



Full wwPDB NMR Structure Validation Report ⓘ

Mar 15, 2026 – 12:59 PM UTC

PDB ID : 7NM5 / pdb_00007nm5
BMRB ID : 34605
Title : Solution structure of MLKL executioner domain in complex with a fragment
Authors : Ruebbelke, M.; Bauer, M.; Hamilton, J.; Binder, F.; Nar, H.; Zeeb, M.
Deposited on : 2021-02-23

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

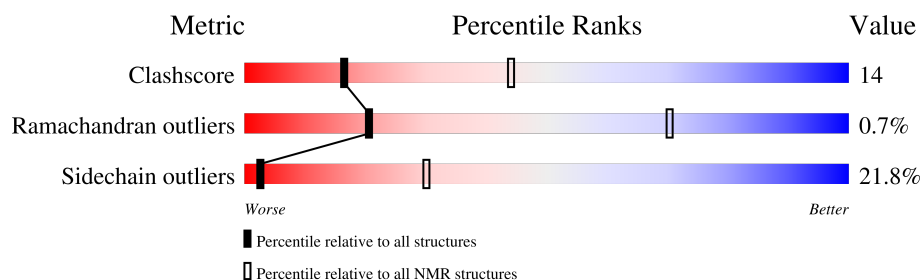
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	58% 27% • 11%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 11 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:2-A:47, A:56-A:149 (140)	0.64	11

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 2 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2609 atoms, of which 1313 are hydrogens and 0 are deuteriums.

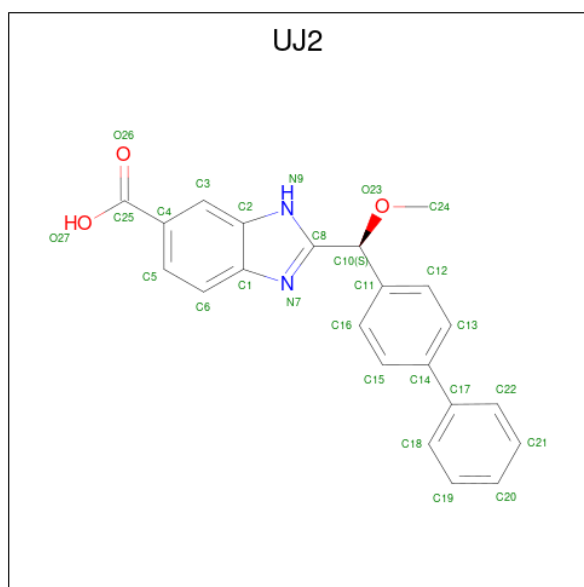
- Molecule 1 is a protein called Mixed lineage kinase domain-like protein.

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

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

- Molecule 2 is 2-[({S})-methoxy-(4-phenylphenyl)methyl]-3 {H}-benzimidazole-5-carboxylic acid (CCD ID: UJ2) (formula: C₂₂H₁₈N₂O₃) (labeled as "Ligand of Interest" by depositor).



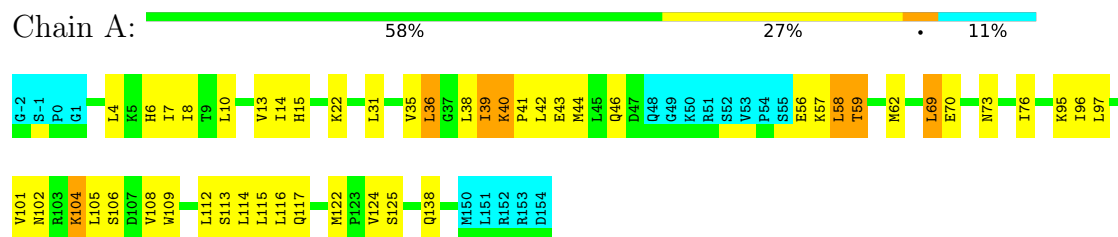
Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	
			45	22	18	2	3	

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

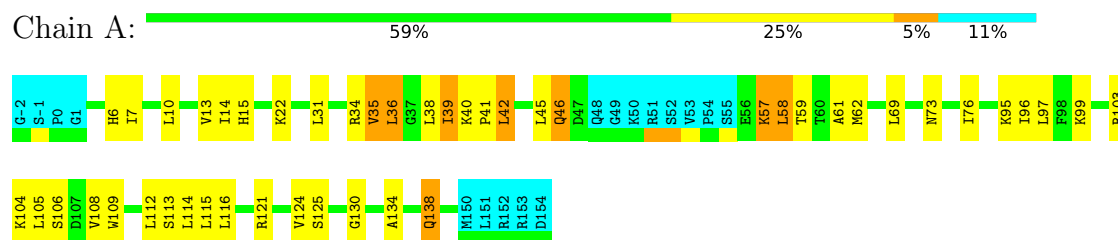


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

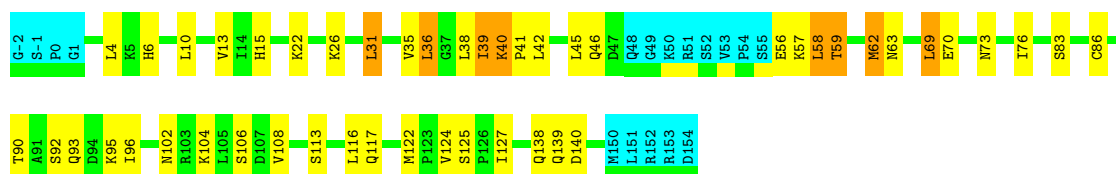
- Molecule 1: Mixed lineage kinase domain-like protein



4.2.2 Score per residue for model 2

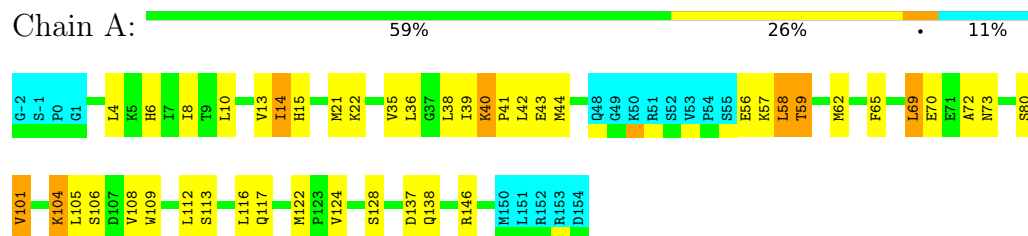
- Molecule 1: Mixed lineage kinase domain-like protein





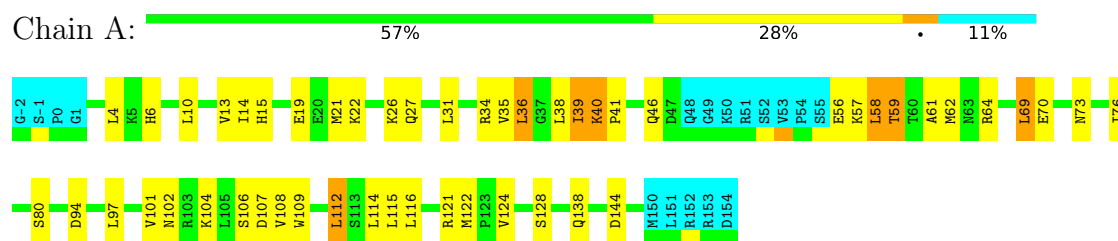
4.2.3 Score per residue for model 3

- Molecule 1: Mixed lineage kinase domain-like protein



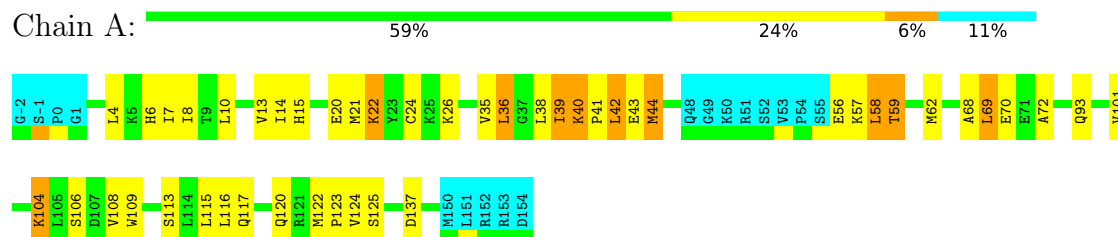
4.2.4 Score per residue for model 4

- Molecule 1: Mixed lineage kinase domain-like protein



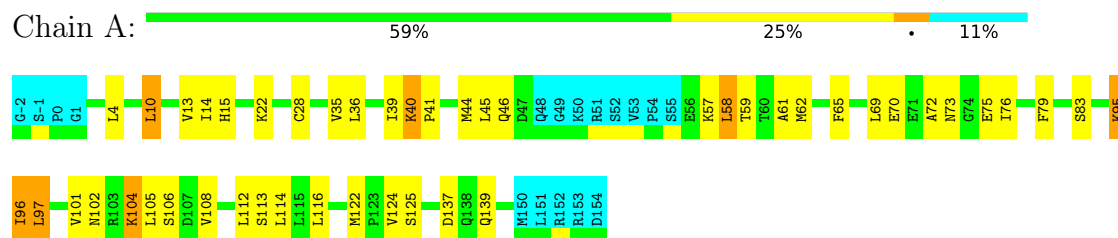
4.2.5 Score per residue for model 5

- Molecule 1: Mixed lineage kinase domain-like protein



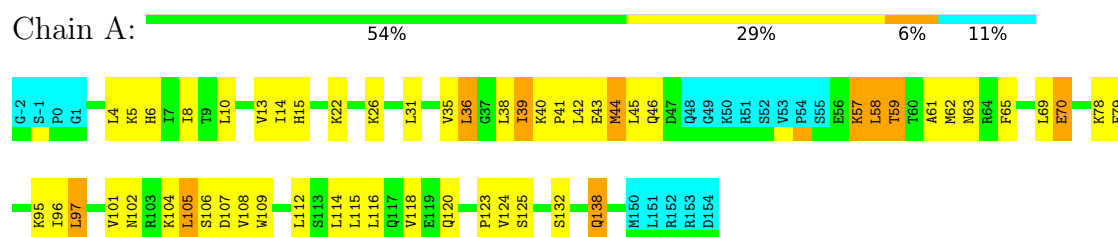
4.2.6 Score per residue for model 6

- Molecule 1: Mixed lineage kinase domain-like protein



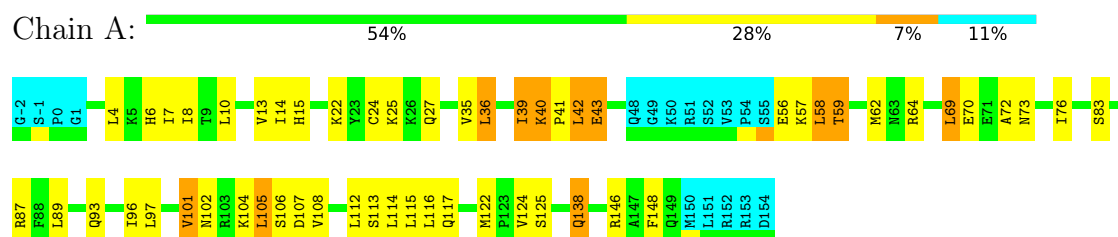
4.2.7 Score per residue for model 7

- Molecule 1: Mixed lineage kinase domain-like protein



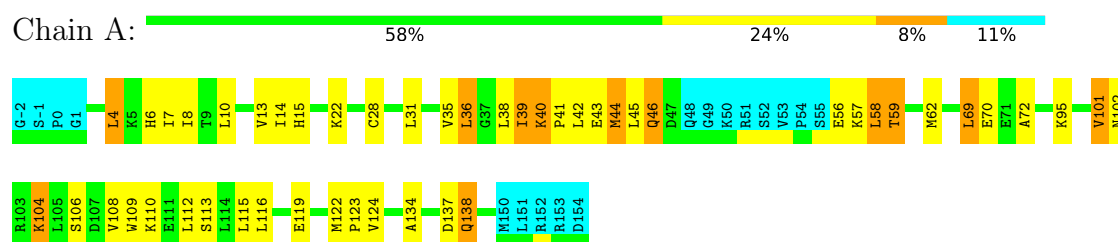
4.2.8 Score per residue for model 8

- Molecule 1: Mixed lineage kinase domain-like protein



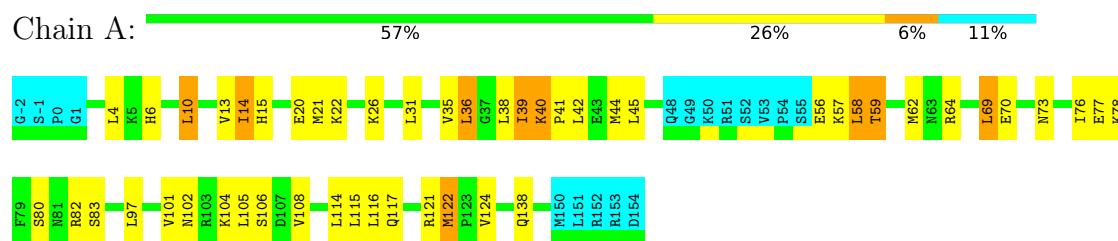
4.2.9 Score per residue for model 9

- Molecule 1: Mixed lineage kinase domain-like protein



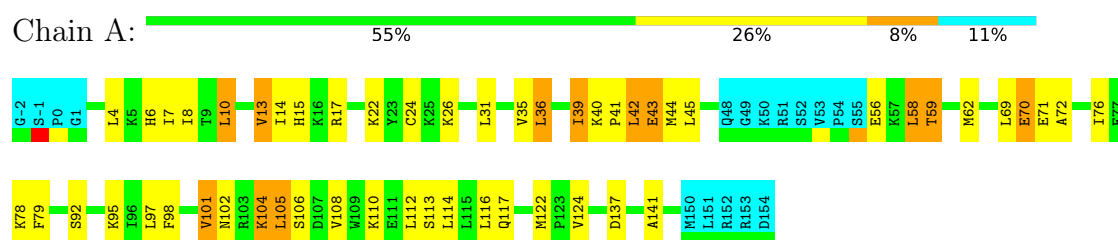
4.2.10 Score per residue for model 10

- Molecule 1: Mixed lineage kinase domain-like protein



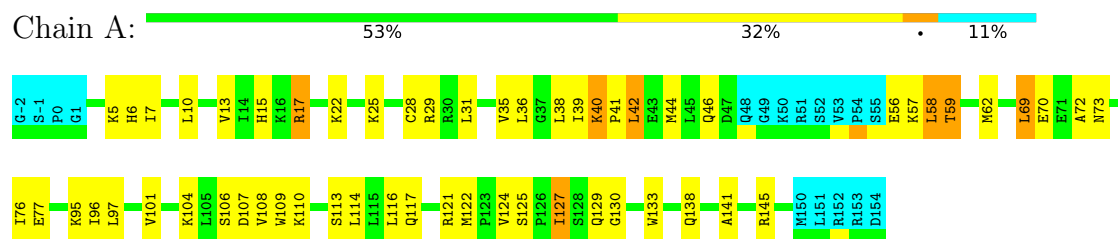
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Mixed lineage kinase domain-like protein



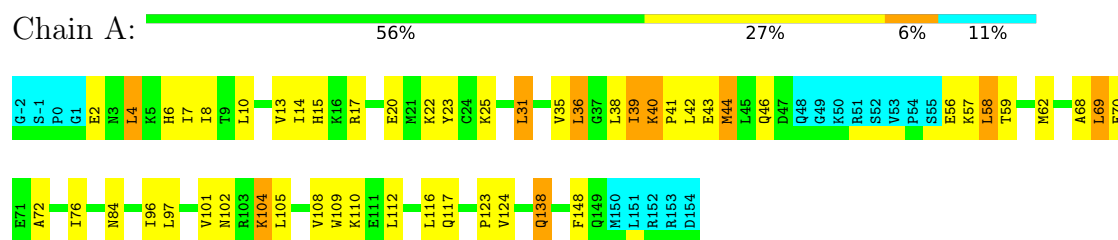
4.2.12 Score per residue for model 12

- Molecule 1: Mixed lineage kinase domain-like protein



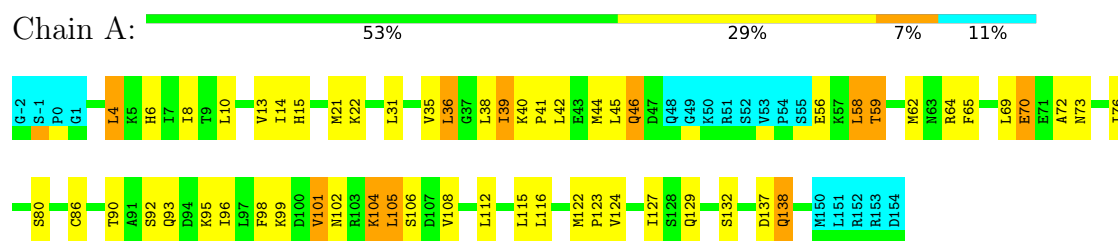
4.2.13 Score per residue for model 13

- Molecule 1: Mixed lineage kinase domain-like protein



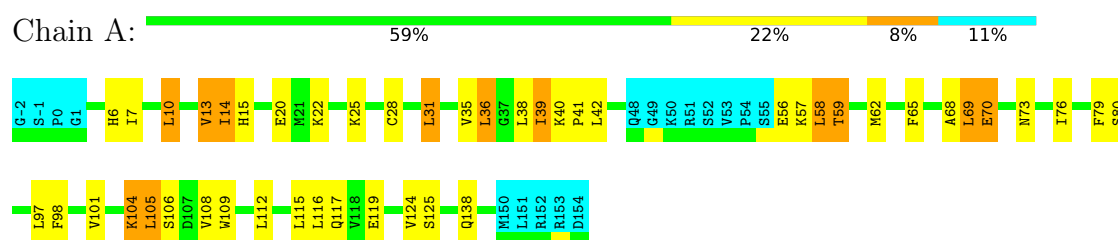
4.2.14 Score per residue for model 14

- Molecule 1: Mixed lineage kinase domain-like protein



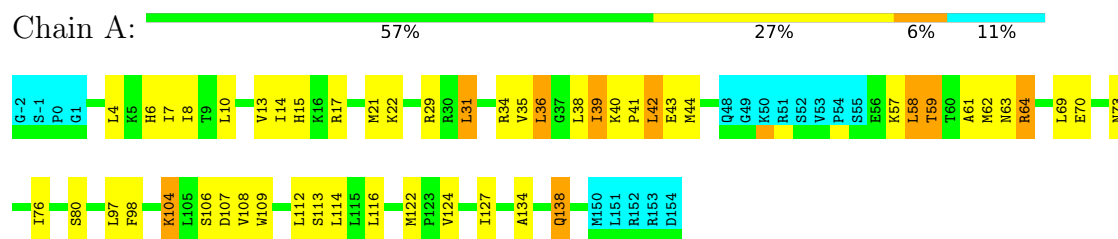
4.2.15 Score per residue for model 15

- Molecule 1: Mixed lineage kinase domain-like protein



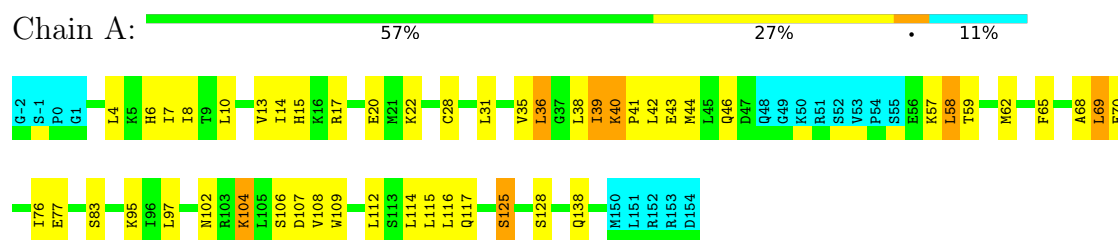
4.2.16 Score per residue for model 16

- Molecule 1: Mixed lineage kinase domain-like protein



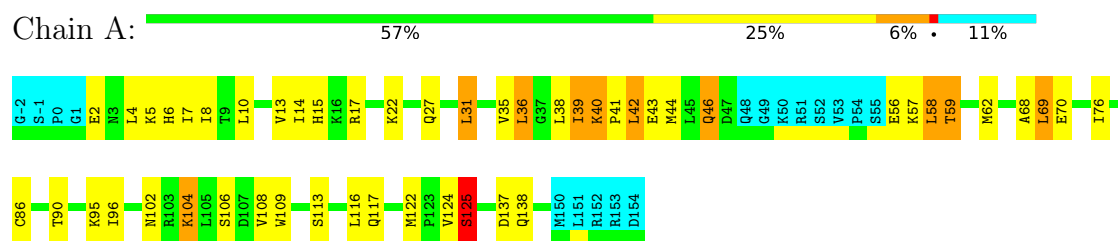
4.2.17 Score per residue for model 17

- Molecule 1: Mixed lineage kinase domain-like protein



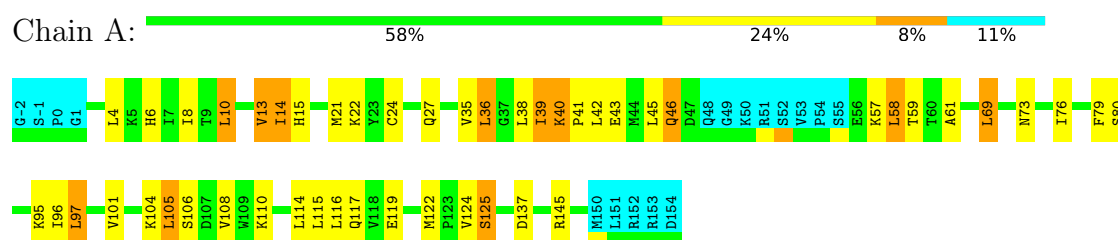
4.2.18 Score per residue for model 18

- Molecule 1: Mixed lineage kinase domain-like protein



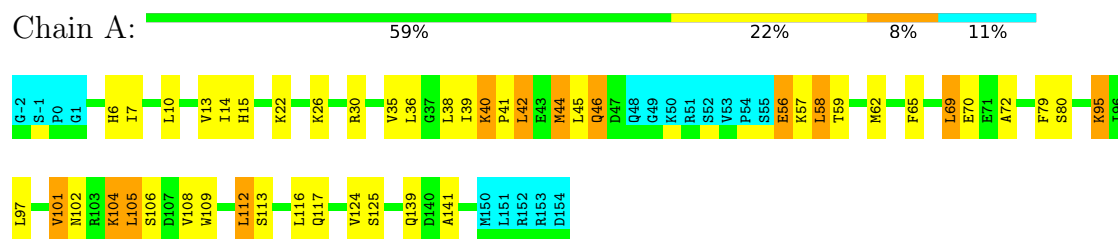
4.2.19 Score per residue for model 19

- 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	1738
Number of shifts mapped to atoms	1738
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UJ2

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

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	1143	1164	1164	33±5
2	A	27	18	0	4±1
All	All	23400	23640	23280	658

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:LEU:HD23	1:A:122:MET:HE2	1.03	1.29	4	4
1:A:61:ALA:HB2	1:A:115:LEU:HD21	0.91	1.41	4	1
1:A:58:LEU:HD13	1:A:59:THR:N	0.90	1.81	14	15
1:A:58:LEU:HD22	1:A:58:LEU:C	0.90	1.92	8	15
1:A:62:MET:HE1	1:A:116:LEU:HD21	0.85	1.47	12	4
1:A:58:LEU:HD22	1:A:58:LEU:O	0.83	1.74	16	15
1:A:7:ILE:HG21	1:A:42:LEU:HD22	0.83	1.49	1	7
1:A:58:LEU:HD23	1:A:116:LEU:HD23	0.78	1.53	2	5
1:A:14:ILE:HD13	1:A:69:LEU:HD12	0.78	1.56	15	2
1:A:116:LEU:HD13	1:A:122:MET:HE2	0.76	1.57	2	5
1:A:134:ALA:HB1	1:A:138:GLN:OE1	0.72	1.85	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:LEU:HD21	1:A:116:LEU:HD23	0.70	1.64	16	1
1:A:79:PHE:CE1	1:A:97:LEU:HD22	0.68	2.24	11	3
1:A:58:LEU:C	1:A:58:LEU:CD2	0.67	2.68	3	15
1:A:38:LEU:O	1:A:42:LEU:HD23	0.67	1.90	19	9
1:A:10:LEU:HD13	1:A:69:LEU:HD11	0.66	1.67	11	1
1:A:104:LYS:O	1:A:108:VAL:HG22	0.66	1.91	20	20
1:A:58:LEU:CD1	1:A:116:LEU:HD23	0.65	2.21	19	1
1:A:58:LEU:HA	1:A:115:LEU:HD13	0.65	1.69	4	1
1:A:36:LEU:HD13	1:A:39:ILE:CG2	0.64	2.22	14	16
1:A:95:LYS:O	1:A:96:ILE:HD13	0.64	1.93	14	3
1:A:62:MET:HE3	2:A:201:UJ2:C14	0.64	2.22	14	18
1:A:62:MET:HE1	1:A:116:LEU:HD11	0.63	1.68	18	3
1:A:10:LEU:HD23	1:A:69:LEU:HD11	0.63	1.71	7	11
1:A:58:LEU:HD12	1:A:116:LEU:HD12	0.63	1.69	6	4
1:A:8:ILE:HD12	1:A:43:GLU:CG	0.63	2.24	18	6
1:A:58:LEU:HD13	1:A:59:THR:H	0.63	1.53	8	13
1:A:6:HIS:NE2	1:A:10:LEU:HD22	0.62	2.10	13	15
1:A:58:LEU:HD12	1:A:116:LEU:CD1	0.62	2.24	6	3
1:A:69:LEU:CA	1:A:105:LEU:HD21	0.62	2.25	19	1
1:A:116:LEU:HD22	2:A:201:UJ2:C21	0.62	2.25	8	3
1:A:58:LEU:HD12	1:A:116:LEU:HD23	0.61	1.70	19	1
1:A:116:LEU:CD1	1:A:122:MET:HE2	0.61	2.24	10	6
1:A:69:LEU:CB	1:A:105:LEU:HD21	0.61	2.25	19	3
1:A:58:LEU:HD22	1:A:119:GLU:CD	0.61	2.20	19	1
1:A:62:MET:HE1	2:A:201:UJ2:C17	0.61	2.26	2	1
1:A:61:ALA:CB	1:A:115:LEU:HD21	0.61	2.23	4	1
1:A:6:HIS:NE2	1:A:10:LEU:HD12	0.61	2.11	15	4
1:A:58:LEU:HD11	2:A:201:UJ2:C21	0.60	2.26	1	4
1:A:73:ASN:HA	1:A:76:ILE:HD12	0.60	1.73	10	11
1:A:10:LEU:O	1:A:13:VAL:HG12	0.60	1.96	16	12
1:A:38:LEU:HD22	1:A:109:TRP:CD1	0.60	2.31	17	3
1:A:116:LEU:HD22	2:A:201:UJ2:C20	0.60	2.25	20	7
1:A:7:ILE:CG2	1:A:42:LEU:HD22	0.60	2.26	8	6
1:A:61:ALA:C	1:A:112:LEU:HD12	0.59	2.22	16	4
1:A:8:ILE:HD12	1:A:43:GLU:HG2	0.59	1.74	7	3
1:A:10:LEU:HD21	1:A:70:GLU:CG	0.59	2.26	14	2
1:A:42:LEU:HD13	1:A:45:LEU:HD21	0.59	1.74	14	4
1:A:61:ALA:O	1:A:112:LEU:HD12	0.58	1.98	6	4
1:A:8:ILE:HD12	1:A:43:GLU:HG3	0.58	1.75	17	5
1:A:8:ILE:HG21	1:A:46:GLN:OE1	0.58	1.99	14	1
1:A:10:LEU:HD22	1:A:69:LEU:HD13	0.57	1.76	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ALA:N	1:A:101:VAL:HG21	0.57	2.13	3	9
1:A:116:LEU:HD12	1:A:122:MET:HE2	0.57	1.75	14	3
1:A:7:ILE:HD11	1:A:62:MET:HG2	0.57	1.76	17	5
1:A:99:LYS:HE2	1:A:134:ALA:HB2	0.57	1.73	1	1
1:A:58:LEU:HD13	1:A:58:LEU:C	0.57	2.25	16	8
1:A:116:LEU:CD2	1:A:122:MET:HE2	0.57	2.29	11	3
1:A:69:LEU:HB3	1:A:105:LEU:HD21	0.56	1.75	10	8
1:A:58:LEU:HD11	2:A:201:UJ2:C22	0.56	2.30	13	4
1:A:14:ILE:CD1	1:A:69:LEU:HD12	0.56	2.29	15	1
1:A:96:ILE:HD11	1:A:138:GLN:HG2	0.55	1.77	13	7
1:A:58:LEU:HD11	2:A:201:UJ2:C18	0.55	2.31	19	1
1:A:31:LEU:HD13	1:A:102:ASN:OD1	0.55	2.02	10	5
1:A:62:MET:HE2	1:A:116:LEU:HD21	0.55	1.77	2	1
1:A:59:THR:HG22	2:A:201:UJ2:C16	0.55	2.32	12	16
1:A:65:PHE:CE1	1:A:69:LEU:HD23	0.55	2.36	7	1
1:A:56:GLU:HA	1:A:59:THR:OG1	0.55	2.02	11	13
1:A:95:LYS:C	1:A:96:ILE:HD13	0.55	2.27	14	3
1:A:116:LEU:HD22	2:A:201:UJ2:C19	0.54	2.32	5	3
1:A:45:LEU:HD22	1:A:120:GLN:NE2	0.54	2.17	7	1
1:A:58:LEU:HD11	2:A:201:UJ2:C19	0.54	2.33	19	1
1:A:72:ALA:CA	1:A:101:VAL:HG21	0.53	2.33	9	7
1:A:101:VAL:HG23	1:A:104:LYS:HE2	0.53	1.78	4	2
1:A:65:PHE:O	1:A:69:LEU:HD23	0.53	2.03	6	1
1:A:10:LEU:HD13	1:A:69:LEU:CD1	0.53	2.33	11	1
1:A:62:MET:SD	1:A:116:LEU:HD11	0.53	2.44	1	1
1:A:115:LEU:HD12	1:A:116:LEU:N	0.53	2.18	4	1
1:A:68:ALA:CB	1:A:108:VAL:HG21	0.53	2.34	18	5
1:A:10:LEU:O	1:A:14:ILE:HD12	0.53	2.04	19	2
1:A:61:ALA:HB1	1:A:112:LEU:HB2	0.52	1.81	4	1
1:A:59:THR:HG22	2:A:201:UJ2:C15	0.52	2.33	12	10
1:A:45:LEU:HD12	1:A:46:GLN:N	0.52	2.19	19	7
1:A:62:MET:HE3	2:A:201:UJ2:C13	0.52	2.34	20	5
1:A:8:ILE:HG23	1:A:43:GLU:HG2	0.52	1.82	11	3
1:A:114:LEU:HD23	1:A:117:GLN:OE1	0.52	2.05	8	1
1:A:14:ILE:HD11	1:A:69:LEU:O	0.52	2.05	19	1
1:A:4:LEU:HD11	1:A:45:LEU:CD1	0.51	2.34	11	1
1:A:69:LEU:HA	1:A:105:LEU:HD21	0.51	1.81	15	2
2:A:201:UJ2:C24	2:A:201:UJ2:C16	0.51	2.89	7	1
1:A:101:VAL:HG22	1:A:105:LEU:HD23	0.51	1.82	15	1
1:A:40:LYS:N	1:A:41:PRO:HD2	0.51	2.21	17	20
1:A:8:ILE:HG23	1:A:43:GLU:CG	0.51	2.35	17	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:LEU:HA	1:A:115:LEU:HD12	0.51	1.82	10	4
1:A:38:LEU:HD22	1:A:109:TRP:CD2	0.51	2.41	1	6
1:A:61:ALA:HB2	1:A:115:LEU:HD12	0.51	1.83	19	1
1:A:116:LEU:HD23	1:A:122:MET:SD	0.50	2.46	9	2
1:A:115:LEU:HD12	1:A:115:LEU:C	0.50	2.31	4	1
1:A:31:LEU:HD22	1:A:98:PHE:HB2	0.50	1.84	11	1
1:A:10:LEU:HG	1:A:69:LEU:HD12	0.50	1.83	12	2
1:A:7:ILE:HD11	1:A:62:MET:CG	0.49	2.37	8	5
1:A:10:LEU:HD21	1:A:70:GLU:HG3	0.49	1.83	7	2
1:A:4:LEU:HD22	1:A:46:GLN:HB2	0.49	1.84	9	3
1:A:95:LYS:O	1:A:141:ALA:HB1	0.49	2.06	12	3
1:A:13:VAL:HG22	1:A:17:ARG:NH1	0.49	2.23	16	1
1:A:109:TRP:CE3	1:A:112:LEU:HD22	0.49	2.42	7	1
1:A:38:LEU:HD23	1:A:125:SER:OG	0.49	2.06	19	1
1:A:4:LEU:O	1:A:4:LEU:HD23	0.49	2.07	4	1
1:A:4:LEU:HD12	1:A:4:LEU:O	0.49	2.07	16	1
1:A:21:MET:HE1	1:A:80:SER:HA	0.48	1.84	14	6
1:A:79:PHE:CD1	1:A:97:LEU:HD23	0.48	2.43	19	1
2:A:201:UJ2:C16	2:A:201:UJ2:N7	0.48	2.75	19	1
1:A:17:ARG:HB3	1:A:76:ILE:HG21	0.48	1.86	13	4
1:A:96:ILE:HD11	1:A:138:GLN:OE1	0.48	2.09	3	1
1:A:58:LEU:CA	1:A:115:LEU:HD13	0.47	2.37	4	1
1:A:6:HIS:CD2	1:A:10:LEU:HD12	0.47	2.44	19	1
1:A:44:MET:HE3	1:A:123:PRO:CD	0.47	2.39	13	1
1:A:21:MET:HE1	1:A:80:SER:CA	0.47	2.39	14	3
1:A:58:LEU:HD23	1:A:116:LEU:HD12	0.47	1.85	11	3
1:A:10:LEU:HD23	1:A:69:LEU:CD1	0.47	2.39	13	5
1:A:127:ILE:HD12	1:A:133:TRP:NE1	0.47	2.25	12	1
1:A:31:LEU:HD12	1:A:98:PHE:CG	0.47	2.45	16	2
1:A:65:PHE:HB2	1:A:112:LEU:HD12	0.47	1.87	20	1
2:A:201:UJ2:C16	2:A:201:UJ2:C24	0.46	2.93	19	1
1:A:69:LEU:HD12	1:A:70:GLU:N	0.46	2.25	11	1
1:A:109:TRP:CE3	1:A:112:LEU:HD23	0.46	2.46	13	3
1:A:7:ILE:HG21	1:A:42:LEU:CD2	0.46	2.40	20	2
1:A:31:LEU:C	1:A:31:LEU:HD13	0.46	2.36	7	2
1:A:44:MET:HE2	1:A:45:LEU:HB3	0.46	1.87	20	1
1:A:58:LEU:CA	1:A:115:LEU:HD12	0.46	2.40	10	2
1:A:58:LEU:HD21	1:A:116:LEU:CD2	0.45	2.38	16	1
1:A:7:ILE:HG21	1:A:42:LEU:CD1	0.45	2.42	17	1
1:A:31:LEU:HD22	1:A:98:PHE:CB	0.45	2.40	11	1
1:A:58:LEU:CD1	1:A:59:THR:HG23	0.45	2.41	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ILE:HG22	1:A:97:LEU:H	0.45	1.72	6	1
1:A:89:LEU:HD12	1:A:148:PHE:CD1	0.45	2.46	8	1
1:A:36:LEU:HD13	1:A:39:ILE:HG23	0.45	1.89	19	3
1:A:56:GLU:O	1:A:59:THR:OG1	0.45	2.29	20	1
1:A:124:VAL:CG2	1:A:125:SER:N	0.45	2.79	18	1
1:A:68:ALA:HB1	1:A:105:LEU:HA	0.45	1.88	13	1
1:A:101:VAL:O	1:A:105:LEU:HD12	0.44	2.13	11	2
1:A:4:LEU:HD12	1:A:46:GLN:HB2	0.44	1.89	14	1
1:A:38:LEU:HD22	1:A:109:TRP:CG	0.44	2.47	7	3
1:A:31:LEU:HD22	1:A:98:PHE:CD2	0.44	2.48	14	1
1:A:96:ILE:HG23	1:A:137:ASP:OD1	0.44	2.11	19	2
1:A:68:ALA:HB2	1:A:108:VAL:HG21	0.44	1.88	13	3
1:A:58:LEU:CD2	1:A:116:LEU:HD23	0.44	2.41	16	1
1:A:79:PHE:CD1	1:A:97:LEU:HD21	0.44	2.47	7	1
1:A:31:LEU:HD13	1:A:102:ASN:ND2	0.44	2.28	9	1
1:A:38:LEU:HD23	1:A:125:SER:HB3	0.44	1.88	7	1
1:A:62:MET:HE3	2:A:201:UJ2:C17	0.44	2.43	18	1
1:A:38:LEU:O	1:A:42:LEU:HD13	0.44	2.12	18	1
1:A:58:LEU:HG	1:A:59:THR:N	0.43	2.26	19	2
1:A:65:PHE:CB	1:A:112:LEU:HD22	0.43	2.43	17	2
1:A:4:LEU:HD22	1:A:46:GLN:CD	0.43	2.37	13	1
1:A:45:LEU:HD12	1:A:45:LEU:C	0.43	2.38	1	1
1:A:14:ILE:HD11	1:A:73:ASN:OD1	0.43	2.13	3	1
1:A:57:LYS:O	1:A:115:LEU:HD12	0.43	2.14	7	1
1:A:62:MET:SD	1:A:112:LEU:HD11	0.43	2.54	8	2
1:A:79:PHE:HE1	1:A:97:LEU:HD22	0.43	1.70	15	1
1:A:101:VAL:O	1:A:105:LEU:HD23	0.43	2.13	15	1
1:A:10:LEU:HD21	1:A:70:GLU:HG2	0.43	1.89	14	1
1:A:65:PHE:CB	1:A:112:LEU:HD12	0.43	2.43	20	1
1:A:36:LEU:HD13	1:A:39:ILE:HG21	0.42	1.89	18	5
1:A:38:LEU:HD22	1:A:109:TRP:CE2	0.42	2.49	3	1
1:A:40:LYS:CB	1:A:41:PRO:CD	0.42	2.96	7	16
1:A:65:PHE:HB2	1:A:112:LEU:HD22	0.42	1.89	14	2
1:A:35:VAL:CG2	1:A:105:LEU:HD13	0.42	2.44	1	1
1:A:58:LEU:C	1:A:58:LEU:HD13	0.42	2.36	20	2
1:A:58:LEU:CD2	1:A:116:LEU:HD12	0.42	2.45	7	1
1:A:124:VAL:O	1:A:125:SER:CB	0.42	2.66	18	1
1:A:44:MET:HE3	1:A:123:PRO:HD2	0.42	1.91	5	3
1:A:112:LEU:HD12	1:A:116:LEU:HD13	0.42	1.91	13	2
1:A:96:ILE:HG23	1:A:137:ASP:CG	0.42	2.39	18	1
1:A:57:LYS:HE2	1:A:115:LEU:HD13	0.41	1.93	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:MET:HE2	1:A:24:CYS:SG	0.41	2.55	5	1
1:A:58:LEU:HD23	1:A:116:LEU:CD2	0.41	2.35	2	1
1:A:14:ILE:HG12	1:A:72:ALA:HB3	0.41	1.92	3	1
1:A:10:LEU:HD22	1:A:69:LEU:CD1	0.41	2.44	11	1
1:A:86:CYS:O	1:A:90:THR:HG23	0.41	2.16	2	3
1:A:17:ARG:HB2	1:A:76:ILE:HG21	0.41	1.92	12	1
1:A:65:PHE:CG	1:A:112:LEU:HD22	0.41	2.51	15	1
1:A:58:LEU:C	1:A:58:LEU:CD1	0.41	2.91	16	1
1:A:40:LYS:N	1:A:41:PRO:CD	0.41	2.84	17	1
1:A:65:PHE:CG	1:A:112:LEU:HD12	0.41	2.51	20	1
1:A:10:LEU:HD11	1:A:70:GLU:HG3	0.40	1.93	15	1
1:A:65:PHE:HB2	1:A:112:LEU:HD13	0.40	1.92	7	1
1:A:64:ARG:NH2	1:A:108:VAL:HG12	0.40	2.31	16	1
1:A:65:PHE:CZ	1:A:69:LEU:HD22	0.40	2.51	6	1
1:A:44:MET:HE2	1:A:123:PRO:HD2	0.40	1.93	14	1
1:A:114:LEU:O	1:A:118:VAL:HG12	0.40	2.16	7	1
1:A:115:LEU:HD23	1:A:115:LEU:N	0.40	2.31	7	1
1:A:116:LEU:HD23	2:A:201:UJ2:C21	0.40	2.47	7	1
1:A:56:GLU:HA	1:A:59:THR:HG1	0.40	1.77	11	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	140/157 (89%)	130±2 (93±2%)	9±2 (7±2%)	1±1 (1±1%)	20	70
All	All	2800/3140 (89%)	2593 (93%)	187 (7%)	20 (1%)	20	70

All 9 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	121	ARG	4
1	A	127	ILE	4
1	A	130	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	92	SER	2
1	A	93	GLN	2
1	A	129	GLN	2
1	A	125	SER	2
1	A	94	ASP	1
1	A	22	LYS	1

6.3.2 Protein sidechains ⓘ

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%)	99±3 (78±3%)	27±3 (22±3%)	2	30
All	All	2520/2800 (90%)	1971 (78%)	549 (22%)	2	30

All 80 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	15	HIS	20
1	A	22	LYS	20
1	A	35	VAL	20
1	A	36	LEU	20
1	A	39	ILE	20
1	A	58	LEU	20
1	A	106	SER	19
1	A	14	ILE	18
1	A	57	LYS	18
1	A	124	VAL	18
1	A	70	GLU	18
1	A	69	LEU	15
1	A	40	LYS	14
1	A	59	THR	14
1	A	44	MET	13
1	A	97	LEU	12
1	A	113	SER	12
1	A	138	GLN	12
1	A	117	GLN	12

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Mol	Chain	Res	Type	Models (Total)
1	A	104	LYS	12
1	A	13	VAL	11
1	A	125	SER	11
1	A	4	LEU	11
1	A	46	GLN	10
1	A	95	LYS	9
1	A	114	LEU	9
1	A	42	LEU	8
1	A	101	VAL	8
1	A	31	LEU	7
1	A	26	LYS	7
1	A	102	ASN	7
1	A	105	LEU	7
1	A	137	ASP	6
1	A	107	ASP	6
1	A	83	SER	5
1	A	64	ARG	5
1	A	20	GLU	5
1	A	10	LEU	5
1	A	28	CYS	5
1	A	110	LYS	5
1	A	27	GLN	4
1	A	25	LYS	4
1	A	34	ARG	3
1	A	63	ASN	3
1	A	139	GLN	3
1	A	128	SER	3
1	A	112	LEU	3
1	A	5	LYS	3
1	A	78	LYS	3
1	A	24	CYS	3
1	A	115	LEU	3
1	A	77	GLU	3
1	A	146	ARG	2
1	A	93	GLN	2
1	A	132	SER	2
1	A	43	GLU	2
1	A	119	GLU	2
1	A	29	ARG	2
1	A	145	ARG	2
1	A	2	GLU	2
1	A	80	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	103	ARG	1
1	A	62	MET	1
1	A	140	ASP	1
1	A	19	GLU	1
1	A	144	ASP	1
1	A	120	GLN	1
1	A	75	GLU	1
1	A	79	PHE	1
1	A	96	ILE	1
1	A	87	ARG	1
1	A	82	ARG	1
1	A	122	MET	1
1	A	71	GLU	1
1	A	92	SER	1
1	A	17	ARG	1
1	A	84	ASN	1
1	A	99	LYS	1
1	A	30	ARG	1
1	A	56	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is

considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	UJ2	A	201	-	29,30,30	0.67±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	UJ2	A	201	-	39,42,42	0.98±0.00	1±0 (1±1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UJ2	A	201	-	-	0±0,17,18,18	0±0,4,4,4

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	201	UJ2	O27-C25-C4	2.03	120.06	114.84	8	15

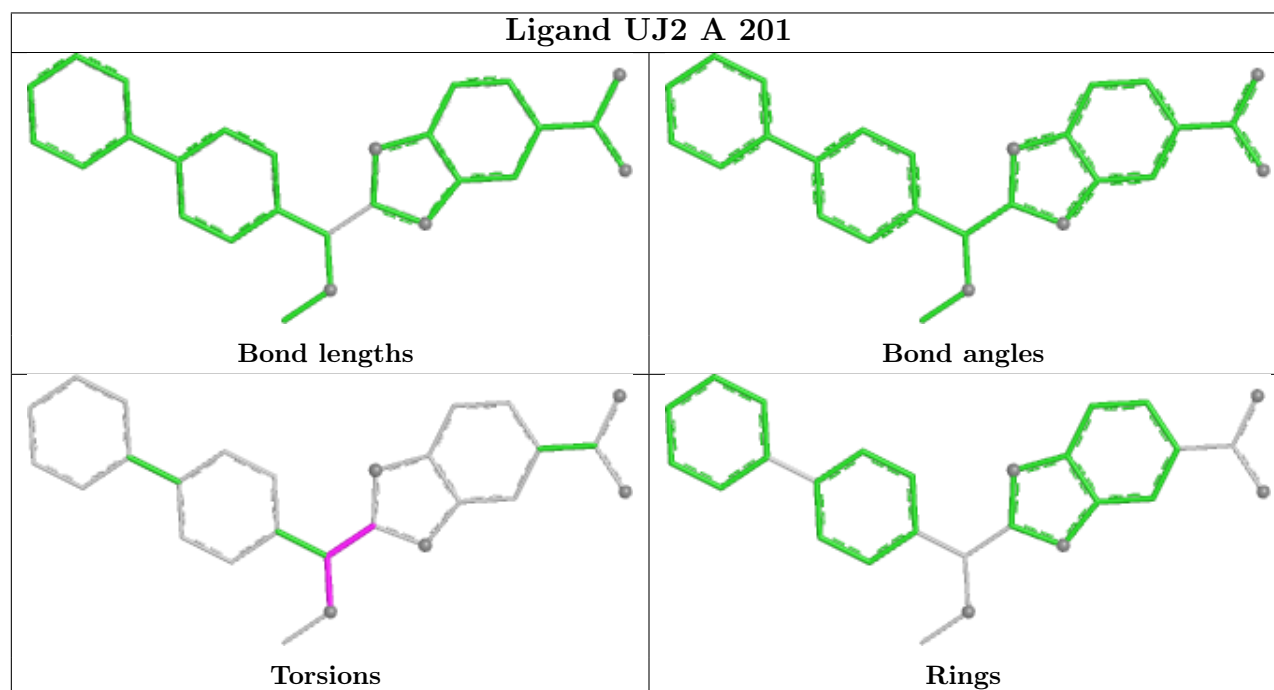
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 79% for the well-defined parts and 78% 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	1738
Number of shifts mapped to atoms	1738
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	153	-0.50 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	144	0.30 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	141	-0.09 ± 0.18	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 79%, i.e. 1581 atoms were assigned a chemical shift out of a possible 2013. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	535/699 (77%)	270/282 (96%)	136/280 (49%)	129/137 (94%)
Sidechain	980/1210 (81%)	665/776 (86%)	300/371 (81%)	15/63 (24%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	66/104 (63%)	33/53 (62%)	31/46 (67%)	2/5 (40%)
Overall	1581/2013 (79%)	968/1111 (87%)	467/697 (67%)	146/205 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1738 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	596/783 (76%)	302/317 (95%)	153/314 (49%)	141/152 (93%)
Sidechain	1076/1351 (80%)	730/866 (84%)	330/411 (80%)	16/74 (22%)
Aromatic	66/104 (63%)	33/53 (62%)	31/46 (67%)	2/5 (40%)
Overall	1738/2238 (78%)	1065/1236 (86%)	514/771 (67%)	159/231 (69%)

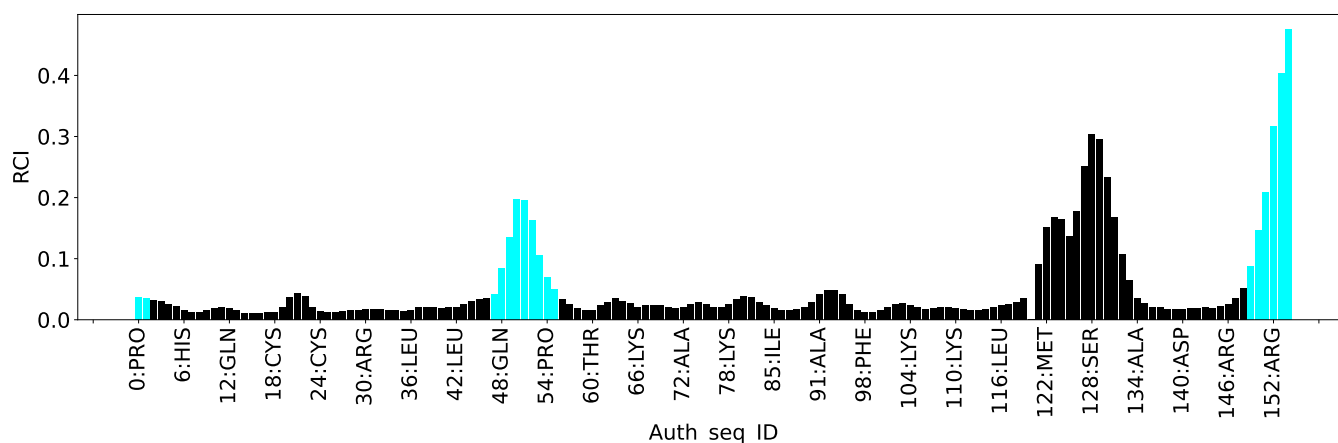
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



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	2557
Intra-residue ($ i-j =0$)	615
Sequential ($ i-j =1$)	592
Medium range ($ i-j >1$ and $ i-j <5$)	652
Long range ($ i-j \geq 5$)	650
Inter-chain	48
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	16.2
Number of long range restraints per residue ¹	4.1

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)	12.9	0.2
0.2-0.5 (Medium)	4.5	0.48
>0.5 (Large)	15.8	7.56

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 ⓘ

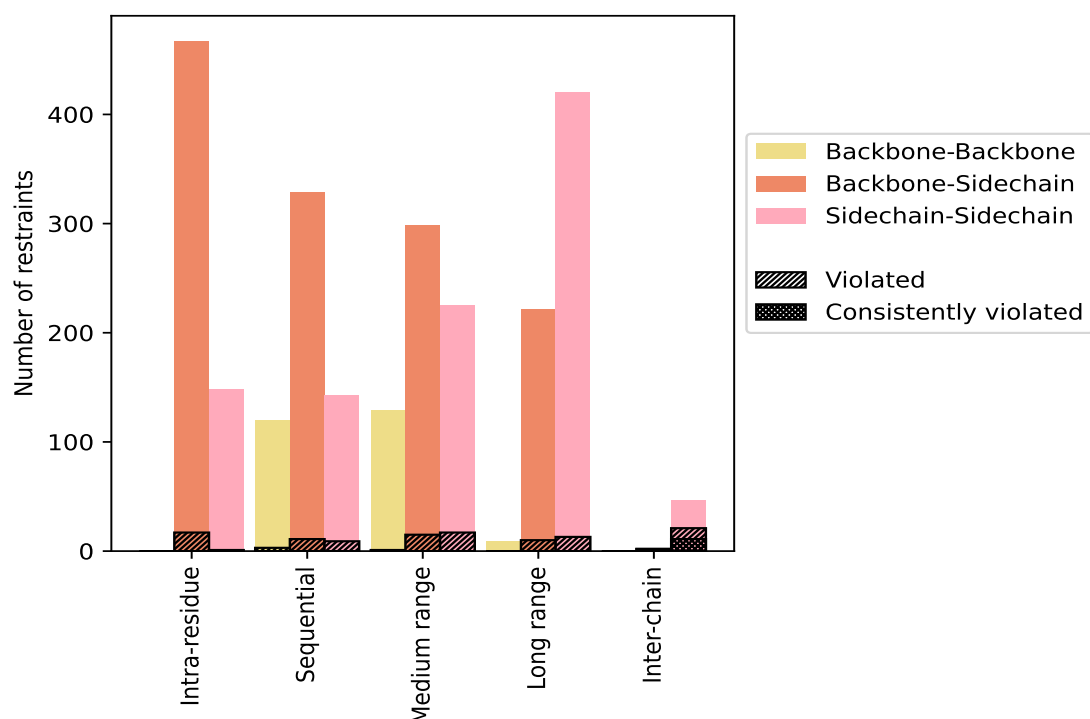
9.1 Summary of distance violations ⓘ

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)	615	24.1	18	2.9	0.7	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	467	18.3	17	3.6	0.7	0	0.0	0.0
Sidechain-Sidechain	148	5.8	1	0.7	0.0	0	0.0	0.0
Sequential (i-j =1)	592	23.2	23	3.9	0.9	0	0.0	0.0
Backbone-Backbone	120	4.7	3	2.5	0.1	0	0.0	0.0
Backbone-Sidechain	329	12.9	11	3.3	0.4	0	0.0	0.0
Sidechain-Sidechain	143	5.6	9	6.3	0.4	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	652	25.5	33	5.1	1.3	0	0.0	0.0
Backbone-Backbone	129	5.0	1	0.8	0.0	0	0.0	0.0
Backbone-Sidechain	298	11.7	15	5.0	0.6	0	0.0	0.0
Sidechain-Sidechain	225	8.8	17	7.6	0.7	0	0.0	0.0
Long range (i-j ≥5)	650	25.4	23	3.5	0.9	0	0.0	0.0
Backbone-Backbone	9	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	221	8.6	10	4.5	0.4	0	0.0	0.0
Sidechain-Sidechain	420	16.4	13	3.1	0.5	0	0.0	0.0
Inter-chain	48	1.9	23	47.9	0.9	13	27.1	0.5
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	0.1	2	100.0	0.1	2	100.0	0.1
Sidechain-Sidechain	46	1.8	21	45.7	0.8	11	23.9	0.4
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	2557	100.0	120	4.7	4.7	13	0.5	0.5
Backbone-Backbone	258	10.1	4	1.6	0.2	0	0.0	0.0
Backbone-Sidechain	1317	51.5	55	4.2	2.2	2	0.2	0.1
Sidechain-Sidechain	982	38.4	61	6.2	2.4	11	1.1	0.4

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	2	6	3	19	33	2.09	6.95	2.46	0.53
2	4	0	10	3	16	33	1.69	6.21	2.07	0.21
3	4	5	4	1	20	34	2.14	7.29	2.57	0.34
4	4	2	4	3	21	34	2.13	6.92	2.44	0.46
5	1	4	7	2	19	33	1.77	6.01	2.03	0.57
6	6	4	9	8	16	43	1.35	6.1	1.93	0.18
7	1	7	10	7	20	45	1.4	6.67	1.91	0.22
8	0	3	5	0	15	23	2.27	6.04	2.06	1.54
9	4	0	6	2	16	28	1.81	5.79	1.89	0.6
10	3	4	5	3	21	36	2.16	7.2	2.53	0.35

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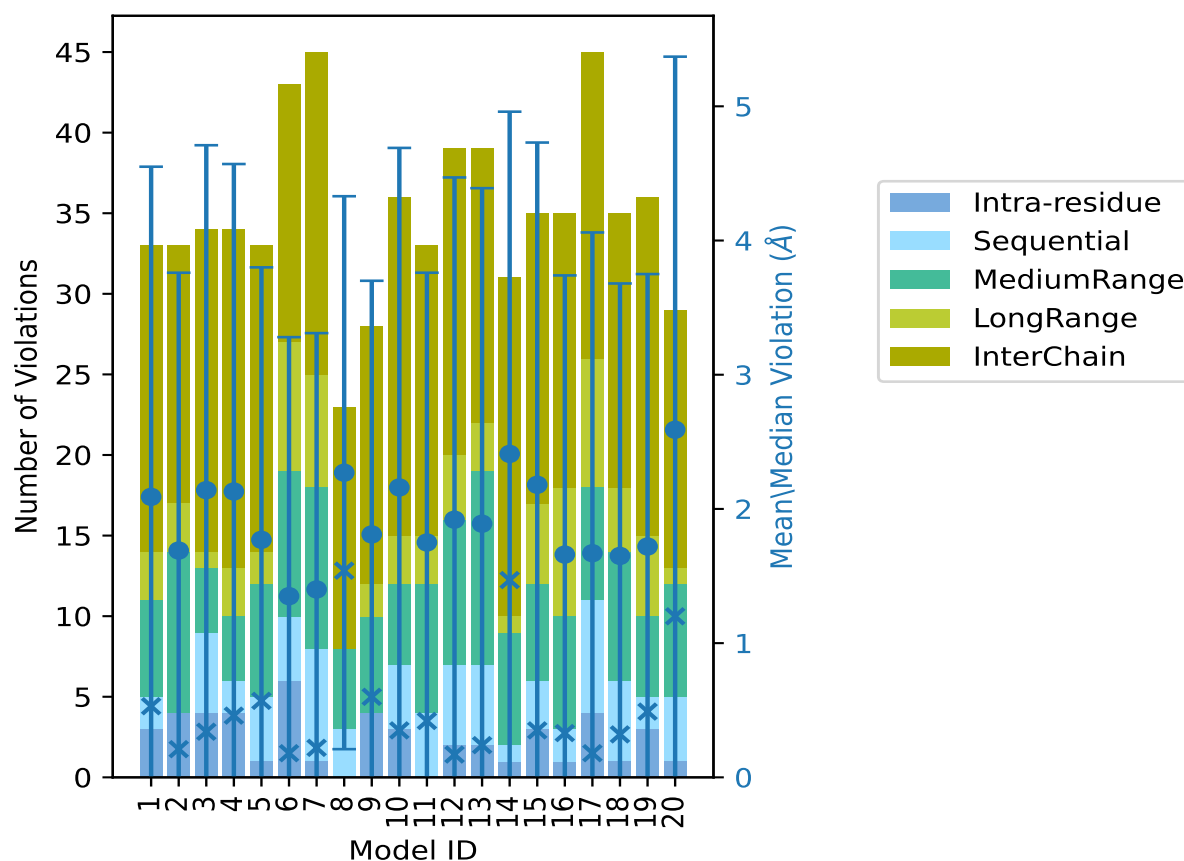
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	4	8	3	18	33	1.75	6.01	2.01	0.42
12	2	5	9	4	19	39	1.92	7.19	2.55	0.17
13	2	5	12	3	17	39	1.89	7.08	2.5	0.24
14	1	1	7	1	21	31	2.41	7.17	2.55	1.47
15	3	3	6	5	18	35	2.18	7.09	2.55	0.35
16	1	2	7	8	17	35	1.66	6.65	2.08	0.33
17	4	7	7	8	19	45	1.67	7.34	2.39	0.18
18	1	5	8	4	17	35	1.65	6.44	2.03	0.32
19	3	2	5	5	21	36	1.72	6.63	2.03	0.49
20	1	4	7	1	16	29	2.59	7.56	2.78	1.2

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 ⓘ



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

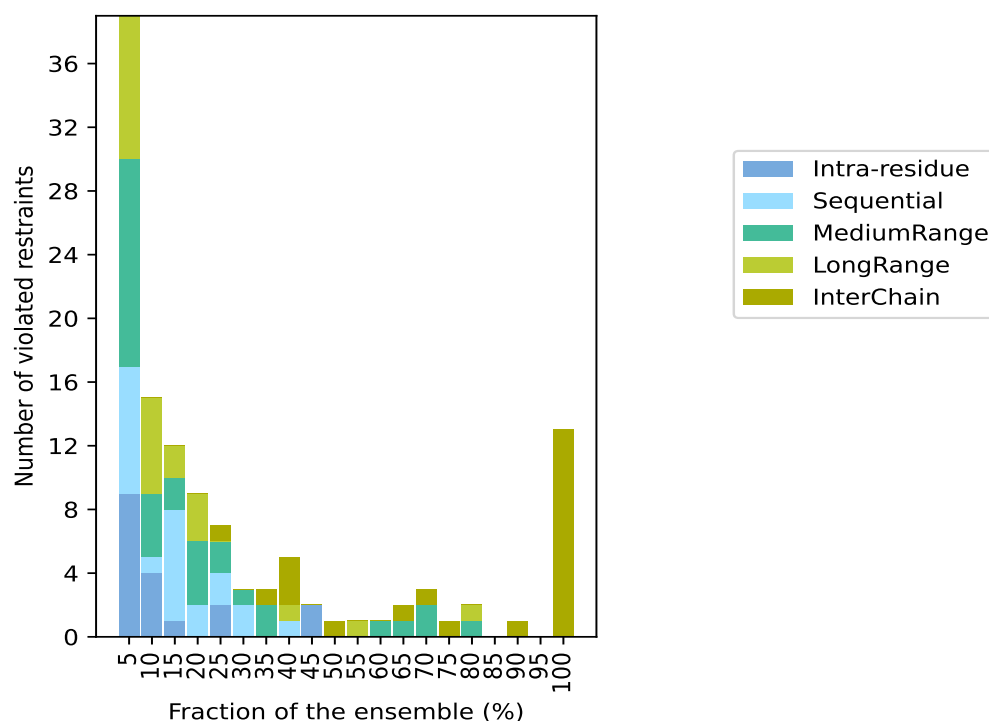
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2437(IR:597, SQ:569, MR:619, LR:627, IC:25) restraints are 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	%
9	8	13	9	0	39	1	5.0
4	1	4	6	0	15	2	10.0
1	7	2	2	0	12	3	15.0
0	2	4	3	0	9	4	20.0
2	2	2	0	1	7	5	25.0
0	2	1	0	0	3	6	30.0
0	0	2	0	1	3	7	35.0
0	1	0	1	3	5	8	40.0
2	0	0	0	0	2	9	45.0
0	0	0	0	1	1	10	50.0
0	0	0	1	0	1	11	55.0
0	0	1	0	0	1	12	60.0
0	0	1	0	1	2	13	65.0
0	0	2	0	1	3	14	70.0
0	0	0	0	1	1	15	75.0
0	0	1	1	0	2	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	1	1	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	13	13	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

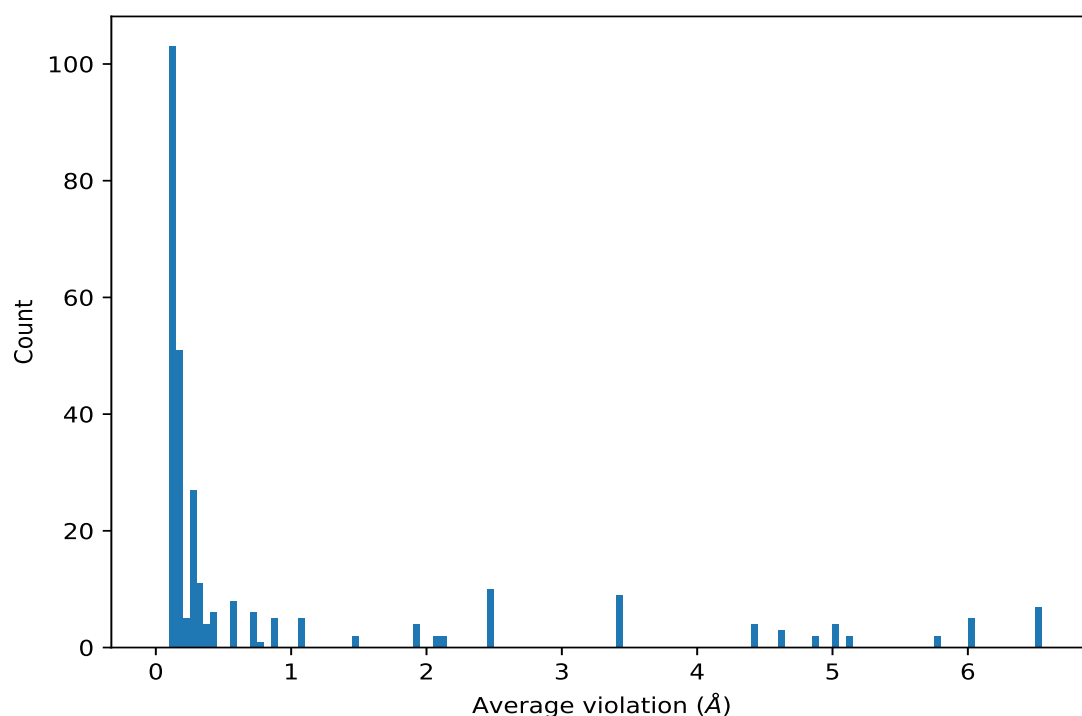
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,2445)	1:116:A:LEU:HD11	2:201:A:UJ2:H28	20	6.51	0.38	6.64
(1,2445)	1:116:A:LEU:HD23	2:201:A:UJ2:H28	20	6.51	0.38	6.64
(1,2445)	1:116:A:LEU:HD12	2:201:A:UJ2:H28	20	6.51	0.38	6.64
(1,2445)	1:116:A:LEU:HD22	2:201:A:UJ2:H28	20	6.51	0.38	6.64
(1,2445)	1:116:A:LEU:HD13	2:201:A:UJ2:H28	20	6.51	0.38	6.64
(1,2445)	1:116:A:LEU:HD21	2:201:A:UJ2:H28	20	6.51	0.38	6.64
(1,2445)	1:116:A:LEU:HD23	2:201:A:UJ2:H29	20	6.51	0.38	6.64
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	20	6.01	1.18	6.01
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H29	20	6.01	1.18	6.01
(1,1832)	1:7:A:ILE:HD12	2:201:A:UJ2:H28	20	6.01	0.28	6.1
(1,1832)	1:7:A:ILE:HD11	2:201:A:UJ2:H28	20	6.01	0.28	6.1
(1,1832)	1:7:A:ILE:HD13	2:201:A:UJ2:H28	20	6.01	0.28	6.1
(1,748)	1:66:A:LYS:HE3	2:201:A:UJ2:H28	20	5.76	0.67	5.78
(1,748)	1:66:A:LYS:HE2	2:201:A:UJ2:H28	20	5.76	0.67	5.78
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H29	20	5.14	1.47	4.96
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H28	20	5.14	1.47	4.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	20	5.0	0.92	5.4
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H29	20	5.0	0.92	5.4
(1,2208)	1:62:A:MET:HB3	2:201:A:UJ2:H28	20	5.0	0.92	5.4
(1,2208)	1:62:A:MET:HB3	2:201:A:UJ2:H29	20	5.0	0.92	5.4
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H29	20	4.85	1.25	4.96
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H28	20	4.85	1.25	4.96
(1,1835)	1:62:A:MET:HE3	2:201:A:UJ2:H28	20	4.62	0.45	4.7
(1,1835)	1:62:A:MET:HE2	2:201:A:UJ2:H28	20	4.62	0.45	4.7
(1,1835)	1:62:A:MET:HE1	2:201:A:UJ2:H28	20	4.62	0.45	4.7
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	20	4.43	0.92	4.84
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H29	20	4.43	0.92	4.84
(1,1849)	1:62:A:MET:HB3	2:201:A:UJ2:H28	20	4.43	0.92	4.84
(1,1849)	1:62:A:MET:HB3	2:201:A:UJ2:H29	20	4.43	0.92	4.84
(1,1868)	1:4:A:LEU:HD12	2:201:A:UJ2:H28	20	3.4	1.23	3.08
(1,1868)	1:4:A:LEU:HD21	2:201:A:UJ2:H28	20	3.4	1.23	3.08
(1,1868)	1:4:A:LEU:HD11	2:201:A:UJ2:H28	20	3.4	1.23	3.08
(1,1868)	1:4:A:LEU:HD13	2:201:A:UJ2:H29	20	3.4	1.23	3.08
(1,1868)	1:4:A:LEU:HD12	2:201:A:UJ2:H29	20	3.4	1.23	3.08
(1,1868)	1:4:A:LEU:HD23	2:201:A:UJ2:H28	20	3.4	1.23	3.08
(1,1868)	1:4:A:LEU:HD22	2:201:A:UJ2:H28	20	3.4	1.23	3.08
(1,1868)	1:4:A:LEU:HD13	2:201:A:UJ2:H28	20	3.4	1.23	3.08
(1,1868)	1:4:A:LEU:HD11	2:201:A:UJ2:H29	20	3.4	1.23	3.08
(1,2191)	1:58:A:LEU:HD22	2:201:A:UJ2:H28	20	2.47	0.43	2.59
(1,2191)	1:58:A:LEU:HD12	2:201:A:UJ2:H28	20	2.47	0.43	2.59
(1,2191)	1:58:A:LEU:HD11	2:201:A:UJ2:H29	20	2.47	0.43	2.59
(1,2191)	1:58:A:LEU:HD12	2:201:A:UJ2:H29	20	2.47	0.43	2.59
(1,2191)	1:58:A:LEU:HD21	2:201:A:UJ2:H28	20	2.47	0.43	2.59
(1,2191)	1:58:A:LEU:HD13	2:201:A:UJ2:H28	20	2.47	0.43	2.59
(1,2191)	1:58:A:LEU:HD11	2:201:A:UJ2:H28	20	2.47	0.43	2.59
(1,2191)	1:58:A:LEU:HD23	2:201:A:UJ2:H29	20	2.47	0.43	2.59
(1,2191)	1:58:A:LEU:HD22	2:201:A:UJ2:H29	20	2.47	0.43	2.59
(1,2191)	1:58:A:LEU:HD13	2:201:A:UJ2:H29	20	2.47	0.43	2.59
(1,814)	1:59:A:THR:HG22	2:201:A:UJ2:H28	20	1.93	0.34	1.98
(1,814)	1:59:A:THR:HG23	2:201:A:UJ2:H28	20	1.93	0.34	1.98
(1,814)	1:59:A:THR:HG21	2:201:A:UJ2:H28	20	1.93	0.34	1.98
(1,814)	1:59:A:THR:HG22	2:201:A:UJ2:H29	20	1.93	0.34	1.98
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	20	1.48	0.66	1.47
(1,1165)	1:3:A:ASN:HB3	2:201:A:UJ2:H28	20	1.48	0.66	1.47
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H29	18	2.06	1.22	2.6
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H28	18	2.06	1.22	2.6
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	16	0.33	0.01	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	16	0.33	0.01	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	16	0.33	0.01	0.33
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	16	0.14	0.02	0.14
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H29	15	2.14	1.18	2.81
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H28	15	2.14	1.18	2.81
(1,1658)	1:7:A:ILE:HG23	2:201:A:UJ2:H37	14	0.34	0.25	0.27
(1,1658)	1:7:A:ILE:HG23	2:201:A:UJ2:H34	14	0.34	0.25	0.27
(1,1658)	1:7:A:ILE:HG22	2:201:A:UJ2:H34	14	0.34	0.25	0.27
(1,1658)	1:7:A:ILE:HG21	2:201:A:UJ2:H37	14	0.34	0.25	0.27
(1,1658)	1:7:A:ILE:HG21	2:201:A:UJ2:H34	14	0.34	0.25	0.27
(1,1658)	1:7:A:ILE:HG22	2:201:A:UJ2:H37	14	0.34	0.25	0.27
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	14	0.18	0.04	0.16
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	14	0.12	0.01	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	14	0.12	0.01	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	14	0.12	0.01	0.12
(1,1836)	1:122:A:MET:HE1	2:201:A:UJ2:H39	13	0.38	0.18	0.33
(1,1836)	1:122:A:MET:HE1	2:201:A:UJ2:H38	13	0.38	0.18	0.33
(1,1836)	1:122:A:MET:HE3	2:201:A:UJ2:H39	13	0.38	0.18	0.33
(1,1836)	1:122:A:MET:HE2	2:201:A:UJ2:H39	13	0.38	0.18	0.33
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	13	0.15	0.03	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	13	0.15	0.03	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	13	0.15	0.03	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	13	0.15	0.03	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	13	0.15	0.03	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	13	0.15	0.03	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	13	0.15	0.03	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	13	0.15	0.03	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	13	0.15	0.03	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	13	0.15	0.03	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	13	0.15	0.03	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	13	0.15	0.03	0.15
(1,2160)	1:56:A:GLU:HG2	1:59:A:THR:HB	12	0.13	0.02	0.13
(1,2160)	1:56:A:GLU:HG3	1:59:A:THR:HB	12	0.13	0.02	0.13
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD11	11	0.13	0.02	0.13
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD12	11	0.13	0.02	0.13
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD13	11	0.13	0.02	0.13
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD11	11	0.13	0.02	0.13
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD12	11	0.13	0.02	0.13
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD13	11	0.13	0.02	0.13
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD11	11	0.13	0.02	0.13
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD12	11	0.13	0.02	0.13
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD13	11	0.13	0.02	0.13
(1,1839)	1:59:A:THR:HG22	2:201:A:UJ2:H28	10	0.27	0.09	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1839)	1:59:A:THR:HG23	2:201:A:UJ2:H28	10	0.27	0.09	0.3
(1,1839)	1:59:A:THR:HG21	2:201:A:UJ2:H28	10	0.27	0.09	0.3
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG2	9	0.16	0.0	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG3	9	0.16	0.0	0.16
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG2	9	0.15	0.03	0.16
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG3	9	0.15	0.03	0.16
(1,1637)	1:42:A:LEU:HD21	2:201:A:UJ2:H38	8	1.07	0.63	1.51
(1,1637)	1:42:A:LEU:HD23	2:201:A:UJ2:H38	8	1.07	0.63	1.51
(1,1637)	1:42:A:LEU:HD22	2:201:A:UJ2:H39	8	1.07	0.63	1.51
(1,1637)	1:42:A:LEU:HD21	2:201:A:UJ2:H39	8	1.07	0.63	1.51
(1,1637)	1:42:A:LEU:HD23	2:201:A:UJ2:H39	8	1.07	0.63	1.51
(1,1842)	1:45:A:LEU:HD13	2:201:A:UJ2:H39	8	0.86	0.29	0.79
(1,1842)	1:45:A:LEU:HD11	2:201:A:UJ2:H39	8	0.86	0.29	0.79
(1,1842)	1:45:A:LEU:HD12	2:201:A:UJ2:H39	8	0.86	0.29	0.79
(1,1842)	1:45:A:LEU:HD13	2:201:A:UJ2:H34	8	0.86	0.29	0.79
(1,1842)	1:45:A:LEU:HD12	2:201:A:UJ2:H34	8	0.86	0.29	0.79
(1,1848)	1:116:A:LEU:HD11	2:201:A:UJ2:H38	8	0.55	0.23	0.54
(1,1848)	1:116:A:LEU:HD12	2:201:A:UJ2:H39	8	0.55	0.23	0.54
(1,1848)	1:116:A:LEU:HD13	2:201:A:UJ2:H37	8	0.55	0.23	0.54
(1,1848)	1:116:A:LEU:HD13	2:201:A:UJ2:H38	8	0.55	0.23	0.54
(1,1848)	1:116:A:LEU:HD12	2:201:A:UJ2:H35	8	0.55	0.23	0.54
(1,1848)	1:116:A:LEU:HD11	2:201:A:UJ2:H37	8	0.55	0.23	0.54
(1,1848)	1:116:A:LEU:HD11	2:201:A:UJ2:H39	8	0.55	0.23	0.54
(1,1848)	1:116:A:LEU:HD13	2:201:A:UJ2:H39	8	0.55	0.23	0.54
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD1	8	0.16	0.01	0.16
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD2	8	0.16	0.01	0.16
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD1	8	0.16	0.01	0.16
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD2	8	0.16	0.01	0.16
(1,279)	1:61:A:ALA:H	1:115:A:LEU:HG	8	0.15	0.04	0.14
(1,1847)	1:42:A:LEU:HD11	2:201:A:UJ2:H38	7	0.73	0.64	0.38
(1,1847)	1:42:A:LEU:HD12	2:201:A:UJ2:H34	7	0.73	0.64	0.38
(1,1847)	1:42:A:LEU:HD12	2:201:A:UJ2:H39	7	0.73	0.64	0.38
(1,1847)	1:42:A:LEU:HD11	2:201:A:UJ2:H39	7	0.73	0.64	0.38
(1,1847)	1:42:A:LEU:HD12	2:201:A:UJ2:H38	7	0.73	0.64	0.38
(1,1847)	1:42:A:LEU:HD13	2:201:A:UJ2:H37	7	0.73	0.64	0.38
(1,153)	1:32:A:GLY:H	1:35:A:VAL:HB	7	0.12	0.02	0.11
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG21	7	0.1	0.0	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG22	7	0.1	0.0	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG23	7	0.1	0.0	0.1
(1,638)	1:151:A:LEU:HA	1:152:A:ARG:H	6	0.16	0.0	0.16
(1,548)	1:123:A:PRO:HB2	1:124:A:VAL:H	6	0.13	0.02	0.12
(1,535)	1:116:A:LEU:HB3	1:118:A:VAL:H	6	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1055)	1:42:A:LEU:HG	2:201:A:UJ2:H34	5	0.76	0.58	0.41
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB1	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB2	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB3	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB1	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB2	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB3	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB1	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB2	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB3	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB1	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB2	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB3	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB1	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB2	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB3	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB1	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB2	5	0.26	0.06	0.28
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB3	5	0.26	0.06	0.28
(1,2347)	1:99:A:LYS:HD2	1:100:A:ASP:HA	5	0.2	0.01	0.21
(1,2347)	1:99:A:LYS:HD3	1:100:A:ASP:HA	5	0.2	0.01	0.21
(1,926)	1:22:A:LYS:HA	1:22:A:LYS:HG3	5	0.19	0.0	0.19
(1,2182)	1:58:A:LEU:HD11	1:61:A:ALA:H	5	0.18	0.03	0.17
(1,2182)	1:58:A:LEU:HD12	1:61:A:ALA:H	5	0.18	0.03	0.17
(1,2182)	1:58:A:LEU:HD13	1:61:A:ALA:H	5	0.18	0.03	0.17
(1,2182)	1:58:A:LEU:HD21	1:61:A:ALA:H	5	0.18	0.03	0.17
(1,2182)	1:58:A:LEU:HD22	1:61:A:ALA:H	5	0.18	0.03	0.17
(1,2182)	1:58:A:LEU:HD23	1:61:A:ALA:H	5	0.18	0.03	0.17
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD11	5	0.13	0.01	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD12	5	0.13	0.01	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD13	5	0.13	0.01	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD21	5	0.13	0.01	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD22	5	0.13	0.01	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD23	5	0.13	0.01	0.13
(1,249)	1:54:A:PRO:HA	1:55:A:SER:H	5	0.1	0.0	0.1
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD11	4	0.25	0.08	0.3
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD12	4	0.25	0.08	0.3
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD13	4	0.25	0.08	0.3
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD21	4	0.25	0.08	0.3
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD22	4	0.25	0.08	0.3
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD23	4	0.25	0.08	0.3
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE1	4	0.15	0.05	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE2	4	0.15	0.05	0.14
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE3	4	0.15	0.05	0.14
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD11	4	0.15	0.02	0.15
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD12	4	0.15	0.02	0.15
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD13	4	0.15	0.02	0.15
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD21	4	0.15	0.02	0.15
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD22	4	0.15	0.02	0.15
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD23	4	0.15	0.02	0.15
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD21	4	0.14	0.01	0.15
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD22	4	0.14	0.01	0.15
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD23	4	0.14	0.01	0.15
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG11	4	0.13	0.01	0.13
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG12	4	0.13	0.01	0.13
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG13	4	0.13	0.01	0.13
(1,2083)	1:36:A:LEU:HD11	1:39:A:ILE:HG12	4	0.13	0.02	0.12
(1,2083)	1:36:A:LEU:HD12	1:39:A:ILE:HG12	4	0.13	0.02	0.12
(1,2083)	1:36:A:LEU:HD13	1:39:A:ILE:HG12	4	0.13	0.02	0.12
(1,2083)	1:36:A:LEU:HD21	1:39:A:ILE:HG12	4	0.13	0.02	0.12
(1,2083)	1:36:A:LEU:HD22	1:39:A:ILE:HG12	4	0.13	0.02	0.12
(1,2083)	1:36:A:LEU:HD23	1:39:A:ILE:HG12	4	0.13	0.02	0.12
(1,2148)	1:52:A:SER:HB2	1:53:A:VAL:HB	4	0.13	0.01	0.12
(1,2148)	1:52:A:SER:HB3	1:53:A:VAL:HB	4	0.13	0.01	0.12
(1,834)	1:9:A:THR:HA	1:13:A:VAL:HA	4	0.11	0.01	0.12
(1,1189)	1:68:A:ALA:HB1	1:70:A:GLU:H	4	0.1	0.0	0.11
(1,1189)	1:68:A:ALA:HB2	1:70:A:GLU:H	4	0.1	0.0	0.11
(1,1189)	1:68:A:ALA:HB3	1:70:A:GLU:H	4	0.1	0.0	0.11
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG11	3	0.16	0.03	0.15
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG12	3	0.16	0.03	0.15
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG13	3	0.16	0.03	0.15
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG21	3	0.16	0.03	0.15
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG22	3	0.16	0.03	0.15
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG23	3	0.16	0.03	0.15
(1,1593)	1:131:A:ALA:HB1	1:132:A:SER:HA	3	0.15	0.01	0.15
(1,1593)	1:131:A:ALA:HB2	1:132:A:SER:HA	3	0.15	0.01	0.15
(1,1593)	1:131:A:ALA:HB3	1:132:A:SER:HA	3	0.15	0.01	0.15
(1,1051)	1:42:A:LEU:HA	1:42:A:LEU:HD11	3	0.13	0.01	0.13
(1,1051)	1:42:A:LEU:HA	1:42:A:LEU:HD12	3	0.13	0.01	0.13
(1,1051)	1:42:A:LEU:HA	1:42:A:LEU:HD13	3	0.13	0.01	0.13
(1,1177)	1:24:A:CYS:H	1:25:A:LYS:HE2	3	0.13	0.02	0.12
(1,1177)	1:24:A:CYS:H	1:25:A:LYS:HE3	3	0.13	0.02	0.12
(1,1347)	1:45:A:LEU:HD21	1:122:A:MET:HA	3	0.13	0.02	0.11
(1,1347)	1:45:A:LEU:HD22	1:122:A:MET:HA	3	0.13	0.02	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1347)	1:45:A:LEU:HD23	1:122:A:MET:HA	3	0.13	0.02	0.11
(1,227)	1:8:A:ILE:HD11	1:44:A:MET:H	3	0.12	0.01	0.11
(1,227)	1:8:A:ILE:HD12	1:44:A:MET:H	3	0.12	0.01	0.11
(1,227)	1:8:A:ILE:HD13	1:44:A:MET:H	3	0.12	0.01	0.11
(1,660)	1:133:A:TRP:HE3	1:134:A:ALA:H	3	0.12	0.01	0.12
(1,1874)	1:5:A:LYS:HG2	1:6:A:HIS:H	3	0.12	0.02	0.12
(1,1874)	1:5:A:LYS:HG3	1:6:A:HIS:H	3	0.12	0.02	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD11	3	0.12	0.0	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD12	3	0.12	0.0	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD13	3	0.12	0.0	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD21	3	0.12	0.0	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD22	3	0.12	0.0	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD23	3	0.12	0.0	0.12
(1,2495)	1:136:A:GLU:HG2	1:137:A:ASP:HB2	3	0.12	0.01	0.11
(1,2495)	1:136:A:GLU:HG2	1:137:A:ASP:HB3	3	0.12	0.01	0.11
(1,2495)	1:136:A:GLU:HG3	1:137:A:ASP:HB2	3	0.12	0.01	0.11
(1,2495)	1:136:A:GLU:HG3	1:137:A:ASP:HB3	3	0.12	0.01	0.11
(1,1813)	1:15:A:HIS:HE1	1:16:A:LYS:HD2	3	0.11	0.01	0.11
(1,1813)	1:15:A:HIS:HE1	1:16:A:LYS:HD3	3	0.11	0.01	0.11
(1,139)	1:56:A:GLU:HB3	1:60:A:THR:H	3	0.11	0.0	0.11
(1,2493)	1:134:A:ALA:HB1	1:138:A:GLN:HG2	2	0.43	0.02	0.43
(1,2493)	1:134:A:ALA:HB1	1:138:A:GLN:HG3	2	0.43	0.02	0.43
(1,2493)	1:134:A:ALA:HB2	1:138:A:GLN:HG2	2	0.43	0.02	0.43
(1,2493)	1:134:A:ALA:HB2	1:138:A:GLN:HG3	2	0.43	0.02	0.43
(1,2493)	1:134:A:ALA:HB3	1:138:A:GLN:HG2	2	0.43	0.02	0.43
(1,2493)	1:134:A:ALA:HB3	1:138:A:GLN:HG3	2	0.43	0.02	0.43
(1,642)	1:153:A:ARG:HA	1:154:A:ASP:H	2	0.34	0.01	0.34
(1,719)	1:114:A:LEU:HA	1:114:A:LEU:HG	2	0.3	0.01	0.3
(1,248)	1:53:A:VAL:H	1:53:A:VAL:HB	2	0.24	0.08	0.24
(1,2392)	1:107:A:ASP:HA	1:110:A:LYS:HG2	2	0.23	0.0	0.23
(1,2392)	1:107:A:ASP:HA	1:110:A:LYS:HG3	2	0.23	0.0	0.23
(1,1582)	1:10:A:LEU:HG	1:69:A:LEU:HD21	2	0.16	0.06	0.16
(1,1582)	1:10:A:LEU:HG	1:69:A:LEU:HD22	2	0.16	0.06	0.16
(1,1582)	1:10:A:LEU:HG	1:69:A:LEU:HD23	2	0.16	0.06	0.16
(1,721)	1:62:A:MET:HB3	1:112:A:LEU:HD21	2	0.14	0.01	0.14
(1,721)	1:62:A:MET:HB3	1:112:A:LEU:HD22	2	0.14	0.01	0.14
(1,721)	1:62:A:MET:HB3	1:112:A:LEU:HD23	2	0.14	0.01	0.14
(1,2450)	1:117:A:GLN:HA	1:122:A:MET:HB2	2	0.14	0.0	0.14
(1,2450)	1:117:A:GLN:HA	1:122:A:MET:HB3	2	0.14	0.0	0.14
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD11	2	0.14	0.02	0.14
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD12	2	0.14	0.02	0.14
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD13	2	0.14	0.02	0.14

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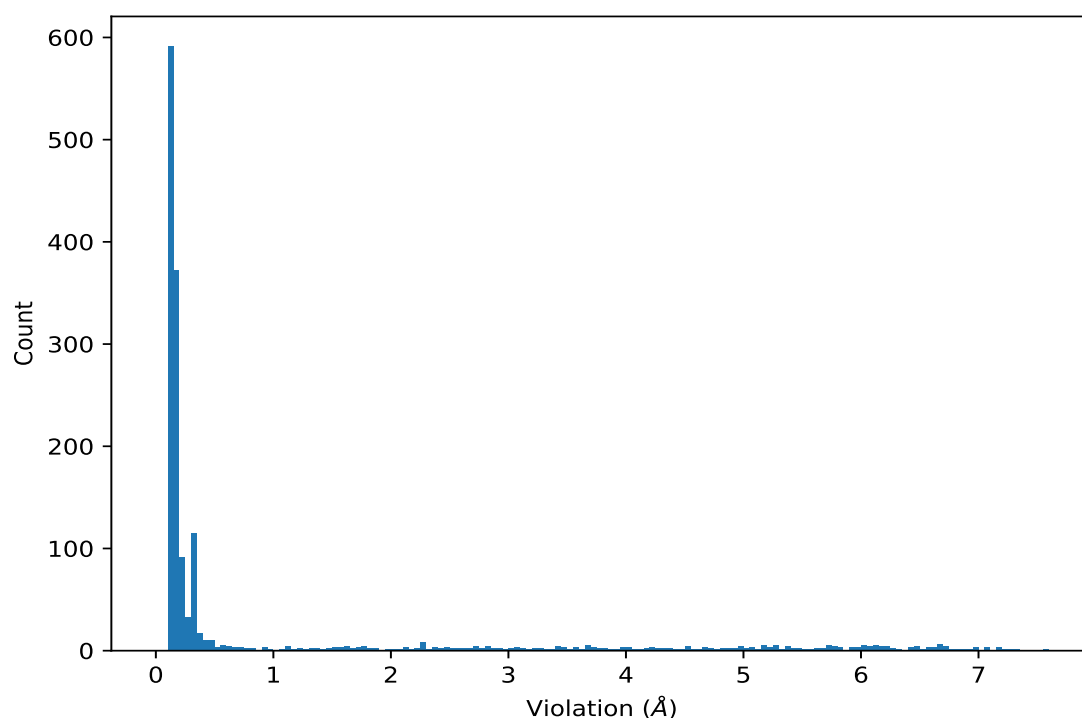
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD21	2	0.14	0.02	0.14
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD22	2	0.14	0.02	0.14
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD23	2	0.14	0.02	0.14
(1,1789)	1:106:A:SER:HA	1:109:A:TRP:HD1	2	0.13	0.02	0.13
(1,1545)	1:109:A:TRP:HZ3	1:122:A:MET:HE1	2	0.12	0.01	0.12
(1,1545)	1:109:A:TRP:HZ3	1:122:A:MET:HE2	2	0.12	0.01	0.12
(1,1545)	1:109:A:TRP:HZ3	1:122:A:MET:HE3	2	0.12	0.01	0.12
(1,1936)	1:13:A:VAL:HG21	1:17:A:ARG:HD2	2	0.12	0.02	0.12
(1,1936)	1:13:A:VAL:HG21	1:17:A:ARG:HD3	2	0.12	0.02	0.12
(1,1936)	1:13:A:VAL:HG22	1:17:A:ARG:HD2	2	0.12	0.02	0.12
(1,1936)	1:13:A:VAL:HG22	1:17:A:ARG:HD3	2	0.12	0.02	0.12
(1,1936)	1:13:A:VAL:HG23	1:17:A:ARG:HD2	2	0.12	0.02	0.12
(1,1936)	1:13:A:VAL:HG23	1:17:A:ARG:HD3	2	0.12	0.02	0.12
(1,2023)	1:26:A:LYS:H	1:26:A:LYS:HG2	2	0.11	0.0	0.11
(1,2023)	1:26:A:LYS:H	1:26:A:LYS:HG3	2	0.11	0.0	0.11
(1,550)	1:124:A:VAL:H	1:124:A:VAL:HB	2	0.11	0.0	0.11
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD11	2	0.11	0.0	0.11
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD12	2	0.11	0.0	0.11
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD13	2	0.11	0.0	0.11
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD21	2	0.11	0.0	0.11
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD22	2	0.11	0.0	0.11
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD23	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)
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	20	7.56
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H29	17	7.34
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	3	7.29
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	10	7.2
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	12	7.19
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	14	7.17
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H29	20	7.15
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	15	7.09
(1,2445)	1:116:A:LEU:HD13	2:201:A:UJ2:H28	15	7.08
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	13	7.08
(1,2445)	1:116:A:LEU:HD11	2:201:A:UJ2:H28	1	6.95
(1,2445)	1:116:A:LEU:HD11	2:201:A:UJ2:H28	17	6.95
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H29	12	6.95
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	4	6.92
(1,2445)	1:116:A:LEU:HD21	2:201:A:UJ2:H28	12	6.86
(1,2445)	1:116:A:LEU:HD11	2:201:A:UJ2:H28	13	6.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H29	13	6.79
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	1	6.73
(1,2445)	1:116:A:LEU:HD22	2:201:A:UJ2:H28	10	6.71
(1,748)	1:66:A:LYS:HE2	2:201:A:UJ2:H28	17	6.71
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H29	3	6.7
(1,2445)	1:116:A:LEU:HD12	2:201:A:UJ2:H28	4	6.69
(1,748)	1:66:A:LYS:HE3	2:201:A:UJ2:H28	20	6.69
(1,2445)	1:116:A:LEU:HD12	2:201:A:UJ2:H28	7	6.67
(1,2445)	1:116:A:LEU:HD22	2:201:A:UJ2:H28	16	6.65
(1,2445)	1:116:A:LEU:HD23	2:201:A:UJ2:H28	20	6.65
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H29	15	6.65
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H29	10	6.64
(1,2445)	1:116:A:LEU:HD23	2:201:A:UJ2:H29	19	6.63
(1,2445)	1:116:A:LEU:HD22	2:201:A:UJ2:H28	14	6.62
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H29	14	6.59
(1,2445)	1:116:A:LEU:HD12	2:201:A:UJ2:H28	3	6.57
(1,748)	1:66:A:LYS:HE3	2:201:A:UJ2:H28	10	6.55
(1,1832)	1:7:A:ILE:HD12	2:201:A:UJ2:H28	10	6.5
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H29	20	6.49
(1,748)	1:66:A:LYS:HE2	2:201:A:UJ2:H28	3	6.48
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H29	13	6.46
(1,748)	1:66:A:LYS:HE3	2:201:A:UJ2:H28	14	6.45
(1,2445)	1:116:A:LEU:HD11	2:201:A:UJ2:H28	18	6.44
(1,1832)	1:7:A:ILE:HD13	2:201:A:UJ2:H28	14	6.44
(1,748)	1:66:A:LYS:HE3	2:201:A:UJ2:H28	15	6.43
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H29	17	6.32
(1,1832)	1:7:A:ILE:HD12	2:201:A:UJ2:H28	1	6.27
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H29	12	6.26
(1,1832)	1:7:A:ILE:HD12	2:201:A:UJ2:H28	2	6.21
(1,1832)	1:7:A:ILE:HD11	2:201:A:UJ2:H28	17	6.21
(1,1832)	1:7:A:ILE:HD11	2:201:A:UJ2:H28	20	6.21
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H29	3	6.2
(1,748)	1:66:A:LYS:HE3	2:201:A:UJ2:H28	13	6.19
(1,1832)	1:7:A:ILE:HD11	2:201:A:UJ2:H28	3	6.18
(1,748)	1:66:A:LYS:HE3	2:201:A:UJ2:H28	1	6.18
(1,1832)	1:7:A:ILE:HD12	2:201:A:UJ2:H28	12	6.15
(1,1832)	1:7:A:ILE:HD13	2:201:A:UJ2:H28	4	6.14
(1,1832)	1:7:A:ILE:HD11	2:201:A:UJ2:H28	15	6.13
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H29	15	6.11
(1,2445)	1:116:A:LEU:HD13	2:201:A:UJ2:H28	6	6.1
(1,748)	1:66:A:LYS:HE3	2:201:A:UJ2:H28	12	6.1
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H29	4	6.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1832)	1:7:A:ILE:HD12	2:201:A:UJ2:H28	13	6.07
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H29	10	6.06
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	20	6.05
(1,2445)	1:116:A:LEU:HD22	2:201:A:UJ2:H28	8	6.04
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H29	14	6.04
(1,748)	1:66:A:LYS:HE3	2:201:A:UJ2:H28	4	6.02
(1,2445)	1:116:A:LEU:HD22	2:201:A:UJ2:H28	5	6.01
(1,2445)	1:116:A:LEU:HD13	2:201:A:UJ2:H28	11	6.01
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	10	5.97
(1,1832)	1:7:A:ILE:HD13	2:201:A:UJ2:H28	6	5.97
(1,2208)	1:62:A:MET:HB3	2:201:A:UJ2:H28	15	5.96
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	12	5.94
(1,2445)	1:116:A:LEU:HD23	2:201:A:UJ2:H28	2	5.93
(1,1832)	1:7:A:ILE:HD11	2:201:A:UJ2:H28	7	5.93
(1,2208)	1:62:A:MET:HB3	2:201:A:UJ2:H29	17	5.84
(1,1832)	1:7:A:ILE:HD12	2:201:A:UJ2:H28	5	5.83
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	3	5.81
(1,2445)	1:116:A:LEU:HD12	2:201:A:UJ2:H28	9	5.79
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	14	5.79
(1,1832)	1:7:A:ILE:HD13	2:201:A:UJ2:H28	11	5.77
(1,1832)	1:7:A:ILE:HD13	2:201:A:UJ2:H28	8	5.76
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H29	4	5.74
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	13	5.74
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	1	5.73
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H29	4	5.72
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H29	17	5.71
(1,1832)	1:7:A:ILE:HD13	2:201:A:UJ2:H28	18	5.66
(1,1832)	1:7:A:ILE:HD12	2:201:A:UJ2:H28	16	5.65
(1,1832)	1:7:A:ILE:HD11	2:201:A:UJ2:H28	19	5.64
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H29	1	5.6
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H29	1	5.57
(1,748)	1:66:A:LYS:HE3	2:201:A:UJ2:H28	5	5.54
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	20	5.48
(1,748)	1:66:A:LYS:HE2	2:201:A:UJ2:H28	6	5.48
(1,1832)	1:7:A:ILE:HD11	2:201:A:UJ2:H28	9	5.41
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	10	5.4
(1,1849)	1:62:A:MET:HB3	2:201:A:UJ2:H28	15	5.39
(1,1835)	1:62:A:MET:HE3	2:201:A:UJ2:H28	12	5.39
(1,1835)	1:62:A:MET:HE1	2:201:A:UJ2:H28	20	5.38
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	12	5.37
(1,1868)	1:4:A:LEU:HD13	2:201:A:UJ2:H29	6	5.31
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	5	5.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,748)	1:66:A:LYS:HE2	2:201:A:UJ2:H28	11	5.28
(1,1849)	1:62:A:MET:HB3	2:201:A:UJ2:H29	17	5.27
(1,748)	1:66:A:LYS:HE2	2:201:A:UJ2:H28	7	5.26
(1,1835)	1:62:A:MET:HE3	2:201:A:UJ2:H28	10	5.25
(1,1868)	1:4:A:LEU:HD11	2:201:A:UJ2:H28	16	5.24
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	3	5.24
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	14	5.22
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	18	5.18
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H29	4	5.17
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	13	5.17
(1,748)	1:66:A:LYS:HE3	2:201:A:UJ2:H28	8	5.17
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	1	5.16
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	11	5.12
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	19	5.08
(1,748)	1:66:A:LYS:HE3	2:201:A:UJ2:H28	18	5.08
(1,748)	1:66:A:LYS:HE2	2:201:A:UJ2:H28	2	5.07
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	7	5.03
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	2	5.0
(1,1835)	1:62:A:MET:HE3	2:201:A:UJ2:H28	15	4.99
(1,1868)	1:4:A:LEU:HD12	2:201:A:UJ2:H29	19	4.98
(1,748)	1:66:A:LYS:HE2	2:201:A:UJ2:H28	16	4.96
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	8	4.95
(1,748)	1:66:A:LYS:HE3	2:201:A:UJ2:H28	9	4.93
(1,1835)	1:62:A:MET:HE2	2:201:A:UJ2:H28	17	4.9
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	6	4.89
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	16	4.85
(1,1835)	1:62:A:MET:HE2	2:201:A:UJ2:H28	19	4.82
(1,1835)	1:62:A:MET:HE3	2:201:A:UJ2:H28	1	4.8
(1,1835)	1:62:A:MET:HE1	2:201:A:UJ2:H28	4	4.76
(1,1835)	1:62:A:MET:HE2	2:201:A:UJ2:H28	14	4.72
(1,1835)	1:62:A:MET:HE3	2:201:A:UJ2:H28	18	4.72
(1,1868)	1:4:A:LEU:HD13	2:201:A:UJ2:H29	9	4.69
(1,1835)	1:62:A:MET:HE3	2:201:A:UJ2:H28	3	4.67
(1,1835)	1:62:A:MET:HE3	2:201:A:UJ2:H28	13	4.67
(1,748)	1:66:A:LYS:HE2	2:201:A:UJ2:H28	19	4.63
(1,1868)	1:4:A:LEU:HD13	2:201:A:UJ2:H29	5	4.58
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	2	4.54
(1,1868)	1:4:A:LEU:HD13	2:201:A:UJ2:H29	11	4.53
(1,1868)	1:4:A:LEU:HD13	2:201:A:UJ2:H29	7	4.51
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	19	4.51
(1,1835)	1:62:A:MET:HE3	2:201:A:UJ2:H28	16	4.48
(1,1835)	1:62:A:MET:HE2	2:201:A:UJ2:H28	7	4.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	16	4.39
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H28	19	4.35
(1,2208)	1:62:A:MET:HB3	2:201:A:UJ2:H28	18	4.33
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H28	5	4.32
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	19	4.29
(1,1835)	1:62:A:MET:HE3	2:201:A:UJ2:H28	8	4.27
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	7	4.23
(1,1868)	1:4:A:LEU:HD21	2:201:A:UJ2:H28	2	4.23
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H28	18	4.2
(1,1835)	1:62:A:MET:HE2	2:201:A:UJ2:H28	2	4.19
(1,1835)	1:62:A:MET:HE3	2:201:A:UJ2:H28	6	4.18
(1,2223)	1:66:A:LYS:HD2	2:201:A:UJ2:H28	9	4.11
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H28	8	4.05
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	6	4.03
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	11	4.02
(1,1835)	1:62:A:MET:HE2	2:201:A:UJ2:H28	9	4.02
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H28	11	3.99
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	2	3.97
(1,1835)	1:62:A:MET:HE3	2:201:A:UJ2:H28	11	3.95
(1,2208)	1:62:A:MET:HB2	2:201:A:UJ2:H28	5	3.92
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H28	18	3.87
(1,1868)	1:4:A:LEU:HD12	2:201:A:UJ2:H29	8	3.83
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	16	3.82
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H28	16	3.79
(1,1849)	1:62:A:MET:HB3	2:201:A:UJ2:H28	18	3.76
(1,1835)	1:62:A:MET:HE3	2:201:A:UJ2:H28	5	3.74
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H29	20	3.74
(1,2208)	1:62:A:MET:HB3	2:201:A:UJ2:H28	8	3.72
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H28	5	3.69
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	7	3.66
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H28	8	3.66
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H28	7	3.65
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H28	11	3.65
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H29	20	3.64
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H28	7	3.59
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H28	19	3.57
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H29	13	3.55
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H28	2	3.54
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	6	3.46
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	11	3.45
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H28	16	3.45
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H28	6	3.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H28	2	3.41
(1,1868)	1:4:A:LEU:HD11	2:201:A:UJ2:H29	18	3.4
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H28	6	3.4
(1,1849)	1:62:A:MET:HB2	2:201:A:UJ2:H28	5	3.35
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H29	12	3.3
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H29	12	3.29
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H29	13	3.27
(1,2208)	1:62:A:MET:HB3	2:201:A:UJ2:H28	9	3.21
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H29	15	3.2
(1,1849)	1:62:A:MET:HB3	2:201:A:UJ2:H28	8	3.15
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H29	3	3.14
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H29	10	3.12
(1,1708)	1:63:A:ASN:HA	2:201:A:UJ2:H28	9	3.08
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H29	15	3.08
(1,2191)	1:58:A:LEU:HD13	2:201:A:UJ2:H28	16	3.07
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H29	10	3.03
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H29	3	3.02
(1,285)	1:63:A:ASN:H	2:201:A:UJ2:H28	9	2.99
(1,2191)	1:58:A:LEU:HD11	2:201:A:UJ2:H29	3	2.94
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H29	14	2.91
(1,2191)	1:58:A:LEU:HD13	2:201:A:UJ2:H28	7	2.88
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H29	17	2.85
(1,2191)	1:58:A:LEU:HD12	2:201:A:UJ2:H29	12	2.84
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H29	14	2.81
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H29	17	2.81
(1,2191)	1:58:A:LEU:HD21	2:201:A:UJ2:H28	13	2.8
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H29	4	2.79
(1,1868)	1:4:A:LEU:HD12	2:201:A:UJ2:H28	4	2.75
(1,2191)	1:58:A:LEU:HD22	2:201:A:UJ2:H28	1	2.73
(1,2191)	1:58:A:LEU:HD12	2:201:A:UJ2:H29	10	2.73
(1,2191)	1:58:A:LEU:HD11	2:201:A:UJ2:H29	15	2.71
(1,1165)	1:3:A:ASN:HB3	2:201:A:UJ2:H28	2	2.7
(1,2191)	1:58:A:LEU:HD11	2:201:A:UJ2:H29	14	2.69
(1,1868)	1:4:A:LEU:HD13	2:201:A:UJ2:H28	17	2.66
(1,1849)	1:62:A:MET:HB3	2:201:A:UJ2:H28	9	2.64
(1,2191)	1:58:A:LEU:HD23	2:201:A:UJ2:H29	17	2.6
(1,2191)	1:58:A:LEU:HD13	2:201:A:UJ2:H29	20	2.58
(1,1165)	1:3:A:ASN:HB3	2:201:A:UJ2:H28	5	2.55
(1,2191)	1:58:A:LEU:HD12	2:201:A:UJ2:H29	4	2.54
(1,2191)	1:58:A:LEU:HD12	2:201:A:UJ2:H28	18	2.5
(1,1868)	1:4:A:LEU:HD12	2:201:A:UJ2:H28	15	2.46
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H29	4	2.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1868)	1:4:A:LEU:HD22	2:201:A:UJ2:H28	12	2.45
(1,1868)	1:4:A:LEU:HD23	2:201:A:UJ2:H28	10	2.42
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H29	1	2.41
(1,1165)	1:3:A:ASN:HB3	2:201:A:UJ2:H28	11	2.38
(1,1868)	1:4:A:LEU:HD23	2:201:A:UJ2:H28	14	2.36
(1,814)	1:59:A:THR:HG22	2:201:A:UJ2:H28	12	2.36
(1,814)	1:59:A:THR:HG21	2:201:A:UJ2:H28	20	2.33
(1,2191)	1:58:A:LEU:HD21	2:201:A:UJ2:H28	6	2.29
(1,2191)	1:58:A:LEU:HD13	2:201:A:UJ2:H28	9	2.29
(1,1165)	1:3:A:ASN:HB3	2:201:A:UJ2:H28	6	2.29
(1,814)	1:59:A:THR:HG23	2:201:A:UJ2:H28	4	2.29
(1,814)	1:59:A:THR:HG22	2:201:A:UJ2:H28	10	2.28
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	7	2.27
(1,814)	1:59:A:THR:HG22	2:201:A:UJ2:H28	15	2.27
(1,814)	1:59:A:THR:HG23	2:201:A:UJ2:H28	3	2.26
(1,814)	1:59:A:THR:HG22	2:201:A:UJ2:H28	14	2.21
(1,2191)	1:58:A:LEU:HD11	2:201:A:UJ2:H28	11	2.2
(1,1868)	1:4:A:LEU:HD12	2:201:A:UJ2:H28	1	2.17
(1,814)	1:59:A:THR:HG21	2:201:A:UJ2:H28	13	2.14
(1,2191)	1:58:A:LEU:HD12	2:201:A:UJ2:H28	2	2.1
(1,814)	1:59:A:THR:HG22	2:201:A:UJ2:H28	17	2.1
(1,814)	1:59:A:THR:HG22	2:201:A:UJ2:H28	1	2.09
(1,1165)	1:3:A:ASN:HB3	2:201:A:UJ2:H28	9	2.0
(1,1868)	1:4:A:LEU:HD11	2:201:A:UJ2:H28	13	1.95
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H29	1	1.89
(1,814)	1:59:A:THR:HG21	2:201:A:UJ2:H28	18	1.87
(1,814)	1:59:A:THR:HG23	2:201:A:UJ2:H28	16	1.81
(1,2191)	1:58:A:LEU:HD12	2:201:A:UJ2:H28	5	1.8
(1,1868)	1:4:A:LEU:HD11	2:201:A:UJ2:H28	3	1.78
(1,814)	1:59:A:THR:HG23	2:201:A:UJ2:H28	6	1.78
(1,1055)	1:42:A:LEU:HG	2:201:A:UJ2:H34	4	1.77
(1,1847)	1:42:A:LEU:HD12	2:201:A:UJ2:H39	5	1.75
(1,814)	1:59:A:THR:HG22	2:201:A:UJ2:H28	7	1.74
(1,1847)	1:42:A:LEU:HD11	2:201:A:UJ2:H39	11	1.73
(1,814)	1:59:A:THR:HG21	2:201:A:UJ2:H28	9	1.71
(1,814)	1:59:A:THR:HG23	2:201:A:UJ2:H28	11	1.68
(1,1868)	1:4:A:LEU:HD13	2:201:A:UJ2:H28	20	1.66
(1,2191)	1:58:A:LEU:HD12	2:201:A:UJ2:H28	8	1.62
(1,1637)	1:42:A:LEU:HD22	2:201:A:UJ2:H39	14	1.61
(1,814)	1:59:A:THR:HG22	2:201:A:UJ2:H28	2	1.61
(1,1637)	1:42:A:LEU:HD21	2:201:A:UJ2:H39	15	1.6
(1,1637)	1:42:A:LEU:HD22	2:201:A:UJ2:H39	10	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1637)	1:42:A:LEU:HD23	2:201:A:UJ2:H39	19	1.58
(1,1165)	1:3:A:ASN:HB3	2:201:A:UJ2:H28	16	1.57
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	8	1.54
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	18	1.53
(1,2191)	1:58:A:LEU:HD22	2:201:A:UJ2:H29	19	1.51
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	14	1.47
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	17	1.47
(1,1637)	1:42:A:LEU:HD22	2:201:A:UJ2:H39	7	1.44
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H28	19	1.39
(1,814)	1:59:A:THR:HG22	2:201:A:UJ2:H28	5	1.37
(1,814)	1:59:A:THR:HG22	2:201:A:UJ2:H28	8	1.31
(1,814)	1:59:A:THR:HG22	2:201:A:UJ2:H29	19	1.31
(1,1842)	1:45:A:LEU:HD13	2:201:A:UJ2:H34	10	1.26
(1,1842)	1:45:A:LEU:HD12	2:201:A:UJ2:H34	14	1.22
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	20	1.2
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	19	1.15
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	10	1.14
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H28	18	1.14
(1,1842)	1:45:A:LEU:HD11	2:201:A:UJ2:H39	15	1.12
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H28	8	1.1
(1,1055)	1:42:A:LEU:HG	2:201:A:UJ2:H34	19	1.05
(1,1658)	1:7:A:ILE:HG22	2:201:A:UJ2:H34	19	0.97
(1,1842)	1:45:A:LEU:HD11	2:201:A:UJ2:H39	5	0.92
(1,1848)	1:116:A:LEU:HD13	2:201:A:UJ2:H38	7	0.91
(1,1836)	1:122:A:MET:HE1	2:201:A:UJ2:H39	7	0.91
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H28	8	0.83
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	12	0.81
(1,1848)	1:116:A:LEU:HD12	2:201:A:UJ2:H35	9	0.79
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	15	0.79
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	1	0.74
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	4	0.71
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	3	0.7
(1,1848)	1:116:A:LEU:HD11	2:201:A:UJ2:H37	17	0.67
(1,1842)	1:45:A:LEU:HD13	2:201:A:UJ2:H39	11	0.66
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H28	18	0.65
(1,1658)	1:7:A:ILE:HG21	2:201:A:UJ2:H34	7	0.64
(1,1848)	1:116:A:LEU:HD11	2:201:A:UJ2:H38	1	0.63
(1,1165)	1:3:A:ASN:HB2	2:201:A:UJ2:H28	13	0.62
(1,1842)	1:45:A:LEU:HD12	2:201:A:UJ2:H34	19	0.6
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H28	5	0.59
(1,1842)	1:45:A:LEU:HD12	2:201:A:UJ2:H39	7	0.57
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H28	5	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1658)	1:7:A:ILE:HG23	2:201:A:UJ2:H37	13	0.56
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H28	6	0.55
(1,1836)	1:122:A:MET:HE1	2:201:A:UJ2:H39	18	0.54
(1,1842)	1:45:A:LEU:HD13	2:201:A:UJ2:H39	4	0.53
(1,1658)	1:7:A:ILE:HG23	2:201:A:UJ2:H37	1	0.53
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H28	11	0.48
(1,2493)	1:134:A:ALA:HB1	1:138:A:GLN:HG2	16	0.45
(1,2493)	1:134:A:ALA:HB1	1:138:A:GLN:HG3	16	0.45
(1,2493)	1:134:A:ALA:HB2	1:138:A:GLN:HG2	16	0.45
(1,2493)	1:134:A:ALA:HB2	1:138:A:GLN:HG3	16	0.45
(1,2493)	1:134:A:ALA:HB3	1:138:A:GLN:HG2	16	0.45
(1,2493)	1:134:A:ALA:HB3	1:138:A:GLN:HG3	16	0.45
(1,1848)	1:116:A:LEU:HD13	2:201:A:UJ2:H37	6	0.45
(1,1658)	1:7:A:ILE:HG21	2:201:A:UJ2:H37	6	0.45
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H28	16	0.45
(1,1836)	1:122:A:MET:HE3	2:201:A:UJ2:H39	9	0.42
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H28	11	0.42
(1,2493)	1:134:A:ALA:HB1	1:138:A:GLN:HG2	9	0.41
(1,2493)	1:134:A:ALA:HB1	1:138:A:GLN:HG3	9	0.41
(1,2493)	1:134:A:ALA:HB2	1:138:A:GLN:HG2	9	0.41
(1,2493)	1:134:A:ALA:HB2	1:138:A:GLN:HG3	9	0.41
(1,2493)	1:134:A:ALA:HB3	1:138:A:GLN:HG2	9	0.41
(1,2493)	1:134:A:ALA:HB3	1:138:A:GLN:HG3	9	0.41
(1,1055)	1:42:A:LEU:HG	2:201:A:UJ2:H34	7	0.41
(1,1839)	1:59:A:THR:HG22	2:201:A:UJ2:H28	12	0.4
(1,1847)	1:42:A:LEU:HD12	2:201:A:UJ2:H38	16	0.39
(1,1836)	1:122:A:MET:HE1	2:201:A:UJ2:H38	3	0.39
(1,1848)	1:116:A:LEU:HD13	2:201:A:UJ2:H39	19	0.38
(1,1847)	1:42:A:LEU:HD11	2:201:A:UJ2:H38	1	0.38
(1,1847)	1:42:A:LEU:HD12	2:201:A:UJ2:H34	4	0.38
(1,1658)	1:7:A:ILE:HG22	2:201:A:UJ2:H37	17	0.38
(1,1839)	1:59:A:THR:HG21	2:201:A:UJ2:H28	20	0.37
(1,1836)	1:122:A:MET:HE3	2:201:A:UJ2:H39	10	0.37
(1,1658)	1:7:A:ILE:HG23	2:201:A:UJ2:H37	9	0.37
(1,1836)	1:122:A:MET:HE3	2:201:A:UJ2:H39	5	0.35
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	15	0.35
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	15	0.35
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	15	0.35
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	16	0.35
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	16	0.35
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	16	0.35
(1,289)	1:63:A:ASN:HD21	2:201:A:UJ2:H28	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1848)	1:116:A:LEU:HD11	2:201:A:UJ2:H39	18	0.34
(1,1637)	1:42:A:LEU:HD23	2:201:A:UJ2:H38	3	0.34
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	17	0.34
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	17	0.34
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	17	0.34
(1,642)	1:153:A:ARG:HA	1:154:A:ASP:H	15	0.34
(1,292)	1:63:A:ASN:HD22	2:201:A:UJ2:H28	19	0.34
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB1	17	0.33
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB2	17	0.33
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB3	17	0.33
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB1	17	0.33
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB2	17	0.33
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB3	17	0.33
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB1	17	0.33
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB2	17	0.33
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB3	17	0.33
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB1	17	0.33
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB2	17	0.33
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB3	17	0.33
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB1	17	0.33
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB2	17	0.33
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB3	17	0.33
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB1	17	0.33
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB2	17	0.33
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB3	17	0.33
(1,1839)	1:59:A:THR:HG23	2:201:A:UJ2:H28	4	0.33
(1,1836)	1:122:A:MET:HE1	2:201:A:UJ2:H39	16	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	1	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	1	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	1	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	2	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	2	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	2	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	4	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	4	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	4	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	5	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	5	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	5	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	7	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	7	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	8	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	8	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	8	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	10	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	10	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	10	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	13	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	13	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	13	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	19	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	19	0.33
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	19	0.33
(1,986)	1:36:A:LEU:HA	1:36:A:LEU:HD21	3	0.33
(1,986)	1:36:A:LEU:HA	1:36:A:LEU:HD22	3	0.33
(1,986)	1:36:A:LEU:HA	1:36:A:LEU:HD23	3	0.33
(1,642)	1:153:A:ARG:HA	1:154:A:ASP:H	17	0.33
(1,1839)	1:59:A:THR:HG22	2:201:A:UJ2:H28	10	0.32
(1,1836)	1:122:A:MET:HE3	2:201:A:UJ2:H39	11	0.32
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	9	0.32
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	9	0.32
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	9	0.32
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	11	0.32
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	11	0.32
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	11	0.32
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	14	0.32
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	14	0.32
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	14	0.32
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG21	18	0.32
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG22	18	0.32
(1,1021)	1:36:A:LEU:HG	1:39:A:ILE:HG23	18	0.32
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD11	19	0.31
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD12	19	0.31
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD13	19	0.31
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD21	19	0.31
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD22	19	0.31
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD23	19	0.31
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB1	13	0.31
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB2	13	0.31
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB3	13	0.31
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB1	13	0.31
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB2	13	0.31
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB3	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB1	13	0.31
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB2	13	0.31
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB3	13	0.31
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB1	13	0.31
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB2	13	0.31
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB3	13	0.31
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB1	13	0.31
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB2	13	0.31
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB3	13	0.31
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB1	13	0.31
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB2	13	0.31
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB3	13	0.31
(1,2178)	1:58:A:LEU:HB2	1:116:A:LEU:HD11	16	0.31
(1,2178)	1:58:A:LEU:HB2	1:116:A:LEU:HD12	16	0.31
(1,2178)	1:58:A:LEU:HB2	1:116:A:LEU:HD13	16	0.31
(1,2178)	1:58:A:LEU:HB2	1:116:A:LEU:HD21	16	0.31
(1,2178)	1:58:A:LEU:HB2	1:116:A:LEU:HD22	16	0.31
(1,2178)	1:58:A:LEU:HB2	1:116:A:LEU:HD23	16	0.31
(1,1839)	1:59:A:THR:HG22	2:201:A:UJ2:H28	15	0.31
(1,248)	1:53:A:VAL:H	1:53:A:VAL:HB	1	0.31
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD11	15	0.3
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD12	15	0.3
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD13	15	0.3
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD21	15	0.3
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD22	15	0.3
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD23	15	0.3
(1,1839)	1:59:A:THR:HG23	2:201:A:UJ2:H28	3	0.3
(1,1836)	1:122:A:MET:HE1	2:201:A:UJ2:H39	2	0.3
(1,1055)	1:42:A:LEU:HG	2:201:A:UJ2:H34	10	0.3
(1,755)	1:50:A:LYS:HA	1:50:A:LYS:HG3	10	0.3
(1,719)	1:114:A:LEU:HA	1:114:A:LEU:HG	4	0.3
(1,2250)	1:75:A:GLU:H	1:75:A:GLU:HG2	6	0.29
(1,2250)	1:75:A:GLU:H	1:75:A:GLU:HG3	6	0.29
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD11	10	0.29
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD12	10	0.29
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD13	10	0.29
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD21	10	0.29
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD22	10	0.29
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD23	10	0.29
(1,719)	1:114:A:LEU:HA	1:114:A:LEU:HG	10	0.29
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB1	6	0.28
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB2	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB3	6	0.28
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB1	6	0.28
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB2	6	0.28
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB3	6	0.28
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB1	6	0.28
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB2	6	0.28
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB3	6	0.28
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB1	6	0.28
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB2	6	0.28
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB3	6	0.28
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB1	6	0.28
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB2	6	0.28
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB3	6	0.28
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB1	6	0.28
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB2	6	0.28
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB3	6	0.28
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	7	0.27
(1,1055)	1:42:A:LEU:HG	2:201:A:UJ2:H34	14	0.27
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	16	0.26
(1,1847)	1:42:A:LEU:HD12	2:201:A:UJ2:H38	12	0.25
(1,1839)	1:59:A:THR:HG22	2:201:A:UJ2:H28	14	0.25
(1,1836)	1:122:A:MET:HE1	2:201:A:UJ2:H39	4	0.25
(1,2505)	1:139:A:GLN:H	1:139:A:GLN:HG2	6	0.24
(1,2505)	1:139:A:GLN:H	1:139:A:GLN:HG3	6	0.24
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	13	0.24
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	13	0.24
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	13	0.24
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	13	0.24
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	13	0.24
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	13	0.24
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	13	0.24
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	13	0.24
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	13	0.24
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	13	0.24
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	13	0.24
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	13	0.24
(1,1847)	1:42:A:LEU:HD13	2:201:A:UJ2:H37	17	0.24
(1,1836)	1:122:A:MET:HE3	2:201:A:UJ2:H39	12	0.24
(1,1836)	1:122:A:MET:HE2	2:201:A:UJ2:H39	14	0.24
(1,1637)	1:42:A:LEU:HD21	2:201:A:UJ2:H38	2	0.24
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	13	0.24
(1,2392)	1:107:A:ASP:HA	1:110:A:LYS:HG2	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2392)	1:107:A:ASP:HA	1:110:A:LYS:HG3	13	0.23
(1,2392)	1:107:A:ASP:HA	1:110:A:LYS:HG2	19	0.23
(1,2392)	1:107:A:ASP:HA	1:110:A:LYS:HG3	19	0.23
(1,1881)	1:7:A:ILE:HA	1:10:A:LEU:HD11	6	0.23
(1,1881)	1:7:A:ILE:HA	1:10:A:LEU:HD12	6	0.23
(1,1881)	1:7:A:ILE:HA	1:10:A:LEU:HD13	6	0.23
(1,1881)	1:7:A:ILE:HA	1:10:A:LEU:HD21	6	0.23
(1,1881)	1:7:A:ILE:HA	1:10:A:LEU:HD22	6	0.23
(1,1881)	1:7:A:ILE:HA	1:10:A:LEU:HD23	6	0.23
(1,1836)	1:122:A:MET:HE2	2:201:A:UJ2:H39	19	0.23
(1,1582)	1:10:A:LEU:HG	1:69:A:LEU:HD21	11	0.23
(1,1582)	1:10:A:LEU:HG	1:69:A:LEU:HD22	11	0.23
(1,1582)	1:10:A:LEU:HG	1:69:A:LEU:HD23	11	0.23
(1,2182)	1:58:A:LEU:HD11	1:61:A:ALA:H	19	0.22
(1,2182)	1:58:A:LEU:HD12	1:61:A:ALA:H	19	0.22
(1,2182)	1:58:A:LEU:HD13	1:61:A:ALA:H	19	0.22
(1,2182)	1:58:A:LEU:HD21	1:61:A:ALA:H	19	0.22
(1,2182)	1:58:A:LEU:HD22	1:61:A:ALA:H	19	0.22
(1,2182)	1:58:A:LEU:HD23	1:61:A:ALA:H	19	0.22
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE1	7	0.22
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE2	7	0.22
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE3	7	0.22
(1,2347)	1:99:A:LYS:HD2	1:100:A:ASP:HA	5	0.21
(1,2347)	1:99:A:LYS:HD3	1:100:A:ASP:HA	5	0.21
(1,2347)	1:99:A:LYS:HD2	1:100:A:ASP:HA	10	0.21
(1,2347)	1:99:A:LYS:HD3	1:100:A:ASP:HA	10	0.21
(1,2347)	1:99:A:LYS:HD2	1:100:A:ASP:HA	12	0.21
(1,2347)	1:99:A:LYS:HD3	1:100:A:ASP:HA	12	0.21
(1,2182)	1:58:A:LEU:HD11	1:61:A:ALA:H	17	0.21
(1,2182)	1:58:A:LEU:HD12	1:61:A:ALA:H	17	0.21
(1,2182)	1:58:A:LEU:HD13	1:61:A:ALA:H	17	0.21
(1,2182)	1:58:A:LEU:HD21	1:61:A:ALA:H	17	0.21
(1,2182)	1:58:A:LEU:HD22	1:61:A:ALA:H	17	0.21
(1,2182)	1:58:A:LEU:HD23	1:61:A:ALA:H	17	0.21
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG2	2	0.21
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG3	2	0.21
(1,1848)	1:116:A:LEU:HD12	2:201:A:UJ2:H39	3	0.21
(1,279)	1:61:A:ALA:H	1:115:A:LEU:HG	7	0.21
(1,2435)	1:115:A:LEU:HA	1:115:A:LEU:HD11	4	0.2
(1,2435)	1:115:A:LEU:HA	1:115:A:LEU:HD12	4	0.2
(1,2435)	1:115:A:LEU:HA	1:115:A:LEU:HD13	4	0.2
(1,2435)	1:115:A:LEU:HA	1:115:A:LEU:HD21	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2435)	1:115:A:LEU:HA	1:115:A:LEU:HD22	4	0.2
(1,2435)	1:115:A:LEU:HA	1:115:A:LEU:HD23	4	0.2
(1,2347)	1:99:A:LYS:HD2	1:100:A:ASP:HA	3	0.2
(1,2347)	1:99:A:LYS:HD3	1:100:A:ASP:HA	3	0.2
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB1	1	0.2
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB2	1	0.2
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB3	1	0.2
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB1	1	0.2
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB2	1	0.2
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB3	1	0.2
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB1	1	0.2
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB2	1	0.2
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB3	1	0.2
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB1	1	0.2
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB2	1	0.2
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB3	1	0.2
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB1	1	0.2
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB2	1	0.2
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB3	1	0.2
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB1	1	0.2
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB2	1	0.2
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB3	1	0.2
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG11	3	0.2
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG12	3	0.2
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG13	3	0.2
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG21	3	0.2
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG22	3	0.2
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG23	3	0.2
(1,279)	1:61:A:ALA:H	1:115:A:LEU:HG	4	0.2
(1,2347)	1:99:A:LYS:HD2	1:100:A:ASP:HA	19	0.19
(1,2347)	1:99:A:LYS:HD3	1:100:A:ASP:HA	19	0.19
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB1	19	0.19
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB2	19	0.19
(1,2183)	1:58:A:LEU:HD11	1:61:A:ALA:HB3	19	0.19
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB1	19	0.19
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB2	19	0.19
(1,2183)	1:58:A:LEU:HD12	1:61:A:ALA:HB3	19	0.19
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB1	19	0.19
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB2	19	0.19
(1,2183)	1:58:A:LEU:HD13	1:61:A:ALA:HB3	19	0.19
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB1	19	0.19
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB2	19	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2183)	1:58:A:LEU:HD21	1:61:A:ALA:HB3	19	0.19
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB1	19	0.19
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB2	19	0.19
(1,2183)	1:58:A:LEU:HD22	1:61:A:ALA:HB3	19	0.19
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB1	19	0.19
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB2	19	0.19
(1,2183)	1:58:A:LEU:HD23	1:61:A:ALA:HB3	19	0.19
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD1	8	0.19
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD2	8	0.19
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD1	8	0.19
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD2	8	0.19
(1,1637)	1:42:A:LEU:HD22	2:201:A:UJ2:H39	4	0.19
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	2	0.19
(1,926)	1:22:A:LYS:HA	1:22:A:LYS:HG3	2	0.19
(1,926)	1:22:A:LYS:HA	1:22:A:LYS:HG3	3	0.19
(1,926)	1:22:A:LYS:HA	1:22:A:LYS:HG3	5	0.19
(1,926)	1:22:A:LYS:HA	1:22:A:LYS:HG3	9	0.19
(1,517)	1:112:A:LEU:HG	1:113:A:SER:H	20	0.19
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	4	0.18
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	4	0.18
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	4	0.18
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	4	0.18
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	4	0.18
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	4	0.18
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	4	0.18
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	4	0.18
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	4	0.18
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	4	0.18
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	4	0.18
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	4	0.18
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG2	6	0.18
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG3	6	0.18
(1,1839)	1:59:A:THR:HG21	2:201:A:UJ2:H28	13	0.18
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD11	10	0.18
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD12	10	0.18
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD13	10	0.18
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD11	10	0.18
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD12	10	0.18
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD13	10	0.18
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD11	10	0.18
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD12	10	0.18
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD13	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	11	0.18
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	6	0.18
(1,926)	1:22:A:LYS:HA	1:22:A:LYS:HG3	15	0.18
(1,279)	1:61:A:ALA:H	1:115:A:LEU:HG	17	0.18
(1,2182)	1:58:A:LEU:HD11	1:61:A:ALA:H	1	0.17
(1,2182)	1:58:A:LEU:HD12	1:61:A:ALA:H	1	0.17
(1,2182)	1:58:A:LEU:HD13	1:61:A:ALA:H	1	0.17
(1,2182)	1:58:A:LEU:HD21	1:61:A:ALA:H	1	0.17
(1,2182)	1:58:A:LEU:HD22	1:61:A:ALA:H	1	0.17
(1,2182)	1:58:A:LEU:HD23	1:61:A:ALA:H	1	0.17
(1,2182)	1:58:A:LEU:HD11	1:61:A:ALA:H	13	0.17
(1,2182)	1:58:A:LEU:HD12	1:61:A:ALA:H	13	0.17
(1,2182)	1:58:A:LEU:HD13	1:61:A:ALA:H	13	0.17
(1,2182)	1:58:A:LEU:HD21	1:61:A:ALA:H	13	0.17
(1,2182)	1:58:A:LEU:HD22	1:61:A:ALA:H	13	0.17
(1,2182)	1:58:A:LEU:HD23	1:61:A:ALA:H	13	0.17
(1,2160)	1:56:A:GLU:HG2	1:59:A:THR:HB	2	0.17
(1,2160)	1:56:A:GLU:HG3	1:59:A:THR:HB	2	0.17
(1,2160)	1:56:A:GLU:HG2	1:59:A:THR:HB	16	0.17
(1,2160)	1:56:A:GLU:HG3	1:59:A:THR:HB	16	0.17
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	9	0.17
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	9	0.17
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	9	0.17
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	9	0.17
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	9	0.17
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	9	0.17
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	9	0.17
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	9	0.17
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	9	0.17
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	9	0.17
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	9	0.17
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	9	0.17
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG2	16	0.17
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG3	16	0.17
(1,2083)	1:36:A:LEU:HD11	1:39:A:ILE:HG12	3	0.17
(1,2083)	1:36:A:LEU:HD12	1:39:A:ILE:HG12	3	0.17
(1,2083)	1:36:A:LEU:HD13	1:39:A:ILE:HG12	3	0.17
(1,2083)	1:36:A:LEU:HD21	1:39:A:ILE:HG12	3	0.17
(1,2083)	1:36:A:LEU:HD22	1:39:A:ILE:HG12	3	0.17
(1,2083)	1:36:A:LEU:HD23	1:39:A:ILE:HG12	3	0.17
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD11	6	0.17
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD12	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD13	6	0.17
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD21	6	0.17
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD22	6	0.17
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD23	6	0.17
(1,2064)	1:31:A:LEU:HD11	1:105:A:LEU:HD11	15	0.17
(1,2064)	1:31:A:LEU:HD11	1:105:A:LEU:HD12	15	0.17
(1,2064)	1:31:A:LEU:HD11	1:105:A:LEU:HD13	15	0.17
(1,2064)	1:31:A:LEU:HD11	1:105:A:LEU:HD21	15	0.17
(1,2064)	1:31:A:LEU:HD11	1:105:A:LEU:HD22	15	0.17
(1,2064)	1:31:A:LEU:HD11	1:105:A:LEU:HD23	15	0.17
(1,2064)	1:31:A:LEU:HD12	1:105:A:LEU:HD11	15	0.17
(1,2064)	1:31:A:LEU:HD12	1:105:A:LEU:HD12	15	0.17
(1,2064)	1:31:A:LEU:HD12	1:105:A:LEU:HD13	15	0.17
(1,2064)	1:31:A:LEU:HD12	1:105:A:LEU:HD21	15	0.17
(1,2064)	1:31:A:LEU:HD12	1:105:A:LEU:HD22	15	0.17
(1,2064)	1:31:A:LEU:HD12	1:105:A:LEU:HD23	15	0.17
(1,2064)	1:31:A:LEU:HD13	1:105:A:LEU:HD11	15	0.17
(1,2064)	1:31:A:LEU:HD13	1:105:A:LEU:HD12	15	0.17
(1,2064)	1:31:A:LEU:HD13	1:105:A:LEU:HD13	15	0.17
(1,2064)	1:31:A:LEU:HD13	1:105:A:LEU:HD21	15	0.17
(1,2064)	1:31:A:LEU:HD13	1:105:A:LEU:HD22	15	0.17
(1,2064)	1:31:A:LEU:HD13	1:105:A:LEU:HD23	15	0.17
(1,2064)	1:31:A:LEU:HD21	1:105:A:LEU:HD11	15	0.17
(1,2064)	1:31:A:LEU:HD21	1:105:A:LEU:HD12	15	0.17
(1,2064)	1:31:A:LEU:HD21	1:105:A:LEU:HD13	15	0.17
(1,2064)	1:31:A:LEU:HD21	1:105:A:LEU:HD21	15	0.17
(1,2064)	1:31:A:LEU:HD21	1:105:A:LEU:HD22	15	0.17
(1,2064)	1:31:A:LEU:HD21	1:105:A:LEU:HD23	15	0.17
(1,2064)	1:31:A:LEU:HD22	1:105:A:LEU:HD11	15	0.17
(1,2064)	1:31:A:LEU:HD22	1:105:A:LEU:HD12	15	0.17
(1,2064)	1:31:A:LEU:HD22	1:105:A:LEU:HD13	15	0.17
(1,2064)	1:31:A:LEU:HD22	1:105:A:LEU:HD21	15	0.17
(1,2064)	1:31:A:LEU:HD22	1:105:A:LEU:HD22	15	0.17
(1,2064)	1:31:A:LEU:HD22	1:105:A:LEU:HD23	15	0.17
(1,2064)	1:31:A:LEU:HD23	1:105:A:LEU:HD11	15	0.17
(1,2064)	1:31:A:LEU:HD23	1:105:A:LEU:HD12	15	0.17
(1,2064)	1:31:A:LEU:HD23	1:105:A:LEU:HD13	15	0.17
(1,2064)	1:31:A:LEU:HD23	1:105:A:LEU:HD21	15	0.17
(1,2064)	1:31:A:LEU:HD23	1:105:A:LEU:HD22	15	0.17
(1,2064)	1:31:A:LEU:HD23	1:105:A:LEU:HD23	15	0.17
(1,1658)	1:7:A:ILE:HG22	2:201:A:UJ2:H34	5	0.17
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG2	7	0.17
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG3	7	0.17
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE1	13	0.17
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE2	13	0.17
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE3	13	0.17
(1,548)	1:123:A:PRO:HB2	1:124:A:VAL:H	12	0.17
(1,2160)	1:56:A:GLU:HG2	1:59:A:THR:HB	7	0.16
(1,2160)	1:56:A:GLU:HG3	1:59:A:THR:HB	7	0.16
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	17	0.16
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	17	0.16
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	17	0.16
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	17	0.16
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	17	0.16
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	17	0.16
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	17	0.16
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	17	0.16
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	17	0.16
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	17	0.16
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	17	0.16
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	17	0.16
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG2	9	0.16
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG3	9	0.16
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG2	13	0.16
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG3	13	0.16
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD11	20	0.16
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD12	20	0.16
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD13	20	0.16
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD21	20	0.16
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD22	20	0.16
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD23	20	0.16
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD1	4	0.16
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD2	4	0.16
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD1	4	0.16
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD2	4	0.16
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD1	11	0.16
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD2	11	0.16
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD1	11	0.16
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD2	11	0.16
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD1	16	0.16
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD2	16	0.16
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD1	16	0.16
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD2	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD1	20	0.16
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD2	20	0.16
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD1	20	0.16
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD2	20	0.16
(1,1658)	1:7:A:ILE:HG22	2:201:A:UJ2:H34	3	0.16
(1,1593)	1:131:A:ALA:HB1	1:132:A:SER:HA	13	0.16
(1,1593)	1:131:A:ALA:HB2	1:132:A:SER:HA	13	0.16
(1,1593)	1:131:A:ALA:HB3	1:132:A:SER:HA	13	0.16
(1,1347)	1:45:A:LEU:HD21	1:122:A:MET:HA	17	0.16
(1,1347)	1:45:A:LEU:HD22	1:122:A:MET:HA	17	0.16
(1,1347)	1:45:A:LEU:HD23	1:122:A:MET:HA	17	0.16
(1,1266)	1:78:A:LYS:HB2	1:78:A:LYS:HE3	9	0.16
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD11	18	0.16
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD12	18	0.16
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD13	18	0.16
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD11	18	0.16
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD12	18	0.16
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD13	18	0.16
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD11	18	0.16
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD12	18	0.16
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD13	18	0.16
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD21	1	0.16
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD22	1	0.16
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD23	1	0.16
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	6	0.16
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	15	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG2	1	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG3	1	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG2	4	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG3	4	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG2	9	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG3	9	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG2	12	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG3	12	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG2	17	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG3	17	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG2	18	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG3	18	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG2	20	0.16
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG3	20	0.16
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	7	0.16
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	17	0.16
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	19	0.16
(1,803)	1:8:A:ILE:HG21	1:46:A:GLN:HG2	14	0.16
(1,803)	1:8:A:ILE:HG21	1:46:A:GLN:HG3	14	0.16
(1,803)	1:8:A:ILE:HG22	1:46:A:GLN:HG2	14	0.16
(1,803)	1:8:A:ILE:HG22	1:46:A:GLN:HG3	14	0.16
(1,803)	1:8:A:ILE:HG23	1:46:A:GLN:HG2	14	0.16
(1,803)	1:8:A:ILE:HG23	1:46:A:GLN:HG3	14	0.16
(1,638)	1:151:A:LEU:HA	1:152:A:ARG:H	1	0.16
(1,638)	1:151:A:LEU:HA	1:152:A:ARG:H	6	0.16
(1,638)	1:151:A:LEU:HA	1:152:A:ARG:H	8	0.16
(1,638)	1:151:A:LEU:HA	1:152:A:ARG:H	11	0.16
(1,638)	1:151:A:LEU:HA	1:152:A:ARG:H	12	0.16
(1,638)	1:151:A:LEU:HA	1:152:A:ARG:H	17	0.16
(1,535)	1:116:A:LEU:HB3	1:118:A:VAL:H	20	0.16
(1,248)	1:53:A:VAL:H	1:53:A:VAL:HB	19	0.16
(1,2182)	1:58:A:LEU:HD11	1:61:A:ALA:H	6	0.15
(1,2182)	1:58:A:LEU:HD12	1:61:A:ALA:H	6	0.15
(1,2182)	1:58:A:LEU:HD13	1:61:A:ALA:H	6	0.15
(1,2182)	1:58:A:LEU:HD21	1:61:A:ALA:H	6	0.15
(1,2182)	1:58:A:LEU:HD22	1:61:A:ALA:H	6	0.15
(1,2182)	1:58:A:LEU:HD23	1:61:A:ALA:H	6	0.15
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD11	19	0.15
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD12	19	0.15
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD13	19	0.15
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD21	19	0.15
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD22	19	0.15
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD23	19	0.15
(1,2160)	1:56:A:GLU:HG2	1:59:A:THR:HB	18	0.15
(1,2160)	1:56:A:GLU:HG3	1:59:A:THR:HB	18	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	2	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	2	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	2	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	2	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	2	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	2	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	2	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	2	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	2	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	2	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	2	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	3	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	3	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	3	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	3	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	3	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	3	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	3	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	3	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	3	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	3	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	3	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	3	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	10	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	10	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	10	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	10	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	10	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	10	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	10	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	10	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	10	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	10	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	10	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	10	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	14	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	14	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	14	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	14	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	14	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	14	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	14	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	14	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	14	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	14	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	14	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	14	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	18	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	18	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	18	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	18	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	18	0.15
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	18	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	18	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	18	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	18	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	18	0.15
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	18	0.15
(1,2148)	1:52:A:SER:HB2	1:53:A:VAL:HB	18	0.15
(1,2148)	1:52:A:SER:HB3	1:53:A:VAL:HB	18	0.15
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG11	11	0.15
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG12	11	0.15
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG13	11	0.15
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG21	11	0.15
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG22	11	0.15
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG23	11	0.15
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD1	10	0.15
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD2	10	0.15
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD1	10	0.15
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD2	10	0.15
(1,1852)	1:2:A:GLU:H	1:2:A:GLU:HG2	17	0.15
(1,1852)	1:2:A:GLU:H	1:2:A:GLU:HG3	17	0.15
(1,1789)	1:106:A:SER:HA	1:109:A:TRP:HD1	7	0.15
(1,1593)	1:131:A:ALA:HB1	1:132:A:SER:HA	18	0.15
(1,1593)	1:131:A:ALA:HB2	1:132:A:SER:HA	18	0.15
(1,1593)	1:131:A:ALA:HB3	1:132:A:SER:HA	18	0.15
(1,1574)	1:126:A:PRO:HG2	1:127:A:ILE:HD11	10	0.15
(1,1574)	1:126:A:PRO:HG2	1:127:A:ILE:HD12	10	0.15
(1,1574)	1:126:A:PRO:HG2	1:127:A:ILE:HD13	10	0.15
(1,1574)	1:126:A:PRO:HG3	1:127:A:ILE:HD11	10	0.15
(1,1574)	1:126:A:PRO:HG3	1:127:A:ILE:HD12	10	0.15
(1,1574)	1:126:A:PRO:HG3	1:127:A:ILE:HD13	10	0.15
(1,1495)	1:112:A:LEU:HD11	1:113:A:SER:HB3	7	0.15
(1,1495)	1:112:A:LEU:HD12	1:113:A:SER:HB3	7	0.15
(1,1495)	1:112:A:LEU:HD13	1:113:A:SER:HB3	7	0.15
(1,1448)	1:108:A:VAL:HB	1:112:A:LEU:HB3	20	0.15
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD11	9	0.15
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD12	9	0.15
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD13	9	0.15
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD11	9	0.15
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD12	9	0.15
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD13	9	0.15
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD11	9	0.15
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD12	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD13	9	0.15
(1,1177)	1:24:A:CYS:H	1:25:A:LYS:HE2	20	0.15
(1,1177)	1:24:A:CYS:H	1:25:A:LYS:HE3	20	0.15
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD21	16	0.15
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD22	16	0.15
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD23	16	0.15
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	3	0.15
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	9	0.15
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	12	0.15
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	17	0.15
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG2	19	0.15
(1,1080)	1:46:A:GLN:HA	1:46:A:GLN:HG3	19	0.15
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	2	0.15
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	15	0.15
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG11	6	0.15
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG12	6	0.15
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG13	6	0.15
(1,721)	1:62:A:MET:HB3	1:112:A:LEU:HD21	7	0.15
(1,721)	1:62:A:MET:HB3	1:112:A:LEU:HD22	7	0.15
(1,721)	1:62:A:MET:HB3	1:112:A:LEU:HD23	7	0.15
(1,548)	1:123:A:PRO:HB2	1:124:A:VAL:H	14	0.15
(1,535)	1:116:A:LEU:HB3	1:118:A:VAL:H	5	0.15
(1,153)	1:32:A:GLY:H	1:35:A:VAL:HB	18	0.15
(1,2468)	1:122:A:MET:HB2	1:124:A:VAL:HA	10	0.14
(1,2468)	1:122:A:MET:HB3	1:124:A:VAL:HA	10	0.14
(1,2450)	1:117:A:GLN:HA	1:122:A:MET:HB2	7	0.14
(1,2450)	1:117:A:GLN:HA	1:122:A:MET:HB3	7	0.14
(1,2450)	1:117:A:GLN:HA	1:122:A:MET:HB2	17	0.14
(1,2450)	1:117:A:GLN:HA	1:122:A:MET:HB3	17	0.14
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD11	6	0.14
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD12	6	0.14
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD13	6	0.14
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD21	6	0.14
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD22	6	0.14
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD23	6	0.14
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD11	13	0.14
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD12	13	0.14
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD13	13	0.14
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD21	13	0.14
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD22	13	0.14
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD23	13	0.14
(1,2160)	1:56:A:GLU:HG2	1:59:A:THR:HB	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2160)	1:56:A:GLU:HG3	1:59:A:THR:HB	11	0.14
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	5	0.14
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	5	0.14
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	5	0.14
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	5	0.14
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	5	0.14
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	5	0.14
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	5	0.14
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	5	0.14
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	5	0.14
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	5	0.14
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	5	0.14
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	5	0.14
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD1	13	0.14
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD2	13	0.14
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD1	13	0.14
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD2	13	0.14
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD1	19	0.14
(1,1999)	1:22:A:LYS:HG2	1:23:A:TYR:HD2	19	0.14
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD1	19	0.14
(1,1999)	1:22:A:LYS:HG3	1:23:A:TYR:HD2	19	0.14
(1,1996)	1:22:A:LYS:HB2	1:23:A:TYR:HE1	5	0.14
(1,1996)	1:22:A:LYS:HB2	1:23:A:TYR:HE2	5	0.14
(1,1996)	1:22:A:LYS:HB3	1:23:A:TYR:HE1	5	0.14
(1,1996)	1:22:A:LYS:HB3	1:23:A:TYR:HE2	5	0.14
(1,1936)	1:13:A:VAL:HG21	1:17:A:ARG:HD2	15	0.14
(1,1936)	1:13:A:VAL:HG21	1:17:A:ARG:HD3	15	0.14
(1,1936)	1:13:A:VAL:HG22	1:17:A:ARG:HD2	15	0.14
(1,1936)	1:13:A:VAL:HG22	1:17:A:ARG:HD3	15	0.14
(1,1936)	1:13:A:VAL:HG23	1:17:A:ARG:HD2	15	0.14
(1,1936)	1:13:A:VAL:HG23	1:17:A:ARG:HD3	15	0.14
(1,1874)	1:5:A:LYS:HG2	1:6:A:HIS:H	12	0.14
(1,1874)	1:5:A:LYS:HG3	1:6:A:HIS:H	12	0.14
(1,1839)	1:59:A:THR:HG22	2:201:A:UJ2:H28	17	0.14
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	20	0.14
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	20	0.14
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	20	0.14
(1,1658)	1:7:A:ILE:HG22	2:201:A:UJ2:H34	14	0.14
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD11	6	0.14
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD12	6	0.14
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD13	6	0.14
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD11	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD12	6	0.14
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD13	6	0.14
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD11	6	0.14
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD12	6	0.14
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD13	6	0.14
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD21	7	0.14
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD22	7	0.14
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD23	7	0.14
(1,1061)	1:7:A:ILE:HB	1:39:A:ILE:HA	19	0.14
(1,1051)	1:42:A:LEU:HA	1:42:A:LEU:HD11	6	0.14
(1,1051)	1:42:A:LEU:HA	1:42:A:LEU:HD12	6	0.14
(1,1051)	1:42:A:LEU:HA	1:42:A:LEU:HD13	6	0.14
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	9	0.14
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG11	12	0.14
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG12	12	0.14
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG13	12	0.14
(1,812)	1:59:A:THR:HG21	1:62:A:MET:HE1	17	0.14
(1,812)	1:59:A:THR:HG21	1:62:A:MET:HE2	17	0.14
(1,812)	1:59:A:THR:HG21	1:62:A:MET:HE3	17	0.14
(1,812)	1:59:A:THR:HG22	1:62:A:MET:HE1	17	0.14
(1,812)	1:59:A:THR:HG22	1:62:A:MET:HE2	17	0.14
(1,812)	1:59:A:THR:HG22	1:62:A:MET:HE3	17	0.14
(1,812)	1:59:A:THR:HG23	1:62:A:MET:HE1	17	0.14
(1,812)	1:59:A:THR:HG23	1:62:A:MET:HE2	17	0.14
(1,812)	1:59:A:THR:HG23	1:62:A:MET:HE3	17	0.14
(1,535)	1:116:A:LEU:HB3	1:118:A:VAL:H	12	0.14
(1,279)	1:61:A:ALA:H	1:115:A:LEU:HG	2	0.14
(1,279)	1:61:A:ALA:H	1:115:A:LEU:HG	12	0.14
(1,227)	1:8:A:ILE:HD11	1:44:A:MET:H	17	0.14
(1,227)	1:8:A:ILE:HD12	1:44:A:MET:H	17	0.14
(1,227)	1:8:A:ILE:HD13	1:44:A:MET:H	17	0.14
(1,2495)	1:136:A:GLU:HG2	1:137:A:ASP:HB2	17	0.13
(1,2495)	1:136:A:GLU:HG2	1:137:A:ASP:HB3	17	0.13
(1,2495)	1:136:A:GLU:HG3	1:137:A:ASP:HB2	17	0.13
(1,2495)	1:136:A:GLU:HG3	1:137:A:ASP:HB3	17	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD11	1	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD12	1	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD13	1	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD21	1	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD22	1	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD23	1	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD11	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD12	19	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD13	19	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD21	19	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD22	19	0.13
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD23	19	0.13
(1,2160)	1:56:A:GLU:HG2	1:59:A:THR:HB	9	0.13
(1,2160)	1:56:A:GLU:HG3	1:59:A:THR:HB	9	0.13
(1,2160)	1:56:A:GLU:HG2	1:59:A:THR:HB	13	0.13
(1,2160)	1:56:A:GLU:HG3	1:59:A:THR:HB	13	0.13
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	6	0.13
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	6	0.13
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	6	0.13
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	6	0.13
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	6	0.13
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	6	0.13
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	6	0.13
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	6	0.13
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	6	0.13
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	6	0.13
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	6	0.13
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	6	0.13
(1,2148)	1:52:A:SER:HB2	1:53:A:VAL:HB	3	0.13
(1,2148)	1:52:A:SER:HB3	1:53:A:VAL:HB	3	0.13
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG11	8	0.13
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG12	8	0.13
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG13	8	0.13
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG21	8	0.13
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG22	8	0.13
(1,2146)	1:52:A:SER:HA	1:53:A:VAL:HG23	8	0.13
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG2	15	0.13
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG3	15	0.13
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD11	12	0.13
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD12	12	0.13
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD13	12	0.13
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD21	12	0.13
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD22	12	0.13
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD23	12	0.13
(1,1839)	1:59:A:THR:HG22	2:201:A:UJ2:H28	1	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	5	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	5	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	5	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	6	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	6	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	8	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	8	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	8	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	12	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	12	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	12	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	18	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	18	0.13
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	18	0.13
(1,1593)	1:131:A:ALA:HB1	1:132:A:SER:HA	7	0.13
(1,1593)	1:131:A:ALA:HB2	1:132:A:SER:HA	7	0.13
(1,1593)	1:131:A:ALA:HB3	1:132:A:SER:HA	7	0.13
(1,1545)	1:109:A:TRP:HZ3	1:122:A:MET:HE1	17	0.13
(1,1545)	1:109:A:TRP:HZ3	1:122:A:MET:HE2	17	0.13
(1,1545)	1:109:A:TRP:HZ3	1:122:A:MET:HE3	17	0.13
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD11	3	0.13
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD12	3	0.13
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD13	3	0.13
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD11	3	0.13
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD12	3	0.13
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD13	3	0.13
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD11	3	0.13
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD12	3	0.13
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD13	3	0.13
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD11	13	0.13
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD12	13	0.13
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD13	13	0.13
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD11	13	0.13
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD12	13	0.13
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD13	13	0.13
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD11	13	0.13
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD12	13	0.13
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD13	13	0.13
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	5	0.13
(1,1131)	1:56:A:GLU:HB3	1:59:A:THR:HB	14	0.13
(1,1124)	1:58:A:LEU:HB2	1:116:A:LEU:HG	16	0.13
(1,1051)	1:42:A:LEU:HA	1:42:A:LEU:HD11	4	0.13
(1,1051)	1:42:A:LEU:HA	1:42:A:LEU:HD12	4	0.13
(1,1051)	1:42:A:LEU:HA	1:42:A:LEU:HD13	4	0.13
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:62:A:MET:HB3	1:112:A:LEU:HD21	16	0.13
(1,721)	1:62:A:MET:HB3	1:112:A:LEU:HD22	16	0.13
(1,721)	1:62:A:MET:HB3	1:112:A:LEU:HD23	16	0.13
(1,660)	1:133:A:TRP:HE3	1:134:A:ALA:H	7	0.13
(1,153)	1:32:A:GLY:H	1:35:A:VAL:HB	7	0.13
(1,2507)	1:139:A:GLN:HA	1:139:A:GLN:HG2	6	0.12
(1,2507)	1:139:A:GLN:HA	1:139:A:GLN:HG3	6	0.12
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD11	17	0.12
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD12	17	0.12
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD13	17	0.12
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD21	17	0.12
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD22	17	0.12
(1,2174)	1:58:A:LEU:HA	1:58:A:LEU:HD23	17	0.12
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD11	4	0.12
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD12	4	0.12
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD13	4	0.12
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD21	4	0.12
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD22	4	0.12
(1,2164)	1:57:A:LYS:H	1:115:A:LEU:HD23	4	0.12
(1,2160)	1:56:A:GLU:HG2	1:59:A:THR:HB	3	0.12
(1,2160)	1:56:A:GLU:HG3	1:59:A:THR:HB	3	0.12
(1,2160)	1:56:A:GLU:HG2	1:59:A:THR:HB	15	0.12
(1,2160)	1:56:A:GLU:HG3	1:59:A:THR:HB	15	0.12
(1,2154)	1:55:A:SER:H	1:58:A:LEU:HD11	7	0.12
(1,2154)	1:55:A:SER:H	1:58:A:LEU:HD12	7	0.12
(1,2154)	1:55:A:SER:H	1:58:A:LEU:HD13	7	0.12
(1,2154)	1:55:A:SER:H	1:58:A:LEU:HD21	7	0.12
(1,2154)	1:55:A:SER:H	1:58:A:LEU:HD22	7	0.12
(1,2154)	1:55:A:SER:H	1:58:A:LEU:HD23	7	0.12
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	11	0.12
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	11	0.12
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	11	0.12
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	11	0.12
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	11	0.12
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	11	0.12
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	11	0.12
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	11	0.12
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	11	0.12
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	11	0.12
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	11	0.12
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	11	0.12
(1,2148)	1:52:A:SER:HB2	1:53:A:VAL:HB	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2148)	1:52:A:SER:HB3	1:53:A:VAL:HB	11	0.12
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG2	10	0.12
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG3	10	0.12
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG2	12	0.12
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG3	12	0.12
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG2	14	0.12
(1,2143)	1:51:A:ARG:HA	1:51:A:ARG:HG3	14	0.12
(1,2098)	1:39:A:ILE:HA	1:69:A:LEU:HD11	11	0.12
(1,2098)	1:39:A:ILE:HA	1:69:A:LEU:HD12	11	0.12
(1,2098)	1:39:A:ILE:HA	1:69:A:LEU:HD13	11	0.12
(1,2098)	1:39:A:ILE:HA	1:69:A:LEU:HD21	11	0.12
(1,2098)	1:39:A:ILE:HA	1:69:A:LEU:HD22	11	0.12
(1,2098)	1:39:A:ILE:HA	1:69:A:LEU:HD23	11	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD11	2	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD12	2	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD13	2	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD21	2	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD22	2	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD23	2	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD11	6	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD12	6	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD13	6	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD21	6	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD22	6	0.12
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD23	6	0.12
(1,2083)	1:36:A:LEU:HD11	1:39:A:ILE:HG12	6	0.12
(1,2083)	1:36:A:LEU:HD12	1:39:A:ILE:HG12	6	0.12
(1,2083)	1:36:A:LEU:HD13	1:39:A:ILE:HG12	6	0.12
(1,2083)	1:36:A:LEU:HD21	1:39:A:ILE:HG12	6	0.12
(1,2083)	1:36:A:LEU:HD22	1:39:A:ILE:HG12	6	0.12
(1,2083)	1:36:A:LEU:HD23	1:39:A:ILE:HG12	6	0.12
(1,2083)	1:36:A:LEU:HD11	1:39:A:ILE:HG12	12	0.12
(1,2083)	1:36:A:LEU:HD12	1:39:A:ILE:HG12	12	0.12
(1,2083)	1:36:A:LEU:HD13	1:39:A:ILE:HG12	12	0.12
(1,2083)	1:36:A:LEU:HD21	1:39:A:ILE:HG12	12	0.12
(1,2083)	1:36:A:LEU:HD22	1:39:A:ILE:HG12	12	0.12
(1,2083)	1:36:A:LEU:HD23	1:39:A:ILE:HG12	12	0.12
(1,2083)	1:36:A:LEU:HD11	1:39:A:ILE:HG12	20	0.12
(1,2083)	1:36:A:LEU:HD12	1:39:A:ILE:HG12	20	0.12
(1,2083)	1:36:A:LEU:HD13	1:39:A:ILE:HG12	20	0.12
(1,2083)	1:36:A:LEU:HD21	1:39:A:ILE:HG12	20	0.12
(1,2083)	1:36:A:LEU:HD22	1:39:A:ILE:HG12	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2083)	1:36:A:LEU:HD23	1:39:A:ILE:HG12	20	0.12
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD11	3	0.12
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD12	3	0.12
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD13	3	0.12
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD21	3	0.12
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD22	3	0.12
(1,2074)	1:35:A:VAL:HB	1:36:A:LEU:HD23	3	0.12
(1,1874)	1:5:A:LYS:HG2	1:6:A:HIS:H	18	0.12
(1,1874)	1:5:A:LYS:HG3	1:6:A:HIS:H	18	0.12
(1,1813)	1:15:A:HIS:HE1	1:16:A:LYS:HD2	7	0.12
(1,1813)	1:15:A:HIS:HE1	1:16:A:LYS:HD3	7	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	1	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	1	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	1	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	2	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	2	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	2	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	13	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	13	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	13	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	14	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	14	0.12
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	14	0.12
(1,1678)	1:37:A:GLY:HA3	1:38:A:LEU:HB2	18	0.12
(1,1658)	1:7:A:ILE:HG23	2:201:A:UJ2:H34	2	0.12
(1,1658)	1:7:A:ILE:HG23	2:201:A:UJ2:H34	16	0.12
(1,1592)	1:129:A:GLN:HG2	1:133:A:TRP:HZ2	18	0.12
(1,1592)	1:129:A:GLN:HG3	1:133:A:TRP:HZ2	18	0.12
(1,1545)	1:109:A:TRP:HZ3	1:122:A:MET:HE1	18	0.12
(1,1545)	1:109:A:TRP:HZ3	1:122:A:MET:HE2	18	0.12
(1,1545)	1:109:A:TRP:HZ3	1:122:A:MET:HE3	18	0.12
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD11	19	0.12
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD12	19	0.12
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD13	19	0.12
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD11	19	0.12
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD12	19	0.12
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD13	19	0.12
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD11	19	0.12
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD12	19	0.12
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD13	19	0.12
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD11	20	0.12
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD12	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD13	20	0.12
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD11	20	0.12
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD12	20	0.12
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD13	20	0.12
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD11	20	0.12
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD12	20	0.12
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD13	20	0.12
(1,1177)	1:24:A:CYS:H	1:25:A:LYS:HE2	13	0.12
(1,1177)	1:24:A:CYS:H	1:25:A:LYS:HE3	13	0.12
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD21	6	0.12
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD22	6	0.12
(1,1150)	1:61:A:ALA:HA	1:112:A:LEU:HD23	6	0.12
(1,1135)	1:60:A:THR:HA	1:64:A:ARG:HD2	11	0.12
(1,1135)	1:60:A:THR:HA	1:64:A:ARG:HD3	11	0.12
(1,1051)	1:42:A:LEU:HA	1:42:A:LEU:HD11	17	0.12
(1,1051)	1:42:A:LEU:HA	1:42:A:LEU:HD12	17	0.12
(1,1051)	1:42:A:LEU:HA	1:42:A:LEU:HD13	17	0.12
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	4	0.12
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	5	0.12
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	10	0.12
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	13	0.12
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG11	15	0.12
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG12	15	0.12
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG13	15	0.12
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG11	20	0.12
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG12	20	0.12
(1,969)	1:32:A:GLY:H	1:35:A:VAL:HG13	20	0.12
(1,928)	1:22:A:LYS:HD2	1:23:A:TYR:HA	5	0.12
(1,928)	1:22:A:LYS:HD3	1:23:A:TYR:HA	5	0.12
(1,834)	1:9:A:THR:HA	1:13:A:VAL:HA	8	0.12
(1,834)	1:9:A:THR:HA	1:13:A:VAL:HA	20	0.12
(1,660)	1:133:A:TRP:HE3	1:134:A:ALA:H	17	0.12
(1,548)	1:123:A:PRO:HB2	1:124:A:VAL:H	3	0.12
(1,548)	1:123:A:PRO:HB2	1:124:A:VAL:H	4	0.12
(1,548)	1:123:A:PRO:HB2	1:124:A:VAL:H	7	0.12
(1,535)	1:116:A:LEU:HB3	1:118:A:VAL:H	8	0.12
(1,279)	1:61:A:ALA:H	1:115:A:LEU:HG	1	0.12
(1,279)	1:61:A:ALA:H	1:115:A:LEU:HG	16	0.12
(1,153)	1:32:A:GLY:H	1:35:A:VAL:HB	1	0.12
(1,2495)	1:136:A:GLU:HG2	1:137:A:ASP:HB2	7	0.11
(1,2495)	1:136:A:GLU:HG2	1:137:A:ASP:HB3	7	0.11
(1,2495)	1:136:A:GLU:HG3	1:137:A:ASP:HB2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2495)	1:136:A:GLU:HG3	1:137:A:ASP:HB3	7	0.11
(1,2495)	1:136:A:GLU:HG2	1:137:A:ASP:HB2	16	0.11
(1,2495)	1:136:A:GLU:HG2	1:137:A:ASP:HB3	16	0.11
(1,2495)	1:136:A:GLU:HG3	1:137:A:ASP:HB2	16	0.11
(1,2495)	1:136:A:GLU:HG3	1:137:A:ASP:HB3	16	0.11
(1,2364)	1:103:A:ARG:HA	1:106:A:SER:HB2	10	0.11
(1,2364)	1:103:A:ARG:HA	1:106:A:SER:HB3	10	0.11
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD11	6	0.11
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD12	6	0.11
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD13	6	0.11
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD21	6	0.11
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD22	6	0.11
(1,2233)	1:69:A:LEU:HG	1:105:A:LEU:HD23	6	0.11
(1,2195)	1:61:A:ALA:H	1:112:A:LEU:HD11	16	0.11
(1,2195)	1:61:A:ALA:H	1:112:A:LEU:HD12	16	0.11
(1,2195)	1:61:A:ALA:H	1:112:A:LEU:HD13	16	0.11
(1,2195)	1:61:A:ALA:H	1:112:A:LEU:HD21	16	0.11
(1,2195)	1:61:A:ALA:H	1:112:A:LEU:HD22	16	0.11
(1,2195)	1:61:A:ALA:H	1:112:A:LEU:HD23	16	0.11
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD11	2	0.11
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD12	2	0.11
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD13	2	0.11
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD21	2	0.11
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD22	2	0.11
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD23	2	0.11
(1,2160)	1:56:A:GLU:HG2	1:59:A:THR:HB	5	0.11
(1,2160)	1:56:A:GLU:HG3	1:59:A:THR:HB	5	0.11
(1,2160)	1:56:A:GLU:HG2	1:59:A:THR:HB	12	0.11
(1,2160)	1:56:A:GLU:HG3	1:59:A:THR:HB	12	0.11
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD11	8	0.11
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD12	8	0.11
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD13	8	0.11
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD21	8	0.11
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD22	8	0.11
(1,2153)	1:54:A:PRO:HB2	1:58:A:LEU:HD23	8	0.11
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD11	8	0.11
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD12	8	0.11
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD13	8	0.11
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD21	8	0.11
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD22	8	0.11
(1,2153)	1:54:A:PRO:HB3	1:58:A:LEU:HD23	8	0.11
(1,2148)	1:52:A:SER:HB2	1:53:A:VAL:HB	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2148)	1:52:A:SER:HB3	1:53:A:VAL:HB	17	0.11
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD11	19	0.11
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD12	19	0.11
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD13	19	0.11
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD21	19	0.11
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD22	19	0.11
(1,2089)	1:38:A:LEU:H	1:42:A:LEU:HD23	19	0.11
(1,2023)	1:26:A:LYS:H	1:26:A:LYS:HG2	2	0.11
(1,2023)	1:26:A:LYS:H	1:26:A:LYS:HG3	2	0.11
(1,2023)	1:26:A:LYS:H	1:26:A:LYS:HG2	3	0.11
(1,2023)	1:26:A:LYS:H	1:26:A:LYS:HG3	3	0.11
(1,1936)	1:13:A:VAL:HG21	1:17:A:ARG:HD2	16	0.11
(1,1936)	1:13:A:VAL:HG21	1:17:A:ARG:HD3	16	0.11
(1,1936)	1:13:A:VAL:HG22	1:17:A:ARG:HD2	16	0.11
(1,1936)	1:13:A:VAL:HG22	1:17:A:ARG:HD3	16	0.11
(1,1936)	1:13:A:VAL:HG23	1:17:A:ARG:HD2	16	0.11
(1,1936)	1:13:A:VAL:HG23	1:17:A:ARG:HD3	16	0.11
(1,1909)	1:10:A:LEU:HD11	1:66:A:LYS:HA	6	0.11
(1,1909)	1:10:A:LEU:HD12	1:66:A:LYS:HA	6	0.11
(1,1909)	1:10:A:LEU:HD13	1:66:A:LYS:HA	6	0.11
(1,1909)	1:10:A:LEU:HD21	1:66:A:LYS:HA	6	0.11
(1,1909)	1:10:A:LEU:HD22	1:66:A:LYS:HA	6	0.11
(1,1909)	1:10:A:LEU:HD23	1:66:A:LYS:HA	6	0.11
(1,1813)	1:15:A:HIS:HE1	1:16:A:LYS:HD2	15	0.11
(1,1813)	1:15:A:HIS:HE1	1:16:A:LYS:HD3	15	0.11
(1,1789)	1:106:A:SER:HA	1:109:A:TRP:HD1	13	0.11
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	9	0.11
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	9	0.11
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	9	0.11
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	11	0.11
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	11	0.11
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	11	0.11
(1,1658)	1:7:A:ILE:HG21	2:201:A:UJ2:H34	10	0.11
(1,1658)	1:7:A:ILE:HG23	2:201:A:UJ2:H34	12	0.11
(1,1384)	1:101:A:VAL:HG11	1:105:A:LEU:HG	10	0.11
(1,1384)	1:101:A:VAL:HG12	1:105:A:LEU:HG	10	0.11
(1,1384)	1:101:A:VAL:HG13	1:105:A:LEU:HG	10	0.11
(1,1347)	1:45:A:LEU:HD21	1:122:A:MET:HA	7	0.11
(1,1347)	1:45:A:LEU:HD22	1:122:A:MET:HA	7	0.11
(1,1347)	1:45:A:LEU:HD23	1:122:A:MET:HA	7	0.11
(1,1347)	1:45:A:LEU:HD21	1:122:A:MET:HA	18	0.11
(1,1347)	1:45:A:LEU:HD22	1:122:A:MET:HA	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1347)	1:45:A:LEU:HD23	1:122:A:MET:HA	18	0.11
(1,1189)	1:68:A:ALA:HB1	1:70:A:GLU:H	13	0.11
(1,1189)	1:68:A:ALA:HB2	1:70:A:GLU:H	13	0.11
(1,1189)	1:68:A:ALA:HB3	1:70:A:GLU:H	13	0.11
(1,1189)	1:68:A:ALA:HB1	1:70:A:GLU:H	14	0.11
(1,1189)	1:68:A:ALA:HB2	1:70:A:GLU:H	14	0.11
(1,1189)	1:68:A:ALA:HB3	1:70:A:GLU:H	14	0.11
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD11	17	0.11
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD12	17	0.11
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD13	17	0.11
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD11	17	0.11
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD12	17	0.11
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD13	17	0.11
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD11	17	0.11
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD12	17	0.11
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD13	17	0.11
(1,1177)	1:24:A:CYS:H	1:25:A:LYS:HE2	5	0.11
(1,1177)	1:24:A:CYS:H	1:25:A:LYS:HE3	5	0.11
(1,1154)	1:125:A:SER:HA	1:126:A:PRO:HB2	18	0.11
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	1	0.11
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	11	0.11
(1,976)	1:15:A:HIS:HD2	1:36:A:LEU:HB2	12	0.11
(1,892)	1:15:A:HIS:HD2	1:19:A:GLU:HG2	12	0.11
(1,892)	1:15:A:HIS:HD2	1:19:A:GLU:HG3	12	0.11
(1,877)	1:15:A:HIS:HB2	1:19:A:GLU:HG2	15	0.11
(1,877)	1:15:A:HIS:HB2	1:19:A:GLU:HG3	15	0.11
(1,877)	1:15:A:HIS:HB3	1:19:A:GLU:HG2	15	0.11
(1,877)	1:15:A:HIS:HB3	1:19:A:GLU:HG3	15	0.11
(1,834)	1:9:A:THR:HA	1:13:A:VAL:HA	1	0.11
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG21	7	0.11
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG22	7	0.11
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG23	7	0.11
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG21	11	0.11
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG22	11	0.11
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG23	11	0.11
(1,752)	1:23:A:TYR:HD1	1:25:A:LYS:HE2	7	0.11
(1,752)	1:23:A:TYR:HD1	1:25:A:LYS:HE3	7	0.11
(1,752)	1:23:A:TYR:HD2	1:25:A:LYS:HE2	7	0.11
(1,752)	1:23:A:TYR:HD2	1:25:A:LYS:HE3	7	0.11
(1,660)	1:133:A:TRP:HE3	1:134:A:ALA:H	6	0.11
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE1	17	0.11
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE2	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE3	17	0.11
(1,550)	1:124:A:VAL:H	1:124:A:VAL:HB	2	0.11
(1,279)	1:61:A:ALA:H	1:115:A:LEU:HG	6	0.11
(1,227)	1:8:A:ILE:HD11	1:44:A:MET:H	6	0.11
(1,227)	1:8:A:ILE:HD12	1:44:A:MET:H	6	0.11
(1,227)	1:8:A:ILE:HD13	1:44:A:MET:H	6	0.11
(1,227)	1:8:A:ILE:HD11	1:44:A:MET:H	15	0.11
(1,227)	1:8:A:ILE:HD12	1:44:A:MET:H	15	0.11
(1,227)	1:8:A:ILE:HD13	1:44:A:MET:H	15	0.11
(1,153)	1:32:A:GLY:H	1:35:A:VAL:HB	5	0.11
(1,139)	1:56:A:GLU:HB3	1:60:A:THR:H	2	0.11
(1,139)	1:56:A:GLU:HB3	1:60:A:THR:H	4	0.11
(1,2423)	1:113:A:SER:HB3	1:116:A:LEU:HD11	11	0.1
(1,2423)	1:113:A:SER:HB3	1:116:A:LEU:HD12	11	0.1
(1,2423)	1:113:A:SER:HB3	1:116:A:LEU:HD13	11	0.1
(1,2423)	1:113:A:SER:HB3	1:116:A:LEU:HD21	11	0.1
(1,2423)	1:113:A:SER:HB3	1:116:A:LEU:HD22	11	0.1
(1,2423)	1:113:A:SER:HB3	1:116:A:LEU:HD23	11	0.1
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD11	12	0.1
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD12	12	0.1
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD13	12	0.1
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD21	12	0.1
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD22	12	0.1
(1,2177)	1:58:A:LEU:HB2	1:115:A:LEU:HD23	12	0.1
(1,2160)	1:56:A:GLU:HG2	1:59:A:THR:HB	14	0.1
(1,2160)	1:56:A:GLU:HG3	1:59:A:THR:HB	14	0.1
(1,1874)	1:5:A:LYS:HG2	1:6:A:HIS:H	7	0.1
(1,1874)	1:5:A:LYS:HG3	1:6:A:HIS:H	7	0.1
(1,1813)	1:15:A:HIS:HE1	1:16:A:LYS:HD2	17	0.1
(1,1813)	1:15:A:HIS:HE1	1:16:A:LYS:HD3	17	0.1
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	4	0.1
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	4	0.1
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	4	0.1
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD11	7	0.1
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD12	7	0.1
(1,1685)	1:36:A:LEU:HA	1:39:A:ILE:HD13	7	0.1
(1,1636)	1:151:A:LEU:HA	1:151:A:LEU:HD11	3	0.1
(1,1636)	1:151:A:LEU:HA	1:151:A:LEU:HD12	3	0.1
(1,1636)	1:151:A:LEU:HA	1:151:A:LEU:HD13	3	0.1
(1,1582)	1:10:A:LEU:HG	1:69:A:LEU:HD21	6	0.1
(1,1582)	1:10:A:LEU:HG	1:69:A:LEU:HD22	6	0.1
(1,1582)	1:10:A:LEU:HG	1:69:A:LEU:HD23	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1281)	1:23:A:TYR:HE1	1:85:A:ILE:HD11	12	0.1
(1,1281)	1:23:A:TYR:HE1	1:85:A:ILE:HD12	12	0.1
(1,1281)	1:23:A:TYR:HE1	1:85:A:ILE:HD13	12	0.1
(1,1281)	1:23:A:TYR:HE2	1:85:A:ILE:HD11	12	0.1
(1,1281)	1:23:A:TYR:HE2	1:85:A:ILE:HD12	12	0.1
(1,1281)	1:23:A:TYR:HE2	1:85:A:ILE:HD13	12	0.1
(1,1189)	1:68:A:ALA:HB1	1:70:A:GLU:H	2	0.1
(1,1189)	1:68:A:ALA:HB2	1:70:A:GLU:H	2	0.1
(1,1189)	1:68:A:ALA:HB3	1:70:A:GLU:H	2	0.1
(1,1189)	1:68:A:ALA:HB1	1:70:A:GLU:H	7	0.1
(1,1189)	1:68:A:ALA:HB2	1:70:A:GLU:H	7	0.1
(1,1189)	1:68:A:ALA:HB3	1:70:A:GLU:H	7	0.1
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD11	5	0.1
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD12	5	0.1
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD13	5	0.1
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD11	5	0.1
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD12	5	0.1
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD13	5	0.1
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD11	5	0.1
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD12	5	0.1
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD13	5	0.1
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD11	16	0.1
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD12	16	0.1
(1,1180)	1:68:A:ALA:HB1	1:105:A:LEU:HD13	16	0.1
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD11	16	0.1
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD12	16	0.1
(1,1180)	1:68:A:ALA:HB2	1:105:A:LEU:HD13	16	0.1
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD11	16	0.1
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD12	16	0.1
(1,1180)	1:68:A:ALA:HB3	1:105:A:LEU:HD13	16	0.1
(1,897)	1:21:A:MET:HE1	1:22:A:LYS:HD2	13	0.1
(1,897)	1:21:A:MET:HE1	1:22:A:LYS:HD3	13	0.1
(1,897)	1:21:A:MET:HE2	1:22:A:LYS:HD2	13	0.1
(1,897)	1:21:A:MET:HE2	1:22:A:LYS:HD3	13	0.1
(1,897)	1:21:A:MET:HE3	1:22:A:LYS:HD2	13	0.1
(1,897)	1:21:A:MET:HE3	1:22:A:LYS:HD3	13	0.1
(1,834)	1:9:A:THR:HA	1:13:A:VAL:HA	12	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG21	13	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG22	13	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG23	13	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG21	16	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG22	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG23	16	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG21	17	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG22	17	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG23	17	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG21	18	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG22	18	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG23	18	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG21	20	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG22	20	0.1
(1,818)	1:6:A:HIS:HD2	1:9:A:THR:HG23	20	0.1
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE1	15	0.1
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE2	15	0.1
(1,656)	1:109:A:TRP:HE1	1:122:A:MET:HE3	15	0.1
(1,550)	1:124:A:VAL:H	1:124:A:VAL:HB	15	0.1
(1,548)	1:123:A:PRO:HB2	1:124:A:VAL:H	6	0.1
(1,535)	1:116:A:LEU:HB3	1:118:A:VAL:H	2	0.1
(1,535)	1:116:A:LEU:HB3	1:118:A:VAL:H	14	0.1
(1,249)	1:54:A:PRO:HA	1:55:A:SER:H	1	0.1
(1,249)	1:54:A:PRO:HA	1:55:A:SER:H	10	0.1
(1,249)	1:54:A:PRO:HA	1:55:A:SER:H	13	0.1
(1,249)	1:54:A:PRO:HA	1:55:A:SER:H	15	0.1
(1,249)	1:54:A:PRO:HA	1:55:A:SER:H	17	0.1
(1,153)	1:32:A:GLY:H	1:35:A:VAL:HB	2	0.1
(1,153)	1:32:A:GLY:H	1:35:A:VAL:HB	13	0.1
(1,153)	1:32:A:GLY:H	1:35:A:VAL:HB	16	0.1
(1,139)	1:56:A:GLU:HB3	1:60:A:THR:H	12	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found