: 67% 23% 6%

G1 K11 Y16 A17 K20 C23 E26 A31 I42 M52 A53 K54 G55 Y59 K63 P64 G65 P66 N67 C68 G69 G79 I80 R81 L82 N83 R84 S85 E86 R87 W88 D89 N94 P95 H96 A97 K98

4.2.7 Score per residue for model 7

• Molecule 1: Tumor necrosis factor-inducible gene 6 protein

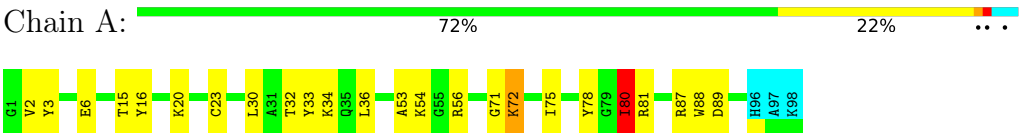
Chain A: 69% 27%

G1 R5 E6 A7 R8 K11 Y12 Y16 A17 K20 C23 T32 Y33 I42 V46 C47 K54 G55 R56 Y59 P60 I61 G71 G74 I75 I76 D77 N83 E86 A90 Y93 N94 P95 H96 A97 K98

4.2.8 Score per residue for model 8

- Molecule 1: Tumor necrosis factor-inducible gene 6 protein

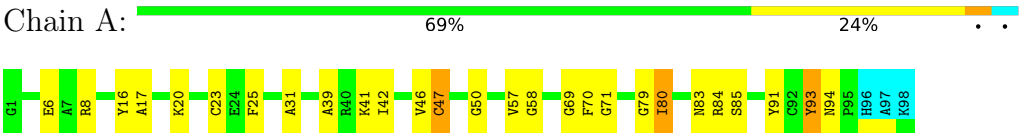
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: Tumor necrosis factor-inducible gene 6 protein

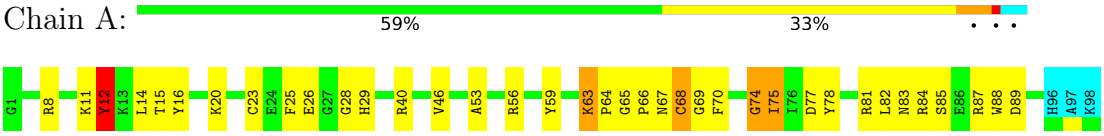
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: Tumor necrosis factor-inducible gene 6 protein

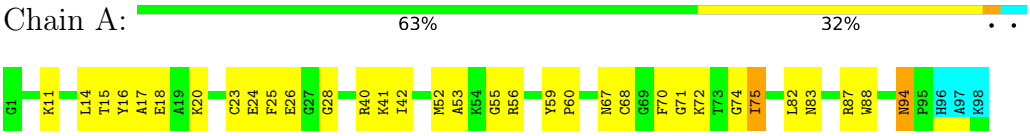
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: Tumor necrosis factor-inducible gene 6 protein

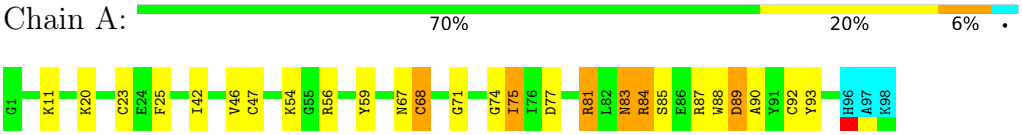
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: Tumor necrosis factor-inducible gene 6 protein

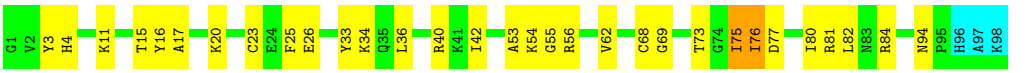
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: Tumor necrosis factor-inducible gene 6 protein

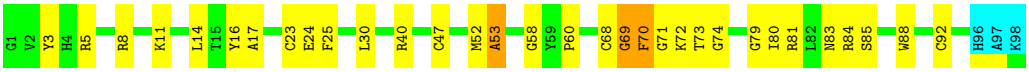
Chain A: 65% 30%



4.2.14 Score per residue for model 14

- Molecule 1: Tumor necrosis factor-inducible gene 6 protein

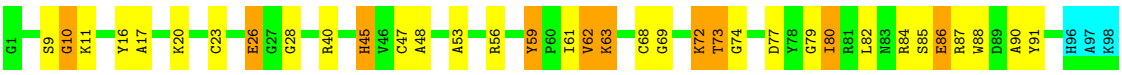
Chain A: 64% 30%



4.2.15 Score per residue for model 15

- Molecule 1: Tumor necrosis factor-inducible gene 6 protein

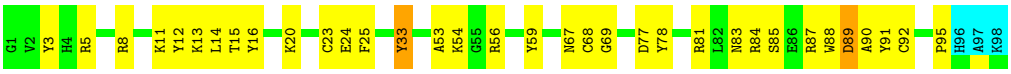
Chain A: 61% 26% 10%



4.2.16 Score per residue for model 16

- Molecule 1: Tumor necrosis factor-inducible gene 6 protein

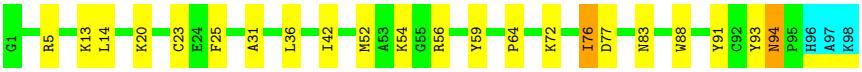
Chain A: 62% 33%



4.2.17 Score per residue for model 17

- Molecule 1: Tumor necrosis factor-inducible gene 6 protein

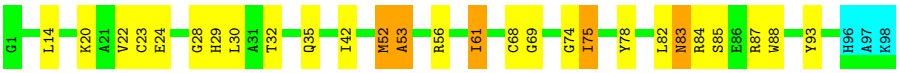
Chain A: 74% 20%



4.2.18 Score per residue for model 18

- Molecule 1: Tumor necrosis factor-inducible gene 6 protein

Chain A:



4.2.19 Score per residue for model 19 (medoid)

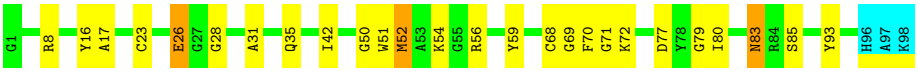
- Molecule 1: Tumor necrosis factor-inducible gene 6 protein

Chain A:

4.2.20 Score per residue for model 20

- Molecule 1: Tumor necrosis factor-inducible gene 6 protein

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	2.8
X-PLOR NIH	structure solution	2.8
CYANA	refinement	3.0
CYANA	structure solution	3.0

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	1114
Number of shifts mapped to atoms	1114
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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	0.76±0.01	0±0/768 (0.0± 0.0%)	0.74±0.02	0±0/1035 (0.0± 0.0%)
All	All	0.76	0/15360 (0.0%)	0.74	1/20700 (0.0%)

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	A	0.0±0.0	0.2±0.4
All	All	0	4

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	56	ARG	NE-CZ-NH2	-5.25	117.67	120.30	3	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	8	ARG	Sidechain	4

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	746	732	729	22±4
All	All	14920	14640	14580	435

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ARG:CZ	1:A:83:ASN:HD21	0.71	1.99	14	4
1:A:80:ILE:N	1:A:80:ILE:HD12	0.69	2.03	5	1
1:A:63:LYS:H	1:A:64:PRO:CD	0.67	2.03	6	2
1:A:81:ARG:NE	1:A:81:ARG:H	0.62	1.93	12	1
1:A:56:ARG:NH2	1:A:78:TYR:H	0.59	1.96	18	1
1:A:81:ARG:N	1:A:81:ARG:HE	0.58	1.96	12	1
1:A:16:TYR:CD2	1:A:17:ALA:N	0.58	2.71	15	8
1:A:20:LYS:O	1:A:23:CYS:O	0.58	2.22	8	14
1:A:42:ILE:HG22	1:A:42:ILE:O	0.58	1.98	18	11
1:A:33:TYR:CG	1:A:34:LYS:N	0.58	2.72	13	2
1:A:61:ILE:H	1:A:61:ILE:HD13	0.58	1.59	18	1
1:A:16:TYR:CG	1:A:17:ALA:N	0.58	2.72	6	6
1:A:81:ARG:H	1:A:81:ARG:CD	0.57	2.11	12	1
1:A:83:ASN:O	1:A:85:SER:N	0.57	2.38	6	13
1:A:70:PHE:CD2	1:A:71:GLY:N	0.57	2.72	11	3
1:A:40:ARG:NH2	1:A:62:VAL:N	0.56	2.53	13	3
1:A:81:ARG:NH1	1:A:88:TRP:NE1	0.56	2.54	14	1
1:A:56:ARG:HH22	1:A:78:TYR:H	0.56	1.40	18	1
1:A:61:ILE:HD13	1:A:61:ILE:N	0.56	2.15	18	1
1:A:32:THR:HG22	1:A:33:TYR:N	0.56	2.16	7	3
1:A:56:ARG:NH2	1:A:77:ASP:OD2	0.56	2.39	7	3
1:A:35:GLN:N	1:A:35:GLN:NE2	0.56	2.54	19	1
1:A:9:SER:O	1:A:10:GLY:C	0.55	2.45	15	1
1:A:83:ASN:C	1:A:85:SER:H	0.55	2.05	6	8
1:A:54:LYS:O	1:A:56:ARG:N	0.55	2.40	13	8
1:A:79:GLY:O	1:A:80:ILE:C	0.54	2.45	6	1
1:A:63:LYS:N	1:A:64:PRO:CD	0.54	2.71	5	2
1:A:40:ARG:NH2	1:A:61:ILE:O	0.54	2.41	5	1
1:A:78:TYR:CZ	1:A:81:ARG:NH2	0.54	2.75	8	1
1:A:87:ARG:O	1:A:88:TRP:CD1	0.53	2.61	12	9
1:A:90:ALA:O	1:A:91:TYR:CD1	0.53	2.61	2	3
1:A:59:TYR:N	1:A:59:TYR:CD1	0.53	2.75	6	2
1:A:33:TYR:CD1	1:A:56:ARG:NH2	0.53	2.76	16	1
1:A:59:TYR:CD1	1:A:59:TYR:N	0.53	2.76	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:THR:HG22	1:A:16:TYR:N	0.53	2.19	3	7
1:A:74:GLY:O	1:A:75:ILE:O	0.53	2.27	18	3
1:A:81:ARG:H	1:A:81:ARG:HE	0.53	1.44	12	1
1:A:26:GLU:CD	1:A:26:GLU:H	0.53	2.07	11	5
1:A:81:ARG:NE	1:A:81:ARG:N	0.53	2.56	12	1
1:A:18:GLU:N	1:A:18:GLU:OE1	0.52	2.42	11	2
1:A:73:THR:HG22	1:A:74:GLY:N	0.52	2.19	3	2
1:A:56:ARG:HH22	1:A:77:ASP:CB	0.52	2.18	20	1
1:A:33:TYR:CD1	1:A:34:LYS:N	0.52	2.78	13	1
1:A:68:CYS:O	1:A:70:PHE:N	0.52	2.43	20	1
1:A:40:ARG:NH2	1:A:61:ILE:C	0.51	2.64	1	2
1:A:56:ARG:HH22	1:A:77:ASP:CG	0.51	2.08	20	2
1:A:29:HIS:CD2	1:A:35:GLN:HE22	0.51	2.24	18	1
1:A:59:TYR:CE2	1:A:61:ILE:HD11	0.51	2.40	7	1
1:A:5:ARG:HH21	1:A:91:TYR:N	0.51	2.03	17	1
1:A:35:GLN:NE2	1:A:93:TYR:CG	0.51	2.78	20	1
1:A:3:TYR:OH	1:A:5:ARG:NH2	0.51	2.43	14	3
1:A:61:ILE:N	1:A:61:ILE:CD1	0.51	2.73	18	1
1:A:80:ILE:N	1:A:80:ILE:CD1	0.51	2.73	5	1
1:A:56:ARG:NH2	1:A:77:ASP:OD1	0.51	2.45	12	1
1:A:54:LYS:C	1:A:56:ARG:H	0.50	2.10	13	4
1:A:30:LEU:CD2	1:A:30:LEU:N	0.50	2.74	1	1
1:A:50:GLY:O	1:A:52:MET:SD	0.50	2.69	3	3
1:A:23:CYS:C	1:A:25:PHE:H	0.50	2.10	9	9
1:A:69:GLY:O	1:A:71:GLY:N	0.50	2.45	14	2
1:A:52:MET:O	1:A:55:GLY:N	0.50	2.45	11	4
1:A:31:ALA:O	1:A:52:MET:SD	0.49	2.70	6	4
1:A:75:ILE:O	1:A:77:ASP:N	0.49	2.44	13	1
1:A:33:TYR:CE1	1:A:56:ARG:NH2	0.49	2.79	8	1
1:A:52:MET:SD	1:A:58:GLY:N	0.49	2.85	14	1
1:A:3:TYR:OH	1:A:5:ARG:CZ	0.49	2.61	16	1
1:A:86:GLU:N	1:A:86:GLU:OE1	0.49	2.46	15	2
1:A:40:ARG:HH12	1:A:60:PRO:CB	0.49	2.21	11	1
1:A:33:TYR:CE1	1:A:56:ARG:CZ	0.48	2.95	8	1
1:A:2:VAL:HG22	1:A:3:TYR:N	0.48	2.23	8	1
1:A:82:LEU:H	1:A:82:LEU:CD2	0.48	2.21	10	2
1:A:82:LEU:N	1:A:82:LEU:CD2	0.48	2.76	15	3
1:A:93:TYR:CD1	1:A:94:ASN:N	0.48	2.81	7	1
1:A:59:TYR:CZ	1:A:76:ILE:O	0.48	2.66	17	1
1:A:59:TYR:O	1:A:59:TYR:CD2	0.48	2.67	10	6
1:A:83:ASN:C	1:A:85:SER:N	0.48	2.67	6	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:TYR:CZ	1:A:78:TYR:CZ	0.48	3.02	3	1
1:A:16:TYR:CD1	1:A:17:ALA:N	0.48	2.81	13	1
1:A:28:GLY:O	1:A:29:HIS:CG	0.48	2.67	10	3
1:A:3:TYR:CE2	1:A:4:HIS:O	0.48	2.67	13	1
1:A:40:ARG:NH2	1:A:61:ILE:N	0.48	2.62	4	1
1:A:32:THR:O	1:A:36:LEU:N	0.47	2.46	4	3
1:A:81:ARG:NE	1:A:83:ASN:HD21	0.47	2.07	6	2
1:A:40:ARG:HE	1:A:60:PRO:HB2	0.47	1.70	14	1
1:A:29:HIS:CD2	1:A:30:LEU:O	0.47	2.67	18	1
1:A:76:ILE:O	1:A:78:TYR:CE2	0.47	2.68	3	1
1:A:65:GLY:N	1:A:66:PRO:CD	0.47	2.77	6	3
1:A:54:LYS:C	1:A:56:ARG:N	0.47	2.68	13	8
1:A:32:THR:OG1	1:A:33:TYR:N	0.47	2.48	19	2
1:A:12:TYR:CD1	1:A:89:ASP:OD2	0.47	2.67	5	1
1:A:52:MET:N	1:A:56:ARG:O	0.47	2.47	17	4
1:A:14:LEU:O	1:A:88:TRP:O	0.47	2.32	10	7
1:A:56:ARG:NH2	1:A:77:ASP:CG	0.47	2.68	20	3
1:A:30:LEU:HD12	1:A:30:LEU:N	0.47	2.25	14	2
1:A:26:GLU:OE1	1:A:28:GLY:N	0.47	2.47	15	2
1:A:94:ASN:ND2	1:A:94:ASN:N	0.47	2.63	17	1
1:A:1:GLY:O	1:A:93:TYR:CD1	0.47	2.68	19	1
1:A:40:ARG:NH2	1:A:61:ILE:CA	0.47	2.78	4	1
1:A:29:HIS:ND1	1:A:30:LEU:O	0.47	2.47	4	1
1:A:67:ASN:OD1	1:A:68:CYS:N	0.47	2.48	16	2
1:A:81:ARG:NH1	1:A:88:TRP:HE1	0.47	2.08	14	1
1:A:45:HIS:CD2	1:A:62:VAL:CG2	0.47	2.98	15	1
1:A:59:TYR:CD2	1:A:59:TYR:O	0.47	2.68	20	1
1:A:40:ARG:HH22	1:A:61:ILE:CA	0.46	2.23	4	1
1:A:81:ARG:NH2	1:A:84:ARG:HE	0.46	2.07	12	1
1:A:33:TYR:CD1	1:A:77:ASP:OD2	0.46	2.68	13	1
1:A:63:LYS:NZ	1:A:63:LYS:CB	0.46	2.78	15	1
1:A:29:HIS:CD2	1:A:35:GLN:NE2	0.46	2.83	18	1
1:A:77:ASP:OD1	1:A:78:TYR:N	0.46	2.48	19	2
1:A:81:ARG:CZ	1:A:83:ASN:ND2	0.46	2.76	14	2
1:A:39:ALA:O	1:A:42:ILE:HG22	0.46	2.10	5	3
1:A:82:LEU:N	1:A:82:LEU:HD22	0.46	2.26	15	3
1:A:75:ILE:H	1:A:75:ILE:HD12	0.46	1.70	19	1
1:A:56:ARG:HH22	1:A:78:TYR:N	0.46	2.06	18	1
1:A:59:TYR:CZ	1:A:91:TYR:CD2	0.46	3.04	15	1
1:A:46:VAL:HG12	1:A:47:CYS:N	0.45	2.26	12	2
1:A:47:CYS:O	1:A:47:CYS:SG	0.45	2.74	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ILE:O	1:A:42:ILE:CG2	0.45	2.64	3	6
1:A:79:GLY:O	1:A:80:ILE:O	0.45	2.34	15	4
1:A:24:GLU:N	1:A:28:GLY:O	0.45	2.45	5	3
1:A:26:GLU:OE2	1:A:94:ASN:ND2	0.45	2.50	13	2
1:A:82:LEU:HD23	1:A:82:LEU:N	0.45	2.27	10	2
1:A:26:GLU:CD	1:A:28:GLY:H	0.45	2.15	15	2
1:A:46:VAL:O	1:A:46:VAL:HG13	0.45	2.12	7	1
1:A:68:CYS:SG	1:A:68:CYS:O	0.45	2.75	16	1
1:A:79:GLY:O	1:A:81:ARG:N	0.45	2.49	6	1
1:A:70:PHE:CG	1:A:71:GLY:N	0.45	2.85	19	2
1:A:47:CYS:SG	1:A:68:CYS:O	0.45	2.74	14	1
1:A:87:ARG:C	1:A:88:TRP:CD1	0.45	2.90	3	6
1:A:52:MET:O	1:A:53:ALA:C	0.45	2.54	4	5
1:A:6:GLU:CD	1:A:6:GLU:N	0.45	2.70	7	2
1:A:23:CYS:O	1:A:25:PHE:N	0.45	2.50	9	2
1:A:61:ILE:O	1:A:73:THR:O	0.45	2.35	15	1
1:A:89:ASP:CG	1:A:90:ALA:H	0.45	2.15	16	3
1:A:77:ASP:OD1	1:A:77:ASP:O	0.45	2.34	12	2
1:A:52:MET:O	1:A:53:ALA:O	0.45	2.35	14	1
1:A:23:CYS:O	1:A:24:GLU:CB	0.45	2.65	18	1
1:A:11:LYS:O	1:A:12:TYR:CG	0.44	2.70	3	1
1:A:52:MET:SD	1:A:56:ARG:O	0.44	2.75	11	1
1:A:35:GLN:NE2	1:A:93:TYR:CD2	0.44	2.86	20	1
1:A:32:THR:CG2	1:A:33:TYR:N	0.44	2.81	2	3
1:A:74:GLY:O	1:A:75:ILE:CB	0.44	2.66	7	1
1:A:20:LYS:NZ	1:A:24:GLU:OE1	0.44	2.48	4	1
1:A:6:GLU:O	1:A:8:ARG:NH1	0.44	2.50	9	1
1:A:83:ASN:C	1:A:83:ASN:HD22	0.44	2.16	12	1
1:A:5:ARG:NE	1:A:92:CYS:SG	0.44	2.90	16	1
1:A:83:ASN:C	1:A:83:ASN:ND2	0.44	2.71	18	1
1:A:50:GLY:O	1:A:57:VAL:HG23	0.44	2.13	9	1
1:A:73:THR:CG2	1:A:74:GLY:N	0.43	2.81	3	2
1:A:83:ASN:O	1:A:86:GLU:OE1	0.43	2.37	7	1
1:A:67:ASN:OD1	1:A:68:CYS:SG	0.43	2.76	10	3
1:A:40:ARG:HH21	1:A:62:VAL:N	0.43	2.10	13	1
1:A:81:ARG:O	1:A:84:ARG:NH1	0.43	2.50	13	1
1:A:15:THR:CG2	1:A:16:TYR:N	0.43	2.81	3	2
1:A:15:THR:OG1	1:A:18:GLU:OE1	0.43	2.36	11	1
1:A:56:ARG:NH2	1:A:78:TYR:N	0.43	2.64	18	1
1:A:69:GLY:O	1:A:70:PHE:CG	0.43	2.71	10	1
1:A:89:ASP:OD1	1:A:90:ALA:N	0.43	2.50	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:THR:HG22	1:A:33:TYR:H	0.43	1.71	7	2
1:A:82:LEU:HD12	1:A:82:LEU:N	0.43	2.27	19	2
1:A:71:GLY:O	1:A:72:LYS:O	0.43	2.37	8	1
1:A:74:GLY:O	1:A:75:ILE:C	0.43	2.57	10	2
1:A:81:ARG:NH1	1:A:88:TRP:CE2	0.43	2.87	14	1
1:A:68:CYS:O	1:A:68:CYS:SG	0.42	2.77	5	1
1:A:48:ALA:HB1	1:A:91:TYR:OH	0.42	2.14	15	1
1:A:81:ARG:NE	1:A:83:ASN:ND2	0.42	2.67	16	1
1:A:56:ARG:NH2	1:A:77:ASP:CB	0.42	2.82	20	1
1:A:11:LYS:C	1:A:13:LYS:N	0.42	2.73	2	1
1:A:58:GLY:C	1:A:59:TYR:CD1	0.42	2.93	4	1
1:A:36:LEU:O	1:A:40:ARG:N	0.42	2.46	5	1
1:A:73:THR:O	1:A:76:ILE:HD11	0.42	2.13	13	1
1:A:52:MET:SD	1:A:58:GLY:O	0.42	2.77	14	1
1:A:59:TYR:OH	1:A:78:TYR:CE1	0.42	2.66	5	1
1:A:63:LYS:N	1:A:64:PRO:HD2	0.42	2.30	10	1
1:A:65:GLY:CA	1:A:68:CYS:SG	0.42	3.08	2	1
1:A:24:GLU:OE1	1:A:24:GLU:N	0.42	2.52	14	1
1:A:30:LEU:N	1:A:30:LEU:HD22	0.42	2.30	1	1
1:A:56:ARG:HE	1:A:77:ASP:CG	0.42	2.18	15	1
1:A:65:GLY:CA	1:A:68:CYS:O	0.42	2.67	10	1
1:A:22:VAL:HG13	1:A:23:CYS:N	0.42	2.30	18	1
1:A:70:PHE:O	1:A:71:GLY:O	0.42	2.37	2	1
1:A:51:TRP:C	1:A:52:MET:SD	0.42	2.97	20	1
1:A:93:TYR:CD1	1:A:93:TYR:C	0.42	2.94	18	1
1:A:32:THR:CG2	1:A:35:GLN:OE1	0.42	2.68	19	1
1:A:51:TRP:CE3	1:A:57:VAL:HG22	0.41	2.50	3	1
1:A:78:TYR:CE1	1:A:81:ARG:NH2	0.41	2.88	8	1
1:A:84:ARG:O	1:A:86:GLU:N	0.41	2.53	15	1
1:A:20:LYS:HZ1	1:A:24:GLU:CD	0.41	2.18	16	1
1:A:51:TRP:CE3	1:A:57:VAL:CG2	0.41	3.03	3	1
1:A:82:LEU:CD2	1:A:82:LEU:N	0.41	2.84	10	1
1:A:59:TYR:O	1:A:59:TYR:CG	0.41	2.73	11	1
1:A:84:ARG:C	1:A:86:GLU:N	0.41	2.73	15	1
1:A:20:LYS:NZ	1:A:24:GLU:CD	0.41	2.74	16	1
1:A:93:TYR:CD1	1:A:94:ASN:O	0.41	2.74	9	1
1:A:2:VAL:HG12	1:A:3:TYR:N	0.41	2.29	1	1
1:A:82:LEU:C	1:A:84:ARG:H	0.41	2.19	3	1
1:A:59:TYR:OH	1:A:91:TYR:CD2	0.41	2.72	15	1
1:A:54:LYS:O	1:A:80:ILE:CG1	0.41	2.68	8	1
1:A:45:HIS:ND1	1:A:45:HIS:C	0.41	2.74	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LYS:H	1:A:64:PRO:HD2	0.41	1.74	6	2
1:A:5:ARG:O	1:A:90:ALA:O	0.41	2.39	7	1
1:A:74:GLY:O	1:A:75:ILE:CG1	0.41	2.69	7	1
1:A:81:ARG:HE	1:A:83:ASN:HD21	0.41	1.59	10	1
1:A:11:LYS:O	1:A:12:TYR:O	0.41	2.39	10	1
1:A:46:VAL:CG1	1:A:47:CYS:N	0.41	2.84	12	1
1:A:11:LYS:O	1:A:13:LYS:N	0.41	2.54	16	1
1:A:59:TYR:CZ	1:A:78:TYR:OH	0.40	2.71	3	1
1:A:73:THR:O	1:A:76:ILE:CD1	0.40	2.69	13	1
1:A:30:LEU:N	1:A:30:LEU:CD1	0.40	2.84	14	1
1:A:40:ARG:HH12	1:A:46:VAL:H	0.40	1.59	10	1
1:A:82:LEU:H	1:A:82:LEU:HD23	0.40	1.75	10	1
1:A:92:CYS:SG	1:A:93:TYR:N	0.40	2.94	12	1
1:A:53:ALA:C	1:A:55:GLY:N	0.40	2.75	5	1
1:A:88:TRP:O	1:A:89:ASP:O	0.40	2.38	12	1
1:A:4:HIS:O	1:A:4:HIS:ND1	0.40	2.55	19	1
1:A:82:LEU:N	1:A:82:LEU:CD1	0.40	2.84	19	1
1:A:75:ILE:CG2	1:A:77:ASP:OD2	0.40	2.70	12	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	94/98 (96%)	75±2 (79±3%)	14±2 (15±2%)	5±2 (6±2%)	3	21
All	All	1880/1960 (96%)	1494 (79%)	277 (15%)	109 (6%)	3	21

All 24 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	84	ARG	12
1	A	53	ALA	11
1	A	80	ILE	9
1	A	11	LYS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	72	LYS	8
1	A	75	ILE	8
1	A	69	GLY	8
1	A	89	ASP	7
1	A	71	GLY	6
1	A	63	LYS	5
1	A	79	GLY	4
1	A	76	ILE	3
1	A	31	ALA	3
1	A	70	PHE	3
1	A	74	GLY	3
1	A	12	TYR	2
1	A	65	GLY	1
1	A	58	GLY	1
1	A	55	GLY	1
1	A	10	GLY	1
1	A	85	SER	1
1	A	95	PRO	1
1	A	64	PRO	1
1	A	28	GLY	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
1	A	71/73 (97%)	68±2 (95±3%)	3±2 (5±3%)	31 80
All	All	1420/1460 (97%)	1356 (95%)	64 (5%)	31 80

All 35 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	68	CYS	8
1	A	83	ASN	5
1	A	8	ARG	3
1	A	59	TYR	3
1	A	23	CYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	92	CYS	2
1	A	81	ARG	2
1	A	63	LYS	2
1	A	78	TYR	2
1	A	12	TYR	2
1	A	47	CYS	2
1	A	41	LYS	2
1	A	94	ASN	2
1	A	36	LEU	2
1	A	26	GLU	2
1	A	40	ARG	2
1	A	52	MET	2
1	A	3	TYR	1
1	A	37	GLU	1
1	A	87	ARG	1
1	A	75	ILE	1
1	A	80	ILE	1
1	A	91	TYR	1
1	A	93	TYR	1
1	A	82	LEU	1
1	A	45	HIS	1
1	A	62	VAL	1
1	A	72	LYS	1
1	A	73	THR	1
1	A	86	GLU	1
1	A	33	TYR	1
1	A	13	LYS	1
1	A	32	THR	1
1	A	61	ILE	1
1	A	35	GLN	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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 84% for the well-defined parts and 84% 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 (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	1114
Number of shifts mapped to atoms	1114
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	97	0.21 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	85	0.22 ± 0.22	None needed (< 0.5 ppm)
$^{13}C'$	82	0.33 ± 0.24	None needed (< 0.5 ppm)
^{15}N	87	0.43 ± 0.58	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 84%, i.e. 1079 atoms were assigned a chemical shift out of a possible 1282. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	451/480 (94%)	193/199 (97%)	174/190 (92%)	84/91 (92%)
Sidechain	570/652 (87%)	393/423 (93%)	173/196 (88%)	4/33 (12%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	58/150 (39%)	56/71 (79%)	0/71 (0%)	2/8 (25%)
Overall	1079/1282 (84%)	642/693 (93%)	347/457 (76%)	90/132 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1113 atoms were assigned a chemical shift out of a possible 1325. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	465/495 (94%)	199/205 (97%)	179/196 (91%)	87/94 (93%)
Sidechain	589/672 (88%)	406/436 (93%)	179/202 (89%)	4/34 (12%)
Aromatic	59/158 (37%)	57/75 (76%)	0/73 (0%)	2/10 (20%)
Overall	1113/1325 (84%)	662/716 (92%)	358/471 (76%)	93/138 (67%)

7.1.4 Statistically unusual chemical shifts (i)

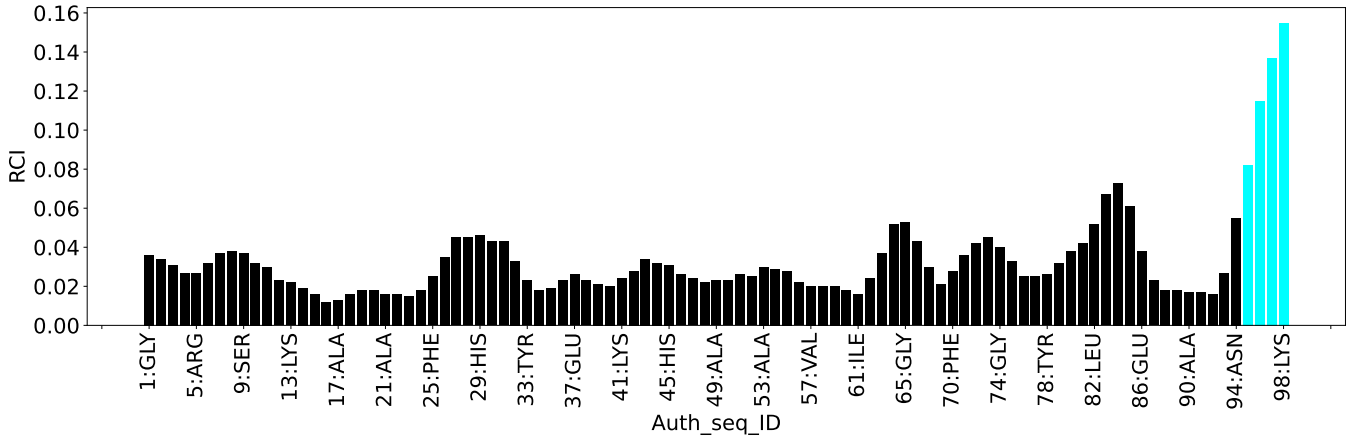
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	32	THR	HG1	5.47	0.08 – 2.19	20.6
1	A	57	VAL	HG21	-0.94	-0.58 – 2.19	-6.3
1	A	57	VAL	HG22	-0.94	-0.58 – 2.19	-6.3
1	A	57	VAL	HG23	-0.94	-0.58 – 2.19	-6.3
1	A	76	ILE	HB	0.19	0.35 – 3.22	-5.6
1	A	16	TYR	HB3	0.83	0.93 – 4.76	-5.2

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
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
1:GLY
5:ARG
9:SER
13:LYS
17:ALA
21:ALA
25:PHE
29:HIS
33:TYR
37:GLU
41:LYS
45:HIS
49:ALA
53:ALA
57:VAL
61:ILE
65:GLY
70:PHE
74:GLY
78:TYR
82:LEU
86:GLU
90:ALA
94:ASN
98:LYS
Auth_seq_ID

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	1443
Intra-residue (|i-j|=0)	345
Sequential (|i-j|=1)	414
Medium range (|i-j|>1 and |i-j|<5)	205
Long range (|i-j|≥5)	467
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	12
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	14.7
Number of long range restraints per residue[1]	4.9

[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)	10.8	0.2
0.2-0.5 (Medium)	7.4	0.5
>0.5 (Large)	0.3	0.88

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)

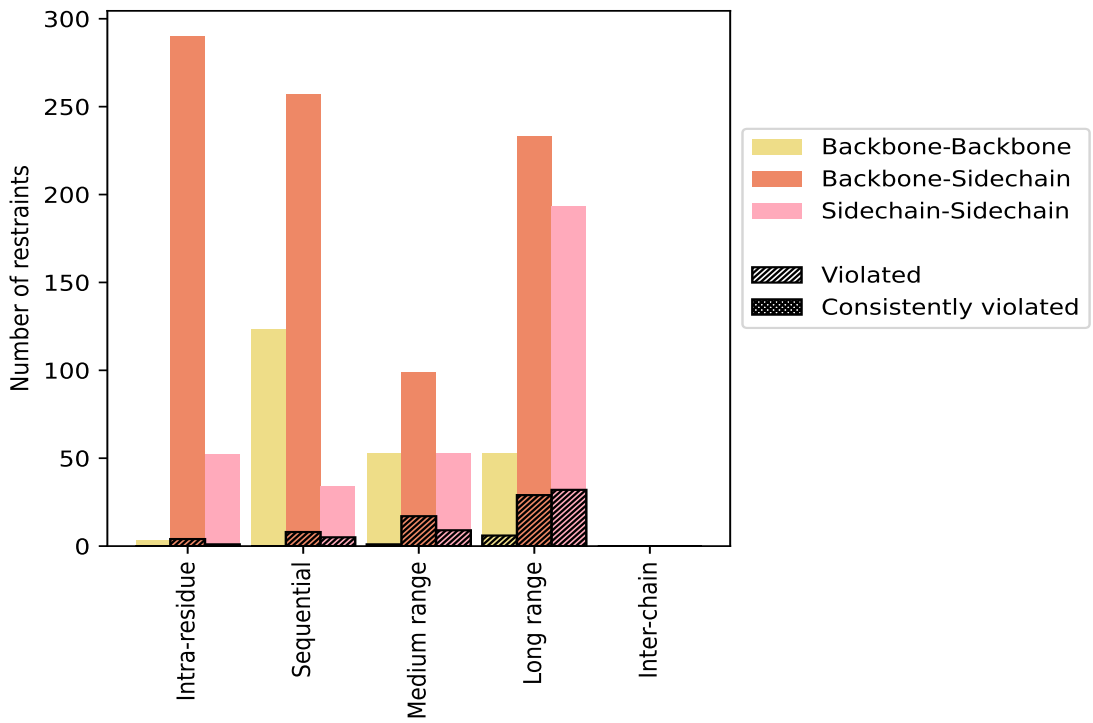
9.1 Summary of distance violations (i)

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)	345	23.9	5	1.4	0.3	0	0.0	0.0
Backbone-Backbone	3	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	290	20.1	4	1.4	0.3	0	0.0	0.0
Sidechain-Sidechain	52	3.6	1	1.9	0.1	0	0.0	0.0
Sequential (|i-j|=1)	414	28.7	13	3.1	0.9	0	0.0	0.0
Backbone-Backbone	123	8.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	257	17.8	8	3.1	0.6	0	0.0	0.0
Sidechain-Sidechain	34	2.4	5	14.7	0.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	205	14.2	27	13.2	1.9	0	0.0	0.0
Backbone-Backbone	53	3.7	1	1.9	0.1	0	0.0	0.0
Backbone-Sidechain	99	6.9	17	17.2	1.2	0	0.0	0.0
Sidechain-Sidechain	53	3.7	9	17.0	0.6	0	0.0	0.0
Long range (|i-j|≥5)	467	32.4	67	14.3	4.6	0	0.0	0.0
Backbone-Backbone	53	3.7	6	11.3	0.4	0	0.0	0.0
Backbone-Sidechain	233	16.1	29	12.4	2.0	0	0.0	0.0
Sidechain-Sidechain	181	12.5	32	17.7	2.2	0	0.0	0.0
Inter-chain	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
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	12	0.8	0	0.0	0.0	0	0.0	0.0
Total	1443	100.0	112	7.8	7.8	0	0.0	0.0
Backbone-Backbone	232	16.1	7	3.0	0.5	0	0.0	0.0
Backbone-Sidechain	879	60.9	58	6.6	4.0	0	0.0	0.0
Sidechain-Sidechain	332	23.0	47	14.2	3.3	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	3	0	6	12	0	21	0.21	0.51	0.11	0.15
2	1	1	3	11	0	16	0.24	0.38	0.08	0.24
3	3	0	3	12	0	18	0.25	0.5	0.12	0.22
4	3	2	7	12	0	24	0.22	0.58	0.11	0.2
5	3	2	5	9	0	19	0.22	0.54	0.12	0.18
6	3	1	5	7	0	16	0.24	0.64	0.12	0.22
7	1	3	3	9	0	16	0.18	0.45	0.08	0.16
8	2	3	6	10	0	21	0.22	0.88	0.17	0.17
9	3	2	5	11	0	21	0.2	0.49	0.1	0.17
10	1	0	4	12	0	17	0.2	0.55	0.1	0.16
11	1	0	6	8	0	15	0.19	0.43	0.09	0.15

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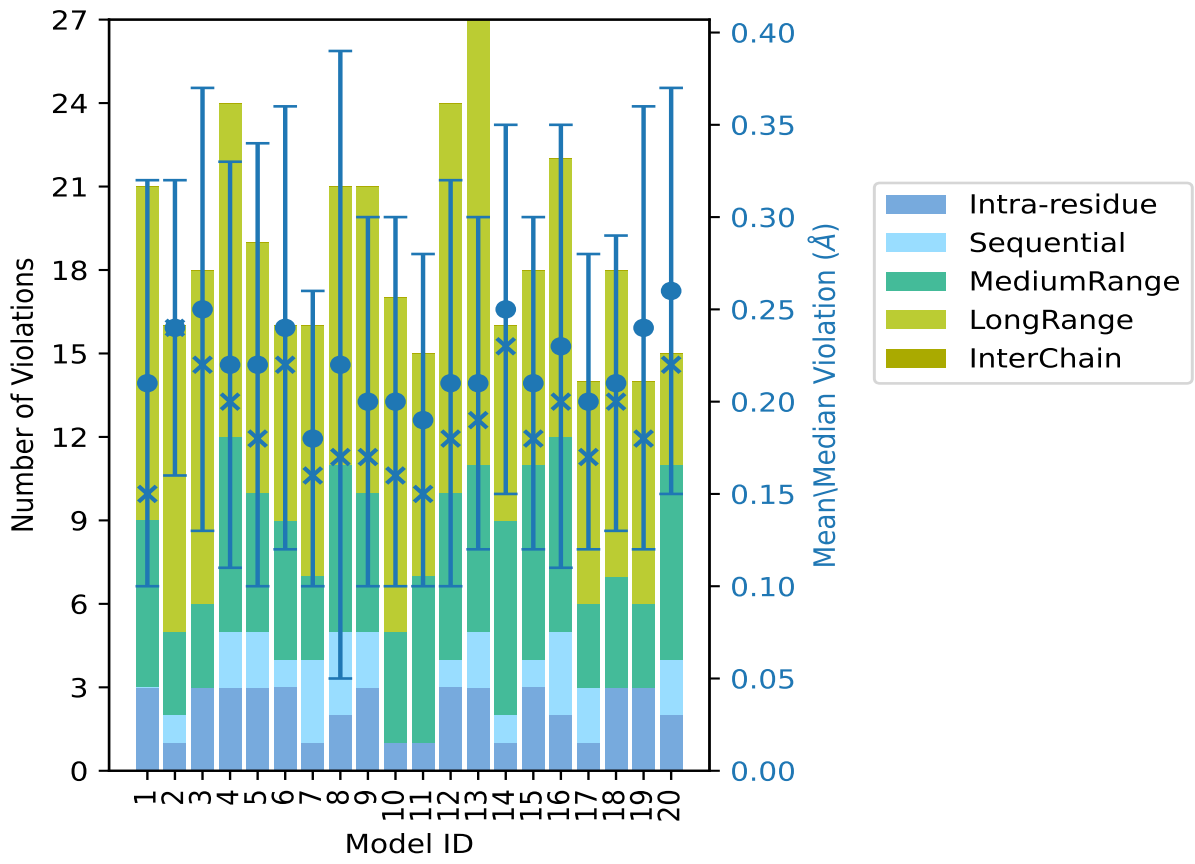
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	3	1	6	14	0	24	0.21	0.49	0.11	0.18
13	3	2	6	16	0	27	0.21	0.47	0.09	0.19
14	1	1	7	7	0	16	0.25	0.47	0.1	0.23
15	3	1	7	7	0	18	0.21	0.43	0.09	0.18
16	2	3	7	10	0	22	0.23	0.65	0.12	0.2
17	1	2	3	8	0	14	0.2	0.39	0.08	0.17
18	3	0	4	11	0	18	0.21	0.38	0.08	0.2
19	3	0	3	8	0	14	0.24	0.46	0.12	0.18
20	2	2	7	4	0	15	0.26	0.42	0.11	0.22

[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

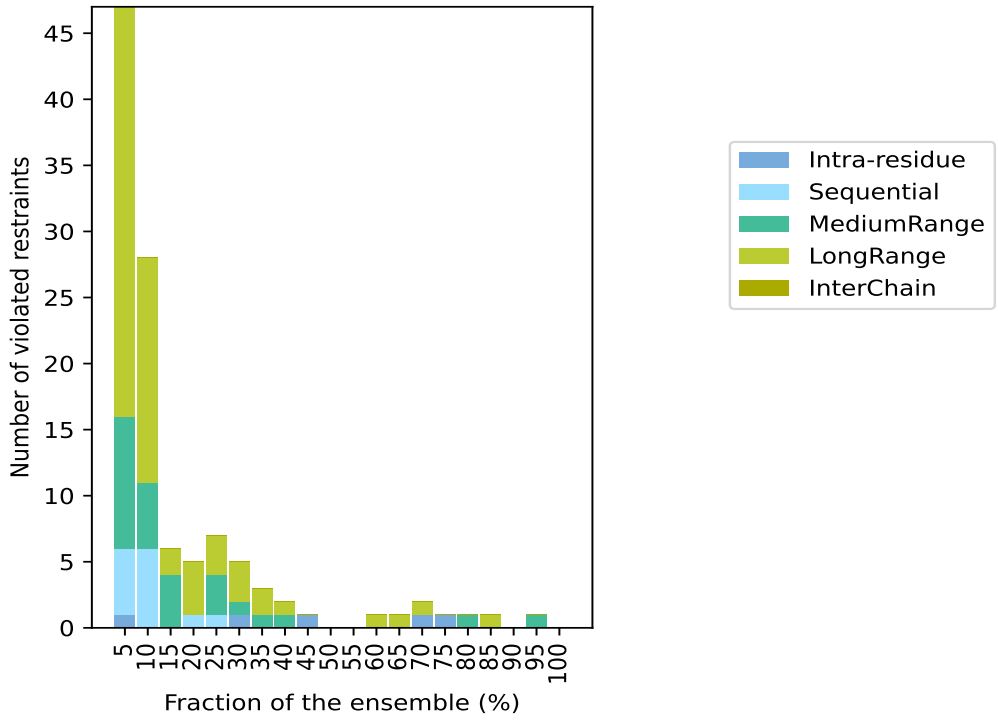
9.3 Distance violation statistics for the ensemble (i)

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, 1319(IR:340, SQ:401, MR:178, LR:400, IC:0) 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]	%
1	5	10	31	0	47	1	5.0
0	6	5	17	0	28	2	10.0
0	0	4	2	0	6	3	15.0
0	1	0	4	0	5	4	20.0
0	1	3	3	0	7	5	25.0
1	0	1	3	0	5	6	30.0
0	0	1	2	0	3	7	35.0
0	0	1	1	0	2	8	40.0
1	0	0	0	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	1	0	1	12	60.0
0	0	0	1	0	1	13	65.0
1	0	0	1	0	2	14	70.0
1	0	0	0	0	1	15	75.0
0	0	1	0	0	1	16	80.0
0	0	0	1	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	1	0	0	1	19	95.0
0	0	0	0	0	0	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

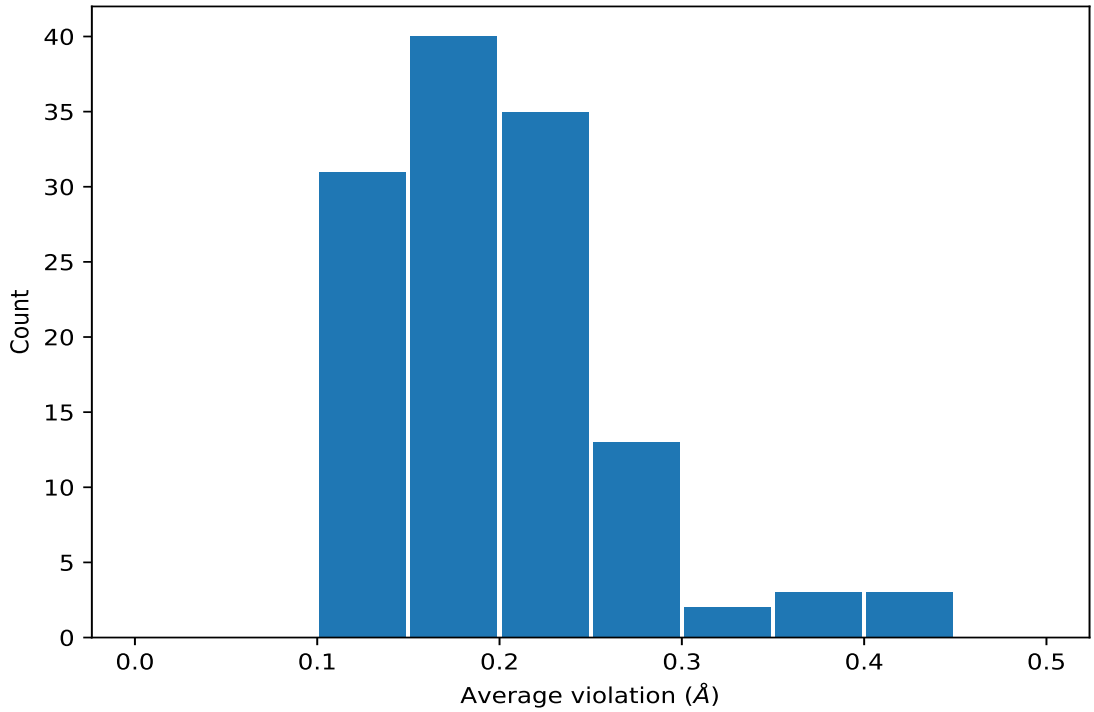
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	19	0.38	0.07	0.39
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	17	0.21	0.07	0.22
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	16	0.19	0.04	0.18
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	16	0.19	0.04	0.18
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	15	0.18	0.09	0.15
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	15	0.18	0.09	0.15
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	14	0.2	0.1	0.16
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	14	0.17	0.04	0.18
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	14	0.17	0.04	0.18
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	14	0.17	0.04	0.18
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	14	0.17	0.04	0.18
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	13	0.26	0.07	0.24
(1,935)	1:A:51:TRP:HE1	1:A:57:VAL:HB	12	0.24	0.07	0.24
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD2	9	0.41	0.14	0.47
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD3	9	0.41	0.14	0.47
(1,426)	1:A:21:ALA:HA	1:A:24:GLU:HB3	8	0.33	0.08	0.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG21	8	0.21	0.07	0.2
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG22	8	0.21	0.07	0.2
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG23	8	0.21	0.07	0.2
(1,1020)	1:A:54:LYS:H	1:A:56:ARG:HB3	7	0.43	0.27	0.41
(1,1144)	1:A:62:VAL:HB	1:A:74:GLY:H	7	0.21	0.11	0.16
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG12	7	0.16	0.04	0.16
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG13	7	0.16	0.04	0.16
(1,104)	1:A:5:ARG:HE	1:A:93:TYR:H	6	0.36	0.17	0.32
(1,272)	1:A:14:LEU:HB2	1:A:18:GLU:H	6	0.3	0.09	0.33
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG2	6	0.28	0.04	0.28
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG3	6	0.28	0.04	0.28
(1,327)	1:A:16:TYR:HB3	1:A:51:TRP:HA	6	0.22	0.04	0.22
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG21	6	0.2	0.09	0.16
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG22	6	0.2	0.09	0.16
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG23	6	0.2	0.09	0.16
(1,219)	1:A:11:LYS:H	1:A:13:LYS:HB2	5	0.27	0.06	0.25
(1,219)	1:A:11:LYS:H	1:A:13:LYS:HB3	5	0.27	0.06	0.25
(1,886)	1:A:49:ALA:HB1	1:A:68:CYS:HB2	5	0.23	0.02	0.23
(1,886)	1:A:49:ALA:HB2	1:A:68:CYS:HB2	5	0.23	0.02	0.23
(1,886)	1:A:49:ALA:HB3	1:A:68:CYS:HB2	5	0.23	0.02	0.23
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB1	5	0.22	0.09	0.18
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB2	5	0.22	0.09	0.18
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB3	5	0.22	0.09	0.18
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB1	5	0.22	0.09	0.18
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB2	5	0.22	0.09	0.18
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB3	5	0.22	0.09	0.18
(1,642)	1:A:33:TYR:H	1:A:56:ARG:HB2	5	0.22	0.06	0.2
(1,816)	1:A:43:GLY:HA3	1:A:45:HIS:HB3	5	0.18	0.05	0.14
(1,310)	1:A:15:THR:HG21	1:A:85:SER:HB2	5	0.13	0.02	0.11
(1,310)	1:A:15:THR:HG21	1:A:85:SER:HB3	5	0.13	0.02	0.11
(1,310)	1:A:15:THR:HG22	1:A:85:SER:HB2	5	0.13	0.02	0.11
(1,310)	1:A:15:THR:HG22	1:A:85:SER:HB3	5	0.13	0.02	0.11
(1,310)	1:A:15:THR:HG23	1:A:85:SER:HB2	5	0.13	0.02	0.11
(1,310)	1:A:15:THR:HG23	1:A:85:SER:HB3	5	0.13	0.02	0.11
(1,410)	1:A:20:LYS:HB2	1:A:24:GLU:HG2	5	0.13	0.02	0.12
(1,410)	1:A:20:LYS:HB3	1:A:24:GLU:HG2	5	0.13	0.02	0.12
(1,355)	1:A:17:ALA:H	1:A:84:ARG:HB3	4	0.26	0.13	0.23
(1,338)	1:A:16:TYR:HD1	1:A:51:TRP:HA	4	0.23	0.09	0.21
(1,338)	1:A:16:TYR:HD2	1:A:51:TRP:HA	4	0.23	0.09	0.21
(1,1115)	1:A:59:TYR:H	1:A:77:ASP:HB2	4	0.2	0.04	0.22
(1,1115)	1:A:59:TYR:H	1:A:77:ASP:HB3	4	0.2	0.04	0.22
(1,1329)	1:A:85:SER:H	1:A:86:GLU:HB3	4	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,288)	1:A:14:LEU:HG	1:A:51:TRP:HE1	4	0.13	0.01	0.13
(1,1027)	1:A:55:GLY:H	1:A:80:ILE:HG21	3	0.18	0.06	0.18
(1,1027)	1:A:55:GLY:H	1:A:80:ILE:HG22	3	0.18	0.06	0.18
(1,1027)	1:A:55:GLY:H	1:A:80:ILE:HG23	3	0.18	0.06	0.18
(1,1280)	1:A:81:ARG:HA	1:A:83:ASN:HB2	3	0.16	0.05	0.14
(1,1280)	1:A:81:ARG:HA	1:A:83:ASN:HB3	3	0.16	0.05	0.14
(1,807)	1:A:42:ILE:HG21	1:A:45:HIS:H	3	0.15	0.03	0.15
(1,807)	1:A:42:ILE:HG22	1:A:45:HIS:H	3	0.15	0.03	0.15
(1,807)	1:A:42:ILE:HG23	1:A:45:HIS:H	3	0.15	0.03	0.15
(1,279)	1:A:14:LEU:HD11	1:A:18:GLU:H	3	0.15	0.02	0.14
(1,279)	1:A:14:LEU:HD12	1:A:18:GLU:H	3	0.15	0.02	0.14
(1,279)	1:A:14:LEU:HD13	1:A:18:GLU:H	3	0.15	0.02	0.14
(1,279)	1:A:14:LEU:HD21	1:A:18:GLU:H	3	0.15	0.02	0.14
(1,279)	1:A:14:LEU:HD22	1:A:18:GLU:H	3	0.15	0.02	0.14
(1,279)	1:A:14:LEU:HD23	1:A:18:GLU:H	3	0.15	0.02	0.14
(1,415)	1:A:20:LYS:HG2	1:A:24:GLU:HG2	3	0.14	0.03	0.12
(1,415)	1:A:20:LYS:HG3	1:A:24:GLU:HG2	3	0.14	0.03	0.12
(1,56)	1:A:3:TYR:HD1	1:A:93:TYR:H	3	0.13	0.01	0.14
(1,56)	1:A:3:TYR:HD2	1:A:93:TYR:H	3	0.13	0.01	0.14
(1,758)	1:A:40:ARG:HE	1:A:74:GLY:H	2	0.36	0.04	0.36
(1,968)	1:A:52:MET:HB3	1:A:56:ARG:HB2	2	0.31	0.07	0.31
(1,760)	1:A:40:ARG:HE	1:A:75:ILE:H	2	0.26	0.08	0.26
(1,483)	1:A:24:GLU:H	1:A:25:PHE:HB2	2	0.26	0.13	0.26
(1,1112)	1:A:59:TYR:H	1:A:76:ILE:HG21	2	0.26	0.04	0.26
(1,1112)	1:A:59:TYR:H	1:A:76:ILE:HG22	2	0.26	0.04	0.26
(1,1112)	1:A:59:TYR:H	1:A:76:ILE:HG23	2	0.26	0.04	0.26
(1,949)	1:A:51:TRP:H	1:A:57:VAL:HB	2	0.25	0.09	0.25
(1,195)	1:A:10:GLY:H	1:A:13:LYS:H	2	0.22	0.08	0.22
(1,20)	1:A:2:VAL:HG11	1:A:93:TYR:HB3	2	0.22	0.07	0.22
(1,20)	1:A:2:VAL:HG12	1:A:93:TYR:HB3	2	0.22	0.07	0.22
(1,20)	1:A:2:VAL:HG13	1:A:93:TYR:HB3	2	0.22	0.07	0.22
(1,1140)	1:A:62:VAL:HB	1:A:63:LYS:HE3	2	0.22	0.07	0.22
(1,1106)	1:A:59:TYR:HB2	1:A:91:TYR:HE1	2	0.21	0.05	0.21
(1,1106)	1:A:59:TYR:HB2	1:A:91:TYR:HE2	2	0.21	0.05	0.21
(1,1127)	1:A:61:ILE:HD11	1:A:76:ILE:HA	2	0.21	0.05	0.21
(1,1127)	1:A:61:ILE:HD12	1:A:76:ILE:HA	2	0.21	0.05	0.21
(1,1127)	1:A:61:ILE:HD13	1:A:76:ILE:HA	2	0.21	0.05	0.21
(1,24)	1:A:2:VAL:HG21	1:A:93:TYR:HB3	2	0.19	0.0	0.19
(1,24)	1:A:2:VAL:HG22	1:A:93:TYR:HB3	2	0.19	0.0	0.19
(1,24)	1:A:2:VAL:HG23	1:A:93:TYR:HB3	2	0.19	0.0	0.19
(1,1310)	1:A:83:ASN:HD22	1:A:86:GLU:HA	2	0.18	0.02	0.18
(1,1323)	1:A:84:ARG:HD2	1:A:85:SER:HB2	2	0.18	0.05	0.18

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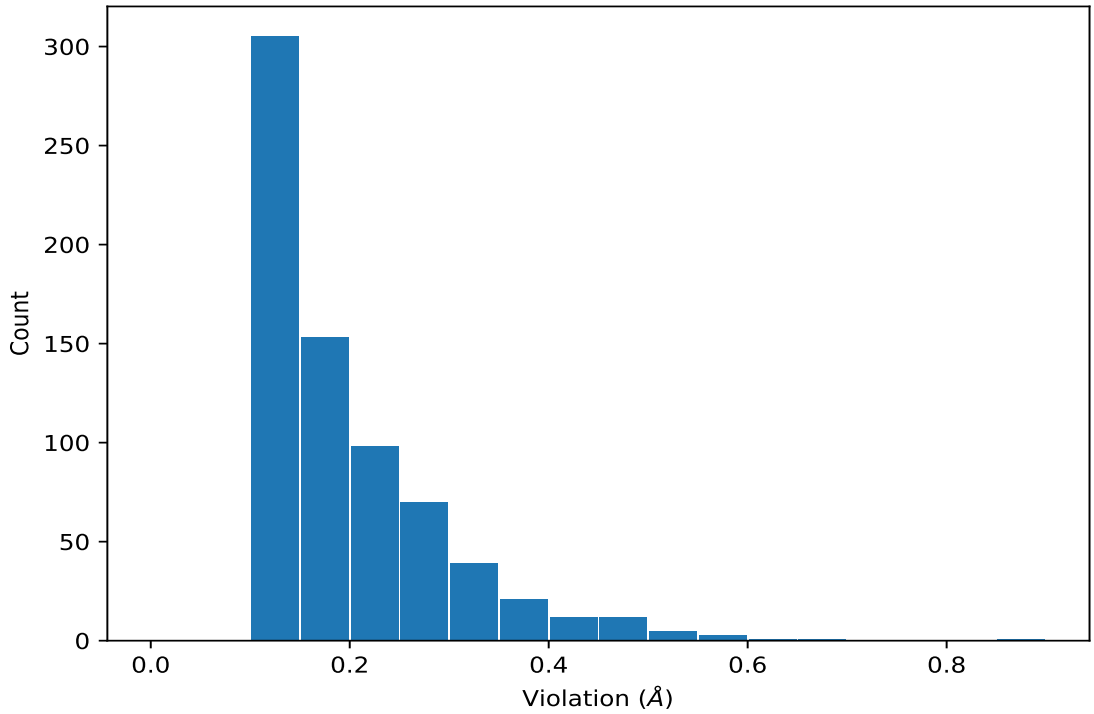
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1323)	1:A:84:ARG:HD2	1:A:85:SER:HB3	2	0.18	0.05	0.18
(1,1323)	1:A:84:ARG:HD3	1:A:85:SER:HB2	2	0.18	0.05	0.18
(1,1323)	1:A:84:ARG:HD3	1:A:85:SER:HB3	2	0.18	0.05	0.18
(1,677)	1:A:35:GLN:H	1:A:36:LEU:HG	2	0.18	0.03	0.18
(1,1057)	1:A:57:VAL:HB	1:A:81:ARG:HG2	2	0.18	0.02	0.18
(1,837)	1:A:45:HIS:HB3	1:A:62:VAL:HB	2	0.17	0.06	0.17
(1,1166)	1:A:64:PRO:HB2	1:A:73:THR:HG21	2	0.17	0.0	0.17
(1,1166)	1:A:64:PRO:HB2	1:A:73:THR:HG22	2	0.17	0.0	0.17
(1,1166)	1:A:64:PRO:HB2	1:A:73:THR:HG23	2	0.17	0.0	0.17
(1,1166)	1:A:64:PRO:HB3	1:A:73:THR:HG21	2	0.17	0.0	0.17
(1,1166)	1:A:64:PRO:HB3	1:A:73:THR:HG22	2	0.17	0.0	0.17
(1,1166)	1:A:64:PRO:HB3	1:A:73:THR:HG23	2	0.17	0.0	0.17
(1,1035)	1:A:56:ARG:HB3	1:A:80:ILE:HD11	2	0.17	0.02	0.17
(1,1035)	1:A:56:ARG:HB3	1:A:80:ILE:HD12	2	0.17	0.02	0.17
(1,1035)	1:A:56:ARG:HB3	1:A:80:ILE:HD13	2	0.17	0.02	0.17
(1,1141)	1:A:62:VAL:HB	1:A:63:LYS:HE2	2	0.16	0.02	0.16
(1,621)	1:A:33:TYR:HB3	1:A:56:ARG:HB2	2	0.16	0.01	0.16
(1,938)	1:A:51:TRP:HE1	1:A:86:GLU:HB3	2	0.16	0.02	0.16
(1,623)	1:A:33:TYR:HB2	1:A:56:ARG:HB2	2	0.16	0.04	0.16
(1,606)	1:A:32:THR:H	1:A:35:GLN:HE22	2	0.15	0.03	0.15
(1,1194)	1:A:72:LYS:H	1:A:73:THR:HB	2	0.14	0.02	0.14
(1,394)	1:A:20:LYS:HA	1:A:24:GLU:HG3	2	0.13	0.01	0.13
(1,567)	1:A:31:ALA:HA	1:A:93:TYR:HE1	2	0.12	0.01	0.12
(1,567)	1:A:31:ALA:HA	1:A:93:TYR:HE2	2	0.12	0.01	0.12
(1,145)	1:A:7:ALA:HB1	1:A:14:LEU:HG	2	0.12	0.0	0.12
(1,145)	1:A:7:ALA:HB2	1:A:14:LEU:HG	2	0.12	0.0	0.12
(1,145)	1:A:7:ALA:HB3	1:A:14:LEU:HG	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)
(1,1020)	1:A:54:LYS:H	1:A:56:ARG:HB3	8	0.88
(1,1020)	1:A:54:LYS:H	1:A:56:ARG:HB3	16	0.65
(1,104)	1:A:5:ARG:HE	1:A:93:TYR:H	6	0.64
(1,1020)	1:A:54:LYS:H	1:A:56:ARG:HB3	4	0.58
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD2	10	0.55
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD3	10	0.55
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD2	5	0.54
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD3	5	0.54
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	1	0.51
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD2	3	0.5
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD3	3	0.5
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	9	0.49
(1,104)	1:A:5:ARG:HE	1:A:93:TYR:H	12	0.49
(1,426)	1:A:21:ALA:HA	1:A:24:GLU:HB3	3	0.47
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD2	12	0.47
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD3	12	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD2	13	0.47
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD3	13	0.47
(1,355)	1:A:17:ALA:H	1:A:84:ARG:HB3	14	0.47
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	5	0.46
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD2	19	0.46
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD3	19	0.46
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	7	0.45
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	8	0.43
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	11	0.43
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	5	0.43
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	5	0.43
(1,1288)	1:A:81:ARG:H	1:A:81:ARG:HE	12	0.43
(1,1144)	1:A:62:VAL:HB	1:A:74:GLY:H	15	0.43
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	4	0.43
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	3	0.42
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	20	0.42
(1,426)	1:A:21:ALA:HA	1:A:24:GLU:HB3	20	0.42
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	1	0.41
(1,1020)	1:A:54:LYS:H	1:A:56:ARG:HB3	13	0.41
(1,758)	1:A:40:ARG:HE	1:A:74:GLY:H	1	0.39
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	4	0.39
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	16	0.39
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	19	0.39
(1,483)	1:A:24:GLU:H	1:A:25:PHE:HB2	20	0.39
(1,272)	1:A:14:LEU:HB2	1:A:18:GLU:H	17	0.39
(1,968)	1:A:52:MET:HB3	1:A:56:ARG:HB2	11	0.38
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	2	0.38
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	12	0.38
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG21	18	0.38
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG22	18	0.38
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG23	18	0.38
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	14	0.38
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	15	0.37
(1,338)	1:A:16:TYR:HD1	1:A:51:TRP:HA	14	0.37
(1,338)	1:A:16:TYR:HD2	1:A:51:TRP:HA	14	0.37
(1,272)	1:A:14:LEU:HB2	1:A:18:GLU:H	20	0.37
(1,219)	1:A:11:LYS:H	1:A:13:LYS:HB2	20	0.37
(1,219)	1:A:11:LYS:H	1:A:13:LYS:HB3	20	0.37
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	14	0.36
(1,104)	1:A:5:ARG:HE	1:A:93:TYR:H	19	0.36
(1,426)	1:A:21:ALA:HA	1:A:24:GLU:HB3	6	0.35
(1,426)	1:A:21:ALA:HA	1:A:24:GLU:HB3	19	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:A:14:LEU:HB2	1:A:18:GLU:H	8	0.35
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	19	0.35
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	19	0.35
(1,949)	1:A:51:TRP:H	1:A:57:VAL:HB	3	0.34
(1,935)	1:A:51:TRP:HE1	1:A:57:VAL:HB	2	0.34
(1,935)	1:A:51:TRP:HE1	1:A:57:VAL:HB	3	0.34
(1,760)	1:A:40:ARG:HE	1:A:75:ILE:H	9	0.34
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	9	0.34
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD2	18	0.34
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD3	18	0.34
(1,758)	1:A:40:ARG:HE	1:A:74:GLY:H	16	0.32
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	10	0.32
(1,426)	1:A:21:ALA:HA	1:A:24:GLU:HB3	2	0.32
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG2	1	0.32
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG3	1	0.32
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG2	6	0.32
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG3	6	0.32
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB1	14	0.32
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB2	14	0.32
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB3	14	0.32
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB1	14	0.32
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB2	14	0.32
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB3	14	0.32
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB1	20	0.32
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB2	20	0.32
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB3	20	0.32
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB1	20	0.32
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB2	20	0.32
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB3	20	0.32
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG21	2	0.32
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG22	2	0.32
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG23	2	0.32
(1,1144)	1:A:62:VAL:HB	1:A:74:GLY:H	13	0.32
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG2	15	0.31
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG3	15	0.31
(1,272)	1:A:14:LEU:HB2	1:A:18:GLU:H	13	0.31
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	1	0.31
(1,935)	1:A:51:TRP:HE1	1:A:57:VAL:HB	18	0.3
(1,642)	1:A:33:TYR:H	1:A:56:ARG:HB2	4	0.3
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	2	0.3
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	16	0.3
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	18	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:A:21:ALA:HA	1:A:24:GLU:HB3	15	0.3
(1,219)	1:A:11:LYS:H	1:A:13:LYS:HB2	16	0.3
(1,219)	1:A:11:LYS:H	1:A:13:LYS:HB3	16	0.3
(1,195)	1:A:10:GLY:H	1:A:13:LYS:H	9	0.3
(1,1112)	1:A:59:TYR:H	1:A:76:ILE:HG21	2	0.3
(1,1112)	1:A:59:TYR:H	1:A:76:ILE:HG22	2	0.3
(1,1112)	1:A:59:TYR:H	1:A:76:ILE:HG23	2	0.3
(1,20)	1:A:2:VAL:HG11	1:A:93:TYR:HB3	18	0.29
(1,20)	1:A:2:VAL:HG12	1:A:93:TYR:HB3	18	0.29
(1,20)	1:A:2:VAL:HG13	1:A:93:TYR:HB3	18	0.29
(1,1140)	1:A:62:VAL:HB	1:A:63:LYS:HE3	2	0.29
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	6	0.28
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	1	0.28
(1,355)	1:A:17:ALA:H	1:A:84:ARG:HB3	3	0.28
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	17	0.28
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	17	0.28
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG21	15	0.28
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG22	15	0.28
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG23	15	0.28
(1,104)	1:A:5:ARG:HE	1:A:93:TYR:H	17	0.28
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	16	0.28
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	19	0.28
(1,935)	1:A:51:TRP:HE1	1:A:57:VAL:HB	7	0.27
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	15	0.27
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	15	0.27
(1,426)	1:A:21:ALA:HA	1:A:24:GLU:HB3	16	0.27
(1,327)	1:A:16:TYR:HB3	1:A:51:TRP:HA	3	0.27
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	17	0.27
(1,935)	1:A:51:TRP:HE1	1:A:57:VAL:HB	12	0.26
(1,816)	1:A:43:GLY:HA3	1:A:45:HIS:HB3	9	0.26
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	14	0.26
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	14	0.26
(1,642)	1:A:33:TYR:H	1:A:56:ARG:HB2	9	0.26
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	14	0.26
(1,338)	1:A:16:TYR:HD1	1:A:51:TRP:HA	7	0.26
(1,338)	1:A:16:TYR:HD2	1:A:51:TRP:HA	7	0.26
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG21	13	0.26
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG22	13	0.26
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG23	13	0.26
(1,1127)	1:A:61:ILE:HD11	1:A:76:ILE:HA	13	0.26
(1,1127)	1:A:61:ILE:HD12	1:A:76:ILE:HA	13	0.26
(1,1127)	1:A:61:ILE:HD13	1:A:76:ILE:HA	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:A:59:TYR:HB2	1:A:91:TYR:HE1	6	0.26
(1,1106)	1:A:59:TYR:HB2	1:A:91:TYR:HE2	6	0.26
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG21	3	0.26
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG22	3	0.26
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG23	3	0.26
(1,886)	1:A:49:ALA:HB1	1:A:68:CYS:HB2	8	0.25
(1,886)	1:A:49:ALA:HB2	1:A:68:CYS:HB2	8	0.25
(1,886)	1:A:49:ALA:HB3	1:A:68:CYS:HB2	8	0.25
(1,886)	1:A:49:ALA:HB1	1:A:68:CYS:HB2	13	0.25
(1,886)	1:A:49:ALA:HB2	1:A:68:CYS:HB2	13	0.25
(1,886)	1:A:49:ALA:HB3	1:A:68:CYS:HB2	13	0.25
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	4	0.25
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	4	0.25
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	18	0.25
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	5	0.25
(1,327)	1:A:16:TYR:HB3	1:A:51:TRP:HA	18	0.25
(1,219)	1:A:11:LYS:H	1:A:13:LYS:HB2	2	0.25
(1,219)	1:A:11:LYS:H	1:A:13:LYS:HB3	2	0.25
(1,1090)	1:A:57:VAL:H	1:A:81:ARG:HD3	20	0.25
(1,1054)	1:A:57:VAL:HB	1:A:81:ARG:HD3	4	0.25
(1,1027)	1:A:55:GLY:H	1:A:80:ILE:HG21	6	0.25
(1,1027)	1:A:55:GLY:H	1:A:80:ILE:HG22	6	0.25
(1,1027)	1:A:55:GLY:H	1:A:80:ILE:HG23	6	0.25
(1,968)	1:A:52:MET:HB3	1:A:56:ARG:HB2	4	0.24
(1,935)	1:A:51:TRP:HE1	1:A:57:VAL:HB	16	0.24
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	8	0.24
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	8	0.24
(1,640)	1:A:33:TYR:H	1:A:36:LEU:HB3	13	0.24
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG2	9	0.24
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG3	9	0.24
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG2	18	0.24
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG3	18	0.24
(1,1323)	1:A:84:ARG:HD2	1:A:85:SER:HB2	16	0.24
(1,1323)	1:A:84:ARG:HD2	1:A:85:SER:HB3	16	0.24
(1,1323)	1:A:84:ARG:HD3	1:A:85:SER:HB2	16	0.24
(1,1323)	1:A:84:ARG:HD3	1:A:85:SER:HB3	16	0.24
(1,1115)	1:A:59:TYR:H	1:A:77:ASP:HB2	5	0.24
(1,1115)	1:A:59:TYR:H	1:A:77:ASP:HB3	5	0.24
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG12	4	0.24
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG13	4	0.24
(1,104)	1:A:5:ARG:HE	1:A:93:TYR:H	10	0.24
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,935)	1:A:51:TRP:HE1	1:A:57:VAL:HB	10	0.23
(1,935)	1:A:51:TRP:HE1	1:A:57:VAL:HB	17	0.23
(1,911)	1:A:50:GLY:H	1:A:59:TYR:HB2	6	0.23
(1,911)	1:A:50:GLY:H	1:A:59:TYR:HB3	6	0.23
(1,886)	1:A:49:ALA:HB1	1:A:68:CYS:HB2	11	0.23
(1,886)	1:A:49:ALA:HB2	1:A:68:CYS:HB2	11	0.23
(1,886)	1:A:49:ALA:HB3	1:A:68:CYS:HB2	11	0.23
(1,837)	1:A:45:HIS:HB3	1:A:62:VAL:HB	15	0.23
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	6	0.23
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	6	0.23
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	8	0.23
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	13	0.23
(1,568)	1:A:31:ALA:HA	1:A:93:TYR:H	15	0.23
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	13	0.23
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG2	16	0.23
(1,367)	1:A:18:GLU:H	1:A:18:GLU:HG3	16	0.23
(1,327)	1:A:16:TYR:HB3	1:A:51:TRP:HA	8	0.23
(1,272)	1:A:14:LEU:HB2	1:A:18:GLU:H	4	0.23
(1,219)	1:A:11:LYS:H	1:A:13:LYS:HB2	14	0.23
(1,219)	1:A:11:LYS:H	1:A:13:LYS:HB3	14	0.23
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	3	0.23
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	3	0.23
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	3	0.23
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	3	0.23
(1,1280)	1:A:81:ARG:HA	1:A:83:ASN:HB2	14	0.23
(1,1280)	1:A:81:ARG:HA	1:A:83:ASN:HB3	14	0.23
(1,1053)	1:A:57:VAL:HB	1:A:78:TYR:HB2	2	0.23
(1,1053)	1:A:57:VAL:HB	1:A:78:TYR:HB3	2	0.23
(1,816)	1:A:43:GLY:HA3	1:A:45:HIS:HB3	10	0.22
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	12	0.22
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	4	0.22
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	7	0.22
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	7	0.22
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	7	0.22
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	7	0.22
(1,1115)	1:A:59:TYR:H	1:A:77:ASP:HB2	3	0.22
(1,1115)	1:A:59:TYR:H	1:A:77:ASP:HB3	3	0.22
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	13	0.22
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	20	0.22
(1,935)	1:A:51:TRP:HE1	1:A:57:VAL:HB	9	0.21
(1,886)	1:A:49:ALA:HB1	1:A:68:CYS:HB2	4	0.21
(1,886)	1:A:49:ALA:HB2	1:A:68:CYS:HB2	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,886)	1:A:49:ALA:HB3	1:A:68:CYS:HB2	4	0.21
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	18	0.21
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	18	0.21
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	20	0.21
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	20	0.21
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	11	0.21
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG21	5	0.21
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG22	5	0.21
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG23	5	0.21
(1,1115)	1:A:59:TYR:H	1:A:77:ASP:HB2	4	0.21
(1,1115)	1:A:59:TYR:H	1:A:77:ASP:HB3	4	0.21
(1,1112)	1:A:59:TYR:H	1:A:76:ILE:HG21	12	0.21
(1,1112)	1:A:59:TYR:H	1:A:76:ILE:HG22	12	0.21
(1,1112)	1:A:59:TYR:H	1:A:76:ILE:HG23	12	0.21
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	6	0.21
(1,942)	1:A:51:TRP:HE1	1:A:88:TRP:H	12	0.2
(1,886)	1:A:49:ALA:HB1	1:A:68:CYS:HB2	12	0.2
(1,886)	1:A:49:ALA:HB2	1:A:68:CYS:HB2	12	0.2
(1,886)	1:A:49:ALA:HB3	1:A:68:CYS:HB2	12	0.2
(1,863)	1:A:47:CYS:H	1:A:61:ILE:HD11	5	0.2
(1,863)	1:A:47:CYS:H	1:A:61:ILE:HD12	5	0.2
(1,863)	1:A:47:CYS:H	1:A:61:ILE:HD13	5	0.2
(1,677)	1:A:35:GLN:H	1:A:36:LEU:HG	12	0.2
(1,642)	1:A:33:TYR:H	1:A:56:ARG:HB2	14	0.2
(1,634)	1:A:33:TYR:HE1	1:A:77:ASP:HB2	2	0.2
(1,634)	1:A:33:TYR:HE2	1:A:77:ASP:HB2	2	0.2
(1,327)	1:A:16:TYR:HB3	1:A:51:TRP:HA	16	0.2
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	5	0.2
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	5	0.2
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	5	0.2
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	5	0.2
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	6	0.2
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	6	0.2
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	6	0.2
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	6	0.2
(1,1310)	1:A:83:ASN:HD22	1:A:86:GLU:HA	1	0.2
(1,1020)	1:A:54:LYS:H	1:A:56:ARG:HB3	11	0.2
(1,807)	1:A:42:ILE:HG21	1:A:45:HIS:H	8	0.19
(1,807)	1:A:42:ILE:HG22	1:A:45:HIS:H	8	0.19
(1,807)	1:A:42:ILE:HG23	1:A:45:HIS:H	8	0.19
(1,760)	1:A:40:ARG:HE	1:A:75:ILE:H	13	0.19
(1,623)	1:A:33:TYR:HB2	1:A:56:ARG:HB2	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	3	0.19
(1,426)	1:A:21:ALA:HA	1:A:24:GLU:HB3	14	0.19
(1,327)	1:A:16:TYR:HB3	1:A:51:TRP:HA	17	0.19
(1,24)	1:A:2:VAL:HG21	1:A:93:TYR:HB3	3	0.19
(1,24)	1:A:2:VAL:HG22	1:A:93:TYR:HB3	3	0.19
(1,24)	1:A:2:VAL:HG23	1:A:93:TYR:HB3	3	0.19
(1,24)	1:A:2:VAL:HG21	1:A:93:TYR:HB3	19	0.19
(1,24)	1:A:2:VAL:HG22	1:A:93:TYR:HB3	19	0.19
(1,24)	1:A:2:VAL:HG23	1:A:93:TYR:HB3	19	0.19
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	14	0.19
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	14	0.19
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	14	0.19
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	14	0.19
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	15	0.19
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	15	0.19
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	15	0.19
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	15	0.19
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	20	0.19
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	20	0.19
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	20	0.19
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	20	0.19
(1,1144)	1:A:62:VAL:HB	1:A:74:GLY:H	18	0.19
(1,1141)	1:A:62:VAL:HB	1:A:63:LYS:HE2	5	0.19
(1,1103)	1:A:58:GLY:H	1:A:78:TYR:H	2	0.19
(1,1057)	1:A:57:VAL:HB	1:A:81:ARG:HG2	13	0.19
(1,1035)	1:A:56:ARG:HB3	1:A:80:ILE:HD11	16	0.19
(1,1035)	1:A:56:ARG:HB3	1:A:80:ILE:HD12	16	0.19
(1,1035)	1:A:56:ARG:HB3	1:A:80:ILE:HD13	16	0.19
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	7	0.19
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	17	0.18
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	17	0.18
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD2	4	0.18
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD3	4	0.18
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD2	20	0.18
(1,419)	1:A:20:LYS:H	1:A:20:LYS:HD3	20	0.18
(1,415)	1:A:20:LYS:HG2	1:A:24:GLU:HG2	7	0.18
(1,415)	1:A:20:LYS:HG3	1:A:24:GLU:HG2	7	0.18
(1,279)	1:A:14:LEU:HD11	1:A:18:GLU:H	5	0.18
(1,279)	1:A:14:LEU:HD12	1:A:18:GLU:H	5	0.18
(1,279)	1:A:14:LEU:HD13	1:A:18:GLU:H	5	0.18
(1,279)	1:A:14:LEU:HD21	1:A:18:GLU:H	5	0.18
(1,279)	1:A:14:LEU:HD22	1:A:18:GLU:H	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,279)	1:A:14:LEU:HD23	1:A:18:GLU:H	5	0.18
(1,219)	1:A:11:LYS:H	1:A:13:LYS:HB2	10	0.18
(1,219)	1:A:11:LYS:H	1:A:13:LYS:HB3	10	0.18
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	1	0.18
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	1	0.18
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	1	0.18
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	1	0.18
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	8	0.18
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	8	0.18
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	8	0.18
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	8	0.18
(1,1343)	1:A:86:GLU:H	1:A:88:TRP:HE1	12	0.18
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB1	16	0.18
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB2	16	0.18
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB3	16	0.18
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB1	16	0.18
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB2	16	0.18
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB3	16	0.18
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG21	6	0.18
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG22	6	0.18
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG23	6	0.18
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	3	0.18
(1,1027)	1:A:55:GLY:H	1:A:80:ILE:HG21	8	0.18
(1,1027)	1:A:55:GLY:H	1:A:80:ILE:HG22	8	0.18
(1,1027)	1:A:55:GLY:H	1:A:80:ILE:HG23	8	0.18
(1,938)	1:A:51:TRP:HE1	1:A:86:GLU:HB3	9	0.17
(1,935)	1:A:51:TRP:HE1	1:A:57:VAL:HB	5	0.17
(1,87)	1:A:5:ARG:HA	1:A:22:VAL:HG11	9	0.17
(1,87)	1:A:5:ARG:HA	1:A:22:VAL:HG12	9	0.17
(1,87)	1:A:5:ARG:HA	1:A:22:VAL:HG13	9	0.17
(1,87)	1:A:5:ARG:HA	1:A:22:VAL:HG21	9	0.17
(1,87)	1:A:5:ARG:HA	1:A:22:VAL:HG22	9	0.17
(1,87)	1:A:5:ARG:HA	1:A:22:VAL:HG23	9	0.17
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	12	0.17
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	12	0.17
(1,621)	1:A:33:TYR:HB3	1:A:56:ARG:HB2	1	0.17
(1,606)	1:A:32:THR:H	1:A:35:GLN:HE22	8	0.17
(1,593)	1:A:32:THR:HB	1:A:35:GLN:HG3	20	0.17
(1,355)	1:A:17:ALA:H	1:A:84:ARG:HB3	12	0.17
(1,310)	1:A:15:THR:HG21	1:A:85:SER:HB2	7	0.17
(1,310)	1:A:15:THR:HG21	1:A:85:SER:HB3	7	0.17
(1,310)	1:A:15:THR:HG22	1:A:85:SER:HB2	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,310)	1:A:15:THR:HG22	1:A:85:SER:HB3	7	0.17
(1,310)	1:A:15:THR:HG23	1:A:85:SER:HB2	7	0.17
(1,310)	1:A:15:THR:HG23	1:A:85:SER:HB3	7	0.17
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	13	0.17
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	13	0.17
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	13	0.17
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	13	0.17
(1,1310)	1:A:83:ASN:HD22	1:A:86:GLU:HA	16	0.17
(1,1247)	1:A:77:ASP:H	1:A:78:TYR:HE1	6	0.17
(1,1247)	1:A:77:ASP:H	1:A:78:TYR:HE2	6	0.17
(1,1166)	1:A:64:PRO:HB2	1:A:73:THR:HG21	2	0.17
(1,1166)	1:A:64:PRO:HB2	1:A:73:THR:HG22	2	0.17
(1,1166)	1:A:64:PRO:HB2	1:A:73:THR:HG23	2	0.17
(1,1166)	1:A:64:PRO:HB3	1:A:73:THR:HG21	2	0.17
(1,1166)	1:A:64:PRO:HB3	1:A:73:THR:HG22	2	0.17
(1,1166)	1:A:64:PRO:HB3	1:A:73:THR:HG23	2	0.17
(1,1166)	1:A:64:PRO:HB2	1:A:73:THR:HG21	13	0.17
(1,1166)	1:A:64:PRO:HB2	1:A:73:THR:HG22	13	0.17
(1,1166)	1:A:64:PRO:HB2	1:A:73:THR:HG23	13	0.17
(1,1166)	1:A:64:PRO:HB3	1:A:73:THR:HG21	13	0.17
(1,1166)	1:A:64:PRO:HB3	1:A:73:THR:HG22	13	0.17
(1,1166)	1:A:64:PRO:HB3	1:A:73:THR:HG23	13	0.17
(1,1135)	1:A:61:ILE:HG21	1:A:73:THR:HB	19	0.17
(1,1135)	1:A:61:ILE:HG22	1:A:73:THR:HB	19	0.17
(1,1135)	1:A:61:ILE:HG23	1:A:73:THR:HB	19	0.17
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG21	13	0.17
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG22	13	0.17
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG23	13	0.17
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG12	9	0.17
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG13	9	0.17
(1,1034)	1:A:56:ARG:HB3	1:A:79:GLY:H	10	0.17
(1,949)	1:A:51:TRP:H	1:A:57:VAL:HB	14	0.16
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	1	0.16
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	1	0.16
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	10	0.16
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	10	0.16
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	13	0.16
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	13	0.16
(1,642)	1:A:33:TYR:H	1:A:56:ARG:HB2	10	0.16
(1,642)	1:A:33:TYR:H	1:A:56:ARG:HB2	11	0.16
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	7	0.16
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	17	0.16
(1,338)	1:A:16:TYR:HD1	1:A:51:TRP:HA	9	0.16
(1,338)	1:A:16:TYR:HD2	1:A:51:TRP:HA	9	0.16
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	16	0.16
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	16	0.16
(1,1409)	1:A:95:PRO:HD2	1:A:97:ALA:H	15	0.16
(1,1409)	1:A:95:PRO:HD3	1:A:97:ALA:H	15	0.16
(1,1329)	1:A:85:SER:H	1:A:86:GLU:HB3	8	0.16
(1,126)	1:A:6:GLU:HG2	1:A:11:LYS:HA	17	0.16
(1,122)	1:A:6:GLU:HA	1:A:89:ASP:HA	2	0.16
(1,1194)	1:A:72:LYS:H	1:A:73:THR:HB	4	0.16
(1,1144)	1:A:62:VAL:HB	1:A:74:GLY:H	19	0.16
(1,1127)	1:A:61:ILE:HD11	1:A:76:ILE:HA	10	0.16
(1,1127)	1:A:61:ILE:HD12	1:A:76:ILE:HA	10	0.16
(1,1127)	1:A:61:ILE:HD13	1:A:76:ILE:HA	10	0.16
(1,1106)	1:A:59:TYR:HB2	1:A:91:TYR:HE1	4	0.16
(1,1106)	1:A:59:TYR:HB2	1:A:91:TYR:HE2	4	0.16
(1,1057)	1:A:57:VAL:HB	1:A:81:ARG:HG2	4	0.16
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG12	11	0.16
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG13	11	0.16
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG12	18	0.16
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG13	18	0.16
(1,807)	1:A:42:ILE:HG21	1:A:45:HIS:H	16	0.15
(1,807)	1:A:42:ILE:HG22	1:A:45:HIS:H	16	0.15
(1,807)	1:A:42:ILE:HG23	1:A:45:HIS:H	16	0.15
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	7	0.15
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	7	0.15
(1,753)	1:A:40:ARG:HD2	1:A:41:LYS:HG2	9	0.15
(1,753)	1:A:40:ARG:HD2	1:A:41:LYS:HG3	9	0.15
(1,753)	1:A:40:ARG:HD3	1:A:41:LYS:HG2	9	0.15
(1,753)	1:A:40:ARG:HD3	1:A:41:LYS:HG3	9	0.15
(1,677)	1:A:35:GLN:H	1:A:36:LEU:HG	13	0.15
(1,621)	1:A:33:TYR:HB3	1:A:56:ARG:HB2	4	0.15
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	10	0.15
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	20	0.15
(1,410)	1:A:20:LYS:HB2	1:A:24:GLU:HG2	5	0.15
(1,410)	1:A:20:LYS:HB3	1:A:24:GLU:HG2	5	0.15
(1,327)	1:A:16:TYR:HB3	1:A:51:TRP:HA	5	0.15
(1,288)	1:A:14:LEU:HG	1:A:51:TRP:HE1	5	0.15
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	1	0.15
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	1	0.15
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	4	0.15
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	6	0.15
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	6	0.15
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	9	0.15
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	9	0.15
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	18	0.15
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	18	0.15
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	19	0.15
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	19	0.15
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	19	0.15
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	19	0.15
(1,1144)	1:A:62:VAL:HB	1:A:74:GLY:H	1	0.15
(1,1122)	1:A:61:ILE:HB	1:A:76:ILE:HD11	13	0.15
(1,1122)	1:A:61:ILE:HB	1:A:76:ILE:HD12	13	0.15
(1,1122)	1:A:61:ILE:HB	1:A:76:ILE:HD13	13	0.15
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG21	11	0.15
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG22	11	0.15
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG23	11	0.15
(1,1100)	1:A:58:GLY:H	1:A:59:TYR:HB2	4	0.15
(1,1100)	1:A:58:GLY:H	1:A:59:TYR:HB3	4	0.15
(1,1081)	1:A:57:VAL:HG11	1:A:88:TRP:HE3	2	0.15
(1,1081)	1:A:57:VAL:HG12	1:A:88:TRP:HE3	2	0.15
(1,1081)	1:A:57:VAL:HG13	1:A:88:TRP:HE3	2	0.15
(1,1081)	1:A:57:VAL:HG21	1:A:88:TRP:HE3	2	0.15
(1,1081)	1:A:57:VAL:HG22	1:A:88:TRP:HE3	2	0.15
(1,1081)	1:A:57:VAL:HG23	1:A:88:TRP:HE3	2	0.15
(1,1035)	1:A:56:ARG:HB3	1:A:80:ILE:HD11	13	0.15
(1,1035)	1:A:56:ARG:HB3	1:A:80:ILE:HD12	13	0.15
(1,1035)	1:A:56:ARG:HB3	1:A:80:ILE:HD13	13	0.15
(1,938)	1:A:51:TRP:HE1	1:A:86:GLU:HB3	1	0.14
(1,922)	1:A:51:TRP:HB3	1:A:90:ALA:HB1	12	0.14
(1,922)	1:A:51:TRP:HB3	1:A:90:ALA:HB2	12	0.14
(1,922)	1:A:51:TRP:HB3	1:A:90:ALA:HB3	12	0.14
(1,819)	1:A:43:GLY:HA3	1:A:62:VAL:HG21	15	0.14
(1,819)	1:A:43:GLY:HA3	1:A:62:VAL:HG22	15	0.14
(1,819)	1:A:43:GLY:HA3	1:A:62:VAL:HG23	15	0.14
(1,816)	1:A:43:GLY:HA3	1:A:45:HIS:HB3	14	0.14
(1,816)	1:A:43:GLY:HA3	1:A:45:HIS:HB3	19	0.14
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	5	0.14
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	5	0.14
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	11	0.14
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:A:40:ARG:HD2	1:A:44:PHE:HB2	16	0.14
(1,755)	1:A:40:ARG:HD3	1:A:44:PHE:HB2	16	0.14
(1,700)	1:A:36:LEU:HG	1:A:75:ILE:HG21	9	0.14
(1,700)	1:A:36:LEU:HG	1:A:75:ILE:HG22	9	0.14
(1,700)	1:A:36:LEU:HG	1:A:75:ILE:HG23	9	0.14
(1,56)	1:A:3:TYR:HD1	1:A:93:TYR:H	2	0.14
(1,56)	1:A:3:TYR:HD2	1:A:93:TYR:H	2	0.14
(1,56)	1:A:3:TYR:HD1	1:A:93:TYR:H	16	0.14
(1,56)	1:A:3:TYR:HD2	1:A:93:TYR:H	16	0.14
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	3	0.14
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	12	0.14
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	19	0.14
(1,410)	1:A:20:LYS:HB2	1:A:24:GLU:HG2	12	0.14
(1,410)	1:A:20:LYS:HB3	1:A:24:GLU:HG2	12	0.14
(1,394)	1:A:20:LYS:HA	1:A:24:GLU:HG3	12	0.14
(1,338)	1:A:16:TYR:HD1	1:A:51:TRP:HA	11	0.14
(1,338)	1:A:16:TYR:HD2	1:A:51:TRP:HA	11	0.14
(1,310)	1:A:15:THR:HG21	1:A:85:SER:HB2	1	0.14
(1,310)	1:A:15:THR:HG21	1:A:85:SER:HB3	1	0.14
(1,310)	1:A:15:THR:HG22	1:A:85:SER:HB2	1	0.14
(1,310)	1:A:15:THR:HG22	1:A:85:SER:HB3	1	0.14
(1,310)	1:A:15:THR:HG23	1:A:85:SER:HB2	1	0.14
(1,310)	1:A:15:THR:HG23	1:A:85:SER:HB3	1	0.14
(1,288)	1:A:14:LEU:HG	1:A:51:TRP:HE1	10	0.14
(1,279)	1:A:14:LEU:HD11	1:A:18:GLU:H	4	0.14
(1,279)	1:A:14:LEU:HD12	1:A:18:GLU:H	4	0.14
(1,279)	1:A:14:LEU:HD13	1:A:18:GLU:H	4	0.14
(1,279)	1:A:14:LEU:HD21	1:A:18:GLU:H	4	0.14
(1,279)	1:A:14:LEU:HD22	1:A:18:GLU:H	4	0.14
(1,279)	1:A:14:LEU:HD23	1:A:18:GLU:H	4	0.14
(1,267)	1:A:14:LEU:HB3	1:A:51:TRP:HE1	8	0.14
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	11	0.14
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	11	0.14
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	13	0.14
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	13	0.14
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	15	0.14
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	15	0.14
(1,20)	1:A:2:VAL:HG11	1:A:93:TYR:HB3	5	0.14
(1,20)	1:A:2:VAL:HG12	1:A:93:TYR:HB3	5	0.14
(1,20)	1:A:2:VAL:HG13	1:A:93:TYR:HB3	5	0.14
(1,195)	1:A:10:GLY:H	1:A:13:LYS:H	1	0.14
(1,180)	1:A:9:SER:HB2	1:A:13:LYS:HB2	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:A:9:SER:HB2	1:A:13:LYS:HB3	9	0.14
(1,1280)	1:A:81:ARG:HA	1:A:83:ASN:HB2	6	0.14
(1,1280)	1:A:81:ARG:HA	1:A:83:ASN:HB3	6	0.14
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG21	10	0.14
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG22	10	0.14
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG23	10	0.14
(1,1159)	1:A:63:LYS:HA	1:A:73:THR:HB	3	0.14
(1,1141)	1:A:62:VAL:HB	1:A:63:LYS:HE2	17	0.14
(1,1140)	1:A:62:VAL:HB	1:A:63:LYS:HE3	15	0.14
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG21	16	0.14
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG22	16	0.14
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG23	16	0.14
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG12	12	0.14
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG13	12	0.14
(1,1020)	1:A:54:LYS:H	1:A:56:ARG:HB3	6	0.14
(1,935)	1:A:51:TRP:HE1	1:A:57:VAL:HB	4	0.13
(1,814)	1:A:43:GLY:HA3	1:A:44:PHE:HB3	16	0.13
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	17	0.13
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	18	0.13
(1,567)	1:A:31:ALA:HA	1:A:93:TYR:HE1	7	0.13
(1,567)	1:A:31:ALA:HA	1:A:93:TYR:HE2	7	0.13
(1,483)	1:A:24:GLU:H	1:A:25:PHE:HB2	7	0.13
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	5	0.13
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	15	0.13
(1,371)	1:A:19:ALA:HA	1:A:30:LEU:HD11	8	0.13
(1,371)	1:A:19:ALA:HA	1:A:30:LEU:HD12	8	0.13
(1,371)	1:A:19:ALA:HA	1:A:30:LEU:HD13	8	0.13
(1,371)	1:A:19:ALA:HA	1:A:30:LEU:HD21	8	0.13
(1,371)	1:A:19:ALA:HA	1:A:30:LEU:HD22	8	0.13
(1,371)	1:A:19:ALA:HA	1:A:30:LEU:HD23	8	0.13
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	3	0.13
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	3	0.13
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	8	0.13
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	8	0.13
(1,191)	1:A:10:GLY:HA2	1:A:13:LYS:HG2	13	0.13
(1,191)	1:A:10:GLY:HA2	1:A:13:LYS:HG3	13	0.13
(1,1329)	1:A:85:SER:H	1:A:86:GLU:HB3	5	0.13
(1,1329)	1:A:85:SER:H	1:A:86:GLU:HB3	7	0.13
(1,1323)	1:A:84:ARG:HD2	1:A:85:SER:HB2	8	0.13
(1,1323)	1:A:84:ARG:HD2	1:A:85:SER:HB3	8	0.13
(1,1323)	1:A:84:ARG:HD3	1:A:85:SER:HB2	8	0.13
(1,1323)	1:A:84:ARG:HD3	1:A:85:SER:HB3	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB1	7	0.13
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB2	7	0.13
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB3	7	0.13
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB1	7	0.13
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB2	7	0.13
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB3	7	0.13
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB1	8	0.13
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB2	8	0.13
(1,129)	1:A:6:GLU:HG2	1:A:7:ALA:HB3	8	0.13
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB1	8	0.13
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB2	8	0.13
(1,129)	1:A:6:GLU:HG3	1:A:7:ALA:HB3	8	0.13
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG21	1	0.13
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG22	1	0.13
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG23	1	0.13
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG21	9	0.13
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG22	9	0.13
(1,1169)	1:A:64:PRO:HD2	1:A:73:THR:HG23	9	0.13
(1,1144)	1:A:62:VAL:HB	1:A:74:GLY:H	20	0.13
(1,1124)	1:A:61:ILE:HD11	1:A:68:CYS:HB3	18	0.13
(1,1124)	1:A:61:ILE:HD12	1:A:68:CYS:HB3	18	0.13
(1,1124)	1:A:61:ILE:HD13	1:A:68:CYS:HB3	18	0.13
(1,1115)	1:A:59:TYR:H	1:A:77:ASP:HB2	10	0.13
(1,1115)	1:A:59:TYR:H	1:A:77:ASP:HB3	10	0.13
(1,1055)	1:A:57:VAL:HB	1:A:81:ARG:HD2	18	0.13
(1,104)	1:A:5:ARG:HE	1:A:93:TYR:H	11	0.13
(1,935)	1:A:51:TRP:HE1	1:A:57:VAL:HB	8	0.12
(1,93)	1:A:5:ARG:HB2	1:A:22:VAL:HB	1	0.12
(1,93)	1:A:5:ARG:HB3	1:A:22:VAL:HB	1	0.12
(1,816)	1:A:43:GLY:HA3	1:A:45:HIS:HB3	18	0.12
(1,623)	1:A:33:TYR:HB2	1:A:56:ARG:HB2	8	0.12
(1,606)	1:A:32:THR:H	1:A:35:GLN:HE22	15	0.12
(1,596)	1:A:32:THR:HB	1:A:52:MET:HE1	16	0.12
(1,596)	1:A:32:THR:HB	1:A:52:MET:HE2	16	0.12
(1,596)	1:A:32:THR:HB	1:A:52:MET:HE3	16	0.12
(1,567)	1:A:31:ALA:HA	1:A:93:TYR:HE1	3	0.12
(1,567)	1:A:31:ALA:HA	1:A:93:TYR:HE2	3	0.12
(1,56)	1:A:3:TYR:HD1	1:A:93:TYR:H	9	0.12
(1,56)	1:A:3:TYR:HD2	1:A:93:TYR:H	9	0.12
(1,415)	1:A:20:LYS:HG2	1:A:24:GLU:HG2	9	0.12
(1,415)	1:A:20:LYS:HG3	1:A:24:GLU:HG2	9	0.12
(1,415)	1:A:20:LYS:HG2	1:A:24:GLU:HG2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,415)	1:A:20:LYS:HG3	1:A:24:GLU:HG2	11	0.12
(1,410)	1:A:20:LYS:HB2	1:A:24:GLU:HG2	4	0.12
(1,410)	1:A:20:LYS:HB3	1:A:24:GLU:HG2	4	0.12
(1,394)	1:A:20:LYS:HA	1:A:24:GLU:HG3	1	0.12
(1,355)	1:A:17:ALA:H	1:A:84:ARG:HB3	10	0.12
(1,346)	1:A:16:TYR:H	1:A:84:ARG:HA	11	0.12
(1,343)	1:A:16:TYR:HD1	1:A:84:ARG:HD3	18	0.12
(1,343)	1:A:16:TYR:HD2	1:A:84:ARG:HD3	18	0.12
(1,288)	1:A:14:LEU:HG	1:A:51:TRP:HE1	1	0.12
(1,288)	1:A:14:LEU:HG	1:A:51:TRP:HE1	15	0.12
(1,279)	1:A:14:LEU:HD11	1:A:18:GLU:H	3	0.12
(1,279)	1:A:14:LEU:HD12	1:A:18:GLU:H	3	0.12
(1,279)	1:A:14:LEU:HD13	1:A:18:GLU:H	3	0.12
(1,279)	1:A:14:LEU:HD21	1:A:18:GLU:H	3	0.12
(1,279)	1:A:14:LEU:HD22	1:A:18:GLU:H	3	0.12
(1,279)	1:A:14:LEU:HD23	1:A:18:GLU:H	3	0.12
(1,272)	1:A:14:LEU:HB2	1:A:18:GLU:H	11	0.12
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD2	12	0.12
(1,235)	1:A:13:LYS:HA	1:A:13:LYS:HD3	12	0.12
(1,149)	1:A:7:ALA:HB1	1:A:9:SER:HB2	12	0.12
(1,149)	1:A:7:ALA:HB2	1:A:9:SER:HB2	12	0.12
(1,149)	1:A:7:ALA:HB3	1:A:9:SER:HB2	12	0.12
(1,145)	1:A:7:ALA:HB1	1:A:14:LEU:HG	8	0.12
(1,145)	1:A:7:ALA:HB2	1:A:14:LEU:HG	8	0.12
(1,145)	1:A:7:ALA:HB3	1:A:14:LEU:HG	8	0.12
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	2	0.12
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	2	0.12
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	2	0.12
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	2	0.12
(1,1329)	1:A:85:SER:H	1:A:86:GLU:HB3	17	0.12
(1,1280)	1:A:81:ARG:HA	1:A:83:ASN:HB2	15	0.12
(1,1280)	1:A:81:ARG:HA	1:A:83:ASN:HB3	15	0.12
(1,1144)	1:A:62:VAL:HB	1:A:74:GLY:H	10	0.12
(1,1132)	1:A:61:ILE:HG21	1:A:63:LYS:HA	20	0.12
(1,1132)	1:A:61:ILE:HG22	1:A:63:LYS:HA	20	0.12
(1,1132)	1:A:61:ILE:HG23	1:A:63:LYS:HA	20	0.12
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG21	12	0.12
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG22	12	0.12
(1,1102)	1:A:58:GLY:H	1:A:75:ILE:HG23	12	0.12
(1,1020)	1:A:54:LYS:H	1:A:56:ARG:HB3	18	0.12
(1,983)	1:A:52:MET:HG2	1:A:56:ARG:HB2	14	0.11
(1,983)	1:A:52:MET:HG3	1:A:56:ARG:HB2	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:A:5:ARG:HB2	1:A:90:ALA:H	4	0.11
(1,98)	1:A:5:ARG:HB3	1:A:90:ALA:H	4	0.11
(1,837)	1:A:45:HIS:HB3	1:A:62:VAL:HB	12	0.11
(1,807)	1:A:42:ILE:HG21	1:A:45:HIS:H	15	0.11
(1,807)	1:A:42:ILE:HG22	1:A:45:HIS:H	15	0.11
(1,807)	1:A:42:ILE:HG23	1:A:45:HIS:H	15	0.11
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	6	0.11
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	7	0.11
(1,612)	1:A:32:THR:H	1:A:52:MET:HB2	19	0.11
(1,465)	1:A:23:CYS:H	1:A:30:LEU:H	8	0.11
(1,412)	1:A:20:LYS:HD2	1:A:30:LEU:HD11	7	0.11
(1,412)	1:A:20:LYS:HD2	1:A:30:LEU:HD12	7	0.11
(1,412)	1:A:20:LYS:HD2	1:A:30:LEU:HD13	7	0.11
(1,412)	1:A:20:LYS:HD2	1:A:30:LEU:HD21	7	0.11
(1,412)	1:A:20:LYS:HD2	1:A:30:LEU:HD22	7	0.11
(1,412)	1:A:20:LYS:HD2	1:A:30:LEU:HD23	7	0.11
(1,412)	1:A:20:LYS:HD3	1:A:30:LEU:HD11	7	0.11
(1,412)	1:A:20:LYS:HD3	1:A:30:LEU:HD12	7	0.11
(1,412)	1:A:20:LYS:HD3	1:A:30:LEU:HD13	7	0.11
(1,412)	1:A:20:LYS:HD3	1:A:30:LEU:HD21	7	0.11
(1,412)	1:A:20:LYS:HD3	1:A:30:LEU:HD22	7	0.11
(1,412)	1:A:20:LYS:HD3	1:A:30:LEU:HD23	7	0.11
(1,410)	1:A:20:LYS:HB2	1:A:24:GLU:HG2	1	0.11
(1,410)	1:A:20:LYS:HB3	1:A:24:GLU:HG2	1	0.11
(1,410)	1:A:20:LYS:HB2	1:A:24:GLU:HG2	13	0.11
(1,410)	1:A:20:LYS:HB3	1:A:24:GLU:HG2	13	0.11
(1,395)	1:A:20:LYS:HA	1:A:24:GLU:HG2	5	0.11
(1,310)	1:A:15:THR:HG21	1:A:85:SER:HB2	12	0.11
(1,310)	1:A:15:THR:HG21	1:A:85:SER:HB3	12	0.11
(1,310)	1:A:15:THR:HG22	1:A:85:SER:HB2	12	0.11
(1,310)	1:A:15:THR:HG22	1:A:85:SER:HB3	12	0.11
(1,310)	1:A:15:THR:HG23	1:A:85:SER:HB2	12	0.11
(1,310)	1:A:15:THR:HG23	1:A:85:SER:HB3	12	0.11
(1,310)	1:A:15:THR:HG21	1:A:85:SER:HB2	13	0.11
(1,310)	1:A:15:THR:HG21	1:A:85:SER:HB3	13	0.11
(1,310)	1:A:15:THR:HG22	1:A:85:SER:HB2	13	0.11
(1,310)	1:A:15:THR:HG22	1:A:85:SER:HB3	13	0.11
(1,310)	1:A:15:THR:HG23	1:A:85:SER:HB2	13	0.11
(1,310)	1:A:15:THR:HG23	1:A:85:SER:HB3	13	0.11
(1,310)	1:A:15:THR:HG21	1:A:85:SER:HB2	19	0.11
(1,310)	1:A:15:THR:HG21	1:A:85:SER:HB3	19	0.11
(1,310)	1:A:15:THR:HG22	1:A:85:SER:HB2	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,310)	1:A:15:THR:HG22	1:A:85:SER:HB3	19	0.11
(1,310)	1:A:15:THR:HG23	1:A:85:SER:HB2	19	0.11
(1,310)	1:A:15:THR:HG23	1:A:85:SER:HB3	19	0.11
(1,255)	1:A:13:LYS:H	1:A:87:ARG:HD2	1	0.11
(1,255)	1:A:13:LYS:H	1:A:87:ARG:HD3	1	0.11
(1,145)	1:A:7:ALA:HB1	1:A:14:LEU:HG	13	0.11
(1,145)	1:A:7:ALA:HB2	1:A:14:LEU:HG	13	0.11
(1,145)	1:A:7:ALA:HB3	1:A:14:LEU:HG	13	0.11
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	4	0.11
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	4	0.11
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	4	0.11
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	4	0.11
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE2	9	0.11
(1,1429)	1:A:98:LYS:HB2	1:A:98:LYS:HE3	9	0.11
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE2	9	0.11
(1,1429)	1:A:98:LYS:HB3	1:A:98:LYS:HE3	9	0.11
(1,1249)	1:A:78:TYR:HB2	1:A:79:GLY:H	13	0.11
(1,1249)	1:A:78:TYR:HB3	1:A:79:GLY:H	13	0.11
(1,1194)	1:A:72:LYS:H	1:A:73:THR:HB	9	0.11
(1,1189)	1:A:72:LYS:HB2	1:A:76:ILE:HG21	17	0.11
(1,1189)	1:A:72:LYS:HB2	1:A:76:ILE:HG22	17	0.11
(1,1189)	1:A:72:LYS:HB2	1:A:76:ILE:HG23	17	0.11
(1,1189)	1:A:72:LYS:HB3	1:A:76:ILE:HG21	17	0.11
(1,1189)	1:A:72:LYS:HB3	1:A:76:ILE:HG22	17	0.11
(1,1189)	1:A:72:LYS:HB3	1:A:76:ILE:HG23	17	0.11
(1,1113)	1:A:59:TYR:H	1:A:76:ILE:H	17	0.11
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG12	7	0.11
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG13	7	0.11
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG12	14	0.11
(1,1040)	1:A:56:ARG:HD2	1:A:80:ILE:HG13	14	0.11
(1,1027)	1:A:55:GLY:H	1:A:80:ILE:HG21	16	0.11
(1,1027)	1:A:55:GLY:H	1:A:80:ILE:HG22	16	0.11
(1,1027)	1:A:55:GLY:H	1:A:80:ILE:HG23	16	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found