



Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 07:43 pm BST

PDB ID : 6ZLE
BMRB ID : 34526
Title : Solution structure of unliganded MLKL executioner domain
Authors : Ruebelke, M.; Bauer, M.; Nar, H.; Zeeb, M.
Deposited on : 2020-06-30

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

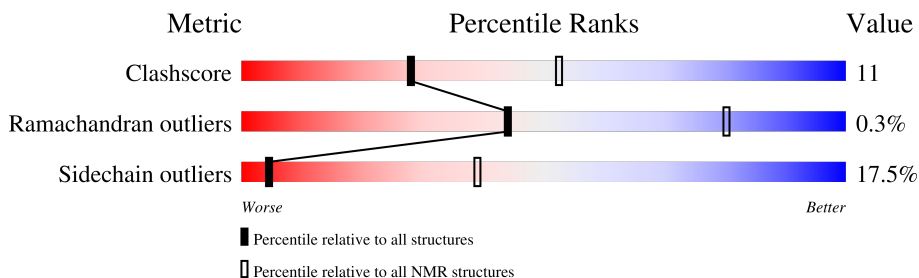
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	157	 64% 23% • 11%

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:47, A:55-A:128, A:132-A:149 (139)	0.75	5

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2564 atoms, of which 1295 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mixed lineage kinase domain-like protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	157	2564	786	1295	239	235	9	0

There are 4 discrepancies between the modelled and reference sequences:

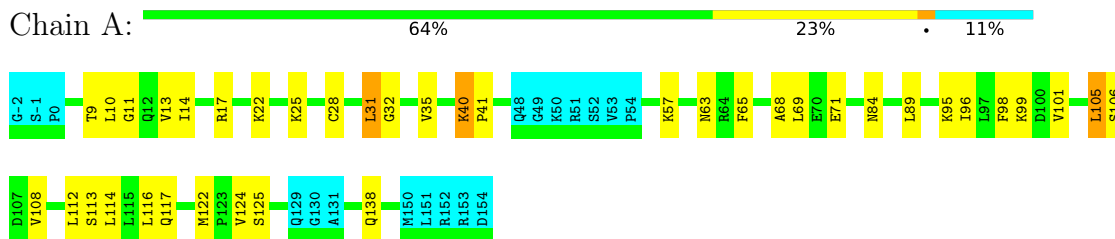
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8NB16
A	-1	SER	-	expression tag	UNP Q8NB16
A	0	PRO	-	expression tag	UNP Q8NB16
A	1	GLY	-	expression tag	UNP Q8NB16

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: Mixed lineage kinase domain-like protein

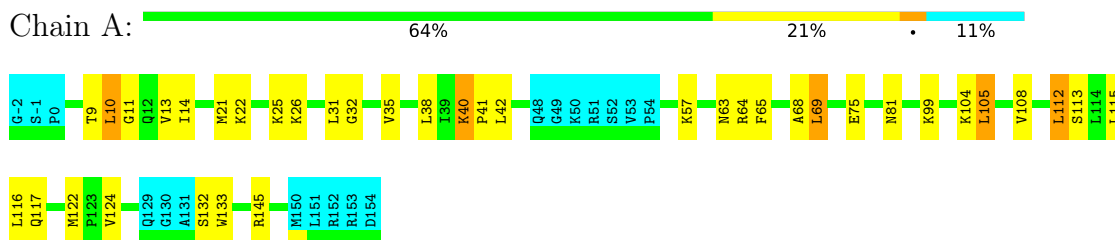


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

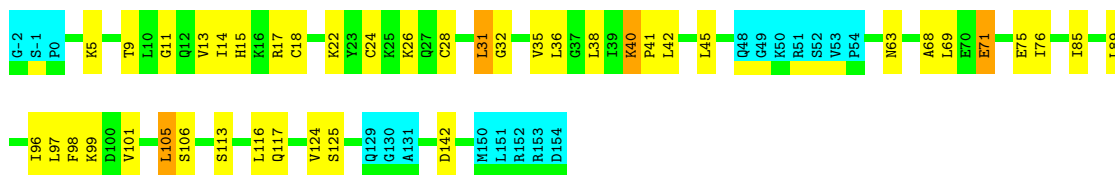
- Molecule 1: Mixed lineage kinase domain-like protein



4.2.2 Score per residue for model 2

- Molecule 1: Mixed lineage kinase domain-like protein





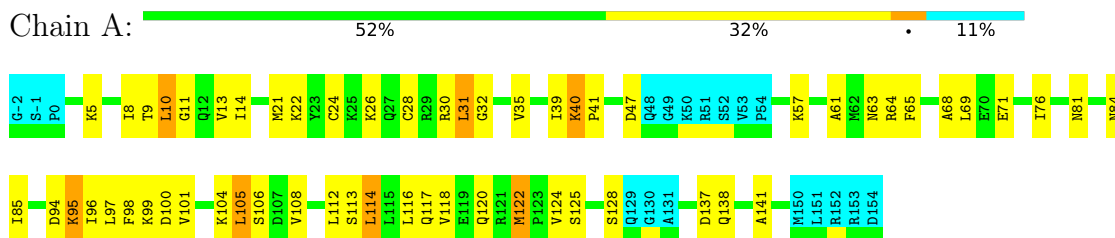
4.2.3 Score per residue for model 3

- Molecule 1: Mixed lineage kinase domain-like protein



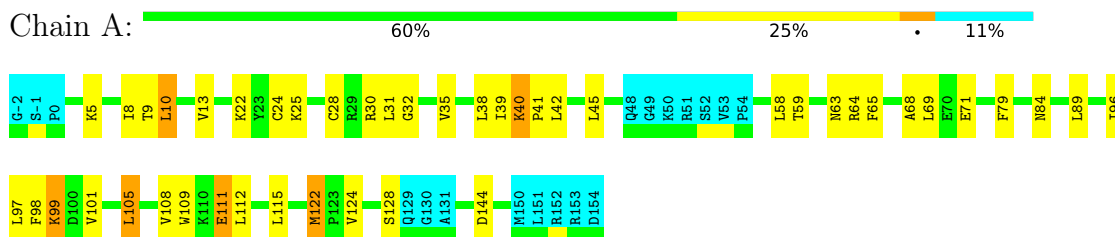
4.2.4 Score per residue for model 4

- Molecule 1: Mixed lineage kinase domain-like protein



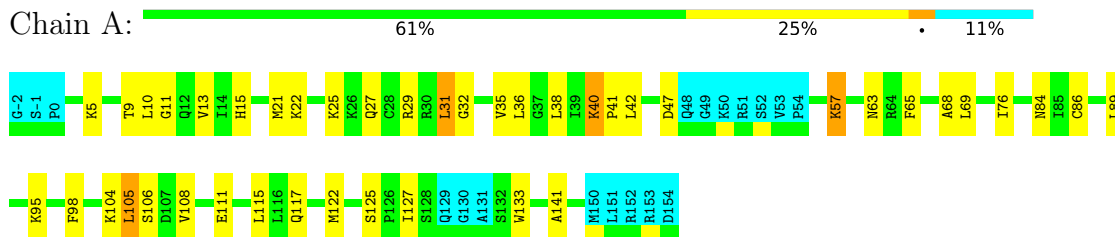
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Mixed lineage kinase domain-like protein



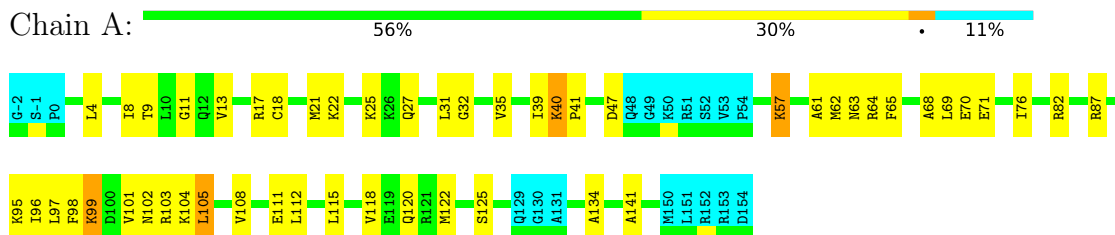
4.2.6 Score per residue for model 6

- Molecule 1: Mixed lineage kinase domain-like protein



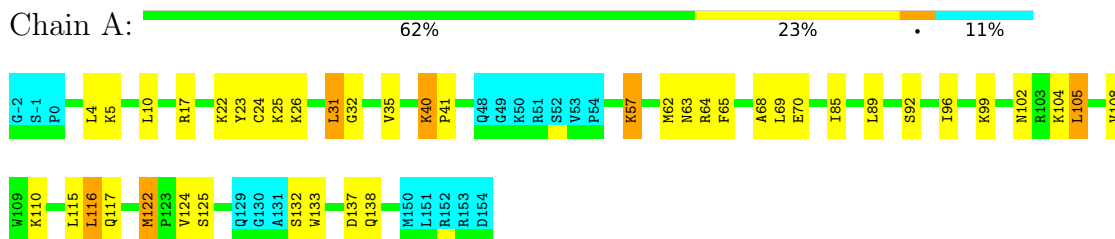
4.2.7 Score per residue for model 7

- Molecule 1: Mixed lineage kinase domain-like protein



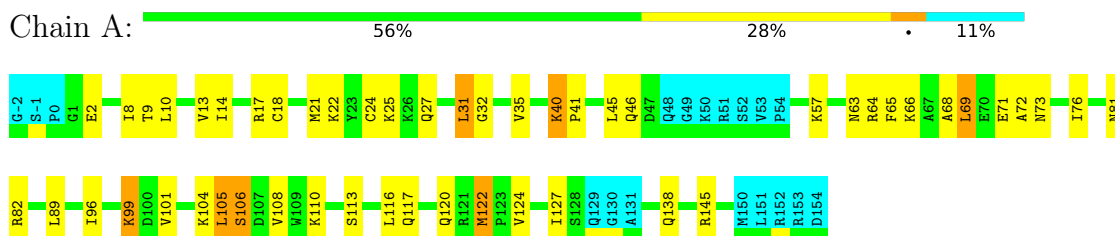
4.2.8 Score per residue for model 8

- Molecule 1: Mixed lineage kinase domain-like protein



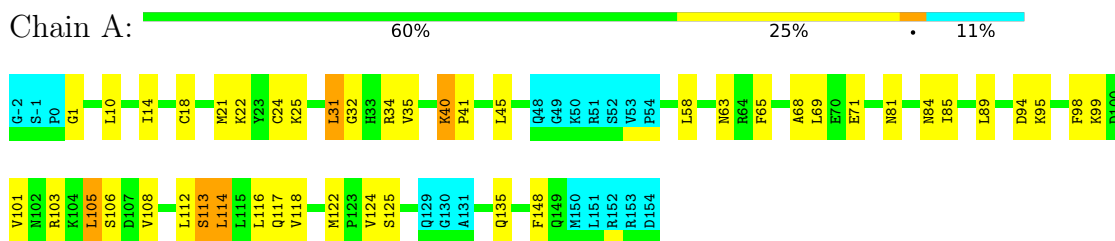
4.2.9 Score per residue for model 9

- Molecule 1: Mixed lineage kinase domain-like protein



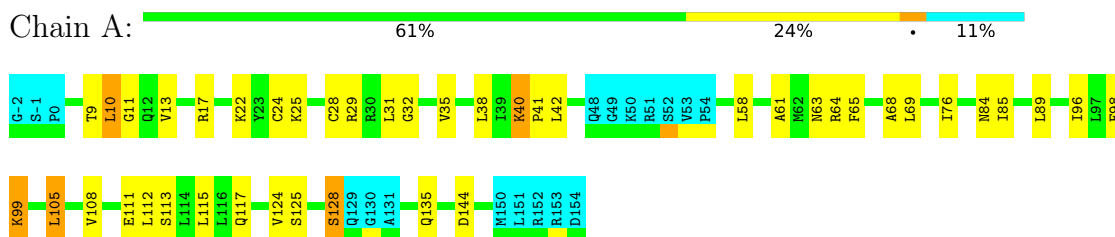
4.2.10 Score per residue for model 10

- Molecule 1: Mixed lineage kinase domain-like protein



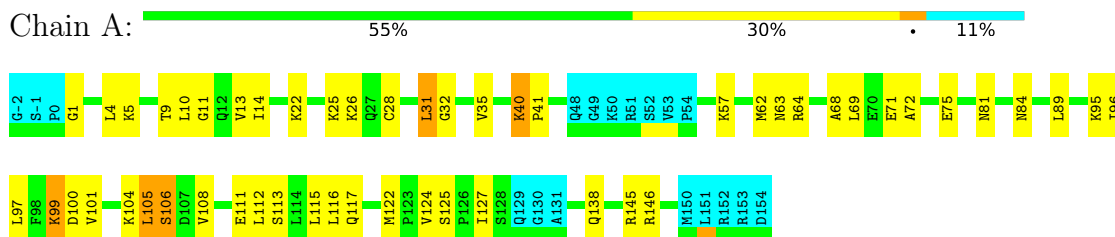
4.2.11 Score per residue for model 11

- Molecule 1: Mixed lineage kinase domain-like protein



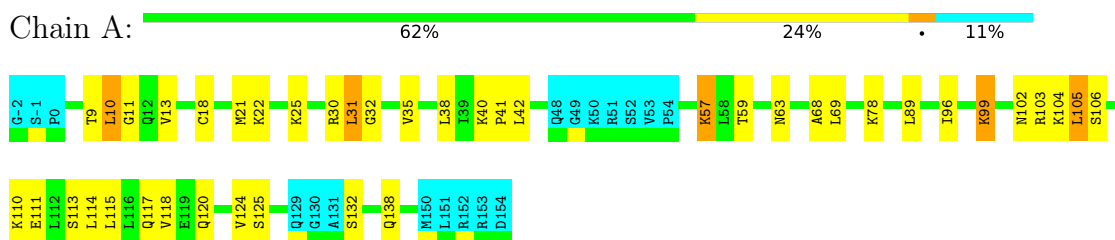
4.2.12 Score per residue for model 12

- Molecule 1: Mixed lineage kinase domain-like protein



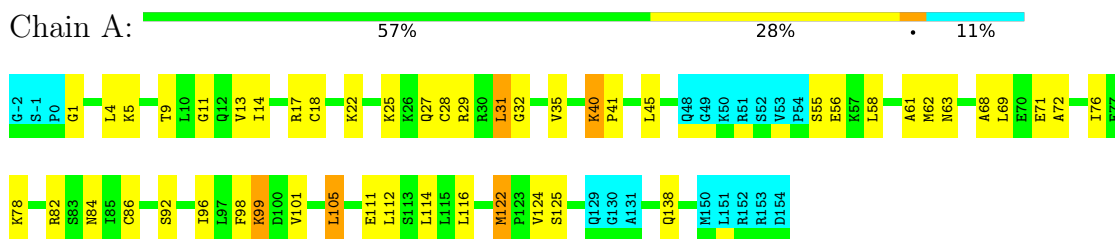
4.2.13 Score per residue for model 13

- Molecule 1: Mixed lineage kinase domain-like protein



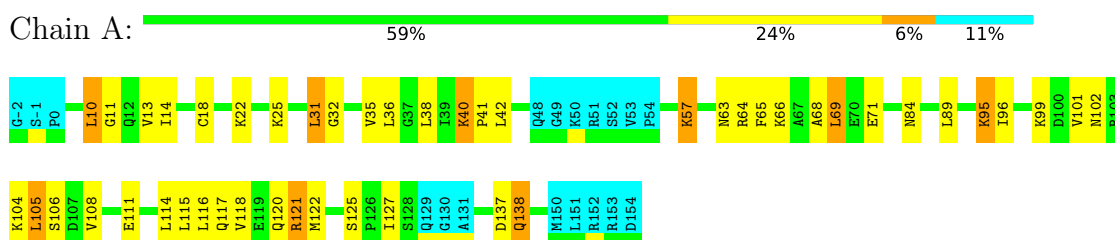
4.2.14 Score per residue for model 14

- Molecule 1: Mixed lineage kinase domain-like protein



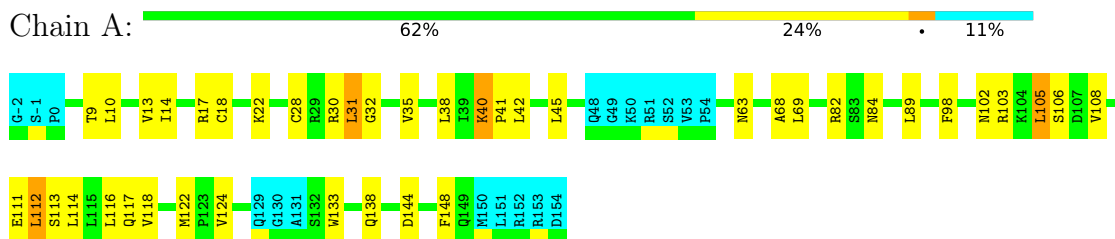
4.2.15 Score per residue for model 15

- Molecule 1: Mixed lineage kinase domain-like protein



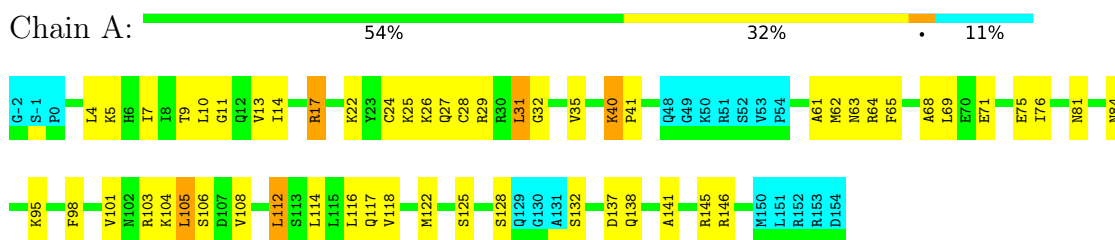
4.2.16 Score per residue for model 16

- Molecule 1: Mixed lineage kinase domain-like protein



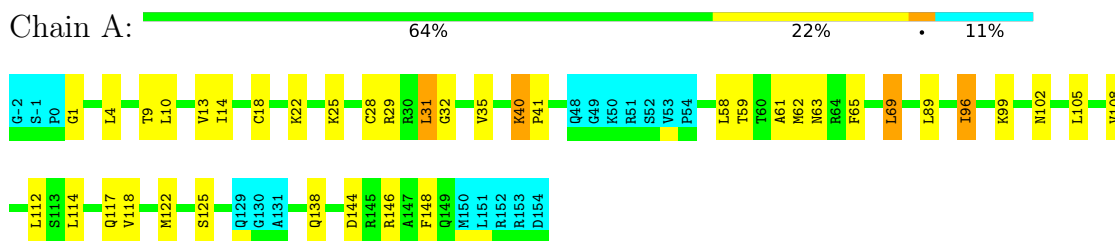
4.2.17 Score per residue for model 17

- Molecule 1: Mixed lineage kinase domain-like protein



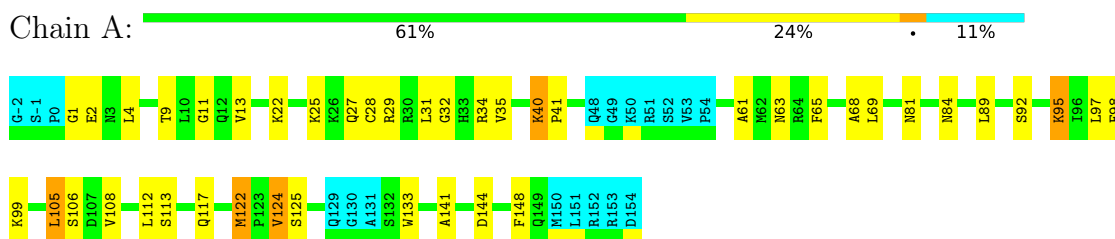
4.2.18 Score per residue for model 18

- Molecule 1: Mixed lineage kinase domain-like protein



4.2.19 Score per residue for model 19

- Molecule 1: Mixed lineage kinase domain-like protein



4.2.20 Score per residue for model 20

- Molecule 1: Mixed lineage kinase domain-like protein



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	3.98.9

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	1796
Number of shifts mapped to atoms	1796
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality i

6.1 Standard geometry i

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1135	1156	1156	24±5
All	All	22700	23120	23120	485

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LEU:HD23	1:A:69:LEU:HD23	0.95	1.35	18	2
1:A:10:LEU:HD23	1:A:69:LEU:HD12	0.76	1.56	16	6
1:A:45:LEU:HD21	1:A:116:LEU:HD11	0.75	1.58	20	1
1:A:116:LEU:HD13	1:A:122:MET:HE3	0.73	1.59	4	2
1:A:31:LEU:HD23	1:A:98:PHE:CD2	0.73	2.19	7	2
1:A:65:PHE:HA	1:A:108:VAL:HG11	0.67	1.67	8	10
1:A:9:THR:O	1:A:13:VAL:HG23	0.67	1.90	9	16
1:A:68:ALA:HB1	1:A:105:LEU:CD2	0.67	2.20	3	15
1:A:120:GLN:O	1:A:121:ARG:C	0.66	2.33	15	1
1:A:11:GLY:CA	1:A:69:LEU:HD22	0.64	2.22	19	8
1:A:68:ALA:HB1	1:A:105:LEU:CD1	0.64	2.22	7	11
1:A:38:LEU:O	1:A:42:LEU:HD13	0.64	1.93	13	9
1:A:71:GLU:HG2	1:A:101:VAL:HG22	0.64	1.68	5	5
1:A:45:LEU:HD23	1:A:58:LEU:HD11	0.64	1.70	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ILE:HD12	1:A:99:LYS:HE2	0.64	1.70	13	3
1:A:11:GLY:HA2	1:A:69:LEU:HD22	0.63	1.68	20	9
1:A:61:ALA:HB1	1:A:112:LEU:CD1	0.63	2.24	14	6
1:A:32:GLY:O	1:A:35:VAL:HG12	0.63	1.94	9	20
1:A:10:LEU:HD22	1:A:69:LEU:HB2	0.63	1.71	1	4
1:A:31:LEU:HD12	1:A:98:PHE:CD2	0.63	2.28	16	6
1:A:9:THR:O	1:A:13:VAL:HG22	0.62	1.94	1	1
1:A:116:LEU:HD13	1:A:122:MET:CE	0.62	2.24	4	7
1:A:61:ALA:HB1	1:A:112:LEU:HD11	0.62	1.71	14	5
1:A:106:SER:O	1:A:127:ILE:HD11	0.61	1.96	6	5
1:A:10:LEU:HD22	1:A:69:LEU:CB	0.60	2.26	11	6
1:A:57:LYS:HD2	1:A:115:LEU:HD21	0.59	1.73	15	2
1:A:113:SER:CB	1:A:124:VAL:HG11	0.59	2.28	4	7
1:A:57:LYS:CD	1:A:115:LEU:HD21	0.58	2.29	15	3
1:A:65:PHE:HA	1:A:108:VAL:HG21	0.58	1.75	5	3
1:A:14:ILE:HD11	1:A:69:LEU:HA	0.58	1.74	9	12
1:A:65:PHE:CA	1:A:108:VAL:HG11	0.57	2.29	8	6
1:A:96:ILE:HD13	1:A:99:LYS:CE	0.57	2.29	4	1
1:A:15:HIS:CG	1:A:36:LEU:HD11	0.57	2.33	2	2
1:A:31:LEU:O	1:A:31:LEU:HD22	0.57	2.00	10	1
1:A:116:LEU:HD13	1:A:122:MET:HE1	0.57	1.76	14	3
1:A:96:ILE:HD12	1:A:99:LYS:HE3	0.56	1.76	20	3
1:A:31:LEU:HD22	1:A:102:ASN:OD1	0.56	2.00	7	1
1:A:45:LEU:HD23	1:A:58:LEU:CD1	0.55	2.31	3	2
1:A:10:LEU:CD2	1:A:69:LEU:HD23	0.55	2.26	9	2
1:A:24:CYS:SG	1:A:85:ILE:HD11	0.55	2.41	2	5
1:A:68:ALA:HB1	1:A:105:LEU:HD21	0.55	1.78	6	12
1:A:31:LEU:HD23	1:A:32:GLY:N	0.55	2.17	20	1
1:A:31:LEU:C	1:A:31:LEU:HD13	0.55	2.22	10	12
1:A:89:LEU:HD11	1:A:95:LYS:HD3	0.54	1.77	15	1
1:A:31:LEU:HD23	1:A:102:ASN:OD1	0.54	2.03	8	3
1:A:117:GLN:NE2	1:A:118:VAL:HG23	0.54	2.18	18	1
1:A:95:LYS:HG3	1:A:141:ALA:HB1	0.54	1.78	19	1
1:A:122:MET:CE	1:A:124:VAL:HG22	0.54	2.32	5	2
1:A:79:PHE:CD1	1:A:97:LEU:HD22	0.54	2.38	5	1
1:A:45:LEU:HD23	1:A:58:LEU:HD13	0.54	1.78	3	1
1:A:10:LEU:HD22	1:A:69:LEU:HB3	0.53	1.79	5	2
1:A:31:LEU:HD22	1:A:31:LEU:O	0.53	2.04	6	13
1:A:24:CYS:SG	1:A:97:LEU:HD21	0.53	2.44	4	2
1:A:31:LEU:HD12	1:A:98:PHE:CE2	0.53	2.39	14	3
1:A:96:ILE:HD12	1:A:99:LYS:CE	0.52	2.34	18	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ILE:HD11	1:A:138:GLN:HG2	0.52	1.81	3	3
1:A:11:GLY:HA3	1:A:69:LEU:HD22	0.52	1.80	17	1
1:A:108:VAL:O	1:A:112:LEU:HD12	0.52	2.04	17	4
1:A:71:GLU:CG	1:A:101:VAL:HG22	0.52	2.34	9	8
1:A:95:LYS:O	1:A:141:ALA:HB1	0.52	2.04	7	2
1:A:72:ALA:HB2	1:A:101:VAL:HG11	0.51	1.82	9	1
1:A:122:MET:HE1	1:A:124:VAL:HG13	0.51	1.82	19	1
1:A:8:ILE:HG23	1:A:39:ILE:HD12	0.51	1.82	4	3
1:A:116:LEU:HD22	1:A:122:MET:CE	0.50	2.36	15	1
1:A:40:LYS:N	1:A:41:PRO:HD2	0.50	2.21	14	20
1:A:113:SER:HB2	1:A:124:VAL:HG11	0.50	1.82	12	5
1:A:31:LEU:HD22	1:A:98:PHE:CD2	0.50	2.41	20	1
1:A:31:LEU:HD23	1:A:98:PHE:CG	0.50	2.40	7	2
1:A:11:GLY:N	1:A:69:LEU:HD22	0.50	2.22	15	5
1:A:68:ALA:HB1	1:A:105:LEU:HD22	0.50	1.84	12	2
1:A:23:TYR:HB3	1:A:85:ILE:HD13	0.50	1.84	8	1
1:A:64:ARG:HG3	1:A:108:VAL:HG13	0.50	1.83	11	9
1:A:17:ARG:HB3	1:A:76:ILE:HD12	0.50	1.84	17	2
1:A:28:CYS:SG	1:A:97:LEU:HD12	0.49	2.47	2	1
1:A:1:GLY:O	1:A:4:LEU:HD12	0.49	2.07	18	4
1:A:96:ILE:HD13	1:A:99:LYS:NZ	0.49	2.22	9	1
1:A:4:LEU:HD23	1:A:62:MET:SD	0.49	2.47	8	4
1:A:114:LEU:O	1:A:118:VAL:HG13	0.49	2.07	13	1
1:A:57:LYS:HG2	1:A:115:LEU:HD21	0.49	1.85	1	2
1:A:57:LYS:HD3	1:A:115:LEU:HD21	0.49	1.85	7	2
1:A:31:LEU:HD13	1:A:32:GLY:N	0.48	2.22	6	15
1:A:31:LEU:HD12	1:A:98:PHE:CE1	0.48	2.43	5	1
1:A:4:LEU:HD23	1:A:62:MET:CE	0.48	2.38	14	3
1:A:113:SER:HB2	1:A:124:VAL:HG21	0.48	1.84	2	1
1:A:45:LEU:HD13	1:A:116:LEU:CD2	0.48	2.38	9	1
1:A:58:LEU:HD23	1:A:59:THR:N	0.48	2.24	18	1
1:A:10:LEU:CB	1:A:69:LEU:HD13	0.47	2.39	5	2
1:A:116:LEU:HD22	1:A:122:MET:HE1	0.47	1.86	15	1
1:A:31:LEU:HD13	1:A:98:PHE:CB	0.47	2.38	20	1
1:A:117:GLN:HE21	1:A:118:VAL:HG23	0.47	1.69	18	1
1:A:11:GLY:HA2	1:A:14:ILE:HD12	0.47	1.86	1	1
1:A:95:LYS:HB2	1:A:141:ALA:HB1	0.47	1.85	4	2
1:A:31:LEU:HD13	1:A:31:LEU:C	0.47	2.30	14	4
1:A:15:HIS:CB	1:A:36:LEU:HD11	0.47	2.39	2	1
1:A:69:LEU:N	1:A:69:LEU:HD13	0.47	2.25	9	2
1:A:69:LEU:HD22	1:A:69:LEU:H	0.47	1.70	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:LEU:HD23	1:A:122:MET:CE	0.46	2.40	8	2
1:A:4:LEU:HD22	1:A:46:GLN:CB	0.46	2.41	3	1
1:A:116:LEU:HD23	1:A:122:MET:HE1	0.46	1.86	8	1
1:A:31:LEU:HD22	1:A:98:PHE:CE2	0.46	2.46	20	1
1:A:31:LEU:HD13	1:A:98:PHE:HB3	0.46	1.88	20	1
1:A:14:ILE:HD13	1:A:72:ALA:HB3	0.45	1.87	12	2
1:A:99:LYS:HE3	1:A:134:ALA:HB1	0.45	1.88	7	1
1:A:61:ALA:HB1	1:A:112:LEU:HG	0.45	1.88	4	2
1:A:68:ALA:HB1	1:A:105:LEU:HD12	0.45	1.88	8	1
1:A:111:GLU:O	1:A:115:LEU:HD12	0.45	2.12	5	2
1:A:1:GLY:HA2	1:A:4:LEU:HD12	0.44	1.88	19	1
1:A:114:LEU:O	1:A:118:VAL:HG23	0.44	2.12	17	5
1:A:101:VAL:HG12	1:A:105:LEU:HD23	0.44	1.90	9	1
1:A:96:ILE:HD12	1:A:99:LYS:HD2	0.44	1.88	7	2
1:A:45:LEU:HD21	1:A:116:LEU:HD21	0.43	1.90	14	1
1:A:38:LEU:HD23	1:A:109:TRP:CD2	0.43	2.48	5	1
1:A:115:LEU:HA	1:A:118:VAL:HG12	0.43	1.90	7	1
1:A:10:LEU:CD2	1:A:69:LEU:HD12	0.43	2.37	16	1
1:A:101:VAL:O	1:A:105:LEU:HD23	0.43	2.14	4	4
1:A:31:LEU:HD22	1:A:98:PHE:CB	0.43	2.44	19	1
1:A:45:LEU:CD2	1:A:116:LEU:HD21	0.42	2.44	14	1
1:A:40:LYS:CB	1:A:41:PRO:CD	0.42	2.97	2	16
1:A:14:ILE:CD1	1:A:72:ALA:HB3	0.42	2.44	14	1
1:A:57:LYS:CE	1:A:115:LEU:HD21	0.42	2.44	13	1
1:A:23:TYR:CB	1:A:85:ILE:HD13	0.42	2.43	8	1
1:A:66:LYS:HA	1:A:69:LEU:HD12	0.42	1.90	15	1
1:A:76:ILE:HG23	1:A:98:PHE:CZ	0.42	2.50	2	4
1:A:76:ILE:HG23	1:A:98:PHE:CE2	0.42	2.49	11	1
1:A:7:ILE:HG23	1:A:69:LEU:HD11	0.42	1.92	17	2
1:A:64:ARG:HG3	1:A:108:VAL:HG23	0.42	1.91	5	1
1:A:8:ILE:HD11	1:A:46:GLN:OE1	0.41	2.14	9	1
1:A:68:ALA:HB1	1:A:105:LEU:HD11	0.41	1.91	11	1
1:A:45:LEU:HD11	1:A:116:LEU:CD2	0.41	2.44	2	1
1:A:115:LEU:HA	1:A:118:VAL:HG22	0.41	1.90	13	1
1:A:31:LEU:HD21	1:A:72:ALA:HB1	0.41	1.91	20	1
1:A:96:ILE:HD12	1:A:99:LYS:CD	0.41	2.45	11	1
1:A:76:ILE:HG22	1:A:97:LEU:HD23	0.41	1.91	7	1
1:A:96:ILE:HD13	1:A:99:LYS:HE2	0.41	1.92	4	1
1:A:94:ASP:HB3	1:A:96:ILE:HD12	0.41	1.91	4	1
1:A:114:LEU:O	1:A:118:VAL:HG22	0.41	2.15	13	1
1:A:106:SER:HA	1:A:127:ILE:HD11	0.41	1.92	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:O	1:A:31:LEU:HD12	0.41	2.16	7	2
1:A:14:ILE:HD11	1:A:69:LEU:CA	0.41	2.45	12	1
1:A:40:LYS:N	1:A:41:PRO:CD	0.40	2.84	14	2
1:A:89:LEU:HD12	1:A:148:PHE:CD1	0.40	2.52	16	1
1:A:89:LEU:HD12	1:A:148:PHE:CE1	0.40	2.52	10	2
1:A:112:LEU:O	1:A:116:LEU:HD23	0.40	2.15	10	1
1:A:122:MET:HE2	1:A:124:VAL:HG22	0.40	1.92	14	1
1:A:13:VAL:HG12	1:A:17:ARG:HD3	0.40	1.92	20	1
1:A:35:VAL:HG13	1:A:36:LEU:HD23	0.40	1.94	15	1
1:A:96:ILE:HD12	1:A:99:LYS:NZ	0.40	2.31	15	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	139/157 (89%)	125±3 (90±2%)	13±2 (10±2%)	0±1 (0±0%)	44	80
All	All	2780/3140 (89%)	2504 (90%)	267 (10%)	9 (0%)	44	80

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

Mol	Chain	Res	Type	Models (Total)
1	A	96	ILE	3
1	A	1	GLY	2
1	A	94	ASP	1
1	A	128	SER	1
1	A	121	ARG	1
1	A	124	VAL	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	126/140 (90%)	104±4 (83±3%)	22±4 (17±3%)	4	39
All	All	2520/2800 (90%)	2080 (83%)	440 (17%)	4	39

All 72 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	22	LYS	20
1	A	63	ASN	20
1	A	105	LEU	19
1	A	40	LYS	18
1	A	25	LYS	17
1	A	117	GLN	16
1	A	125	SER	16
1	A	99	LYS	14
1	A	31	LEU	14
1	A	89	LEU	11
1	A	122	MET	11
1	A	84	ASN	11
1	A	104	LYS	10
1	A	28	CYS	10
1	A	5	LYS	9
1	A	18	CYS	9
1	A	106	SER	9
1	A	138	GLN	9
1	A	17	ARG	8
1	A	57	LYS	8
1	A	111	GLU	8
1	A	21	MET	7
1	A	26	LYS	7
1	A	81	ASN	7
1	A	133	TRP	7
1	A	27	GLN	7
1	A	10	LEU	6
1	A	75	GLU	6
1	A	132	SER	6
1	A	95	LYS	6
1	A	29	ARG	6
1	A	112	LEU	5
1	A	30	ARG	5
1	A	82	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	114	LEU	5
1	A	144	ASP	5
1	A	103	ARG	5
1	A	69	LEU	4
1	A	145	ARG	4
1	A	110	LYS	4
1	A	120	GLN	4
1	A	128	SER	4
1	A	137	ASP	4
1	A	102	ASN	3
1	A	47	ASP	3
1	A	24	CYS	3
1	A	92	SER	3
1	A	146	ARG	3
1	A	71	GLU	2
1	A	87	ARG	2
1	A	100	ASP	2
1	A	59	THR	2
1	A	86	CYS	2
1	A	70	GLU	2
1	A	124	VAL	2
1	A	2	GLU	2
1	A	34	ARG	2
1	A	45	LEU	2
1	A	113	SER	2
1	A	135	GLN	2
1	A	97	LEU	2
1	A	78	LYS	2
1	A	58	LEU	2
1	A	142	ASP	1
1	A	116	LEU	1
1	A	66	LYS	1
1	A	73	ASN	1
1	A	115	LEU	1
1	A	55	SER	1
1	A	56	GLU	1
1	A	13	VAL	1
1	A	39	ILE	1

6.3.3 RNA

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

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *molecule_1*

7.1.1 Bookkeeping

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

Total number of shifts	1796
Number of shifts mapped to atoms	1796
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	156	-0.44 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	144	0.17 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	144	0.01 ± 0.17	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 1608 atoms were assigned a chemical shift out of a possible 1997. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	541/694 (78%)	273/280 (98%)	138/278 (50%)	130/136 (96%)
Sidechain	995/1199 (83%)	677/769 (88%)	302/368 (82%)	16/62 (26%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	72/104 (69%)	36/53 (68%)	34/46 (74%)	2/5 (40%)
Overall	1608/1997 (81%)	986/1102 (89%)	474/692 (68%)	148/203 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1796 atoms were assigned a chemical shift out of a possible 2238. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	608/783 (78%)	308/317 (97%)	156/314 (50%)	144/152 (95%)
Sidechain	1116/1351 (83%)	759/866 (88%)	339/411 (82%)	18/74 (24%)
Aromatic	72/104 (69%)	36/53 (68%)	34/46 (74%)	2/5 (40%)
Overall	1796/2238 (80%)	1103/1236 (89%)	529/771 (69%)	164/231 (71%)

7.1.4 Statistically unusual chemical shifts [i](#)

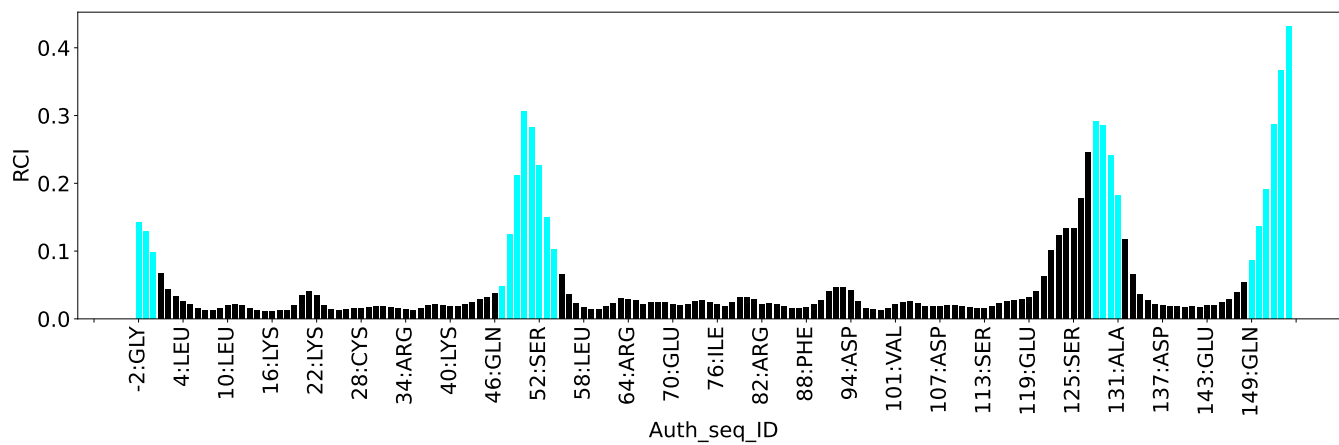
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	113	SER	HB2	2.61	2.61 – 5.13	-5.0

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2618
Intra-residue ($ i-j =0$)	614
Sequential ($ i-j =1$)	617
Medium range ($ i-j >1$ and $ i-j <5$)	761
Long range ($ i-j \geq 5$)	626
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	16.7
Number of long range restraints per residue ¹	4.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	11.2	0.2
0.2-0.5 (Medium)	3.6	0.48
>0.5 (Large)	0.2	0.65

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis [i](#)

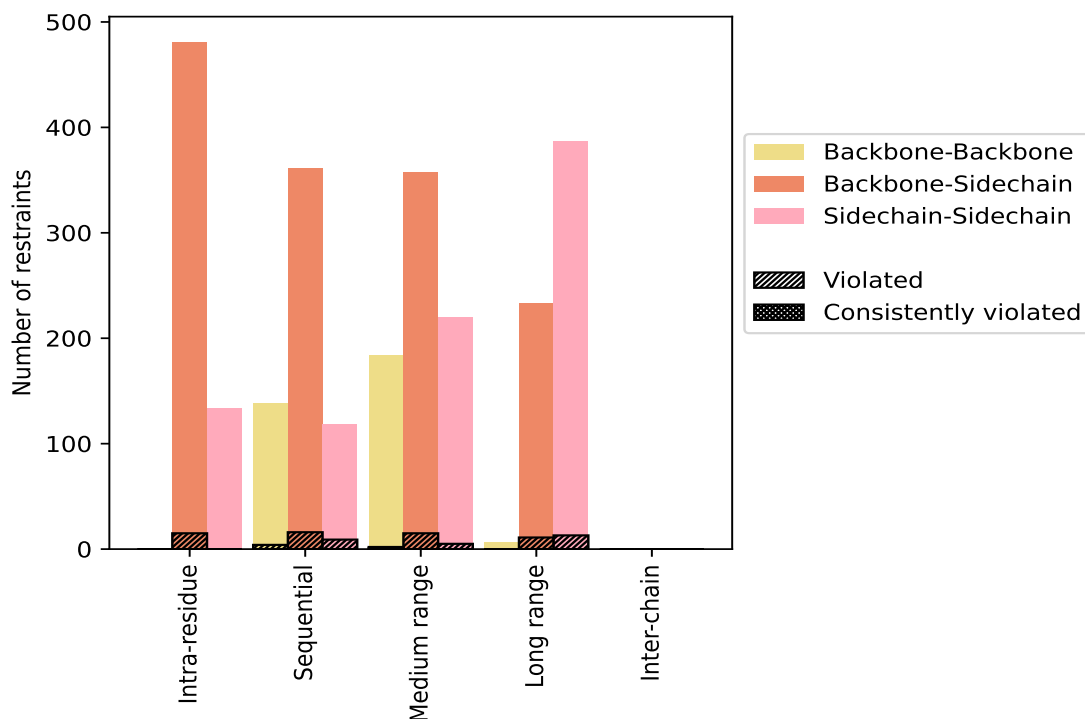
9.1 Summary of distance violations [i](#)

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	614	23.5	15	2.4	0.6	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	481	18.4	15	3.1	0.6	0	0.0	0.0
Sidechain-Sidechain	133	5.1	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	617	23.6	29	4.7	1.1	0	0.0	0.0
Backbone-Backbone	138	5.3	4	2.9	0.2	0	0.0	0.0
Backbone-Sidechain	361	13.8	16	4.4	0.6	0	0.0	0.0
Sidechain-Sidechain	118	4.5	9	7.6	0.3	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	761	29.1	22	2.9	0.8	1	0.1	0.0
Backbone-Backbone	184	7.0	2	1.1	0.1	1	0.5	0.0
Backbone-Sidechain	357	13.6	15	4.2	0.6	0	0.0	0.0
Sidechain-Sidechain	220	8.4	5	2.3	0.2	0	0.0	0.0
Long range ($i-j \geq 5$)	626	23.9	24	3.8	0.9	0	0.0	0.0
Backbone-Backbone	6	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	233	8.9	11	4.7	0.4	0	0.0	0.0
Sidechain-Sidechain	387	14.8	13	3.4	0.5	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	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2618	100.0	90	3.4	3.4	1	0.0	0.0
Backbone-Backbone	328	12.5	6	1.8	0.2	1	0.3	0.0
Backbone-Sidechain	1432	54.7	57	4.0	2.2	0	0.0	0.0
Sidechain-Sidechain	858	32.8	27	3.1	1.0	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 disulfid 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	0	4	4	1	0	9	0.18	0.33	0.09	0.14
2	0	2	5	3	0	10	0.18	0.36	0.08	0.16
3	1	4	4	4	0	13	0.2	0.4	0.08	0.15
4	0	4	5	3	0	12	0.18	0.35	0.08	0.14
5	2	3	3	4	0	12	0.19	0.39	0.09	0.16
6	2	4	4	2	0	12	0.2	0.39	0.09	0.15
7	2	6	8	3	0	19	0.17	0.4	0.07	0.15
8	3	8	9	5	0	25	0.15	0.3	0.04	0.14
9	1	3	8	4	0	16	0.19	0.61	0.12	0.16
10	1	4	6	4	0	15	0.2	0.36	0.08	0.18
11	1	5	3	3	0	12	0.16	0.33	0.06	0.15

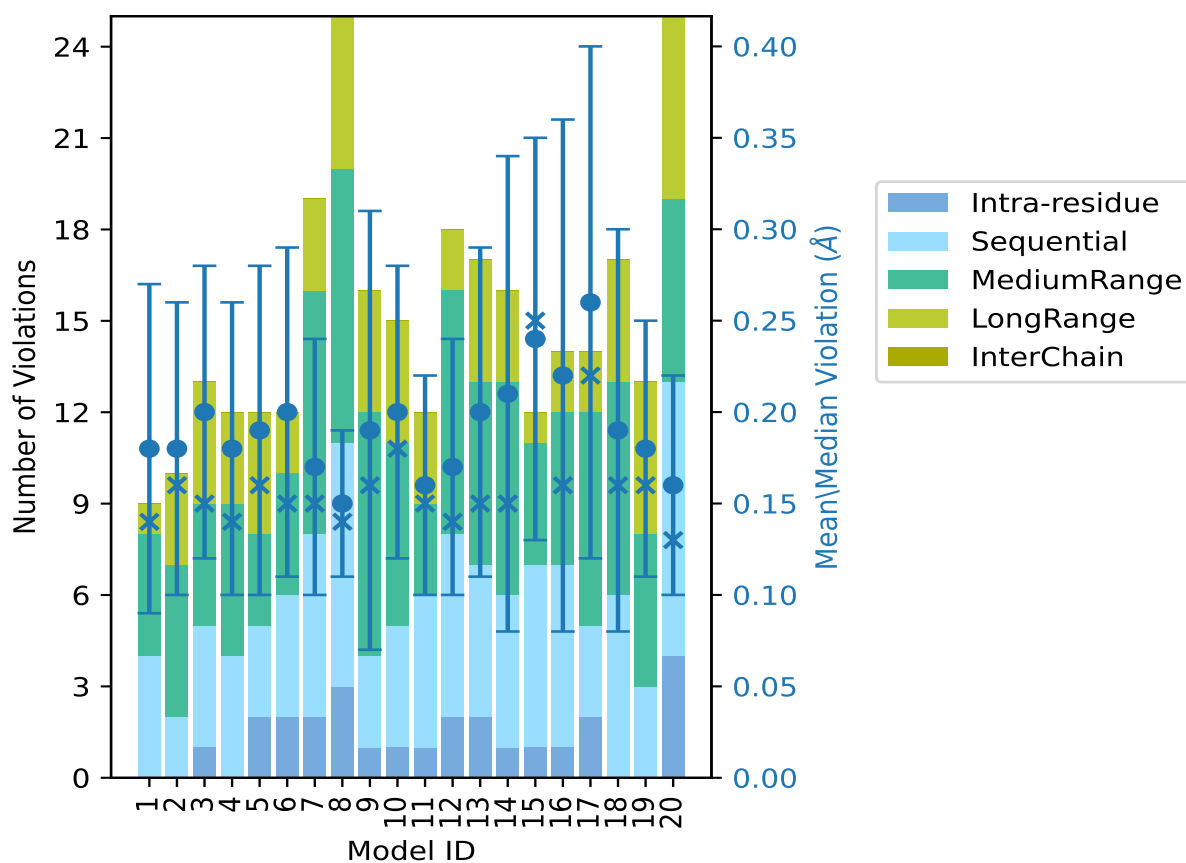
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
12	2	6	8	2	0	18	0.17	0.38	0.07	0.14
13	2	5	6	4	0	17	0.2	0.38	0.09	0.15
14	1	5	7	3	0	16	0.21	0.57	0.13	0.15
15	1	6	4	1	0	12	0.24	0.48	0.11	0.25
16	1	6	5	2	0	14	0.22	0.65	0.14	0.16
17	2	3	7	2	0	14	0.26	0.59	0.14	0.22
18	0	6	7	4	0	17	0.19	0.58	0.11	0.16
19	0	3	5	5	0	13	0.18	0.33	0.07	0.16
20	4	9	6	6	0	25	0.16	0.33	0.06	0.13

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

9.2.1 Bar graph : Distance Violation statistics for each model [\(i\)](#)



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

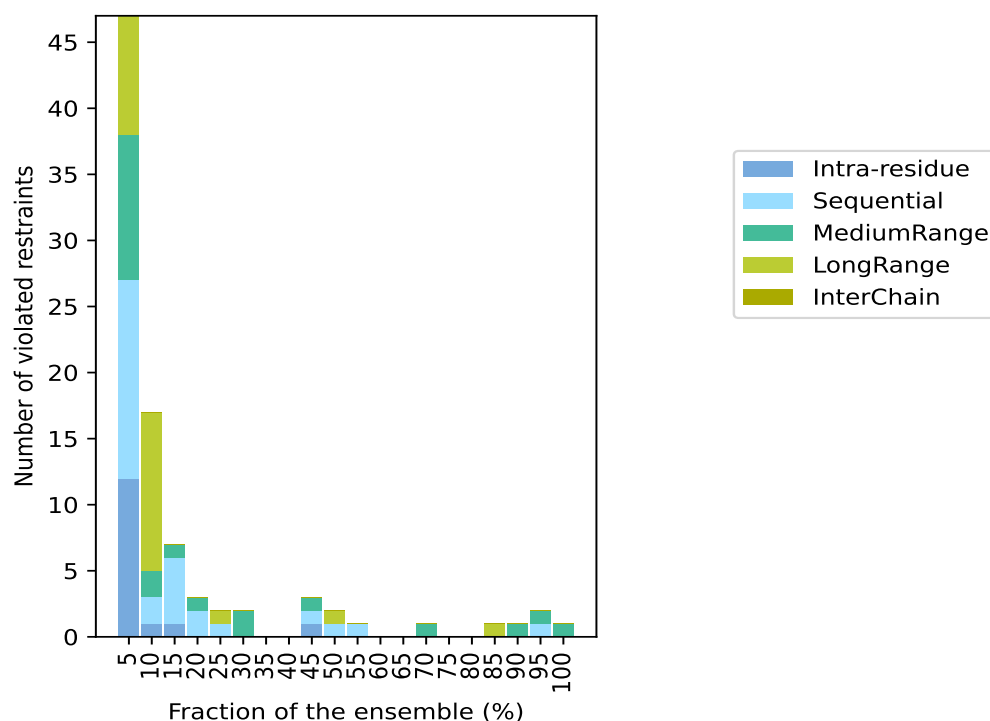
9.3 Distance violation statistics for the ensemble

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, 2528(IR:599, SQ:588, MR:739, LR:602, 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	%
12	15	11	9	0	47	1	5.0
1	2	2	12	0	17	2	10.0
1	5	1	0	0	7	3	15.0
0	2	1	0	0	3	4	20.0
0	1	0	1	0	2	5	25.0
0	0	2	0	0	2	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
1	1	1	0	0	3	9	45.0
0	1	0	1	0	2	10	50.0
0	1	0	0	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	1	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	1	0	1	17	85.0
0	0	1	0	0	1	18	90.0
0	1	1	0	0	2	19	95.0
0	0	1	0	0	1	20	100.0

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

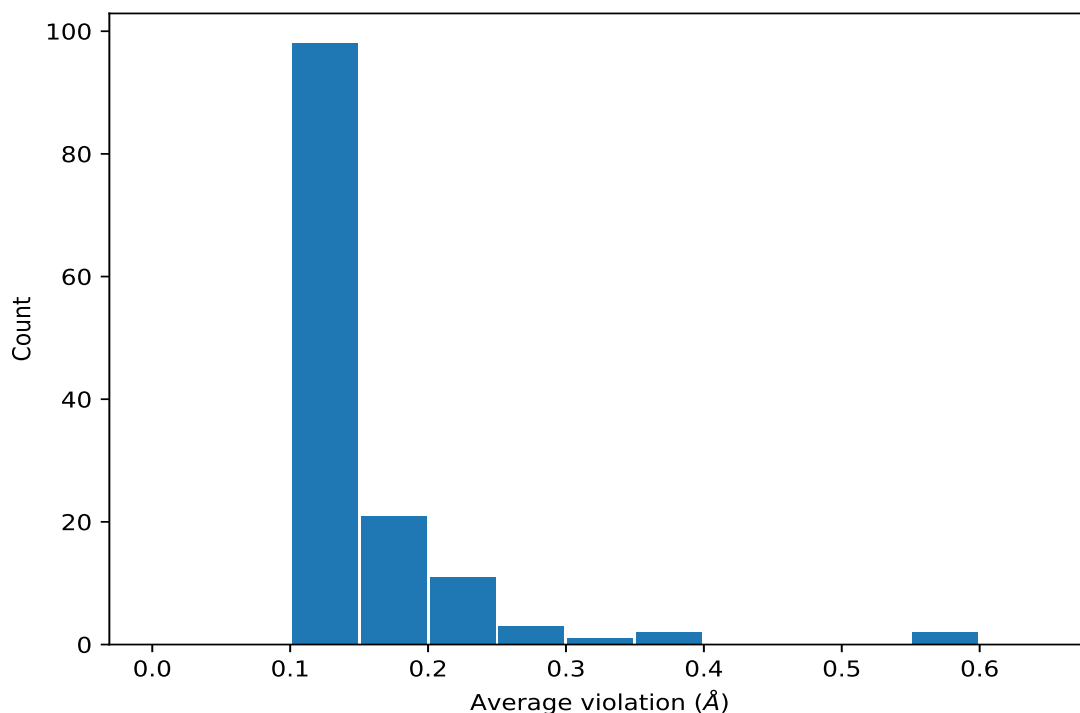
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	20	0.16	0.03	0.15
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	19	0.31	0.01	0.31
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	19	0.14	0.03	0.14
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	18	0.16	0.03	0.15
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	17	0.3	0.05	0.3
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	17	0.3	0.05	0.3
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	17	0.3	0.05	0.3
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	14	0.15	0.02	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	14	0.15	0.02	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	14	0.15	0.02	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	14	0.15	0.02	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	14	0.15	0.02	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	14	0.15	0.02	0.15
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB2	11	0.13	0.01	0.13
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB3	11	0.13	0.01	0.13
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB2	11	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB3	11	0.13	0.01	0.13
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB2	11	0.13	0.01	0.13
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB3	11	0.13	0.01	0.13
(1,1612)	1:A:118:VAL:HG21	1:A:119:GLU:HA	10	0.18	0.06	0.16
(1,1612)	1:A:118:VAL:HG22	1:A:119:GLU:HA	10	0.18	0.06	0.16
(1,1612)	1:A:118:VAL:HG23	1:A:119:GLU:HA	10	0.18	0.06	0.16
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD1	10	0.13	0.02	0.14
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD2	10	0.13	0.02	0.14
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG2	9	0.38	0.02	0.39
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG3	9	0.38	0.02	0.39
(1,649)	1:A:103:ARG:HG2	1:A:104:LYS:H	9	0.16	0.06	0.13
(1,649)	1:A:103:ARG:HG3	1:A:104:LYS:H	9	0.16	0.06	0.13
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD21	9	0.15	0.01	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD22	9	0.15	0.01	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD23	9	0.15	0.01	0.16
(1,1517)	1:A:94:ASP:HA	1:A:96:ILE:HB	6	0.14	0.02	0.15
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD11	6	0.12	0.01	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD12	6	0.12	0.01	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD13	6	0.12	0.01	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD21	6	0.12	0.01	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD22	6	0.12	0.01	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD23	6	0.12	0.01	0.12
(1,1235)	1:A:41:PRO:HA	1:A:42:LEU:HB2	5	0.13	0.01	0.13
(1,1402)	1:A:31:LEU:HD21	1:A:72:ALA:HA	5	0.12	0.01	0.11
(1,1402)	1:A:31:LEU:HD22	1:A:72:ALA:HA	5	0.12	0.01	0.11
(1,1402)	1:A:31:LEU:HD23	1:A:72:ALA:HA	5	0.12	0.01	0.11
(1,358)	1:A:47:ASP:HB2	1:A:48:GLN:H	4	0.17	0.01	0.16
(1,358)	1:A:47:ASP:HB3	1:A:48:GLN:H	4	0.17	0.01	0.16
(1,742)	1:A:116:LEU:HA	1:A:120:GLN:HE22	4	0.15	0.02	0.15
(1,1987)	1:A:18:CYS:HB2	1:A:19:GLU:HA	4	0.15	0.02	0.15
(1,1987)	1:A:18:CYS:HB3	1:A:19:GLU:HA	4	0.15	0.02	0.15
(1,871)	1:A:153:ARG:HA	1:A:154:ASP:H	3	0.6	0.03	0.59
(1,19)	1:A:134:ALA:HB1	1:A:135:GLN:HE22	3	0.23	0.13	0.18
(1,19)	1:A:134:ALA:HB2	1:A:135:GLN:HE22	3	0.23	0.13	0.18
(1,19)	1:A:134:ALA:HB3	1:A:135:GLN:HE22	3	0.23	0.13	0.18
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG11	3	0.18	0.06	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG12	3	0.18	0.06	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG13	3	0.18	0.06	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG21	3	0.18	0.06	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG22	3	0.18	0.06	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG23	3	0.18	0.06	0.14
(1,595)	1:A:97:LEU:H	1:A:98:PHE:HD1	3	0.17	0.01	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,595)	1:A:97:LEU:H	1:A:98:PHE:HD2	3	0.17	0.01	0.18
(1,776)	1:A:124:VAL:HA	1:A:125:SER:H	3	0.17	0.01	0.18
(1,1598)	1:A:105:LEU:H	1:A:105:LEU:HD21	3	0.15	0.01	0.15
(1,1598)	1:A:105:LEU:H	1:A:105:LEU:HD22	3	0.15	0.01	0.15
(1,1598)	1:A:105:LEU:H	1:A:105:LEU:HD23	3	0.15	0.01	0.15
(1,1181)	1:A:36:LEU:HD21	1:A:39:ILE:H	3	0.12	0.01	0.12
(1,1181)	1:A:36:LEU:HD22	1:A:39:ILE:H	3	0.12	0.01	0.12
(1,1181)	1:A:36:LEU:HD23	1:A:39:ILE:H	3	0.12	0.01	0.12
(1,7)	1:A:68:ALA:H	1:A:69:LEU:HG	2	0.6	0.02	0.6
(1,449)	1:A:86:CYS:HB2	1:A:87:ARG:H	2	0.22	0.05	0.22
(1,449)	1:A:86:CYS:HB3	1:A:87:ARG:H	2	0.22	0.05	0.22
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD11	2	0.2	0.02	0.2
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD12	2	0.2	0.02	0.2
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD13	2	0.2	0.02	0.2
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD21	2	0.2	0.02	0.2
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD22	2	0.2	0.02	0.2
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD23	2	0.2	0.02	0.2
(1,988)	1:A:10:LEU:HD11	1:A:69:LEU:H	2	0.17	0.01	0.17
(1,988)	1:A:10:LEU:HD12	1:A:69:LEU:H	2	0.17	0.01	0.17
(1,988)	1:A:10:LEU:HD13	1:A:69:LEU:H	2	0.17	0.01	0.17
(1,564)	1:A:116:LEU:H	1:A:116:LEU:HG	2	0.15	0.04	0.15
(1,168)	1:A:21:MET:H	1:A:76:ILE:HG21	2	0.14	0.01	0.14
(1,168)	1:A:21:MET:H	1:A:76:ILE:HG22	2	0.14	0.01	0.14
(1,168)	1:A:21:MET:H	1:A:76:ILE:HG23	2	0.14	0.01	0.14
(1,1696)	1:A:109:TRP:HZ3	1:A:122:MET:HE1	2	0.14	0.02	0.14
(1,1696)	1:A:109:TRP:HZ3	1:A:122:MET:HE2	2	0.14	0.02	0.14
(1,1696)	1:A:109:TRP:HZ3	1:A:122:MET:HE3	2	0.14	0.02	0.14
(1,2072)	1:A:31:LEU:HD11	1:A:73:ASN:HA	2	0.14	0.01	0.14
(1,2072)	1:A:31:LEU:HD12	1:A:73:ASN:HA	2	0.14	0.01	0.14
(1,2072)	1:A:31:LEU:HD13	1:A:73:ASN:HA	2	0.14	0.01	0.14
(1,2072)	1:A:31:LEU:HD21	1:A:73:ASN:HA	2	0.14	0.01	0.14
(1,2072)	1:A:31:LEU:HD22	1:A:73:ASN:HA	2	0.14	0.01	0.14
(1,2072)	1:A:31:LEU:HD23	1:A:73:ASN:HA	2	0.14	0.01	0.14
(1,68)	1:A:8:ILE:HB	1:A:11:GLY:H	2	0.14	0.02	0.14
(1,1010)	1:A:14:ILE:HD11	1:A:68:ALA:HA	2	0.14	0.02	0.14
(1,1010)	1:A:14:ILE:HD12	1:A:68:ALA:HA	2	0.14	0.02	0.14
(1,1010)	1:A:14:ILE:HD13	1:A:68:ALA:HA	2	0.14	0.02	0.14
(1,2511)	1:A:116:LEU:HD11	1:A:122:MET:HB2	2	0.13	0.02	0.13
(1,2511)	1:A:116:LEU:HD12	1:A:122:MET:HB2	2	0.13	0.02	0.13
(1,2511)	1:A:116:LEU:HD13	1:A:122:MET:HB2	2	0.13	0.02	0.13
(1,2511)	1:A:116:LEU:HD21	1:A:122:MET:HB2	2	0.13	0.02	0.13
(1,2511)	1:A:116:LEU:HD22	1:A:122:MET:HB2	2	0.13	0.02	0.13

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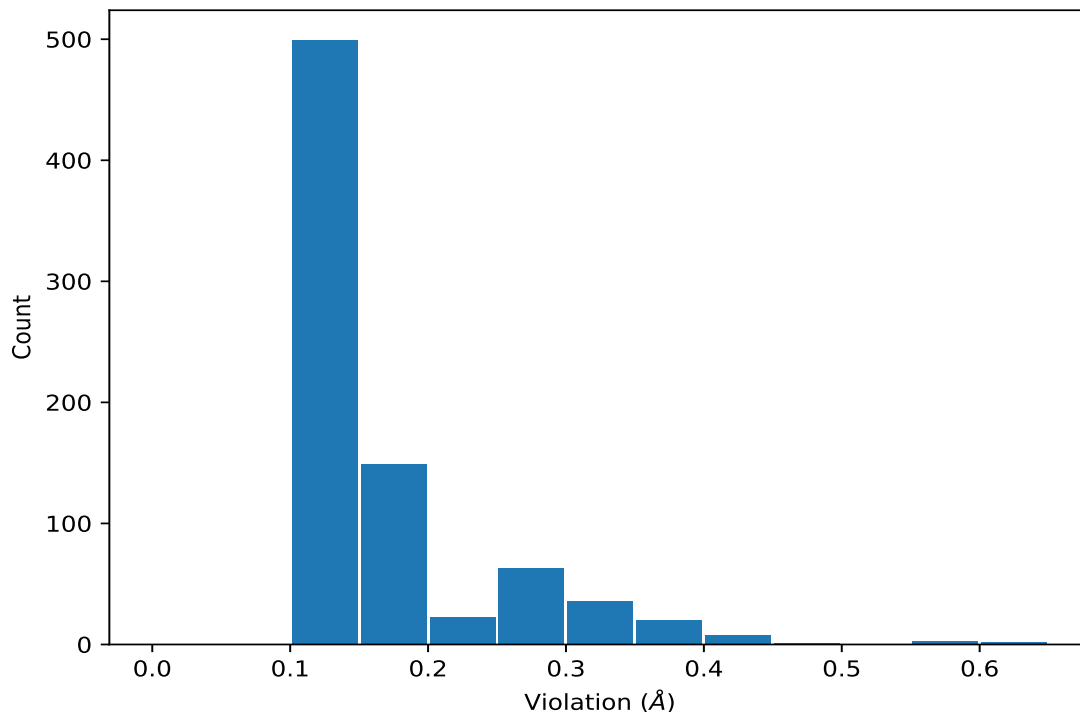
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2511)	1:A:116:LEU:HD23	1:A:122:MET:HB2	2	0.13	0.02	0.13
(1,1702)	1:A:116:LEU:HD11	1:A:122:MET:HE1	2	0.12	0.01	0.12
(1,1702)	1:A:116:LEU:HD11	1:A:122:MET:HE2	2	0.12	0.01	0.12
(1,1702)	1:A:116:LEU:HD11	1:A:122:MET:HE3	2	0.12	0.01	0.12
(1,1702)	1:A:116:LEU:HD12	1:A:122:MET:HE1	2	0.12	0.01	0.12
(1,1702)	1:A:116:LEU:HD12	1:A:122:MET:HE2	2	0.12	0.01	0.12
(1,1702)	1:A:116:LEU:HD12	1:A:122:MET:HE3	2	0.12	0.01	0.12
(1,1702)	1:A:116:LEU:HD13	1:A:122:MET:HE1	2	0.12	0.01	0.12
(1,1702)	1:A:116:LEU:HD13	1:A:122:MET:HE2	2	0.12	0.01	0.12
(1,1702)	1:A:116:LEU:HD13	1:A:122:MET:HE3	2	0.12	0.01	0.12
(1,1851)	1:A:31:LEU:HD11	1:A:98:PHE:HD1	2	0.12	0.01	0.12
(1,1851)	1:A:31:LEU:HD11	1:A:98:PHE:HD2	2	0.12	0.01	0.12
(1,1851)	1:A:31:LEU:HD12	1:A:98:PHE:HD1	2	0.12	0.01	0.12
(1,1851)	1:A:31:LEU:HD12	1:A:98:PHE:HD2	2	0.12	0.01	0.12
(1,1851)	1:A:31:LEU:HD13	1:A:98:PHE:HD1	2	0.12	0.01	0.12
(1,1851)	1:A:31:LEU:HD13	1:A:98:PHE:HD2	2	0.12	0.01	0.12
(1,547)	1:A:85:ILE:H	1:A:148:PHE:HE1	2	0.12	0.0	0.12
(1,547)	1:A:85:ILE:H	1:A:148:PHE:HE2	2	0.12	0.0	0.12
(1,1581)	1:A:72:ALA:HB1	1:A:101:VAL:HG21	2	0.12	0.0	0.12
(1,1581)	1:A:72:ALA:HB1	1:A:101:VAL:HG22	2	0.12	0.0	0.12
(1,1581)	1:A:72:ALA:HB1	1:A:101:VAL:HG23	2	0.12	0.0	0.12
(1,1581)	1:A:72:ALA:HB2	1:A:101:VAL:HG21	2	0.12	0.0	0.12
(1,1581)	1:A:72:ALA:HB2	1:A:101:VAL:HG22	2	0.12	0.0	0.12
(1,1581)	1:A:72:ALA:HB2	1:A:101:VAL:HG23	2	0.12	0.0	0.12
(1,1581)	1:A:72:ALA:HB3	1:A:101:VAL:HG21	2	0.12	0.0	0.12
(1,1581)	1:A:72:ALA:HB3	1:A:101:VAL:HG22	2	0.12	0.0	0.12
(1,1581)	1:A:72:ALA:HB3	1:A:101:VAL:HG23	2	0.12	0.0	0.12
(1,1669)	1:A:116:LEU:HD21	1:A:122:MET:HE1	2	0.12	0.0	0.12
(1,1669)	1:A:116:LEU:HD21	1:A:122:MET:HE2	2	0.12	0.0	0.12
(1,1669)	1:A:116:LEU:HD21	1:A:122:MET:HE3	2	0.12	0.0	0.12
(1,1669)	1:A:116:LEU:HD22	1:A:122:MET:HE1	2	0.12	0.0	0.12
(1,1669)	1:A:116:LEU:HD22	1:A:122:MET:HE2	2	0.12	0.0	0.12
(1,1669)	1:A:116:LEU:HD22	1:A:122:MET:HE3	2	0.12	0.0	0.12
(1,1669)	1:A:116:LEU:HD23	1:A:122:MET:HE1	2	0.12	0.0	0.12
(1,1669)	1:A:116:LEU:HD23	1:A:122:MET:HE2	2	0.12	0.0	0.12
(1,1669)	1:A:116:LEU:HD23	1:A:122:MET:HE3	2	0.12	0.0	0.12
(1,800)	1:A:38:LEU:H	1:A:40:LYS:HE2	2	0.11	0.0	0.11
(1,800)	1:A:38:LEU:H	1:A:40:LYS:HE3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,871)	1:A:153:ARG:HA	1:A:154:ASP:H	16	0.65
(1,7)	1:A:68:ALA:H	1:A:69:LEU:HG	9	0.61
(1,871)	1:A:153:ARG:HA	1:A:154:ASP:H	17	0.59
(1,7)	1:A:68:ALA:H	1:A:69:LEU:HG	18	0.58
(1,871)	1:A:153:ARG:HA	1:A:154:ASP:H	14	0.57
(1,1003)	1:A:13:VAL:HB	1:A:14:ILE:HA	15	0.48
(1,14)	1:A:135:GLN:HA	1:A:135:GLN:HE22	17	0.42
(1,19)	1:A:134:ALA:HB1	1:A:135:GLN:HE22	17	0.41
(1,19)	1:A:134:ALA:HB2	1:A:135:GLN:HE22	17	0.41
(1,19)	1:A:134:ALA:HB3	1:A:135:GLN:HE22	17	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG2	3	0.4
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG3	3	0.4
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG2	7	0.4
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG3	7	0.4
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG2	5	0.39
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG3	5	0.39
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG2	6	0.39
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG3	6	0.39
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG2	14	0.39
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG3	14	0.39
(1,754)	1:A:118:VAL:H	1:A:118:VAL:HB	13	0.38
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	12	0.38
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	12	0.38
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	12	0.38
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG2	15	0.37
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG3	15	0.37
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG2	17	0.37
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG3	17	0.37
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG2	10	0.36
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG3	10	0.36
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	2	0.36
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	2	0.36
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	2	0.36
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	10	0.36
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG2	16	0.35
(1,2513)	1:A:117:GLN:H	1:A:117:GLN:HG3	16	0.35
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	4	0.35
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	4	0.35
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	4	0.35
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	13	0.34
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	13	0.34
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	13	0.34
(1,927)	1:A:50:LYS:HA	1:A:50:LYS:HG3	20	0.33
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	1	0.33
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	1	0.33
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	1	0.33
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	14	0.33
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	14	0.33
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	14	0.33
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	17	0.33
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	17	0.33
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	17	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	19	0.33
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	19	0.33
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	19	0.33
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	5	0.33
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	11	0.33
(1,1277)	1:A:50:LYS:HA	1:A:50:LYS:HG2	6	0.32
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	3	0.32
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	6	0.32
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	19	0.32
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	1	0.31
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	2	0.31
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	4	0.31
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	7	0.31
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	9	0.31
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	12	0.31
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	13	0.31
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	14	0.31
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	15	0.31
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	16	0.3
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	16	0.3
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	16	0.3
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	20	0.3
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	20	0.3
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	20	0.3
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	8	0.3
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	18	0.3
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	20	0.3
(1,2610)	1:A:151:LEU:HA	1:A:151:LEU:HD11	12	0.29
(1,2610)	1:A:151:LEU:HA	1:A:151:LEU:HD12	12	0.29
(1,2610)	1:A:151:LEU:HA	1:A:151:LEU:HD13	12	0.29
(1,2610)	1:A:151:LEU:HA	1:A:151:LEU:HD21	12	0.29
(1,2610)	1:A:151:LEU:HA	1:A:151:LEU:HD22	12	0.29
(1,2610)	1:A:151:LEU:HA	1:A:151:LEU:HD23	12	0.29
(1,1685)	1:A:115:LEU:HA	1:A:118:VAL:HB	13	0.29
(1,10)	1:A:132:SER:HA	1:A:135:GLN:HE22	16	0.29
(1,768)	1:A:121:ARG:H	1:A:122:MET:H	15	0.28
(1,649)	1:A:103:ARG:HG2	1:A:104:LYS:H	10	0.28
(1,649)	1:A:103:ARG:HG3	1:A:104:LYS:H	10	0.28
(1,1686)	1:A:118:VAL:HG11	1:A:119:GLU:HA	13	0.28
(1,1686)	1:A:118:VAL:HG12	1:A:119:GLU:HA	13	0.28
(1,1686)	1:A:118:VAL:HG13	1:A:119:GLU:HA	13	0.28
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	15	0.28
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	15	0.28
(1,449)	1:A:86:CYS:HB2	1:A:87:ARG:H	1	0.27
(1,449)	1:A:86:CYS:HB3	1:A:87:ARG:H	1	0.27
(1,1677)	1:A:133:TRP:HB2	1:A:135:GLN:HG2	17	0.27
(1,1677)	1:A:133:TRP:HB2	1:A:135:GLN:HG3	17	0.27
(1,1677)	1:A:133:TRP:HB3	1:A:135:GLN:HG2	17	0.27
(1,1677)	1:A:133:TRP:HB3	1:A:135:GLN:HG3	17	0.27
(1,1612)	1:A:118:VAL:HG21	1:A:119:GLU:HA	10	0.27
(1,1612)	1:A:118:VAL:HG22	1:A:119:GLU:HA	10	0.27
(1,1612)	1:A:118:VAL:HG23	1:A:119:GLU:HA	10	0.27
(1,1612)	1:A:118:VAL:HG21	1:A:119:GLU:HA	15	0.27
(1,1612)	1:A:118:VAL:HG22	1:A:119:GLU:HA	15	0.27
(1,1612)	1:A:118:VAL:HG23	1:A:119:GLU:HA	15	0.27
(1,1612)	1:A:118:VAL:HG21	1:A:119:GLU:HA	17	0.27
(1,1612)	1:A:118:VAL:HG22	1:A:119:GLU:HA	17	0.27
(1,1612)	1:A:118:VAL:HG23	1:A:119:GLU:HA	17	0.27
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG11	14	0.27
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG12	14	0.27
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG13	14	0.27
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG21	14	0.27
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG22	14	0.27
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG23	14	0.27
(1,371)	1:A:52:SER:HA	1:A:53:VAL:H	4	0.26
(1,228)	1:A:31:LEU:H	1:A:98:PHE:HD1	19	0.26
(1,228)	1:A:31:LEU:H	1:A:98:PHE:HD2	19	0.26
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	3	0.26
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	3	0.26
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	3	0.26
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	7	0.25
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	5	0.25
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	5	0.25
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	5	0.25
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	6	0.25
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	6	0.25
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	6	0.25
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	18	0.25
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	18	0.25
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	18	0.25
(1,649)	1:A:103:ARG:HG2	1:A:104:LYS:H	15	0.23
(1,649)	1:A:103:ARG:HG3	1:A:104:LYS:H	15	0.23
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	10	0.23
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	10	0.23
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	10	0.23
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	10	0.22
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	3	0.22
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	11	0.21
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD11	9	0.21
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD12	9	0.21
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD13	9	0.21
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD21	9	0.21
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD22	9	0.21
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD23	9	0.21
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	7	0.21
(1,1785)	1:A:146:ARG:HD2	1:A:147:ALA:HB1	13	0.21
(1,1785)	1:A:146:ARG:HD2	1:A:147:ALA:HB2	13	0.21
(1,1785)	1:A:146:ARG:HD2	1:A:147:ALA:HB3	13	0.21
(1,1785)	1:A:146:ARG:HD3	1:A:147:ALA:HB1	13	0.21
(1,1785)	1:A:146:ARG:HD3	1:A:147:ALA:HB2	13	0.21
(1,1785)	1:A:146:ARG:HD3	1:A:147:ALA:HB3	13	0.21
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	5	0.2
(1,649)	1:A:103:ARG:HG2	1:A:104:LYS:H	18	0.19
(1,649)	1:A:103:ARG:HG3	1:A:104:LYS:H	18	0.19
(1,564)	1:A:116:LEU:H	1:A:116:LEU:HG	8	0.19
(1,358)	1:A:47:ASP:HB2	1:A:48:GLN:H	3	0.19
(1,358)	1:A:47:ASP:HB3	1:A:48:GLN:H	3	0.19
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	20	0.19
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	8	0.19
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	8	0.19
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	8	0.19
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	8	0.19
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	8	0.19
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	8	0.19
(1,988)	1:A:10:LEU:HD11	1:A:69:LEU:H	18	0.18
(1,988)	1:A:10:LEU:HD12	1:A:69:LEU:H	18	0.18
(1,988)	1:A:10:LEU:HD13	1:A:69:LEU:H	18	0.18
(1,776)	1:A:124:VAL:HA	1:A:125:SER:H	8	0.18
(1,776)	1:A:124:VAL:HA	1:A:125:SER:H	19	0.18
(1,743)	1:A:117:GLN:HE21	1:A:118:VAL:HB	16	0.18
(1,742)	1:A:116:LEU:HA	1:A:120:GLN:HE22	12	0.18
(1,595)	1:A:97:LEU:H	1:A:98:PHE:HD1	12	0.18
(1,595)	1:A:97:LEU:H	1:A:98:PHE:HD2	12	0.18
(1,595)	1:A:97:LEU:H	1:A:98:PHE:HD1	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,595)	1:A:97:LEU:H	1:A:98:PHE:HD2	20	0.18
(1,449)	1:A:86:CYS:HB2	1:A:87:ARG:H	14	0.18
(1,449)	1:A:86:CYS:HB3	1:A:87:ARG:H	14	0.18
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	19	0.18
(1,1987)	1:A:18:CYS:HB2	1:A:19:GLU:HA	7	0.18
(1,1987)	1:A:18:CYS:HB3	1:A:19:GLU:HA	7	0.18
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD11	18	0.18
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD12	18	0.18
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD13	18	0.18
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD21	18	0.18
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD22	18	0.18
(1,1931)	1:A:10:LEU:HA	1:A:69:LEU:HD23	18	0.18
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	10	0.18
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	10	0.18
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	10	0.18
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	10	0.18
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	10	0.18
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	10	0.18
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	16	0.18
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	16	0.18
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	16	0.18
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	16	0.18
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	16	0.18
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	16	0.18
(1,19)	1:A:134:ALA:HB1	1:A:135:GLN:HE22	10	0.18
(1,19)	1:A:134:ALA:HB2	1:A:135:GLN:HE22	10	0.18
(1,19)	1:A:134:ALA:HB3	1:A:135:GLN:HE22	10	0.18
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	8	0.18
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	10	0.18
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	13	0.18
(1,141)	1:A:16:LYS:HB2	1:A:17:ARG:H	7	0.18
(1,141)	1:A:16:LYS:HB3	1:A:17:ARG:H	7	0.18
(1,1385)	1:A:68:ALA:HB1	1:A:105:LEU:HG	9	0.18
(1,1385)	1:A:68:ALA:HB2	1:A:105:LEU:HG	9	0.18
(1,1385)	1:A:68:ALA:HB3	1:A:105:LEU:HG	9	0.18
(1,747)	1:A:117:GLN:HA	1:A:117:GLN:HE22	13	0.17
(1,657)	1:A:104:LYS:HE2	1:A:105:LEU:H	5	0.17
(1,657)	1:A:104:LYS:HE3	1:A:105:LEU:H	5	0.17
(1,358)	1:A:47:ASP:HB2	1:A:48:GLN:H	6	0.17
(1,358)	1:A:47:ASP:HB3	1:A:48:GLN:H	6	0.17
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	9	0.17
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	18	0.17
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	9	0.17
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	9	0.17
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	9	0.17
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	9	0.17
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	9	0.17
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	9	0.17
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	15	0.17
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD1	5	0.17
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD2	5	0.17
(1,1038)	1:A:50:LYS:HA	1:A:50:LYS:HD2	20	0.17
(1,1038)	1:A:50:LYS:HA	1:A:50:LYS:HD3	20	0.17
(1,988)	1:A:10:LEU:HD11	1:A:69:LEU:H	9	0.16
(1,988)	1:A:10:LEU:HD12	1:A:69:LEU:H	9	0.16
(1,988)	1:A:10:LEU:HD13	1:A:69:LEU:H	9	0.16
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	19	0.16
(1,773)	1:A:124:VAL:H	1:A:124:VAL:HB	8	0.16
(1,742)	1:A:116:LEU:HA	1:A:120:GLN:HE22	19	0.16
(1,68)	1:A:8:ILE:HB	1:A:11:GLY:H	9	0.16
(1,595)	1:A:97:LEU:H	1:A:98:PHE:HD1	18	0.16
(1,595)	1:A:97:LEU:H	1:A:98:PHE:HD2	18	0.16
(1,358)	1:A:47:ASP:HB2	1:A:48:GLN:H	7	0.16
(1,358)	1:A:47:ASP:HB3	1:A:48:GLN:H	7	0.16
(1,358)	1:A:47:ASP:HB2	1:A:48:GLN:H	8	0.16
(1,358)	1:A:47:ASP:HB3	1:A:48:GLN:H	8	0.16
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	2	0.16
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	8	0.16
(1,1974)	1:A:15:HIS:HB2	1:A:16:LYS:HG2	7	0.16
(1,1974)	1:A:15:HIS:HB2	1:A:16:LYS:HG3	7	0.16
(1,1974)	1:A:15:HIS:HB3	1:A:16:LYS:HG2	7	0.16
(1,1974)	1:A:15:HIS:HB3	1:A:16:LYS:HG3	7	0.16
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	2	0.16
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	2	0.16
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	2	0.16
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	2	0.16
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	2	0.16
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	2	0.16
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	19	0.16
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	19	0.16
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	19	0.16
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	19	0.16
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	19	0.16
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	14	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD21	4	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD22	4	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD23	4	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD21	9	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD22	9	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD23	9	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD21	10	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD22	10	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD23	10	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD21	17	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD22	17	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD23	17	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD21	18	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD22	18	0.16
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD23	18	0.16
(1,1696)	1:A:109:TRP:HZ3	1:A:122:MET:HE1	8	0.16
(1,1696)	1:A:109:TRP:HZ3	1:A:122:MET:HE2	8	0.16
(1,1696)	1:A:109:TRP:HZ3	1:A:122:MET:HE3	8	0.16
(1,1660)	1:A:115:LEU:HA	1:A:115:LEU:HD11	9	0.16
(1,1660)	1:A:115:LEU:HA	1:A:115:LEU:HD12	9	0.16
(1,1660)	1:A:115:LEU:HA	1:A:115:LEU:HD13	9	0.16
(1,1612)	1:A:118:VAL:HG21	1:A:119:GLU:HA	2	0.16
(1,1612)	1:A:118:VAL:HG22	1:A:119:GLU:HA	2	0.16
(1,1612)	1:A:118:VAL:HG23	1:A:119:GLU:HA	2	0.16
(1,1612)	1:A:118:VAL:HG21	1:A:119:GLU:HA	8	0.16
(1,1612)	1:A:118:VAL:HG22	1:A:119:GLU:HA	8	0.16
(1,1612)	1:A:118:VAL:HG23	1:A:119:GLU:HA	8	0.16
(1,1612)	1:A:118:VAL:HG21	1:A:119:GLU:HA	11	0.16
(1,1612)	1:A:118:VAL:HG22	1:A:119:GLU:HA	11	0.16
(1,1612)	1:A:118:VAL:HG23	1:A:119:GLU:HA	11	0.16
(1,1612)	1:A:118:VAL:HG21	1:A:119:GLU:HA	19	0.16
(1,1612)	1:A:118:VAL:HG22	1:A:119:GLU:HA	19	0.16
(1,1612)	1:A:118:VAL:HG23	1:A:119:GLU:HA	19	0.16
(1,1598)	1:A:105:LEU:H	1:A:105:LEU:HD21	7	0.16
(1,1598)	1:A:105:LEU:H	1:A:105:LEU:HD22	7	0.16
(1,1598)	1:A:105:LEU:H	1:A:105:LEU:HD23	7	0.16
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD1	2	0.16
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD2	2	0.16
(1,1010)	1:A:14:ILE:HD11	1:A:68:ALA:HA	8	0.16
(1,1010)	1:A:14:ILE:HD12	1:A:68:ALA:HA	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1010)	1:A:14:ILE:HD13	1:A:68:ALA:HA	8	0.16
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	4	0.15
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	5	0.15
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	9	0.15
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	14	0.15
(1,776)	1:A:124:VAL:HA	1:A:125:SER:H	20	0.15
(1,2511)	1:A:116:LEU:HD11	1:A:122:MET:HB2	8	0.15
(1,2511)	1:A:116:LEU:HD12	1:A:122:MET:HB2	8	0.15
(1,2511)	1:A:116:LEU:HD13	1:A:122:MET:HB2	8	0.15
(1,2511)	1:A:116:LEU:HD21	1:A:122:MET:HB2	8	0.15
(1,2511)	1:A:116:LEU:HD22	1:A:122:MET:HB2	8	0.15
(1,2511)	1:A:116:LEU:HD23	1:A:122:MET:HB2	8	0.15
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	5	0.15
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	6	0.15
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	10	0.15
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	11	0.15
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	13	0.15
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	15	0.15
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	17	0.15
(1,2072)	1:A:31:LEU:HD11	1:A:73:ASN:HA	3	0.15
(1,2072)	1:A:31:LEU:HD12	1:A:73:ASN:HA	3	0.15
(1,2072)	1:A:31:LEU:HD13	1:A:73:ASN:HA	3	0.15
(1,2072)	1:A:31:LEU:HD21	1:A:73:ASN:HA	3	0.15
(1,2072)	1:A:31:LEU:HD22	1:A:73:ASN:HA	3	0.15
(1,2072)	1:A:31:LEU:HD23	1:A:73:ASN:HA	3	0.15
(1,1987)	1:A:18:CYS:HB2	1:A:19:GLU:HA	11	0.15
(1,1987)	1:A:18:CYS:HB3	1:A:19:GLU:HA	11	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	3	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	3	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	3	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	3	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	3	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	3	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	6	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	6	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	6	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	6	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	6	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	6	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	7	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	7	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	7	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	7	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	7	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	12	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	12	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	12	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	12	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	12	0.15
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	12	0.15
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	18	0.15
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD21	7	0.15
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD22	7	0.15
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD23	7	0.15
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD21	20	0.15
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD22	20	0.15
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD23	20	0.15
(1,168)	1:A:21:MET:H	1:A:76:ILE:HG21	11	0.15
(1,168)	1:A:21:MET:H	1:A:76:ILE:HG22	11	0.15
(1,168)	1:A:21:MET:H	1:A:76:ILE:HG23	11	0.15
(1,1598)	1:A:105:LEU:H	1:A:105:LEU:HD21	11	0.15
(1,1598)	1:A:105:LEU:H	1:A:105:LEU:HD22	11	0.15
(1,1598)	1:A:105:LEU:H	1:A:105:LEU:HD23	11	0.15
(1,1517)	1:A:94:ASP:HA	1:A:96:ILE:HB	11	0.15
(1,1517)	1:A:94:ASP:HA	1:A:96:ILE:HB	12	0.15
(1,1517)	1:A:94:ASP:HA	1:A:96:ILE:HB	18	0.15
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD1	16	0.15
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD2	16	0.15
(1,1263)	1:A:151:LEU:HA	1:A:151:LEU:HD21	12	0.15
(1,1263)	1:A:151:LEU:HA	1:A:151:LEU:HD22	12	0.15
(1,1263)	1:A:151:LEU:HA	1:A:151:LEU:HD23	12	0.15
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	2	0.14
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	12	0.14
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	13	0.14
(1,742)	1:A:116:LEU:HA	1:A:120:GLN:HE22	1	0.14
(1,649)	1:A:103:ARG:HG2	1:A:104:LYS:H	3	0.14
(1,649)	1:A:103:ARG:HG3	1:A:104:LYS:H	3	0.14
(1,519)	1:A:76:ILE:H	1:A:98:PHE:HD1	13	0.14
(1,519)	1:A:76:ILE:H	1:A:98:PHE:HD2	13	0.14
(1,2558)	1:A:132:SER:HB2	1:A:135:GLN:HG2	17	0.14
(1,2558)	1:A:132:SER:HB2	1:A:135:GLN:HG3	17	0.14
(1,2558)	1:A:132:SER:HB3	1:A:135:GLN:HG2	17	0.14
(1,2558)	1:A:132:SER:HB3	1:A:135:GLN:HG3	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	1	0.14
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	12	0.14
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	14	0.14
(1,1987)	1:A:18:CYS:HB2	1:A:19:GLU:HA	20	0.14
(1,1987)	1:A:18:CYS:HB3	1:A:19:GLU:HA	20	0.14
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	17	0.14
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	17	0.14
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	17	0.14
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	17	0.14
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	17	0.14
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	17	0.14
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	4	0.14
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	12	0.14
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	20	0.14
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD21	12	0.14
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD22	12	0.14
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD23	12	0.14
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD21	14	0.14
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD22	14	0.14
(1,1816)	1:A:39:ILE:H	1:A:42:LEU:HD23	14	0.14
(1,1726)	1:A:124:VAL:HA	1:A:125:SER:HB2	16	0.14
(1,1726)	1:A:124:VAL:HA	1:A:125:SER:HB3	16	0.14
(1,1598)	1:A:105:LEU:H	1:A:105:LEU:HD21	8	0.14
(1,1598)	1:A:105:LEU:H	1:A:105:LEU:HD22	8	0.14
(1,1598)	1:A:105:LEU:H	1:A:105:LEU:HD23	8	0.14
(1,1517)	1:A:94:ASP:HA	1:A:96:ILE:HB	9	0.14
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD1	11	0.14
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD2	11	0.14
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD1	13	0.14
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD2	13	0.14
(1,1402)	1:A:31:LEU:HD21	1:A:72:ALA:HA	6	0.14
(1,1402)	1:A:31:LEU:HD22	1:A:72:ALA:HA	6	0.14
(1,1402)	1:A:31:LEU:HD23	1:A:72:ALA:HA	6	0.14
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB2	3	0.14
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB3	3	0.14
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB2	3	0.14
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB3	3	0.14
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB2	3	0.14
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB3	3	0.14
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB2	18	0.14
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB3	18	0.14
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB2	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB3	18	0.14
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB2	18	0.14
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB3	18	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG11	13	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG12	13	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG13	13	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG21	13	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG22	13	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG23	13	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG11	20	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG12	20	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG13	20	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG21	20	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG22	20	0.14
(1,1288)	1:A:52:SER:HA	1:A:53:VAL:HG23	20	0.14
(1,1235)	1:A:41:PRO:HA	1:A:42:LEU:HB2	12	0.14
(1,1235)	1:A:41:PRO:HA	1:A:42:LEU:HB2	14	0.14
(1,1137)	1:A:31:LEU:HG	1:A:72:ALA:HA	20	0.14
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	15	0.13
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	18	0.13
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	20	0.13
(1,742)	1:A:116:LEU:HA	1:A:120:GLN:HE22	20	0.13
(1,649)	1:A:103:ARG:HG2	1:A:104:LYS:H	8	0.13
(1,649)	1:A:103:ARG:HG3	1:A:104:LYS:H	8	0.13
(1,649)	1:A:103:ARG:HG2	1:A:104:LYS:H	20	0.13
(1,649)	1:A:103:ARG:HG3	1:A:104:LYS:H	20	0.13
(1,630)	1:A:102:ASN:H	1:A:105:LEU:HB2	8	0.13
(1,2311)	1:A:84:ASN:HD21	1:A:85:ILE:HB	18	0.13
(1,2311)	1:A:84:ASN:HD22	1:A:85:ILE:HB	18	0.13
(1,212)	1:A:28:CYS:H	1:A:31:LEU:H	4	0.13
(1,2072)	1:A:31:LEU:HD11	1:A:73:ASN:HA	7	0.13
(1,2072)	1:A:31:LEU:HD12	1:A:73:ASN:HA	7	0.13
(1,2072)	1:A:31:LEU:HD13	1:A:73:ASN:HA	7	0.13
(1,2072)	1:A:31:LEU:HD21	1:A:73:ASN:HA	7	0.13
(1,2072)	1:A:31:LEU:HD22	1:A:73:ASN:HA	7	0.13
(1,2072)	1:A:31:LEU:HD23	1:A:73:ASN:HA	7	0.13
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD11	14	0.13
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD12	14	0.13
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD13	14	0.13
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD21	14	0.13
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD22	14	0.13
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD23	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD11	17	0.13
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD12	17	0.13
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD13	17	0.13
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD21	17	0.13
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD22	17	0.13
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD23	17	0.13
(1,1987)	1:A:18:CYS:HB2	1:A:19:GLU:HA	12	0.13
(1,1987)	1:A:18:CYS:HB3	1:A:19:GLU:HA	12	0.13
(1,1975)	1:A:15:HIS:HB2	1:A:18:CYS:HB2	7	0.13
(1,1975)	1:A:15:HIS:HB2	1:A:18:CYS:HB3	7	0.13
(1,1975)	1:A:15:HIS:HB3	1:A:18:CYS:HB2	7	0.13
(1,1975)	1:A:15:HIS:HB3	1:A:18:CYS:HB3	7	0.13
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	14	0.13
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	14	0.13
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	14	0.13
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	14	0.13
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	14	0.13
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	14	0.13
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	18	0.13
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	18	0.13
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	18	0.13
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	18	0.13
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	18	0.13
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	18	0.13
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	6	0.13
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	16	0.13
(1,1851)	1:A:31:LEU:HD11	1:A:98:PHE:HD1	7	0.13
(1,1851)	1:A:31:LEU:HD11	1:A:98:PHE:HD2	7	0.13
(1,1851)	1:A:31:LEU:HD12	1:A:98:PHE:HD1	7	0.13
(1,1851)	1:A:31:LEU:HD12	1:A:98:PHE:HD2	7	0.13
(1,1851)	1:A:31:LEU:HD13	1:A:98:PHE:HD1	7	0.13
(1,1851)	1:A:31:LEU:HD13	1:A:98:PHE:HD2	7	0.13
(1,1719)	1:A:125:SER:HB2	1:A:126:PRO:HG2	8	0.13
(1,1719)	1:A:125:SER:HB2	1:A:126:PRO:HG3	8	0.13
(1,1719)	1:A:125:SER:HB3	1:A:126:PRO:HG2	8	0.13
(1,1719)	1:A:125:SER:HB3	1:A:126:PRO:HG3	8	0.13
(1,1702)	1:A:116:LEU:HD11	1:A:122:MET:HE1	8	0.13
(1,1702)	1:A:116:LEU:HD11	1:A:122:MET:HE2	8	0.13
(1,1702)	1:A:116:LEU:HD11	1:A:122:MET:HE3	8	0.13
(1,1702)	1:A:116:LEU:HD12	1:A:122:MET:HE1	8	0.13
(1,1702)	1:A:116:LEU:HD12	1:A:122:MET:HE2	8	0.13
(1,1702)	1:A:116:LEU:HD12	1:A:122:MET:HE3	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1702)	1:A:116:LEU:HD13	1:A:122:MET:HE1	8	0.13
(1,1702)	1:A:116:LEU:HD13	1:A:122:MET:HE2	8	0.13
(1,1702)	1:A:116:LEU:HD13	1:A:122:MET:HE3	8	0.13
(1,168)	1:A:21:MET:H	1:A:76:ILE:HG21	8	0.13
(1,168)	1:A:21:MET:H	1:A:76:ILE:HG22	8	0.13
(1,168)	1:A:21:MET:H	1:A:76:ILE:HG23	8	0.13
(1,1612)	1:A:118:VAL:HG21	1:A:119:GLU:HA	4	0.13
(1,1612)	1:A:118:VAL:HG22	1:A:119:GLU:HA	4	0.13
(1,1612)	1:A:118:VAL:HG23	1:A:119:GLU:HA	4	0.13
(1,1612)	1:A:118:VAL:HG21	1:A:119:GLU:HA	16	0.13
(1,1612)	1:A:118:VAL:HG22	1:A:119:GLU:HA	16	0.13
(1,1612)	1:A:118:VAL:HG23	1:A:119:GLU:HA	16	0.13
(1,1612)	1:A:118:VAL:HG21	1:A:119:GLU:HA	20	0.13
(1,1612)	1:A:118:VAL:HG22	1:A:119:GLU:HA	20	0.13
(1,1612)	1:A:118:VAL:HG23	1:A:119:GLU:HA	20	0.13
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD1	12	0.13
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD2	12	0.13
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB2	6	0.13
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB3	6	0.13
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB2	6	0.13
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB3	6	0.13
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB2	6	0.13
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB3	6	0.13
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB2	7	0.13
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB3	7	0.13
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB2	7	0.13
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB3	7	0.13
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB2	7	0.13
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB3	7	0.13
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB2	16	0.13
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB3	16	0.13
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB2	16	0.13
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB3	16	0.13
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB2	16	0.13
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB3	16	0.13
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB2	20	0.13
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB3	20	0.13
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB2	20	0.13
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB3	20	0.13
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB2	20	0.13
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB3	20	0.13
(1,1235)	1:A:41:PRO:HA	1:A:42:LEU:HB2	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1181)	1:A:36:LEU:HD21	1:A:39:ILE:H	7	0.13
(1,1181)	1:A:36:LEU:HD22	1:A:39:ILE:H	7	0.13
(1,1181)	1:A:36:LEU:HD23	1:A:39:ILE:H	7	0.13
(1,1154)	1:A:15:HIS:HB2	1:A:35:VAL:HG21	10	0.13
(1,1154)	1:A:15:HIS:HB2	1:A:35:VAL:HG22	10	0.13
(1,1154)	1:A:15:HIS:HB2	1:A:35:VAL:HG23	10	0.13
(1,1154)	1:A:15:HIS:HB3	1:A:35:VAL:HG21	10	0.13
(1,1154)	1:A:15:HIS:HB3	1:A:35:VAL:HG22	10	0.13
(1,1154)	1:A:15:HIS:HB3	1:A:35:VAL:HG23	10	0.13
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	1	0.12
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	3	0.12
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	6	0.12
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	7	0.12
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	8	0.12
(1,741)	1:A:114:LEU:HA	1:A:117:GLN:HE21	13	0.12
(1,649)	1:A:103:ARG:HG2	1:A:104:LYS:H	1	0.12
(1,649)	1:A:103:ARG:HG3	1:A:104:LYS:H	1	0.12
(1,547)	1:A:85:ILE:H	1:A:148:PHE:HE1	9	0.12
(1,547)	1:A:85:ILE:H	1:A:148:PHE:HE2	9	0.12
(1,547)	1:A:85:ILE:H	1:A:148:PHE:HE1	11	0.12
(1,547)	1:A:85:ILE:H	1:A:148:PHE:HE2	11	0.12
(1,2564)	1:A:136:GLU:HA	1:A:136:GLU:HG2	5	0.12
(1,2564)	1:A:136:GLU:HA	1:A:136:GLU:HG3	5	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD11	9	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD12	9	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD13	9	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD21	9	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD22	9	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD23	9	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD11	10	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD12	10	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD13	10	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD21	10	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD22	10	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD23	10	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD11	15	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD12	15	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD13	15	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD21	15	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD22	15	0.12
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD23	15	0.12
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	17	0.12
(1,1851)	1:A:31:LEU:HD11	1:A:98:PHE:HD1	3	0.12
(1,1851)	1:A:31:LEU:HD11	1:A:98:PHE:HD2	3	0.12
(1,1851)	1:A:31:LEU:HD12	1:A:98:PHE:HD1	3	0.12
(1,1851)	1:A:31:LEU:HD12	1:A:98:PHE:HD2	3	0.12
(1,1851)	1:A:31:LEU:HD13	1:A:98:PHE:HD1	3	0.12
(1,1851)	1:A:31:LEU:HD13	1:A:98:PHE:HD2	3	0.12
(1,1760)	1:A:147:ALA:HA	1:A:149:GLN:HG2	12	0.12
(1,1702)	1:A:116:LEU:HD11	1:A:122:MET:HE1	20	0.12
(1,1702)	1:A:116:LEU:HD11	1:A:122:MET:HE2	20	0.12
(1,1702)	1:A:116:LEU:HD11	1:A:122:MET:HE3	20	0.12
(1,1702)	1:A:116:LEU:HD12	1:A:122:MET:HE1	20	0.12
(1,1702)	1:A:116:LEU:HD12	1:A:122:MET:HE2	20	0.12
(1,1702)	1:A:116:LEU:HD12	1:A:122:MET:HE3	20	0.12
(1,1702)	1:A:116:LEU:HD13	1:A:122:MET:HE1	20	0.12
(1,1702)	1:A:116:LEU:HD13	1:A:122:MET:HE2	20	0.12
(1,1702)	1:A:116:LEU:HD13	1:A:122:MET:HE3	20	0.12
(1,1696)	1:A:109:TRP:HZ3	1:A:122:MET:HE1	20	0.12
(1,1696)	1:A:109:TRP:HZ3	1:A:122:MET:HE2	20	0.12
(1,1696)	1:A:109:TRP:HZ3	1:A:122:MET:HE3	20	0.12
(1,1669)	1:A:116:LEU:HD21	1:A:122:MET:HE1	19	0.12
(1,1669)	1:A:116:LEU:HD21	1:A:122:MET:HE2	19	0.12
(1,1669)	1:A:116:LEU:HD21	1:A:122:MET:HE3	19	0.12
(1,1669)	1:A:116:LEU:HD22	1:A:122:MET:HE1	19	0.12
(1,1669)	1:A:116:LEU:HD22	1:A:122:MET:HE2	19	0.12
(1,1669)	1:A:116:LEU:HD22	1:A:122:MET:HE3	19	0.12
(1,1669)	1:A:116:LEU:HD23	1:A:122:MET:HE1	19	0.12
(1,1669)	1:A:116:LEU:HD23	1:A:122:MET:HE2	19	0.12
(1,1669)	1:A:116:LEU:HD23	1:A:122:MET:HE3	19	0.12
(1,1581)	1:A:72:ALA:HB1	1:A:101:VAL:HG21	4	0.12
(1,1581)	1:A:72:ALA:HB1	1:A:101:VAL:HG22	4	0.12
(1,1581)	1:A:72:ALA:HB1	1:A:101:VAL:HG23	4	0.12
(1,1581)	1:A:72:ALA:HB2	1:A:101:VAL:HG21	4	0.12
(1,1581)	1:A:72:ALA:HB2	1:A:101:VAL:HG22	4	0.12
(1,1581)	1:A:72:ALA:HB2	1:A:101:VAL:HG23	4	0.12
(1,1581)	1:A:72:ALA:HB3	1:A:101:VAL:HG21	4	0.12
(1,1581)	1:A:72:ALA:HB3	1:A:101:VAL:HG22	4	0.12
(1,1581)	1:A:72:ALA:HB3	1:A:101:VAL:HG23	4	0.12
(1,1581)	1:A:72:ALA:HB1	1:A:101:VAL:HG21	5	0.12
(1,1581)	1:A:72:ALA:HB1	1:A:101:VAL:HG22	5	0.12
(1,1581)	1:A:72:ALA:HB1	1:A:101:VAL:HG23	5	0.12
(1,1581)	1:A:72:ALA:HB2	1:A:101:VAL:HG21	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1581)	1:A:72:ALA:HB2	1:A:101:VAL:HG22	5	0.12
(1,1581)	1:A:72:ALA:HB2	1:A:101:VAL:HG23	5	0.12
(1,1581)	1:A:72:ALA:HB3	1:A:101:VAL:HG21	5	0.12
(1,1581)	1:A:72:ALA:HB3	1:A:101:VAL:HG22	5	0.12
(1,1581)	1:A:72:ALA:HB3	1:A:101:VAL:HG23	5	0.12
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD1	18	0.12
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD2	18	0.12
(1,1432)	1:A:76:ILE:HD11	1:A:98:PHE:HD1	19	0.12
(1,1432)	1:A:76:ILE:HD11	1:A:98:PHE:HD2	19	0.12
(1,1432)	1:A:76:ILE:HD12	1:A:98:PHE:HD1	19	0.12
(1,1432)	1:A:76:ILE:HD12	1:A:98:PHE:HD2	19	0.12
(1,1432)	1:A:76:ILE:HD13	1:A:98:PHE:HD1	19	0.12
(1,1432)	1:A:76:ILE:HD13	1:A:98:PHE:HD2	19	0.12
(1,1402)	1:A:31:LEU:HD21	1:A:72:ALA:HA	10	0.12
(1,1402)	1:A:31:LEU:HD22	1:A:72:ALA:HA	10	0.12
(1,1402)	1:A:31:LEU:HD23	1:A:72:ALA:HA	10	0.12
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB2	1	0.12
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB3	1	0.12
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB2	1	0.12
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB3	1	0.12
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB2	1	0.12
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB3	1	0.12
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB2	8	0.12
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB3	8	0.12
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB2	8	0.12
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB3	8	0.12
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB2	8	0.12
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB3	8	0.12
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB2	13	0.12
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB3	13	0.12
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB2	13	0.12
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB3	13	0.12
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB2	13	0.12
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB3	13	0.12
(1,1235)	1:A:41:PRO:HA	1:A:42:LEU:HB2	20	0.12
(1,1181)	1:A:36:LEU:HD21	1:A:39:ILE:H	14	0.12
(1,1181)	1:A:36:LEU:HD22	1:A:39:ILE:H	14	0.12
(1,1181)	1:A:36:LEU:HD23	1:A:39:ILE:H	14	0.12
(1,1099)	1:A:24:CYS:HA	1:A:97:LEU:HD21	2	0.12
(1,1099)	1:A:24:CYS:HA	1:A:97:LEU:HD22	2	0.12
(1,1099)	1:A:24:CYS:HA	1:A:97:LEU:HD23	2	0.12
(1,800)	1:A:38:LEU:H	1:A:40:LYS:HE2	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:A:38:LEU:H	1:A:40:LYS:HE3	13	0.11
(1,800)	1:A:38:LEU:H	1:A:40:LYS:HE2	19	0.11
(1,800)	1:A:38:LEU:H	1:A:40:LYS:HE3	19	0.11
(1,796)	1:A:135:GLN:HE21	1:A:136:GLU:HA	16	0.11
(1,708)	1:A:111:GLU:H	1:A:111:GLU:HG2	20	0.11
(1,708)	1:A:111:GLU:H	1:A:111:GLU:HG3	20	0.11
(1,68)	1:A:8:ILE:HB	1:A:11:GLY:H	18	0.11
(1,677)	1:A:104:LYS:HB2	1:A:106:SER:H	8	0.11
(1,66)	1:A:10:LEU:HG	1:A:11:GLY:H	5	0.11
(1,649)	1:A:103:ARG:HG2	1:A:104:LYS:H	6	0.11
(1,649)	1:A:103:ARG:HG3	1:A:104:LYS:H	6	0.11
(1,649)	1:A:103:ARG:HG2	1:A:104:LYS:H	11	0.11
(1,649)	1:A:103:ARG:HG3	1:A:104:LYS:H	11	0.11
(1,564)	1:A:116:LEU:H	1:A:116:LEU:HG	20	0.11
(1,2547)	1:A:127:ILE:HG13	1:A:128:SER:HB2	8	0.11
(1,2547)	1:A:127:ILE:HG13	1:A:128:SER:HB3	8	0.11
(1,2511)	1:A:116:LEU:HD11	1:A:122:MET:HB2	20	0.11
(1,2511)	1:A:116:LEU:HD12	1:A:122:MET:HB2	20	0.11
(1,2511)	1:A:116:LEU:HD13	1:A:122:MET:HB2	20	0.11
(1,2511)	1:A:116:LEU:HD21	1:A:122:MET:HB2	20	0.11
(1,2511)	1:A:116:LEU:HD22	1:A:122:MET:HB2	20	0.11
(1,2511)	1:A:116:LEU:HD23	1:A:122:MET:HB2	20	0.11
(1,2506)	1:A:116:LEU:HG	1:A:124:VAL:HG11	17	0.11
(1,2506)	1:A:116:LEU:HG	1:A:124:VAL:HG12	17	0.11
(1,2506)	1:A:116:LEU:HG	1:A:124:VAL:HG13	17	0.11
(1,2506)	1:A:116:LEU:HG	1:A:124:VAL:HG21	17	0.11
(1,2506)	1:A:116:LEU:HG	1:A:124:VAL:HG22	17	0.11
(1,2506)	1:A:116:LEU:HG	1:A:124:VAL:HG23	17	0.11
(1,2441)	1:A:109:TRP:HZ2	1:A:116:LEU:HD11	19	0.11
(1,2441)	1:A:109:TRP:HZ2	1:A:116:LEU:HD12	19	0.11
(1,2441)	1:A:109:TRP:HZ2	1:A:116:LEU:HD13	19	0.11
(1,2441)	1:A:109:TRP:HZ2	1:A:116:LEU:HD21	19	0.11
(1,2441)	1:A:109:TRP:HZ2	1:A:116:LEU:HD22	19	0.11
(1,2441)	1:A:109:TRP:HZ2	1:A:116:LEU:HD23	19	0.11
(1,2267)	1:A:71:GLU:HG2	1:A:98:PHE:HD1	5	0.11
(1,2267)	1:A:71:GLU:HG2	1:A:98:PHE:HD2	5	0.11
(1,2267)	1:A:71:GLU:HG3	1:A:98:PHE:HD1	5	0.11
(1,2267)	1:A:71:GLU:HG3	1:A:98:PHE:HD2	5	0.11
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD11	8	0.11
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD12	8	0.11
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD13	8	0.11
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD21	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD22	8	0.11
(1,2053)	1:A:28:CYS:HA	1:A:31:LEU:HD23	8	0.11
(1,1958)	1:A:13:VAL:HG11	1:A:16:LYS:HB2	8	0.11
(1,1958)	1:A:13:VAL:HG11	1:A:16:LYS:HB3	8	0.11
(1,1958)	1:A:13:VAL:HG12	1:A:16:LYS:HB2	8	0.11
(1,1958)	1:A:13:VAL:HG12	1:A:16:LYS:HB3	8	0.11
(1,1958)	1:A:13:VAL:HG13	1:A:16:LYS:HB2	8	0.11
(1,1958)	1:A:13:VAL:HG13	1:A:16:LYS:HB3	8	0.11
(1,1958)	1:A:13:VAL:HG21	1:A:16:LYS:HB2	8	0.11
(1,1958)	1:A:13:VAL:HG21	1:A:16:LYS:HB3	8	0.11
(1,1958)	1:A:13:VAL:HG22	1:A:16:LYS:HB2	8	0.11
(1,1958)	1:A:13:VAL:HG22	1:A:16:LYS:HB3	8	0.11
(1,1958)	1:A:13:VAL:HG23	1:A:16:LYS:HB2	8	0.11
(1,1958)	1:A:13:VAL:HG23	1:A:16:LYS:HB3	8	0.11
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD11	20	0.11
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD12	20	0.11
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD13	20	0.11
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD21	20	0.11
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD22	20	0.11
(1,1909)	1:A:7:ILE:H	1:A:10:LEU:HD23	20	0.11
(1,19)	1:A:134:ALA:HB1	1:A:135:GLN:HE22	11	0.11
(1,19)	1:A:134:ALA:HB2	1:A:135:GLN:HE22	11	0.11
(1,19)	1:A:134:ALA:HB3	1:A:135:GLN:HE22	11	0.11
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	1	0.11
(1,189)	1:A:23:TYR:H	1:A:25:LYS:HA	9	0.11
(1,1752)	1:A:133:TRP:HA	1:A:135:GLN:HG2	16	0.11
(1,1752)	1:A:133:TRP:HA	1:A:135:GLN:HG3	16	0.11
(1,1669)	1:A:116:LEU:HD21	1:A:122:MET:HE1	3	0.11
(1,1669)	1:A:116:LEU:HD21	1:A:122:MET:HE2	3	0.11
(1,1669)	1:A:116:LEU:HD21	1:A:122:MET:HE3	3	0.11
(1,1669)	1:A:116:LEU:HD22	1:A:122:MET:HE1	3	0.11
(1,1669)	1:A:116:LEU:HD22	1:A:122:MET:HE2	3	0.11
(1,1669)	1:A:116:LEU:HD22	1:A:122:MET:HE3	3	0.11
(1,1669)	1:A:116:LEU:HD23	1:A:122:MET:HE1	3	0.11
(1,1669)	1:A:116:LEU:HD23	1:A:122:MET:HE2	3	0.11
(1,1669)	1:A:116:LEU:HD23	1:A:122:MET:HE3	3	0.11
(1,1563)	1:A:98:PHE:HD1	1:A:101:VAL:HG11	7	0.11
(1,1563)	1:A:98:PHE:HD1	1:A:101:VAL:HG12	7	0.11
(1,1563)	1:A:98:PHE:HD1	1:A:101:VAL:HG13	7	0.11
(1,1563)	1:A:98:PHE:HD2	1:A:101:VAL:HG11	7	0.11
(1,1563)	1:A:98:PHE:HD2	1:A:101:VAL:HG12	7	0.11
(1,1563)	1:A:98:PHE:HD2	1:A:101:VAL:HG13	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1548)	1:A:97:LEU:HG	1:A:98:PHE:HD1	12	0.11
(1,1548)	1:A:97:LEU:HG	1:A:98:PHE:HD2	12	0.11
(1,1517)	1:A:94:ASP:HA	1:A:96:ILE:HB	2	0.11
(1,1517)	1:A:94:ASP:HA	1:A:96:ILE:HB	8	0.11
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD1	10	0.11
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD2	10	0.11
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD1	14	0.11
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD2	14	0.11
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD1	20	0.11
(1,1442)	1:A:76:ILE:HG12	1:A:98:PHE:HD2	20	0.11
(1,1402)	1:A:31:LEU:HD21	1:A:72:ALA:HA	4	0.11
(1,1402)	1:A:31:LEU:HD22	1:A:72:ALA:HA	4	0.11
(1,1402)	1:A:31:LEU:HD23	1:A:72:ALA:HA	4	0.11
(1,1402)	1:A:31:LEU:HD21	1:A:72:ALA:HA	13	0.11
(1,1402)	1:A:31:LEU:HD22	1:A:72:ALA:HA	13	0.11
(1,1402)	1:A:31:LEU:HD23	1:A:72:ALA:HA	13	0.11
(1,1402)	1:A:31:LEU:HD21	1:A:72:ALA:HA	14	0.11
(1,1402)	1:A:31:LEU:HD22	1:A:72:ALA:HA	14	0.11
(1,1402)	1:A:31:LEU:HD23	1:A:72:ALA:HA	14	0.11
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB2	12	0.11
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB3	12	0.11
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB2	12	0.11
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB3	12	0.11
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB2	12	0.11
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB3	12	0.11
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB2	15	0.11
(1,1384)	1:A:134:ALA:HB1	1:A:135:GLN:HB3	15	0.11
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB2	15	0.11
(1,1384)	1:A:134:ALA:HB2	1:A:135:GLN:HB3	15	0.11
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB2	15	0.11
(1,1384)	1:A:134:ALA:HB3	1:A:135:GLN:HB3	15	0.11
(1,1235)	1:A:41:PRO:HA	1:A:42:LEU:HB2	9	0.11
(1,1181)	1:A:36:LEU:HD21	1:A:39:ILE:H	4	0.11
(1,1181)	1:A:36:LEU:HD22	1:A:39:ILE:H	4	0.11
(1,1181)	1:A:36:LEU:HD23	1:A:39:ILE:H	4	0.11
(1,1010)	1:A:14:ILE:HD11	1:A:68:ALA:HA	7	0.11
(1,1010)	1:A:14:ILE:HD12	1:A:68:ALA:HA	7	0.11
(1,1010)	1:A:14:ILE:HD13	1:A:68:ALA:HA	7	0.11

10 Dihedral-angle violation analysis

No dihedral-angle restraints found