Full wwPDB NMR Structure Validation Report (i)

Dec 24, 2024 – 08:29 PM EST

PDB ID	:	2M5V
BMRB ID	:	18242
Title	:	Three-dimensional structure of human NLRP10/PYNOD pyrin domain
Authors	:	Su, M.Y.; Chang, C.F.; Chang, C.I.
Deposited on	:	2013-03-11

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

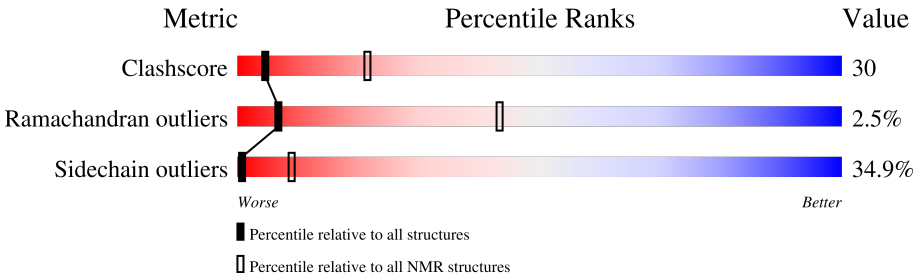
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 89%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	102	28% 37% 8% 26%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:12-A:39, A:49-A:95 (75)	0.38	2

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 5 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1658 atoms, of which 848 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NACHT, LRR and PYD domains-containing protein 10.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	102	1658	521	848	136	148	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q86W26
A	2	ALA	-	expression tag	UNP Q86W26

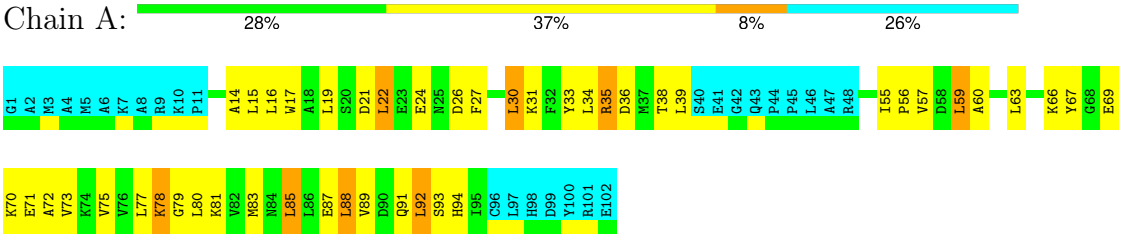
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

Chain A:



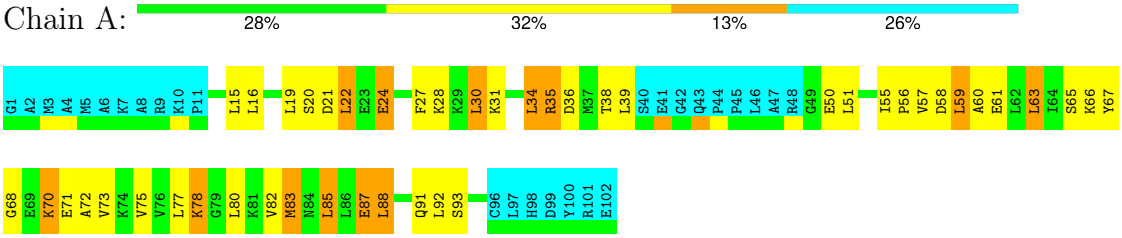
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

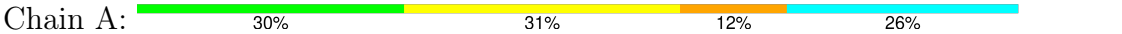
Chain A:

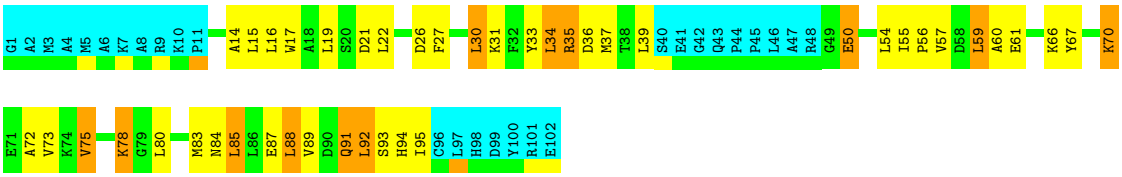


4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

Chain A:

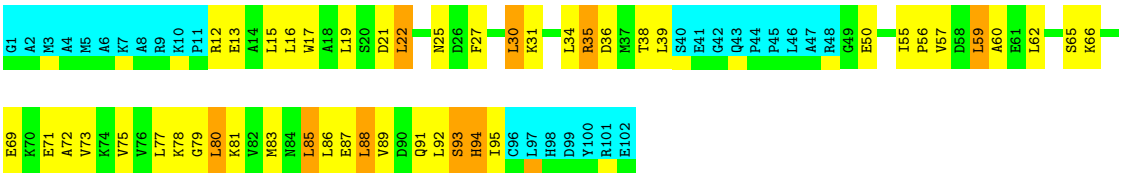




4.2.3 Score per residue for model 3

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

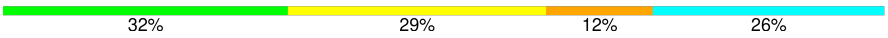
Chain A:

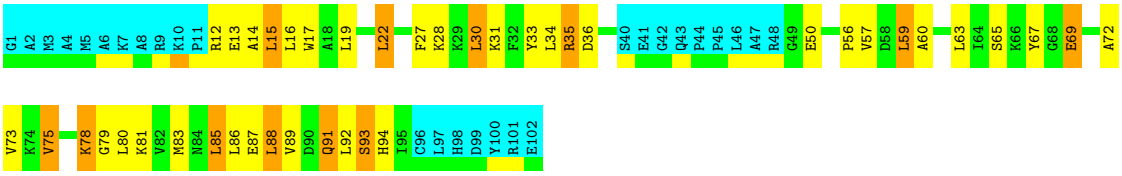


4.2.4 Score per residue for model 4

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

Chain A:

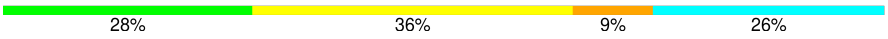


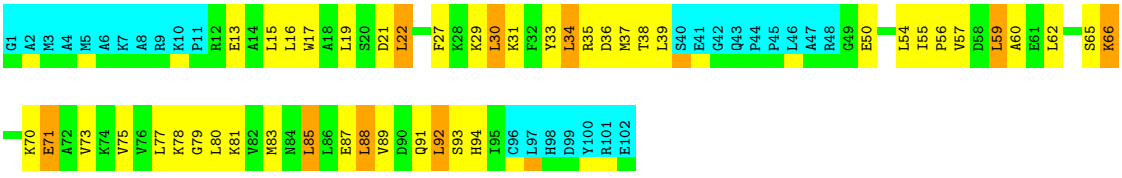


4.2.5 Score per residue for model 5

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

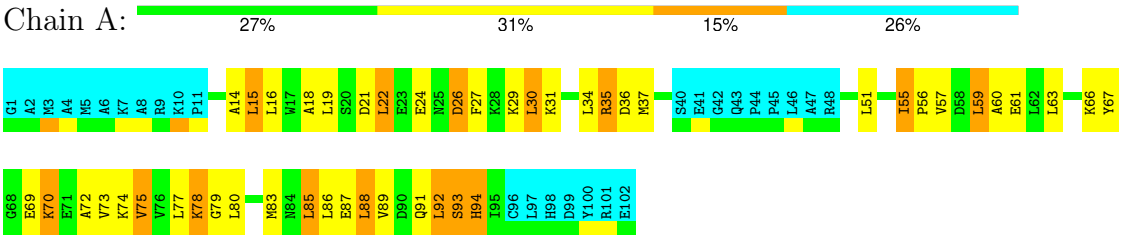
Chain A:





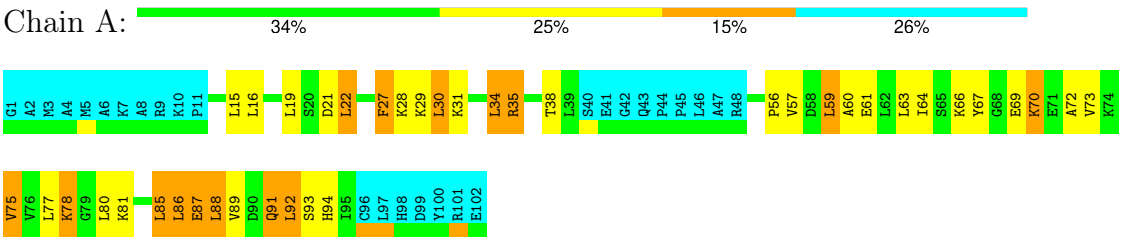
4.2.6 Score per residue for model 6

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10



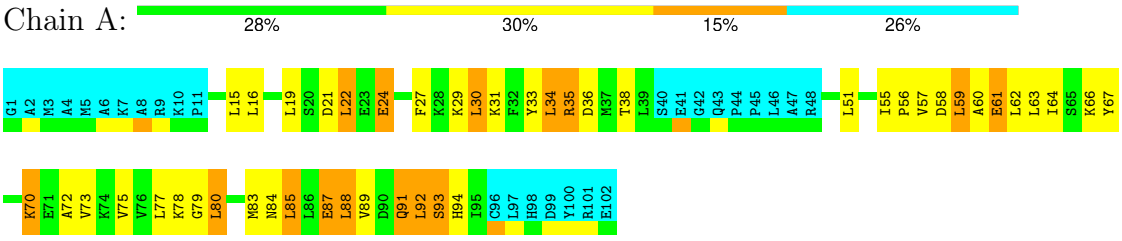
4.2.7 Score per residue for model 7

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10



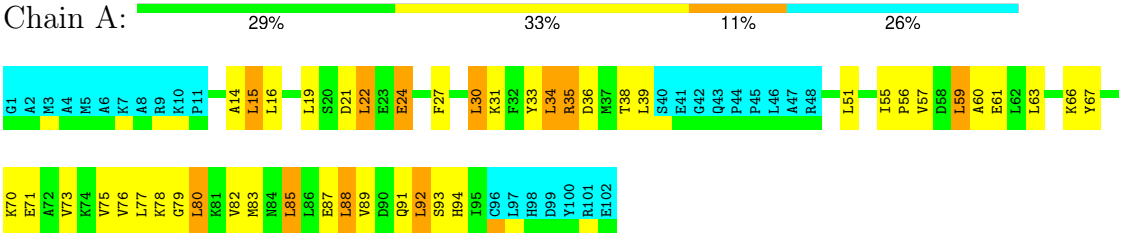
4.2.8 Score per residue for model 8

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10



4.2.9 Score per residue for model 9

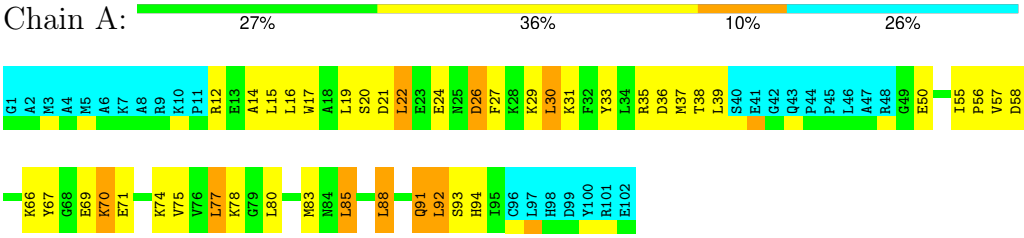
• Molecule 1: NACHT, LRR and PYD domains-containing protein 10



4.2.10 Score per residue for model 10

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

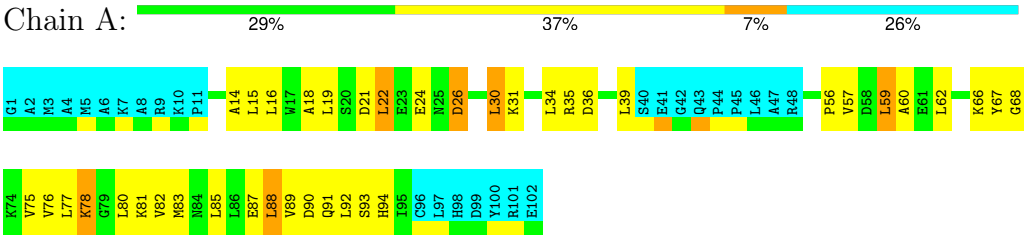
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

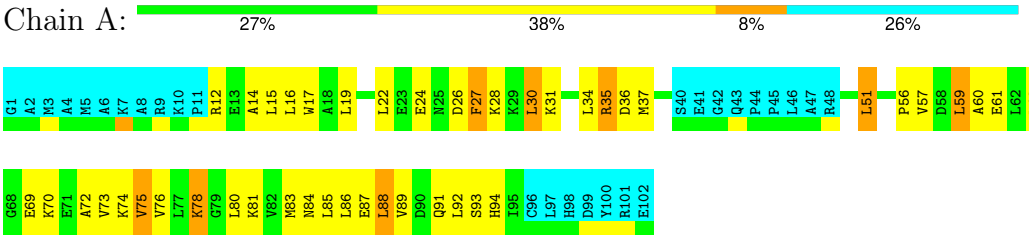
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

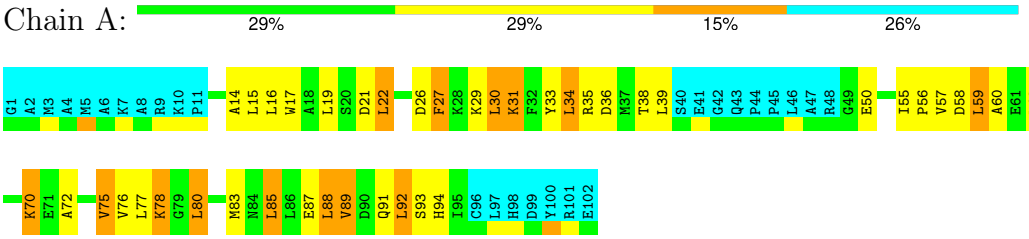
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

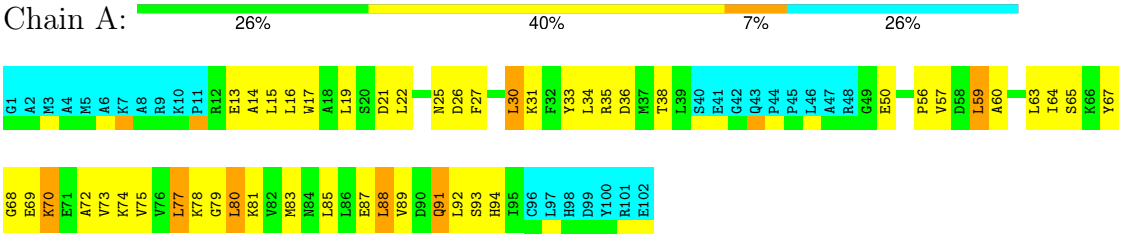
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

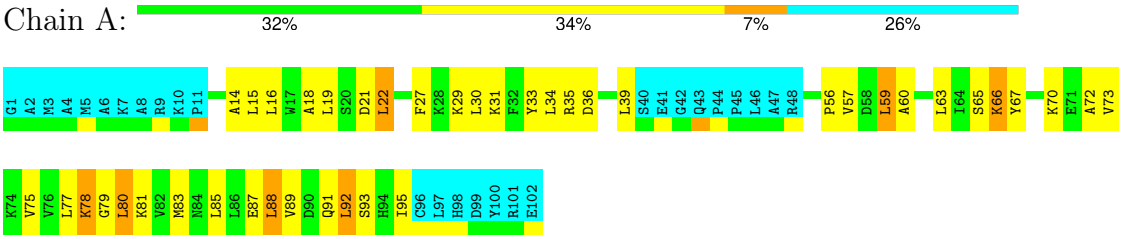
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

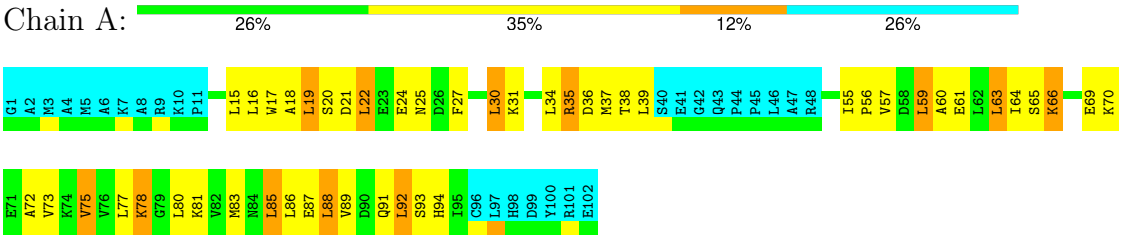
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

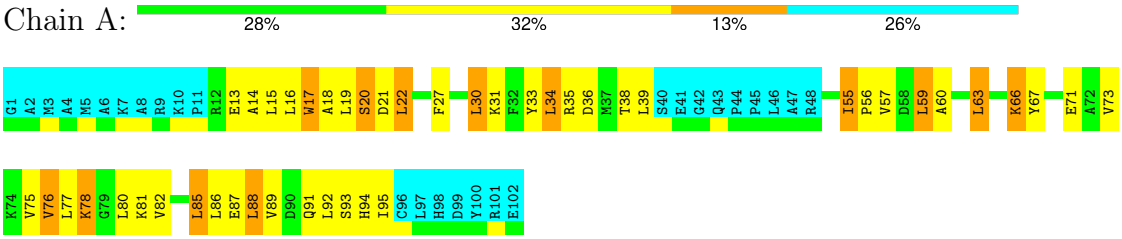
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

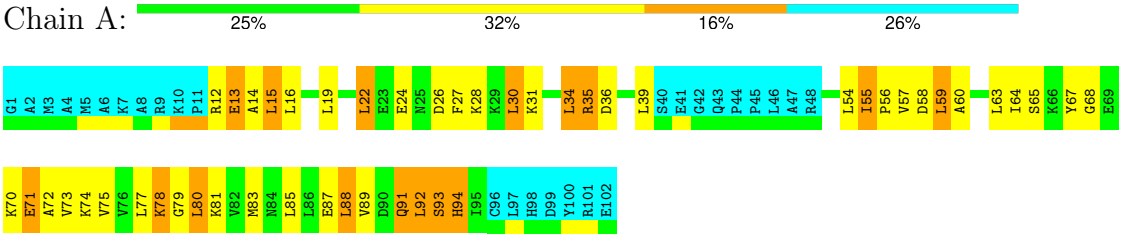
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

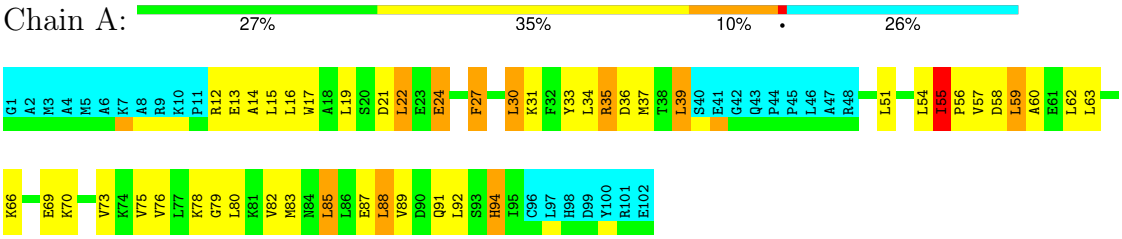
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

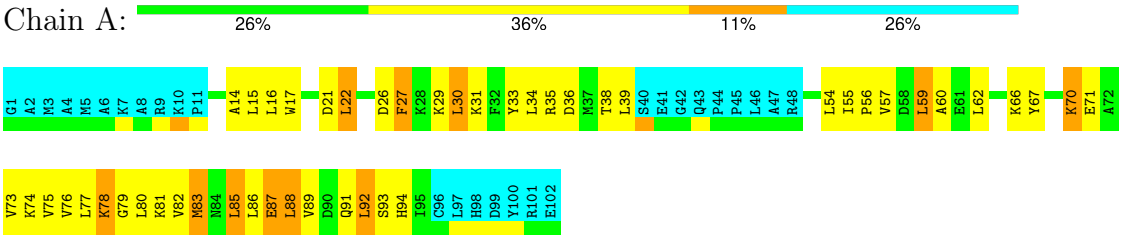
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: NACHT, LRR and PYD domains-containing protein 10

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1240
Number of shifts mapped to atoms	1240
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

6 Model quality

6.1 Standard geometry

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	604	641	641	38±6
All	All	12080	12820	12820	752

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 30.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LEU:HD13	1:A:57:VAL:HG22	1.07	1.22	16	17
1:A:19:LEU:HD13	1:A:20:SER:N	0.99	1.73	16	1
1:A:16:LEU:HD22	1:A:57:VAL:HG22	0.84	1.48	10	2
1:A:88:LEU:HD22	1:A:88:LEU:C	0.83	1.93	18	15
1:A:15:LEU:HD13	1:A:19:LEU:HD23	0.83	1.49	11	6
1:A:88:LEU:HD13	1:A:89:VAL:N	0.81	1.91	13	12
1:A:54:LEU:O	1:A:55:ILE:O	0.80	1.99	18	2
1:A:18:ALA:HB1	1:A:88:LEU:HD23	0.78	1.54	17	2
1:A:59:LEU:HD23	1:A:60:ALA:N	0.77	1.94	1	20
1:A:72:ALA:O	1:A:75:VAL:HG12	0.75	1.80	8	7
1:A:73:VAL:HG13	1:A:92:LEU:HD21	0.75	1.57	17	2
1:A:15:LEU:O	1:A:19:LEU:HD12	0.73	1.82	16	1
1:A:30:LEU:CD1	1:A:80:LEU:HD12	0.72	2.14	13	4
1:A:80:LEU:HD23	1:A:85:LEU:CB	0.72	2.13	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:LEU:HD22	1:A:89:VAL:N	0.71	2.00	20	13
1:A:15:LEU:HB2	1:A:73:VAL:HG22	0.70	1.62	2	9
1:A:15:LEU:HD12	1:A:19:LEU:HD23	0.70	1.62	18	7
1:A:88:LEU:HD13	1:A:89:VAL:H	0.69	1.48	4	12
1:A:22:LEU:HD22	1:A:80:LEU:HD21	0.68	1.66	3	6
1:A:16:LEU:CD1	1:A:57:VAL:HG22	0.68	2.18	1	3
1:A:88:LEU:HD22	1:A:88:LEU:H	0.67	1.48	11	5
1:A:30:LEU:HD21	1:A:83:MET:SD	0.67	2.29	15	1
1:A:71:GLU:O	1:A:75:VAL:HG23	0.65	1.91	3	7
1:A:30:LEU:HD11	1:A:80:LEU:HD12	0.64	1.68	8	4
1:A:80:LEU:HD22	1:A:85:LEU:CB	0.64	2.23	2	10
1:A:30:LEU:HD13	1:A:79:GLY:C	0.63	2.13	20	6
1:A:34:LEU:HD13	1:A:38:THR:HG21	0.63	1.70	7	2
1:A:18:ALA:HB1	1:A:88:LEU:CD2	0.63	2.22	17	2
1:A:39:LEU:HD11	1:A:75:VAL:HG21	0.63	1.69	3	5
1:A:83:MET:HB3	1:A:85:LEU:HD23	0.62	1.71	15	3
1:A:19:LEU:HD13	1:A:19:LEU:C	0.62	2.13	16	1
1:A:22:LEU:HD13	1:A:80:LEU:HD21	0.62	1.71	5	8
1:A:34:LEU:HD21	1:A:78:LYS:HE2	0.62	1.72	13	1
1:A:15:LEU:CB	1:A:73:VAL:HG22	0.61	2.24	18	7
1:A:62:LEU:C	1:A:62:LEU:HD13	0.61	2.15	20	4
1:A:30:LEU:HD21	1:A:83:MET:HG3	0.61	1.72	19	6
1:A:30:LEU:HD21	1:A:83:MET:CE	0.61	2.25	9	2
1:A:22:LEU:HD22	1:A:80:LEU:HD11	0.61	1.71	7	3
1:A:88:LEU:C	1:A:88:LEU:CD2	0.60	2.69	6	15
1:A:19:LEU:HD12	1:A:20:SER:N	0.60	2.11	17	2
1:A:39:LEU:HD23	1:A:66:LYS:HG3	0.60	1.71	20	2
1:A:34:LEU:HD11	1:A:79:GLY:CA	0.60	2.27	3	1
1:A:92:LEU:C	1:A:92:LEU:HD13	0.60	2.17	19	15
1:A:39:LEU:CD1	1:A:75:VAL:HG21	0.60	2.27	15	9
1:A:34:LEU:HB3	1:A:75:VAL:HG22	0.59	1.74	12	2
1:A:16:LEU:HD12	1:A:17:TRP:N	0.59	2.13	10	2
1:A:34:LEU:HD11	1:A:78:LYS:HE2	0.59	1.73	15	3
1:A:16:LEU:HD22	1:A:57:VAL:HA	0.59	1.73	15	13
1:A:30:LEU:HD11	1:A:80:LEU:CD1	0.59	2.28	3	1
1:A:19:LEU:HD11	1:A:56:PRO:HB3	0.59	1.73	19	17
1:A:80:LEU:HD22	1:A:85:LEU:CG	0.59	2.28	7	8
1:A:39:LEU:HD23	1:A:66:LYS:CG	0.59	2.28	20	5
1:A:27:PHE:CD1	1:A:51:LEU:HD13	0.59	2.33	12	2
1:A:16:LEU:C	1:A:16:LEU:HD12	0.59	2.18	17	1
1:A:91:GLN:O	1:A:94:HIS:N	0.58	2.37	20	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:LEU:HD23	1:A:85:LEU:HB2	0.58	1.75	15	1
1:A:15:LEU:HD22	1:A:73:VAL:CG2	0.58	2.28	17	5
1:A:15:LEU:CD1	1:A:19:LEU:HD23	0.57	2.29	14	5
1:A:15:LEU:HD23	1:A:73:VAL:HG22	0.57	1.76	14	2
1:A:24:GLU:HA	1:A:51:LEU:HD22	0.57	1.74	19	1
1:A:39:LEU:HD23	1:A:66:LYS:HG2	0.57	1.75	15	2
1:A:19:LEU:HD12	1:A:19:LEU:C	0.57	2.19	10	1
1:A:22:LEU:CD2	1:A:80:LEU:HD21	0.57	2.29	18	2
1:A:16:LEU:CD2	1:A:57:VAL:HG22	0.57	2.27	10	1
1:A:30:LEU:HD22	1:A:79:GLY:O	0.57	2.00	19	5
1:A:80:LEU:HD23	1:A:89:VAL:CG2	0.57	2.30	11	4
1:A:87:GLU:HG3	1:A:88:LEU:HD13	0.56	1.77	11	2
1:A:88:LEU:HD22	1:A:88:LEU:O	0.56	2.00	13	9
1:A:38:THR:OG1	1:A:39:LEU:HD12	0.56	2.00	5	3
1:A:77:LEU:HD12	1:A:78:LYS:N	0.56	2.15	7	8
1:A:54:LEU:O	1:A:55:ILE:C	0.56	2.43	19	2
1:A:80:LEU:HD23	1:A:85:LEU:HB3	0.56	1.76	15	2
1:A:15:LEU:HD22	1:A:73:VAL:HG23	0.56	1.75	20	1
1:A:30:LEU:HD21	1:A:83:MET:HE2	0.56	1.75	9	2
1:A:80:LEU:HD23	1:A:89:VAL:HG23	0.55	1.78	9	2
1:A:16:LEU:HD12	1:A:16:LEU:C	0.55	2.21	10	1
1:A:31:LYS:O	1:A:35:ARG:HB2	0.55	2.01	9	10
1:A:73:VAL:CG1	1:A:92:LEU:HD21	0.55	2.30	17	2
1:A:30:LEU:O	1:A:34:LEU:N	0.54	2.41	9	18
1:A:14:ALA:HB2	1:A:95:ILE:HG21	0.54	1.77	15	1
1:A:24:GLU:HA	1:A:51:LEU:HD13	0.54	1.79	6	1
1:A:34:LEU:HD21	1:A:78:LYS:CE	0.54	2.31	13	2
1:A:76:VAL:O	1:A:80:LEU:HD13	0.54	2.02	9	2
1:A:34:LEU:HD11	1:A:78:LYS:HD3	0.54	1.78	17	2
1:A:15:LEU:HG	1:A:73:VAL:HG22	0.53	1.79	11	2
1:A:31:LYS:O	1:A:35:ARG:CB	0.53	2.56	14	18
1:A:87:GLU:HG2	1:A:88:LEU:HD13	0.53	1.81	8	1
1:A:34:LEU:CD1	1:A:38:THR:HG21	0.53	2.33	7	3
1:A:15:LEU:HD21	1:A:76:VAL:HG21	0.53	1.80	13	1
1:A:15:LEU:HD13	1:A:73:VAL:HG22	0.53	1.78	20	1
1:A:15:LEU:CG	1:A:73:VAL:HG22	0.53	2.34	14	4
1:A:19:LEU:C	1:A:19:LEU:HD12	0.53	2.24	3	16
1:A:30:LEU:HD21	1:A:83:MET:CG	0.53	2.34	18	3
1:A:76:VAL:O	1:A:80:LEU:HB2	0.53	2.04	12	2
1:A:13:GLU:HA	1:A:16:LEU:HD12	0.52	1.81	19	2
1:A:92:LEU:HD22	1:A:92:LEU:O	0.52	2.04	5	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:GLU:HA	1:A:51:LEU:HD23	0.52	1.80	1	2
1:A:35:ARG:HG2	1:A:39:LEU:HD22	0.52	1.81	15	1
1:A:35:ARG:CD	1:A:63:LEU:HD21	0.52	2.35	17	1
1:A:56:PRO:HA	1:A:59:LEU:HD22	0.52	1.82	20	19
1:A:86:LEU:HD12	1:A:87:GLU:N	0.52	2.20	7	1
1:A:92:LEU:HD13	1:A:93:SER:N	0.51	2.20	15	18
1:A:34:LEU:HD11	1:A:79:GLY:HA3	0.51	1.82	3	1
1:A:34:LEU:HD11	1:A:78:LYS:CE	0.51	2.35	6	3
1:A:34:LEU:HD11	1:A:78:LYS:HE3	0.51	1.81	6	3
1:A:15:LEU:CD2	1:A:73:VAL:HG22	0.51	2.35	14	2
1:A:22:LEU:HD12	1:A:27:PHE:HB3	0.51	1.83	20	3
1:A:34:LEU:HD13	1:A:38:THR:CG2	0.51	2.34	7	2
1:A:80:LEU:HD22	1:A:85:LEU:HG	0.51	1.83	6	5
1:A:39:LEU:HD23	1:A:67:TYR:HB2	0.51	1.80	9	2
1:A:35:ARG:CG	1:A:39:LEU:HD22	0.51	2.34	15	1
1:A:18:ALA:CB	1:A:88:LEU:HD23	0.51	2.32	17	2
1:A:34:LEU:HD12	1:A:75:VAL:CG2	0.51	2.36	13	1
1:A:30:LEU:O	1:A:34:LEU:HB2	0.51	2.06	15	17
1:A:69:GLU:O	1:A:72:ALA:HB3	0.51	2.06	12	4
1:A:92:LEU:HD13	1:A:92:LEU:C	0.50	2.26	8	5
1:A:35:ARG:HG3	1:A:39:LEU:HD13	0.50	1.82	17	1
1:A:26:ASP:O	1:A:30:LEU:HG	0.50	2.07	20	6
1:A:22:LEU:CD1	1:A:27:PHE:HB2	0.50	2.36	3	1
1:A:50:GLU:HA	1:A:54:LEU:HD12	0.50	1.82	2	1
1:A:22:LEU:HD12	1:A:27:PHE:HB2	0.50	1.84	15	2
1:A:22:LEU:HD13	1:A:80:LEU:HD11	0.50	1.82	18	2
1:A:35:ARG:HG2	1:A:39:LEU:HD13	0.49	1.83	2	3
1:A:31:LYS:HD2	1:A:63:LEU:HD11	0.49	1.84	16	1
1:A:85:LEU:HD12	1:A:88:LEU:HD12	0.49	1.84	6	1
1:A:15:LEU:O	1:A:15:LEU:HD12	0.49	2.07	16	1
1:A:91:GLN:O	1:A:92:LEU:C	0.49	2.51	20	20
1:A:88:LEU:HD13	1:A:88:LEU:N	0.48	2.23	11	1
1:A:34:LEU:HD12	1:A:75:VAL:O	0.48	2.08	3	1
1:A:30:LEU:N	1:A:30:LEU:HD23	0.48	2.23	13	5
1:A:83:MET:CB	1:A:85:LEU:HD23	0.48	2.37	15	2
1:A:22:LEU:CD1	1:A:80:LEU:HD11	0.48	2.38	18	1
1:A:39:LEU:HD21	1:A:71:GLU:OE2	0.47	2.09	5	1
1:A:14:ALA:CB	1:A:95:ILE:HD13	0.47	2.39	17	1
1:A:68:GLY:O	1:A:72:ALA:HB2	0.47	2.10	1	4
1:A:83:MET:CG	1:A:85:LEU:HD23	0.47	2.40	13	5
1:A:34:LEU:HD12	1:A:79:GLY:HA3	0.47	1.87	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LEU:O	1:A:19:LEU:CD1	0.47	2.63	16	1
1:A:31:LYS:NZ	1:A:76:VAL:HG23	0.47	2.25	11	2
1:A:19:LEU:HD11	1:A:56:PRO:CB	0.47	2.40	8	2
1:A:18:ALA:HA	1:A:88:LEU:HD23	0.47	1.87	16	1
1:A:35:ARG:HE	1:A:63:LEU:HD21	0.46	1.69	1	1
1:A:60:ALA:O	1:A:64:ILE:HG23	0.46	2.11	18	2
1:A:34:LEU:O	1:A:38:THR:OG1	0.46	2.32	20	3
1:A:15:LEU:HG	1:A:16:LEU:N	0.46	2.25	4	2
1:A:58:ASP:O	1:A:61:GLU:HG2	0.46	2.11	1	2
1:A:80:LEU:HD22	1:A:85:LEU:HB2	0.46	1.85	2	1
1:A:15:LEU:HG	1:A:19:LEU:HD23	0.46	1.88	7	1
1:A:63:LEU:HD12	1:A:72:ALA:HB1	0.45	1.87	15	1
1:A:56:PRO:O	1:A:60:ALA:CB	0.45	2.65	15	2
1:A:30:LEU:O	1:A:34:LEU:CB	0.45	2.64	9	1
1:A:34:LEU:HD23	1:A:75:VAL:HG13	0.45	1.88	9	1
1:A:15:LEU:HD13	1:A:15:LEU:O	0.45	2.10	1	1
1:A:24:GLU:HG3	1:A:51:LEU:HD22	0.45	1.88	9	1
1:A:18:ALA:O	1:A:22:LEU:HD23	0.45	2.12	11	2
1:A:19:LEU:HD22	1:A:19:LEU:O	0.45	2.12	16	1
1:A:19:LEU:HA	1:A:22:LEU:HD21	0.45	1.88	6	1
1:A:59:LEU:HD23	1:A:60:ALA:H	0.44	1.70	17	4
1:A:15:LEU:HD12	1:A:19:LEU:CD2	0.44	2.39	19	2
1:A:22:LEU:CD2	1:A:80:LEU:HD11	0.44	2.43	19	1
1:A:55:ILE:HB	1:A:56:PRO:HD2	0.44	1.90	17	13
1:A:35:ARG:HD3	1:A:39:LEU:HD22	0.44	1.88	16	1
1:A:34:LEU:O	1:A:38:THR:HG23	0.44	2.13	9	3
1:A:30:LEU:HD11	1:A:80:LEU:HD13	0.43	1.90	14	1
1:A:24:GLU:CA	1:A:51:LEU:HD23	0.43	2.43	1	1
1:A:15:LEU:HB3	1:A:73:VAL:HG22	0.43	1.89	15	1
1:A:54:LEU:C	1:A:55:ILE:O	0.43	2.56	18	2
1:A:26:ASP:O	1:A:30:LEU:CD2	0.43	2.66	11	1
1:A:83:MET:HG2	1:A:85:LEU:HD23	0.43	1.91	2	1
1:A:16:LEU:HD13	1:A:57:VAL:CG2	0.43	2.22	11	1
1:A:19:LEU:HD22	1:A:59:LEU:HD21	0.43	1.90	13	2
1:A:35:ARG:HG2	1:A:39:LEU:HB2	0.42	1.90	17	1
1:A:80:LEU:HD12	1:A:85:LEU:HB2	0.42	1.90	14	1
1:A:77:LEU:HD23	1:A:92:LEU:HD11	0.42	1.91	17	1
1:A:64:ILE:HD12	1:A:65:SER:N	0.42	2.29	16	1
1:A:18:ALA:O	1:A:22:LEU:CD2	0.42	2.68	11	1
1:A:73:VAL:O	1:A:77:LEU:HD23	0.42	2.15	14	1
1:A:13:GLU:O	1:A:16:LEU:HG	0.42	2.15	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LYS:HA	1:A:35:ARG:HB2	0.42	1.91	9	1
1:A:34:LEU:CD2	1:A:38:THR:HG21	0.42	2.45	8	1
1:A:15:LEU:HD22	1:A:15:LEU:O	0.42	2.15	10	1
1:A:12:ARG:O	1:A:16:LEU:HG	0.42	2.15	4	1
1:A:34:LEU:HD11	1:A:78:LYS:CG	0.41	2.45	2	1
1:A:26:ASP:HA	1:A:83:MET:CE	0.41	2.45	13	1
1:A:14:ALA:HB1	1:A:95:ILE:HD13	0.41	1.91	17	1
1:A:20:SER:HA	1:A:51:LEU:HD11	0.41	1.91	1	1
1:A:34:LEU:HD21	1:A:78:LYS:HD3	0.41	1.93	17	1
1:A:22:LEU:HD12	1:A:27:PHE:CB	0.41	2.45	13	2
1:A:64:ILE:HG22	1:A:69:GLU:HA	0.41	1.93	7	2
1:A:63:LEU:O	1:A:66:LYS:HB3	0.41	2.15	15	2
1:A:34:LEU:HD11	1:A:78:LYS:HG3	0.41	1.93	2	1
1:A:19:LEU:C	1:A:19:LEU:CD1	0.41	2.90	10	1
1:A:80:LEU:O	1:A:83:MET:HB2	0.41	2.15	15	1
1:A:92:LEU:C	1:A:92:LEU:CD1	0.41	2.89	19	1
1:A:51:LEU:C	1:A:51:LEU:HD23	0.41	2.37	9	1
1:A:88:LEU:CD1	1:A:88:LEU:H	0.41	2.29	12	3
1:A:30:LEU:HD11	1:A:80:LEU:HD23	0.40	1.92	10	1
1:A:19:LEU:C	1:A:19:LEU:HD22	0.40	2.37	16	1
1:A:58:ASP:O	1:A:61:GLU:HG3	0.40	2.16	8	1
1:A:61:GLU:HG3	1:A:62:LEU:N	0.40	2.31	8	1
1:A:30:LEU:HD23	1:A:30:LEU:N	0.40	2.32	14	1
1:A:55:ILE:HD11	1:A:58:ASP:OD2	0.40	2.17	13	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	75/102 (74%)	64±1 (86±2%)	9±1 (12±2%)	2±1 (2±1%)	7	43
All	All	1500/2040 (74%)	1284 (86%)	179 (12%)	37 (2%)	7	43

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

Mol	Chain	Res	Type	Models (Total)
1	A	87	GLU	18
1	A	70	LYS	15
1	A	55	ILE	2
1	A	50	GLU	1
1	A	54	LEU	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	67/87 (77%)	44±3 (65±4%)	23±3 (35±4%)	1 9
All	All	1340/1740 (77%)	872 (65%)	468 (35%)	1 9

All 58 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	22	LEU	20
1	A	59	LEU	20
1	A	88	LEU	20
1	A	30	LEU	19
1	A	36	ASP	19
1	A	78	LYS	19
1	A	21	ASP	17
1	A	27	PHE	17
1	A	85	LEU	17
1	A	66	LYS	15
1	A	63	LEU	14
1	A	67	TYR	14
1	A	35	ARG	12
1	A	70	LYS	12
1	A	33	TYR	12
1	A	92	LEU	12
1	A	81	LYS	12
1	A	17	TRP	11
1	A	94	HIS	10
1	A	24	GLU	9
1	A	34	LEU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	75	VAL	9
1	A	65	SER	8
1	A	77	LEU	8
1	A	86	LEU	8
1	A	29	LYS	8
1	A	37	MET	7
1	A	61	GLU	7
1	A	91	GLN	7
1	A	80	LEU	7
1	A	82	VAL	6
1	A	83	MET	6
1	A	93	SER	6
1	A	74	LYS	6
1	A	28	LYS	5
1	A	50	GLU	5
1	A	26	ASP	5
1	A	12	ARG	5
1	A	13	GLU	5
1	A	69	GLU	5
1	A	15	LEU	4
1	A	84	ASN	3
1	A	89	VAL	3
1	A	25	ASN	3
1	A	71	GLU	3
1	A	55	ILE	3
1	A	95	ILE	2
1	A	62	LEU	2
1	A	76	VAL	2
1	A	58	ASP	2
1	A	90	ASP	1
1	A	51	LEU	1
1	A	31	LYS	1
1	A	19	LEU	1
1	A	20	SER	1
1	A	39	LEU	1
1	A	54	LEU	1
1	A	87	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

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1240
Number of shifts mapped to atoms	1240
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	101	-0.45 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	95	0.16 ± 0.06	None needed (< 0.5 ppm)
$^{13}C'$	96	-0.35 ± 0.10	None needed (< 0.5 ppm)
^{15}N	93	0.63 ± 0.23	Should be applied

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 89%, i.e. 967 atoms were assigned a chemical shift out of a possible 1092. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	373/377 (99%)	152/153 (99%)	148/150 (99%)	73/74 (99%)
Sidechain	594/658 (90%)	412/431 (96%)	182/210 (87%)	0/17 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/57 (0%)	0/28 (0%)	0/27 (0%)	0/2 (0%)
Overall	967/1092 (89%)	564/612 (92%)	330/387 (85%)	73/93 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1240 atoms were assigned a chemical shift out of a possible 1452. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	489/508 (96%)	199/206 (97%)	197/204 (97%)	93/98 (95%)
Sidechain	751/871 (86%)	520/569 (91%)	231/273 (85%)	0/29 (0%)
Aromatic	0/73 (0%)	0/36 (0%)	0/34 (0%)	0/3 (0%)
Overall	1240/1452 (85%)	719/811 (89%)	428/511 (84%)	93/130 (72%)

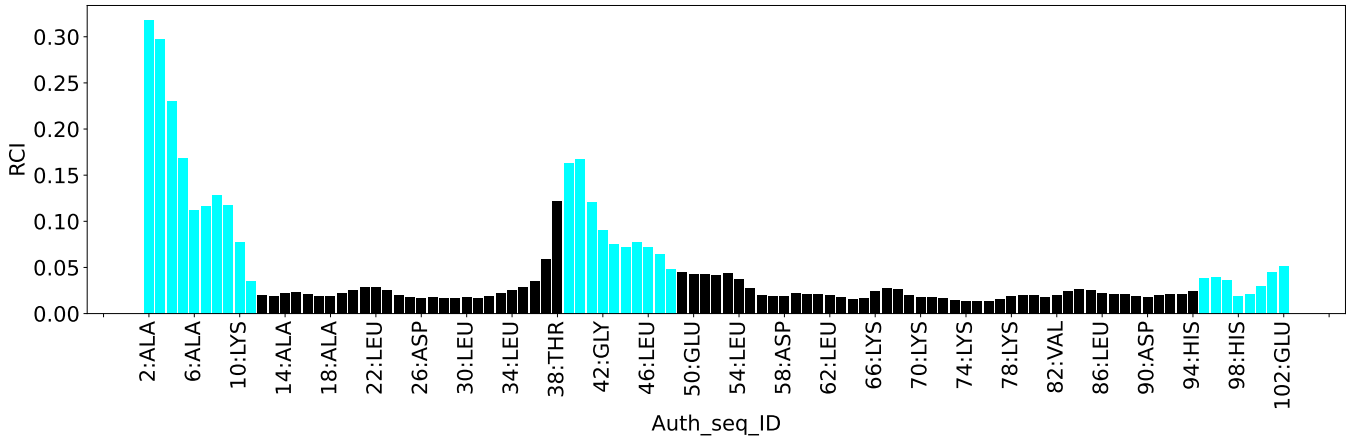
7.1.4 Statistically unusual chemical shifts (i)

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	910
Intra-residue (|i-j|=0)	274
Sequential (|i-j|=1)	243
Medium range (|i-j|>1 and |i-j|<5)	187
Long range (|i-j|≥5)	130
Inter-chain	0
Hydrogen bond restraints	76
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	8.9
Number of long range restraints per residue[1]	1.3

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	12.2	0.2
0.2-0.5 (Medium)	2.1	0.5
>0.5 (Large)	None	None

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

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

9 Distance violation analysis (i)

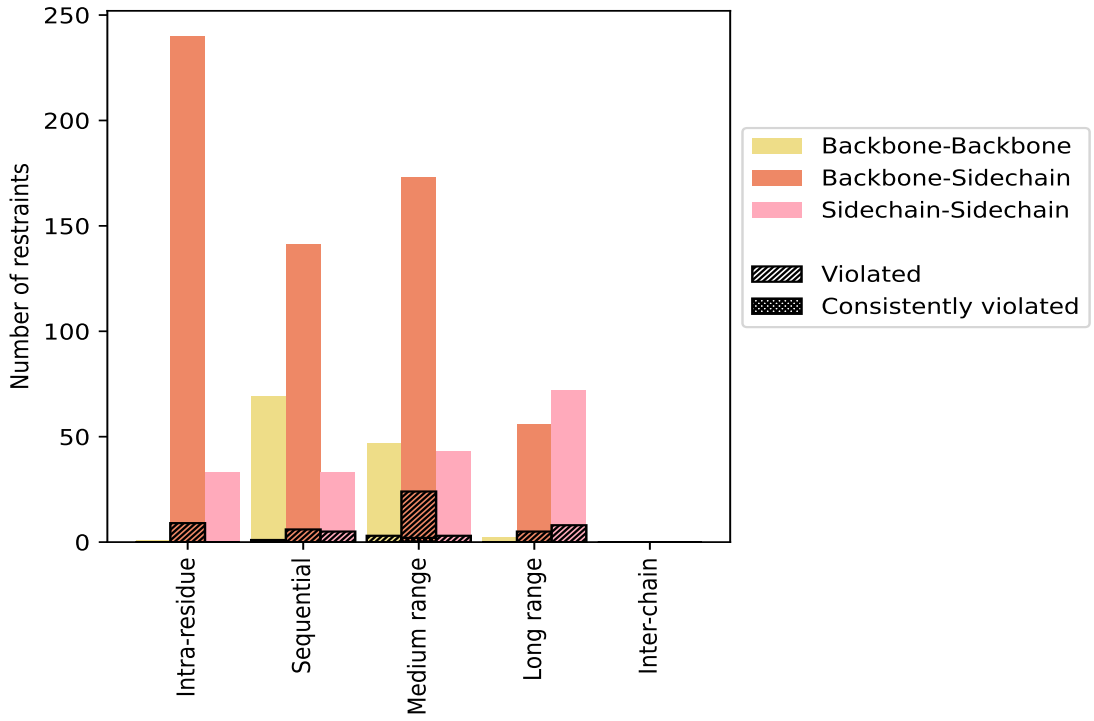
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	274	30.1	9	3.3	1.0	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	240	26.4	9	3.8	1.0	0	0.0	0.0
Sidechain-Sidechain	33	3.6	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	243	26.7	12	4.9	1.3	0	0.0	0.0
Backbone-Backbone	69	7.6	1	1.4	0.1	0	0.0	0.0
Backbone-Sidechain	141	15.5	6	4.3	0.7	0	0.0	0.0
Sidechain-Sidechain	33	3.6	5	15.2	0.5	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	187	20.5	21	11.2	2.3	1	0.5	0.1
Backbone-Backbone	47	5.2	3	6.4	0.3	0	0.0	0.0
Backbone-Sidechain	97	10.7	15	15.5	1.6	1	1.0	0.1
Sidechain-Sidechain	43	4.7	3	7.0	0.3	0	0.0	0.0
Long range (|i-j|≥5)	130	14.3	13	10.0	1.4	0	0.0	0.0
Backbone-Backbone	2	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	56	6.2	5	8.9	0.5	0	0.0	0.0
Sidechain-Sidechain	72	7.9	8	11.1	0.9	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	76	8.4	9	11.8	1.0	1	1.3	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	910	100.0	64	7.0	7.0	2	0.2	0.2
Backbone-Backbone	119	13.1	4	3.4	0.4	0	0.0	0.0
Backbone-Sidechain	610	67.0	44	7.2	4.8	2	0.3	0.2
Sidechain-Sidechain	181	19.9	16	8.8	1.8	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	1	3	9	2	0	15	0.16	0.38	0.06	0.15
2	1	3	11	1	0	16	0.15	0.28	0.04	0.15
3	3	2	10	2	0	17	0.17	0.5	0.09	0.16
4	2	1	9	2	0	14	0.14	0.26	0.04	0.13
5	1	0	6	3	0	10	0.14	0.23	0.04	0.14
6	2	1	8	4	0	15	0.14	0.24	0.04	0.13
7	2	1	11	4	0	18	0.14	0.25	0.04	0.12
8	0	3	9	3	0	15	0.16	0.24	0.04	0.15
9	1	2	10	2	0	15	0.17	0.35	0.07	0.16
10	1	3	11	2	0	17	0.15	0.22	0.04	0.14

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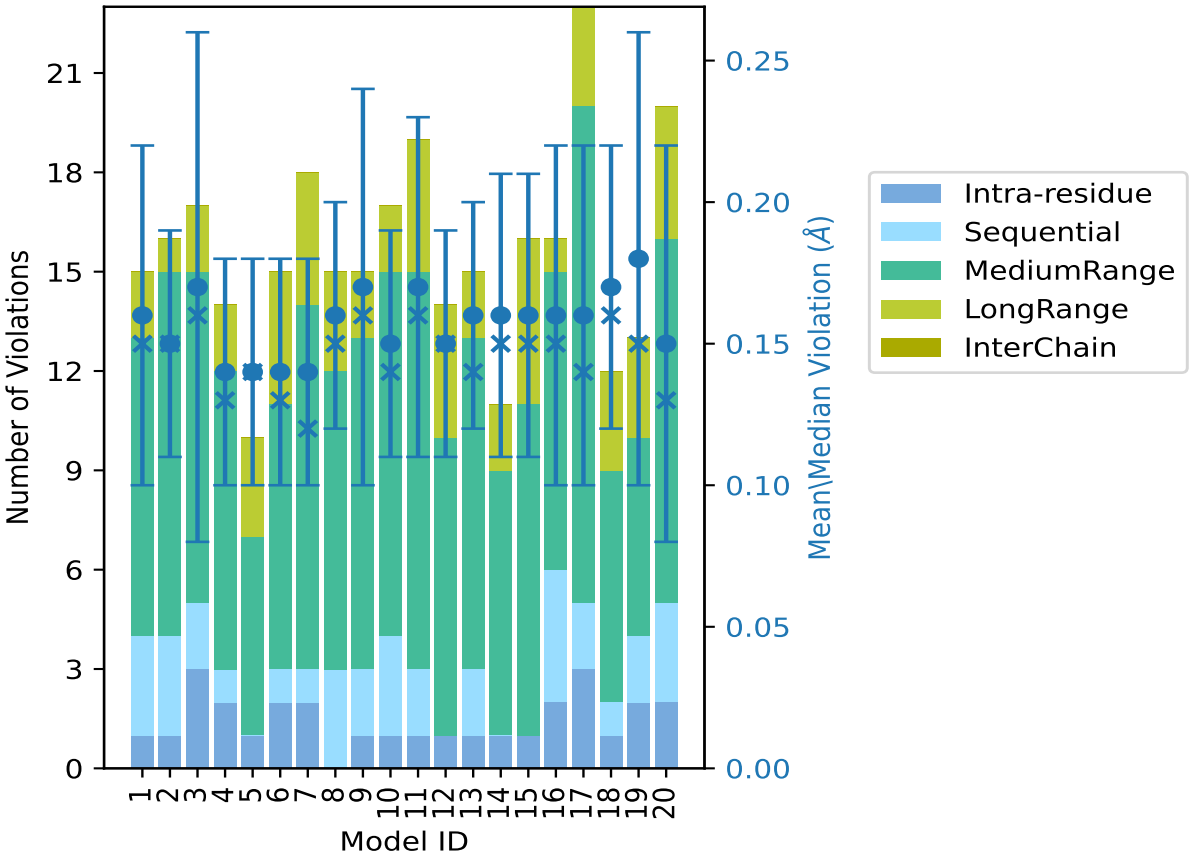
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	1	2	12	4	0	19	0.17	0.37	0.06	0.16
12	1	0	9	4	0	14	0.15	0.22	0.04	0.15
13	1	2	10	2	0	15	0.16	0.26	0.04	0.14
14	1	0	8	2	0	11	0.16	0.31	0.05	0.15
15	1	0	10	5	0	16	0.16	0.3	0.05	0.15
16	2	4	9	1	0	16	0.16	0.3	0.06	0.15
17	3	2	15	3	0	23	0.16	0.39	0.06	0.14
18	1	1	7	3	0	12	0.17	0.29	0.05	0.16
19	2	2	6	3	0	13	0.18	0.41	0.08	0.15
20	2	3	11	4	0	20	0.15	0.41	0.07	0.13

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

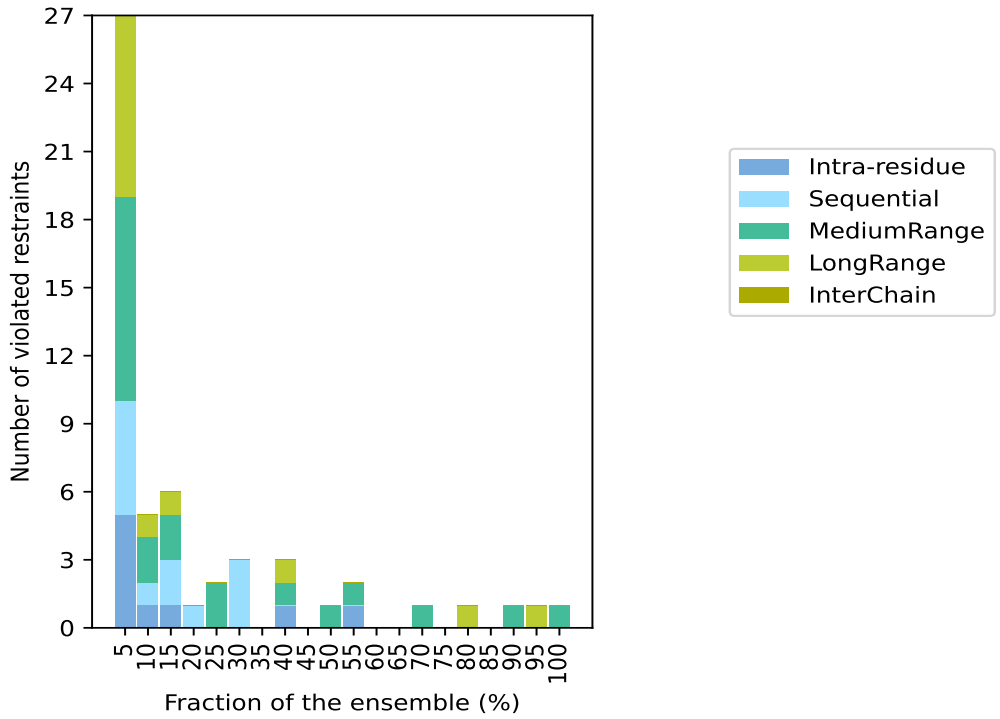
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 779(IR:265, SQ:231, MR:166, LR:117, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
5	5	9	8	0	27	1	5.0
1	1	2	1	0	5	2	10.0
1	2	2	1	0	6	3	15.0
0	1	0	0	0	1	4	20.0
0	0	2	0	0	2	5	25.0
0	3	0	0	0	3	6	30.0
0	0	0	0	0	0	7	35.0
1	0	1	1	0	3	8	40.0
0	0	0	0	0	0	9	45.0
0	0	1	0	0	1	10	50.0
1	0	1	0	0	2	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	1	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	1	0	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	1	0	0	1	18	90.0
0	0	0	1	0	1	19	95.0
0	0	1	0	0	1	20	100.0

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

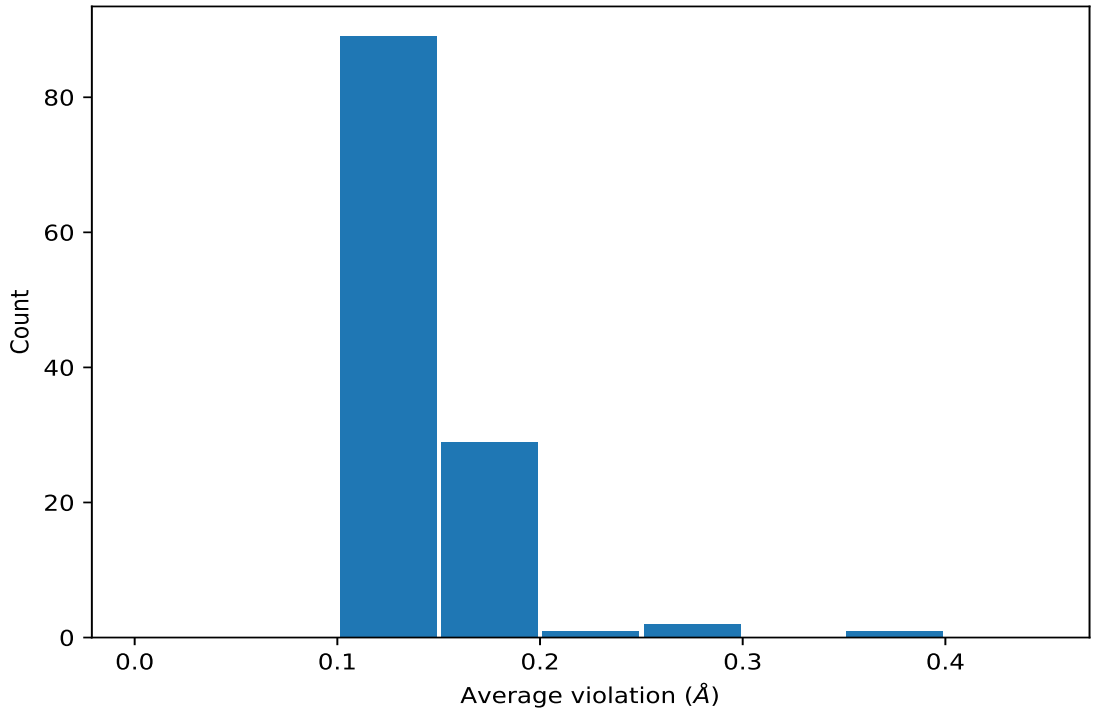
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of theviolation 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)
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	20	0.24	0.03	0.23
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	20	0.15	0.02	0.15
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	19	0.16	0.04	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	19	0.16	0.04	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	19	0.16	0.04	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	19	0.16	0.04	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	19	0.16	0.04	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	19	0.16	0.04	0.16
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	19	0.15	0.03	0.15
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	18	0.16	0.02	0.16
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	18	0.16	0.02	0.16
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	17	0.16	0.02	0.16
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	16	0.14	0.03	0.13
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	16	0.14	0.03	0.13
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	16	0.14	0.03	0.13
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	16	0.14	0.03	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	16	0.14	0.03	0.13
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	16	0.14	0.03	0.13
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	14	0.15	0.04	0.14
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	14	0.15	0.04	0.14
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD11	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD12	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD13	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD21	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD22	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD23	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD11	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD12	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD13	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD21	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD22	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD23	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD11	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD12	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD13	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD21	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD22	11	0.15	0.03	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD23	11	0.15	0.03	0.15
(2,69)	1:88:A:LEU:O	1:92:A:LEU:H	11	0.13	0.02	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD11	11	0.12	0.01	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD12	11	0.12	0.01	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD13	11	0.12	0.01	0.12
(1,372)	1:25:A:ASN:HA	1:29:A:LYS:H	10	0.14	0.03	0.13
(1,578)	1:31:A:LYS:HG2	1:35:A:ARG:H	8	0.14	0.02	0.14
(1,578)	1:31:A:LYS:HG3	1:35:A:ARG:H	8	0.14	0.02	0.14
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG21	8	0.13	0.01	0.12
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG22	8	0.13	0.01	0.12
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG23	8	0.13	0.01	0.12
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG21	8	0.13	0.01	0.12
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG22	8	0.13	0.01	0.12
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG23	8	0.13	0.01	0.12
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG21	8	0.13	0.01	0.12
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG22	8	0.13	0.01	0.12
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG23	8	0.13	0.01	0.12
(1,546)	1:88:A:LEU:H	1:88:A:LEU:HG	8	0.12	0.02	0.12
(1,497)	1:82:A:VAL:HB	1:83:A:MET:H	6	0.38	0.02	0.38
(1,621)	1:82:A:VAL:HG21	1:83:A:MET:H	6	0.14	0.01	0.14
(1,621)	1:82:A:VAL:HG22	1:83:A:MET:H	6	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,621)	1:82:A:VAL:HG23	1:83:A:MET:H	6	0.14	0.01	0.14
(1,500)	1:31:A:LYS:HD2	1:32:A:PHE:H	6	0.11	0.01	0.11
(1,500)	1:31:A:LYS:HD3	1:32:A:PHE:H	6	0.11	0.01	0.11
(1,612)	1:88:A:LEU:HD11	1:90:A:ASP:H	5	0.17	0.02	0.17
(1,612)	1:88:A:LEU:HD12	1:90:A:ASP:H	5	0.17	0.02	0.17
(1,612)	1:88:A:LEU:HD13	1:90:A:ASP:H	5	0.17	0.02	0.17
(1,53)	1:81:A:LYS:HA	1:84:A:ASN:HA	5	0.16	0.04	0.14
(1,469)	1:61:A:GLU:HB2	1:62:A:LEU:H	4	0.16	0.01	0.16
(1,469)	1:61:A:GLU:HB3	1:62:A:LEU:H	4	0.16	0.01	0.16
(2,35)	1:58:A:ASP:O	1:62:A:LEU:H	4	0.14	0.02	0.14
(1,139)	1:60:A:ALA:HB1	1:61:A:GLU:HG2	3	0.17	0.03	0.15
(1,139)	1:60:A:ALA:HB1	1:61:A:GLU:HG3	3	0.17	0.03	0.15
(1,139)	1:60:A:ALA:HB2	1:61:A:GLU:HG2	3	0.17	0.03	0.15
(1,139)	1:60:A:ALA:HB2	1:61:A:GLU:HG3	3	0.17	0.03	0.15
(1,139)	1:60:A:ALA:HB3	1:61:A:GLU:HG2	3	0.17	0.03	0.15
(1,139)	1:60:A:ALA:HB3	1:61:A:GLU:HG3	3	0.17	0.03	0.15
(1,575)	1:74:A:LYS:H	1:74:A:LYS:HG2	3	0.17	0.01	0.18
(1,575)	1:74:A:LYS:H	1:74:A:LYS:HG3	3	0.17	0.01	0.18
(2,11)	1:16:A:LEU:O	1:20:A:SER:H	3	0.15	0.04	0.12
(2,1)	1:11:A:PRO:O	1:15:A:LEU:H	3	0.14	0.04	0.12
(1,482)	1:23:A:GLU:HB2	1:26:A:ASP:H	3	0.13	0.03	0.11
(1,46)	1:22:A:LEU:HA	1:26:A:ASP:HB2	3	0.13	0.03	0.12
(1,397)	1:10:A:LYS:H	1:11:A:PRO:HD2	3	0.13	0.01	0.13
(1,397)	1:10:A:LYS:H	1:11:A:PRO:HD3	3	0.13	0.01	0.13
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD11	3	0.12	0.01	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD12	3	0.12	0.01	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD13	3	0.12	0.01	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD21	3	0.12	0.01	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD22	3	0.12	0.01	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD23	3	0.12	0.01	0.11
(1,432)	1:55:A:ILE:H	1:58:A:ASP:HB2	2	0.3	0.01	0.3
(1,432)	1:55:A:ILE:H	1:58:A:ASP:HB3	2	0.3	0.01	0.3
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD11	2	0.18	0.01	0.18
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD12	2	0.18	0.01	0.18
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD13	2	0.18	0.01	0.18
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD21	2	0.18	0.01	0.18
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD22	2	0.18	0.01	0.18
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD23	2	0.18	0.01	0.18
(2,3)	1:12:A:ARG:O	1:16:A:LEU:H	2	0.14	0.01	0.14
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG11	2	0.13	0.02	0.13
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG12	2	0.13	0.02	0.13
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG13	2	0.13	0.02	0.13

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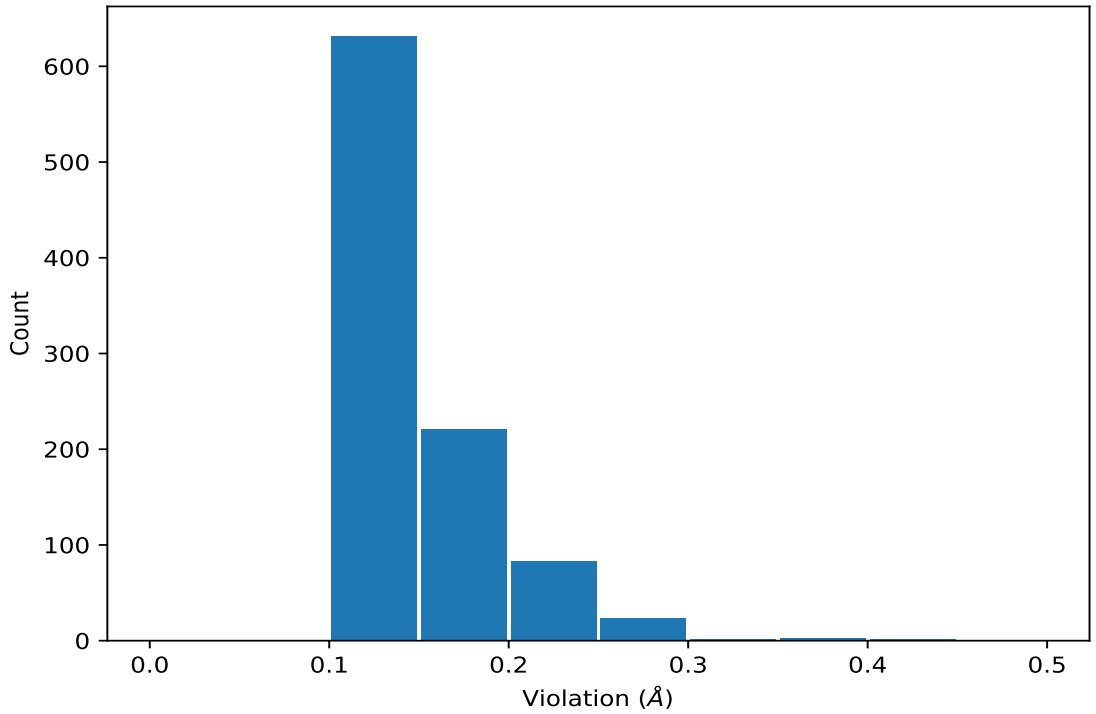
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG21	2	0.13	0.02	0.13
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG22	2	0.13	0.02	0.13
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG23	2	0.13	0.02	0.13
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG11	2	0.12	0.0	0.12
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG12	2	0.12	0.0	0.12
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG13	2	0.12	0.0	0.12
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG21	2	0.12	0.0	0.12
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG22	2	0.12	0.0	0.12
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG23	2	0.12	0.0	0.12
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG11	2	0.12	0.0	0.12
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG12	2	0.12	0.0	0.12
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG13	2	0.12	0.0	0.12
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG21	2	0.12	0.0	0.12
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG22	2	0.12	0.0	0.12
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG23	2	0.12	0.0	0.12
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG11	2	0.11	0.0	0.11
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG12	2	0.11	0.0	0.11
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG13	2	0.11	0.0	0.11
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG21	2	0.11	0.0	0.11
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG22	2	0.11	0.0	0.11
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG23	2	0.11	0.0	0.11
(2,65)	1:90:A:ASP:O	1:94:A:HIS:H	2	0.1	0.0	0.1

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:28:A:LYS:H	1:28:A:LYS:HB3	3	0.5
(1,497)	1:82:A:VAL:HB	1:83:A:MET:H	19	0.41
(1,497)	1:82:A:VAL:HB	1:83:A:MET:H	20	0.41
(1,497)	1:82:A:VAL:HB	1:83:A:MET:H	17	0.39
(1,497)	1:82:A:VAL:HB	1:83:A:MET:H	1	0.38
(1,497)	1:82:A:VAL:HB	1:83:A:MET:H	11	0.37
(1,497)	1:82:A:VAL:HB	1:83:A:MET:H	9	0.35
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	14	0.31
(1,432)	1:55:A:ILE:H	1:58:A:ASP:HB2	19	0.3
(1,432)	1:55:A:ILE:H	1:58:A:ASP:HB3	19	0.3
(1,160)	1:18:A:ALA:HB1	1:19:A:LEU:HG	16	0.3
(1,160)	1:18:A:ALA:HB2	1:19:A:LEU:HG	16	0.3
(1,160)	1:18:A:ALA:HB3	1:19:A:LEU:HG	16	0.3
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	15	0.3
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	15	0.3
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	15	0.3
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	15	0.3
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	15	0.3
(1,432)	1:55:A:ILE:H	1:58:A:ASP:HB2	18	0.29
(1,432)	1:55:A:ILE:H	1:58:A:ASP:HB3	18	0.29
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	2	0.28
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	20	0.27
(1,572)	1:31:A:LYS:HG2	1:32:A:PHE:H	13	0.26
(1,572)	1:31:A:LYS:HG3	1:32:A:PHE:H	13	0.26
(1,468)	1:19:A:LEU:H	1:19:A:LEU:HG	16	0.26
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	4	0.26
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	18	0.26
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	9	0.26
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	9	0.26
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	7	0.25
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	9	0.25
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	11	0.24
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	11	0.24
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	11	0.24
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	11	0.24
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	11	0.24
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	11	0.24
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	6	0.24
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	8	0.24
(1,238)	1:11:A:PRO:HA	1:14:A:ALA:HB1	17	0.23
(1,238)	1:11:A:PRO:HA	1:14:A:ALA:HB2	17	0.23
(1,238)	1:11:A:PRO:HA	1:14:A:ALA:HB3	17	0.23
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	5	0.23
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	19	0.23
(1,68)	1:11:A:PRO:HA	1:95:A:ILE:HG21	17	0.23
(1,68)	1:11:A:PRO:HA	1:95:A:ILE:HG22	17	0.23
(1,68)	1:11:A:PRO:HA	1:95:A:ILE:HG23	17	0.23
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	8	0.23
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	8	0.23
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	8	0.23
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	8	0.23
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	8	0.23
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	8	0.23
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD11	9	0.22
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD12	9	0.22
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD13	9	0.22
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD21	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD22	9	0.22
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD23	9	0.22
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD11	9	0.22
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD12	9	0.22
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD13	9	0.22
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD21	9	0.22
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD22	9	0.22
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD23	9	0.22
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD11	9	0.22
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD12	9	0.22
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD13	9	0.22
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD21	9	0.22
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD22	9	0.22
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD23	9	0.22
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	11	0.22
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	12	0.22
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	13	0.22
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	17	0.22
(1,139)	1:60:A:ALA:HB1	1:61:A:GLU:HG2	10	0.22
(1,139)	1:60:A:ALA:HB1	1:61:A:GLU:HG3	10	0.22
(1,139)	1:60:A:ALA:HB2	1:61:A:GLU:HG2	10	0.22
(1,139)	1:60:A:ALA:HB2	1:61:A:GLU:HG3	10	0.22
(1,139)	1:60:A:ALA:HB3	1:61:A:GLU:HG2	10	0.22
(1,139)	1:60:A:ALA:HB3	1:61:A:GLU:HG3	10	0.22
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	16	0.21
(2,11)	1:16:A:LEU:O	1:20:A:SER:H	16	0.21
(1,612)	1:88:A:LEU:HD11	1:90:A:ASP:H	10	0.21
(1,612)	1:88:A:LEU:HD12	1:90:A:ASP:H	10	0.21
(1,612)	1:88:A:LEU:HD13	1:90:A:ASP:H	10	0.21
(1,372)	1:25:A:ASN:HA	1:29:A:LYS:H	11	0.21
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	1	0.21
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	15	0.21
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	16	0.21
(1,53)	1:81:A:LYS:HA	1:84:A:ASN:HA	11	0.21
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	8	0.2
(2,1)	1:11:A:PRO:O	1:15:A:LEU:H	17	0.2
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	3	0.2
(1,147)	1:70:A:LYS:HA	1:73:A:VAL:HB	10	0.2
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	10	0.2
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	10	0.2
(1,113)	1:27:A:PHE:HB2	1:30:A:LEU:HG	11	0.2
(1,113)	1:27:A:PHE:HB3	1:30:A:LEU:HG	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	13	0.2
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	13	0.2
(1,53)	1:81:A:LYS:HA	1:84:A:ASN:HA	12	0.2
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	12	0.2
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	12	0.2
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	12	0.2
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	12	0.2
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	12	0.2
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	12	0.2
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	13	0.2
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	13	0.2
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	13	0.2
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	13	0.2
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	13	0.2
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	13	0.2
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	11	0.19
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	13	0.19
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	4	0.19
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	15	0.19
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	17	0.19
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD11	17	0.19
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD12	17	0.19
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD13	17	0.19
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD21	17	0.19
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD22	17	0.19
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD23	17	0.19
(1,217)	1:78:A:LYS:HA	1:78:A:LYS:HD2	9	0.19
(1,217)	1:78:A:LYS:HA	1:78:A:LYS:HD3	9	0.19
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	16	0.19
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	16	0.19
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	15	0.18
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	6	0.18
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	3	0.18
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	9	0.18
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	18	0.18
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	19	0.18
(1,827)	1:88:A:LEU:HA	1:91:A:GLN:HB2	14	0.18
(1,827)	1:88:A:LEU:HA	1:91:A:GLN:HB3	14	0.18
(1,612)	1:88:A:LEU:HD11	1:90:A:ASP:H	8	0.18
(1,612)	1:88:A:LEU:HD12	1:90:A:ASP:H	8	0.18
(1,612)	1:88:A:LEU:HD13	1:90:A:ASP:H	8	0.18
(1,575)	1:74:A:LYS:H	1:74:A:LYS:HG2	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,575)	1:74:A:LYS:H	1:74:A:LYS:HG3	6	0.18
(1,575)	1:74:A:LYS:H	1:74:A:LYS:HG2	20	0.18
(1,575)	1:74:A:LYS:H	1:74:A:LYS:HG3	20	0.18
(1,482)	1:23:A:GLU:HB2	1:26:A:ASP:H	3	0.18
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD11	7	0.18
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD12	7	0.18
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD13	7	0.18
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD21	7	0.18
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD22	7	0.18
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD23	7	0.18
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD11	7	0.18
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD12	7	0.18
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD13	7	0.18
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD21	7	0.18
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD22	7	0.18
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD23	7	0.18
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD11	7	0.18
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD12	7	0.18
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD13	7	0.18
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD21	7	0.18
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD22	7	0.18
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD23	7	0.18
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD11	13	0.18
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD12	13	0.18
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD13	13	0.18
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD21	13	0.18
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD22	13	0.18
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD23	13	0.18
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD11	13	0.18
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD12	13	0.18
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD13	13	0.18
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD21	13	0.18
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD22	13	0.18
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD23	13	0.18
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD11	13	0.18
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD12	13	0.18
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD13	13	0.18
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD21	13	0.18
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD22	13	0.18
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD23	13	0.18
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	18	0.18
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	18	0.18
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	18	0.18
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	18	0.18
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	18	0.18
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	20	0.18
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	20	0.18
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	20	0.18
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	20	0.18
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	20	0.18
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	20	0.18
(2,69)	1:88:A:LEU:O	1:92:A:LEU:H	2	0.17
(2,69)	1:88:A:LEU:O	1:92:A:LEU:H	11	0.17
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	3	0.17
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	8	0.17
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	14	0.17
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	9	0.17
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	20	0.17
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	14	0.17
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	15	0.17
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	3	0.17
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	3	0.17
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	3	0.17
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	3	0.17
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	3	0.17
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	3	0.17
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD11	10	0.17
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD12	10	0.17
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD13	10	0.17
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD21	10	0.17
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD22	10	0.17
(1,647)	1:16:A:LEU:HA	1:16:A:LEU:HD23	10	0.17
(1,612)	1:88:A:LEU:HD11	1:90:A:ASP:H	2	0.17
(1,612)	1:88:A:LEU:HD12	1:90:A:ASP:H	2	0.17
(1,612)	1:88:A:LEU:HD13	1:90:A:ASP:H	2	0.17
(1,578)	1:31:A:LYS:HG2	1:35:A:ARG:H	12	0.17
(1,578)	1:31:A:LYS:HG3	1:35:A:ARG:H	12	0.17
(1,469)	1:61:A:GLU:HB2	1:62:A:LEU:H	16	0.17
(1,469)	1:61:A:GLU:HB3	1:62:A:LEU:H	16	0.17
(1,372)	1:25:A:ASN:HA	1:29:A:LYS:H	15	0.17
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	8	0.17
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	8	0.17
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	12	0.17
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	13	0.17
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	13	0.17
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	7	0.17
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	7	0.17
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	15	0.17
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	15	0.17
(1,46)	1:22:A:LEU:HA	1:26:A:ASP:HB2	3	0.17
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	10	0.17
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	10	0.17
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	10	0.17
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	10	0.17
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	10	0.17
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	10	0.17
(2,69)	1:88:A:LEU:O	1:92:A:LEU:H	1	0.16
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	1	0.16
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	5	0.16
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	10	0.16
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	18	0.16
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	1	0.16
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	12	0.16
(2,35)	1:58:A:ASP:O	1:62:A:LEU:H	18	0.16
(2,35)	1:58:A:ASP:O	1:62:A:LEU:H	19	0.16
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	5	0.16
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	5	0.16
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	5	0.16
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	5	0.16
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	5	0.16
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	5	0.16
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	15	0.16
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	15	0.16
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	15	0.16
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	15	0.16
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	15	0.16
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	15	0.16
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	17	0.16
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	17	0.16
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	17	0.16
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	17	0.16
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	17	0.16
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	17	0.16
(1,612)	1:88:A:LEU:HD11	1:90:A:ASP:H	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,612)	1:88:A:LEU:HD12	1:90:A:ASP:H	11	0.16
(1,612)	1:88:A:LEU:HD13	1:90:A:ASP:H	11	0.16
(1,578)	1:31:A:LYS:HG2	1:35:A:ARG:H	9	0.16
(1,578)	1:31:A:LYS:HG3	1:35:A:ARG:H	9	0.16
(1,575)	1:74:A:LYS:H	1:74:A:LYS:HG2	2	0.16
(1,575)	1:74:A:LYS:H	1:74:A:LYS:HG3	2	0.16
(1,469)	1:61:A:GLU:HB2	1:62:A:LEU:H	8	0.16
(1,469)	1:61:A:GLU:HB3	1:62:A:LEU:H	8	0.16
(1,469)	1:61:A:GLU:HB2	1:62:A:LEU:H	10	0.16
(1,469)	1:61:A:GLU:HB3	1:62:A:LEU:H	10	0.16
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD11	2	0.16
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD12	2	0.16
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD13	2	0.16
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD21	2	0.16
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD22	2	0.16
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD23	2	0.16
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD11	2	0.16
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD12	2	0.16
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD13	2	0.16
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD21	2	0.16
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD22	2	0.16
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD23	2	0.16
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD11	2	0.16
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD12	2	0.16
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD13	2	0.16
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD21	2	0.16
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD22	2	0.16
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD23	2	0.16
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	2	0.16
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	2	0.16
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	3	0.16
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	3	0.16
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	14	0.16
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	14	0.16
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	17	0.16
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	17	0.16
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	20	0.16
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	20	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	3	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	3	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	3	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	3	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	3	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	4	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	4	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	4	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	4	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	4	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	4	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	5	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	5	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	5	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	5	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	5	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	5	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	11	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	11	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	11	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	11	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	11	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	11	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	19	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	19	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	19	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	19	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	19	0.16
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	19	0.16
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	2	0.15
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	14	0.15
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	19	0.15
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	2	0.15
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	6	0.15
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	12	0.15
(2,3)	1:12:A:ARG:O	1:16:A:LEU:H	4	0.15
(1,811)	1:78:A:LYS:HB2	1:101:A:ARG:HB2	7	0.15
(1,811)	1:78:A:LYS:HB2	1:101:A:ARG:HB3	7	0.15
(1,811)	1:78:A:LYS:HB3	1:101:A:ARG:HB2	7	0.15
(1,811)	1:78:A:LYS:HB3	1:101:A:ARG:HB3	7	0.15
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	1	0.15
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	1	0.15
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	1	0.15
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	1	0.15
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	1	0.15
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG11	8	0.15
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG12	8	0.15
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG13	8	0.15
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG21	8	0.15
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG22	8	0.15
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG23	8	0.15
(1,621)	1:82:A:VAL:HG21	1:83:A:MET:H	11	0.15
(1,621)	1:82:A:VAL:HG22	1:83:A:MET:H	11	0.15
(1,621)	1:82:A:VAL:HG23	1:83:A:MET:H	11	0.15
(1,612)	1:88:A:LEU:HD11	1:90:A:ASP:H	1	0.15
(1,612)	1:88:A:LEU:HD12	1:90:A:ASP:H	1	0.15
(1,612)	1:88:A:LEU:HD13	1:90:A:ASP:H	1	0.15
(1,578)	1:31:A:LYS:HG2	1:35:A:ARG:H	17	0.15
(1,578)	1:31:A:LYS:HG3	1:35:A:ARG:H	17	0.15
(1,469)	1:61:A:GLU:HB2	1:62:A:LEU:H	1	0.15
(1,469)	1:61:A:GLU:HB3	1:62:A:LEU:H	1	0.15
(1,447)	1:23:A:GLU:HB3	1:26:A:ASP:H	3	0.15
(1,372)	1:25:A:ASN:HA	1:29:A:LYS:H	6	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD11	8	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD12	8	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD13	8	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD21	8	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD22	8	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD23	8	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD11	8	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD12	8	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD13	8	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD21	8	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD22	8	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD23	8	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD11	8	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD12	8	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD13	8	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD21	8	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD22	8	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD23	8	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD11	20	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD12	20	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD13	20	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD21	20	0.15
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD22	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD23	20	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD11	20	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD12	20	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD13	20	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD21	20	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD22	20	0.15
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD23	20	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD11	20	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD12	20	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD13	20	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD21	20	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD22	20	0.15
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD23	20	0.15
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG21	14	0.15
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG22	14	0.15
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG23	14	0.15
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG21	14	0.15
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG22	14	0.15
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG23	14	0.15
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG21	14	0.15
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG22	14	0.15
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG23	14	0.15
(1,139)	1:60:A:ALA:HB1	1:61:A:GLU:HG2	8	0.15
(1,139)	1:60:A:ALA:HB1	1:61:A:GLU:HG3	8	0.15
(1,139)	1:60:A:ALA:HB2	1:61:A:GLU:HG2	8	0.15
(1,139)	1:60:A:ALA:HB2	1:61:A:GLU:HG3	8	0.15
(1,139)	1:60:A:ALA:HB3	1:61:A:GLU:HG2	8	0.15
(1,139)	1:60:A:ALA:HB3	1:61:A:GLU:HG3	8	0.15
(1,139)	1:60:A:ALA:HB1	1:61:A:GLU:HG2	16	0.15
(1,139)	1:60:A:ALA:HB1	1:61:A:GLU:HG3	16	0.15
(1,139)	1:60:A:ALA:HB2	1:61:A:GLU:HG2	16	0.15
(1,139)	1:60:A:ALA:HB2	1:61:A:GLU:HG3	16	0.15
(1,139)	1:60:A:ALA:HB3	1:61:A:GLU:HG2	16	0.15
(1,139)	1:60:A:ALA:HB3	1:61:A:GLU:HG3	16	0.15
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	6	0.15
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	6	0.15
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	7	0.15
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	7	0.15
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	11	0.15
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	11	0.15
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	2	0.15
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	18	0.15
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	18	0.15
(2,69)	1:88:A:LEU:O	1:92:A:LEU:H	20	0.14
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	7	0.14
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	9	0.14
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	12	0.14
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	16	0.14
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	17	0.14
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	7	0.14
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	1	0.14
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	5	0.14
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	10	0.14
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	11	0.14
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	13	0.14
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	17	0.14
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	10	0.14
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	10	0.14
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	10	0.14
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	10	0.14
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	10	0.14
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	10	0.14
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	13	0.14
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	13	0.14
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	13	0.14
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	13	0.14
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	13	0.14
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	13	0.14
(1,621)	1:82:A:VAL:HG21	1:83:A:MET:H	9	0.14
(1,621)	1:82:A:VAL:HG22	1:83:A:MET:H	9	0.14
(1,621)	1:82:A:VAL:HG23	1:83:A:MET:H	9	0.14
(1,621)	1:82:A:VAL:HG21	1:83:A:MET:H	17	0.14
(1,621)	1:82:A:VAL:HG22	1:83:A:MET:H	17	0.14
(1,621)	1:82:A:VAL:HG23	1:83:A:MET:H	17	0.14
(1,578)	1:31:A:LYS:HG2	1:35:A:ARG:H	2	0.14
(1,578)	1:31:A:LYS:HG3	1:35:A:ARG:H	2	0.14
(1,546)	1:88:A:LEU:H	1:88:A:LEU:HG	13	0.14
(1,546)	1:88:A:LEU:H	1:88:A:LEU:HG	15	0.14
(1,546)	1:88:A:LEU:H	1:88:A:LEU:HG	18	0.14
(1,397)	1:10:A:LYS:H	1:11:A:PRO:HD2	2	0.14
(1,397)	1:10:A:LYS:H	1:11:A:PRO:HD3	2	0.14
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG21	15	0.14
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG22	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG23	15	0.14
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG21	15	0.14
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG22	15	0.14
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG23	15	0.14
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG21	15	0.14
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG22	15	0.14
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG23	15	0.14
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG21	19	0.14
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG22	19	0.14
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG23	19	0.14
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG21	19	0.14
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG22	19	0.14
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG23	19	0.14
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG21	19	0.14
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG22	19	0.14
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG23	19	0.14
(1,203)	1:28:A:LYS:HG2	1:29:A:LYS:HD2	3	0.14
(1,203)	1:28:A:LYS:HG2	1:29:A:LYS:HD3	3	0.14
(1,203)	1:28:A:LYS:HG3	1:29:A:LYS:HD2	3	0.14
(1,203)	1:28:A:LYS:HG3	1:29:A:LYS:HD3	3	0.14
(1,200)	1:10:A:LYS:HA	1:10:A:LYS:HD2	17	0.14
(1,200)	1:10:A:LYS:HA	1:10:A:LYS:HD3	17	0.14
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	1	0.14
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	1	0.14
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	9	0.14
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	9	0.14
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	15	0.14
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	15	0.14
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	17	0.14
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	17	0.14
(1,82)	1:19:A:LEU:HA	1:22:A:LEU:HB3	11	0.14
(1,53)	1:81:A:LYS:HA	1:84:A:ASN:HA	1	0.14
(1,42)	1:92:A:LEU:HD21	1:96:A:CYS:HA	17	0.14
(1,42)	1:92:A:LEU:HD22	1:96:A:CYS:HA	17	0.14
(1,42)	1:92:A:LEU:HD23	1:96:A:CYS:HA	17	0.14
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	1	0.14
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	1	0.14
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	1	0.14
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	1	0.14
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	1	0.14
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	1	0.14
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	6	0.14
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	6	0.14
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	6	0.14
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	6	0.14
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	6	0.14
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD11	19	0.14
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD12	19	0.14
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD13	19	0.14
(2,69)	1:88:A:LEU:O	1:92:A:LEU:H	10	0.13
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	4	0.13
(2,57)	1:75:A:VAL:O	1:79:A:GLY:H	6	0.13
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	3	0.13
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	11	0.13
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	18	0.13
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	4	0.13
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	7	0.13
(2,3)	1:12:A:ARG:O	1:16:A:LEU:H	20	0.13
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD11	6	0.13
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD12	6	0.13
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD13	6	0.13
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD21	6	0.13
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD22	6	0.13
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD23	6	0.13
(1,621)	1:82:A:VAL:HG21	1:83:A:MET:H	1	0.13
(1,621)	1:82:A:VAL:HG22	1:83:A:MET:H	1	0.13
(1,621)	1:82:A:VAL:HG23	1:83:A:MET:H	1	0.13
(1,621)	1:82:A:VAL:HG21	1:83:A:MET:H	19	0.13
(1,621)	1:82:A:VAL:HG22	1:83:A:MET:H	19	0.13
(1,621)	1:82:A:VAL:HG23	1:83:A:MET:H	19	0.13
(1,621)	1:82:A:VAL:HG21	1:83:A:MET:H	20	0.13
(1,621)	1:82:A:VAL:HG22	1:83:A:MET:H	20	0.13
(1,621)	1:82:A:VAL:HG23	1:83:A:MET:H	20	0.13
(1,578)	1:31:A:LYS:HG2	1:35:A:ARG:H	14	0.13
(1,578)	1:31:A:LYS:HG3	1:35:A:ARG:H	14	0.13
(1,578)	1:31:A:LYS:HG2	1:35:A:ARG:H	19	0.13
(1,578)	1:31:A:LYS:HG3	1:35:A:ARG:H	19	0.13
(1,549)	1:70:A:LYS:H	1:70:A:LYS:HD2	19	0.13
(1,549)	1:70:A:LYS:H	1:70:A:LYS:HD3	19	0.13
(1,397)	1:10:A:LYS:H	1:11:A:PRO:HD2	18	0.13
(1,397)	1:10:A:LYS:H	1:11:A:PRO:HD3	18	0.13
(1,372)	1:25:A:ASN:HA	1:29:A:LYS:H	7	0.13
(1,372)	1:25:A:ASN:HA	1:29:A:LYS:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,372)	1:25:A:ASN:HA	1:29:A:LYS:H	13	0.13
(1,300)	1:31:A:LYS:HD2	1:75:A:VAL:HG21	5	0.13
(1,300)	1:31:A:LYS:HD2	1:75:A:VAL:HG22	5	0.13
(1,300)	1:31:A:LYS:HD2	1:75:A:VAL:HG23	5	0.13
(1,300)	1:31:A:LYS:HD3	1:75:A:VAL:HG21	5	0.13
(1,300)	1:31:A:LYS:HD3	1:75:A:VAL:HG22	5	0.13
(1,300)	1:31:A:LYS:HD3	1:75:A:VAL:HG23	5	0.13
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD11	10	0.13
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD12	10	0.13
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD13	10	0.13
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD21	10	0.13
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD22	10	0.13
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD23	10	0.13
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD11	10	0.13
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD12	10	0.13
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD13	10	0.13
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD21	10	0.13
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD22	10	0.13
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD23	10	0.13
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD11	10	0.13
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD12	10	0.13
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD13	10	0.13
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD21	10	0.13
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD22	10	0.13
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD23	10	0.13
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	4	0.13
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	4	0.13
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	4	0.13
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	4	0.13
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	14	0.13
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	14	0.13
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	20	0.13
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	20	0.13
(1,53)	1:81:A:LYS:HA	1:84:A:ASN:HA	15	0.13
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	14	0.13
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	14	0.13
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	14	0.13
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	14	0.13
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	14	0.13
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	14	0.13
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	16	0.13
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	16	0.13
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	16	0.13
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	16	0.13
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	16	0.13
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD11	1	0.13
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD12	1	0.13
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD13	1	0.13
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD11	17	0.13
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD12	17	0.13
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD13	17	0.13
(2,69)	1:88:A:LEU:O	1:92:A:LEU:H	7	0.12
(2,69)	1:88:A:LEU:O	1:92:A:LEU:H	8	0.12
(2,69)	1:88:A:LEU:O	1:92:A:LEU:H	15	0.12
(2,35)	1:58:A:ASP:O	1:62:A:LEU:H	13	0.12
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	20	0.12
(2,11)	1:16:A:LEU:O	1:20:A:SER:H	10	0.12
(2,11)	1:16:A:LEU:O	1:20:A:SER:H	17	0.12
(2,1)	1:11:A:PRO:O	1:15:A:LEU:H	6	0.12
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG11	6	0.12
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG12	6	0.12
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG13	6	0.12
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG21	6	0.12
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG22	6	0.12
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG23	6	0.12
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG11	6	0.12
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG12	6	0.12
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG13	6	0.12
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG21	6	0.12
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG22	6	0.12
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG23	6	0.12
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	6	0.12
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	6	0.12
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	6	0.12
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	6	0.12
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	6	0.12
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	6	0.12
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	8	0.12
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	8	0.12
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	8	0.12
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	8	0.12
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	8	0.12
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	18	0.12
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	18	0.12
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	18	0.12
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	18	0.12
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	18	0.12
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	18	0.12
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	19	0.12
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	19	0.12
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	19	0.12
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	19	0.12
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	19	0.12
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	19	0.12
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	20	0.12
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	20	0.12
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	20	0.12
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	20	0.12
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	20	0.12
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	20	0.12
(1,546)	1:88:A:LEU:H	1:88:A:LEU:HG	4	0.12
(1,500)	1:31:A:LYS:HD2	1:32:A:PHE:H	8	0.12
(1,500)	1:31:A:LYS:HD3	1:32:A:PHE:H	8	0.12
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD11	3	0.12
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD12	3	0.12
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD13	3	0.12
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD21	3	0.12
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD22	3	0.12
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD23	3	0.12
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD11	3	0.12
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD12	3	0.12
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD13	3	0.12
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD21	3	0.12
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD22	3	0.12
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD23	3	0.12
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD11	3	0.12
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD12	3	0.12
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD13	3	0.12
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD21	3	0.12
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD22	3	0.12
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD23	3	0.12
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD11	17	0.12
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD12	17	0.12
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD13	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD21	17	0.12
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD22	17	0.12
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD23	17	0.12
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD11	17	0.12
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD12	17	0.12
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD13	17	0.12
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD21	17	0.12
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD22	17	0.12
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD23	17	0.12
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD11	17	0.12
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD12	17	0.12
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD13	17	0.12
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD21	17	0.12
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD22	17	0.12
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD23	17	0.12
(1,250)	1:30:A:LEU:HD11	1:80:A:LEU:HG	12	0.12
(1,250)	1:30:A:LEU:HD12	1:80:A:LEU:HG	12	0.12
(1,250)	1:30:A:LEU:HD13	1:80:A:LEU:HG	12	0.12
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG21	7	0.12
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG22	7	0.12
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG23	7	0.12
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG21	7	0.12
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG22	7	0.12
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG23	7	0.12
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG21	7	0.12
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG22	7	0.12
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG23	7	0.12
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG21	11	0.12
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG22	11	0.12
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG23	11	0.12
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG21	11	0.12
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG22	11	0.12
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG23	11	0.12
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG21	11	0.12
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG22	11	0.12
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG23	11	0.12
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG21	12	0.12
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG22	12	0.12
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG23	12	0.12
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG21	12	0.12
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG22	12	0.12
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG23	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG21	12	0.12
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG22	12	0.12
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG23	12	0.12
(1,166)	1:30:A:LEU:HG	1:83:A:MET:HE1	15	0.12
(1,166)	1:30:A:LEU:HG	1:83:A:MET:HE2	15	0.12
(1,166)	1:30:A:LEU:HG	1:83:A:MET:HE3	15	0.12
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB2	5	0.12
(1,131)	1:54:A:LEU:HA	1:58:A:ASP:HB3	5	0.12
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	3	0.12
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	3	0.12
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	16	0.12
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	16	0.12
(1,46)	1:22:A:LEU:HA	1:26:A:ASP:HB2	7	0.12
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	2	0.12
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	2	0.12
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	2	0.12
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	2	0.12
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	2	0.12
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	2	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD11	3	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD12	3	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD13	3	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD11	7	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD12	7	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD13	7	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD11	11	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD12	11	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD13	11	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD11	20	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD12	20	0.12
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD13	20	0.12
(2,69)	1:88:A:LEU:O	1:92:A:LEU:H	12	0.11
(2,69)	1:88:A:LEU:O	1:92:A:LEU:H	13	0.11
(2,69)	1:88:A:LEU:O	1:92:A:LEU:H	17	0.11
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	5	0.11
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	13	0.11
(2,51)	1:72:A:ALA:O	1:76:A:VAL:H	16	0.11
(2,35)	1:58:A:ASP:O	1:62:A:LEU:H	20	0.11
(2,28)	1:32:A:PHE:O	1:36:A:ASP:N	8	0.11
(2,1)	1:11:A:PRO:O	1:15:A:LEU:H	9	0.11
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG11	20	0.11
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG12	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG13	20	0.11
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG21	20	0.11
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG22	20	0.11
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG23	20	0.11
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG11	2	0.11
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG12	2	0.11
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG13	2	0.11
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG21	2	0.11
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG22	2	0.11
(1,799)	1:74:A:LYS:HB2	1:75:A:VAL:HG23	2	0.11
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG11	2	0.11
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG12	2	0.11
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG13	2	0.11
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG21	2	0.11
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG22	2	0.11
(1,799)	1:74:A:LYS:HB3	1:75:A:VAL:HG23	2	0.11
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	12	0.11
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	12	0.11
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	12	0.11
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	12	0.11
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	12	0.11
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	12	0.11
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG11	7	0.11
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG12	7	0.11
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG13	7	0.11
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG21	7	0.11
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG22	7	0.11
(1,711)	1:31:A:LYS:HA	1:75:A:VAL:HG23	7	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD11	11	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD12	11	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD13	11	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD21	11	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD22	11	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD23	11	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD11	15	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD12	15	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD13	15	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD21	15	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD22	15	0.11
(1,676)	1:22:A:LEU:HB2	1:51:A:LEU:HD23	15	0.11
(1,627)	1:9:A:ARG:HB2	1:95:A:ILE:HG21	17	0.11
(1,627)	1:9:A:ARG:HB2	1:95:A:ILE:HG22	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,627)	1:9:A:ARG:HB2	1:95:A:ILE:HG23	17	0.11
(1,627)	1:9:A:ARG:HB3	1:95:A:ILE:HG21	17	0.11
(1,627)	1:9:A:ARG:HB3	1:95:A:ILE:HG22	17	0.11
(1,627)	1:9:A:ARG:HB3	1:95:A:ILE:HG23	17	0.11
(1,578)	1:31:A:LYS:HG2	1:35:A:ARG:H	7	0.11
(1,578)	1:31:A:LYS:HG3	1:35:A:ARG:H	7	0.11
(1,546)	1:88:A:LEU:H	1:88:A:LEU:HG	16	0.11
(1,500)	1:31:A:LYS:HD2	1:32:A:PHE:H	7	0.11
(1,500)	1:31:A:LYS:HD3	1:32:A:PHE:H	7	0.11
(1,500)	1:31:A:LYS:HD2	1:32:A:PHE:H	20	0.11
(1,500)	1:31:A:LYS:HD3	1:32:A:PHE:H	20	0.11
(1,482)	1:23:A:GLU:HB2	1:26:A:ASP:H	4	0.11
(1,482)	1:23:A:GLU:HB2	1:26:A:ASP:H	15	0.11
(1,397)	1:10:A:LYS:H	1:11:A:PRO:HD2	13	0.11
(1,397)	1:10:A:LYS:H	1:11:A:PRO:HD3	13	0.11
(1,375)	1:9:A:ARG:HA	1:10:A:LYS:H	3	0.11
(1,372)	1:25:A:ASN:HA	1:29:A:LYS:H	4	0.11
(1,372)	1:25:A:ASN:HA	1:29:A:LYS:H	5	0.11
(1,372)	1:25:A:ASN:HA	1:29:A:LYS:H	10	0.11
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD11	1	0.11
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD12	1	0.11
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD13	1	0.11
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD21	1	0.11
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD22	1	0.11
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD23	1	0.11
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD11	1	0.11
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD12	1	0.11
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD13	1	0.11
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD21	1	0.11
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD22	1	0.11
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD23	1	0.11
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD11	1	0.11
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD12	1	0.11
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD13	1	0.11
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD21	1	0.11
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD22	1	0.11
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD23	1	0.11
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG21	18	0.11
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG22	18	0.11
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG23	18	0.11
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG21	18	0.11
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG22	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG23	18	0.11
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG21	18	0.11
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG22	18	0.11
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG23	18	0.11
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG21	20	0.11
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG22	20	0.11
(1,242)	1:18:A:ALA:HB1	1:76:A:VAL:HG23	20	0.11
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG21	20	0.11
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG22	20	0.11
(1,242)	1:18:A:ALA:HB2	1:76:A:VAL:HG23	20	0.11
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG21	20	0.11
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG22	20	0.11
(1,242)	1:18:A:ALA:HB3	1:76:A:VAL:HG23	20	0.11
(1,237)	1:18:A:ALA:HB1	1:92:A:LEU:HA	20	0.11
(1,237)	1:18:A:ALA:HB2	1:92:A:LEU:HA	20	0.11
(1,237)	1:18:A:ALA:HB3	1:92:A:LEU:HA	20	0.11
(1,163)	1:58:A:ASP:HA	1:61:A:GLU:HB2	10	0.11
(1,163)	1:58:A:ASP:HA	1:61:A:GLU:HB3	10	0.11
(1,156)	1:88:A:LEU:HD21	1:89:A:VAL:HB	10	0.11
(1,156)	1:88:A:LEU:HD22	1:89:A:VAL:HB	10	0.11
(1,156)	1:88:A:LEU:HD23	1:89:A:VAL:HB	10	0.11
(1,93)	1:11:A:PRO:HD2	1:95:A:ILE:HG21	6	0.11
(1,93)	1:11:A:PRO:HD2	1:95:A:ILE:HG22	6	0.11
(1,93)	1:11:A:PRO:HD2	1:95:A:ILE:HG23	6	0.11
(1,93)	1:11:A:PRO:HD3	1:95:A:ILE:HG21	6	0.11
(1,93)	1:11:A:PRO:HD3	1:95:A:ILE:HG22	6	0.11
(1,93)	1:11:A:PRO:HD3	1:95:A:ILE:HG23	6	0.11
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	9	0.11
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	9	0.11
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	9	0.11
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	9	0.11
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	9	0.11
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	9	0.11
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD11	4	0.11
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD12	4	0.11
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD13	4	0.11
(2,65)	1:90:A:ASP:O	1:94:A:HIS:H	17	0.1
(2,65)	1:90:A:ASP:O	1:94:A:HIS:H	20	0.1
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG11	17	0.1
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG12	17	0.1
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG13	17	0.1
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG21	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG22	17	0.1
(1,815)	1:80:A:LEU:H	1:82:A:VAL:HG23	17	0.1
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	4	0.1
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	4	0.1
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	4	0.1
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	4	0.1
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	4	0.1
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	4	0.1
(1,738)	1:39:A:LEU:HD11	1:75:A:VAL:H	9	0.1
(1,738)	1:39:A:LEU:HD12	1:75:A:VAL:H	9	0.1
(1,738)	1:39:A:LEU:HD13	1:75:A:VAL:H	9	0.1
(1,738)	1:39:A:LEU:HD21	1:75:A:VAL:H	9	0.1
(1,738)	1:39:A:LEU:HD22	1:75:A:VAL:H	9	0.1
(1,738)	1:39:A:LEU:HD23	1:75:A:VAL:H	9	0.1
(1,578)	1:31:A:LYS:HG2	1:35:A:ARG:H	16	0.1
(1,578)	1:31:A:LYS:HG3	1:35:A:ARG:H	16	0.1
(1,546)	1:88:A:LEU:H	1:88:A:LEU:HG	3	0.1
(1,546)	1:88:A:LEU:H	1:88:A:LEU:HG	5	0.1
(1,546)	1:88:A:LEU:H	1:88:A:LEU:HG	7	0.1
(1,500)	1:31:A:LYS:HD2	1:32:A:PHE:H	2	0.1
(1,500)	1:31:A:LYS:HD3	1:32:A:PHE:H	2	0.1
(1,500)	1:31:A:LYS:HD2	1:32:A:PHE:H	4	0.1
(1,500)	1:31:A:LYS:HD3	1:32:A:PHE:H	4	0.1
(1,500)	1:31:A:LYS:HD2	1:32:A:PHE:H	16	0.1
(1,500)	1:31:A:LYS:HD3	1:32:A:PHE:H	16	0.1
(1,372)	1:25:A:ASN:HA	1:29:A:LYS:H	2	0.1
(1,315)	1:28:A:LYS:H	1:30:A:LEU:H	11	0.1
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD11	16	0.1
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD12	16	0.1
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD13	16	0.1
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD21	16	0.1
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD22	16	0.1
(1,272)	1:83:A:MET:HE1	1:85:A:LEU:HD23	16	0.1
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD11	16	0.1
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD12	16	0.1
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD13	16	0.1
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD21	16	0.1
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD22	16	0.1
(1,272)	1:83:A:MET:HE2	1:85:A:LEU:HD23	16	0.1
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD11	16	0.1
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD12	16	0.1
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD13	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD21	16	0.1
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD22	16	0.1
(1,272)	1:83:A:MET:HE3	1:85:A:LEU:HD23	16	0.1
(1,178)	1:55:A:ILE:HG21	1:57:A:VAL:HB	10	0.1
(1,178)	1:55:A:ILE:HG22	1:57:A:VAL:HB	10	0.1
(1,178)	1:55:A:ILE:HG23	1:57:A:VAL:HB	10	0.1
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	6	0.1
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	6	0.1
(1,92)	1:31:A:LYS:HB2	1:35:A:ARG:HA	8	0.1
(1,92)	1:31:A:LYS:HB3	1:35:A:ARG:HA	8	0.1
(1,53)	1:81:A:LYS:HA	1:84:A:ASN:HA	2	0.1
(1,46)	1:22:A:LEU:HA	1:26:A:ASP:HB2	9	0.1
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD11	7	0.1
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD12	7	0.1
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD13	7	0.1
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD21	7	0.1
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD22	7	0.1
(1,30)	1:26:A:ASP:H	1:85:A:LEU:HD23	7	0.1
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD11	6	0.1
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD12	6	0.1
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD13	6	0.1
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD11	12	0.1
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD12	12	0.1
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD13	12	0.1
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD11	14	0.1
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD12	14	0.1
(1,7)	1:92:A:LEU:H	1:92:A:LEU:HD13	14	0.1

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found