Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2LMS
BMRB ID	:	18135
Title	:	A single GalNAc residue on Threonine-106 modifies the dynamics and the structure of Interferon alpha-2a around the glycosylation site
Authors	:	Ghasriani, H.; Belcourt, P.J.F.; Sauve, S.; Hodgson, D.J.; Gingras, G.; Brochu, D.; Gilbert, M.; Aubin, Y.
Deposited on	:	2011-12-12

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

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

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

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

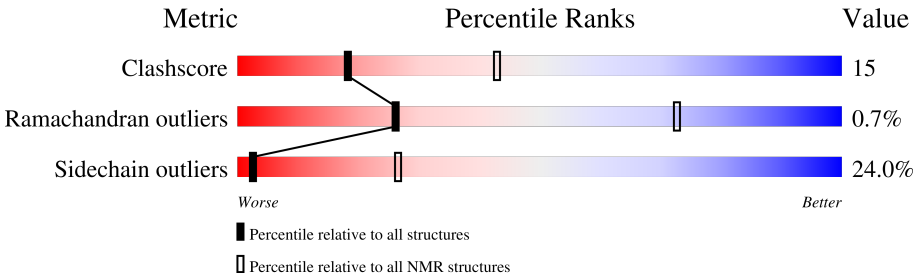
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 90%.

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	166	50% 31% 5% 13% .

2 Ensemble composition and analysis

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

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:3-A:38, A:49-A:156 (144)	0.41	2

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2722 atoms, of which 1358 are hydrogens and 0 are deuteriums.

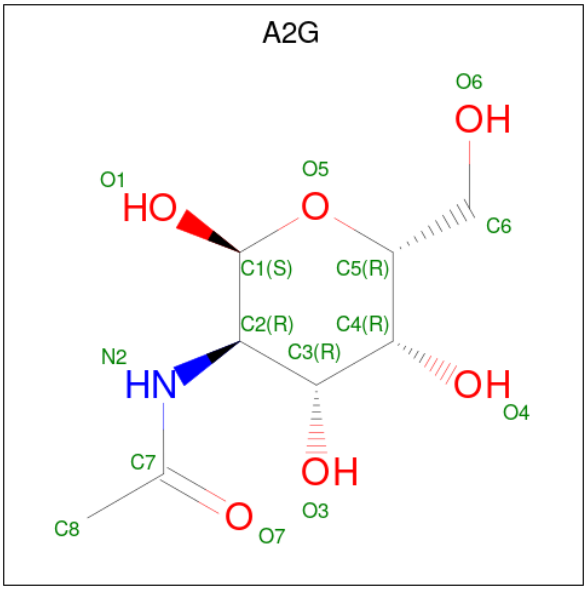
- Molecule 1 is a protein called Interferon alpha-2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	165	2694	860	1344	227	254	9	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01563

- Molecule 2 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
2	A	1	28	8	14	1	5

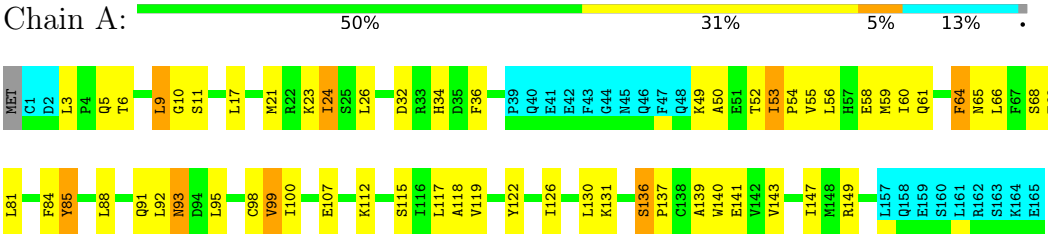
4 Residue-property plots

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: Interferon alpha-2

Chain A:



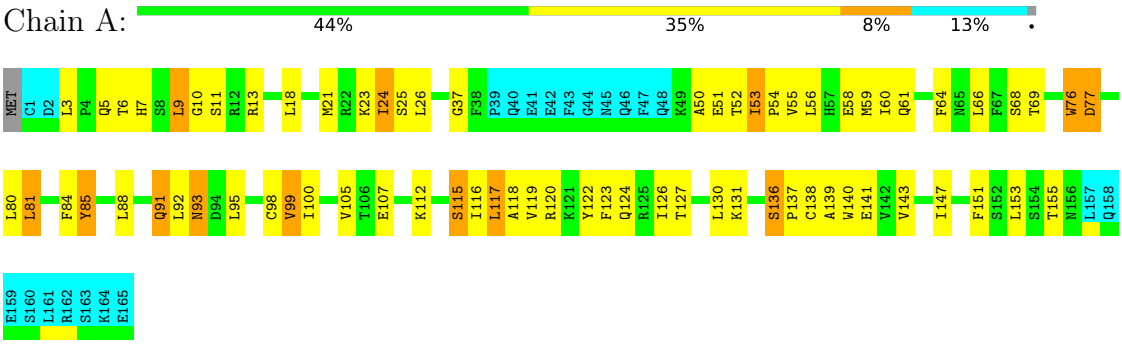
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

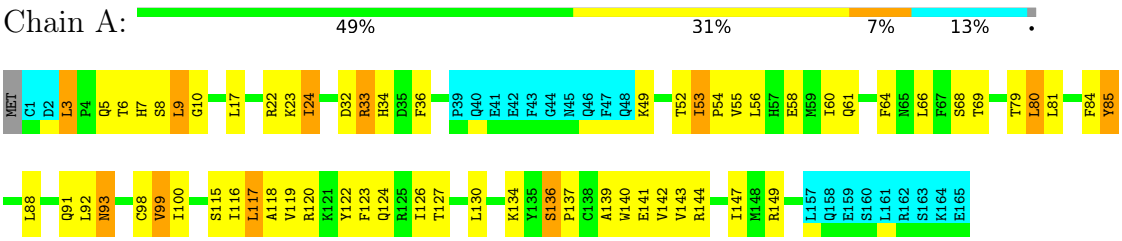
• Molecule 1: Interferon alpha-2

Chain A:



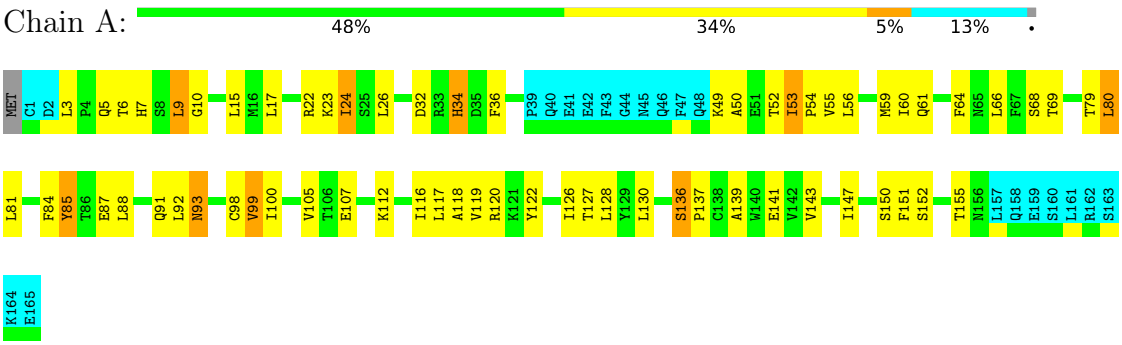
4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Interferon alpha-2



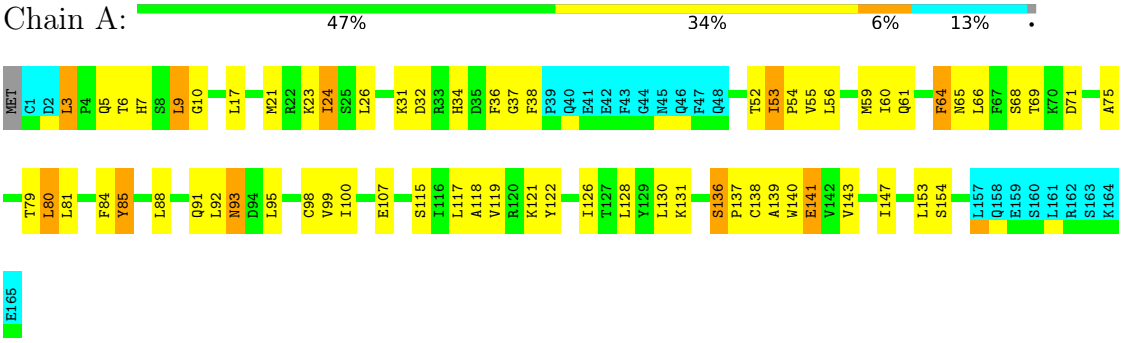
4.2.3 Score per residue for model 3

• Molecule 1: Interferon alpha-2



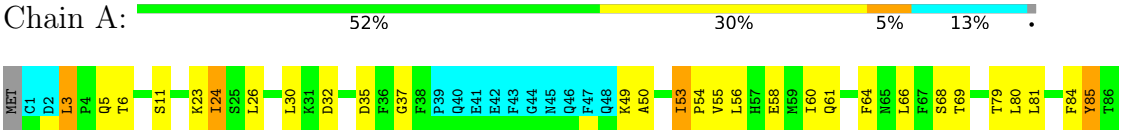
4.2.4 Score per residue for model 4

• Molecule 1: Interferon alpha-2



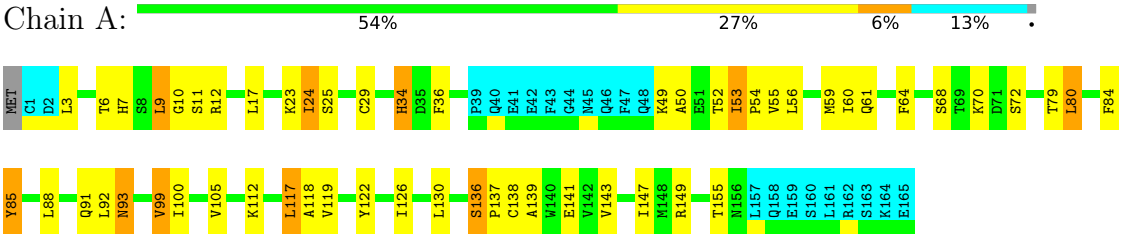
4.2.5 Score per residue for model 5

• Molecule 1: Interferon alpha-2



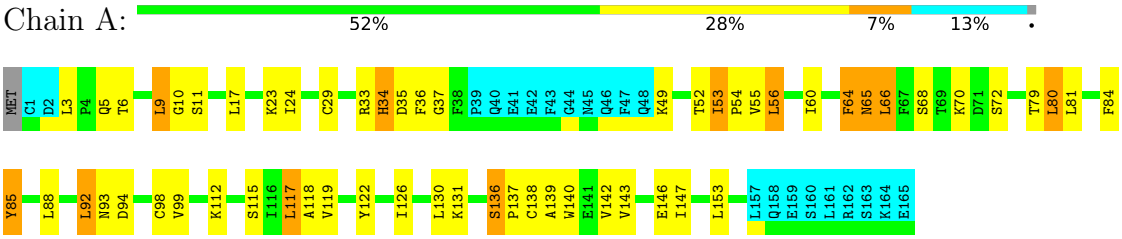
4.2.6 Score per residue for model 6

• Molecule 1: Interferon alpha-2



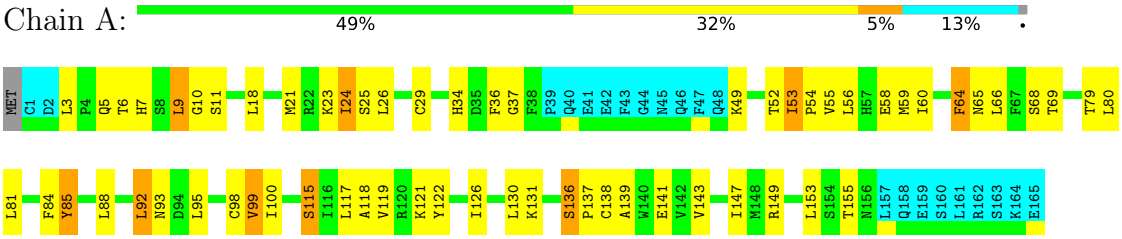
4.2.7 Score per residue for model 7

• Molecule 1: Interferon alpha-2



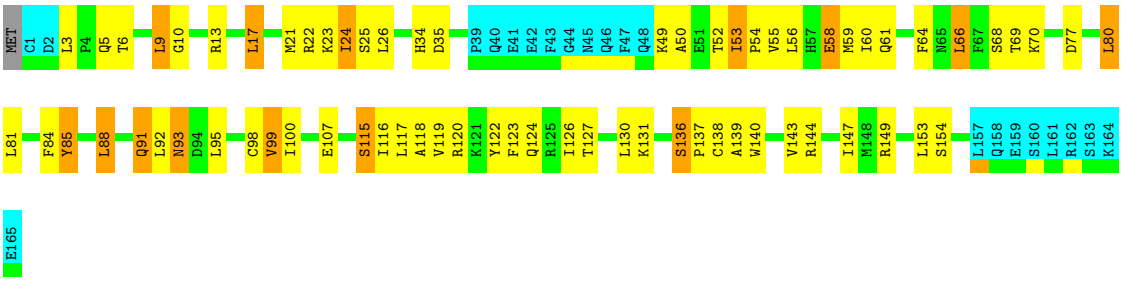
4.2.8 Score per residue for model 8

• Molecule 1: Interferon alpha-2



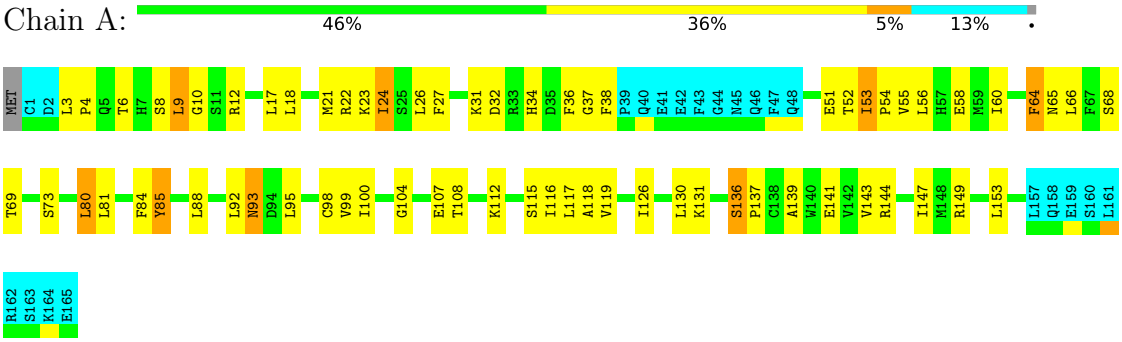
4.2.9 Score per residue for model 9

• Molecule 1: Interferon alpha-2



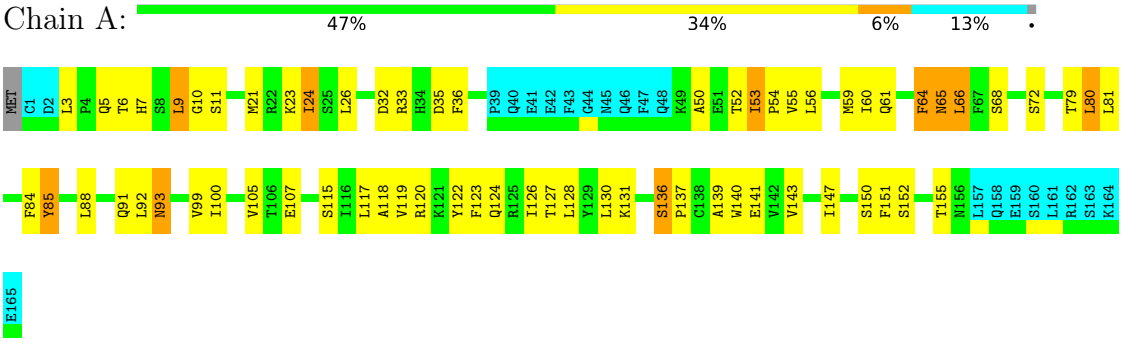
4.2.10 Score per residue for model 10

• Molecule 1: Interferon alpha-2



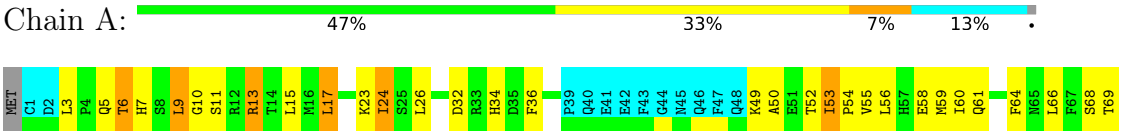
4.2.11 Score per residue for model 11

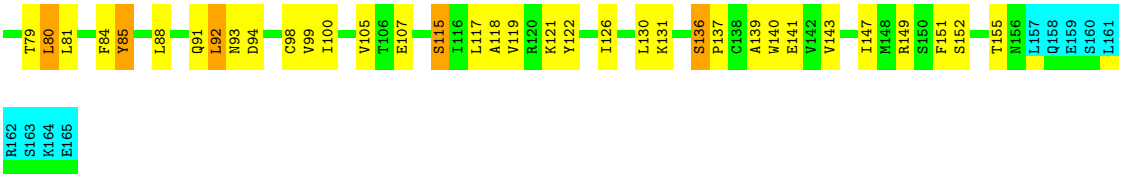
• Molecule 1: Interferon alpha-2



4.2.12 Score per residue for model 12

• Molecule 1: Interferon alpha-2

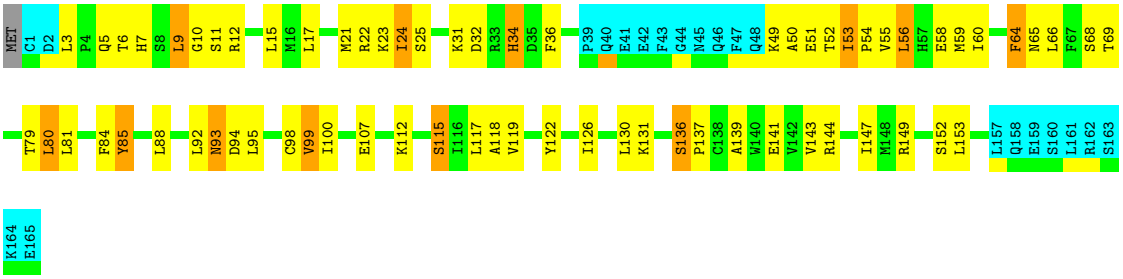




4.2.13 Score per residue for model 13

• Molecule 1: Interferon alpha-2

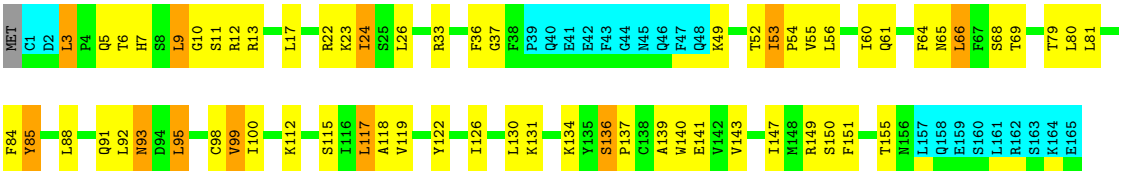
Chain A: 46% 34% 7% 13%



4.2.14 Score per residue for model 14

• Molecule 1: Interferon alpha-2

Chain A: 48% 32% 7% 13%



4.2.15 Score per residue for model 15

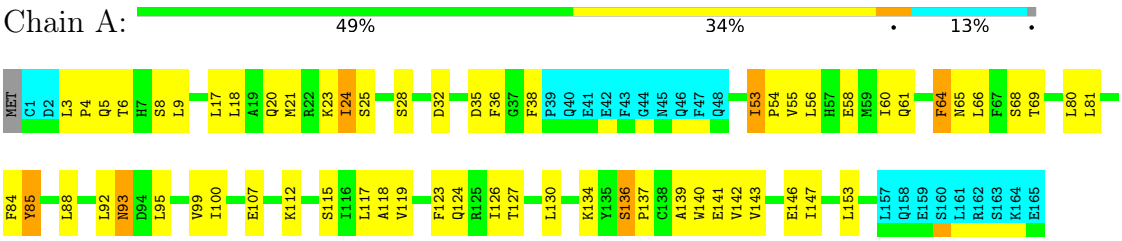
• Molecule 1: Interferon alpha-2

Chain A: 46% 34% 7% 13%

4.2.16 Score per residue for model 16

• Molecule 1: Interferon alpha-2

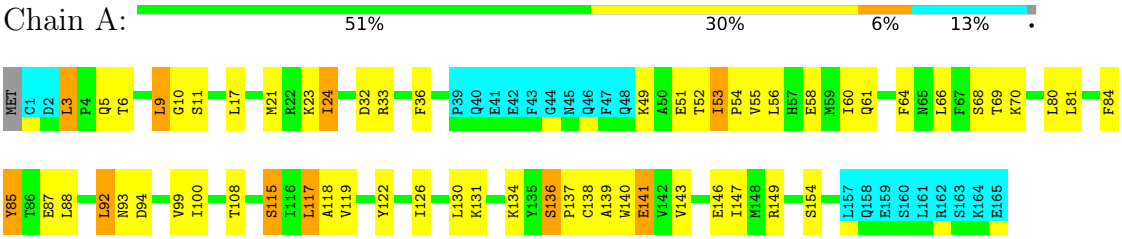
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Interferon alpha-2

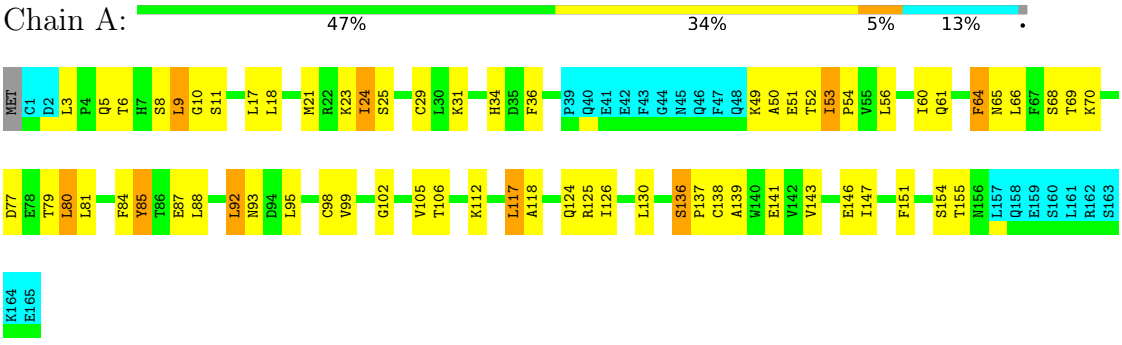
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Interferon alpha-2

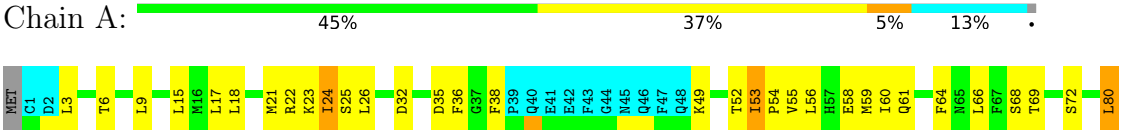
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Interferon alpha-2

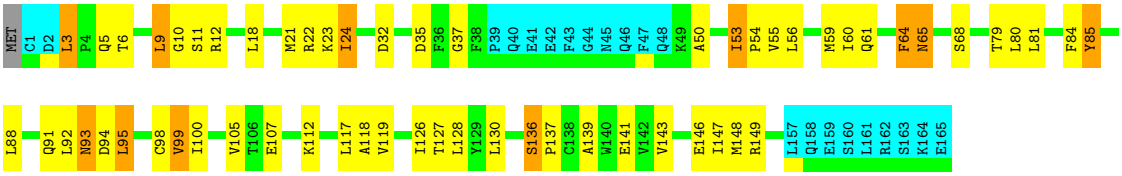
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Interferon alpha-2

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2106
Number of shifts mapped to atoms	2106
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A2G

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1175	1188	1188	35±5
2	A	14	14	11	0±0
All	All	23780	24040	23980	703

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:LEU:HD22	1:A:80:LEU:HD21	0.91	1.42	19	2
1:A:17:LEU:HD12	1:A:80:LEU:HD21	0.88	1.43	4	7
1:A:53:ILE:N	1:A:54:PRO:HD2	0.75	1.96	17	20
1:A:17:LEU:HD23	1:A:80:LEU:HD21	0.74	1.58	9	3
1:A:60:ILE:HG22	1:A:92:LEU:HD23	0.71	1.60	20	12
1:A:32:ASP:O	1:A:142:VAL:HG21	0.70	1.87	16	1
1:A:118:ALA:HB1	1:A:122:TYR:OH	0.68	1.89	19	13
1:A:66:LEU:HD22	1:A:140:TRP:CH2	0.68	2.23	17	12
1:A:55:VAL:HA	1:A:119:VAL:HG11	0.65	1.67	11	14
1:A:24:ILE:HD13	1:A:141:GLU:CD	0.65	2.11	17	2
1:A:53:ILE:N	1:A:54:PRO:CD	0.64	2.60	14	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:O	1:A:69:THR:HG22	0.64	1.92	17	16
1:A:56:LEU:HD23	1:A:95:LEU:HD21	0.64	1.69	19	2
1:A:53:ILE:HD12	1:A:100:ILE:HD12	0.64	1.70	11	18
1:A:38:PHE:CZ	1:A:153:LEU:HD23	0.64	2.28	4	1
1:A:24:ILE:HD13	1:A:141:GLU:HB2	0.63	1.71	19	16
1:A:85:TYR:C	1:A:85:TYR:CD1	0.63	2.71	1	20
1:A:126:ILE:HD12	1:A:143:VAL:HG13	0.63	1.71	8	18
1:A:24:ILE:HD13	1:A:141:GLU:CG	0.63	2.24	4	2
1:A:56:LEU:HD22	1:A:60:ILE:HD11	0.63	1.70	13	1
1:A:17:LEU:HD22	1:A:80:LEU:CD2	0.62	2.24	19	1
1:A:50:ALA:HB2	1:A:105:VAL:HG13	0.62	1.71	5	9
1:A:116:ILE:HG22	1:A:120:ARG:NE	0.62	2.10	15	2
1:A:56:LEU:O	1:A:60:ILE:HD12	0.60	1.97	15	16
1:A:56:LEU:HD11	1:A:95:LEU:HD23	0.60	1.71	18	1
1:A:112:LYS:HE3	1:A:116:ILE:HD11	0.60	1.72	19	2
1:A:56:LEU:HD12	1:A:95:LEU:HD22	0.59	1.73	20	1
1:A:50:ALA:HB2	1:A:105:VAL:CG1	0.59	2.28	11	7
1:A:115:SER:O	1:A:119:VAL:HG22	0.59	1.98	10	6
1:A:17:LEU:CD1	1:A:80:LEU:HD21	0.59	2.26	4	5
1:A:36:PHE:CZ	1:A:126:ILE:HD13	0.59	2.32	15	12
1:A:56:LEU:HD22	1:A:95:LEU:HD22	0.58	1.75	15	1
1:A:118:ALA:HB1	1:A:122:TYR:CZ	0.58	2.34	2	11
1:A:24:ILE:HG21	1:A:141:GLU:HG3	0.58	1.76	17	3
1:A:151:PHE:O	1:A:155:THR:HG23	0.57	1.99	1	6
1:A:130:LEU:HD23	1:A:143:VAL:HG21	0.57	1.76	19	17
1:A:21:MET:HB2	1:A:80:LEU:HD12	0.56	1.77	16	7
1:A:58:GLU:HG3	1:A:119:VAL:HG21	0.55	1.78	10	4
1:A:13:ARG:O	1:A:17:LEU:HD12	0.55	2.01	12	1
1:A:55:VAL:HA	1:A:119:VAL:HG21	0.55	1.79	8	4
1:A:126:ILE:HD11	1:A:146:GLU:CD	0.55	2.22	5	3
1:A:123:PHE:O	1:A:127:THR:HG22	0.54	2.01	16	6
1:A:84:PHE:O	1:A:88:LEU:HD22	0.54	2.03	9	20
1:A:9:LEU:HD23	1:A:10:GLY:N	0.53	2.19	11	9
1:A:77:ASP:O	1:A:81:LEU:HD23	0.53	2.03	1	1
1:A:15:LEU:HD21	1:A:152:SER:OG	0.53	2.03	19	2
1:A:56:LEU:CD1	1:A:95:LEU:HD22	0.53	2.33	20	1
1:A:58:GLU:HG2	1:A:119:VAL:HG21	0.53	1.81	9	2
1:A:15:LEU:HD21	1:A:152:SER:HB2	0.53	1.80	15	3
1:A:38:PHE:CZ	1:A:153:LEU:HD13	0.52	2.39	16	2
1:A:56:LEU:CD2	1:A:95:LEU:HD22	0.52	2.34	15	1
1:A:18:LEU:HD12	1:A:21:MET:SD	0.52	2.44	16	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:SER:O	1:A:119:VAL:HG23	0.52	2.05	12	5
1:A:117:LEU:HD23	1:A:118:ALA:N	0.52	2.20	18	16
1:A:24:ILE:HG21	1:A:141:GLU:CG	0.51	2.36	13	2
1:A:52:THR:HG22	1:A:56:LEU:HB2	0.50	1.82	12	8
1:A:21:MET:CE	1:A:81:LEU:HD22	0.50	2.37	1	1
1:A:126:ILE:HG23	1:A:143:VAL:HG13	0.50	1.82	8	12
1:A:130:LEU:HD12	1:A:131:LYS:N	0.50	2.22	9	14
1:A:116:ILE:HG22	1:A:120:ARG:HD3	0.49	1.85	1	3
1:A:52:THR:C	1:A:54:PRO:HD2	0.49	2.28	13	6
1:A:117:LEU:HD13	1:A:118:ALA:N	0.49	2.23	10	2
1:A:55:VAL:HG12	1:A:119:VAL:CG2	0.48	2.37	5	2
1:A:58:GLU:CB	1:A:119:VAL:HG11	0.48	2.38	13	5
1:A:92:LEU:HD12	1:A:93:ASN:N	0.48	2.23	11	15
1:A:126:ILE:HD11	1:A:146:GLU:OE1	0.48	2.08	15	1
1:A:52:THR:HG22	1:A:52:THR:O	0.48	2.09	6	13
1:A:56:LEU:HD11	1:A:95:LEU:HD13	0.48	1.86	20	1
1:A:76:TRP:CD1	1:A:81:LEU:HD21	0.48	2.44	1	1
1:A:50:ALA:HB1	1:A:107:GLU:HG2	0.48	1.84	9	3
1:A:53:ILE:CG2	1:A:99:VAL:HG21	0.47	2.39	9	17
1:A:130:LEU:HA	1:A:139:ALA:HB1	0.47	1.86	2	20
1:A:33:ARG:HA	1:A:142:VAL:HG13	0.47	1.86	2	2
1:A:7:HIS:ND1	1:A:155:THR:HG22	0.47	2.25	6	2
1:A:56:LEU:CD2	1:A:60:ILE:HD11	0.47	2.39	20	3
1:A:80:LEU:O	1:A:80:LEU:HD13	0.46	2.10	1	2
1:A:38:PHE:HZ	1:A:153:LEU:HD23	0.46	1.69	4	1
1:A:56:LEU:CD2	1:A:95:LEU:HD21	0.46	2.40	14	1
1:A:56:LEU:HD21	1:A:95:LEU:HD11	0.46	1.87	5	4
1:A:36:PHE:CE2	1:A:126:ILE:HD13	0.46	2.46	4	3
1:A:56:LEU:HD21	1:A:95:LEU:HD13	0.46	1.89	15	1
1:A:60:ILE:CG2	1:A:92:LEU:HD23	0.45	2.39	20	1
1:A:102:GLY:HA2	1:A:106:THR:HG23	0.45	1.88	18	1
1:A:56:LEU:HD13	1:A:95:LEU:CD2	0.45	2.42	13	1
1:A:116:ILE:HG22	1:A:120:ARG:CD	0.45	2.41	3	2
1:A:91:GLN:O	1:A:95:LEU:HD12	0.45	2.10	1	2
1:A:3:LEU:HD12	1:A:3:LEU:O	0.45	2.12	20	5
1:A:60:ILE:HG21	1:A:92:LEU:HB3	0.45	1.89	8	4
1:A:64:PHE:CD1	1:A:65:ASN:N	0.44	2.85	8	10
1:A:21:MET:HE3	1:A:81:LEU:HD22	0.44	1.87	1	1
1:A:122:TYR:CD1	1:A:122:TYR:N	0.44	2.85	9	1
1:A:122:TYR:N	1:A:122:TYR:CD1	0.44	2.81	19	4
1:A:56:LEU:HD21	1:A:95:LEU:CD1	0.44	2.42	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:LEU:C	1:A:92:LEU:HD12	0.44	2.33	8	5
1:A:153:LEU:HD13	1:A:154:SER:N	0.44	2.27	9	1
1:A:53:ILE:HG23	1:A:54:PRO:HD3	0.44	1.90	4	17
1:A:6:THR:HG23	1:A:91:GLN:OE1	0.44	2.13	12	1
1:A:136:SER:CB	1:A:137:PRO:HD2	0.44	2.43	19	20
1:A:36:PHE:CE1	1:A:126:ILE:HD13	0.44	2.48	16	1
1:A:91:GLN:C	1:A:95:LEU:HD12	0.44	2.33	9	2
1:A:58:GLU:CG	1:A:119:VAL:HG21	0.44	2.43	19	3
1:A:56:LEU:HD23	1:A:95:LEU:CD2	0.43	2.41	19	1
1:A:52:THR:O	1:A:52:THR:CG2	0.43	2.67	6	1
1:A:13:ARG:O	1:A:17:LEU:HD13	0.43	2.13	14	1
1:A:15:LEU:HD11	1:A:152:SER:OG	0.43	2.13	15	1
1:A:153:LEU:C	1:A:153:LEU:HD13	0.43	2.34	7	2
1:A:9:LEU:HD23	1:A:10:GLY:H	0.43	1.74	2	14
1:A:55:VAL:HG13	1:A:115:SER:HB2	0.43	1.91	2	1
1:A:112:LYS:CE	1:A:116:ILE:HD11	0.43	2.44	19	1
1:A:117:LEU:HD22	1:A:117:LEU:O	0.43	2.12	17	1
1:A:21:MET:CB	1:A:80:LEU:HD12	0.42	2.43	16	1
1:A:53:ILE:HG12	1:A:54:PRO:N	0.42	2.29	19	7
1:A:53:ILE:HD12	1:A:100:ILE:CD1	0.42	2.44	5	1
1:A:60:ILE:CG2	1:A:92:LEU:HB3	0.42	2.45	8	4
1:A:24:ILE:HG23	1:A:25:SER:N	0.42	2.30	9	1
1:A:55:VAL:HG23	1:A:56:LEU:N	0.42	2.29	7	14
1:A:52:THR:O	1:A:52:THR:HG22	0.42	2.15	13	1
1:A:18:LEU:HD21	1:A:148:MET:HG2	0.42	1.91	20	1
1:A:52:THR:HA	1:A:55:VAL:HG22	0.42	1.91	13	2
1:A:119:VAL:HG23	1:A:120:ARG:N	0.42	2.29	11	2
1:A:52:THR:O	1:A:56:LEU:HB2	0.42	2.13	13	1
1:A:17:LEU:HG	1:A:80:LEU:HD21	0.42	1.91	17	1
1:A:117:LEU:HD13	1:A:117:LEU:C	0.41	2.35	17	1
1:A:17:LEU:CD2	1:A:80:LEU:HD21	0.41	2.30	19	1
2:A:500:A2G:H3	2:A:500:A2G:H8B	0.41	1.91	5	1
1:A:126:ILE:HG23	1:A:143:VAL:CG1	0.41	2.45	18	2
1:A:38:PHE:HB2	1:A:122:TYR:CE1	0.41	2.49	19	1
1:A:3:LEU:O	1:A:3:LEU:HD12	0.41	2.16	2	1
1:A:56:LEU:HD21	1:A:60:ILE:HD11	0.41	1.92	20	1
1:A:71:ASP:O	1:A:75:ALA:HB2	0.41	2.15	4	1
1:A:26:LEU:HD11	1:A:27:PHE:CE2	0.41	2.50	10	1
1:A:127:THR:HG23	1:A:128:LEU:N	0.41	2.31	3	3
1:A:128:LEU:C	1:A:128:LEU:HD13	0.41	2.35	4	1
1:A:26:LEU:H	1:A:26:LEU:HD22	0.41	1.75	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:VAL:HG13	1:A:115:SER:HB3	0.41	1.92	16	1
1:A:30:LEU:HD22	1:A:30:LEU:N	0.40	2.32	5	1
1:A:17:LEU:HD23	1:A:20:GLN:NE2	0.40	2.31	16	1
1:A:80:LEU:HD13	1:A:80:LEU:O	0.40	2.16	4	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/166 (87%)	123±2 (85±1%)	20±2 (14±1%)	1±1 (1±1%)	26	73
All	All	2880/3320 (87%)	2451 (85%)	408 (14%)	21 (1%)	26	73

All 4 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	37	GLY	8
1	A	34	HIS	7
1	A	35	ASP	5
1	A	104	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	132/153 (86%)	100±3 (76±3%)	32±3 (24±3%)	2	26
All	All	2640/3060 (86%)	2006 (76%)	634 (24%)	2	26

All 73 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	3	LEU	20
1	A	6	THR	20
1	A	23	LYS	20
1	A	24	ILE	20
1	A	53	ILE	20
1	A	64	PHE	20
1	A	68	SER	20
1	A	85	TYR	20
1	A	93	ASN	20
1	A	136	SER	20
1	A	147	ILE	20
1	A	9	LEU	19
1	A	81	LEU	19
1	A	5	GLN	17
1	A	80	LEU	17
1	A	61	GLN	16
1	A	98	CYS	15
1	A	99	VAL	15
1	A	49	LYS	14
1	A	79	THR	14
1	A	11	SER	12
1	A	59	MET	12
1	A	32	ASP	12
1	A	149	ARG	12
1	A	91	GLN	11
1	A	115	SER	11
1	A	117	LEU	11
1	A	107	GLU	10
1	A	26	LEU	9
1	A	112	LYS	9
1	A	124	GLN	9
1	A	138	CYS	9
1	A	22	ARG	9
1	A	34	HIS	8
1	A	25	SER	7
1	A	51	GLU	6
1	A	144	ARG	6
1	A	94	ASP	6
1	A	146	GLU	6
1	A	33	ARG	5
1	A	87	GLU	5
1	A	12	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	70	LYS	5
1	A	92	LEU	5
1	A	134	LYS	4
1	A	31	LYS	4
1	A	121	LYS	4
1	A	95	LEU	4
1	A	29	CYS	4
1	A	72	SER	4
1	A	65	ASN	4
1	A	66	LEU	4
1	A	13	ARG	3
1	A	77	ASP	3
1	A	150	SER	3
1	A	122	TYR	3
1	A	141	GLU	2
1	A	35	ASP	2
1	A	56	LEU	2
1	A	17	LEU	2
1	A	58	GLU	2
1	A	108	THR	2
1	A	154	SER	2
1	A	76	TRP	1
1	A	21	MET	1
1	A	88	LEU	1
1	A	73	SER	1
1	A	152	SER	1
1	A	83	LYS	1
1	A	28	SER	1
1	A	8	SER	1
1	A	36	PHE	1
1	A	125	ARG	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	A2G	A	500	1	14,14,15	1.22±0.00	2±0 (14±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	A2G	A	500	1	17,19,21	1.27±0.00	3±0 (17±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2G	A	500	1	-	0±0,6,23,26	0±0,1,1,1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	500	A2G	O6-C6	2.96	1.29	1.42	16	20
2	A	500	A2G	C1-C2	2.24	1.55	1.52	2	20

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	500	A2G	C6-C5-C4	2.70	106.69	113.00	10	20
2	A	500	A2G	O3-C3-C4	2.45	104.68	110.35	15	20
2	A	500	A2G	O3-C3-C2	2.10	113.82	109.47	15	20

There are no chirality outliers.

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	500	A2G	O7-C7-N2-C2	1

There are no ring outliers.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	2106
Number of shifts mapped to atoms	2106
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	165	-0.45 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	160	0.45 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	159	-0.33 ± 0.08	None needed (< 0.5 ppm)
^{15}N	160	-0.06 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1847 atoms were assigned a chemical shift out of a possible 2057. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	711/716 (99%)	288/288 (100%)	283/288 (98%)	140/140 (100%)
Sidechain	1015/1171 (87%)	693/763 (91%)	311/363 (86%)	11/45 (24%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	121/170 (71%)	69/84 (82%)	50/81 (62%)	2/5 (40%)
Overall	1847/2057 (90%)	1050/1135 (93%)	644/732 (88%)	153/190 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 2101 atoms were assigned a chemical shift out of a possible 2341. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	814/820 (99%)	330/330 (100%)	324/330 (98%)	160/160 (100%)
Sidechain	1150/1331 (86%)	785/862 (91%)	349/415 (84%)	16/54 (30%)
Aromatic	137/190 (72%)	78/94 (83%)	57/91 (63%)	2/5 (40%)
Overall	2101/2341 (90%)	1193/1286 (93%)	730/836 (87%)	178/219 (81%)

7.1.4 Statistically unusual chemical shifts (i)

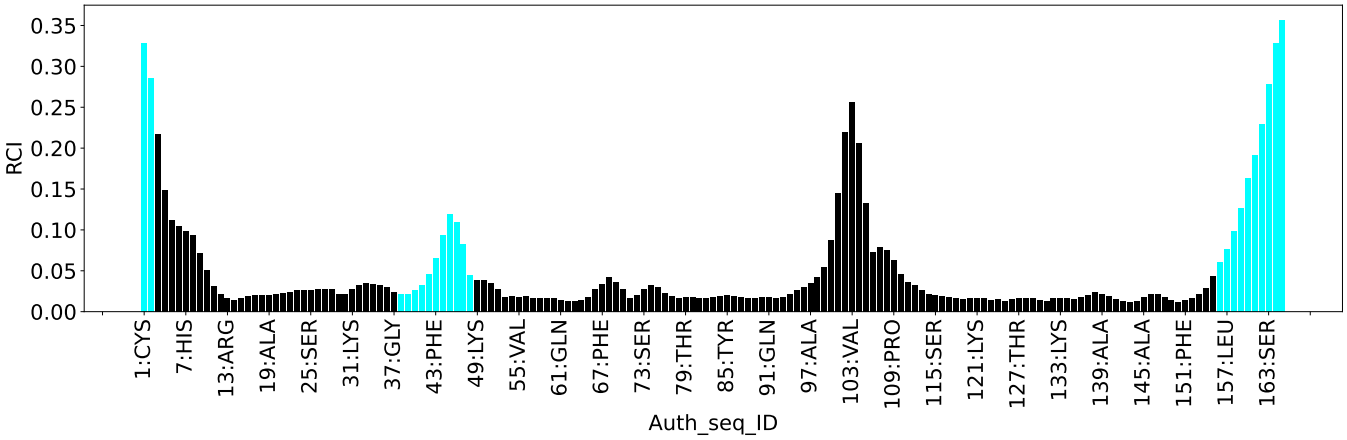
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	75	ALA	HB1	-0.29	0.14 – 2.58	-6.7
1	A	75	ALA	HB2	-0.29	0.14 – 2.58	-6.7
1	A	75	ALA	HB3	-0.29	0.14 – 2.58	-6.7
1	A	150	SER	HB2	2.18	2.61 – 5.13	-6.7
1	A	62	GLN	HB2	0.51	0.80 – 3.29	-6.2
1	A	106	THR	CB	79.54	61.12 – 78.27	5.7
1	A	76	TRP	HE1	6.77	6.88 – 13.28	-5.2

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1:CYS
7:HIS
13:ARG
19:ALA
25:SER
31:LYS
37:GLY
43:PHE
49:LYS
55:VAL
61:GLN
67:PHE
73:SER
79:THR
85:TYR
91:GLN
97:ALA
103:VAL
109:PRO
115:SER
121:LYS
127:THR
133:LYS
139:ALA
145:ALA
151:PHE
157:LEU
163:SER
Auth_seq_ID

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	2486
Intra-residue (|i-j|=0)	547
Sequential (|i-j|=1)	659
Medium range (|i-j|>1 and |i-j|<5)	657
Long range (|i-j|≥5)	623
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	15.0
Number of long range restraints per residue[1]	3.8

[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)	14.2	0.2
0.2-0.5 (Medium)	4.2	0.49
>0.5 (Large)	2.7	2.1

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

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

9 Distance violation analysis (i)

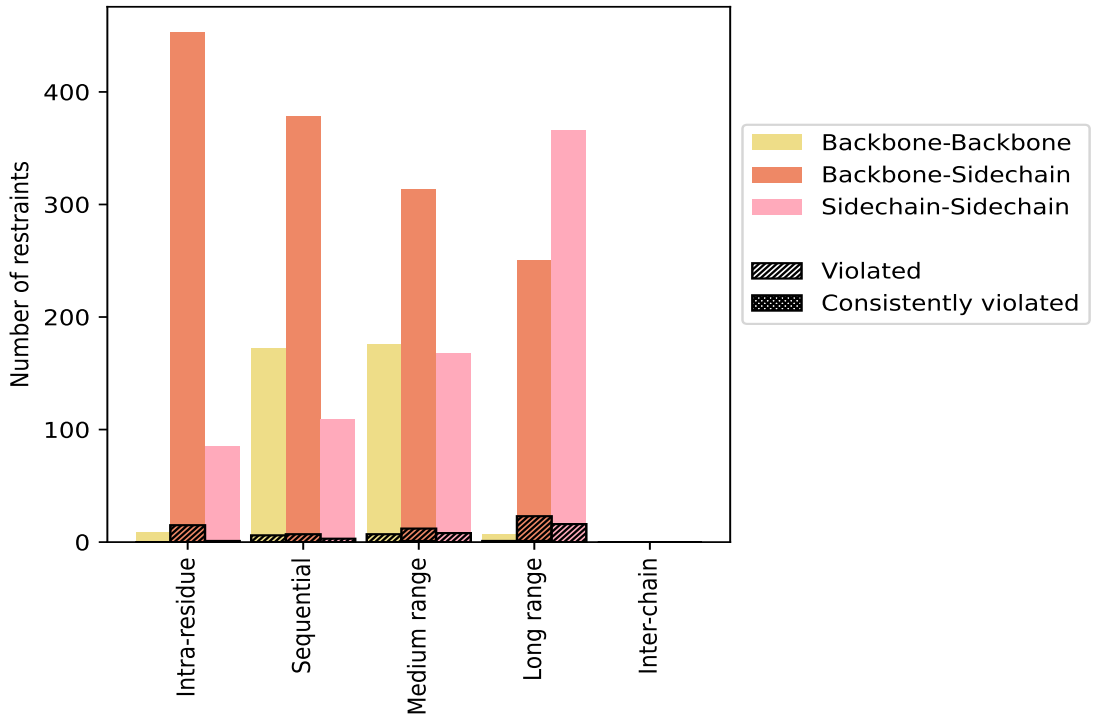
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	547	22.0	16	2.9	0.6	0	0.0	0.0
Backbone-Backbone	9	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	453	18.2	15	3.3	0.6	0	0.0	0.0
Sidechain-Sidechain	85	3.4	1	1.2	0.0	0	0.0	0.0
Sequential (|i-j|=1)	659	26.5	16	2.4	0.6	0	0.0	0.0
Backbone-Backbone	172	6.9	6	3.5	0.2	0	0.0	0.0
Backbone-Sidechain	378	15.2	7	1.9	0.3	0	0.0	0.0
Sidechain-Sidechain	109	4.4	3	2.8	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	657	26.4	27	4.1	1.1	1	0.2	0.0
Backbone-Backbone	176	7.1	7	4.0	0.3	0	0.0	0.0
Backbone-Sidechain	313	12.6	12	3.8	0.5	1	0.3	0.0
Sidechain-Sidechain	168	6.8	8	4.8	0.3	0	0.0	0.0
Long range (|i-j|≥5)	623	25.1	40	6.4	1.6	1	0.2	0.0
Backbone-Backbone	7	0.3	1	14.3	0.0	0	0.0	0.0
Backbone-Sidechain	250	10.1	23	9.2	0.9	1	0.4	0.0
Sidechain-Sidechain	366	14.7	16	4.4	0.6	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2486	100.0	99	4.0	4.0	2	0.1	0.1
Backbone-Backbone	364	14.6	14	3.8	0.6	0	0.0	0.0
Backbone-Sidechain	1394	56.1	57	4.1	2.3	2	0.1	0.1
Sidechain-Sidechain	728	29.3	28	3.8	1.1	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	2	2	5	8	0	17	0.19	0.69	0.13	0.16
2	4	2	5	8	0	19	0.16	0.35	0.07	0.13
3	1	1	4	7	0	13	0.2	0.49	0.11	0.13
4	2	0	8	7	0	17	0.16	0.36	0.07	0.12
5	2	2	9	14	0	27	0.38	1.32	0.42	0.15
6	2	2	6	8	0	18	0.17	0.34	0.06	0.14
7	4	1	4	14	0	23	0.36	1.44	0.34	0.2
8	0	2	5	11	0	18	0.24	1.09	0.24	0.15
9	1	1	7	8	0	17	0.26	0.94	0.24	0.14
10	4	4	7	15	0	30	0.34	2.1	0.45	0.15
11	1	2	1	10	0	14	0.34	0.98	0.27	0.26

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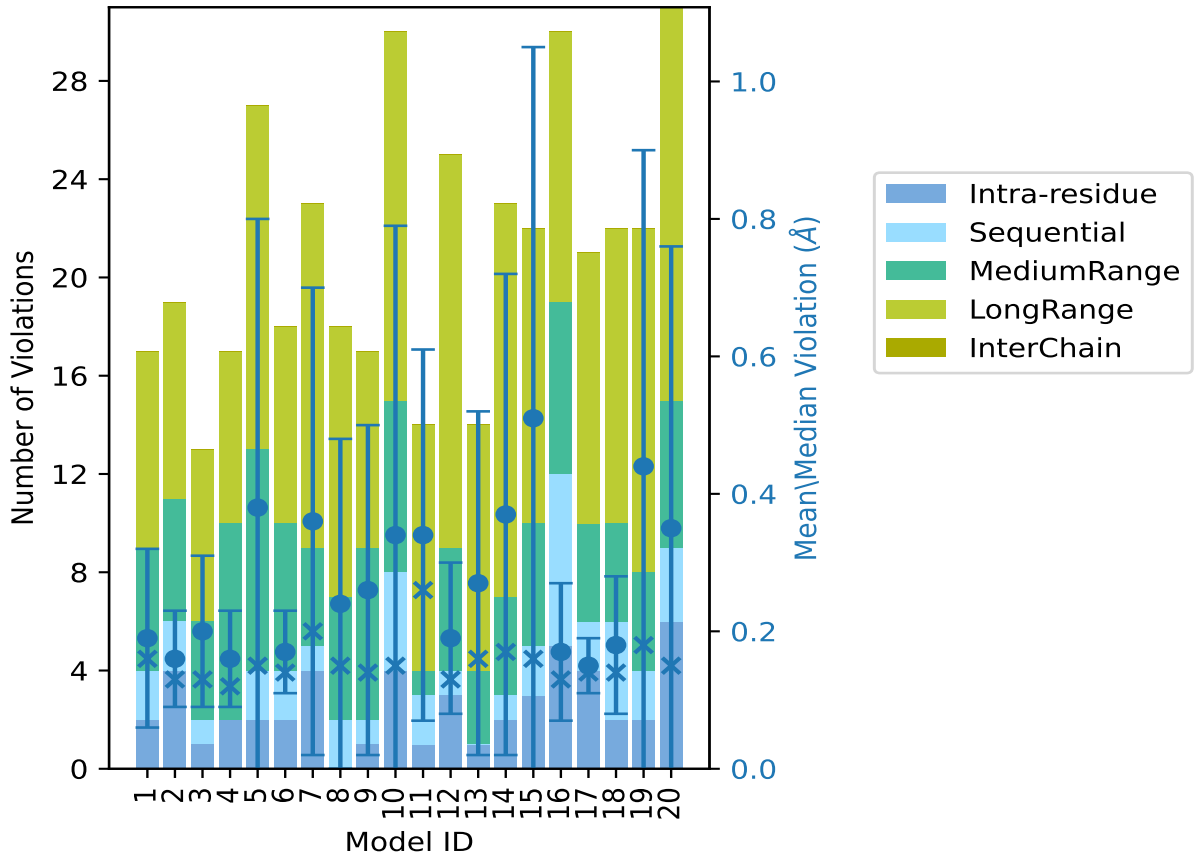
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	3	1	5	16	0	25	0.19	0.56	0.11	0.13
13	1	0	3	10	0	14	0.27	0.92	0.25	0.16
14	2	1	4	16	0	23	0.37	1.28	0.35	0.17
15	3	2	5	12	0	22	0.51	1.63	0.54	0.16
16	5	7	7	11	0	30	0.17	0.58	0.1	0.13
17	4	2	4	11	0	21	0.15	0.25	0.04	0.14
18	2	4	4	12	0	22	0.18	0.48	0.1	0.14
19	2	2	4	14	0	22	0.44	1.53	0.46	0.18
20	6	3	6	16	0	31	0.35	1.6	0.41	0.15

[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

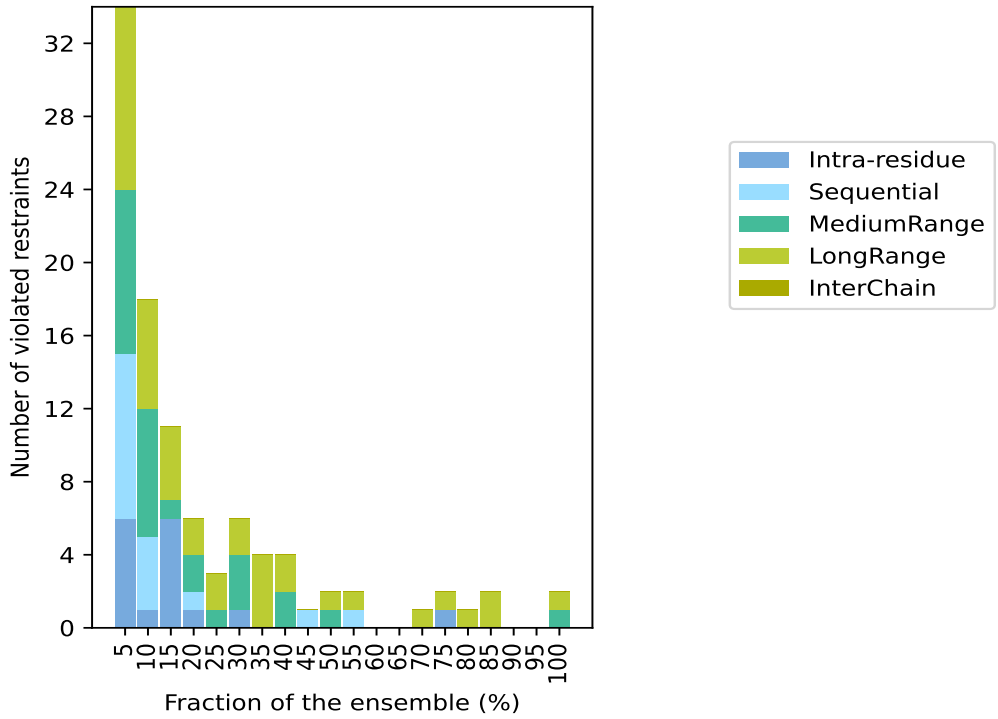
9.3 Distance violation statistics for the ensemble (i)

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, 2387(IR:531, SQ:643, MR:630, LR:583, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
6	9	9	10	0	34	1	5.0
1	4	7	6	0	18	2	10.0
6	0	1	4	0	11	3	15.0
1	1	2	2	0	6	4	20.0
0	0	1	2	0	3	5	25.0
1	0	3	2	0	6	6	30.0
0	0	0	4	0	4	7	35.0
0	0	2	2	0	4	8	40.0
0	1	0	0	0	1	9	45.0
0	0	1	1	0	2	10	50.0
0	1	0	1	0	2	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	1	0	1	14	70.0
1	0	0	1	0	2	15	75.0
0	0	0	1	0	1	16	80.0
0	0	0	2	0	2	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	1	1	0	2	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

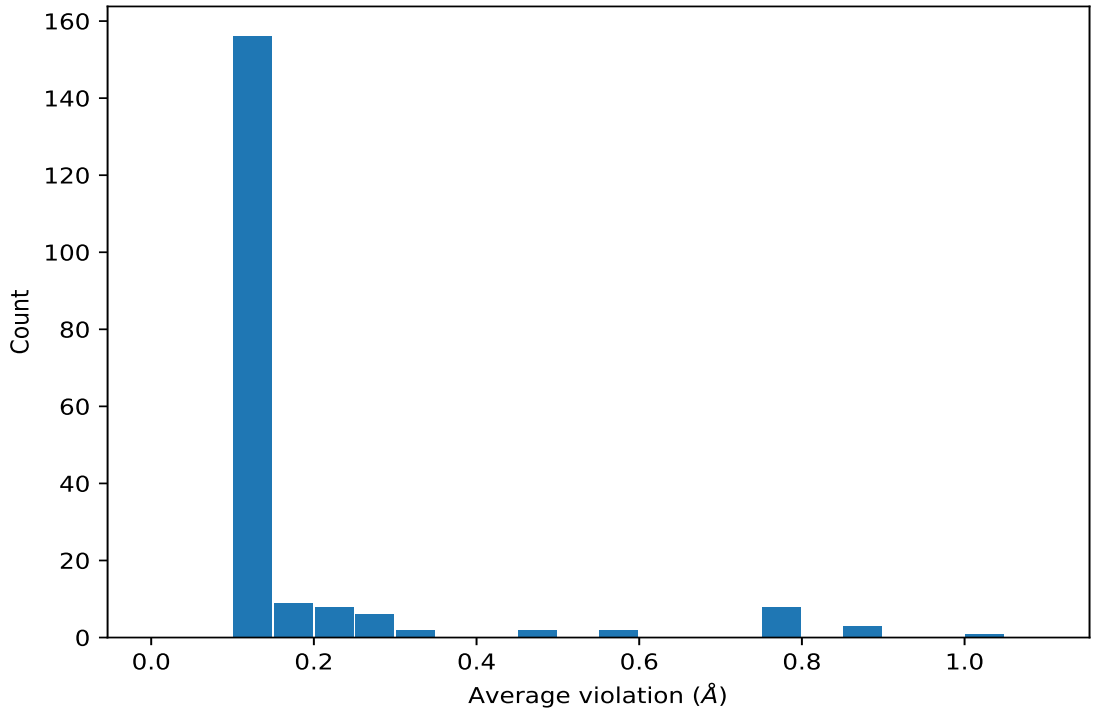
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	20	0.31	0.04	0.3
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	20	0.31	0.04	0.3
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	20	0.25	0.03	0.25
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	17	0.78	0.52	0.69
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	17	0.12	0.01	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	17	0.12	0.01	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	17	0.12	0.01	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	17	0.12	0.01	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	17	0.12	0.01	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	17	0.12	0.01	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	17	0.12	0.01	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	17	0.12	0.01	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	17	0.12	0.01	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	16	0.13	0.02	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	16	0.13	0.02	0.12
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	15	0.75	0.42	0.6

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	15	0.75	0.42	0.6
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	15	0.75	0.42	0.6
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	15	0.75	0.42	0.6
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	15	0.75	0.42	0.6
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	15	0.75	0.42	0.6
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	15	0.14	0.02	0.15
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	15	0.14	0.02	0.15
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	14	0.75	0.51	0.68
(1,714)	1:A:50:ALA:HB1	2:A:500:A2G:H81	11	0.89	0.4	0.97
(1,714)	1:A:50:ALA:HB2	2:A:500:A2G:H81	11	0.89	0.4	0.97
(1,714)	1:A:50:ALA:HB3	2:A:500:A2G:H81	11	0.89	0.4	0.97
(1,2312)	1:A:161:LEU:HA	1:A:162:ARG:H	11	0.12	0.01	0.12
(1,1578)	1:A:106:THR:HB	2:A:500:A2G:H81	10	1.03	0.41	1.13
(1,1036)	1:A:66:LEU:HD11	1:A:69:THR:H	10	0.15	0.03	0.16
(1,1036)	1:A:66:LEU:HD12	1:A:69:THR:H	10	0.15	0.03	0.16
(1,1036)	1:A:66:LEU:HD13	1:A:69:THR:H	10	0.15	0.03	0.16
(1,1036)	1:A:66:LEU:HD21	1:A:69:THR:H	10	0.15	0.03	0.16
(1,1036)	1:A:66:LEU:HD22	1:A:69:THR:H	10	0.15	0.03	0.16
(1,1036)	1:A:66:LEU:HD23	1:A:69:THR:H	10	0.15	0.03	0.16
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE1	9	0.13	0.02	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE2	9	0.13	0.02	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE3	9	0.13	0.02	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE1	9	0.13	0.02	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE2	9	0.13	0.02	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE3	9	0.13	0.02	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE1	9	0.13	0.02	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE2	9	0.13	0.02	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE3	9	0.13	0.02	0.12
(2,60)	1:A:61:GLN:HE21	1:A:65:ASN:HA	8	0.21	0.02	0.21
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG21	8	0.17	0.02	0.16
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG22	8	0.17	0.02	0.16
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG23	8	0.17	0.02	0.16
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG21	8	0.13	0.02	0.12
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG22	8	0.13	0.02	0.12
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG23	8	0.13	0.02	0.12
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD11	8	0.12	0.01	0.12
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD12	8	0.12	0.01	0.12
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD13	8	0.12	0.01	0.12
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD21	8	0.12	0.01	0.12
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD22	8	0.12	0.01	0.12
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD23	8	0.12	0.01	0.12
(1,1570)	1:A:106:THR:H	2:A:500:A2G:H81	7	0.59	0.16	0.58

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,102)	1:A:106:THR:HA	2:A:500:A2G:H81	7	0.57	0.13	0.55
(1,365)	1:A:23:LYS:HG2	1:A:76:TRP:HA	7	0.13	0.02	0.12
(1,365)	1:A:23:LYS:HG3	1:A:76:TRP:HA	7	0.13	0.02	0.12
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE1	7	0.13	0.01	0.13
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE2	7	0.13	0.01	0.13
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG21	6	0.15	0.05	0.13
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG22	6	0.15	0.05	0.13
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG23	6	0.15	0.05	0.13
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG21	6	0.15	0.05	0.13
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG22	6	0.15	0.05	0.13
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG23	6	0.15	0.05	0.13
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG21	6	0.15	0.05	0.13
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG22	6	0.15	0.05	0.13
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG23	6	0.15	0.05	0.13
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD1	6	0.15	0.02	0.15
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD2	6	0.15	0.02	0.15
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD1	6	0.15	0.02	0.15
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD2	6	0.15	0.02	0.15
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD1	6	0.15	0.02	0.15
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD2	6	0.15	0.02	0.15
(1,900)	1:A:61:GLN:HE22	1:A:64:PHE:HB3	6	0.14	0.02	0.15
(1,788)	1:A:55:VAL:HG21	1:A:115:SER:HA	6	0.12	0.01	0.12
(1,788)	1:A:55:VAL:HG22	1:A:115:SER:HA	6	0.12	0.01	0.12
(1,788)	1:A:55:VAL:HG23	1:A:115:SER:HA	6	0.12	0.01	0.12
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG2	6	0.12	0.01	0.12
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG3	6	0.12	0.01	0.12
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB2	6	0.12	0.01	0.12
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB3	6	0.12	0.01	0.12
(1,857)	1:A:60:ILE:HB	1:A:92:LEU:HA	5	0.16	0.03	0.16
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD11	5	0.13	0.01	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD12	5	0.13	0.01	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD13	5	0.13	0.01	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD21	5	0.13	0.01	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD22	5	0.13	0.01	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD23	5	0.13	0.01	0.13
(2,135)	1:A:135:TYR:H	1:A:139:ALA:H	5	0.12	0.01	0.12
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD21	4	0.15	0.02	0.15
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD22	4	0.15	0.02	0.15
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD23	4	0.15	0.02	0.15
(1,878)	1:A:60:ILE:HG21	1:A:92:LEU:HG	4	0.14	0.01	0.15
(1,878)	1:A:60:ILE:HG22	1:A:92:LEU:HG	4	0.14	0.01	0.15
(1,878)	1:A:60:ILE:HG23	1:A:92:LEU:HG	4	0.14	0.01	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD11	4	0.13	0.01	0.12
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD12	4	0.13	0.01	0.12
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD13	4	0.13	0.01	0.12
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD21	4	0.13	0.01	0.12
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD22	4	0.13	0.01	0.12
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD23	4	0.13	0.01	0.12
(1,2048)	1:A:134:LYS:HA	1:A:134:LYS:HD2	4	0.13	0.01	0.12
(1,2048)	1:A:134:LYS:HA	1:A:134:LYS:HD3	4	0.13	0.01	0.12
(1,1278)	1:A:81:LEU:HB3	1:A:85:TYR:HD1	4	0.12	0.01	0.12
(1,1278)	1:A:81:LEU:HB3	1:A:85:TYR:HD2	4	0.12	0.01	0.12
(2,115)	1:A:127:THR:H	1:A:129:TYR:HD1	4	0.12	0.0	0.12
(2,115)	1:A:127:THR:H	1:A:129:TYR:HD2	4	0.12	0.0	0.12
(1,46)	1:A:5:GLN:HA	1:A:5:GLN:HG2	3	0.47	0.0	0.47
(1,46)	1:A:5:GLN:HA	1:A:5:GLN:HG3	3	0.47	0.0	0.47
(1,1372)	1:A:87:GLU:H	1:A:87:GLU:HG2	3	0.29	0.07	0.34
(1,1372)	1:A:87:GLU:H	1:A:87:GLU:HG3	3	0.29	0.07	0.34
(1,55)	1:A:5:GLN:HG2	1:A:10:GLY:H	3	0.26	0.02	0.27
(1,55)	1:A:5:GLN:HG3	1:A:10:GLY:H	3	0.26	0.02	0.27
(2,1)	1:A:1:CYS:H	1:A:98:CYS:H	3	0.26	0.01	0.26
(1,1729)	1:A:122:TYR:H	1:A:122:TYR:HD1	3	0.18	0.04	0.18
(1,1729)	1:A:122:TYR:H	1:A:122:TYR:HD2	3	0.18	0.04	0.18
(1,1394)	1:A:88:LEU:HB2	1:A:92:LEU:HD21	3	0.14	0.02	0.13
(1,1394)	1:A:88:LEU:HB2	1:A:92:LEU:HD22	3	0.14	0.02	0.13
(1,1394)	1:A:88:LEU:HB2	1:A:92:LEU:HD23	3	0.14	0.02	0.13
(1,643)	1:A:45:ASN:H	1:A:45:ASN:HB2	3	0.12	0.01	0.12
(1,643)	1:A:45:ASN:H	1:A:45:ASN:HB3	3	0.12	0.01	0.12
(1,681)	1:A:48:GLN:H	1:A:48:GLN:HB2	3	0.12	0.01	0.12
(1,681)	1:A:48:GLN:H	1:A:48:GLN:HB3	3	0.12	0.01	0.12
(1,743)	1:A:53:ILE:HG13	1:A:100:ILE:HA	3	0.12	0.01	0.12
(1,2043)	1:A:134:LYS:H	1:A:134:LYS:HG2	3	0.12	0.01	0.11
(1,2043)	1:A:134:LYS:H	1:A:134:LYS:HG3	3	0.12	0.01	0.11
(1,366)	1:A:23:LYS:HG2	1:A:76:TRP:HB3	3	0.11	0.0	0.11
(1,366)	1:A:23:LYS:HG3	1:A:76:TRP:HB3	3	0.11	0.0	0.11
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD11	2	0.24	0.03	0.24
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD12	2	0.24	0.03	0.24
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD13	2	0.24	0.03	0.24
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD21	2	0.24	0.03	0.24
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD22	2	0.24	0.03	0.24
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD23	2	0.24	0.03	0.24
(1,1524)	1:A:101:GLN:HA	1:A:103:VAL:H	2	0.23	0.01	0.23
(1,501)	1:A:33:ARG:HB2	1:A:34:HIS:HE1	2	0.19	0.06	0.19
(1,501)	1:A:33:ARG:HB3	1:A:34:HIS:HE1	2	0.19	0.06	0.19

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,651)	1:A:45:ASN:HA	1:A:47:PHE:H	2	0.17	0.01	0.17
(1,706)	1:A:50:ALA:HB1	1:A:105:VAL:HB	2	0.14	0.01	0.14
(1,706)	1:A:50:ALA:HB2	1:A:105:VAL:HB	2	0.14	0.01	0.14
(1,706)	1:A:50:ALA:HB3	1:A:105:VAL:HB	2	0.14	0.01	0.14
(1,224)	1:A:18:LEU:HD21	1:A:84:PHE:HD1	2	0.13	0.01	0.13
(1,224)	1:A:18:LEU:HD21	1:A:84:PHE:HD2	2	0.13	0.01	0.13
(1,224)	1:A:18:LEU:HD22	1:A:84:PHE:HD1	2	0.13	0.01	0.13
(1,224)	1:A:18:LEU:HD22	1:A:84:PHE:HD2	2	0.13	0.01	0.13
(1,224)	1:A:18:LEU:HD23	1:A:84:PHE:HD1	2	0.13	0.01	0.13
(1,224)	1:A:18:LEU:HD23	1:A:84:PHE:HD2	2	0.13	0.01	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG11	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG12	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG13	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG21	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG22	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG23	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG11	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG12	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG13	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG21	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG22	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG23	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG11	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG12	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG13	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG21	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG22	2	0.13	0.0	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG23	2	0.13	0.0	0.13
(1,521)	1:A:35:ASP:HA	1:A:37:GLY:H	2	0.12	0.01	0.12
(1,656)	1:A:46:GLN:H	1:A:46:GLN:HB2	2	0.12	0.0	0.12
(1,656)	1:A:46:GLN:H	1:A:46:GLN:HB3	2	0.12	0.0	0.12
(1,1411)	1:A:89:TYR:HB2	1:A:92:LEU:HD21	2	0.12	0.0	0.12
(1,1411)	1:A:89:TYR:HB2	1:A:92:LEU:HD22	2	0.12	0.0	0.12
(1,1411)	1:A:89:TYR:HB2	1:A:92:LEU:HD23	2	0.12	0.0	0.12
(1,1738)	1:A:123:PHE:H	1:A:126:ILE:HG21	2	0.12	0.01	0.12
(1,1738)	1:A:123:PHE:H	1:A:126:ILE:HG22	2	0.12	0.01	0.12
(1,1738)	1:A:123:PHE:H	1:A:126:ILE:HG23	2	0.12	0.01	0.12
(2,41)	1:A:38:PHE:H	1:A:40:GLN:HB3	2	0.12	0.01	0.12
(1,2323)	1:A:162:ARG:HG2	1:A:163:SER:H	2	0.12	0.0	0.12
(1,2323)	1:A:162:ARG:HG3	1:A:163:SER:H	2	0.12	0.0	0.12
(2,140)	1:A:140:TRP:H	1:A:144:ARG:H	2	0.12	0.0	0.12
(1,508)	1:A:34:HIS:H	1:A:35:ASP:H	2	0.11	0.0	0.11

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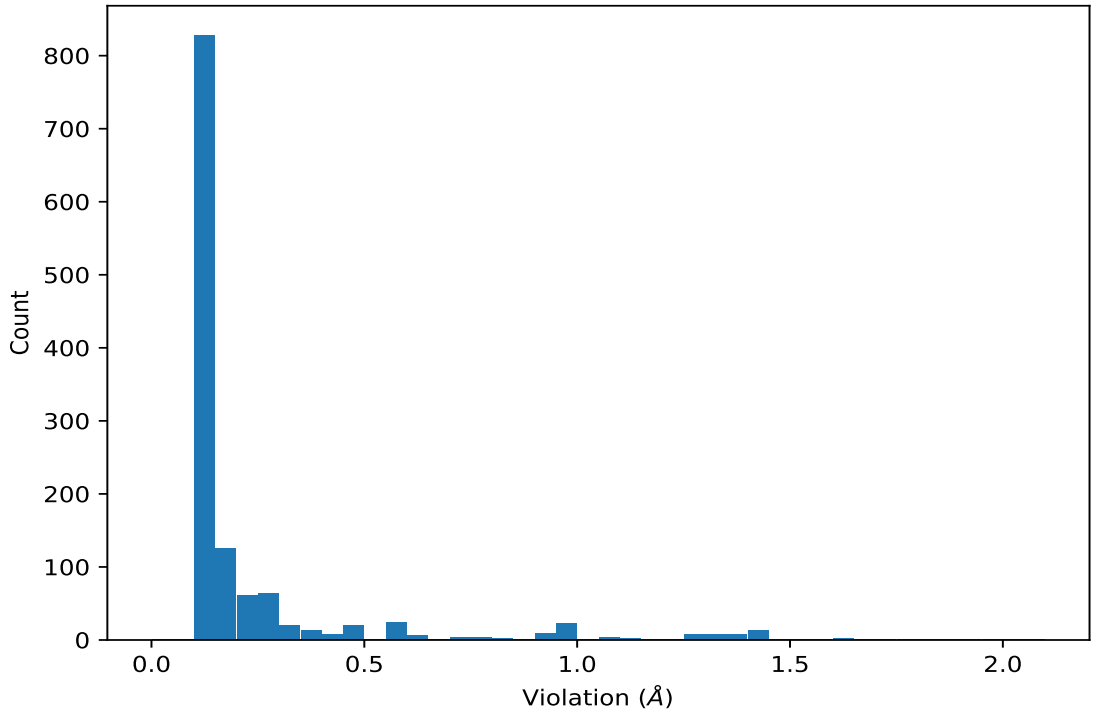
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,544)	1:A:36:PHE:HD1	1:A:126:ILE:HG21	2	0.11	0.0	0.11
(1,544)	1:A:36:PHE:HD1	1:A:126:ILE:HG22	2	0.11	0.0	0.11
(1,544)	1:A:36:PHE:HD1	1:A:126:ILE:HG23	2	0.11	0.0	0.11
(1,544)	1:A:36:PHE:HD2	1:A:126:ILE:HG21	2	0.11	0.0	0.11
(1,544)	1:A:36:PHE:HD2	1:A:126:ILE:HG22	2	0.11	0.0	0.11
(1,544)	1:A:36:PHE:HD2	1:A:126:ILE:HG23	2	0.11	0.0	0.11
(1,547)	1:A:36:PHE:HD1	1:A:143:VAL:HG21	2	0.11	0.0	0.11
(1,547)	1:A:36:PHE:HD1	1:A:143:VAL:HG22	2	0.11	0.0	0.11
(1,547)	1:A:36:PHE:HD1	1:A:143:VAL:HG23	2	0.11	0.0	0.11
(1,547)	1:A:36:PHE:HD2	1:A:143:VAL:HG21	2	0.11	0.0	0.11
(1,547)	1:A:36:PHE:HD2	1:A:143:VAL:HG22	2	0.11	0.0	0.11
(1,547)	1:A:36:PHE:HD2	1:A:143:VAL:HG23	2	0.11	0.0	0.11
(1,771)	1:A:54:PRO:HG2	1:A:55:VAL:HA	2	0.11	0.0	0.11

[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 (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	10	2.1
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	15	1.63
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	20	1.6
(1,1578)	1:A:106:THR:HB	2:A:500:A2G:H81	10	1.59
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	19	1.53
(1,1578)	1:A:106:THR:HB	2:A:500:A2G:H81	7	1.44
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	19	1.43
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	19	1.43
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	19	1.43
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	19	1.43
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	19	1.43
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	19	1.43
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	15	1.41
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	15	1.41
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	15	1.41
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	15	1.41
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	15	1.41
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	15	1.41
(1,714)	1:A:50:ALA:HB1	2:A:500:A2G:H81	15	1.4
(1,714)	1:A:50:ALA:HB2	2:A:500:A2G:H81	15	1.4
(1,714)	1:A:50:ALA:HB3	2:A:500:A2G:H81	15	1.4
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	20	1.4
(1,1578)	1:A:106:THR:HB	2:A:500:A2G:H81	15	1.36
(1,714)	1:A:50:ALA:HB1	2:A:500:A2G:H81	19	1.35
(1,714)	1:A:50:ALA:HB2	2:A:500:A2G:H81	19	1.35
(1,714)	1:A:50:ALA:HB3	2:A:500:A2G:H81	19	1.35
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	5	1.32
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	5	1.32
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	5	1.32
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	5	1.32
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	5	1.32
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	5	1.32
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	15	1.32
(1,714)	1:A:50:ALA:HB1	2:A:500:A2G:H81	14	1.28
(1,714)	1:A:50:ALA:HB2	2:A:500:A2G:H81	14	1.28
(1,714)	1:A:50:ALA:HB3	2:A:500:A2G:H81	14	1.28
(1,714)	1:A:50:ALA:HB1	2:A:500:A2G:H81	5	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:A:50:ALA:HB2	2:A:500:A2G:H81	5	1.26
(1,714)	1:A:50:ALA:HB3	2:A:500:A2G:H81	5	1.26
(1,1578)	1:A:106:THR:HB	2:A:500:A2G:H81	14	1.26
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	5	1.25
(1,1578)	1:A:106:THR:HB	2:A:500:A2G:H81	20	1.16
(1,1578)	1:A:106:THR:HB	2:A:500:A2G:H81	5	1.1
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	5	1.1
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	8	1.09
(1,714)	1:A:50:ALA:HB1	2:A:500:A2G:H81	7	1.08
(1,714)	1:A:50:ALA:HB2	2:A:500:A2G:H81	7	1.08
(1,714)	1:A:50:ALA:HB3	2:A:500:A2G:H81	7	1.08
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	11	0.98
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	11	0.98
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	11	0.98
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	11	0.98
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	11	0.98
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	11	0.98
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	14	0.98
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	14	0.98
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	14	0.98
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	14	0.98
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	14	0.98
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	14	0.98
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	20	0.98
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	20	0.98
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	20	0.98
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	20	0.98
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	20	0.98
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	20	0.98
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	19	0.98
(1,714)	1:A:50:ALA:HB1	2:A:500:A2G:H81	20	0.97
(1,714)	1:A:50:ALA:HB2	2:A:500:A2G:H81	20	0.97
(1,714)	1:A:50:ALA:HB3	2:A:500:A2G:H81	20	0.97
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	9	0.94
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	9	0.94
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	9	0.94
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	9	0.94
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	9	0.94
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	9	0.94
(1,1570)	1:A:106:THR:H	2:A:500:A2G:H81	15	0.92
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	10	0.92
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	13	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,102)	1:A:106:THR:HA	2:A:500:A2G:H81	15	0.88
(1,1578)	1:A:106:THR:HB	2:A:500:A2G:H81	19	0.81
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	11	0.8
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	14	0.77
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	7	0.77
(1,1578)	1:A:106:THR:HB	2:A:500:A2G:H81	13	0.76
(1,714)	1:A:50:ALA:HB1	2:A:500:A2G:H81	9	0.72
(1,714)	1:A:50:ALA:HB2	2:A:500:A2G:H81	9	0.72
(1,714)	1:A:50:ALA:HB3	2:A:500:A2G:H81	9	0.72
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	1	0.69
(1,1570)	1:A:106:THR:H	2:A:500:A2G:H81	5	0.64
(1,1578)	1:A:106:THR:HB	2:A:500:A2G:H81	8	0.63
(1,1570)	1:A:106:THR:H	2:A:500:A2G:H81	19	0.62
(1,714)	1:A:50:ALA:HB1	2:A:500:A2G:H81	11	0.61
(1,714)	1:A:50:ALA:HB2	2:A:500:A2G:H81	11	0.61
(1,714)	1:A:50:ALA:HB3	2:A:500:A2G:H81	11	0.61
(2,102)	1:A:106:THR:HA	2:A:500:A2G:H81	5	0.6
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	7	0.6
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	7	0.6
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	7	0.6
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	7	0.6
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	7	0.6
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	7	0.6
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	7	0.6
(1,1570)	1:A:106:THR:H	2:A:500:A2G:H81	20	0.58
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	16	0.58
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	16	0.58
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	16	0.58
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	16	0.58
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	16	0.58
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	16	0.58
(2,102)	1:A:106:THR:HA	2:A:500:A2G:H81	20	0.56
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	12	0.56
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	12	0.56
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	12	0.56
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	12	0.56
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	12	0.56
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	12	0.56
(2,102)	1:A:106:THR:HA	2:A:500:A2G:H81	10	0.55
(1,1570)	1:A:106:THR:H	2:A:500:A2G:H81	10	0.55
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	9	0.53
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:A:5:GLN:HA	1:A:5:GLN:HG2	7	0.48
(1,46)	1:A:5:GLN:HA	1:A:5:GLN:HG3	7	0.48
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	18	0.48
(2,102)	1:A:106:THR:HA	2:A:500:A2G:H81	7	0.47
(2,102)	1:A:106:THR:HA	2:A:500:A2G:H81	14	0.47
(2,102)	1:A:106:THR:HA	2:A:500:A2G:H81	19	0.47
(1,46)	1:A:5:GLN:HA	1:A:5:GLN:HG2	11	0.47
(1,46)	1:A:5:GLN:HA	1:A:5:GLN:HG3	11	0.47
(1,46)	1:A:5:GLN:HA	1:A:5:GLN:HG2	14	0.47
(1,46)	1:A:5:GLN:HA	1:A:5:GLN:HG3	14	0.47
(1,714)	1:A:50:ALA:HB1	2:A:500:A2G:H81	16	0.45
(1,714)	1:A:50:ALA:HB2	2:A:500:A2G:H81	16	0.45
(1,714)	1:A:50:ALA:HB3	2:A:500:A2G:H81	16	0.45
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	10	0.45
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	10	0.45
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	10	0.45
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	10	0.45
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	10	0.45
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	10	0.45
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	13	0.43
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	13	0.43
(1,1570)	1:A:106:THR:H	2:A:500:A2G:H81	14	0.42
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	14	0.42
(1,714)	1:A:50:ALA:HB1	2:A:500:A2G:H81	10	0.41
(1,714)	1:A:50:ALA:HB2	2:A:500:A2G:H81	10	0.41
(1,714)	1:A:50:ALA:HB3	2:A:500:A2G:H81	10	0.41
(1,1570)	1:A:106:THR:H	2:A:500:A2G:H81	7	0.41
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	15	0.38
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	15	0.38
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	12	0.37
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	3	0.36
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	3	0.36
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	9	0.36
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	9	0.36
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	4	0.36
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	4	0.36
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	4	0.36
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	4	0.36
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	4	0.36
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	4	0.36
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	2	0.35
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	2	0.35
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	20	0.34
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	20	0.34
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	18	0.34
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	6	0.34
(1,1372)	1:A:87:GLU:H	1:A:87:GLU:HG2	12	0.34
(1,1372)	1:A:87:GLU:H	1:A:87:GLU:HG3	12	0.34
(1,1372)	1:A:87:GLU:H	1:A:87:GLU:HG2	20	0.34
(1,1372)	1:A:87:GLU:H	1:A:87:GLU:HG3	20	0.34
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	18	0.33
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	7	0.32
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	7	0.32
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	11	0.32
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	11	0.32
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	14	0.32
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	14	0.32
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	12	0.31
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	12	0.31
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	8	0.3
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	8	0.3
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	10	0.3
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	10	0.3
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	18	0.3
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	18	0.3
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	19	0.3
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	19	0.3
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	4	0.29
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	4	0.29
(2,1)	1:A:1:CYS:H	1:A:98:CYS:H	12	0.28
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	12	0.28
(1,55)	1:A:5:GLN:HG2	1:A:10:GLY:H	11	0.28
(1,55)	1:A:5:GLN:HG3	1:A:10:GLY:H	11	0.28
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	1	0.28
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	1	0.28
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	6	0.28
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	6	0.28
(1,714)	1:A:50:ALA:HB1	2:A:500:A2G:H81	12	0.27
(1,714)	1:A:50:ALA:HB2	2:A:500:A2G:H81	12	0.27
(1,714)	1:A:50:ALA:HB3	2:A:500:A2G:H81	12	0.27
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	6	0.27
(1,55)	1:A:5:GLN:HG2	1:A:10:GLY:H	14	0.27
(1,55)	1:A:5:GLN:HG3	1:A:10:GLY:H	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG21	5	0.27
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG22	5	0.27
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG23	5	0.27
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG21	5	0.27
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG22	5	0.27
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG23	5	0.27
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG21	5	0.27
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG22	5	0.27
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG23	5	0.27
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD11	19	0.27
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD12	19	0.27
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD13	19	0.27
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD21	19	0.27
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD22	19	0.27
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD23	19	0.27
(1,1525)	1:A:101:GLN:HA	1:A:106:THR:HG21	10	0.27
(1,1525)	1:A:101:GLN:HA	1:A:106:THR:HG22	10	0.27
(1,1525)	1:A:101:GLN:HA	1:A:106:THR:HG23	10	0.27
(2,60)	1:A:61:GLN:HE21	1:A:65:ASN:HA	3	0.26
(2,1)	1:A:1:CYS:H	1:A:98:CYS:H	13	0.26
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	8	0.26
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	11	0.26
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	14	0.26
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	19	0.26
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	20	0.26
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	16	0.26
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	16	0.26
(2,1)	1:A:1:CYS:H	1:A:98:CYS:H	11	0.25
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	3	0.25
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	4	0.25
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	13	0.25
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	15	0.25
(1,501)	1:A:33:ARG:HB2	1:A:34:HIS:HE1	16	0.25
(1,501)	1:A:33:ARG:HB3	1:A:34:HIS:HE1	16	0.25
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	5	0.25
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	5	0.25
(1,343)	1:A:22:ARG:HD2	1:A:26:LEU:H	17	0.25
(1,343)	1:A:22:ARG:HD3	1:A:26:LEU:H	17	0.25
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	12	0.25
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	1	0.24
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	7	0.24
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:A:5:GLN:HG2	1:A:10:GLY:H	7	0.24
(1,55)	1:A:5:GLN:HG3	1:A:10:GLY:H	7	0.24
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	2	0.24
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	2	0.24
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	2	0.24
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	2	0.24
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	2	0.24
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	2	0.24
(1,1524)	1:A:101:GLN:HA	1:A:103:VAL:H	10	0.24
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	9	0.23
(2,60)	1:A:61:GLN:HE21	1:A:65:ASN:HA	5	0.22
(2,60)	1:A:61:GLN:HE21	1:A:65:ASN:HA	17	0.22
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	5	0.22
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	17	0.22
(1,1729)	1:A:122:TYR:H	1:A:122:TYR:HD1	16	0.22
(1,1729)	1:A:122:TYR:H	1:A:122:TYR:HD2	16	0.22
(1,1524)	1:A:101:GLN:HA	1:A:103:VAL:H	18	0.22
(2,60)	1:A:61:GLN:HE21	1:A:65:ASN:HA	1	0.21
(2,60)	1:A:61:GLN:HE21	1:A:65:ASN:HA	12	0.21
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	2	0.21
(1,505)	1:A:33:ARG:HG2	1:A:34:HIS:HA	17	0.21
(1,505)	1:A:33:ARG:HG3	1:A:34:HIS:HA	17	0.21
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD11	16	0.21
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD12	16	0.21
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD13	16	0.21
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD21	16	0.21
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD22	16	0.21
(1,181)	1:A:17:LEU:HG	1:A:80:LEU:HD23	16	0.21
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	6	0.21
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	6	0.21
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	6	0.21
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	6	0.21
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	6	0.21
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	6	0.21
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG21	10	0.21
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG22	10	0.21
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG23	10	0.21
(2,60)	1:A:61:GLN:HE21	1:A:65:ASN:HA	2	0.2
(2,60)	1:A:61:GLN:HE21	1:A:65:ASN:HA	9	0.2
(1,857)	1:A:60:ILE:HB	1:A:92:LEU:HA	18	0.2
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	11	0.2
(1,1372)	1:A:87:GLU:H	1:A:87:GLU:HG2	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1372)	1:A:87:GLU:H	1:A:87:GLU:HG3	7	0.2
(1,1036)	1:A:66:LEU:HD11	1:A:69:THR:H	6	0.2
(1,1036)	1:A:66:LEU:HD12	1:A:69:THR:H	6	0.2
(1,1036)	1:A:66:LEU:HD13	1:A:69:THR:H	6	0.2
(1,1036)	1:A:66:LEU:HD21	1:A:69:THR:H	6	0.2
(1,1036)	1:A:66:LEU:HD22	1:A:69:THR:H	6	0.2
(1,1036)	1:A:66:LEU:HD23	1:A:69:THR:H	6	0.2
(1,1036)	1:A:66:LEU:HD11	1:A:69:THR:H	8	0.2
(1,1036)	1:A:66:LEU:HD12	1:A:69:THR:H	8	0.2
(1,1036)	1:A:66:LEU:HD13	1:A:69:THR:H	8	0.2
(1,1036)	1:A:66:LEU:HD21	1:A:69:THR:H	8	0.2
(1,1036)	1:A:66:LEU:HD22	1:A:69:THR:H	8	0.2
(1,1036)	1:A:66:LEU:HD23	1:A:69:THR:H	8	0.2
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG21	3	0.2
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG22	3	0.2
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG23	3	0.2
(1,702)	1:A:50:ALA:HA	1:A:99:VAL:HB	10	0.19
(1,518)	1:A:35:ASP:H	1:A:36:PHE:HE1	16	0.19
(1,518)	1:A:35:ASP:H	1:A:36:PHE:HE2	16	0.19
(1,1566)	1:A:105:VAL:HG11	2:A:500:A2G:H81	17	0.19
(1,1566)	1:A:105:VAL:HG12	2:A:500:A2G:H81	17	0.19
(1,1566)	1:A:105:VAL:HG13	2:A:500:A2G:H81	17	0.19
(1,1566)	1:A:105:VAL:HG21	2:A:500:A2G:H81	17	0.19
(1,1566)	1:A:105:VAL:HG22	2:A:500:A2G:H81	17	0.19
(1,1566)	1:A:105:VAL:HG23	2:A:500:A2G:H81	17	0.19
(1,1564)	1:A:105:VAL:HG11	1:A:107:GLU:HG2	10	0.19
(1,1564)	1:A:105:VAL:HG11	1:A:107:GLU:HG3	10	0.19
(1,1564)	1:A:105:VAL:HG12	1:A:107:GLU:HG2	10	0.19
(1,1564)	1:A:105:VAL:HG12	1:A:107:GLU:HG3	10	0.19
(1,1564)	1:A:105:VAL:HG13	1:A:107:GLU:HG2	10	0.19
(1,1564)	1:A:105:VAL:HG13	1:A:107:GLU:HG3	10	0.19
(1,1564)	1:A:105:VAL:HG21	1:A:107:GLU:HG2	10	0.19
(1,1564)	1:A:105:VAL:HG21	1:A:107:GLU:HG3	10	0.19
(1,1564)	1:A:105:VAL:HG22	1:A:107:GLU:HG2	10	0.19
(1,1564)	1:A:105:VAL:HG22	1:A:107:GLU:HG3	10	0.19
(1,1564)	1:A:105:VAL:HG23	1:A:107:GLU:HG2	10	0.19
(1,1564)	1:A:105:VAL:HG23	1:A:107:GLU:HG3	10	0.19
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG21	19	0.18
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG22	19	0.18
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG23	19	0.18
(1,900)	1:A:61:GLN:HE22	1:A:64:PHE:HB3	1	0.18
(1,651)	1:A:45:ASN:HA	1:A:47:PHE:H	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1729)	1:A:122:TYR:H	1:A:122:TYR:HD1	20	0.18
(1,1729)	1:A:122:TYR:H	1:A:122:TYR:HD2	20	0.18
(1,1280)	1:A:81:LEU:HG	1:A:85:TYR:HD1	1	0.18
(1,1280)	1:A:81:LEU:HG	1:A:85:TYR:HD2	1	0.18
(1,1036)	1:A:66:LEU:HD11	1:A:69:THR:H	13	0.18
(1,1036)	1:A:66:LEU:HD12	1:A:69:THR:H	13	0.18
(1,1036)	1:A:66:LEU:HD13	1:A:69:THR:H	13	0.18
(1,1036)	1:A:66:LEU:HD21	1:A:69:THR:H	13	0.18
(1,1036)	1:A:66:LEU:HD22	1:A:69:THR:H	13	0.18
(1,1036)	1:A:66:LEU:HD23	1:A:69:THR:H	13	0.18
(1,1036)	1:A:66:LEU:HD11	1:A:69:THR:H	15	0.18
(1,1036)	1:A:66:LEU:HD12	1:A:69:THR:H	15	0.18
(1,1036)	1:A:66:LEU:HD13	1:A:69:THR:H	15	0.18
(1,1036)	1:A:66:LEU:HD21	1:A:69:THR:H	15	0.18
(1,1036)	1:A:66:LEU:HD22	1:A:69:THR:H	15	0.18
(1,1036)	1:A:66:LEU:HD23	1:A:69:THR:H	15	0.18
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG21	20	0.18
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG22	20	0.18
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG23	20	0.18
(2,60)	1:A:61:GLN:HE21	1:A:65:ASN:HA	14	0.17
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD21	8	0.17
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD22	8	0.17
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD23	8	0.17
(1,857)	1:A:60:ILE:HB	1:A:92:LEU:HA	7	0.17
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	18	0.17
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	18	0.17
(1,601)	1:A:40:GLN:HB3	1:A:40:GLN:HG2	5	0.17
(1,601)	1:A:40:GLN:HB3	1:A:40:GLN:HG3	5	0.17
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD1	10	0.17
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD2	10	0.17
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD1	10	0.17
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD2	10	0.17
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD1	10	0.17
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD2	10	0.17
(1,1578)	1:A:106:THR:HB	2:A:500:A2G:H81	17	0.17
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	6	0.17
(1,1394)	1:A:88:LEU:HB2	1:A:92:LEU:HD21	8	0.17
(1,1394)	1:A:88:LEU:HB2	1:A:92:LEU:HD22	8	0.17
(1,1394)	1:A:88:LEU:HB2	1:A:92:LEU:HD23	8	0.17
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG21	13	0.17
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG22	13	0.17
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG23	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	1	0.16
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	1	0.16
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	16	0.16
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	16	0.16
(1,857)	1:A:60:ILE:HB	1:A:92:LEU:HA	17	0.16
(1,651)	1:A:45:ASN:HA	1:A:47:PHE:H	4	0.16
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	5	0.16
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	5	0.16
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	7	0.16
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	7	0.16
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	15	0.16
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	15	0.16
(1,365)	1:A:23:LYS:HG2	1:A:76:TRP:HA	3	0.16
(1,365)	1:A:23:LYS:HG3	1:A:76:TRP:HA	3	0.16
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE1	1	0.16
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE2	1	0.16
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE3	1	0.16
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE1	1	0.16
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE2	1	0.16
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE3	1	0.16
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE1	1	0.16
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE2	1	0.16
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE3	1	0.16
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE1	8	0.16
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE2	8	0.16
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE3	8	0.16
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE1	8	0.16
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE2	8	0.16
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE3	8	0.16
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE1	8	0.16
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE2	8	0.16
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE3	8	0.16
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG21	1	0.16
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG22	1	0.16
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG23	1	0.16
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG21	1	0.16
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG22	1	0.16
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG23	1	0.16
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG21	1	0.16
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG22	1	0.16
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG23	1	0.16
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD1	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD2	20	0.16
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD1	20	0.16
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD2	20	0.16
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD1	20	0.16
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD2	20	0.16
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	2	0.16
(1,1036)	1:A:66:LEU:HD11	1:A:69:THR:H	18	0.16
(1,1036)	1:A:66:LEU:HD12	1:A:69:THR:H	18	0.16
(1,1036)	1:A:66:LEU:HD13	1:A:69:THR:H	18	0.16
(1,1036)	1:A:66:LEU:HD21	1:A:69:THR:H	18	0.16
(1,1036)	1:A:66:LEU:HD22	1:A:69:THR:H	18	0.16
(1,1036)	1:A:66:LEU:HD23	1:A:69:THR:H	18	0.16
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG21	8	0.16
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG22	8	0.16
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG23	8	0.16
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG21	20	0.15
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG22	20	0.15
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG23	20	0.15
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	4	0.15
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	4	0.15
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD21	12	0.15
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD22	12	0.15
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD23	12	0.15
(1,900)	1:A:61:GLN:HE22	1:A:64:PHE:HB3	2	0.15
(1,900)	1:A:61:GLN:HE22	1:A:64:PHE:HB3	9	0.15
(1,878)	1:A:60:ILE:HG21	1:A:92:LEU:HG	7	0.15
(1,878)	1:A:60:ILE:HG22	1:A:92:LEU:HG	7	0.15
(1,878)	1:A:60:ILE:HG23	1:A:92:LEU:HG	7	0.15
(1,878)	1:A:60:ILE:HG21	1:A:92:LEU:HG	12	0.15
(1,878)	1:A:60:ILE:HG22	1:A:92:LEU:HG	12	0.15
(1,878)	1:A:60:ILE:HG23	1:A:92:LEU:HG	12	0.15
(1,878)	1:A:60:ILE:HG21	1:A:92:LEU:HG	17	0.15
(1,878)	1:A:60:ILE:HG22	1:A:92:LEU:HG	17	0.15
(1,878)	1:A:60:ILE:HG23	1:A:92:LEU:HG	17	0.15
(1,688)	1:A:49:LYS:H	1:A:49:LYS:HD2	9	0.15
(1,688)	1:A:49:LYS:H	1:A:49:LYS:HD3	9	0.15
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	10	0.15
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	10	0.15
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	13	0.15
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	13	0.15
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	16	0.15
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	17	0.15
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	17	0.15
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	20	0.15
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	20	0.15
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD11	14	0.15
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD12	14	0.15
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD13	14	0.15
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD21	14	0.15
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD22	14	0.15
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD23	14	0.15
(1,519)	1:A:35:ASP:H	1:A:37:GLY:H	16	0.15
(1,499)	1:A:33:ARG:HB2	1:A:34:HIS:H	19	0.15
(1,499)	1:A:33:ARG:HB3	1:A:34:HIS:H	19	0.15
(1,365)	1:A:23:LYS:HG2	1:A:76:TRP:HA	5	0.15
(1,365)	1:A:23:LYS:HG3	1:A:76:TRP:HA	5	0.15
(1,365)	1:A:23:LYS:HG2	1:A:76:TRP:HA	6	0.15
(1,365)	1:A:23:LYS:HG3	1:A:76:TRP:HA	6	0.15
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD1	5	0.15
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD2	5	0.15
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD1	5	0.15
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD2	5	0.15
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD1	5	0.15
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD2	5	0.15
(1,1550)	1:A:104:GLY:HA3	1:A:105:VAL:H	18	0.15
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD11	7	0.15
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD12	7	0.15
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD13	7	0.15
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD21	7	0.15
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD22	7	0.15
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD23	7	0.15
(1,1036)	1:A:66:LEU:HD11	1:A:69:THR:H	20	0.15
(1,1036)	1:A:66:LEU:HD12	1:A:69:THR:H	20	0.15
(1,1036)	1:A:66:LEU:HD13	1:A:69:THR:H	20	0.15
(1,1036)	1:A:66:LEU:HD21	1:A:69:THR:H	20	0.15
(1,1036)	1:A:66:LEU:HD22	1:A:69:THR:H	20	0.15
(1,1036)	1:A:66:LEU:HD23	1:A:69:THR:H	20	0.15
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG21	15	0.15
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG22	15	0.15
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG23	15	0.15
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG21	18	0.15
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG22	18	0.15
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG23	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD11	6	0.15
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD12	6	0.15
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD13	6	0.15
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD21	6	0.15
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD22	6	0.15
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD23	6	0.15
(2,135)	1:A:135:TYR:H	1:A:139:ALA:H	17	0.14
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	19	0.14
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	19	0.14
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD21	17	0.14
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD22	17	0.14
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD23	17	0.14
(1,900)	1:A:61:GLN:HE22	1:A:64:PHE:HB3	14	0.14
(1,788)	1:A:55:VAL:HG21	1:A:115:SER:HA	9	0.14
(1,788)	1:A:55:VAL:HG22	1:A:115:SER:HA	9	0.14
(1,788)	1:A:55:VAL:HG23	1:A:115:SER:HA	9	0.14
(1,788)	1:A:55:VAL:HG21	1:A:115:SER:HA	11	0.14
(1,788)	1:A:55:VAL:HG22	1:A:115:SER:HA	11	0.14
(1,788)	1:A:55:VAL:HG23	1:A:115:SER:HA	11	0.14
(1,706)	1:A:50:ALA:HB1	1:A:105:VAL:HB	18	0.14
(1,706)	1:A:50:ALA:HB2	1:A:105:VAL:HB	18	0.14
(1,706)	1:A:50:ALA:HB3	1:A:105:VAL:HB	18	0.14
(1,682)	1:A:48:GLN:H	1:A:48:GLN:HG2	6	0.14
(1,682)	1:A:48:GLN:H	1:A:48:GLN:HG3	6	0.14
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	1	0.14
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	1	0.14
(1,570)	1:A:38:PHE:H	1:A:38:PHE:HE1	4	0.14
(1,570)	1:A:38:PHE:H	1:A:38:PHE:HE2	4	0.14
(1,558)	1:A:36:PHE:HE1	1:A:130:LEU:H	16	0.14
(1,558)	1:A:36:PHE:HE2	1:A:130:LEU:H	16	0.14
(1,224)	1:A:18:LEU:HD21	1:A:84:PHE:HD1	1	0.14
(1,224)	1:A:18:LEU:HD21	1:A:84:PHE:HD2	1	0.14
(1,224)	1:A:18:LEU:HD22	1:A:84:PHE:HD1	1	0.14
(1,224)	1:A:18:LEU:HD22	1:A:84:PHE:HD2	1	0.14
(1,224)	1:A:18:LEU:HD23	1:A:84:PHE:HD1	1	0.14
(1,224)	1:A:18:LEU:HD23	1:A:84:PHE:HD2	1	0.14
(1,2048)	1:A:134:LYS:HA	1:A:134:LYS:HD2	16	0.14
(1,2048)	1:A:134:LYS:HA	1:A:134:LYS:HD3	16	0.14
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	2	0.14
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	2	0.14
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	2	0.14
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	2	0.14
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	2	0.14
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	2	0.14
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	2	0.14
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	2	0.14
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	14	0.14
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	14	0.14
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	14	0.14
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	14	0.14
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	14	0.14
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	14	0.14
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	14	0.14
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	14	0.14
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	14	0.14
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	20	0.14
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	20	0.14
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	20	0.14
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	20	0.14
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	20	0.14
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	20	0.14
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	20	0.14
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	20	0.14
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	20	0.14
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD1	16	0.14
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD2	16	0.14
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD1	16	0.14
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD2	16	0.14
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD1	16	0.14
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD2	16	0.14
(1,1560)	1:A:105:VAL:HA	2:A:500:A2G:H81	13	0.14
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD11	6	0.14
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD12	6	0.14
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD13	6	0.14
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD21	6	0.14
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD22	6	0.14
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD23	6	0.14
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE1	9	0.14
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE2	9	0.14
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE1	14	0.14
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE2	14	0.14
(1,1036)	1:A:66:LEU:HD11	1:A:69:THR:H	10	0.14
(1,1036)	1:A:66:LEU:HD12	1:A:69:THR:H	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:A:66:LEU:HD13	1:A:69:THR:H	10	0.14
(1,1036)	1:A:66:LEU:HD21	1:A:69:THR:H	10	0.14
(1,1036)	1:A:66:LEU:HD22	1:A:69:THR:H	10	0.14
(1,1036)	1:A:66:LEU:HD23	1:A:69:THR:H	10	0.14
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG21	6	0.14
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG22	6	0.14
(1,1019)	1:A:66:LEU:HG	1:A:126:ILE:HG23	6	0.14
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG21	1	0.13
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG22	1	0.13
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG23	1	0.13
(2,41)	1:A:38:PHE:H	1:A:40:GLN:HB3	19	0.13
(2,145)	1:A:151:PHE:H	1:A:155:THR:H	16	0.13
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	13	0.13
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	13	0.13
(1,900)	1:A:61:GLN:HE22	1:A:64:PHE:HB3	5	0.13
(1,878)	1:A:60:ILE:HG21	1:A:92:LEU:HG	18	0.13
(1,878)	1:A:60:ILE:HG22	1:A:92:LEU:HG	18	0.13
(1,878)	1:A:60:ILE:HG23	1:A:92:LEU:HG	18	0.13
(1,857)	1:A:60:ILE:HB	1:A:92:LEU:HA	12	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG11	10	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG12	10	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG13	10	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG21	10	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG22	10	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG23	10	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG11	10	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG12	10	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG13	10	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG21	10	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG22	10	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG23	10	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG11	10	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG12	10	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG13	10	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG21	10	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG22	10	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG23	10	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG11	20	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG12	20	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG13	20	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG21	20	0.13
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG22	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,790)	1:A:55:VAL:HG21	1:A:119:VAL:HG23	20	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG11	20	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG12	20	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG13	20	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG21	20	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG22	20	0.13
(1,790)	1:A:55:VAL:HG22	1:A:119:VAL:HG23	20	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG11	20	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG12	20	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG13	20	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG21	20	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG22	20	0.13
(1,790)	1:A:55:VAL:HG23	1:A:119:VAL:HG23	20	0.13
(1,788)	1:A:55:VAL:HG21	1:A:115:SER:HA	1	0.13
(1,788)	1:A:55:VAL:HG22	1:A:115:SER:HA	1	0.13
(1,788)	1:A:55:VAL:HG23	1:A:115:SER:HA	1	0.13
(1,743)	1:A:53:ILE:HG13	1:A:100:ILE:HA	18	0.13
(1,706)	1:A:50:ALA:HB1	1:A:105:VAL:HB	20	0.13
(1,706)	1:A:50:ALA:HB2	1:A:105:VAL:HB	20	0.13
(1,706)	1:A:50:ALA:HB3	1:A:105:VAL:HB	20	0.13
(1,681)	1:A:48:GLN:H	1:A:48:GLN:HB2	7	0.13
(1,681)	1:A:48:GLN:H	1:A:48:GLN:HB3	7	0.13
(1,643)	1:A:45:ASN:H	1:A:45:ASN:HB2	15	0.13
(1,643)	1:A:45:ASN:H	1:A:45:ASN:HB3	15	0.13
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	3	0.13
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	3	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD11	4	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD12	4	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD13	4	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD21	4	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD22	4	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD23	4	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD11	8	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD12	8	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD13	8	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD21	8	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD22	8	0.13
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD23	8	0.13
(1,521)	1:A:35:ASP:HA	1:A:37:GLY:H	4	0.13
(1,501)	1:A:33:ARG:HB2	1:A:34:HIS:HE1	19	0.13
(1,501)	1:A:33:ARG:HB3	1:A:34:HIS:HE1	19	0.13
(1,478)	1:A:31:LYS:H	1:A:33:ARG:HD2	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:A:31:LYS:H	1:A:33:ARG:HD3	17	0.13
(1,2312)	1:A:161:LEU:HA	1:A:162:ARG:H	1	0.13
(1,2312)	1:A:161:LEU:HA	1:A:162:ARG:H	10	0.13
(1,2312)	1:A:161:LEU:HA	1:A:162:ARG:H	14	0.13
(1,2312)	1:A:161:LEU:HA	1:A:162:ARG:H	16	0.13
(1,2048)	1:A:134:LYS:HA	1:A:134:LYS:HD2	2	0.13
(1,2048)	1:A:134:LYS:HA	1:A:134:LYS:HD3	2	0.13
(1,2043)	1:A:134:LYS:H	1:A:134:LYS:HG2	2	0.13
(1,2043)	1:A:134:LYS:H	1:A:134:LYS:HG3	2	0.13
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	7	0.13
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	7	0.13
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	7	0.13
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	7	0.13
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	7	0.13
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	7	0.13
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	7	0.13
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	7	0.13
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	7	0.13
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	12	0.13
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	12	0.13
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	12	0.13
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	12	0.13
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	12	0.13
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	12	0.13
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	12	0.13
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	12	0.13
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	12	0.13
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG21	9	0.13
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG22	9	0.13
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG23	9	0.13
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG21	9	0.13
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG22	9	0.13
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG23	9	0.13
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG21	9	0.13
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG22	9	0.13
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG23	9	0.13
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG21	11	0.13
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG22	11	0.13
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG23	11	0.13
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG21	11	0.13
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG22	11	0.13
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG23	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG21	11	0.13
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG22	11	0.13
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG23	11	0.13
(1,1738)	1:A:123:PHE:H	1:A:126:ILE:HG21	8	0.13
(1,1738)	1:A:123:PHE:H	1:A:126:ILE:HG22	8	0.13
(1,1738)	1:A:123:PHE:H	1:A:126:ILE:HG23	8	0.13
(1,1729)	1:A:122:TYR:H	1:A:122:TYR:HD1	10	0.13
(1,1729)	1:A:122:TYR:H	1:A:122:TYR:HD2	10	0.13
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD1	7	0.13
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD2	7	0.13
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD1	7	0.13
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD2	7	0.13
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD1	7	0.13
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD2	7	0.13
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG2	15	0.13
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG3	15	0.13
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG2	16	0.13
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG3	16	0.13
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG2	20	0.13
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG3	20	0.13
(1,1523)	1:A:101:GLN:HA	1:A:102:GLY:H	10	0.13
(1,1394)	1:A:88:LEU:HB2	1:A:92:LEU:HD21	7	0.13
(1,1394)	1:A:88:LEU:HB2	1:A:92:LEU:HD22	7	0.13
(1,1394)	1:A:88:LEU:HB2	1:A:92:LEU:HD23	7	0.13
(1,1278)	1:A:81:LEU:HB3	1:A:85:TYR:HD1	6	0.13
(1,1278)	1:A:81:LEU:HB3	1:A:85:TYR:HD2	6	0.13
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD11	20	0.13
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD12	20	0.13
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD13	20	0.13
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD21	20	0.13
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD22	20	0.13
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD23	20	0.13
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE1	2	0.13
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE2	2	0.13
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE1	12	0.13
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE2	12	0.13
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE1	17	0.13
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE2	17	0.13
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB2	6	0.13
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB3	6	0.13
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD11	18	0.13
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD12	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD13	18	0.13
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD21	18	0.13
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD22	18	0.13
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD23	18	0.13
(1,1001)	1:A:65:ASN:H	1:A:92:LEU:HD21	8	0.13
(1,1001)	1:A:65:ASN:H	1:A:92:LEU:HD22	8	0.13
(1,1001)	1:A:65:ASN:H	1:A:92:LEU:HD23	8	0.13
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG21	13	0.12
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG22	13	0.12
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG23	13	0.12
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG21	16	0.12
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG22	16	0.12
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG23	16	0.12
(2,140)	1:A:140:TRP:H	1:A:144:ARG:H	20	0.12
(2,135)	1:A:135:TYR:H	1:A:139:ALA:H	9	0.12
(2,135)	1:A:135:TYR:H	1:A:139:ALA:H	12	0.12
(2,124)	1:A:129:TYR:HD1	1:A:142:VAL:H	16	0.12
(2,124)	1:A:129:TYR:HD2	1:A:142:VAL:H	16	0.12
(2,115)	1:A:127:THR:H	1:A:129:TYR:HD1	6	0.12
(2,115)	1:A:127:THR:H	1:A:129:TYR:HD2	6	0.12
(2,115)	1:A:127:THR:H	1:A:129:TYR:HD1	8	0.12
(2,115)	1:A:127:THR:H	1:A:129:TYR:HD2	8	0.12
(2,115)	1:A:127:THR:H	1:A:129:TYR:HD1	16	0.12
(2,115)	1:A:127:THR:H	1:A:129:TYR:HD2	16	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	2	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	2	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	6	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	6	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	7	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	7	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	8	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	8	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	11	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	11	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	17	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	17	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	18	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	18	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	20	0.12
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	20	0.12
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD21	18	0.12
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD22	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,913)	1:A:62:GLN:H	1:A:92:LEU:HD23	18	0.12
(1,900)	1:A:61:GLN:HE22	1:A:64:PHE:HB3	3	0.12
(1,857)	1:A:60:ILE:HB	1:A:92:LEU:HA	14	0.12
(1,817)	1:A:57:HIS:HD2	1:A:92:LEU:HA	8	0.12
(1,788)	1:A:55:VAL:HG21	1:A:115:SER:HA	4	0.12
(1,788)	1:A:55:VAL:HG22	1:A:115:SER:HA	4	0.12
(1,788)	1:A:55:VAL:HG23	1:A:115:SER:HA	4	0.12
(1,743)	1:A:53:ILE:HG13	1:A:100:ILE:HA	10	0.12
(1,726)	1:A:52:THR:HG21	1:A:57:HIS:H	16	0.12
(1,726)	1:A:52:THR:HG22	1:A:57:HIS:H	16	0.12
(1,726)	1:A:52:THR:HG23	1:A:57:HIS:H	16	0.12
(1,681)	1:A:48:GLN:H	1:A:48:GLN:HB2	2	0.12
(1,681)	1:A:48:GLN:H	1:A:48:GLN:HB3	2	0.12
(1,656)	1:A:46:GLN:H	1:A:46:GLN:HB2	4	0.12
(1,656)	1:A:46:GLN:H	1:A:46:GLN:HB3	4	0.12
(1,656)	1:A:46:GLN:H	1:A:46:GLN:HB2	19	0.12
(1,656)	1:A:46:GLN:H	1:A:46:GLN:HB3	19	0.12
(1,653)	1:A:45:ASN:HA	1:A:48:GLN:HG2	14	0.12
(1,653)	1:A:45:ASN:HA	1:A:48:GLN:HG3	14	0.12
(1,643)	1:A:45:ASN:H	1:A:45:ASN:HB2	10	0.12
(1,643)	1:A:45:ASN:H	1:A:45:ASN:HB3	10	0.12
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	12	0.12
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	12	0.12
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	14	0.12
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	14	0.12
(1,511)	1:A:34:HIS:HA	1:A:35:ASP:HA	16	0.12
(1,438)	1:A:28:SER:H	1:A:29:CYS:HB2	5	0.12
(1,366)	1:A:23:LYS:HG2	1:A:76:TRP:HB3	19	0.12
(1,366)	1:A:23:LYS:HG3	1:A:76:TRP:HB3	19	0.12
(1,365)	1:A:23:LYS:HG2	1:A:76:TRP:HA	8	0.12
(1,365)	1:A:23:LYS:HG3	1:A:76:TRP:HA	8	0.12
(1,365)	1:A:23:LYS:HG2	1:A:76:TRP:HA	20	0.12
(1,365)	1:A:23:LYS:HG3	1:A:76:TRP:HA	20	0.12
(1,2323)	1:A:162:ARG:HG2	1:A:163:SER:H	17	0.12
(1,2323)	1:A:162:ARG:HG3	1:A:163:SER:H	17	0.12
(1,2312)	1:A:161:LEU:HA	1:A:162:ARG:H	3	0.12
(1,2312)	1:A:161:LEU:HA	1:A:162:ARG:H	8	0.12
(1,2312)	1:A:161:LEU:HA	1:A:162:ARG:H	15	0.12
(1,224)	1:A:18:LEU:HD21	1:A:84:PHE:HD1	7	0.12
(1,224)	1:A:18:LEU:HD21	1:A:84:PHE:HD2	7	0.12
(1,224)	1:A:18:LEU:HD22	1:A:84:PHE:HD1	7	0.12
(1,224)	1:A:18:LEU:HD22	1:A:84:PHE:HD2	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:A:18:LEU:HD23	1:A:84:PHE:HD1	7	0.12
(1,224)	1:A:18:LEU:HD23	1:A:84:PHE:HD2	7	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE1	10	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE2	10	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE3	10	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE1	10	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE2	10	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE3	10	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE1	10	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE2	10	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE3	10	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE1	12	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE2	12	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE3	12	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE1	12	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE2	12	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE3	12	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE1	12	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE2	12	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE3	12	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE1	15	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE2	15	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE3	15	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE1	15	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE2	15	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE3	15	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE1	15	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE2	15	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE3	15	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE1	16	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE2	16	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE3	16	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE1	16	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE2	16	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE3	16	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE1	16	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE2	16	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE3	16	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE1	20	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE2	20	0.12
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE3	20	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE1	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE2	20	0.12
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE3	20	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE1	20	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE2	20	0.12
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE3	20	0.12
(1,2173)	1:A:145:ALA:H	1:A:148:MET:HE1	5	0.12
(1,2173)	1:A:145:ALA:H	1:A:148:MET:HE2	5	0.12
(1,2173)	1:A:145:ALA:H	1:A:148:MET:HE3	5	0.12
(1,2048)	1:A:134:LYS:HA	1:A:134:LYS:HD2	17	0.12
(1,2048)	1:A:134:LYS:HA	1:A:134:LYS:HD3	17	0.12
(1,2048)	1:A:134:LYS:HA	1:A:134:LYS:HD2	20	0.12
(1,2048)	1:A:134:LYS:HA	1:A:134:LYS:HD3	20	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	1	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	1	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	1	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	1	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	1	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	1	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	1	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	1	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	1	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	3	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	3	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	3	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	3	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	3	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	3	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	3	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	3	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	3	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	4	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	4	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	4	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	4	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	4	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	4	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	4	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	4	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	4	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	8	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	8	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	8	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	8	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	8	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	8	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	8	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	8	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	13	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	13	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	13	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	13	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	13	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	13	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	13	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	13	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	13	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	19	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	19	0.12
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	19	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	19	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	19	0.12
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	19	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	19	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	19	0.12
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	19	0.12
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG21	12	0.12
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG22	12	0.12
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG23	12	0.12
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG21	12	0.12
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG22	12	0.12
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG23	12	0.12
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG21	12	0.12
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG22	12	0.12
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG23	12	0.12
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD1	4	0.12
(1,1698)	1:A:118:ALA:HB1	1:A:122:TYR:HD2	4	0.12
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD1	4	0.12
(1,1698)	1:A:118:ALA:HB2	1:A:122:TYR:HD2	4	0.12
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD1	4	0.12
(1,1698)	1:A:118:ALA:HB3	1:A:122:TYR:HD2	4	0.12
(1,1681)	1:A:117:LEU:HA	1:A:117:LEU:HG	17	0.12
(1,1645)	1:A:113:GLU:HB2	1:A:114:ASP:H	2	0.12
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG2	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG3	12	0.12
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG2	19	0.12
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG3	19	0.12
(1,1411)	1:A:89:TYR:HB2	1:A:92:LEU:HD21	1	0.12
(1,1411)	1:A:89:TYR:HB2	1:A:92:LEU:HD22	1	0.12
(1,1411)	1:A:89:TYR:HB2	1:A:92:LEU:HD23	1	0.12
(1,1411)	1:A:89:TYR:HB2	1:A:92:LEU:HD21	4	0.12
(1,1411)	1:A:89:TYR:HB2	1:A:92:LEU:HD22	4	0.12
(1,1411)	1:A:89:TYR:HB2	1:A:92:LEU:HD23	4	0.12
(1,1278)	1:A:81:LEU:HB3	1:A:85:TYR:HD1	2	0.12
(1,1278)	1:A:81:LEU:HB3	1:A:85:TYR:HD2	2	0.12
(1,1278)	1:A:81:LEU:HB3	1:A:85:TYR:HD1	20	0.12
(1,1278)	1:A:81:LEU:HB3	1:A:85:TYR:HD2	20	0.12
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD11	9	0.12
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD12	9	0.12
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD13	9	0.12
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD21	9	0.12
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD22	9	0.12
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD23	9	0.12
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB2	2	0.12
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB3	2	0.12
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB2	10	0.12
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB3	10	0.12
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB2	15	0.12
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB3	15	0.12
(1,1036)	1:A:66:LEU:HD11	1:A:69:THR:H	3	0.12
(1,1036)	1:A:66:LEU:HD12	1:A:69:THR:H	3	0.12
(1,1036)	1:A:66:LEU:HD13	1:A:69:THR:H	3	0.12
(1,1036)	1:A:66:LEU:HD21	1:A:69:THR:H	3	0.12
(1,1036)	1:A:66:LEU:HD22	1:A:69:THR:H	3	0.12
(1,1036)	1:A:66:LEU:HD23	1:A:69:THR:H	3	0.12
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD11	10	0.12
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD12	10	0.12
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD13	10	0.12
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD21	10	0.12
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD22	10	0.12
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD23	10	0.12
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG21	2	0.11
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG22	2	0.11
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG23	2	0.11
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG21	10	0.11
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG22	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG23	10	0.11
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG21	12	0.11
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG22	12	0.11
(2,5)	1:A:5:GLN:HE22	1:A:60:ILE:HG23	12	0.11
(2,44)	1:A:43:PHE:HD1	1:A:45:ASN:H	16	0.11
(2,44)	1:A:43:PHE:HD2	1:A:45:ASN:H	16	0.11
(2,41)	1:A:38:PHE:H	1:A:40:GLN:HB3	9	0.11
(2,140)	1:A:140:TRP:H	1:A:144:ARG:H	5	0.11
(2,135)	1:A:135:TYR:H	1:A:139:ALA:H	4	0.11
(2,135)	1:A:135:TYR:H	1:A:139:ALA:H	15	0.11
(2,128)	1:A:130:LEU:HD21	1:A:132:GLU:H	9	0.11
(2,128)	1:A:130:LEU:HD22	1:A:132:GLU:H	9	0.11
(2,128)	1:A:130:LEU:HD23	1:A:132:GLU:H	9	0.11
(2,115)	1:A:127:THR:H	1:A:129:TYR:HD1	18	0.11
(2,115)	1:A:127:THR:H	1:A:129:TYR:HD2	18	0.11
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	10	0.11
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	10	0.11
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	14	0.11
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	14	0.11
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD1	15	0.11
(1,974)	1:A:64:PHE:HA	1:A:85:TYR:HD2	15	0.11
(1,788)	1:A:55:VAL:HG21	1:A:115:SER:HA	5	0.11
(1,788)	1:A:55:VAL:HG22	1:A:115:SER:HA	5	0.11
(1,788)	1:A:55:VAL:HG23	1:A:115:SER:HA	5	0.11
(1,788)	1:A:55:VAL:HG21	1:A:115:SER:HA	19	0.11
(1,788)	1:A:55:VAL:HG22	1:A:115:SER:HA	19	0.11
(1,788)	1:A:55:VAL:HG23	1:A:115:SER:HA	19	0.11
(1,771)	1:A:54:PRO:HG2	1:A:55:VAL:HA	2	0.11
(1,771)	1:A:54:PRO:HG2	1:A:55:VAL:HA	18	0.11
(1,743)	1:A:53:ILE:HG13	1:A:100:ILE:HA	20	0.11
(1,681)	1:A:48:GLN:H	1:A:48:GLN:HB2	10	0.11
(1,681)	1:A:48:GLN:H	1:A:48:GLN:HB3	10	0.11
(1,643)	1:A:45:ASN:H	1:A:45:ASN:HB2	18	0.11
(1,643)	1:A:45:ASN:H	1:A:45:ASN:HB3	18	0.11
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	2	0.11
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	2	0.11
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE1	6	0.11
(1,616)	1:A:43:PHE:H	1:A:43:PHE:HE2	6	0.11
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD11	5	0.11
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD12	5	0.11
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD13	5	0.11
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD21	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD22	5	0.11
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD23	5	0.11
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD11	16	0.11
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD12	16	0.11
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD13	16	0.11
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD21	16	0.11
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD22	16	0.11
(1,595)	1:A:40:GLN:HA	1:A:153:LEU:HD23	16	0.11
(1,568)	1:A:37:GLY:H	1:A:38:PHE:H	16	0.11
(1,565)	1:A:36:PHE:HE1	1:A:146:GLU:H	18	0.11
(1,565)	1:A:36:PHE:HE2	1:A:146:GLU:H	18	0.11
(1,547)	1:A:36:PHE:HD1	1:A:143:VAL:HG21	12	0.11
(1,547)	1:A:36:PHE:HD1	1:A:143:VAL:HG22	12	0.11
(1,547)	1:A:36:PHE:HD1	1:A:143:VAL:HG23	12	0.11
(1,547)	1:A:36:PHE:HD2	1:A:143:VAL:HG21	12	0.11
(1,547)	1:A:36:PHE:HD2	1:A:143:VAL:HG22	12	0.11
(1,547)	1:A:36:PHE:HD2	1:A:143:VAL:HG23	12	0.11
(1,547)	1:A:36:PHE:HD1	1:A:143:VAL:HG21	14	0.11
(1,547)	1:A:36:PHE:HD1	1:A:143:VAL:HG22	14	0.11
(1,547)	1:A:36:PHE:HD1	1:A:143:VAL:HG23	14	0.11
(1,547)	1:A:36:PHE:HD2	1:A:143:VAL:HG21	14	0.11
(1,547)	1:A:36:PHE:HD2	1:A:143:VAL:HG22	14	0.11
(1,547)	1:A:36:PHE:HD2	1:A:143:VAL:HG23	14	0.11
(1,544)	1:A:36:PHE:HD1	1:A:126:ILE:HG21	3	0.11
(1,544)	1:A:36:PHE:HD1	1:A:126:ILE:HG22	3	0.11
(1,544)	1:A:36:PHE:HD1	1:A:126:ILE:HG23	3	0.11
(1,544)	1:A:36:PHE:HD2	1:A:126:ILE:HG21	3	0.11
(1,544)	1:A:36:PHE:HD2	1:A:126:ILE:HG22	3	0.11
(1,544)	1:A:36:PHE:HD2	1:A:126:ILE:HG23	3	0.11
(1,544)	1:A:36:PHE:HD1	1:A:126:ILE:HG21	13	0.11
(1,544)	1:A:36:PHE:HD1	1:A:126:ILE:HG22	13	0.11
(1,544)	1:A:36:PHE:HD1	1:A:126:ILE:HG23	13	0.11
(1,544)	1:A:36:PHE:HD2	1:A:126:ILE:HG21	13	0.11
(1,544)	1:A:36:PHE:HD2	1:A:126:ILE:HG22	13	0.11
(1,544)	1:A:36:PHE:HD2	1:A:126:ILE:HG23	13	0.11
(1,521)	1:A:35:ASP:HA	1:A:37:GLY:H	5	0.11
(1,508)	1:A:34:HIS:H	1:A:35:ASP:H	11	0.11
(1,508)	1:A:34:HIS:H	1:A:35:ASP:H	20	0.11
(1,485)	1:A:32:ASP:H	1:A:142:VAL:HG21	16	0.11
(1,485)	1:A:32:ASP:H	1:A:142:VAL:HG22	16	0.11
(1,485)	1:A:32:ASP:H	1:A:142:VAL:HG23	16	0.11
(1,366)	1:A:23:LYS:HG2	1:A:76:TRP:HB3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:A:23:LYS:HG3	1:A:76:TRP:HB3	4	0.11
(1,366)	1:A:23:LYS:HG2	1:A:76:TRP:HB3	17	0.11
(1,366)	1:A:23:LYS:HG3	1:A:76:TRP:HB3	17	0.11
(1,365)	1:A:23:LYS:HG2	1:A:76:TRP:HA	12	0.11
(1,365)	1:A:23:LYS:HG3	1:A:76:TRP:HA	12	0.11
(1,365)	1:A:23:LYS:HG2	1:A:76:TRP:HA	14	0.11
(1,365)	1:A:23:LYS:HG3	1:A:76:TRP:HA	14	0.11
(1,266)	1:A:19:ALA:H	1:A:148:MET:HE1	12	0.11
(1,266)	1:A:19:ALA:H	1:A:148:MET:HE2	12	0.11
(1,266)	1:A:19:ALA:H	1:A:148:MET:HE3	12	0.11
(1,247)	1:A:18:LEU:HD11	1:A:144:ARG:H	5	0.11
(1,247)	1:A:18:LEU:HD12	1:A:144:ARG:H	5	0.11
(1,247)	1:A:18:LEU:HD13	1:A:144:ARG:H	5	0.11
(1,247)	1:A:18:LEU:HD21	1:A:144:ARG:H	5	0.11
(1,247)	1:A:18:LEU:HD22	1:A:144:ARG:H	5	0.11
(1,247)	1:A:18:LEU:HD23	1:A:144:ARG:H	5	0.11
(1,2323)	1:A:162:ARG:HG2	1:A:163:SER:H	9	0.11
(1,2323)	1:A:162:ARG:HG3	1:A:163:SER:H	9	0.11
(1,2312)	1:A:161:LEU:HA	1:A:162:ARG:H	5	0.11
(1,2312)	1:A:161:LEU:HA	1:A:162:ARG:H	7	0.11
(1,2312)	1:A:161:LEU:HA	1:A:162:ARG:H	11	0.11
(1,2312)	1:A:161:LEU:HA	1:A:162:ARG:H	20	0.11
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE1	6	0.11
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE2	6	0.11
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE3	6	0.11
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE1	6	0.11
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE2	6	0.11
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE3	6	0.11
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE1	6	0.11
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE2	6	0.11
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE3	6	0.11
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE1	18	0.11
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE2	18	0.11
(1,2210)	1:A:147:ILE:HG21	1:A:148:MET:HE3	18	0.11
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE1	18	0.11
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE2	18	0.11
(1,2210)	1:A:147:ILE:HG22	1:A:148:MET:HE3	18	0.11
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE1	18	0.11
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE2	18	0.11
(1,2210)	1:A:147:ILE:HG23	1:A:148:MET:HE3	18	0.11
(1,2043)	1:A:134:LYS:H	1:A:134:LYS:HG2	16	0.11
(1,2043)	1:A:134:LYS:H	1:A:134:LYS:HG3	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2043)	1:A:134:LYS:H	1:A:134:LYS:HG2	20	0.11
(1,2043)	1:A:134:LYS:H	1:A:134:LYS:HG3	20	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	6	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	6	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	6	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	6	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	6	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	6	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	6	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	6	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	6	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	9	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	9	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	9	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	9	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	9	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	9	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	9	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	9	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	9	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	10	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	10	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	10	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	10	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	10	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	10	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	10	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	10	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	10	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	15	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	15	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	15	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	15	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	15	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	15	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	15	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	15	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	15	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	17	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	17	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	17	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	17	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	17	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	17	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	17	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	17	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB1	18	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB2	18	0.11
(1,1942)	1:A:130:LEU:HD11	1:A:139:ALA:HB3	18	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB1	18	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB2	18	0.11
(1,1942)	1:A:130:LEU:HD12	1:A:139:ALA:HB3	18	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB1	18	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB2	18	0.11
(1,1942)	1:A:130:LEU:HD13	1:A:139:ALA:HB3	18	0.11
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG21	15	0.11
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG22	15	0.11
(1,1812)	1:A:126:ILE:HD11	1:A:147:ILE:HG23	15	0.11
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG21	15	0.11
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG22	15	0.11
(1,1812)	1:A:126:ILE:HD12	1:A:147:ILE:HG23	15	0.11
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG21	15	0.11
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG22	15	0.11
(1,1812)	1:A:126:ILE:HD13	1:A:147:ILE:HG23	15	0.11
(1,1738)	1:A:123:PHE:H	1:A:126:ILE:HG21	10	0.11
(1,1738)	1:A:123:PHE:H	1:A:126:ILE:HG22	10	0.11
(1,1738)	1:A:123:PHE:H	1:A:126:ILE:HG23	10	0.11
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG2	1	0.11
(1,1584)	1:A:107:GLU:HA	1:A:107:GLU:HG3	1	0.11
(1,1537)	1:A:102:GLY:HA2	2:A:500:A2G:H81	17	0.11
(1,1405)	1:A:89:TYR:H	1:A:89:TYR:HE1	17	0.11
(1,1405)	1:A:89:TYR:H	1:A:89:TYR:HE2	17	0.11
(1,1394)	1:A:88:LEU:HB2	1:A:92:LEU:HD21	12	0.11
(1,1394)	1:A:88:LEU:HB2	1:A:92:LEU:HD22	12	0.11
(1,1394)	1:A:88:LEU:HB2	1:A:92:LEU:HD23	12	0.11
(1,1278)	1:A:81:LEU:HB3	1:A:85:TYR:HD1	5	0.11
(1,1278)	1:A:81:LEU:HB3	1:A:85:TYR:HD2	5	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD11	5	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD12	5	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD13	5	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD21	5	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD22	5	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD23	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD11	13	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD12	13	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD13	13	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD21	13	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD22	13	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD23	13	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD11	15	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD12	15	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD13	15	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD21	15	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD22	15	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD23	15	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD11	19	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD12	19	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD13	19	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD21	19	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD22	19	0.11
(1,1219)	1:A:78:GLU:H	1:A:81:LEU:HD23	19	0.11
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE1	3	0.11
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE2	3	0.11
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE1	5	0.11
(1,1087)	1:A:68:SER:HB3	1:A:89:TYR:HE2	5	0.11
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB2	4	0.11
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB3	4	0.11
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB2	12	0.11
(1,104)	1:A:9:LEU:HG	1:A:12:ARG:HB3	12	0.11
(1,1036)	1:A:66:LEU:HD11	1:A:69:THR:H	4	0.11
(1,1036)	1:A:66:LEU:HD12	1:A:69:THR:H	4	0.11
(1,1036)	1:A:66:LEU:HD13	1:A:69:THR:H	4	0.11
(1,1036)	1:A:66:LEU:HD21	1:A:69:THR:H	4	0.11
(1,1036)	1:A:66:LEU:HD22	1:A:69:THR:H	4	0.11
(1,1036)	1:A:66:LEU:HD23	1:A:69:THR:H	4	0.11
(1,1036)	1:A:66:LEU:HD11	1:A:69:THR:H	16	0.11
(1,1036)	1:A:66:LEU:HD12	1:A:69:THR:H	16	0.11
(1,1036)	1:A:66:LEU:HD13	1:A:69:THR:H	16	0.11
(1,1036)	1:A:66:LEU:HD21	1:A:69:THR:H	16	0.11
(1,1036)	1:A:66:LEU:HD22	1:A:69:THR:H	16	0.11
(1,1036)	1:A:66:LEU:HD23	1:A:69:THR:H	16	0.11
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD11	16	0.11
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD12	16	0.11
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD13	16	0.11
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD21	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD22	16	0.11
(1,1005)	1:A:65:ASN:HD21	1:A:66:LEU:HD23	16	0.11

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value