Full wwPDB NMR Structure Validation Report ⓘ

Jun 4, 2023 – 10:08 AM EDT

PDB ID	:	2N9P
BMRB ID	:	25914
Title	:	Solution structure of RNF126 N-terminal zinc finger domain in complex with BAG6 Ubiquitin-like domain
Authors	:	Martinez-Lumbreras, S.; Krysztofinska, E.M.; Thapaliya, A.; Isaacson, R.L.
Deposited on	:	2015-12-01

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

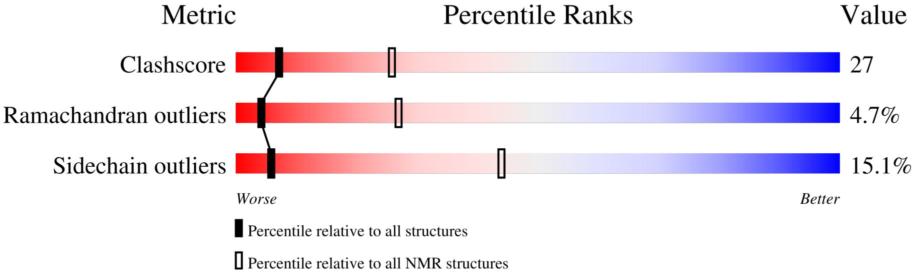
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

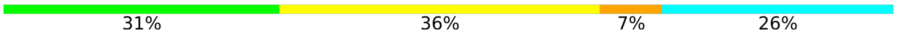
The overall completeness of chemical shifts assignment is 86%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	42	
2	C	100	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 10 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:10-A:40, C:16-C:23, C:28-C:85 (97)	0.61	10

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

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

The models can be grouped into 2 clusters and 5 single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2220 atoms, of which 1101 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase RNF126.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	42	630	204	304	55	61	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9BV68
A	0	SER	-	expression tag	UNP Q9BV68

- Molecule 2 is a protein called Large proline-rich protein BAG6.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	C	100	1589	493	797	147	149	3	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	MET	-	expression tag	UNP P46379
C	3	ALA	-	expression tag	UNP P46379
C	4	HIS	-	expression tag	UNP P46379
C	5	HIS	-	expression tag	UNP P46379
C	6	HIS	-	expression tag	UNP P46379
C	7	HIS	-	expression tag	UNP P46379
C	8	HIS	-	expression tag	UNP P46379
C	9	HIS	-	expression tag	UNP P46379
C	10	VAL	-	expression tag	UNP P46379
C	11	ASP	-	expression tag	UNP P46379
C	12	ASP	-	expression tag	UNP P46379
C	13	ASP	-	expression tag	UNP P46379
C	14	ASP	-	expression tag	UNP P46379
C	15	LYS	-	expression tag	UNP P46379
C	16	MET	-	expression tag	UNP P46379

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

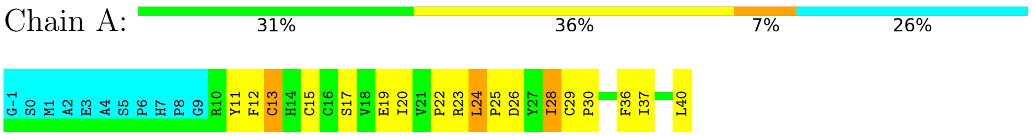
Mol	Chain	Residues	Atoms	
			Total	Zn
3	A	1	1	1

4 Residue-property plots ⓘ

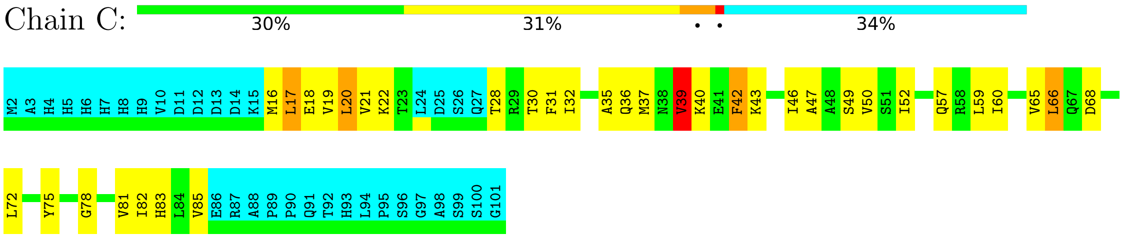
4.1 Average score per residue in the NMR ensemble

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: E3 ubiquitin-protein ligase RNF126



- Molecule 2: Large proline-rich protein BAG6

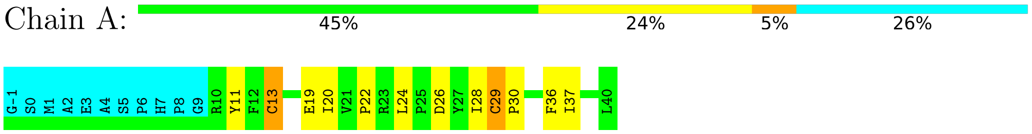


4.2 Scores per residue for each member of the ensemble

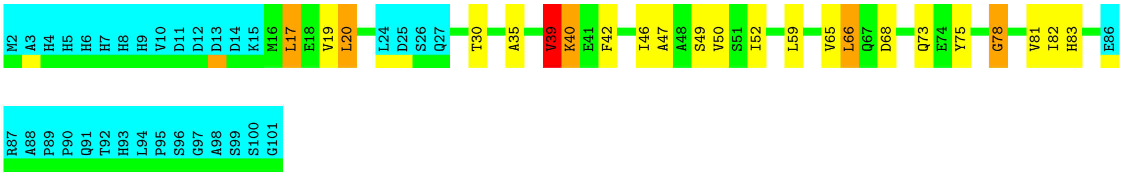
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: E3 ubiquitin-protein ligase RNF126

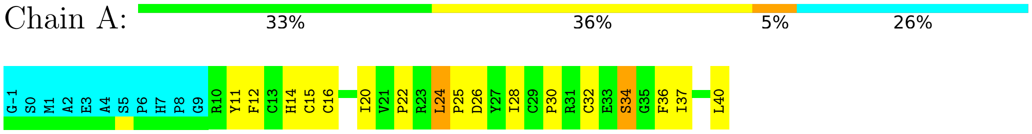


- Molecule 2: Large proline-rich protein BAG6

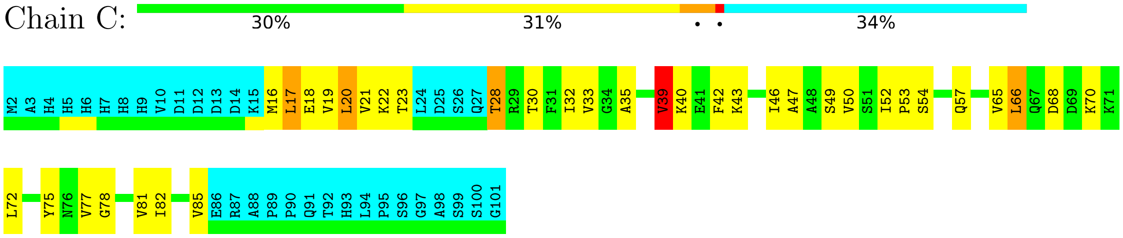


4.2.2 Score per residue for model 2

- Molecule 1: E3 ubiquitin-protein ligase RNF126

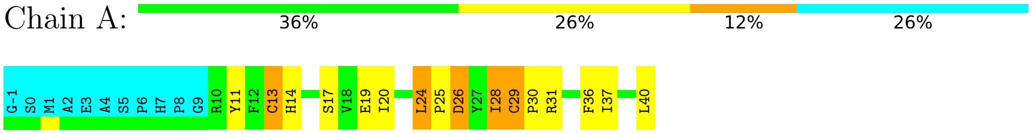


- Molecule 2: Large proline-rich protein BAG6

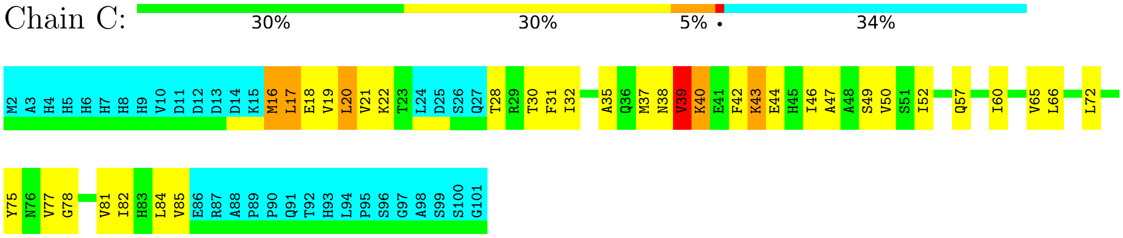


4.2.3 Score per residue for model 3

- Molecule 1: E3 ubiquitin-protein ligase RNF126

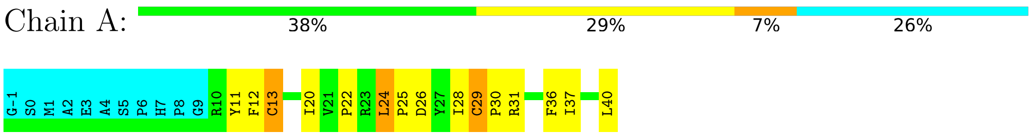


- Molecule 2: Large proline-rich protein BAG6

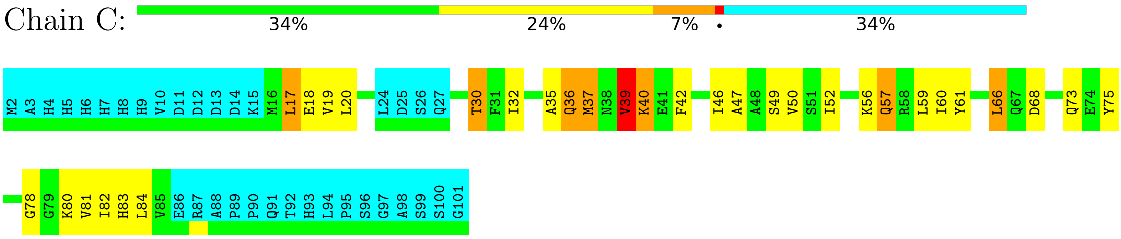


4.2.4 Score per residue for model 4

- Molecule 1: E3 ubiquitin-protein ligase RNF126

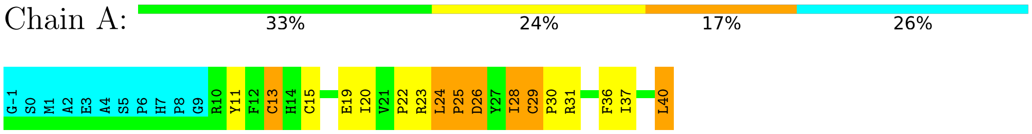


- Molecule 2: Large proline-rich protein BAG6

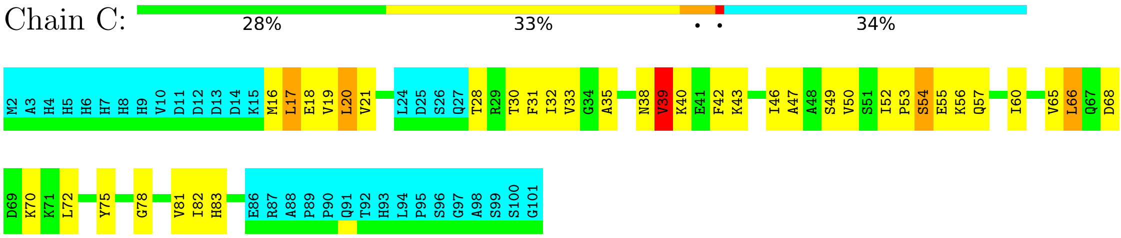


4.2.5 Score per residue for model 5

- Molecule 1: E3 ubiquitin-protein ligase RNF126

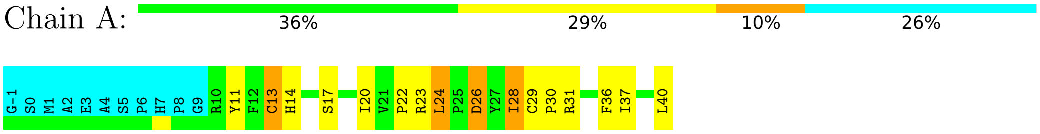


- Molecule 2: Large proline-rich protein BAG6

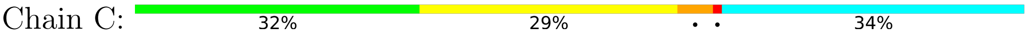


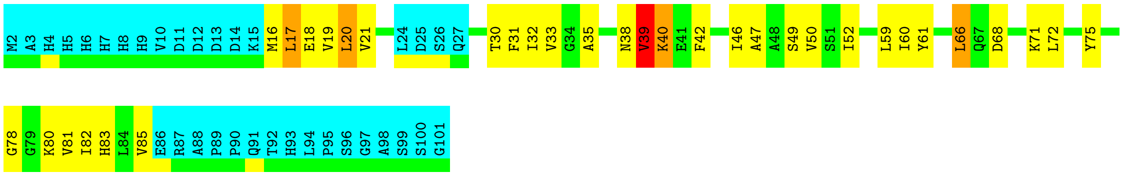
4.2.6 Score per residue for model 6

- Molecule 1: E3 ubiquitin-protein ligase RNF126



- Molecule 2: Large proline-rich protein BAG6

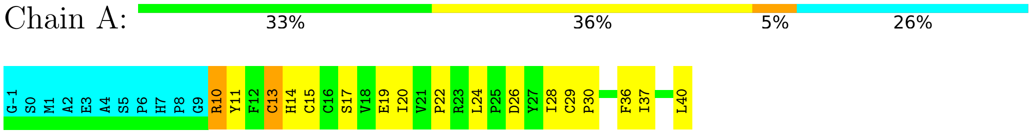




4.2.7 Score per residue for model 7

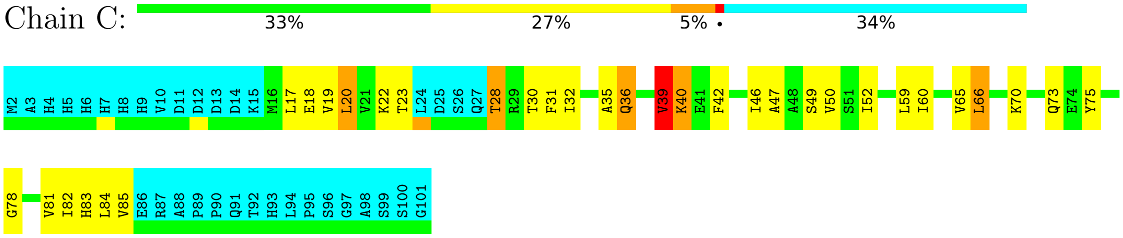
- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:



- Molecule 2: Large proline-rich protein BAG6

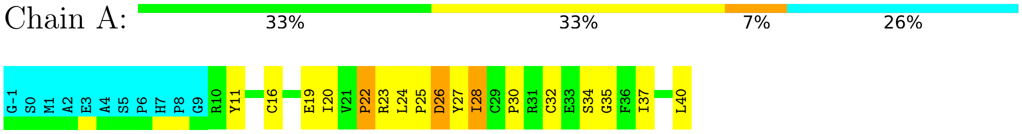
Chain C:



4.2.8 Score per residue for model 8

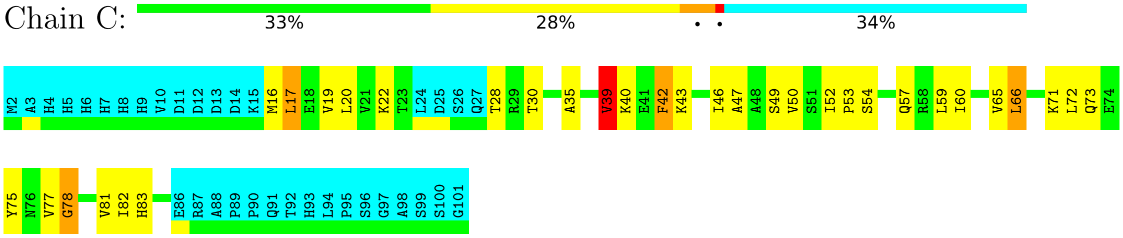
- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:



- Molecule 2: Large proline-rich protein BAG6

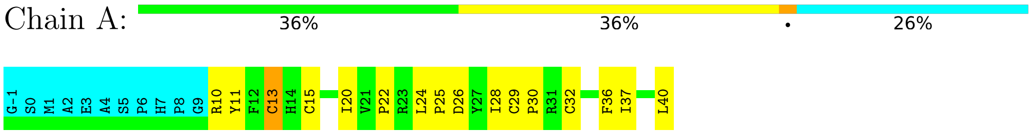
Chain C:



4.2.9 Score per residue for model 9

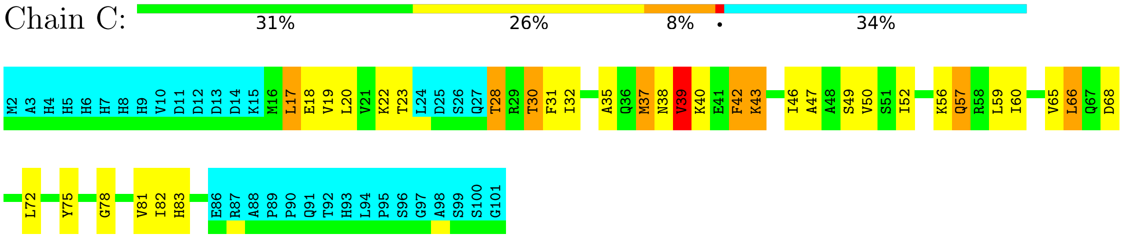
- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:



- Molecule 2: Large proline-rich protein BAG6

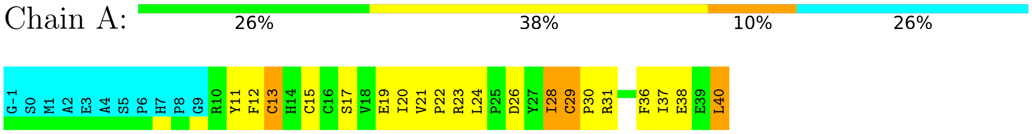
Chain C:



4.2.10 Score per residue for model 10 (medoid)

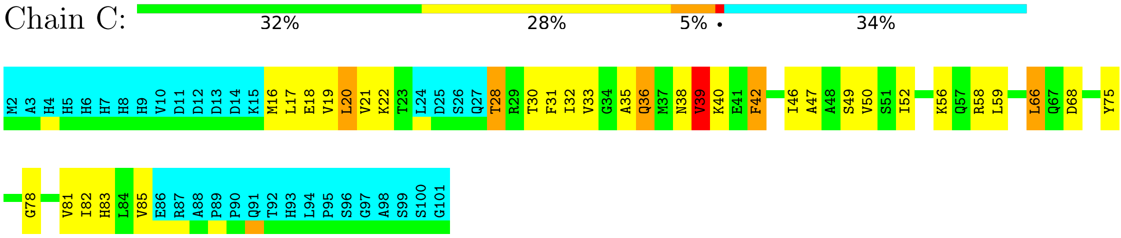
- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:



- Molecule 2: Large proline-rich protein BAG6

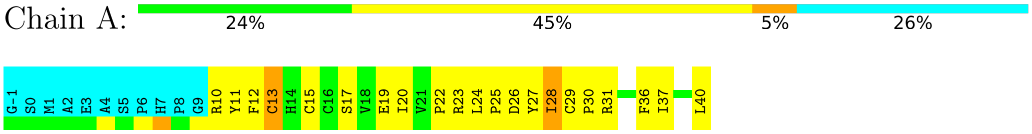
Chain C:



4.2.11 Score per residue for model 11

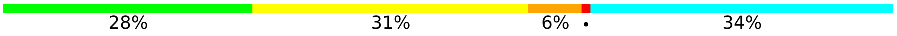
- Molecule 1: E3 ubiquitin-protein ligase RNF126

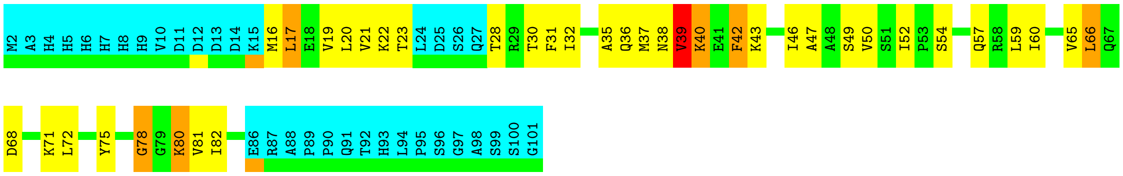
Chain A:



- Molecule 2: Large proline-rich protein BAG6

Chain C:

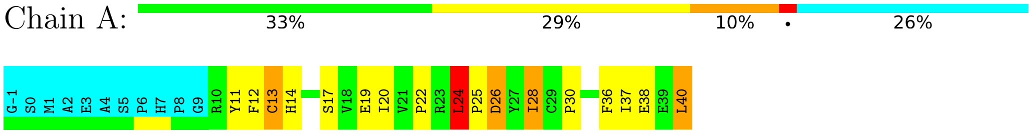




4.2.12 Score per residue for model 12

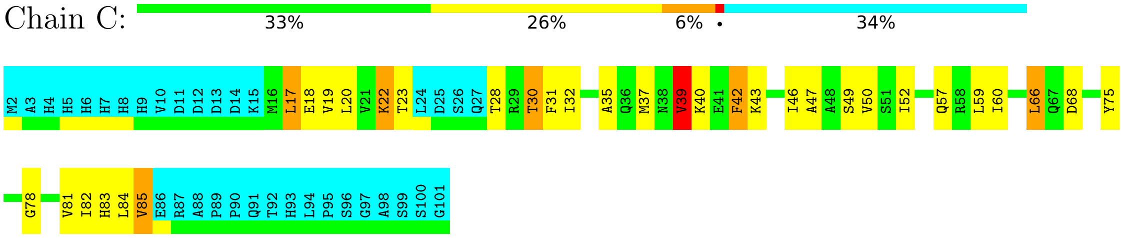
- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:



- Molecule 2: Large proline-rich protein BAG6

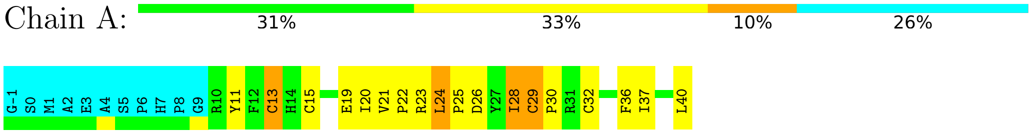
Chain C:



4.2.13 Score per residue for model 13

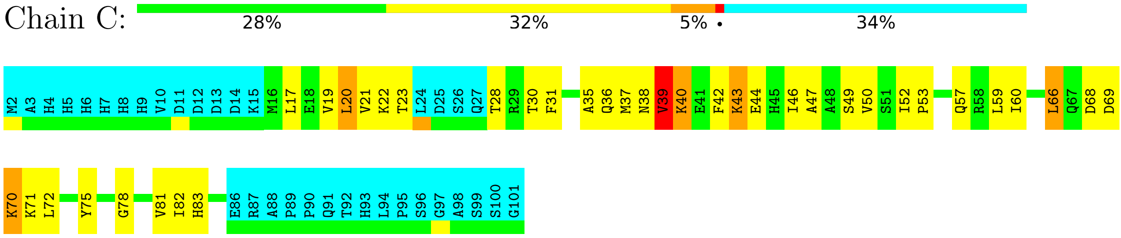
- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:



- Molecule 2: Large proline-rich protein BAG6

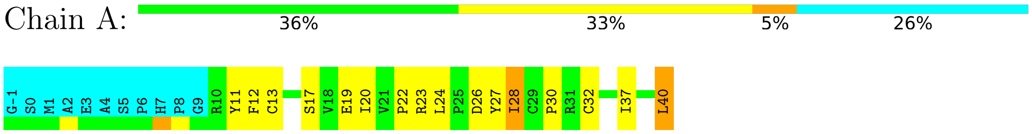
Chain C:



4.2.14 Score per residue for model 14

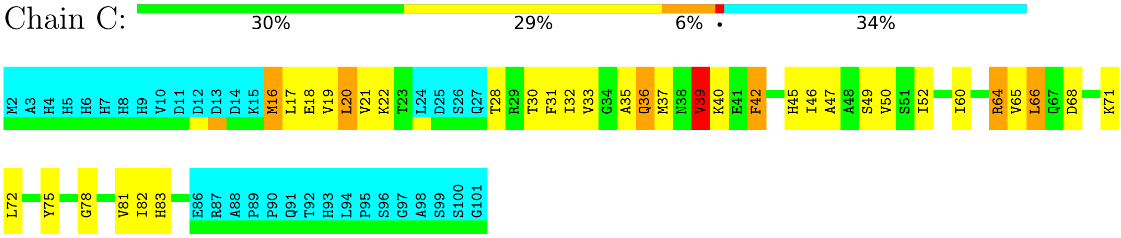
- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:



- Molecule 2: Large proline-rich protein BAG6

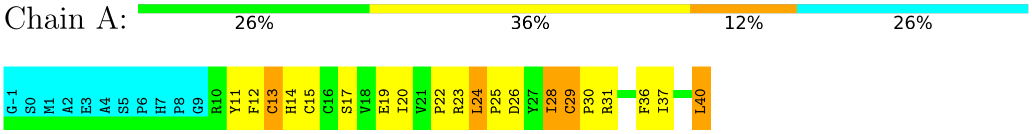
Chain C:



4.2.15 Score per residue for model 15

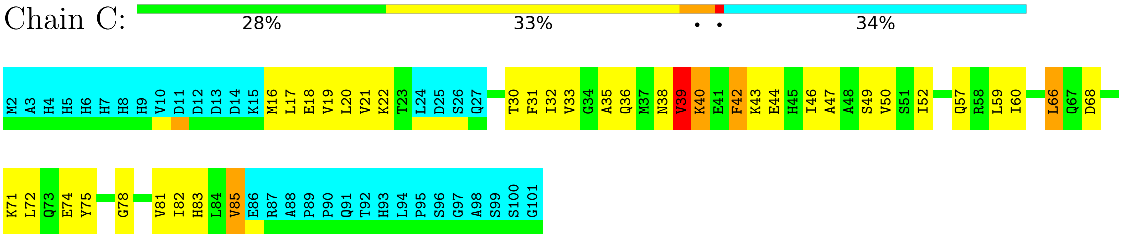
- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:



- Molecule 2: Large proline-rich protein BAG6

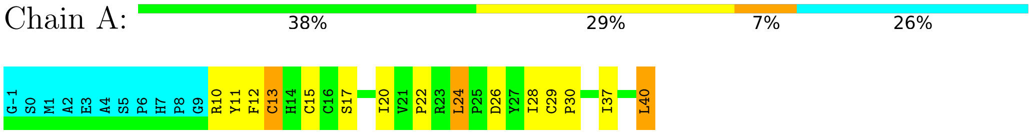
Chain C:



4.2.16 Score per residue for model 16

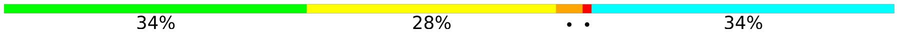
- Molecule 1: E3 ubiquitin-protein ligase RNF126

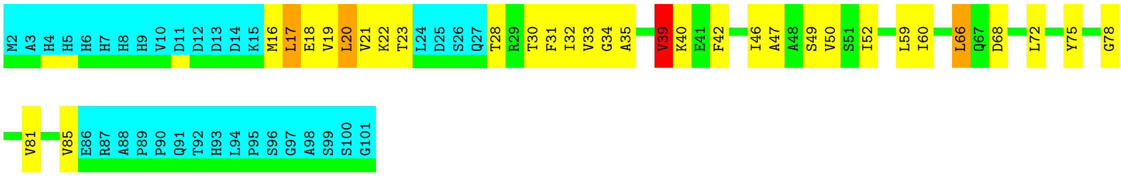
Chain A:



- Molecule 2: Large proline-rich protein BAG6

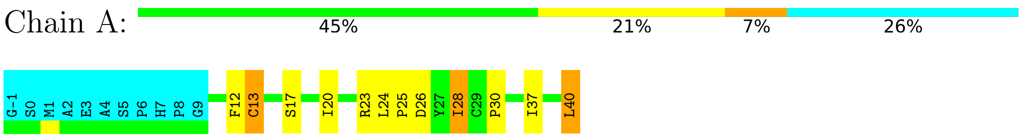
Chain C:



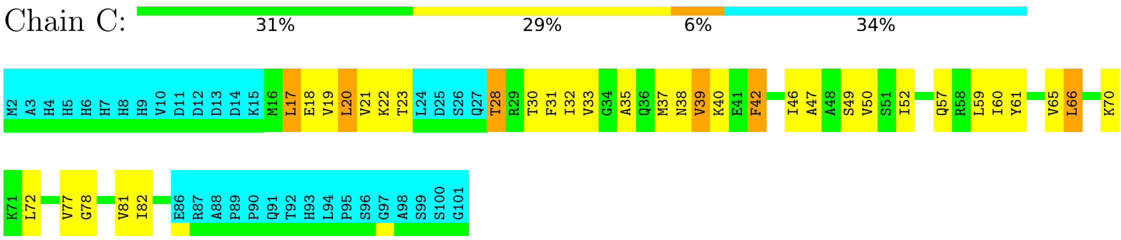


4.2.17 Score per residue for model 17

- Molecule 1: E3 ubiquitin-protein ligase RNF126

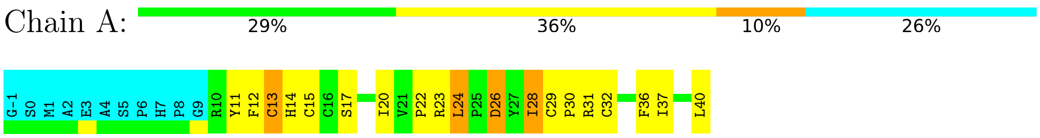


- Molecule 2: Large proline-rich protein BAG6

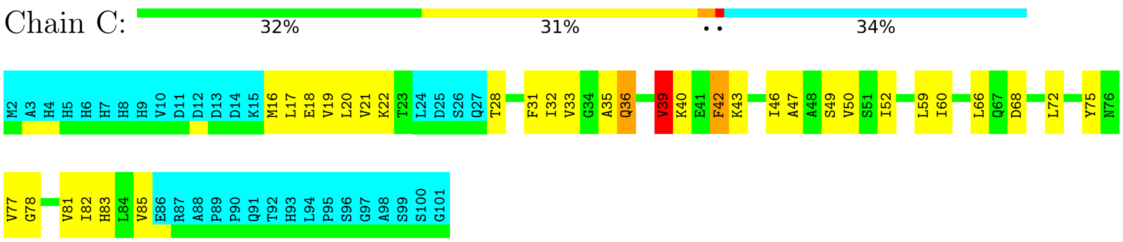


4.2.18 Score per residue for model 18

- Molecule 1: E3 ubiquitin-protein ligase RNF126



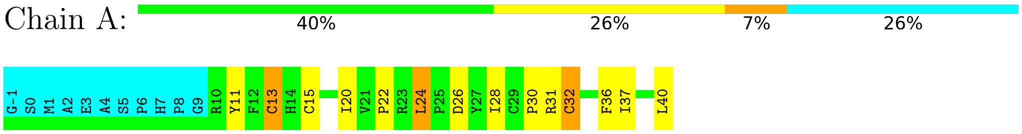
- Molecule 2: Large proline-rich protein BAG6



4.2.19 Score per residue for model 19

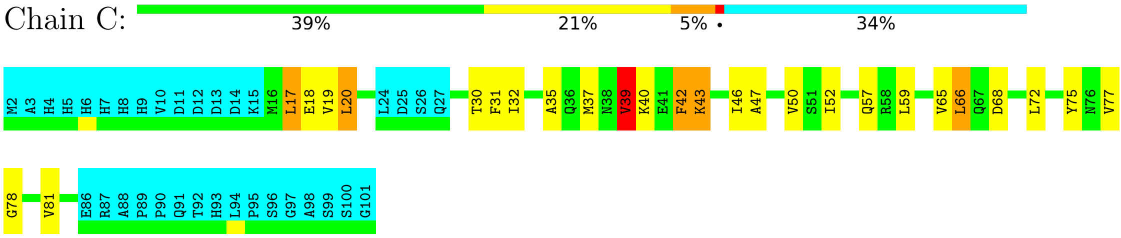
- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:



- Molecule 2: Large proline-rich protein BAG6

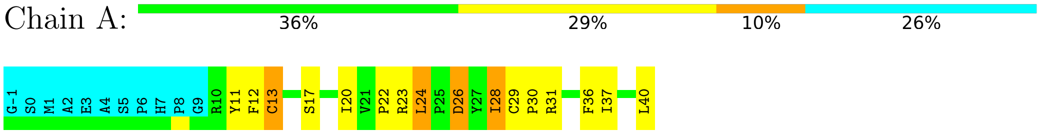
Chain C:



4.2.20 Score per residue for model 20

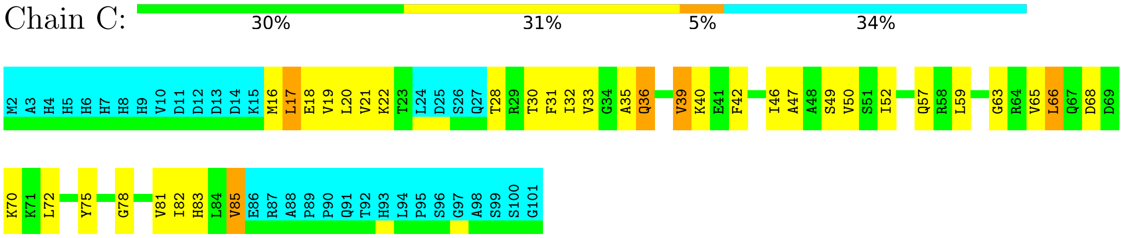
- Molecule 1: E3 ubiquitin-protein ligase RNF126

Chain A:



- Molecule 2: Large proline-rich protein BAG6

Chain C:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *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**
ARIA	structure solution	2.1
ARIA	refinement	2.1
CcpNmr Analysis	structure solution	2.3

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	1547
Number of shifts mapped to atoms	1547
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

6 Model quality (i)

6.1 Standard geometry (i)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	255	239	238	14±2
2	C	528	562	560	30±5
All	All	15680	16020	15960	844

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:20:LEU:HB3	2:C:81:VAL:HG12	0.83	1.50	11	6
1:A:20:ILE:HD11	1:A:37:ILE:HG21	0.79	1.51	8	18
2:C:21:VAL:O	2:C:28:THR:HA	0.79	1.78	17	6
2:C:17:LEU:HD11	2:C:35:ALA:HA	0.76	1.56	3	13
2:C:17:LEU:HD22	2:C:35:ALA:HA	0.74	1.57	8	5
2:C:35:ALA:O	2:C:36:GLN:HB2	0.73	1.82	4	5
1:A:20:ILE:CD1	1:A:37:ILE:HG21	0.72	2.13	8	20
2:C:17:LEU:CD2	2:C:35:ALA:HA	0.69	2.18	6	7
2:C:20:LEU:HB3	2:C:81:VAL:CG1	0.67	2.20	11	3
1:A:20:ILE:HD12	1:A:30:PRO:HD3	0.66	1.67	17	20
1:A:15:CYS:SG	1:A:36:PHE:HB2	0.65	2.32	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:17:LEU:HD21	2:C:35:ALA:HA	0.64	1.68	11	2
2:C:59:LEU:O	2:C:66:LEU:HG	0.64	1.92	16	11
2:C:42:PHE:O	2:C:46:ILE:HG23	0.64	1.93	10	7
2:C:36:GLN:H	2:C:72:LEU:HD12	0.64	1.52	14	1
1:A:11:TYR:CG	1:A:22:PRO:HG3	0.63	2.29	6	18
1:A:13:CYS:SG	1:A:15:CYS:SG	0.62	2.96	15	4
1:A:14:HIS:CG	2:C:85:VAL:HG13	0.62	2.30	6	1
2:C:22:LYS:HG2	2:C:28:THR:OG1	0.62	1.94	8	5
2:C:35:ALA:O	2:C:72:LEU:HB2	0.61	1.95	8	7
2:C:39:VAL:O	2:C:43:LYS:HD2	0.60	1.96	3	3
2:C:46:ILE:HD11	2:C:57:GLN:OE1	0.60	1.96	19	6
1:A:22:PRO:HB3	1:A:37:ILE:CD1	0.59	2.27	8	8
1:A:20:ILE:HB	1:A:30:PRO:CD	0.59	2.28	16	20
2:C:17:LEU:HB3	2:C:78:GLY:HA2	0.59	1.74	20	15
2:C:17:LEU:HD21	2:C:35:ALA:HB2	0.58	1.74	20	1
2:C:35:ALA:O	2:C:36:GLN:HB3	0.58	1.97	18	1
1:A:11:TYR:O	1:A:19:GLU:HG3	0.58	1.97	11	11
2:C:39:VAL:CA	2:C:42:PHE:HB3	0.58	2.28	18	20
2:C:66:LEU:HD22	2:C:75:TYR:CD1	0.58	2.34	3	17
2:C:20:LEU:CB	2:C:81:VAL:HG12	0.58	2.29	14	15
2:C:46:ILE:O	2:C:50:VAL:HG22	0.58	1.97	9	19
2:C:43:LYS:HG3	2:C:57:GLN:OE1	0.57	1.99	19	3
2:C:47:ALA:HA	2:C:52:ILE:O	0.57	1.98	3	20
1:A:23:ARG:HB2	1:A:28:ILE:HG13	0.57	1.75	10	9
2:C:16:MET:HA	2:C:33:VAL:O	0.56	2.00	2	8
2:C:33:VAL:HG21	2:C:72:LEU:HD13	0.56	1.74	2	4
2:C:19:VAL:O	2:C:30:THR:HA	0.56	2.00	6	19
2:C:19:VAL:HB	2:C:31:PHE:O	0.56	2.01	16	10
2:C:20:LEU:HB2	2:C:81:VAL:HG12	0.56	1.76	14	6
2:C:20:LEU:O	2:C:81:VAL:HA	0.56	2.01	3	13
1:A:13:CYS:SG	1:A:15:CYS:HB3	0.56	2.41	7	4
2:C:43:LYS:HB2	2:C:57:GLN:OE1	0.55	2.01	13	2
1:A:29:CYS:SG	1:A:31:ARG:HB2	0.55	2.41	15	9
1:A:13:CYS:HB2	1:A:37:ILE:HG22	0.55	1.76	9	7
2:C:61:TYR:CD2	2:C:77:VAL:HG12	0.55	2.36	17	1
1:A:13:CYS:HB2	1:A:37:ILE:CG2	0.55	2.32	19	12
2:C:20:LEU:HB2	2:C:81:VAL:CG1	0.55	2.32	17	4
2:C:33:VAL:HG11	2:C:42:PHE:CD1	0.55	2.37	20	1
2:C:39:VAL:HG23	2:C:72:LEU:HD21	0.54	1.77	13	4
2:C:39:VAL:HA	2:C:42:PHE:CD2	0.54	2.38	15	5
2:C:40:LYS:O	2:C:43:LYS:HG2	0.54	2.03	11	3

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:12:PHE:CB	1:A:40:LEU:HD11	0.54	2.31	15	6
2:C:17:LEU:HB3	2:C:78:GLY:CA	0.54	2.33	2	14
2:C:38:ASN:O	2:C:39:VAL:HG12	0.53	2.04	11	6
1:A:20:ILE:HD13	1:A:37:ILE:HG21	0.53	1.81	19	7
2:C:43:LYS:HB3	2:C:57:GLN:OE1	0.53	2.04	5	1
2:C:21:VAL:HG21	2:C:31:PHE:CE2	0.53	2.39	18	3
2:C:20:LEU:C	2:C:81:VAL:HA	0.53	2.24	7	13
1:A:12:PHE:HB2	1:A:40:LEU:HD21	0.53	1.81	2	1
1:A:22:PRO:HG2	1:A:24:LEU:CD2	0.53	2.34	6	1
1:A:14:HIS:CE1	2:C:85:VAL:HB	0.53	2.39	15	1
1:A:11:TYR:CD2	1:A:22:PRO:HG3	0.52	2.39	1	9
2:C:21:VAL:HG22	2:C:82:ILE:HB	0.52	1.82	14	7
1:A:37:ILE:O	2:C:60:ILE:HG21	0.52	2.04	9	15
2:C:19:VAL:CG1	2:C:31:PHE:HB2	0.52	2.34	14	12
2:C:33:VAL:HG11	2:C:42:PHE:CD2	0.52	2.40	14	4
2:C:54:SER:HA	2:C:57:GLN:OE1	0.52	2.04	5	1
1:A:12:PHE:CB	1:A:40:LEU:HD21	0.51	2.34	2	5
2:C:43:LYS:HG2	2:C:57:GLN:OE1	0.51	2.04	12	3
2:C:39:VAL:HG13	2:C:68:ASP:HA	0.51	1.82	9	13
2:C:35:ALA:O	2:C:36:GLN:CB	0.51	2.57	4	2
2:C:50:VAL:HG21	2:C:57:GLN:OE1	0.51	2.04	20	1
1:A:10:ARG:O	1:A:10:ARG:HG3	0.51	2.04	11	1
2:C:19:VAL:O	2:C:19:VAL:HG12	0.51	2.06	9	2
2:C:59:LEU:O	2:C:66:LEU:HB2	0.50	2.06	18	1
2:C:20:LEU:HB2	2:C:81:VAL:HA	0.50	1.83	14	12
2:C:35:ALA:C	2:C:72:LEU:HB2	0.50	2.27	20	1
1:A:22:PRO:HB3	1:A:37:ILE:HD12	0.50	1.84	2	2
1:A:23:ARG:HB2	1:A:28:ILE:CD1	0.50	2.36	20	3
2:C:39:VAL:H	2:C:42:PHE:HB3	0.49	1.67	15	5
2:C:40:LYS:HE2	2:C:70:LYS:O	0.49	2.07	7	1
2:C:40:LYS:HA	2:C:68:ASP:CB	0.49	2.37	6	3
2:C:39:VAL:N	2:C:42:PHE:HB3	0.49	2.23	18	11
2:C:38:ASN:O	2:C:40:LYS:HD2	0.49	2.08	6	1
2:C:66:LEU:HG	2:C:75:TYR:CD1	0.49	2.42	18	1
2:C:82:ILE:HG22	2:C:83:HIS:N	0.49	2.23	18	14
2:C:22:LYS:HG3	2:C:81:VAL:CG2	0.48	2.38	11	10
2:C:66:LEU:HB3	2:C:75:TYR:CD2	0.48	2.42	10	1
2:C:22:LYS:HG3	2:C:81:VAL:CB	0.48	2.37	11	3
2:C:38:ASN:O	2:C:39:VAL:HB	0.48	2.08	17	1
1:A:13:CYS:HA	1:A:36:PHE:O	0.48	2.07	13	10
1:A:10:ARG:HG2	1:A:40:LEU:HD12	0.48	1.86	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:22:LYS:HG3	2:C:81:VAL:HB	0.48	1.86	12	6
2:C:61:TYR:OH	2:C:80:LYS:HD3	0.47	2.09	4	1
2:C:17:LEU:HG	2:C:78:GLY:CA	0.47	2.38	6	2
2:C:21:VAL:HG21	2:C:31:PHE:HE2	0.47	1.68	20	4
2:C:39:VAL:HA	2:C:42:PHE:HB3	0.47	1.86	3	15
2:C:42:PHE:C	2:C:42:PHE:CD1	0.47	2.87	14	6
2:C:20:LEU:CD2	2:C:30:THR:HG22	0.47	2.40	5	11
1:A:12:PHE:HB2	1:A:40:LEU:HD11	0.47	1.86	15	5
2:C:64:ARG:HD3	2:C:65:VAL:N	0.47	2.24	14	1
2:C:17:LEU:O	2:C:32:ILE:HG23	0.47	2.10	11	1
2:C:52:ILE:HG22	2:C:57:GLN:HB2	0.47	1.86	17	1
2:C:18:GLU:HA	2:C:32:ILE:HG13	0.47	1.86	14	15
2:C:66:LEU:HD12	2:C:82:ILE:HD13	0.47	1.85	3	2
2:C:36:GLN:HG3	2:C:73:GLN:CB	0.47	2.40	4	1
2:C:36:GLN:N	2:C:72:LEU:HD12	0.47	2.24	14	1
1:A:15:CYS:SG	1:A:34:SER:HB2	0.47	2.49	2	1
1:A:14:HIS:CD2	2:C:85:VAL:HG12	0.47	2.44	7	1
1:A:26:ASP:HB3	1:A:28:ILE:HG12	0.46	1.87	12	6
1:A:15:CYS:SG	1:A:32:CYS:SG	0.46	3.13	13	3
2:C:52:ILE:CG2	2:C:57:GLN:HB3	0.46	2.41	11	2
1:A:10:ARG:HG2	1:A:10:ARG:O	0.46	2.10	7	1
2:C:18:GLU:HG2	2:C:32:ILE:HG12	0.46	1.86	12	1
2:C:22:LYS:HE3	2:C:81:VAL:HG21	0.46	1.88	15	3
2:C:53:PRO:O	2:C:57:GLN:HG3	0.46	2.11	5	1
1:A:11:TYR:CD1	1:A:22:PRO:HG3	0.46	2.46	6	3
2:C:35:ALA:O	2:C:73:GLN:HB2	0.46	2.11	7	1
2:C:20:LEU:HB2	2:C:80:LYS:C	0.46	2.31	11	1
1:A:31:ARG:O	1:A:32:CYS:HB3	0.46	2.10	19	1
1:A:29:CYS:SG	1:A:30:PRO:HD2	0.46	2.51	20	7
2:C:17:LEU:CD1	2:C:35:ALA:HA	0.46	2.40	18	2
2:C:19:VAL:O	2:C:31:PHE:N	0.46	2.48	18	8
2:C:52:ILE:HG22	2:C:57:GLN:HG3	0.46	1.88	5	1
2:C:43:LYS:HA	2:C:57:GLN:OE1	0.45	2.11	3	1
2:C:16:MET:H	2:C:34:GLY:HA2	0.45	1.71	16	1
2:C:46:ILE:HG13	2:C:57:GLN:NE2	0.45	2.26	5	1
2:C:18:GLU:HA	2:C:32:ILE:CG1	0.45	2.42	10	4
2:C:66:LEU:HD21	2:C:77:VAL:HG11	0.45	1.89	18	1
2:C:22:LYS:HE3	2:C:28:THR:OG1	0.45	2.11	3	1
1:A:23:ARG:C	1:A:25:PRO:HD2	0.45	2.32	5	1
1:A:14:HIS:HD2	1:A:38:GLU:OE1	0.45	1.94	12	1
2:C:59:LEU:HB3	2:C:82:ILE:HG21	0.44	1.88	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:39:VAL:HG11	2:C:70:LYS:HA	0.44	1.89	17	1
2:C:37:MET:HG3	2:C:38:ASN:OD1	0.44	2.11	3	2
2:C:19:VAL:HG11	2:C:42:PHE:CZ	0.44	2.47	4	1
2:C:59:LEU:O	2:C:66:LEU:N	0.44	2.51	11	5
2:C:52:ILE:HG22	2:C:57:GLN:CG	0.44	2.43	5	1
1:A:10:ARG:HD3	1:A:10:ARG:H	0.43	1.72	7	1
1:A:11:TYR:HB2	1:A:22:PRO:HD3	0.43	1.90	8	4
2:C:72:LEU:HA	2:C:75:TYR:CD2	0.43	2.48	5	2
1:A:37:ILE:O	2:C:63:GLY:HA2	0.43	2.13	20	1
2:C:35:ALA:O	2:C:73:GLN:N	0.43	2.51	1	2
2:C:19:VAL:HG22	2:C:77:VAL:HG23	0.43	1.90	2	1
2:C:59:LEU:HD23	2:C:84:LEU:HD21	0.43	1.90	7	1
1:A:14:HIS:CD2	2:C:85:VAL:HG21	0.43	2.48	18	2
2:C:20:LEU:HB2	2:C:81:VAL:CA	0.43	2.44	5	4
1:A:14:HIS:CE1	2:C:85:VAL:HG13	0.43	2.48	2	1
2:C:53:PRO:O	2:C:57:GLN:HB2	0.43	2.14	8	3
2:C:55:GLU:HG3	2:C:56:LYS:HG3	0.42	1.91	5	1
1:A:27:TYR:C	1:A:37:ILE:HD11	0.42	2.35	14	2
1:A:12:PHE:CZ	1:A:17:SER:HA	0.42	2.48	20	1
2:C:54:SER:HA	2:C:57:GLN:HG2	0.42	1.90	11	1
2:C:69:ASP:O	2:C:70:LYS:HB2	0.42	2.14	13	1
1:A:27:TYR:O	1:A:35:GLY:HA2	0.42	2.14	8	1
2:C:71:LYS:HB3	2:C:74:GLU:CG	0.42	2.45	15	1
2:C:22:LYS:HE2	2:C:28:THR:OG1	0.42	2.14	18	1
2:C:39:VAL:O	2:C:43:LYS:HG3	0.42	2.14	18	1
2:C:36:GLN:HG3	2:C:73:GLN:HB3	0.42	1.92	4	1
2:C:66:LEU:HA	2:C:75:TYR:CZ	0.42	2.50	6	1
2:C:23:THR:HG22	2:C:84:LEU:O	0.42	2.15	12	1
2:C:40:LYS:O	2:C:43:LYS:HB2	0.41	2.15	3	1
2:C:50:VAL:HG11	2:C:84:LEU:CD1	0.41	2.46	12	1
2:C:39:VAL:CG1	2:C:70:LYS:HA	0.41	2.44	2	1
2:C:22:LYS:HA	2:C:28:THR:HA	0.41	1.90	3	1
2:C:39:VAL:H	2:C:42:PHE:CB	0.41	2.28	8	3
2:C:61:TYR:CZ	2:C:80:LYS:HB3	0.41	2.50	6	1
2:C:42:PHE:CD1	2:C:42:PHE:C	0.41	2.94	10	2
2:C:33:VAL:CG2	2:C:72:LEU:HD13	0.41	2.46	18	1
2:C:22:LYS:HG3	2:C:81:VAL:HG21	0.41	1.92	11	1
1:A:26:ASP:CB	1:A:28:ILE:HG12	0.41	2.46	20	1
2:C:22:LYS:N	2:C:82:ILE:O	0.41	2.48	11	2
2:C:59:LEU:HB2	2:C:66:LEU:HB2	0.41	1.92	18	1
1:A:26:ASP:HB3	1:A:28:ILE:CG1	0.40	2.46	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:43:LYS:HE3	2:C:54:SER:OG	0.40	2.16	2	2
1:A:24:LEU:O	1:A:26:ASP:N	0.40	2.49	12	1
2:C:22:LYS:CD	2:C:81:VAL:HG21	0.40	2.46	15	1
2:C:66:LEU:HG	2:C:75:TYR:CG	0.40	2.51	18	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	30/42 (71%)	23±1 (76±3%)	5±1 (18±2%)	2±1 (6±2%)	3	20
2	C	66/100 (66%)	51±2 (77±3%)	12±2 (19±3%)	3±1 (4±2%)	5	30
All	All	1920/2840 (68%)	1472 (77%)	357 (19%)	91 (5%)	4	27

All 14 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	24	LEU	20
2	C	39	VAL	20
1	A	25	PRO	11
2	C	28	THR	8
2	C	36	GLN	7
2	C	16	MET	4
2	C	37	MET	4
2	C	78	GLY	3
2	C	70	LYS	3
1	A	32	CYS	3
2	C	71	LYS	3
2	C	85	VAL	3
1	A	22	PRO	1
1	A	26	ASP	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	30/37 (81%)	25±1 (82±3%)	5±1 (18±3%)	4	37
2	C	59/88 (67%)	51±2 (86±3%)	8±2 (14±3%)	7	47
All	All	1780/2500 (71%)	1511 (85%)	269 (15%)	6	44

All 37 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	28	ILE	20
2	C	40	LYS	20
1	A	26	ASP	19
2	C	49	SER	19
1	A	13	CYS	18
2	C	39	VAL	18
2	C	66	LEU	18
2	C	17	LEU	14
1	A	40	LEU	13
2	C	20	LEU	12
2	C	65	VAL	11
1	A	24	LEU	11
1	A	17	SER	11
2	C	42	PHE	10
1	A	29	CYS	8
2	C	37	MET	5
2	C	23	THR	4
2	C	43	LYS	4
2	C	44	GLU	3
2	C	77	VAL	3
2	C	30	THR	3
1	A	16	CYS	2
1	A	32	CYS	2
1	A	34	SER	2
2	C	84	LEU	2
2	C	57	GLN	2
2	C	71	LYS	2
1	A	10	ARG	2

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Mol	Chain	Res	Type	Models (Total)
2	C	36	GLN	2
2	C	85	VAL	2
2	C	16	MET	1
2	C	54	SER	1
1	A	38	GLU	1
2	C	80	LYS	1
2	C	22	LYS	1
2	C	45	HIS	1
2	C	64	ARG	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 monosaccharides in this entry.

6.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 (i)

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	486
Number of shifts mapped to atoms	486
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 (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	42	-0.10 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	39	0.01 ± 0.27	None needed (< 0.5 ppm)
$^{13}C'$	40	0.07 ± 0.20	None needed (< 0.5 ppm)
^{15}N	35	0.11 ± 1.36	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 28%, i.e. 390 atoms were assigned a chemical shift out of a possible 1387. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	149/482 (31%)	60/195 (31%)	61/194 (31%)	28/93 (30%)
Sidechain	203/805 (25%)	136/524 (26%)	64/249 (26%)	3/32 (9%)

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	Total	^{1}**H**	^{13}**C**	^{15}**N**
Aromatic	38/100 (38%)	19/48 (40%)	19/46 (41%)	0/6 (0%)
Overall	390/1387 (28%)	215/767 (28%)	144/489 (29%)	31/131 (24%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 25%, i.e. 486 atoms were assigned a chemical shift out of a possible 1924. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}**H**	^{13}**C**	^{15}**N**
Backbone	196/701 (28%)	79/284 (28%)	82/284 (29%)	35/133 (26%)
Sidechain	251/1059 (24%)	168/689 (24%)	80/332 (24%)	3/38 (8%)
Aromatic	39/164 (24%)	20/80 (25%)	19/62 (31%)	0/22 (0%)
Overall	486/1924 (25%)	267/1053 (25%)	181/678 (27%)	38/193 (20%)

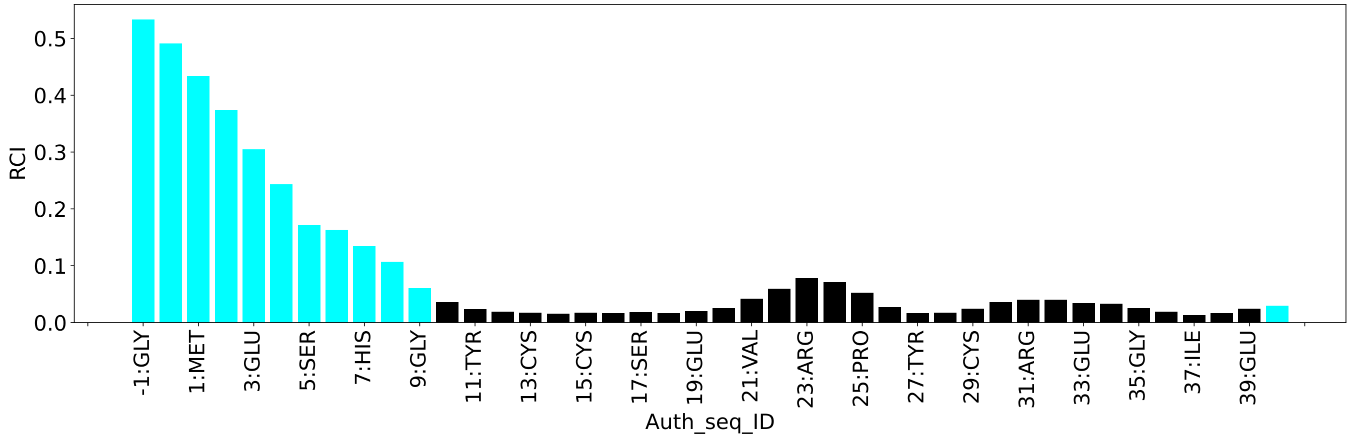
7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	1061
Number of shifts mapped to atoms	1061
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	**# values**	**Correction ± precision, *ppm***	**Suggested action**
$^{13}C_{\alpha}$	89	-0.30 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	81	0.14 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	77	-0.10 ± 0.13	None needed (< 0.5 ppm)
^{15}N	87	-0.42 ± 0.79	None needed (< 0.5 ppm)

7.2.3 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 58%, i.e. 807 atoms were assigned a chemical shift out of a possible 1387. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	322/482 (67%)	133/195 (68%)	124/194 (64%)	65/93 (70%)
Sidechain	453/805 (56%)	304/524 (58%)	140/249 (56%)	9/32 (28%)
Aromatic	32/100 (32%)	16/48 (33%)	16/46 (35%)	0/6 (0%)
Overall	807/1387 (58%)	453/767 (59%)	280/489 (57%)	74/131 (56%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 55%, i.e. 1061 atoms were assigned a chemical shift out of a possible 1924. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	434/701 (62%)	181/284 (64%)	166/284 (58%)	87/133 (65%)
Sidechain	595/1059 (56%)	398/689 (58%)	186/332 (56%)	11/38 (29%)
Aromatic	32/164 (20%)	16/80 (20%)	16/62 (26%)	0/22 (0%)
Overall	1061/1924 (55%)	595/1053 (57%)	368/678 (54%)	98/193 (51%)

7.2.4 Statistically unusual chemical shifts ⓘ

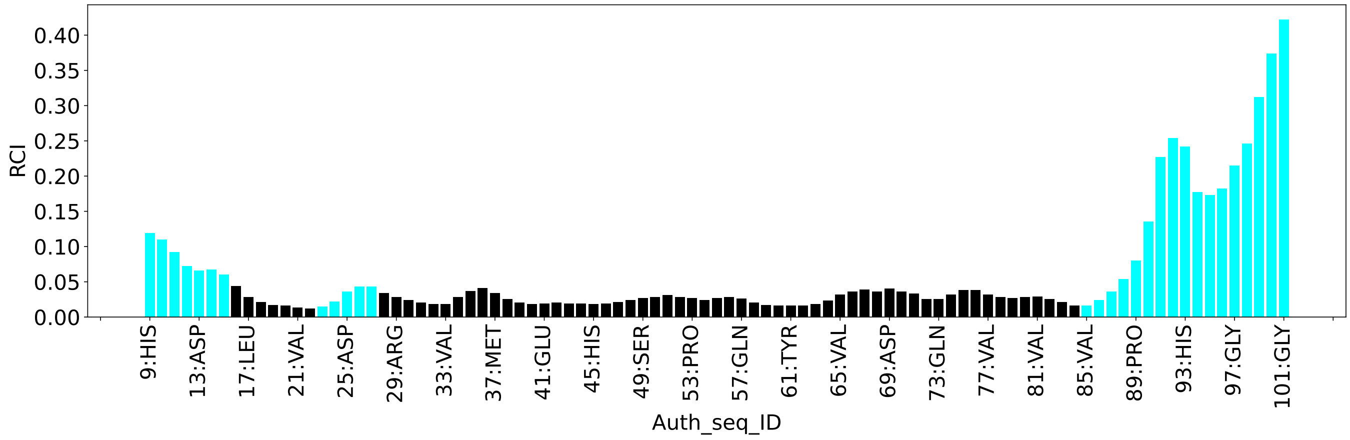
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
2	C	46	ILE	HG21	-0.87	-0.56 – 2.11	-6.2
2	C	46	ILE	HG22	-0.87	-0.56 – 2.11	-6.2
2	C	46	ILE	HG23	-0.87	-0.56 – 2.11	-6.2
2	C	57	GLN	NE2	102.88	103.38 – 120.35	-5.3
2	C	70	LYS	CG	30.63	19.35 – 30.45	5.2

7.2.5 Random Coil Index (RCI) plots ⓘ

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 C:



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	7225
Intra-residue ($\lvert i-j\rvert=0$)	3771
Sequential ($\lvert i-j\rvert=1$)	1315
Medium range ($\lvert i-j\rvert>1$ and $\lvert i-j\rvert<5$)	561
Long range ($\lvert i-j\rvert\geq5$)	1386
Inter-chain	192
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	50.9
Number of long range restraints per residue[1]	9.8

[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)	38.8	0.2
0.2-0.5 (Medium)	12.8	0.48
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model ⓘ

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

9 Distance violation analysis ⓘ

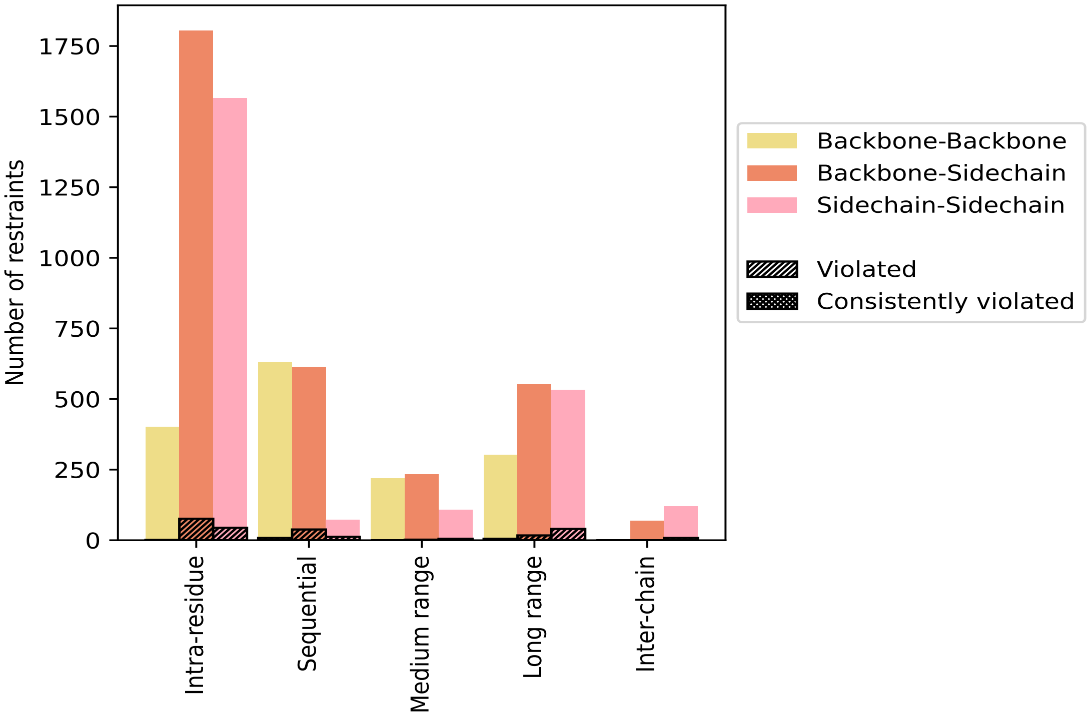
9.1 Summary of distance violations ⓘ

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

Restraints type	**Count**	%[1]	**Violated**[3]			**Consistently Violated**[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue ($\lvert i-j \rvert=0$)	3771	52.2	121	3.2	1.7	0	0.0	0.0
Backbone-Backbone	401	5.6	1	0.2	0.0	0	0.0	0.0
Backbone-Sidechain	1804	25.0	76	4.2	1.1	0	0.0	0.0
Sidechain-Sidechain	1566	21.7	44	2.8	0.6	0	0.0	0.0
Sequential ($\lvert i-j \rvert=1$)	1315	18.2	58	4.4	0.8	0	0.0	0.0
Backbone-Backbone	629	8.7	8	1.3	0.1	0	0.0	0.0
Backbone-Sidechain	613	8.5	38	6.2	0.5	0	0.0	0.0
Sidechain-Sidechain	73	1.0	12	16.4	0.2	0	0.0	0.0
Medium range ($\lvert i-j \rvert>1$ & $\lvert i-j \rvert<5$)	561	7.8	7	1.2	0.1	0	0.0	0.0
Backbone-Backbone	220	3.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	234	3.2	2	0.9	0.0	0	0.0	0.0
Sidechain-Sidechain	107	1.5	5	4.7	0.1	0	0.0	0.0
Long range ($\lvert i-j \rvert\geq5$)	1386	19.2	62	4.5	0.9	0	0.0	0.0
Backbone-Backbone	302	4.2	5	1.7	0.1	0	0.0	0.0
Backbone-Sidechain	552	7.6	17	3.1	0.2	0	0.0	0.0
Sidechain-Sidechain	532	7.4	40	7.5	0.6	0	0.0	0.0
Inter-chain	192	2.7	8	4.2	0.1	0	0.0	0.0
Backbone-Backbone	4	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	68	0.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	120	1.7	8	6.7	0.1	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	7225	100.0	256	3.5	3.5	0	0.0	0.0
Backbone-Backbone	1556	21.5	14	0.9	0.2	0	0.0	0.0
Backbone-Sidechain	3271	45.3	133	4.1	1.8	0	0.0	0.0
Sidechain-Sidechain	2398	33.2	109	4.5	1.5	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	20	12	1	17	0	50	0.16	0.27	0.06	0.14
2	28	8	5	25	0	66	0.19	0.33	0.07	0.16
3	24	8	2	9	0	43	0.2	0.39	0.1	0.15
4	20	4	5	17	4	50	0.18	0.33	0.07	0.16
5	28	8	1	17	0	54	0.15	0.25	0.05	0.12
6	28	16	0	13	4	61	0.17	0.37	0.07	0.15
7	17	16	4	9	0	46	0.15	0.34	0.06	0.11
8	24	8	2	21	4	59	0.19	0.48	0.09	0.15
9	20	24	5	8	0	57	0.17	0.37	0.08	0.14
10	28	4	1	9	0	42	0.17	0.27	0.05	0.16
11	32	12	0	13	4	61	0.16	0.29	0.05	0.15

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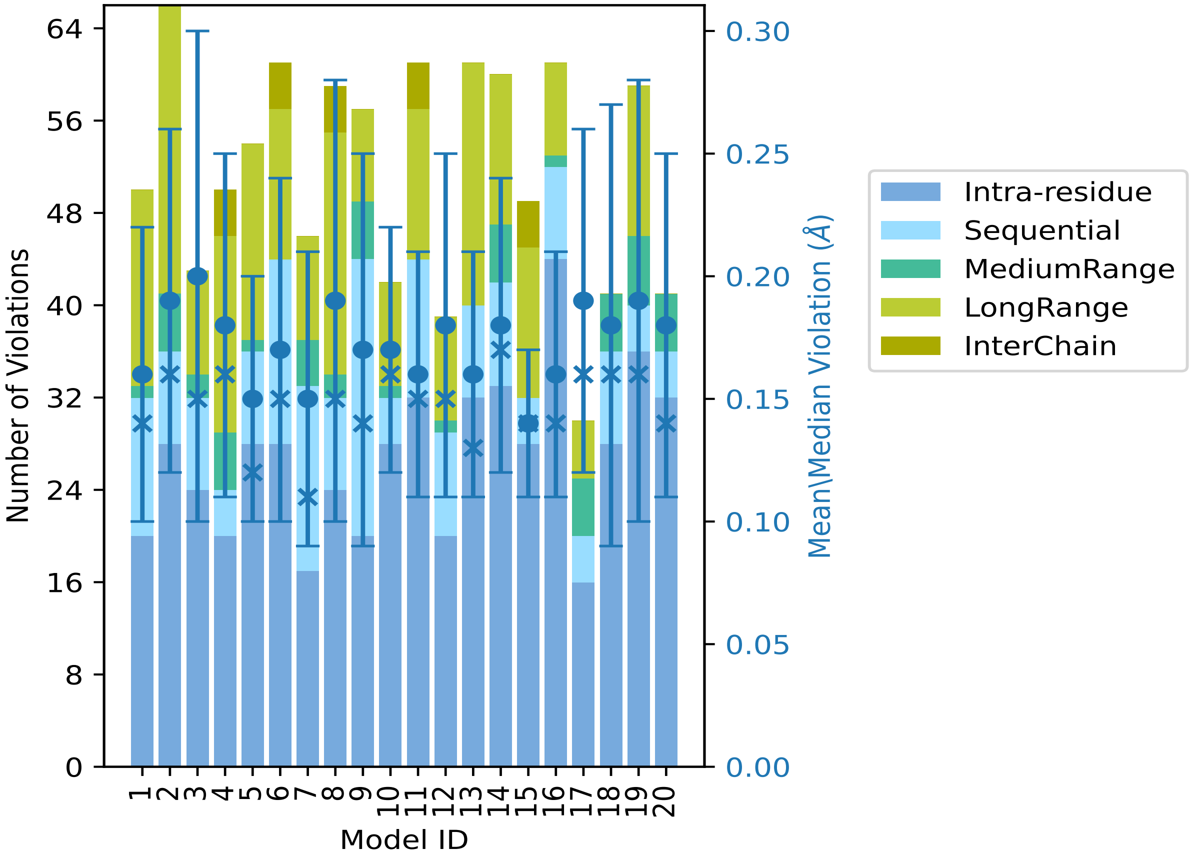
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	20	9	1	9	0	39	0.18	0.36	0.07	0.15
13	32	8	0	21	0	61	0.16	0.25	0.05	0.13
14	33	9	5	13	0	60	0.18	0.33	0.06	0.17
15	28	4	0	13	4	49	0.14	0.21	0.03	0.14
16	44	8	1	8	0	61	0.16	0.28	0.05	0.14
17	16	4	5	5	0	30	0.19	0.34	0.07	0.16
18	28	8	5	0	0	41	0.18	0.34	0.09	0.16
19	36	4	6	13	0	59	0.19	0.41	0.09	0.16
20	32	4	5	0	0	41	0.18	0.32	0.07	0.14

[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

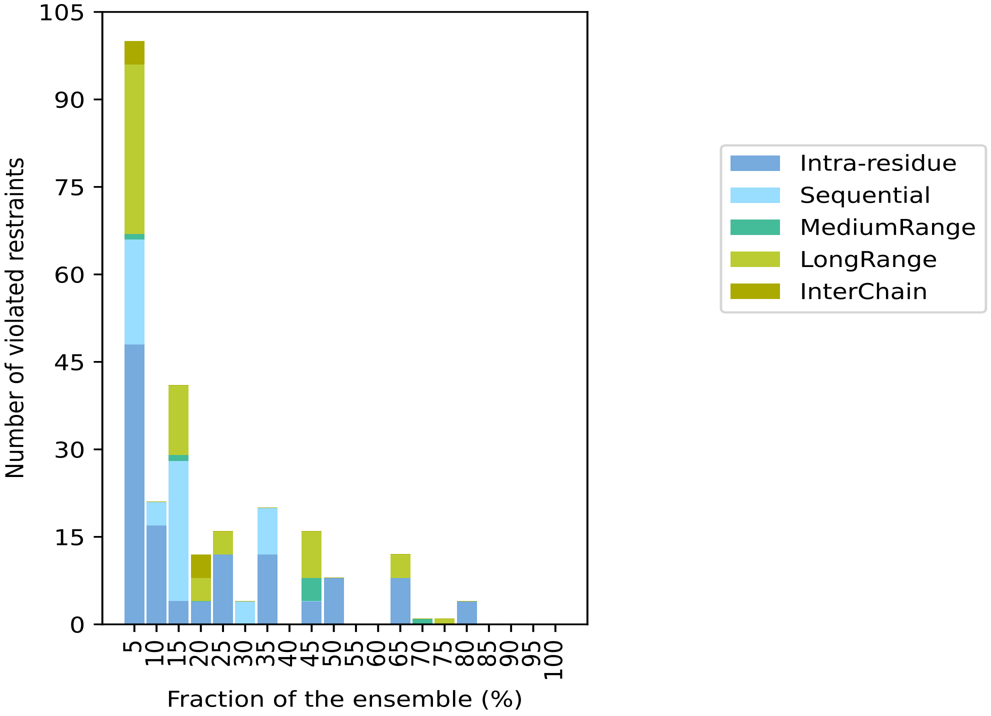
9.3 Distance violation statistics for the ensemble (i)

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, 6969(IR:3650, SQ:1257, MR:554, LR:1324, IC:184) 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]	%
48	18	1	29	4	100	1	5.0
17	4	0	0	0	21	2	10.0
4	24	1	12	0	41	3	15.0
4	0	0	4	4	12	4	20.0
12	0	0	4	0	16	5	25.0
0	4	0	0	0	4	6	30.0
12	8	0	0	0	20	7	35.0
0	0	0	0	0	0	8	40.0
4	0	4	8	0	16	9	45.0
8	0	0	0	0	8	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
8	0	0	4	0	12	13	65.0
0	0	1	0	0	1	14	70.0
0	0	0	1	0	1	15	75.0
4	0	0	0	0	4	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

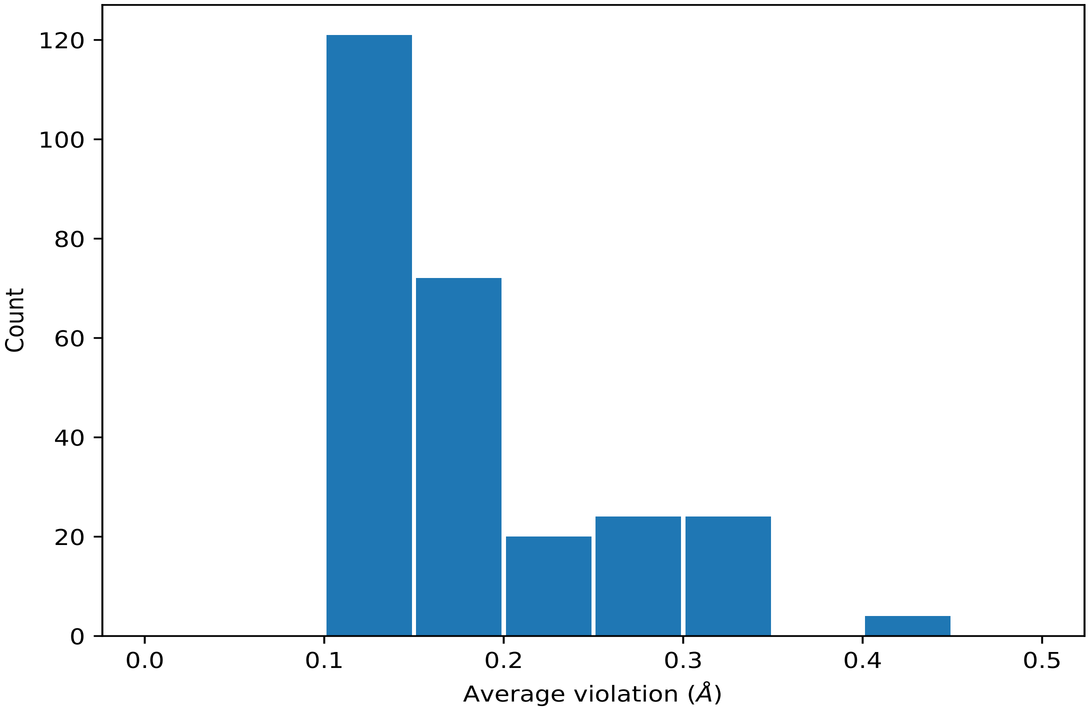
9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ



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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	16	0.14	0.02	0.14
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	16	0.14	0.02	0.14
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	16	0.14	0.02	0.14
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	16	0.14	0.02	0.14
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	15	0.14	0.02	0.13
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	15	0.14	0.02	0.13
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	14	0.15	0.03	0.13
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	14	0.15	0.03	0.13
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	14	0.15	0.03	0.13
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	14	0.15	0.03	0.13
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	14	0.15	0.03	0.13
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	14	0.15	0.03	0.13
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	14	0.15	0.03	0.13
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	14	0.15	0.03	0.13
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	14	0.15	0.03	0.13
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	13	0.21	0.04	0.22

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Key	Atom-1	Atom-2	Models^1	Mean (Å)	SD^1 (Å)	Median (Å)
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	13	0.21	0.04	0.22
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	13	0.21	0.04	0.22
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	13	0.21	0.04	0.22
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	13	0.12	0.01	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	13	0.12	0.01	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	13	0.12	0.01	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	13	0.12	0.01	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	13	0.12	0.01	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	13	0.12	0.01	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	13	0.12	0.01	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	13	0.12	0.01	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	13	0.12	0.01	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	13	0.12	0.01	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	13	0.12	0.01	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	13	0.12	0.01	0.12
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	13	0.11	0.0	0.11
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	13	0.11	0.0	0.11
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	13	0.11	0.0	0.11
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	13	0.11	0.0	0.11
(1,1187)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	10	0.16	0.01	0.17
(1,1187)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	10	0.16	0.01	0.17
(1,1187)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	10	0.16	0.01	0.17
(1,2980)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	10	0.16	0.01	0.17
(1,2980)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	10	0.16	0.01	0.17
(1,2980)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	10	0.16	0.01	0.17
(1,4773)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	10	0.16	0.01	0.17
(1,4773)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	10	0.16	0.01	0.17
(1,4773)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	10	0.16	0.01	0.17
(1,6566)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	10	0.16	0.01	0.17
(1,6566)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	10	0.16	0.01	0.17
(1,6566)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	10	0.16	0.01	0.17
(1,501)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	10	0.14	0.01	0.15
(1,501)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	10	0.14	0.01	0.15
(1,501)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	10	0.14	0.01	0.15
(1,2294)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	10	0.14	0.01	0.15
(1,2294)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	10	0.14	0.01	0.15
(1,2294)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	10	0.14	0.01	0.15
(1,4087)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	10	0.14	0.01	0.15
(1,4087)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	10	0.14	0.01	0.15
(1,4087)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	10	0.14	0.01	0.15
(1,5880)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	10	0.14	0.01	0.15
(1,5880)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	10	0.14	0.01	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,5880)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	10	0.14	0.01	0.15
(1,293)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	9	0.34	0.01	0.34
(1,293)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	9	0.34	0.01	0.34
(1,293)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	9	0.34	0.01	0.34
(1,2086)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	9	0.34	0.01	0.34
(1,2086)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	9	0.34	0.01	0.34
(1,2086)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	9	0.34	0.01	0.34
(1,3879)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	9	0.34	0.01	0.34
(1,3879)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	9	0.34	0.01	0.34
(1,3879)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	9	0.34	0.01	0.34
(1,5672)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	9	0.34	0.01	0.34
(1,5672)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	9	0.34	0.01	0.34
(1,5672)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	9	0.34	0.01	0.34
(1,1816)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	9	0.26	0.07	0.26
(1,1816)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	9	0.26	0.07	0.26
(1,1816)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	9	0.26	0.07	0.26
(1,3609)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	9	0.26	0.07	0.26
(1,3609)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	9	0.26	0.07	0.26
(1,3609)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	9	0.26	0.07	0.26
(1,5402)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	9	0.26	0.07	0.26
(1,5402)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	9	0.26	0.07	0.26
(1,5402)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	9	0.26	0.07	0.26
(1,7195)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	9	0.26	0.07	0.26
(1,7195)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	9	0.26	0.07	0.26
(1,7195)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	9	0.26	0.07	0.26
(1,122)	2:C:19:VAL:H	2:C:31:PHE:HB3	9	0.25	0.05	0.24
(1,1915)	2:C:19:VAL:H	2:C:31:PHE:HB3	9	0.25	0.05	0.24
(1,3708)	2:C:19:VAL:H	2:C:31:PHE:HB3	9	0.25	0.05	0.24
(1,5501)	2:C:19:VAL:H	2:C:31:PHE:HB3	9	0.25	0.05	0.24
(1,1019)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	9	0.12	0.01	0.12
(1,1019)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	9	0.12	0.01	0.12
(1,1019)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	9	0.12	0.01	0.12
(1,2812)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	9	0.12	0.01	0.12
(1,2812)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	9	0.12	0.01	0.12
(1,2812)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	9	0.12	0.01	0.12
(1,4605)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	9	0.12	0.01	0.12
(1,4605)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	9	0.12	0.01	0.12
(1,4605)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	9	0.12	0.01	0.12
(1,6398)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	9	0.12	0.01	0.12
(1,6398)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	9	0.12	0.01	0.12
(1,6398)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	9	0.12	0.01	0.12
(1,526)	2:C:46:ILE:H	2:C:46:ILE:HG13	7	0.24	0.05	0.27

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2319)	2:C:46:ILE:H	2:C:46:ILE:HG13	7	0.24	0.05	0.27
(1,4112)	2:C:46:ILE:H	2:C:46:ILE:HG13	7	0.24	0.05	0.27
(1,5905)	2:C:46:ILE:H	2:C:46:ILE:HG13	7	0.24	0.05	0.27
(1,746)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	7	0.24	0.03	0.25
(1,2539)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	7	0.24	0.03	0.25
(1,4332)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	7	0.24	0.03	0.25
(1,6125)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	7	0.24	0.03	0.25
(1,1414)	2:C:70:LYS:H	2:C:69:ASP:HB2	7	0.17	0.03	0.16
(1,3207)	2:C:70:LYS:H	2:C:69:ASP:HB2	7	0.17	0.03	0.16
(1,5000)	2:C:70:LYS:H	2:C:69:ASP:HB2	7	0.17	0.03	0.16
(1,6793)	2:C:70:LYS:H	2:C:69:ASP:HB2	7	0.17	0.03	0.16
(1,1407)	2:C:42:PHE:H	2:C:41:GLU:HB3	7	0.12	0.0	0.12
(1,3200)	2:C:42:PHE:H	2:C:41:GLU:HB3	7	0.12	0.0	0.12
(1,4993)	2:C:42:PHE:H	2:C:41:GLU:HB3	7	0.12	0.0	0.12
(1,6786)	2:C:42:PHE:H	2:C:41:GLU:HB3	7	0.12	0.0	0.12
(1,1776)	1:A:25:PRO:HA	1:A:25:PRO:HD2	7	0.12	0.0	0.12
(1,3569)	1:A:25:PRO:HA	1:A:25:PRO:HD2	7	0.12	0.0	0.12
(1,5362)	1:A:25:PRO:HA	1:A:25:PRO:HD2	7	0.12	0.0	0.12
(1,7155)	1:A:25:PRO:HA	1:A:25:PRO:HD2	7	0.12	0.0	0.12
(1,1273)	2:C:18:GLU:H	2:C:17:LEU:HB2	6	0.12	0.01	0.12
(1,3066)	2:C:18:GLU:H	2:C:17:LEU:HB2	6	0.12	0.01	0.12
(1,4859)	2:C:18:GLU:H	2:C:17:LEU:HB2	6	0.12	0.01	0.12
(1,6652)	2:C:18:GLU:H	2:C:17:LEU:HB2	6	0.12	0.01	0.12
(1,785)	1:A:8:PRO:HA	1:A:8:PRO:HD3	5	0.19	0.04	0.16
(1,2578)	1:A:8:PRO:HA	1:A:8:PRO:HD3	5	0.19	0.04	0.16
(1,4371)	1:A:8:PRO:HA	1:A:8:PRO:HD3	5	0.19	0.04	0.16
(1,6164)	1:A:8:PRO:HA	1:A:8:PRO:HD3	5	0.19	0.04	0.16
(1,980)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	5	0.18	0.02	0.18
(1,2773)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	5	0.18	0.02	0.18
(1,4566)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	5	0.18	0.02	0.18
(1,6359)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	5	0.18	0.02	0.18
(1,1812)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	5	0.18	0.01	0.18
(1,1812)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	5	0.18	0.01	0.18
(1,3605)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	5	0.18	0.01	0.18
(1,3605)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	5	0.18	0.01	0.18
(1,5398)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	5	0.18	0.01	0.18
(1,5398)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	5	0.18	0.01	0.18
(1,7191)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	5	0.18	0.01	0.18
(1,7191)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	5	0.18	0.01	0.18
(1,734)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	5	0.12	0.01	0.11
(1,734)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	5	0.12	0.01	0.11
(1,2527)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	5	0.12	0.01	0.11

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Key	Atom-1	Atom-2	Models^1	Mean (Å)	SD^1 (Å)	Median (Å)
(1,2527)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	5	0.12	0.01	0.11
(1,4320)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	5	0.12	0.01	0.11
(1,4320)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	5	0.12	0.01	0.11
(1,6113)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	5	0.12	0.01	0.11
(1,6113)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	5	0.12	0.01	0.11
(1,1569)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	4	0.2	0.05	0.18
(1,3362)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	4	0.2	0.05	0.18
(1,5155)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	4	0.2	0.05	0.18
(1,6948)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	4	0.2	0.05	0.18
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	4	0.17	0.04	0.17
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	4	0.17	0.04	0.17
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	4	0.17	0.04	0.17
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	4	0.17	0.04	0.17
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	4	0.17	0.04	0.17
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	4	0.17	0.04	0.17
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	4	0.17	0.04	0.17
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	4	0.17	0.04	0.17
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	4	0.17	0.04	0.17
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	4	0.17	0.04	0.17
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	4	0.17	0.04	0.17
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	4	0.17	0.04	0.17
(1,86)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	4	0.15	0.0	0.15
(1,86)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	4	0.15	0.0	0.15
(1,1879)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	4	0.15	0.0	0.15
(1,1879)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	4	0.15	0.0	0.15
(1,3672)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	4	0.15	0.0	0.15
(1,3672)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	4	0.15	0.0	0.15
(1,5465)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	4	0.15	0.0	0.15
(1,5465)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	4	0.15	0.0	0.15
(1,1782)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	3	0.35	0.08	0.39
(1,1782)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	3	0.35	0.08	0.39
(1,1782)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	3	0.35	0.08	0.39
(1,3575)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	3	0.35	0.08	0.39
(1,3575)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	3	0.35	0.08	0.39
(1,3575)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	3	0.35	0.08	0.39
(1,5368)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	3	0.35	0.08	0.39
(1,5368)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	3	0.35	0.08	0.39
(1,5368)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	3	0.35	0.08	0.39
(1,7161)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	3	0.35	0.08	0.39
(1,7161)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	3	0.35	0.08	0.39
(1,7161)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	3	0.35	0.08	0.39
(1,521)	2:C:25:ASP:H	2:C:24:LEU:HB3	3	0.26	0.07	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2314)	2:C:25:ASP:H	2:C:24:LEU:HB3	3	0.26	0.07	0.29
(1,4107)	2:C:25:ASP:H	2:C:24:LEU:HB3	3	0.26	0.07	0.29
(1,5900)	2:C:25:ASP:H	2:C:24:LEU:HB3	3	0.26	0.07	0.29
(1,847)	2:C:36:GLN:H	2:C:37:MET:HG2	3	0.22	0.1	0.16
(1,2640)	2:C:36:GLN:H	2:C:37:MET:HG2	3	0.22	0.1	0.16
(1,4433)	2:C:36:GLN:H	2:C:37:MET:HG2	3	0.22	0.1	0.16
(1,6226)	2:C:36:GLN:H	2:C:37:MET:HG2	3	0.22	0.1	0.16
(1,38)	2:C:77:VAL:HG11	2:C:75:TYR:HA	3	0.19	0.04	0.18
(1,38)	2:C:77:VAL:HG12	2:C:75:TYR:HA	3	0.19	0.04	0.18
(1,38)	2:C:77:VAL:HG13	2:C:75:TYR:HA	3	0.19	0.04	0.18
(1,38)	2:C:77:VAL:HG21	2:C:75:TYR:HA	3	0.19	0.04	0.18
(1,38)	2:C:77:VAL:HG22	2:C:75:TYR:HA	3	0.19	0.04	0.18
(1,38)	2:C:77:VAL:HG23	2:C:75:TYR:HA	3	0.19	0.04	0.18
(1,38)	2:C:77:VAL:HG11	2:C:76:ASN:HA	3	0.19	0.04	0.18
(1,38)	2:C:77:VAL:HG12	2:C:76:ASN:HA	3	0.19	0.04	0.18
(1,38)	2:C:77:VAL:HG13	2:C:76:ASN:HA	3	0.19	0.04	0.18
(1,38)	2:C:77:VAL:HG21	2:C:76:ASN:HA	3	0.19	0.04	0.18
(1,38)	2:C:77:VAL:HG22	2:C:76:ASN:HA	3	0.19	0.04	0.18
(1,38)	2:C:77:VAL:HG23	2:C:76:ASN:HA	3	0.19	0.04	0.18
(1,1532)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	3	0.19	0.02	0.2
(1,1532)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	3	0.19	0.02	0.2
(1,1532)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	3	0.19	0.02	0.2
(1,3325)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	3	0.19	0.02	0.2
(1,3325)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	3	0.19	0.02	0.2
(1,3325)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	3	0.19	0.02	0.2
(1,5118)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	3	0.19	0.02	0.2
(1,5118)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	3	0.19	0.02	0.2
(1,5118)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	3	0.19	0.02	0.2
(1,6911)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	3	0.19	0.02	0.2
(1,6911)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	3	0.19	0.02	0.2
(1,6911)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	3	0.19	0.02	0.2
(1,1234)	2:C:27:GLN:HG3	2:C:27:GLN:HA	3	0.14	0.04	0.12
(1,3027)	2:C:27:GLN:HG3	2:C:27:GLN:HA	3	0.14	0.04	0.12
(1,4820)	2:C:27:GLN:HG3	2:C:27:GLN:HA	3	0.14	0.04	0.12
(1,6613)	2:C:27:GLN:HG3	2:C:27:GLN:HA	3	0.14	0.04	0.12
(1,833)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	3	0.14	0.01	0.14
(1,833)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	3	0.14	0.01	0.14
(1,2626)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	3	0.14	0.01	0.14
(1,2626)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	3	0.14	0.01	0.14
(1,4419)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	3	0.14	0.01	0.14
(1,4419)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	3	0.14	0.01	0.14
(1,6212)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	3	0.14	0.01	0.14

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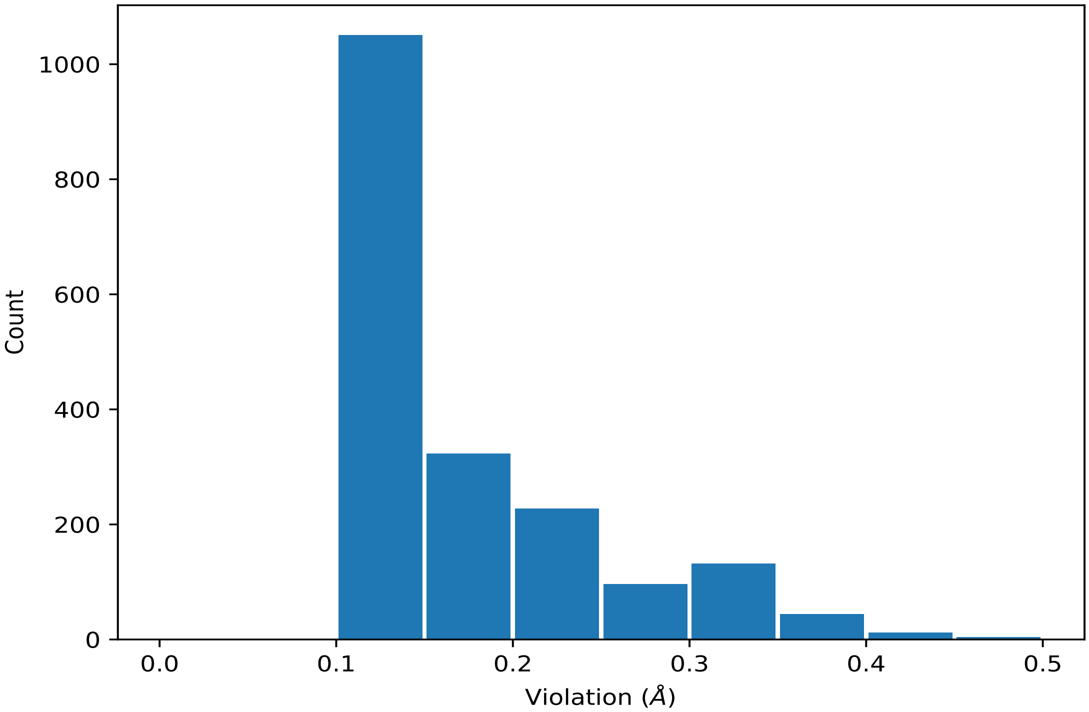
Key	Atom-1	Atom-2	Models^1	Mean (Å)	SD^1 (Å)	Median (Å)
(1,6212)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	3	0.14	0.01	0.14
(1,393)	1:A:10:ARG:H	1:A:9:GLY:HA3	3	0.13	0.02	0.12
(1,2186)	1:A:10:ARG:H	1:A:9:GLY:HA3	3	0.13	0.02	0.12
(1,3979)	1:A:10:ARG:H	1:A:9:GLY:HA3	3	0.13	0.02	0.12
(1,5772)	1:A:10:ARG:H	1:A:9:GLY:HA3	3	0.13	0.02	0.12
(1,1694)	2:C:39:VAL:HB	2:C:38:ASN:HB2	3	0.12	0.01	0.12
(1,3487)	2:C:39:VAL:HB	2:C:38:ASN:HB2	3	0.12	0.01	0.12
(1,5280)	2:C:39:VAL:HB	2:C:38:ASN:HB2	3	0.12	0.01	0.12
(1,7073)	2:C:39:VAL:HB	2:C:38:ASN:HB2	3	0.12	0.01	0.12
(1,1789)	2:C:30:THR:H	2:C:29:ARG:HB2	3	0.12	0.0	0.12
(1,3582)	2:C:30:THR:H	2:C:29:ARG:HB2	3	0.12	0.0	0.12
(1,5375)	2:C:30:THR:H	2:C:29:ARG:HB2	3	0.12	0.0	0.12
(1,7168)	2:C:30:THR:H	2:C:29:ARG:HB2	3	0.12	0.0	0.12
(1,566)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	3	0.11	0.0	0.11
(1,2359)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	3	0.11	0.0	0.11
(1,4152)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	3	0.11	0.0	0.11
(1,5945)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	3	0.11	0.0	0.11
(1,1788)	2:C:27:GLN:H	2:C:27:GLN:HG2	2	0.42	0.06	0.42
(1,3581)	2:C:27:GLN:H	2:C:27:GLN:HG2	2	0.42	0.06	0.42
(1,5374)	2:C:27:GLN:H	2:C:27:GLN:HG2	2	0.42	0.06	0.42
(1,7167)	2:C:27:GLN:H	2:C:27:GLN:HG2	2	0.42	0.06	0.42
(1,1286)	2:C:70:LYS:H	2:C:70:LYS:HG2	2	0.25	0.0	0.25
(1,3079)	2:C:70:LYS:H	2:C:70:LYS:HG2	2	0.25	0.0	0.25
(1,4872)	2:C:70:LYS:H	2:C:70:LYS:HG2	2	0.25	0.0	0.25
(1,6665)	2:C:70:LYS:H	2:C:70:LYS:HG2	2	0.25	0.0	0.25
(1,1053)	2:C:87:ARG:H	2:C:87:ARG:HG2	2	0.19	0.02	0.19
(1,2846)	2:C:87:ARG:H	2:C:87:ARG:HG2	2	0.19	0.02	0.19
(1,4639)	2:C:87:ARG:H	2:C:87:ARG:HG2	2	0.19	0.02	0.19
(1,6432)	2:C:87:ARG:H	2:C:87:ARG:HG2	2	0.19	0.02	0.19
(1,24)	2:C:91:GLN:H	2:C:91:GLN:HA	2	0.12	0.01	0.12
(1,24)	2:C:91:GLN:H	2:C:90:PRO:HA	2	0.12	0.01	0.12
(1,1659)	1:A:16:CYS:H	1:A:15:CYS:HB3	2	0.12	0.01	0.12
(1,3452)	1:A:16:CYS:H	1:A:15:CYS:HB3	2	0.12	0.01	0.12
(1,5245)	1:A:16:CYS:H	1:A:15:CYS:HB3	2	0.12	0.01	0.12
(1,7038)	1:A:16:CYS:H	1:A:15:CYS:HB3	2	0.12	0.01	0.12
(1,111)	1:A:28:ILE:HG13	1:A:28:ILE:HA	2	0.12	0.0	0.12
(1,1904)	1:A:28:ILE:HG13	1:A:28:ILE:HA	2	0.12	0.0	0.12
(1,3697)	1:A:28:ILE:HG13	1:A:28:ILE:HA	2	0.12	0.0	0.12
(1,5490)	1:A:28:ILE:HG13	1:A:28:ILE:HA	2	0.12	0.0	0.12

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

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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 ⓘ

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)
(1,7167)	2:C:27:GLN:H	2:C:27:GLN:HG2	8	0.48
(1,5374)	2:C:27:GLN:H	2:C:27:GLN:HG2	8	0.48
(1,3581)	2:C:27:GLN:H	2:C:27:GLN:HG2	8	0.48
(1,1788)	2:C:27:GLN:H	2:C:27:GLN:HG2	8	0.48
(1,7161)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	19	0.41
(1,7161)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	19	0.41
(1,7161)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	19	0.41
(1,5368)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	19	0.41
(1,5368)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	19	0.41
(1,5368)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	19	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3575)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	19	0.41
(1,3575)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	19	0.41
(1,3575)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	19	0.41
(1,1782)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	19	0.41
(1,1782)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	19	0.41
(1,1782)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	19	0.41
(1,7161)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	3	0.39
(1,7161)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	3	0.39
(1,7161)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	3	0.39
(1,5368)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	3	0.39
(1,5368)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	3	0.39
(1,5368)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	3	0.39
(1,3575)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	3	0.39
(1,3575)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	3	0.39
(1,3575)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	3	0.39
(1,1782)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	3	0.39
(1,1782)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	3	0.39
(1,1782)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	3	0.39
(1,847)	2:C:36:GLN:H	2:C:37:MET:HG2	6	0.37
(1,7195)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	9	0.37
(1,7195)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	9	0.37
(1,7195)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	9	0.37
(1,6226)	2:C:36:GLN:H	2:C:37:MET:HG2	6	0.37
(1,5402)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	9	0.37
(1,5402)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	9	0.37
(1,5402)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	9	0.37
(1,4433)	2:C:36:GLN:H	2:C:37:MET:HG2	6	0.37
(1,3609)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	9	0.37
(1,3609)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	9	0.37
(1,3609)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	9	0.37
(1,2640)	2:C:36:GLN:H	2:C:37:MET:HG2	6	0.37
(1,1816)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	9	0.37
(1,1816)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	9	0.37
(1,1816)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	9	0.37
(1,7195)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	12	0.36
(1,7195)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	12	0.36
(1,7195)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	12	0.36
(1,7167)	2:C:27:GLN:H	2:C:27:GLN:HG2	3	0.36
(1,5402)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	12	0.36
(1,5402)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	12	0.36
(1,5402)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	12	0.36
(1,5374)	2:C:27:GLN:H	2:C:27:GLN:HG2	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3609)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	12	0.36
(1,3609)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	12	0.36
(1,3609)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	12	0.36
(1,3581)	2:C:27:GLN:H	2:C:27:GLN:HG2	3	0.36
(1,1816)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	12	0.36
(1,1816)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	12	0.36
(1,1816)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	12	0.36
(1,1788)	2:C:27:GLN:H	2:C:27:GLN:HG2	3	0.36
(1,5672)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	9	0.35
(1,5672)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	9	0.35
(1,5672)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	9	0.35
(1,3879)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	9	0.35
(1,3879)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	9	0.35
(1,3879)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	9	0.35
(1,293)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	9	0.35
(1,293)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	9	0.35
(1,293)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	9	0.35
(1,2086)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	9	0.35
(1,2086)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	9	0.35
(1,2086)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	9	0.35
(1,5672)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	7	0.34
(1,5672)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	7	0.34
(1,5672)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	7	0.34
(1,5672)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	17	0.34
(1,5672)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	17	0.34
(1,5672)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	17	0.34
(1,5672)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	18	0.34
(1,5672)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	18	0.34
(1,5672)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	18	0.34
(1,5672)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	19	0.34
(1,5672)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	19	0.34
(1,5672)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	19	0.34
(1,3879)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	7	0.34
(1,3879)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	7	0.34
(1,3879)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	7	0.34
(1,3879)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	17	0.34
(1,3879)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	17	0.34
(1,3879)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	17	0.34
(1,3879)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	18	0.34
(1,3879)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	18	0.34
(1,3879)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	18	0.34
(1,3879)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	19	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3879)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	19	0.34
(1,3879)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	19	0.34
(1,293)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	7	0.34
(1,293)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	7	0.34
(1,293)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	7	0.34
(1,293)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	17	0.34
(1,293)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	17	0.34
(1,293)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	17	0.34
(1,293)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	18	0.34
(1,293)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	18	0.34
(1,293)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	18	0.34
(1,293)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	19	0.34
(1,293)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	19	0.34
(1,293)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	19	0.34
(1,2086)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	7	0.34
(1,2086)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	7	0.34
(1,2086)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	7	0.34
(1,2086)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	17	0.34
(1,2086)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	17	0.34
(1,2086)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	17	0.34
(1,2086)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	18	0.34
(1,2086)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	18	0.34
(1,2086)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	18	0.34
(1,2086)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	19	0.34
(1,2086)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	19	0.34
(1,2086)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	19	0.34
(1,5900)	2:C:25:ASP:H	2:C:24:LEU:HB3	18	0.33
(1,5672)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	2	0.33
(1,5672)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	2	0.33
(1,5672)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	2	0.33
(1,5672)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	4	0.33
(1,5672)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	4	0.33
(1,5672)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	4	0.33
(1,5672)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	14	0.33
(1,5672)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	14	0.33
(1,5672)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	14	0.33
(1,5501)	2:C:19:VAL:H	2:C:31:PHE:HB3	2	0.33
(1,521)	2:C:25:ASP:H	2:C:24:LEU:HB3	18	0.33
(1,4107)	2:C:25:ASP:H	2:C:24:LEU:HB3	18	0.33
(1,3879)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	2	0.33
(1,3879)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	2	0.33
(1,3879)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3879)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	4	0.33
(1,3879)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	4	0.33
(1,3879)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	4	0.33
(1,3879)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	14	0.33
(1,3879)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	14	0.33
(1,3879)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	14	0.33
(1,3708)	2:C:19:VAL:H	2:C:31:PHE:HB3	2	0.33
(1,293)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	2	0.33
(1,293)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	2	0.33
(1,293)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	2	0.33
(1,293)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	4	0.33
(1,293)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	4	0.33
(1,293)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	4	0.33
(1,293)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	14	0.33
(1,293)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	14	0.33
(1,293)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	14	0.33
(1,2314)	2:C:25:ASP:H	2:C:24:LEU:HB3	18	0.33
(1,2086)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	2	0.33
(1,2086)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	2	0.33
(1,2086)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	2	0.33
(1,2086)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	4	0.33
(1,2086)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	4	0.33
(1,2086)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	4	0.33
(1,2086)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	14	0.33
(1,2086)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	14	0.33
(1,2086)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	14	0.33
(1,1915)	2:C:19:VAL:H	2:C:31:PHE:HB3	2	0.33
(1,122)	2:C:19:VAL:H	2:C:31:PHE:HB3	2	0.33
(1,5672)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	20	0.32
(1,5672)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	20	0.32
(1,5672)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	20	0.32
(1,5501)	2:C:19:VAL:H	2:C:31:PHE:HB3	6	0.32
(1,3879)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	20	0.32
(1,3879)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	20	0.32
(1,3879)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	20	0.32
(1,3708)	2:C:19:VAL:H	2:C:31:PHE:HB3	6	0.32
(1,293)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	20	0.32
(1,293)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	20	0.32
(1,293)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	20	0.32
(1,2086)	1:A:28:ILE:HD11	1:A:26:ASP:HB3	20	0.32
(1,2086)	1:A:28:ILE:HD12	1:A:26:ASP:HB3	20	0.32
(1,2086)	1:A:28:ILE:HD13	1:A:26:ASP:HB3	20	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1915)	2:C:19:VAL:H	2:C:31:PHE:HB3	6	0.32
(1,122)	2:C:19:VAL:H	2:C:31:PHE:HB3	6	0.32
(1,7195)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	2	0.31
(1,7195)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	2	0.31
(1,7195)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	2	0.31
(1,5402)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	2	0.31
(1,5402)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	2	0.31
(1,5402)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	2	0.31
(1,3609)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	2	0.31
(1,3609)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	2	0.31
(1,3609)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	2	0.31
(1,1816)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	2	0.31
(1,1816)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	2	0.31
(1,1816)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	2	0.31
(1,5900)	2:C:25:ASP:H	2:C:24:LEU:HB3	11	0.29
(1,521)	2:C:25:ASP:H	2:C:24:LEU:HB3	11	0.29
(1,4107)	2:C:25:ASP:H	2:C:24:LEU:HB3	11	0.29
(1,2314)	2:C:25:ASP:H	2:C:24:LEU:HB3	11	0.29
(1,5905)	2:C:46:ILE:H	2:C:46:ILE:HG13	16	0.28
(1,526)	2:C:46:ILE:H	2:C:46:ILE:HG13	16	0.28
(1,4112)	2:C:46:ILE:H	2:C:46:ILE:HG13	16	0.28
(1,2319)	2:C:46:ILE:H	2:C:46:ILE:HG13	16	0.28
(1,7195)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	4	0.27
(1,7195)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	4	0.27
(1,7195)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	4	0.27
(1,5905)	2:C:46:ILE:H	2:C:46:ILE:HG13	10	0.27
(1,5905)	2:C:46:ILE:H	2:C:46:ILE:HG13	18	0.27
(1,5905)	2:C:46:ILE:H	2:C:46:ILE:HG13	20	0.27
(1,5501)	2:C:19:VAL:H	2:C:31:PHE:HB3	1	0.27
(1,5501)	2:C:19:VAL:H	2:C:31:PHE:HB3	11	0.27
(1,5402)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	4	0.27
(1,5402)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	4	0.27
(1,5402)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	4	0.27
(1,526)	2:C:46:ILE:H	2:C:46:ILE:HG13	10	0.27
(1,526)	2:C:46:ILE:H	2:C:46:ILE:HG13	18	0.27
(1,526)	2:C:46:ILE:H	2:C:46:ILE:HG13	20	0.27
(1,4112)	2:C:46:ILE:H	2:C:46:ILE:HG13	10	0.27
(1,4112)	2:C:46:ILE:H	2:C:46:ILE:HG13	18	0.27
(1,4112)	2:C:46:ILE:H	2:C:46:ILE:HG13	20	0.27
(1,3708)	2:C:19:VAL:H	2:C:31:PHE:HB3	1	0.27
(1,3708)	2:C:19:VAL:H	2:C:31:PHE:HB3	11	0.27
(1,3609)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3609)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	4	0.27
(1,3609)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	4	0.27
(1,2319)	2:C:46:ILE:H	2:C:46:ILE:HG13	10	0.27
(1,2319)	2:C:46:ILE:H	2:C:46:ILE:HG13	18	0.27
(1,2319)	2:C:46:ILE:H	2:C:46:ILE:HG13	20	0.27
(1,1915)	2:C:19:VAL:H	2:C:31:PHE:HB3	1	0.27
(1,1915)	2:C:19:VAL:H	2:C:31:PHE:HB3	11	0.27
(1,1816)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	4	0.27
(1,1816)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	4	0.27
(1,1816)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	4	0.27
(1,122)	2:C:19:VAL:H	2:C:31:PHE:HB3	1	0.27
(1,122)	2:C:19:VAL:H	2:C:31:PHE:HB3	11	0.27
(1,746)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	14	0.26
(1,746)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	20	0.26
(1,7195)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	1	0.26
(1,7195)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	1	0.26
(1,7195)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	1	0.26
(1,6948)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	3	0.26
(1,6125)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	14	0.26
(1,6125)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	20	0.26
(1,5905)	2:C:46:ILE:H	2:C:46:ILE:HG13	8	0.26
(1,5402)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	1	0.26
(1,5402)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	1	0.26
(1,5402)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	1	0.26
(1,526)	2:C:46:ILE:H	2:C:46:ILE:HG13	8	0.26
(1,5155)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	3	0.26
(1,4332)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	14	0.26
(1,4332)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	20	0.26
(1,4112)	2:C:46:ILE:H	2:C:46:ILE:HG13	8	0.26
(1,3609)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	1	0.26
(1,3609)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	1	0.26
(1,3609)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	1	0.26
(1,3362)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	3	0.26
(1,2539)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	14	0.26
(1,2539)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	20	0.26
(1,2319)	2:C:46:ILE:H	2:C:46:ILE:HG13	8	0.26
(1,1816)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	1	0.26
(1,1816)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	1	0.26
(1,1816)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	1	0.26
(1,1569)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	3	0.26
(1,785)	1:A:8:PRO:HA	1:A:8:PRO:HD3	10	0.25
(1,746)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,746)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	5	0.25
(1,746)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	16	0.25
(1,6665)	2:C:70:LYS:H	2:C:70:LYS:HG2	5	0.25
(1,6665)	2:C:70:LYS:H	2:C:70:LYS:HG2	13	0.25
(1,6164)	1:A:8:PRO:HA	1:A:8:PRO:HD3	10	0.25
(1,6125)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	2	0.25
(1,6125)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	5	0.25
(1,6125)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	16	0.25
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	1	0.25
(1,4872)	2:C:70:LYS:H	2:C:70:LYS:HG2	5	0.25
(1,4872)	2:C:70:LYS:H	2:C:70:LYS:HG2	13	0.25
(1,4371)	1:A:8:PRO:HA	1:A:8:PRO:HD3	10	0.25
(1,4332)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	2	0.25
(1,4332)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	5	0.25
(1,4332)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	16	0.25
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	1	0.25
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	1	0.25
(1,3079)	2:C:70:LYS:H	2:C:70:LYS:HG2	5	0.25
(1,3079)	2:C:70:LYS:H	2:C:70:LYS:HG2	13	0.25
(1,2578)	1:A:8:PRO:HA	1:A:8:PRO:HD3	10	0.25
(1,2539)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	2	0.25
(1,2539)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	5	0.25
(1,2539)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	16	0.25
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	1	0.25
(1,1286)	2:C:70:LYS:H	2:C:70:LYS:HG2	5	0.25
(1,1286)	2:C:70:LYS:H	2:C:70:LYS:HG2	13	0.25
(1,7195)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	8	0.24
(1,7195)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	8	0.24
(1,7195)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	8	0.24
(1,7161)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	17	0.24
(1,7161)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	17	0.24
(1,7161)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	17	0.24
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	13	0.24
(1,5501)	2:C:19:VAL:H	2:C:31:PHE:HB3	19	0.24
(1,5402)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	8	0.24
(1,5402)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	8	0.24
(1,5402)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	8	0.24
(1,5368)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	17	0.24
(1,5368)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	17	0.24
(1,5368)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	17	0.24
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	19	0.24
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	19	0.24
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	19	0.24
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	19	0.24
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	19	0.24
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	19	0.24
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	19	0.24
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	19	0.24
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	13	0.24
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	13	0.24
(1,38)	2:C:77:VAL:HG11	2:C:75:TYR:HA	8	0.24
(1,38)	2:C:77:VAL:HG12	2:C:75:TYR:HA	8	0.24
(1,38)	2:C:77:VAL:HG13	2:C:75:TYR:HA	8	0.24
(1,38)	2:C:77:VAL:HG21	2:C:75:TYR:HA	8	0.24
(1,38)	2:C:77:VAL:HG22	2:C:75:TYR:HA	8	0.24
(1,38)	2:C:77:VAL:HG23	2:C:75:TYR:HA	8	0.24
(1,38)	2:C:77:VAL:HG11	2:C:76:ASN:HA	8	0.24
(1,38)	2:C:77:VAL:HG12	2:C:76:ASN:HA	8	0.24
(1,38)	2:C:77:VAL:HG13	2:C:76:ASN:HA	8	0.24
(1,38)	2:C:77:VAL:HG21	2:C:76:ASN:HA	8	0.24
(1,38)	2:C:77:VAL:HG22	2:C:76:ASN:HA	8	0.24
(1,38)	2:C:77:VAL:HG23	2:C:76:ASN:HA	8	0.24
(1,3708)	2:C:19:VAL:H	2:C:31:PHE:HB3	19	0.24
(1,3609)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	8	0.24
(1,3609)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	8	0.24
(1,3609)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	8	0.24
(1,3575)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	17	0.24
(1,3575)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	17	0.24
(1,3575)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	17	0.24
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	13	0.24
(1,1915)	2:C:19:VAL:H	2:C:31:PHE:HB3	19	0.24
(1,1816)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	8	0.24
(1,1816)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	8	0.24
(1,1816)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	8	0.24
(1,1782)	1:A:30:PRO:HG3	1:A:20:ILE:HG21	17	0.24
(1,1782)	1:A:30:PRO:HG3	1:A:20:ILE:HG22	17	0.24
(1,1782)	1:A:30:PRO:HG3	1:A:20:ILE:HG23	17	0.24
(1,122)	2:C:19:VAL:H	2:C:31:PHE:HB3	19	0.24
(1,7066)	2:C:44:GLU:HA	2:C:54:SER:HB3	2	0.23
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	2	0.23
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	4	0.23
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	5	0.23
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5273)	2:C:44:GLU:HA	2:C:54:SER:HB3	2	0.23
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	2	0.23
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	4	0.23
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	5	0.23
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	16	0.23
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	2	0.23
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	4	0.23
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	5	0.23
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	16	0.23
(1,3480)	2:C:44:GLU:HA	2:C:54:SER:HB3	2	0.23
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	2	0.23
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	4	0.23
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	5	0.23
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	16	0.23
(1,1687)	2:C:44:GLU:HA	2:C:54:SER:HB3	2	0.23
(1,785)	1:A:8:PRO:HA	1:A:8:PRO:HD3	3	0.22
(1,7195)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	19	0.22
(1,7195)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	19	0.22
(1,7195)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	19	0.22
(1,6948)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	14	0.22
(1,6164)	1:A:8:PRO:HA	1:A:8:PRO:HD3	3	0.22
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	11	0.22
(1,5501)	2:C:19:VAL:H	2:C:31:PHE:HB3	12	0.22
(1,5501)	2:C:19:VAL:H	2:C:31:PHE:HB3	13	0.22
(1,5402)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	19	0.22
(1,5402)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	19	0.22
(1,5402)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	19	0.22
(1,5155)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	14	0.22
(1,4371)	1:A:8:PRO:HA	1:A:8:PRO:HD3	3	0.22
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	11	0.22
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	11	0.22
(1,3708)	2:C:19:VAL:H	2:C:31:PHE:HB3	12	0.22
(1,3708)	2:C:19:VAL:H	2:C:31:PHE:HB3	13	0.22
(1,3609)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	19	0.22
(1,3609)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	19	0.22
(1,3609)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	19	0.22
(1,3362)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	14	0.22
(1,2578)	1:A:8:PRO:HA	1:A:8:PRO:HD3	3	0.22
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	11	0.22
(1,1915)	2:C:19:VAL:H	2:C:31:PHE:HB3	12	0.22
(1,1915)	2:C:19:VAL:H	2:C:31:PHE:HB3	13	0.22
(1,19)	2:C:75:TYR:H	2:C:74:GLU:HG2	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	2:C:75:TYR:H	2:C:74:GLU:HG3	14	0.22
(1,1816)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	19	0.22
(1,1816)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	19	0.22
(1,1816)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	19	0.22
(1,1569)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	14	0.22
(1,122)	2:C:19:VAL:H	2:C:31:PHE:HB3	12	0.22
(1,122)	2:C:19:VAL:H	2:C:31:PHE:HB3	13	0.22
(1,871)	1:A:17:SER:HB3	1:A:12:PHE:HZ	4	0.21
(1,7195)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	13	0.21
(1,7195)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	13	0.21
(1,7195)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	13	0.21
(1,6793)	2:C:70:LYS:H	2:C:69:ASP:HB2	8	0.21
(1,6568)	2:C:52:ILE:HD11	2:C:53:PRO:HD2	16	0.21
(1,6568)	2:C:52:ILE:HD12	2:C:53:PRO:HD2	16	0.21
(1,6568)	2:C:52:ILE:HD13	2:C:53:PRO:HD2	16	0.21
(1,6432)	2:C:87:ARG:H	2:C:87:ARG:HG2	14	0.21
(1,6250)	1:A:17:SER:HB3	1:A:12:PHE:HZ	4	0.21
(1,5905)	2:C:46:ILE:H	2:C:46:ILE:HG13	12	0.21
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	15	0.21
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	6	0.21
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	6	0.21
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	6	0.21
(1,5402)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	13	0.21
(1,5402)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	13	0.21
(1,5402)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	13	0.21
(1,526)	2:C:46:ILE:H	2:C:46:ILE:HG13	12	0.21
(1,5000)	2:C:70:LYS:H	2:C:69:ASP:HB2	8	0.21
(1,4775)	2:C:52:ILE:HD11	2:C:53:PRO:HD2	16	0.21
(1,4775)	2:C:52:ILE:HD12	2:C:53:PRO:HD2	16	0.21
(1,4775)	2:C:52:ILE:HD13	2:C:53:PRO:HD2	16	0.21
(1,4639)	2:C:87:ARG:H	2:C:87:ARG:HG2	14	0.21
(1,4457)	1:A:17:SER:HB3	1:A:12:PHE:HZ	4	0.21
(1,4112)	2:C:46:ILE:H	2:C:46:ILE:HG13	12	0.21
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	15	0.21
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	15	0.21
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	6	0.21
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	6	0.21
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	6	0.21
(1,3609)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	13	0.21
(1,3609)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	13	0.21
(1,3609)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	13	0.21
(1,3207)	2:C:70:LYS:H	2:C:69:ASP:HB2	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2982)	2:C:52:ILE:HD11	2:C:53:PRO:HD2	16	0.21
(1,2982)	2:C:52:ILE:HD12	2:C:53:PRO:HD2	16	0.21
(1,2982)	2:C:52:ILE:HD13	2:C:53:PRO:HD2	16	0.21
(1,2846)	2:C:87:ARG:H	2:C:87:ARG:HG2	14	0.21
(1,2664)	1:A:17:SER:HB3	1:A:12:PHE:HZ	4	0.21
(1,2319)	2:C:46:ILE:H	2:C:46:ILE:HG13	12	0.21
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	15	0.21
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	6	0.21
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	6	0.21
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	6	0.21
(1,1816)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	13	0.21
(1,1816)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	13	0.21
(1,1816)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	13	0.21
(1,1414)	2:C:70:LYS:H	2:C:69:ASP:HB2	8	0.21
(1,1189)	2:C:52:ILE:HD11	2:C:53:PRO:HD2	16	0.21
(1,1189)	2:C:52:ILE:HD12	2:C:53:PRO:HD2	16	0.21
(1,1189)	2:C:52:ILE:HD13	2:C:53:PRO:HD2	16	0.21
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	6	0.21
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	6	0.21
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	6	0.21
(1,1053)	2:C:87:ARG:H	2:C:87:ARG:HG2	14	0.21
(1,980)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	10	0.2
(1,980)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	11	0.2
(1,746)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	17	0.2
(1,6911)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	2	0.2
(1,6911)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	2	0.2
(1,6911)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	2	0.2
(1,6911)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	14	0.2
(1,6911)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	14	0.2
(1,6911)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	14	0.2
(1,6793)	2:C:70:LYS:H	2:C:69:ASP:HB2	15	0.2
(1,6613)	2:C:27:GLN:HG3	2:C:27:GLN:HA	3	0.2
(1,6359)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	10	0.2
(1,6359)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	11	0.2
(1,6125)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	17	0.2
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	10	0.2
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	14	0.2
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	8	0.2
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	8	0.2
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	8	0.2
(1,5118)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	2	0.2
(1,5118)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5118)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	2	0.2
(1,5118)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	14	0.2
(1,5118)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	14	0.2
(1,5118)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	14	0.2
(1,5000)	2:C:70:LYS:H	2:C:69:ASP:HB2	15	0.2
(1,4820)	2:C:27:GLN:HG3	2:C:27:GLN:HA	3	0.2
(1,4566)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	10	0.2
(1,4566)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	11	0.2
(1,4332)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	17	0.2
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	10	0.2
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	14	0.2
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	10	0.2
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	14	0.2
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	8	0.2
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	8	0.2
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	8	0.2
(1,3325)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	2	0.2
(1,3325)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	2	0.2
(1,3325)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	2	0.2
(1,3325)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	14	0.2
(1,3325)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	14	0.2
(1,3325)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	14	0.2
(1,3207)	2:C:70:LYS:H	2:C:69:ASP:HB2	15	0.2
(1,3027)	2:C:27:GLN:HG3	2:C:27:GLN:HA	3	0.2
(1,2773)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	10	0.2
(1,2773)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	11	0.2
(1,2539)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	17	0.2
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	10	0.2
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	14	0.2
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	8	0.2
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	8	0.2
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	8	0.2
(1,1532)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	2	0.2
(1,1532)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	2	0.2
(1,1532)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	2	0.2
(1,1532)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	14	0.2
(1,1532)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	14	0.2
(1,1532)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	14	0.2
(1,1414)	2:C:70:LYS:H	2:C:69:ASP:HB2	15	0.2
(1,1234)	2:C:27:GLN:HG3	2:C:27:GLN:HA	3	0.2
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	8	0.2
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	8	0.2
(1,746)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	7	0.19
(1,7191)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	11	0.19
(1,7191)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	11	0.19
(1,7191)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	13	0.19
(1,7191)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	13	0.19
(1,6125)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	7	0.19
(1,5501)	2:C:19:VAL:H	2:C:31:PHE:HB3	4	0.19
(1,5398)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	11	0.19
(1,5398)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	11	0.19
(1,5398)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	13	0.19
(1,5398)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	13	0.19
(1,4332)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	7	0.19
(1,3708)	2:C:19:VAL:H	2:C:31:PHE:HB3	4	0.19
(1,3605)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	11	0.19
(1,3605)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	11	0.19
(1,3605)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	13	0.19
(1,3605)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	13	0.19
(1,2539)	2:C:36:GLN:HE21	2:C:36:GLN:HB3	7	0.19
(1,1915)	2:C:19:VAL:H	2:C:31:PHE:HB3	4	0.19
(1,1812)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	11	0.19
(1,1812)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	11	0.19
(1,1812)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	13	0.19
(1,1812)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	13	0.19
(1,122)	2:C:19:VAL:H	2:C:31:PHE:HB3	4	0.19
(1,980)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	6	0.18
(1,7191)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	12	0.18
(1,7191)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	12	0.18
(1,6793)	2:C:70:LYS:H	2:C:69:ASP:HB2	6	0.18
(1,6566)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	14	0.18
(1,6566)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	14	0.18
(1,6566)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	14	0.18
(1,6566)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	20	0.18
(1,6566)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	20	0.18
(1,6566)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	20	0.18
(1,6544)	2:C:79:GLY:H	2:C:78:GLY:HA3	20	0.18
(1,6359)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	6	0.18
(1,5501)	2:C:19:VAL:H	2:C:31:PHE:HB3	8	0.18
(1,5398)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	12	0.18
(1,5398)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	12	0.18
(1,5000)	2:C:70:LYS:H	2:C:69:ASP:HB2	6	0.18
(1,4773)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4773)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	14	0.18
(1,4773)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	14	0.18
(1,4773)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	20	0.18
(1,4773)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	20	0.18
(1,4773)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	20	0.18
(1,4751)	2:C:79:GLY:H	2:C:78:GLY:HA3	20	0.18
(1,4566)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	6	0.18
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	9	0.18
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	9	0.18
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	9	0.18
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	9	0.18
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	9	0.18
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	9	0.18
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	9	0.18
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	9	0.18
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	9	0.18
(1,38)	2:C:77:VAL:HG11	2:C:75:TYR:HA	19	0.18
(1,38)	2:C:77:VAL:HG12	2:C:75:TYR:HA	19	0.18
(1,38)	2:C:77:VAL:HG13	2:C:75:TYR:HA	19	0.18
(1,38)	2:C:77:VAL:HG21	2:C:75:TYR:HA	19	0.18
(1,38)	2:C:77:VAL:HG22	2:C:75:TYR:HA	19	0.18
(1,38)	2:C:77:VAL:HG23	2:C:75:TYR:HA	19	0.18
(1,38)	2:C:77:VAL:HG11	2:C:76:ASN:HA	19	0.18
(1,38)	2:C:77:VAL:HG12	2:C:76:ASN:HA	19	0.18
(1,38)	2:C:77:VAL:HG13	2:C:76:ASN:HA	19	0.18
(1,38)	2:C:77:VAL:HG21	2:C:76:ASN:HA	19	0.18
(1,38)	2:C:77:VAL:HG22	2:C:76:ASN:HA	19	0.18
(1,38)	2:C:77:VAL:HG23	2:C:76:ASN:HA	19	0.18
(1,3708)	2:C:19:VAL:H	2:C:31:PHE:HB3	8	0.18
(1,3605)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	12	0.18
(1,3605)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	12	0.18
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	1	0.18
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	1	0.18
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	12	0.18
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	12	0.18
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	14	0.18
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	14	0.18
(1,3207)	2:C:70:LYS:H	2:C:69:ASP:HB2	6	0.18
(1,2980)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	14	0.18
(1,2980)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	14	0.18
(1,2980)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	14	0.18
(1,2980)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2980)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	20	0.18
(1,2980)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	20	0.18
(1,2958)	2:C:79:GLY:H	2:C:78:GLY:HA3	20	0.18
(1,2773)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	6	0.18
(1,1915)	2:C:19:VAL:H	2:C:31:PHE:HB3	8	0.18
(1,1812)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	12	0.18
(1,1812)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	12	0.18
(1,1414)	2:C:70:LYS:H	2:C:69:ASP:HB2	6	0.18
(1,122)	2:C:19:VAL:H	2:C:31:PHE:HB3	8	0.18
(1,1187)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	14	0.18
(1,1187)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	14	0.18
(1,1187)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	14	0.18
(1,1187)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	20	0.18
(1,1187)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	20	0.18
(1,1187)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	20	0.18
(1,1165)	2:C:79:GLY:H	2:C:78:GLY:HA3	20	0.18
(1,980)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	15	0.17
(1,7191)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	6	0.17
(1,7191)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	6	0.17
(1,7191)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	19	0.17
(1,7191)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	19	0.17
(1,6566)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	2	0.17
(1,6566)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	2	0.17
(1,6566)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	2	0.17
(1,6566)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	4	0.17
(1,6566)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	4	0.17
(1,6566)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	4	0.17
(1,6566)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	10	0.17
(1,6566)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	10	0.17
(1,6566)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	10	0.17
(1,6566)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	16	0.17
(1,6566)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	16	0.17
(1,6566)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	16	0.17
(1,6566)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	19	0.17
(1,6566)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	19	0.17
(1,6566)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	19	0.17
(1,6432)	2:C:87:ARG:H	2:C:87:ARG:HG2	5	0.17
(1,6359)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	15	0.17
(1,5900)	2:C:25:ASP:H	2:C:24:LEU:HB3	9	0.17
(1,5398)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	6	0.17
(1,5398)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	6	0.17
(1,5398)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5398)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	19	0.17
(1,521)	2:C:25:ASP:H	2:C:24:LEU:HB3	9	0.17
(1,4773)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	2	0.17
(1,4773)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	2	0.17
(1,4773)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	2	0.17
(1,4773)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	4	0.17
(1,4773)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	4	0.17
(1,4773)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	4	0.17
(1,4773)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	10	0.17
(1,4773)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	10	0.17
(1,4773)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	10	0.17
(1,4773)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	16	0.17
(1,4773)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	16	0.17
(1,4773)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	16	0.17
(1,4773)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	19	0.17
(1,4773)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	19	0.17
(1,4773)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	19	0.17
(1,4639)	2:C:87:ARG:H	2:C:87:ARG:HG2	5	0.17
(1,4566)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	15	0.17
(1,4107)	2:C:25:ASP:H	2:C:24:LEU:HB3	9	0.17
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	10	0.17
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	10	0.17
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	10	0.17
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	10	0.17
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	10	0.17
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	10	0.17
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	10	0.17
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	10	0.17
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	10	0.17
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	16	0.17
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	16	0.17
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	16	0.17
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	16	0.17
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	16	0.17
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	16	0.17
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	16	0.17
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	16	0.17
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	16	0.17
(1,3605)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	6	0.17
(1,3605)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	6	0.17
(1,3605)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	19	0.17
(1,3605)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	6	0.17
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	6	0.17
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	7	0.17
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	7	0.17
(1,2980)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	2	0.17
(1,2980)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	2	0.17
(1,2980)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	2	0.17
(1,2980)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	4	0.17
(1,2980)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	4	0.17
(1,2980)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	4	0.17
(1,2980)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	10	0.17
(1,2980)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	10	0.17
(1,2980)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	10	0.17
(1,2980)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	16	0.17
(1,2980)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	16	0.17
(1,2980)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	16	0.17
(1,2980)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	19	0.17
(1,2980)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	19	0.17
(1,2980)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	19	0.17
(1,2846)	2:C:87:ARG:H	2:C:87:ARG:HG2	5	0.17
(1,2773)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	15	0.17
(1,2314)	2:C:25:ASP:H	2:C:24:LEU:HB3	9	0.17
(1,1812)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	6	0.17
(1,1812)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	6	0.17
(1,1812)	2:C:36:GLN:HG2	2:C:36:GLN:HB3	19	0.17
(1,1812)	2:C:36:GLN:HG3	2:C:36:GLN:HB3	19	0.17
(1,1187)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	2	0.17
(1,1187)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	2	0.17
(1,1187)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	2	0.17
(1,1187)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	4	0.17
(1,1187)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	4	0.17
(1,1187)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	4	0.17
(1,1187)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	10	0.17
(1,1187)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	10	0.17
(1,1187)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	10	0.17
(1,1187)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	16	0.17
(1,1187)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	16	0.17
(1,1187)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	16	0.17
(1,1187)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	19	0.17
(1,1187)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	19	0.17
(1,1187)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	19	0.17
(1,1053)	2:C:87:ARG:H	2:C:87:ARG:HG2	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,980)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	13	0.16
(1,847)	2:C:36:GLN:H	2:C:37:MET:HG2	7	0.16
(1,785)	1:A:8:PRO:HA	1:A:8:PRO:HD3	2	0.16
(1,785)	1:A:8:PRO:HA	1:A:8:PRO:HD3	19	0.16
(1,6911)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	9	0.16
(1,6911)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	9	0.16
(1,6911)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	9	0.16
(1,6793)	2:C:70:LYS:H	2:C:69:ASP:HB2	4	0.16
(1,6566)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	17	0.16
(1,6566)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	17	0.16
(1,6566)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	17	0.16
(1,6507)	1:A:24:LEU:HD21	1:A:24:LEU:HA	16	0.16
(1,6507)	1:A:24:LEU:HD22	1:A:24:LEU:HA	16	0.16
(1,6507)	1:A:24:LEU:HD23	1:A:24:LEU:HA	16	0.16
(1,6359)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	13	0.16
(1,6226)	2:C:36:GLN:H	2:C:37:MET:HG2	7	0.16
(1,6164)	1:A:8:PRO:HA	1:A:8:PRO:HD3	2	0.16
(1,6164)	1:A:8:PRO:HA	1:A:8:PRO:HD3	19	0.16
(1,5880)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	9	0.16
(1,5880)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	9	0.16
(1,5880)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	9	0.16
(1,5880)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	18	0.16
(1,5880)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	18	0.16
(1,5880)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	18	0.16
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	14	0.16
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	18	0.16
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	19	0.16
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	8	0.16
(1,5118)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	9	0.16
(1,5118)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	9	0.16
(1,5118)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	9	0.16
(1,501)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	9	0.16
(1,501)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	9	0.16
(1,501)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	9	0.16
(1,501)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	18	0.16
(1,501)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	18	0.16
(1,501)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	18	0.16
(1,5000)	2:C:70:LYS:H	2:C:69:ASP:HB2	4	0.16
(1,4773)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	17	0.16
(1,4773)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	17	0.16
(1,4773)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	17	0.16
(1,4714)	1:A:24:LEU:HD21	1:A:24:LEU:HA	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4714)	1:A:24:LEU:HD22	1:A:24:LEU:HA	16	0.16
(1,4714)	1:A:24:LEU:HD23	1:A:24:LEU:HA	16	0.16
(1,4566)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	13	0.16
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	14	0.16
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	18	0.16
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	19	0.16
(1,4433)	2:C:36:GLN:H	2:C:37:MET:HG2	7	0.16
(1,4371)	1:A:8:PRO:HA	1:A:8:PRO:HD3	2	0.16
(1,4371)	1:A:8:PRO:HA	1:A:8:PRO:HD3	19	0.16
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	2	0.16
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	2	0.16
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	2	0.16
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	2	0.16
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	2	0.16
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	2	0.16
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	2	0.16
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	2	0.16
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	2	0.16
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	18	0.16
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	18	0.16
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	18	0.16
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	18	0.16
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	18	0.16
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	18	0.16
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	18	0.16
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	18	0.16
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	18	0.16
(1,4087)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	9	0.16
(1,4087)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	9	0.16
(1,4087)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	9	0.16
(1,4087)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	18	0.16
(1,4087)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	18	0.16
(1,4087)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	18	0.16
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	14	0.16
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	18	0.16
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	19	0.16
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	8	0.16
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	8	0.16
(1,3325)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	9	0.16
(1,3325)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	9	0.16
(1,3325)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	9	0.16
(1,3207)	2:C:70:LYS:H	2:C:69:ASP:HB2	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2980)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	17	0.16
(1,2980)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	17	0.16
(1,2980)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	17	0.16
(1,2921)	1:A:24:LEU:HD21	1:A:24:LEU:HA	16	0.16
(1,2921)	1:A:24:LEU:HD22	1:A:24:LEU:HA	16	0.16
(1,2921)	1:A:24:LEU:HD23	1:A:24:LEU:HA	16	0.16
(1,2773)	1:A:23:ARG:HB2	1:A:28:ILE:HG13	13	0.16
(1,2640)	2:C:36:GLN:H	2:C:37:MET:HG2	7	0.16
(1,2578)	1:A:8:PRO:HA	1:A:8:PRO:HD3	2	0.16
(1,2578)	1:A:8:PRO:HA	1:A:8:PRO:HD3	19	0.16
(1,2294)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	9	0.16
(1,2294)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	9	0.16
(1,2294)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	9	0.16
(1,2294)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	18	0.16
(1,2294)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	18	0.16
(1,2294)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	18	0.16
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	14	0.16
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	18	0.16
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	19	0.16
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	8	0.16
(1,1532)	2:C:53:PRO:HD3	2:C:52:ILE:HG21	9	0.16
(1,1532)	2:C:53:PRO:HD3	2:C:52:ILE:HG22	9	0.16
(1,1532)	2:C:53:PRO:HD3	2:C:52:ILE:HG23	9	0.16
(1,1414)	2:C:70:LYS:H	2:C:69:ASP:HB2	4	0.16
(1,1187)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	17	0.16
(1,1187)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	17	0.16
(1,1187)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	17	0.16
(1,1128)	1:A:24:LEU:HD21	1:A:24:LEU:HA	16	0.16
(1,1128)	1:A:24:LEU:HD22	1:A:24:LEU:HA	16	0.16
(1,1128)	1:A:24:LEU:HD23	1:A:24:LEU:HA	16	0.16
(1,86)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	6	0.15
(1,86)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	6	0.15
(1,86)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	11	0.15
(1,86)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	11	0.15
(1,833)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	8	0.15
(1,833)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	8	0.15
(1,6948)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	1	0.15
(1,6948)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	2	0.15
(1,6894)	2:C:54:SER:H	2:C:54:SER:HB2	11	0.15
(1,6874)	1:A:28:ILE:HA	1:A:35:GLY:HA3	16	0.15
(1,6793)	2:C:70:LYS:H	2:C:69:ASP:HB2	7	0.15
(1,6566)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6566)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	8	0.15
(1,6566)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	8	0.15
(1,6514)	2:C:24:LEU:HD11	1:A:14:HIS:HB3	11	0.15
(1,6514)	2:C:24:LEU:HD12	1:A:14:HIS:HB3	11	0.15
(1,6514)	2:C:24:LEU:HD13	1:A:14:HIS:HB3	11	0.15
(1,6212)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	8	0.15
(1,6212)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	8	0.15
(1,5880)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	3	0.15
(1,5880)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	3	0.15
(1,5880)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	3	0.15
(1,5880)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	13	0.15
(1,5880)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	13	0.15
(1,5880)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	13	0.15
(1,5880)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	15	0.15
(1,5880)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	15	0.15
(1,5880)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	15	0.15
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	2	0.15
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	6	0.15
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	10	0.15
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	12	0.15
(1,5772)	1:A:10:ARG:H	1:A:9:GLY:HA3	17	0.15
(1,5465)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	6	0.15
(1,5465)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	6	0.15
(1,5465)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	11	0.15
(1,5465)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	11	0.15
(1,52)	1:A:26:ASP:H	1:A:25:PRO:HB2	12	0.15
(1,52)	1:A:26:ASP:H	1:A:25:PRO:HB3	12	0.15
(1,52)	1:A:26:ASP:H	1:A:26:ASP:HB2	12	0.15
(1,52)	1:A:26:ASP:H	1:A:26:ASP:HB3	12	0.15
(1,5155)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	1	0.15
(1,5155)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	2	0.15
(1,5101)	2:C:54:SER:H	2:C:54:SER:HB2	11	0.15
(1,5081)	1:A:28:ILE:HA	1:A:35:GLY:HA3	16	0.15
(1,501)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	3	0.15
(1,501)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	3	0.15
(1,501)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	3	0.15
(1,501)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	13	0.15
(1,501)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	13	0.15
(1,501)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	13	0.15
(1,501)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	15	0.15
(1,501)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	15	0.15
(1,501)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5000)	2:C:70:LYS:H	2:C:69:ASP:HB2	7	0.15
(1,4773)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	8	0.15
(1,4773)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	8	0.15
(1,4773)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	8	0.15
(1,4721)	2:C:24:LEU:HD11	1:A:14:HIS:HB3	11	0.15
(1,4721)	2:C:24:LEU:HD12	1:A:14:HIS:HB3	11	0.15
(1,4721)	2:C:24:LEU:HD13	1:A:14:HIS:HB3	11	0.15
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	2	0.15
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	6	0.15
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	10	0.15
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	12	0.15
(1,4419)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	8	0.15
(1,4419)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	8	0.15
(1,4087)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	3	0.15
(1,4087)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	3	0.15
(1,4087)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	3	0.15
(1,4087)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	13	0.15
(1,4087)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	13	0.15
(1,4087)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	13	0.15
(1,4087)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	15	0.15
(1,4087)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	15	0.15
(1,4087)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	15	0.15
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	2	0.15
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	6	0.15
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	10	0.15
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	12	0.15
(1,3979)	1:A:10:ARG:H	1:A:9:GLY:HA3	17	0.15
(1,393)	1:A:10:ARG:H	1:A:9:GLY:HA3	17	0.15
(1,38)	2:C:77:VAL:HG11	2:C:75:TYR:HA	3	0.15
(1,38)	2:C:77:VAL:HG12	2:C:75:TYR:HA	3	0.15
(1,38)	2:C:77:VAL:HG13	2:C:75:TYR:HA	3	0.15
(1,38)	2:C:77:VAL:HG21	2:C:75:TYR:HA	3	0.15
(1,38)	2:C:77:VAL:HG22	2:C:75:TYR:HA	3	0.15
(1,38)	2:C:77:VAL:HG23	2:C:75:TYR:HA	3	0.15
(1,38)	2:C:77:VAL:HG11	2:C:76:ASN:HA	3	0.15
(1,38)	2:C:77:VAL:HG12	2:C:76:ASN:HA	3	0.15
(1,38)	2:C:77:VAL:HG13	2:C:76:ASN:HA	3	0.15
(1,38)	2:C:77:VAL:HG21	2:C:76:ASN:HA	3	0.15
(1,38)	2:C:77:VAL:HG22	2:C:76:ASN:HA	3	0.15
(1,38)	2:C:77:VAL:HG23	2:C:76:ASN:HA	3	0.15
(1,3672)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	6	0.15
(1,3672)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3672)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	11	0.15
(1,3672)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	11	0.15
(1,3362)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	1	0.15
(1,3362)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	2	0.15
(1,3308)	2:C:54:SER:H	2:C:54:SER:HB2	11	0.15
(1,3288)	1:A:28:ILE:HA	1:A:35:GLY:HA3	16	0.15
(1,3207)	2:C:70:LYS:H	2:C:69:ASP:HB2	7	0.15
(1,2980)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	8	0.15
(1,2980)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	8	0.15
(1,2980)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	8	0.15
(1,2928)	2:C:24:LEU:HD11	1:A:14:HIS:HB3	11	0.15
(1,2928)	2:C:24:LEU:HD12	1:A:14:HIS:HB3	11	0.15
(1,2928)	2:C:24:LEU:HD13	1:A:14:HIS:HB3	11	0.15
(1,2626)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	8	0.15
(1,2626)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	8	0.15
(1,2294)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	3	0.15
(1,2294)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	3	0.15
(1,2294)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	3	0.15
(1,2294)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	13	0.15
(1,2294)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	13	0.15
(1,2294)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	13	0.15
(1,2294)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	15	0.15
(1,2294)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	15	0.15
(1,2294)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	15	0.15
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	2	0.15
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	6	0.15
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	10	0.15
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	12	0.15
(1,2186)	1:A:10:ARG:H	1:A:9:GLY:HA3	17	0.15
(1,1879)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	6	0.15
(1,1879)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	6	0.15
(1,1879)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	11	0.15
(1,1879)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	11	0.15
(1,1569)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	1	0.15
(1,1569)	2:C:57:GLN:HE22	2:C:46:ILE:HG13	2	0.15
(1,1515)	2:C:54:SER:H	2:C:54:SER:HB2	11	0.15
(1,1495)	1:A:28:ILE:HA	1:A:35:GLY:HA3	16	0.15
(1,1414)	2:C:70:LYS:H	2:C:69:ASP:HB2	7	0.15
(1,12)	2:C:58:ARG:H	2:C:86:GLU:HG2	3	0.15
(1,12)	2:C:58:ARG:H	2:C:86:GLU:HG3	3	0.15
(1,12)	2:C:58:ARG:H	2:C:56:LYS:HB2	3	0.15
(1,12)	2:C:58:ARG:H	2:C:56:LYS:HB3	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1187)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	8	0.15
(1,1187)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	8	0.15
(1,1187)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	8	0.15
(1,1135)	2:C:24:LEU:HD11	1:A:14:HIS:HB3	11	0.15
(1,1135)	2:C:24:LEU:HD12	1:A:14:HIS:HB3	11	0.15
(1,1135)	2:C:24:LEU:HD13	1:A:14:HIS:HB3	11	0.15
(1,86)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	15	0.14
(1,86)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	15	0.14
(1,86)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	19	0.14
(1,86)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	19	0.14
(1,847)	2:C:36:GLN:H	2:C:37:MET:HG2	9	0.14
(1,833)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	5	0.14
(1,833)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	5	0.14
(1,785)	1:A:8:PRO:HA	1:A:8:PRO:HD3	1	0.14
(1,734)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	2	0.14
(1,734)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	2	0.14
(1,7195)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	6	0.14
(1,7195)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	6	0.14
(1,7195)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	6	0.14
(1,7116)	2:C:49:SER:H	2:C:49:SER:HB2	9	0.14
(1,7073)	2:C:39:VAL:HB	2:C:38:ASN:HB2	12	0.14
(1,6793)	2:C:70:LYS:H	2:C:69:ASP:HB2	1	0.14
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	20	0.14
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	20	0.14
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	20	0.14
(1,6226)	2:C:36:GLN:H	2:C:37:MET:HG2	9	0.14
(1,6212)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	5	0.14
(1,6212)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	5	0.14
(1,6164)	1:A:8:PRO:HA	1:A:8:PRO:HD3	1	0.14
(1,6113)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	2	0.14
(1,6113)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	2	0.14
(1,5880)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	6	0.14
(1,5880)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	6	0.14
(1,5880)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	6	0.14
(1,5880)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	8	0.14
(1,5880)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	8	0.14
(1,5880)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	8	0.14
(1,5880)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	11	0.14
(1,5880)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	11	0.14
(1,5880)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	11	0.14
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	4	0.14
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	16	0.14
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	7	0.14
(1,5777)	1:A:20:ILE:HG13	1:A:29:CYS:HA	9	0.14
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	15	0.14
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	15	0.14
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	15	0.14
(1,5465)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	15	0.14
(1,5465)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	15	0.14
(1,5465)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	19	0.14
(1,5465)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	19	0.14
(1,5402)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	6	0.14
(1,5402)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	6	0.14
(1,5402)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	6	0.14
(1,5323)	2:C:49:SER:H	2:C:49:SER:HB2	9	0.14
(1,5280)	2:C:39:VAL:HB	2:C:38:ASN:HB2	12	0.14
(1,501)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	6	0.14
(1,501)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	6	0.14
(1,501)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	6	0.14
(1,501)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	8	0.14
(1,501)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	8	0.14
(1,501)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	8	0.14
(1,501)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	11	0.14
(1,501)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	11	0.14
(1,501)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	11	0.14
(1,5000)	2:C:70:LYS:H	2:C:69:ASP:HB2	1	0.14
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	20	0.14
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	20	0.14
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	20	0.14
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	4	0.14
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	15	0.14
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	16	0.14
(1,4433)	2:C:36:GLN:H	2:C:37:MET:HG2	9	0.14
(1,4419)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	5	0.14
(1,4419)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	5	0.14
(1,4371)	1:A:8:PRO:HA	1:A:8:PRO:HD3	1	0.14
(1,4320)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	2	0.14
(1,4320)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	2	0.14
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	4	0.14
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	4	0.14
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	4	0.14
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	4	0.14
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	4	0.14
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	4	0.14
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	4	0.14
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	4	0.14
(1,4087)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	6	0.14
(1,4087)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	6	0.14
(1,4087)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	6	0.14
(1,4087)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	8	0.14
(1,4087)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	8	0.14
(1,4087)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	8	0.14
(1,4087)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	11	0.14
(1,4087)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	11	0.14
(1,4087)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	11	0.14
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	4	0.14
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	15	0.14
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	16	0.14
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	7	0.14
(1,3984)	1:A:20:ILE:HG13	1:A:29:CYS:HA	9	0.14
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	7	0.14
(1,398)	1:A:20:ILE:HG13	1:A:29:CYS:HA	9	0.14
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	15	0.14
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	15	0.14
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	15	0.14
(1,3672)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	15	0.14
(1,3672)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	15	0.14
(1,3672)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	19	0.14
(1,3672)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	19	0.14
(1,3609)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	6	0.14
(1,3609)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	6	0.14
(1,3609)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	6	0.14
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	2	0.14
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	2	0.14
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	15	0.14
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	15	0.14
(1,3530)	2:C:49:SER:H	2:C:49:SER:HB2	9	0.14
(1,3487)	2:C:39:VAL:HB	2:C:38:ASN:HB2	12	0.14
(1,3207)	2:C:70:LYS:H	2:C:69:ASP:HB2	1	0.14
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	20	0.14
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	20	0.14
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	20	0.14
(1,2640)	2:C:36:GLN:H	2:C:37:MET:HG2	9	0.14
(1,2626)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2626)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	5	0.14
(1,2578)	1:A:8:PRO:HA	1:A:8:PRO:HD3	1	0.14
(1,2527)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	2	0.14
(1,2527)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	2	0.14
(1,2294)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	6	0.14
(1,2294)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	6	0.14
(1,2294)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	6	0.14
(1,2294)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	8	0.14
(1,2294)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	8	0.14
(1,2294)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	8	0.14
(1,2294)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	11	0.14
(1,2294)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	11	0.14
(1,2294)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	11	0.14
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	4	0.14
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	15	0.14
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	16	0.14
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	7	0.14
(1,2191)	1:A:20:ILE:HG13	1:A:29:CYS:HA	9	0.14
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	15	0.14
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	15	0.14
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	15	0.14
(1,1879)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	15	0.14
(1,1879)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	15	0.14
(1,1879)	2:C:55:GLU:HG3	2:C:55:GLU:HB2	19	0.14
(1,1879)	2:C:55:GLU:HG3	2:C:55:GLU:HB3	19	0.14
(1,1816)	2:C:19:VAL:HG21	2:C:31:PHE:HB3	6	0.14
(1,1816)	2:C:19:VAL:HG22	2:C:31:PHE:HB3	6	0.14
(1,1816)	2:C:19:VAL:HG23	2:C:31:PHE:HB3	6	0.14
(1,1737)	2:C:49:SER:H	2:C:49:SER:HB2	9	0.14
(1,1694)	2:C:39:VAL:HB	2:C:38:ASN:HB2	12	0.14
(1,1414)	2:C:70:LYS:H	2:C:69:ASP:HB2	1	0.14
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	15	0.14
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	15	0.14
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	15	0.14
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	20	0.14
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	20	0.14
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	20	0.14
(1,959)	2:C:96:SER:H	2:C:95:PRO:HB3	3	0.13
(1,927)	1:A:19:GLU:HG2	1:A:10:ARG:HA	15	0.13
(1,919)	2:C:59:LEU:HB2	2:C:59:LEU:HD11	5	0.13
(1,919)	2:C:59:LEU:HB2	2:C:59:LEU:HD12	5	0.13
(1,919)	2:C:59:LEU:HB2	2:C:59:LEU:HD13	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,833)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	14	0.13
(1,833)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	14	0.13
(1,7038)	1:A:16:CYS:H	1:A:15:CYS:HB3	18	0.13
(1,6793)	2:C:70:LYS:H	2:C:69:ASP:HB2	11	0.13
(1,6652)	2:C:18:GLU:H	2:C:17:LEU:HB2	8	0.13
(1,6576)	1:A:24:LEU:HA	1:A:24:LEU:HD11	16	0.13
(1,6576)	1:A:24:LEU:HA	1:A:24:LEU:HD12	16	0.13
(1,6576)	1:A:24:LEU:HA	1:A:24:LEU:HD13	16	0.13
(1,6566)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	11	0.13
(1,6566)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	11	0.13
(1,6566)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	11	0.13
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	9	0.13
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	9	0.13
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	9	0.13
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	17	0.13
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	17	0.13
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	17	0.13
(1,6403)	1:A:15:CYS:HA	1:A:15:CYS:HB2	14	0.13
(1,6398)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	14	0.13
(1,6398)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	14	0.13
(1,6398)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	14	0.13
(1,6338)	2:C:96:SER:H	2:C:95:PRO:HB3	3	0.13
(1,6306)	1:A:19:GLU:HG2	1:A:10:ARG:HA	15	0.13
(1,6298)	2:C:59:LEU:HB2	2:C:59:LEU:HD11	5	0.13
(1,6298)	2:C:59:LEU:HB2	2:C:59:LEU:HD12	5	0.13
(1,6298)	2:C:59:LEU:HB2	2:C:59:LEU:HD13	5	0.13
(1,6212)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	14	0.13
(1,6212)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	14	0.13
(1,5905)	2:C:46:ILE:H	2:C:46:ILE:HG13	13	0.13
(1,5880)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	1	0.13
(1,5880)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	1	0.13
(1,5880)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	1	0.13
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	20	0.13
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	4	0.13
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	4	0.13
(1,5497)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	4	0.13
(1,526)	2:C:46:ILE:H	2:C:46:ILE:HG13	13	0.13
(1,5245)	1:A:16:CYS:H	1:A:15:CYS:HB3	18	0.13
(1,501)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	1	0.13
(1,501)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	1	0.13
(1,501)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	1	0.13
(1,5000)	2:C:70:LYS:H	2:C:69:ASP:HB2	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4859)	2:C:18:GLU:H	2:C:17:LEU:HB2	8	0.13
(1,4783)	1:A:24:LEU:HA	1:A:24:LEU:HD11	16	0.13
(1,4783)	1:A:24:LEU:HA	1:A:24:LEU:HD12	16	0.13
(1,4783)	1:A:24:LEU:HA	1:A:24:LEU:HD13	16	0.13
(1,4773)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	11	0.13
(1,4773)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	11	0.13
(1,4773)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	11	0.13
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	9	0.13
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	9	0.13
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	9	0.13
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	17	0.13
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	17	0.13
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	17	0.13
(1,4610)	1:A:15:CYS:HA	1:A:15:CYS:HB2	14	0.13
(1,4605)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	14	0.13
(1,4605)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	14	0.13
(1,4605)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	14	0.13
(1,4545)	2:C:96:SER:H	2:C:95:PRO:HB3	3	0.13
(1,4513)	1:A:19:GLU:HG2	1:A:10:ARG:HA	15	0.13
(1,4505)	2:C:59:LEU:HB2	2:C:59:LEU:HD11	5	0.13
(1,4505)	2:C:59:LEU:HB2	2:C:59:LEU:HD12	5	0.13
(1,4505)	2:C:59:LEU:HB2	2:C:59:LEU:HD13	5	0.13
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	20	0.13
(1,4419)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	14	0.13
(1,4419)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	14	0.13
(1,4112)	2:C:46:ILE:H	2:C:46:ILE:HG13	13	0.13
(1,4087)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	1	0.13
(1,4087)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	1	0.13
(1,4087)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	1	0.13
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	20	0.13
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	4	0.13
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	4	0.13
(1,3704)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	4	0.13
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	4	0.13
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	4	0.13
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	8	0.13
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	8	0.13
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	10	0.13
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	10	0.13
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	13	0.13
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	13	0.13
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	17	0.13
(1,3452)	1:A:16:CYS:H	1:A:15:CYS:HB3	18	0.13
(1,3207)	2:C:70:LYS:H	2:C:69:ASP:HB2	11	0.13
(1,3066)	2:C:18:GLU:H	2:C:17:LEU:HB2	8	0.13
(1,2990)	1:A:24:LEU:HA	1:A:24:LEU:HD11	16	0.13
(1,2990)	1:A:24:LEU:HA	1:A:24:LEU:HD12	16	0.13
(1,2990)	1:A:24:LEU:HA	1:A:24:LEU:HD13	16	0.13
(1,2980)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	11	0.13
(1,2980)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	11	0.13
(1,2980)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	11	0.13
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	9	0.13
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	9	0.13
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	9	0.13
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	17	0.13
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	17	0.13
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	17	0.13
(1,2817)	1:A:15:CYS:HA	1:A:15:CYS:HB2	14	0.13
(1,2812)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	14	0.13
(1,2812)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	14	0.13
(1,2812)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	14	0.13
(1,2752)	2:C:96:SER:H	2:C:95:PRO:HB3	3	0.13
(1,2720)	1:A:19:GLU:HG2	1:A:10:ARG:HA	15	0.13
(1,2712)	2:C:59:LEU:HB2	2:C:59:LEU:HD11	5	0.13
(1,2712)	2:C:59:LEU:HB2	2:C:59:LEU:HD12	5	0.13
(1,2712)	2:C:59:LEU:HB2	2:C:59:LEU:HD13	5	0.13
(1,2626)	1:A:37:ILE:HG12	1:A:11:TYR:HD1	14	0.13
(1,2626)	1:A:37:ILE:HG12	1:A:11:TYR:HD2	14	0.13
(1,24)	2:C:91:GLN:H	2:C:91:GLN:HA	7	0.13
(1,24)	2:C:91:GLN:H	2:C:90:PRO:HA	7	0.13
(1,2319)	2:C:46:ILE:H	2:C:46:ILE:HG13	13	0.13
(1,2294)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	1	0.13
(1,2294)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	1	0.13
(1,2294)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	1	0.13
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	20	0.13
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	4	0.13
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	4	0.13
(1,1911)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	4	0.13
(1,1659)	1:A:16:CYS:H	1:A:15:CYS:HB3	18	0.13
(1,1414)	2:C:70:LYS:H	2:C:69:ASP:HB2	11	0.13
(1,1273)	2:C:18:GLU:H	2:C:17:LEU:HB2	8	0.13
(1,1197)	1:A:24:LEU:HA	1:A:24:LEU:HD11	16	0.13
(1,1197)	1:A:24:LEU:HA	1:A:24:LEU:HD12	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1197)	1:A:24:LEU:HA	1:A:24:LEU:HD13	16	0.13
(1,1187)	2:C:59:LEU:HD21	2:C:59:LEU:HB2	11	0.13
(1,1187)	2:C:59:LEU:HD22	2:C:59:LEU:HB2	11	0.13
(1,1187)	2:C:59:LEU:HD23	2:C:59:LEU:HB2	11	0.13
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD11	4	0.13
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD12	4	0.13
(1,118)	1:A:38:GLU:HB2	2:C:60:ILE:HD13	4	0.13
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	9	0.13
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	9	0.13
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	9	0.13
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	17	0.13
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	17	0.13
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	17	0.13
(1,1024)	1:A:15:CYS:HA	1:A:15:CYS:HB2	14	0.13
(1,1019)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	14	0.13
(1,1019)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	14	0.13
(1,1019)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	14	0.13
(1,734)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	1	0.12
(1,734)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	1	0.12
(1,7168)	2:C:30:THR:H	2:C:29:ARG:HB2	9	0.12
(1,7168)	2:C:30:THR:H	2:C:29:ARG:HB2	13	0.12
(1,7155)	1:A:25:PRO:HA	1:A:25:PRO:HD2	1	0.12
(1,7155)	1:A:25:PRO:HA	1:A:25:PRO:HD2	6	0.12
(1,7155)	1:A:25:PRO:HA	1:A:25:PRO:HD2	14	0.12
(1,7155)	1:A:25:PRO:HA	1:A:25:PRO:HD2	18	0.12
(1,7155)	1:A:25:PRO:HA	1:A:25:PRO:HD2	19	0.12
(1,7114)	2:C:45:HIS:H	2:C:45:HIS:HB3	12	0.12
(1,7073)	2:C:39:VAL:HB	2:C:38:ASN:HB2	16	0.12
(1,6786)	2:C:42:PHE:H	2:C:41:GLU:HB3	1	0.12
(1,6786)	2:C:42:PHE:H	2:C:41:GLU:HB3	2	0.12
(1,6786)	2:C:42:PHE:H	2:C:41:GLU:HB3	3	0.12
(1,6786)	2:C:42:PHE:H	2:C:41:GLU:HB3	5	0.12
(1,6786)	2:C:42:PHE:H	2:C:41:GLU:HB3	6	0.12
(1,6786)	2:C:42:PHE:H	2:C:41:GLU:HB3	9	0.12
(1,6786)	2:C:42:PHE:H	2:C:41:GLU:HB3	10	0.12
(1,6652)	2:C:18:GLU:H	2:C:17:LEU:HB2	1	0.12
(1,6652)	2:C:18:GLU:H	2:C:17:LEU:HB2	9	0.12
(1,6652)	2:C:18:GLU:H	2:C:17:LEU:HB2	19	0.12
(1,6613)	2:C:27:GLN:HG3	2:C:27:GLN:HA	16	0.12
(1,6570)	1:A:15:CYS:HB2	1:A:36:PHE:HD1	13	0.12
(1,6570)	1:A:15:CYS:HB2	1:A:36:PHE:HD2	13	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	5	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	5	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	10	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	10	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	10	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	14	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	14	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	14	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	16	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	16	0.12
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	16	0.12
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	2	0.12
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	6	0.12
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	11	0.12
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	16	0.12
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	19	0.12
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	20	0.12
(1,6398)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	5	0.12
(1,6398)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	5	0.12
(1,6398)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	5	0.12
(1,6398)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	10	0.12
(1,6398)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	10	0.12
(1,6398)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	10	0.12
(1,6398)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	13	0.12
(1,6398)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	13	0.12
(1,6398)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	13	0.12
(1,6398)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	18	0.12
(1,6398)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	18	0.12
(1,6398)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	18	0.12
(1,6398)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	19	0.12
(1,6398)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	19	0.12
(1,6398)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	19	0.12
(1,6398)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	20	0.12
(1,6398)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	20	0.12
(1,6398)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	20	0.12
(1,6113)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	1	0.12
(1,6113)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	1	0.12
(1,5945)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	5	0.12
(1,5880)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	20	0.12
(1,5880)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	20	0.12
(1,5880)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	20	0.12
(1,5772)	1:A:10:ARG:H	1:A:9:GLY:HA3	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	5	0.12
(1,5490)	1:A:28:ILE:HG13	1:A:28:ILE:HA	15	0.12
(1,5375)	2:C:30:THR:H	2:C:29:ARG:HB2	9	0.12
(1,5375)	2:C:30:THR:H	2:C:29:ARG:HB2	13	0.12
(1,5362)	1:A:25:PRO:HA	1:A:25:PRO:HD2	1	0.12
(1,5362)	1:A:25:PRO:HA	1:A:25:PRO:HD2	6	0.12
(1,5362)	1:A:25:PRO:HA	1:A:25:PRO:HD2	14	0.12
(1,5362)	1:A:25:PRO:HA	1:A:25:PRO:HD2	18	0.12
(1,5362)	1:A:25:PRO:HA	1:A:25:PRO:HD2	19	0.12
(1,5321)	2:C:45:HIS:H	2:C:45:HIS:HB3	12	0.12
(1,5280)	2:C:39:VAL:HB	2:C:38:ASN:HB2	16	0.12
(1,501)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	20	0.12
(1,501)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	20	0.12
(1,501)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	20	0.12
(1,4993)	2:C:42:PHE:H	2:C:41:GLU:HB3	1	0.12
(1,4993)	2:C:42:PHE:H	2:C:41:GLU:HB3	2	0.12
(1,4993)	2:C:42:PHE:H	2:C:41:GLU:HB3	3	0.12
(1,4993)	2:C:42:PHE:H	2:C:41:GLU:HB3	5	0.12
(1,4993)	2:C:42:PHE:H	2:C:41:GLU:HB3	6	0.12
(1,4993)	2:C:42:PHE:H	2:C:41:GLU:HB3	9	0.12
(1,4993)	2:C:42:PHE:H	2:C:41:GLU:HB3	10	0.12
(1,4859)	2:C:18:GLU:H	2:C:17:LEU:HB2	1	0.12
(1,4859)	2:C:18:GLU:H	2:C:17:LEU:HB2	9	0.12
(1,4859)	2:C:18:GLU:H	2:C:17:LEU:HB2	19	0.12
(1,4820)	2:C:27:GLN:HG3	2:C:27:GLN:HA	16	0.12
(1,4777)	1:A:15:CYS:HB2	1:A:36:PHE:HD1	13	0.12
(1,4777)	1:A:15:CYS:HB2	1:A:36:PHE:HD2	13	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	5	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	5	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	5	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	10	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	10	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	10	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	14	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	14	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	14	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	16	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	16	0.12
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	16	0.12
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	2	0.12
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	6	0.12
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	16	0.12
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	19	0.12
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	20	0.12
(1,4605)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	5	0.12
(1,4605)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	5	0.12
(1,4605)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	5	0.12
(1,4605)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	10	0.12
(1,4605)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	10	0.12
(1,4605)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	10	0.12
(1,4605)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	13	0.12
(1,4605)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	13	0.12
(1,4605)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	13	0.12
(1,4605)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	18	0.12
(1,4605)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	18	0.12
(1,4605)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	18	0.12
(1,4605)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	19	0.12
(1,4605)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	19	0.12
(1,4605)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	19	0.12
(1,4605)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	20	0.12
(1,4605)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	20	0.12
(1,4605)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	20	0.12
(1,4320)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	1	0.12
(1,4320)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	1	0.12
(1,4152)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	5	0.12
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	1	0.12
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	1	0.12
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	1	0.12
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	1	0.12
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	1	0.12
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	1	0.12
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	1	0.12
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	1	0.12
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	1	0.12
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	3	0.12
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	3	0.12
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	3	0.12
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	3	0.12
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	3	0.12
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	3	0.12
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	3	0.12
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	3	0.12
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	5	0.12
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	5	0.12
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	5	0.12
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	5	0.12
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	5	0.12
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	5	0.12
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	5	0.12
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	5	0.12
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	5	0.12
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	12	0.12
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	12	0.12
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	12	0.12
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	12	0.12
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	12	0.12
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	12	0.12
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	12	0.12
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	12	0.12
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	12	0.12
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	14	0.12
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	14	0.12
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	14	0.12
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	14	0.12
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	14	0.12
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	14	0.12
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	14	0.12
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	14	0.12
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	14	0.12
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	17	0.12
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	17	0.12
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	17	0.12
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	17	0.12
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	17	0.12
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	17	0.12
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	17	0.12
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	17	0.12
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	17	0.12
(1,4087)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	20	0.12
(1,4087)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	20	0.12
(1,4087)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	20	0.12
(1,3979)	1:A:10:ARG:H	1:A:9:GLY:HA3	11	0.12
(1,393)	1:A:10:ARG:H	1:A:9:GLY:HA3	11	0.12
(1,3697)	1:A:28:ILE:HG13	1:A:28:ILE:HA	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	11	0.12
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	11	0.12
(1,3582)	2:C:30:THR:H	2:C:29:ARG:HB2	9	0.12
(1,3582)	2:C:30:THR:H	2:C:29:ARG:HB2	13	0.12
(1,3569)	1:A:25:PRO:HA	1:A:25:PRO:HD2	1	0.12
(1,3569)	1:A:25:PRO:HA	1:A:25:PRO:HD2	6	0.12
(1,3569)	1:A:25:PRO:HA	1:A:25:PRO:HD2	14	0.12
(1,3569)	1:A:25:PRO:HA	1:A:25:PRO:HD2	18	0.12
(1,3569)	1:A:25:PRO:HA	1:A:25:PRO:HD2	19	0.12
(1,3528)	2:C:45:HIS:H	2:C:45:HIS:HB3	12	0.12
(1,3487)	2:C:39:VAL:HB	2:C:38:ASN:HB2	16	0.12
(1,3200)	2:C:42:PHE:H	2:C:41:GLU:HB3	1	0.12
(1,3200)	2:C:42:PHE:H	2:C:41:GLU:HB3	2	0.12
(1,3200)	2:C:42:PHE:H	2:C:41:GLU:HB3	3	0.12
(1,3200)	2:C:42:PHE:H	2:C:41:GLU:HB3	5	0.12
(1,3200)	2:C:42:PHE:H	2:C:41:GLU:HB3	6	0.12
(1,3200)	2:C:42:PHE:H	2:C:41:GLU:HB3	9	0.12
(1,3200)	2:C:42:PHE:H	2:C:41:GLU:HB3	10	0.12
(1,3066)	2:C:18:GLU:H	2:C:17:LEU:HB2	1	0.12
(1,3066)	2:C:18:GLU:H	2:C:17:LEU:HB2	9	0.12
(1,3066)	2:C:18:GLU:H	2:C:17:LEU:HB2	19	0.12
(1,3027)	2:C:27:GLN:HG3	2:C:27:GLN:HA	16	0.12
(1,2984)	1:A:15:CYS:HB2	1:A:36:PHE:HD1	13	0.12
(1,2984)	1:A:15:CYS:HB2	1:A:36:PHE:HD2	13	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	5	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	5	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	5	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	10	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	10	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	10	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	14	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	14	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	14	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	16	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	16	0.12
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	16	0.12
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	2	0.12
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	6	0.12
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	11	0.12
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	16	0.12
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	19	0.12
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2812)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	5	0.12
(1,2812)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	5	0.12
(1,2812)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	5	0.12
(1,2812)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	10	0.12
(1,2812)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	10	0.12
(1,2812)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	10	0.12
(1,2812)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	13	0.12
(1,2812)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	13	0.12
(1,2812)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	13	0.12
(1,2812)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	18	0.12
(1,2812)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	18	0.12
(1,2812)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	18	0.12
(1,2812)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	19	0.12
(1,2812)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	19	0.12
(1,2812)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	19	0.12
(1,2812)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	20	0.12
(1,2812)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	20	0.12
(1,2812)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	20	0.12
(1,2527)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	1	0.12
(1,2527)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	1	0.12
(1,24)	2:C:91:GLN:H	2:C:91:GLN:HA	14	0.12
(1,24)	2:C:91:GLN:H	2:C:90:PRO:HA	14	0.12
(1,2359)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	5	0.12
(1,2294)	2:C:24:LEU:HD21	2:C:24:LEU:HB3	20	0.12
(1,2294)	2:C:24:LEU:HD22	2:C:24:LEU:HB3	20	0.12
(1,2294)	2:C:24:LEU:HD23	2:C:24:LEU:HB3	20	0.12
(1,2186)	1:A:10:ARG:H	1:A:9:GLY:HA3	11	0.12
(1,1904)	1:A:28:ILE:HG13	1:A:28:ILE:HA	15	0.12
(1,1789)	2:C:30:THR:H	2:C:29:ARG:HB2	9	0.12
(1,1789)	2:C:30:THR:H	2:C:29:ARG:HB2	13	0.12
(1,1776)	1:A:25:PRO:HA	1:A:25:PRO:HD2	1	0.12
(1,1776)	1:A:25:PRO:HA	1:A:25:PRO:HD2	6	0.12
(1,1776)	1:A:25:PRO:HA	1:A:25:PRO:HD2	14	0.12
(1,1776)	1:A:25:PRO:HA	1:A:25:PRO:HD2	18	0.12
(1,1776)	1:A:25:PRO:HA	1:A:25:PRO:HD2	19	0.12
(1,1735)	2:C:45:HIS:H	2:C:45:HIS:HB3	12	0.12
(1,1694)	2:C:39:VAL:HB	2:C:38:ASN:HB2	16	0.12
(1,1407)	2:C:42:PHE:H	2:C:41:GLU:HB3	1	0.12
(1,1407)	2:C:42:PHE:H	2:C:41:GLU:HB3	2	0.12
(1,1407)	2:C:42:PHE:H	2:C:41:GLU:HB3	3	0.12
(1,1407)	2:C:42:PHE:H	2:C:41:GLU:HB3	5	0.12
(1,1407)	2:C:42:PHE:H	2:C:41:GLU:HB3	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1407)	2:C:42:PHE:H	2:C:41:GLU:HB3	9	0.12
(1,1407)	2:C:42:PHE:H	2:C:41:GLU:HB3	10	0.12
(1,1273)	2:C:18:GLU:H	2:C:17:LEU:HB2	1	0.12
(1,1273)	2:C:18:GLU:H	2:C:17:LEU:HB2	9	0.12
(1,1273)	2:C:18:GLU:H	2:C:17:LEU:HB2	19	0.12
(1,1234)	2:C:27:GLN:HG3	2:C:27:GLN:HA	16	0.12
(1,1191)	1:A:15:CYS:HB2	1:A:36:PHE:HD1	13	0.12
(1,1191)	1:A:15:CYS:HB2	1:A:36:PHE:HD2	13	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	5	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	5	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	5	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	10	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	10	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	10	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	14	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	14	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	14	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	16	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	16	0.12
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	16	0.12
(1,111)	1:A:28:ILE:HG13	1:A:28:ILE:HA	15	0.12
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	2	0.12
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	6	0.12
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	11	0.12
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	16	0.12
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	19	0.12
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	20	0.12
(1,1019)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	5	0.12
(1,1019)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	5	0.12
(1,1019)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	5	0.12
(1,1019)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	10	0.12
(1,1019)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	10	0.12
(1,1019)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	10	0.12
(1,1019)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	13	0.12
(1,1019)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	13	0.12
(1,1019)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	13	0.12
(1,1019)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	18	0.12
(1,1019)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	18	0.12
(1,1019)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	18	0.12
(1,1019)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	19	0.12
(1,1019)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	19	0.12
(1,1019)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1019)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	20	0.12
(1,1019)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	20	0.12
(1,1019)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	20	0.12
(1,734)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	4	0.11
(1,734)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	4	0.11
(1,734)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	13	0.11
(1,734)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	13	0.11
(1,734)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	16	0.11
(1,734)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	16	0.11
(1,7168)	2:C:30:THR:H	2:C:29:ARG:HB2	12	0.11
(1,7155)	1:A:25:PRO:HA	1:A:25:PRO:HD2	4	0.11
(1,7155)	1:A:25:PRO:HA	1:A:25:PRO:HD2	7	0.11
(1,7073)	2:C:39:VAL:HB	2:C:38:ASN:HB2	7	0.11
(1,7038)	1:A:16:CYS:H	1:A:15:CYS:HB3	13	0.11
(1,6950)	2:C:62:GLN:H	2:C:62:GLN:HG3	4	0.11
(1,6929)	1:A:22:PRO:HG3	1:A:21:VAL:HA	14	0.11
(1,6876)	1:A:37:ILE:HG21	1:A:11:TYR:HB2	5	0.11
(1,6876)	1:A:37:ILE:HG22	1:A:11:TYR:HB2	5	0.11
(1,6876)	1:A:37:ILE:HG23	1:A:11:TYR:HB2	5	0.11
(1,6652)	2:C:18:GLU:H	2:C:17:LEU:HB2	5	0.11
(1,6652)	2:C:18:GLU:H	2:C:17:LEU:HB2	6	0.11
(1,6613)	2:C:27:GLN:HG3	2:C:27:GLN:HA	8	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	2	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	2	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	2	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	8	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	8	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	8	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	11	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	11	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	11	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	13	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	13	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	13	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	15	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	15	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	15	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG11	18	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG12	18	0.11
(1,6557)	2:C:39:VAL:HA	2:C:39:VAL:HG13	18	0.11
(1,6484)	2:C:76:ASN:H	2:C:76:ASN:HB3	16	0.11
(1,648)	2:C:91:GLN:HE22	2:C:91:GLN:HG2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	1	0.11
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	3	0.11
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	9	0.11
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	13	0.11
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	15	0.11
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	17	0.11
(1,6412)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	18	0.11
(1,6398)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	7	0.11
(1,6398)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	7	0.11
(1,6398)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	7	0.11
(1,6398)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	15	0.11
(1,6398)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	15	0.11
(1,6398)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	15	0.11
(1,6113)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	4	0.11
(1,6113)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	4	0.11
(1,6113)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	13	0.11
(1,6113)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	13	0.11
(1,6113)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	16	0.11
(1,6113)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	16	0.11
(1,6027)	2:C:91:GLN:HE22	2:C:91:GLN:HG2	6	0.11
(1,5976)	2:C:49:SER:HB2	2:C:49:SER:HA	12	0.11
(1,597)	2:C:49:SER:HB2	2:C:49:SER:HA	12	0.11
(1,5945)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	2	0.11
(1,5945)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	8	0.11
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	3	0.11
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	5	0.11
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	7	0.11
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	9	0.11
(1,5828)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	11	0.11
(1,5806)	2:C:55:GLU:HG3	2:C:55:GLU:HA	19	0.11
(1,5772)	1:A:10:ARG:H	1:A:9:GLY:HA3	7	0.11
(1,566)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	2	0.11
(1,566)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	8	0.11
(1,5592)	2:C:61:TYR:HB2	2:C:66:LEU:HD21	7	0.11
(1,5592)	2:C:61:TYR:HB2	2:C:66:LEU:HD22	7	0.11
(1,5592)	2:C:61:TYR:HB2	2:C:66:LEU:HD23	7	0.11
(1,5490)	1:A:28:ILE:HG13	1:A:28:ILE:HA	10	0.11
(1,5375)	2:C:30:THR:H	2:C:29:ARG:HB2	12	0.11
(1,5362)	1:A:25:PRO:HA	1:A:25:PRO:HD2	4	0.11
(1,5362)	1:A:25:PRO:HA	1:A:25:PRO:HD2	7	0.11
(1,5280)	2:C:39:VAL:HB	2:C:38:ASN:HB2	7	0.11
(1,5245)	1:A:16:CYS:H	1:A:15:CYS:HB3	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5157)	2:C:62:GLN:H	2:C:62:GLN:HG3	4	0.11
(1,5136)	1:A:22:PRO:HG3	1:A:21:VAL:HA	14	0.11
(1,5083)	1:A:37:ILE:HG21	1:A:11:TYR:HB2	5	0.11
(1,5083)	1:A:37:ILE:HG22	1:A:11:TYR:HB2	5	0.11
(1,5083)	1:A:37:ILE:HG23	1:A:11:TYR:HB2	5	0.11
(1,4859)	2:C:18:GLU:H	2:C:17:LEU:HB2	5	0.11
(1,4859)	2:C:18:GLU:H	2:C:17:LEU:HB2	6	0.11
(1,4820)	2:C:27:GLN:HG3	2:C:27:GLN:HA	8	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	2	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	2	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	2	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	8	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	8	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	8	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	11	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	11	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	11	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	13	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	13	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	13	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	15	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	15	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	15	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG11	18	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG12	18	0.11
(1,4764)	2:C:39:VAL:HA	2:C:39:VAL:HG13	18	0.11
(1,4691)	2:C:76:ASN:H	2:C:76:ASN:HB3	16	0.11
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	1	0.11
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	3	0.11
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	9	0.11
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	13	0.11
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	15	0.11
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	17	0.11
(1,4619)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	18	0.11
(1,4605)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	7	0.11
(1,4605)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	7	0.11
(1,4605)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	7	0.11
(1,4605)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	15	0.11
(1,4605)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	15	0.11
(1,4605)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	15	0.11
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	3	0.11
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	7	0.11
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	9	0.11
(1,449)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	11	0.11
(1,4320)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	4	0.11
(1,4320)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	4	0.11
(1,4320)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	13	0.11
(1,4320)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	13	0.11
(1,4320)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	16	0.11
(1,4320)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	16	0.11
(1,427)	2:C:55:GLU:HG3	2:C:55:GLU:HA	19	0.11
(1,4234)	2:C:91:GLN:HE22	2:C:91:GLN:HG2	6	0.11
(1,4183)	2:C:49:SER:HB2	2:C:49:SER:HA	12	0.11
(1,4152)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	2	0.11
(1,4152)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	8	0.11
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB2	8	0.11
(1,41)	2:C:46:ILE:HG21	2:C:43:LYS:HB3	8	0.11
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB2	8	0.11
(1,41)	2:C:46:ILE:HG22	2:C:43:LYS:HB3	8	0.11
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB2	8	0.11
(1,41)	2:C:46:ILE:HG23	2:C:43:LYS:HB3	8	0.11
(1,41)	2:C:46:ILE:HG21	2:C:21:VAL:HB	8	0.11
(1,41)	2:C:46:ILE:HG22	2:C:21:VAL:HB	8	0.11
(1,41)	2:C:46:ILE:HG23	2:C:21:VAL:HB	8	0.11
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	3	0.11
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	5	0.11
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	7	0.11
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	9	0.11
(1,4035)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	11	0.11
(1,4013)	2:C:55:GLU:HG3	2:C:55:GLU:HA	19	0.11
(1,3979)	1:A:10:ARG:H	1:A:9:GLY:HA3	7	0.11
(1,393)	1:A:10:ARG:H	1:A:9:GLY:HA3	7	0.11
(1,3799)	2:C:61:TYR:HB2	2:C:66:LEU:HD21	7	0.11
(1,3799)	2:C:61:TYR:HB2	2:C:66:LEU:HD22	7	0.11
(1,3799)	2:C:61:TYR:HB2	2:C:66:LEU:HD23	7	0.11
(1,3697)	1:A:28:ILE:HG13	1:A:28:ILE:HA	10	0.11
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	5	0.11
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	5	0.11
(1,36)	2:C:39:VAL:HA	2:C:68:ASP:HA	19	0.11
(1,36)	2:C:39:VAL:HA	2:C:42:PHE:HA	19	0.11
(1,3582)	2:C:30:THR:H	2:C:29:ARG:HB2	12	0.11
(1,3569)	1:A:25:PRO:HA	1:A:25:PRO:HD2	4	0.11
(1,3569)	1:A:25:PRO:HA	1:A:25:PRO:HD2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3487)	2:C:39:VAL:HB	2:C:38:ASN:HB2	7	0.11
(1,3452)	1:A:16:CYS:H	1:A:15:CYS:HB3	13	0.11
(1,3364)	2:C:62:GLN:H	2:C:62:GLN:HG3	4	0.11
(1,3343)	1:A:22:PRO:HG3	1:A:21:VAL:HA	14	0.11
(1,3290)	1:A:37:ILE:HG21	1:A:11:TYR:HB2	5	0.11
(1,3290)	1:A:37:ILE:HG22	1:A:11:TYR:HB2	5	0.11
(1,3290)	1:A:37:ILE:HG23	1:A:11:TYR:HB2	5	0.11
(1,31)	2:C:38:ASN:HA	2:C:40:LYS:HG2	20	0.11
(1,31)	2:C:38:ASN:HA	2:C:40:LYS:HG3	20	0.11
(1,3066)	2:C:18:GLU:H	2:C:17:LEU:HB2	5	0.11
(1,3066)	2:C:18:GLU:H	2:C:17:LEU:HB2	6	0.11
(1,3027)	2:C:27:GLN:HG3	2:C:27:GLN:HA	8	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	2	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	2	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	2	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	8	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	8	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	8	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	11	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	11	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	11	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	13	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	13	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	13	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	15	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	15	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	15	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG11	18	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG12	18	0.11
(1,2971)	2:C:39:VAL:HA	2:C:39:VAL:HG13	18	0.11
(1,2898)	2:C:76:ASN:H	2:C:76:ASN:HB3	16	0.11
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	1	0.11
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	3	0.11
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	9	0.11
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	13	0.11
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	15	0.11
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	17	0.11
(1,2826)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	18	0.11
(1,2812)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	7	0.11
(1,2812)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	7	0.11
(1,2812)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	7	0.11
(1,2812)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2812)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	15	0.11
(1,2812)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	15	0.11
(1,2527)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	4	0.11
(1,2527)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	4	0.11
(1,2527)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	13	0.11
(1,2527)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	13	0.11
(1,2527)	1:A:23:ARG:HD3	1:A:23:ARG:HG2	16	0.11
(1,2527)	1:A:23:ARG:HD3	1:A:23:ARG:HG3	16	0.11
(1,2441)	2:C:91:GLN:HE22	2:C:91:GLN:HG2	6	0.11
(1,2390)	2:C:49:SER:HB2	2:C:49:SER:HA	12	0.11
(1,2359)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	2	0.11
(1,2359)	1:A:22:PRO:HD3	1:A:11:TYR:HB2	8	0.11
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	3	0.11
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	5	0.11
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	7	0.11
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	9	0.11
(1,2242)	1:A:19:GLU:HG2	1:A:19:GLU:HB2	11	0.11
(1,2220)	2:C:55:GLU:HG3	2:C:55:GLU:HA	19	0.11
(1,2186)	1:A:10:ARG:H	1:A:9:GLY:HA3	7	0.11
(1,213)	2:C:61:TYR:HB2	2:C:66:LEU:HD21	7	0.11
(1,213)	2:C:61:TYR:HB2	2:C:66:LEU:HD22	7	0.11
(1,213)	2:C:61:TYR:HB2	2:C:66:LEU:HD23	7	0.11
(1,2006)	2:C:61:TYR:HB2	2:C:66:LEU:HD21	7	0.11
(1,2006)	2:C:61:TYR:HB2	2:C:66:LEU:HD22	7	0.11
(1,2006)	2:C:61:TYR:HB2	2:C:66:LEU:HD23	7	0.11
(1,1904)	1:A:28:ILE:HG13	1:A:28:ILE:HA	10	0.11
(1,1789)	2:C:30:THR:H	2:C:29:ARG:HB2	12	0.11
(1,1776)	1:A:25:PRO:HA	1:A:25:PRO:HD2	4	0.11
(1,1776)	1:A:25:PRO:HA	1:A:25:PRO:HD2	7	0.11
(1,1694)	2:C:39:VAL:HB	2:C:38:ASN:HB2	7	0.11
(1,1659)	1:A:16:CYS:H	1:A:15:CYS:HB3	13	0.11
(1,1571)	2:C:62:GLN:H	2:C:62:GLN:HG3	4	0.11
(1,1550)	1:A:22:PRO:HG3	1:A:21:VAL:HA	14	0.11
(1,1497)	1:A:37:ILE:HG21	1:A:11:TYR:HB2	5	0.11
(1,1497)	1:A:37:ILE:HG22	1:A:11:TYR:HB2	5	0.11
(1,1497)	1:A:37:ILE:HG23	1:A:11:TYR:HB2	5	0.11
(1,1273)	2:C:18:GLU:H	2:C:17:LEU:HB2	5	0.11
(1,1273)	2:C:18:GLU:H	2:C:17:LEU:HB2	6	0.11
(1,1234)	2:C:27:GLN:HG3	2:C:27:GLN:HA	8	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	2	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	2	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	8	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	8	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	8	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	11	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	11	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	11	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	13	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	13	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	13	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	15	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	15	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	15	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG11	18	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG12	18	0.11
(1,1178)	2:C:39:VAL:HA	2:C:39:VAL:HG13	18	0.11
(1,111)	1:A:28:ILE:HG13	1:A:28:ILE:HA	10	0.11
(1,1105)	2:C:76:ASN:H	2:C:76:ASN:HB3	16	0.11
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	1	0.11
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	3	0.11
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	9	0.11
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	13	0.11
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	15	0.11
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	17	0.11
(1,1033)	1:A:39:GLU:HB2	1:A:39:GLU:HG2	18	0.11
(1,1019)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	7	0.11
(1,1019)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	7	0.11
(1,1019)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	7	0.11
(1,1019)	2:C:72:LEU:HD21	2:C:72:LEU:HB2	15	0.11
(1,1019)	2:C:72:LEU:HD22	2:C:72:LEU:HB2	15	0.11
(1,1019)	2:C:72:LEU:HD23	2:C:72:LEU:HB2	15	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found