Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2LRE
BMRB ID	:	18358
Title	:	The solution structure of the dimeric Acanthaporin
Authors	:	Michalek, M.; Soennichsen, F.D.; Wechselberger, R.; Dingley, A.J.; Wienk, H.; Simanski, M.; Herbst, R.; Lorenzen, I.; Marciano-Cabral, F.; Gelhaus, C.; Groetzinger, J.; Leippe, M.
Deposited on	:	2012-03-28

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 (1)) were used in the production of this report:

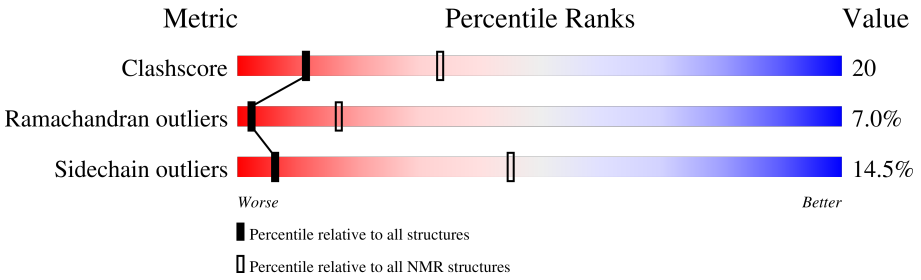
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 22%.

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	61	49% 28% • 20%
1	B	61	46% 25% • 26%

2 Ensemble composition and analysis (i)

This entry contains 17 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:13-A:61, B:74-B:98, B:103-B:122 (94)	1.98	16

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1634 atoms, of which 816 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Acanthaporin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	61	817	252	408	72	74	11	0
1	B	61	817	252	408	72	74	11	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

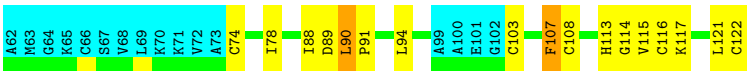
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for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

• Molecule 1: Acanthaporin

Chain A: 49% 28% • 20%

• Molecule 1: Acanthaporin

Chain B: 46% 25% • 26%



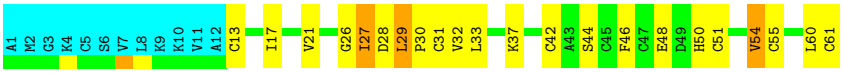
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

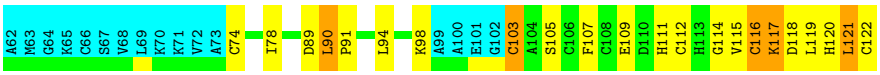
• Molecule 1: Acanthaporin

Chain A: 44% 31% 5% 20%



• Molecule 1: Acanthaporin

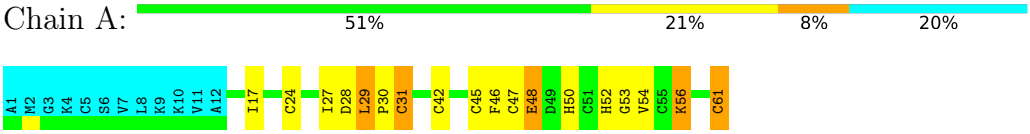
Chain B: 38% 28% 8% 26%



4.2.2 Score per residue for model 2

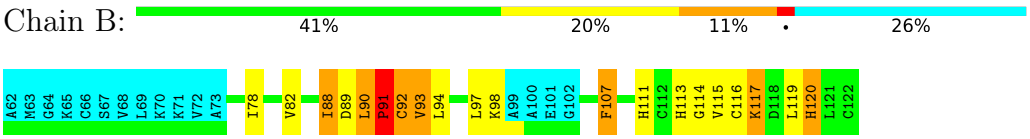
- Molecule 1: Acanthaporin

Chain A:



- Molecule 1: Acanthaporin

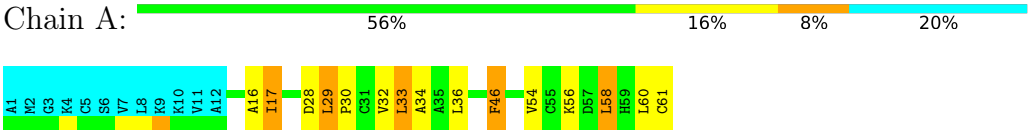
Chain B:



4.2.3 Score per residue for model 3

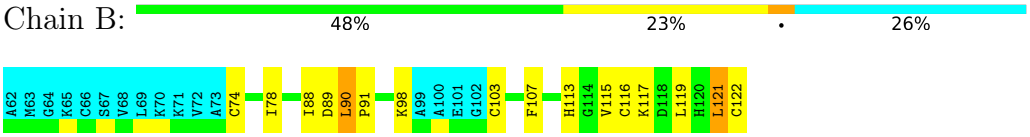
- Molecule 1: Acanthaporin

Chain A:



- Molecule 1: Acanthaporin

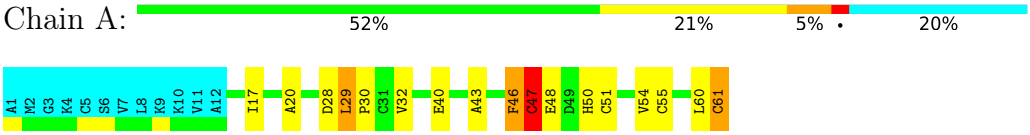
Chain B:



4.2.4 Score per residue for model 4

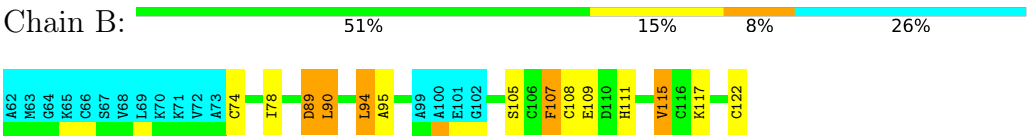
- Molecule 1: Acanthaporin

Chain A:



- Molecule 1: Acanthaporin

Chain B:



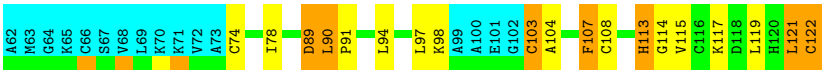
4.2.5 Score per residue for model 5

- Molecule 1: Acanthaporin

Chain A: 56% 16% 8% 20%

- Molecule 1: Acanthaporin

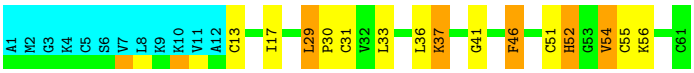
Chain B: 43% 20% 11% 26%



4.2.6 Score per residue for model 6

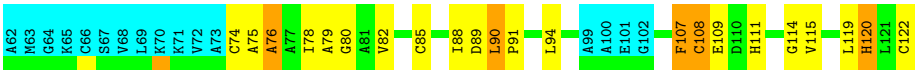
- Molecule 1: Acanthaporin

Chain A: 56% 16% 8% 20%



- Molecule 1: Acanthaporin

Chain B: 38% 28% 8% 26%



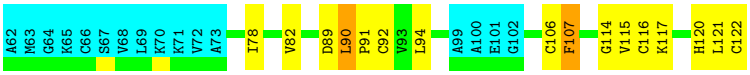
4.2.7 Score per residue for model 7

- Molecule 1: Acanthaporin

Chain A: 49% 23% 8% 20%

- Molecule 1: Acanthaporin

Chain B: 48% 23% • 26%



4.2.8 Score per residue for model 8

- Molecule 1: Acanthaporin

Chain A: 52% 20% 8% 20%

A1 M2 G3 K4 C5 S6 V7 L8 K9 K10 V11 A12 C13 I17 D28 L29 P30 C31 K37 A43 F46 H50 C51 H52 G53 V54 C55 K56 D57 L58 H59 L60 C61

- Molecule 1: Acanthaporin

Chain B: 51% 18% • • 26%

A62 M63 G64 K65 C66 S67 V68 L69 K70 K71 V72 A73 C74 I78 D89 L90 P91 C92 V93 K98 A99 A100 E101 G102 F107 C108 E109 H113 G114 V115 C116 C122

4.2.9 Score per residue for model 9

- Molecule 1: Acanthaporin

Chain A: 39% 31% 10% 20%

A1 M2 G3 K4 C5 S6 V7 L8 K9 K10 V11 A12 C13 A14 I17 A18 G19 A20 C24 I27 D28 L29 P30 C31 V32 L33 A39 E40 G41 C42 F46 C47 E48 D49 H50 V54 C55 L58 H59 L60 C61

- Molecule 1: Acanthaporin

Chain B: 41% 23% 8% • 26%

A62 M63 G64 K65 C66 S67 V68 L69 K70 K71 V72 A73 C74 A75 I78 A79 G80 A81 L90 P91 C92 V93 L97 K98 A99 A100 E101 G102 C103 A104 S105 C106 F107 C108 E109 D110 H111 G114 V115 C116 L119 H120 L121 C122

4.2.10 Score per residue for model 10

- Molecule 1: Acanthaporin

Chain A: 56% 18% 7% 20%

A1 M2 G3 K4 C5 S6 V7 L8 K9 K10 V11 A12 I17 I27 D28 L29 P30 C31 E40 A43 S44 C45 F46 V54 C55 K56 D57 L58 H59 L60 C61

- Molecule 1: Acanthaporin

Chain B: 41% 28% 5% 26%

A62 M63 G64 K65 C66 S67 V68 L69 K70 K71 V72 A73 C74 I78 G86 G87 I88 D89 L90 P91 L94 K98 A99 A100 E101 G102 C103 A104 S105 C106 F107 C108 C112 H113 G114 V115 C116 K117 L121 C122

4.2.11 Score per residue for model 11

- Molecule 1: Acanthaporin

Chain A: 56% 16% 8% 20%

A1 M2 G3 K4 C5 S6 V7 L8 K9 K10 V11 A12 I17 C24 L29 P30 C31 V32 L36 C42 F46 C47 E48 D49 H50 C51 H52 G53 V54 C55 C61

- Molecule 1: Acanthaporin

Chain B: 41% 30% • 26%

A62 M63 G64 K65 C66 S67 V68 L69 K70 K71 V72 A73 I78 V82 C85 I88 D89 L90 P91 C92 V93 L94 L97 K98 A99 A100 E101 G102 C103 A104 S105 C106 F107 C108 H111 C112 H113 G114 V115 C116 K117 L121 C122

4.2.12 Score per residue for model 12

- Molecule 1: Acanthaporin

Chain A: 49% 28% • 20%

A1 M2 G3 K4 C5 S6 V7 L8 K9 K10 V11 A12 C13 I17 I27 D28 L29 P30 L33 K37 A38 F46 C47 E48 H52 G53 V54 C55 K56 D57 L58 H59 L60 C61

- Molecule 1: Acanthaporin

Chain B: 51% 18% 5% 26%

A62 M63 G64 K65 C66 S67 V68 L69 K70 K71 V72 A73 C74 A77 I78 D89 L90 P91 L94 K98 A99 A100 E101 G102 F107 H113 G114 V115 C116 L121 C122

4.2.13 Score per residue for model 13

- Molecule 1: Acanthaporin

Chain A: 52% 21% 7% 20%

A1 M2 G3 K4 C5 S6 V7 L8 K9 K10 V11 A12 C13 I17 I27 D28 L29 P30 C31 V32 L33 G41 C45 F46 H52 G53 V54 C55 K56 L60 C61

- Molecule 1: Acanthaporin

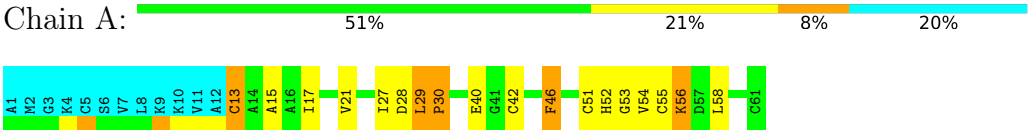
Chain B: 48% 18% 8% 26%

A62 M63 G64 K65 C66 S67 V68 L69 K70 K71 V72 A73 A77 I78 A81 I88 D89 L90 P91 C92 V93 L94 A95 A96 A99 A100 E101 G102 S105 C106 F107 H113 G114 V115 C116 C122

4.2.14 Score per residue for model 14

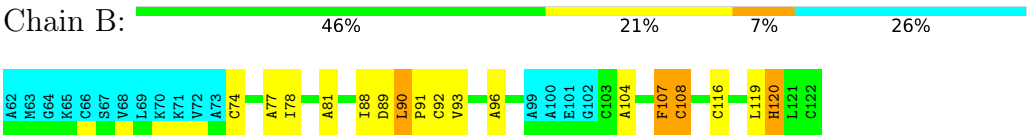
- Molecule 1: Acanthaporin

Chain A:



- Molecule 1: Acanthaporin

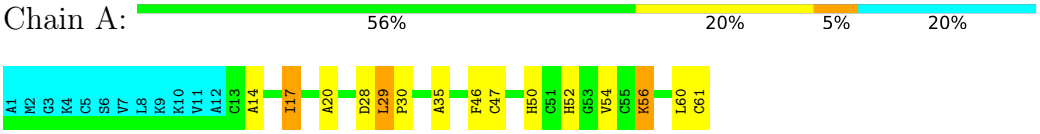
Chain B:



4.2.15 Score per residue for model 15

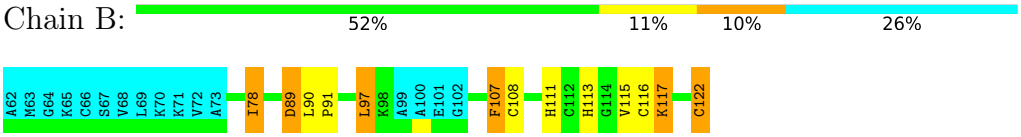
- Molecule 1: Acanthaporin

Chain A:



- Molecule 1: Acanthaporin

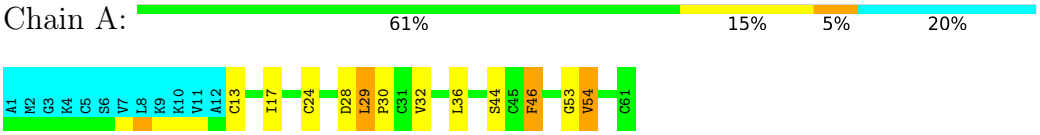
Chain B:



4.2.16 Score per residue for model 16 (medoid)

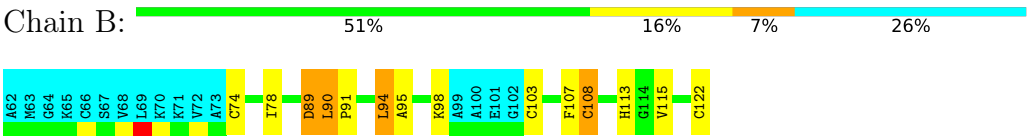
- Molecule 1: Acanthaporin

Chain A:



- Molecule 1: Acanthaporin

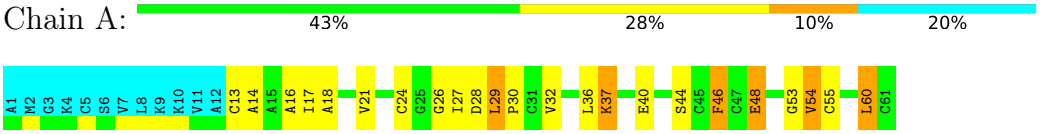
Chain B:



4.2.17 Score per residue for model 17

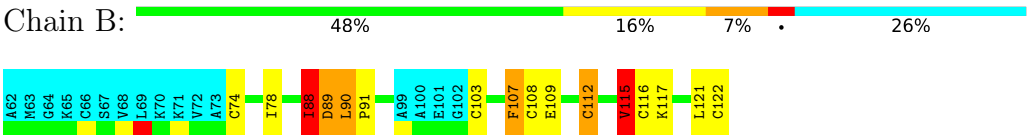
- Molecule 1: Acanthaporin

Chain A:



- Molecule 1: Acanthaporin

Chain B:



5 Refinement protocol and experimental data overview (i)

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

Of the 400 calculated structures, 17 were deposited, based on the following criterion: *target function.*

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

Software name	**Classification**	**Version**
CYANA	structure solution	
X-PLOR NIH	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	263
Number of shifts mapped to atoms	262
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	22%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	326	307	307	14±4
1	B	303	288	288	13±5
All	All	10693	10115	10115	419

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 20.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:74:CYS:HB2	1:B:78:ILE:HD12	0.89	1.44	1	2
1:A:13:CYS:HB2	1:A:17:ILE:HD12	0.84	1.47	6	3
1:A:30:PRO:HA	1:A:54:VAL:HG11	0.82	1.49	6	8
1:B:91:PRO:HA	1:B:115:VAL:HG11	0.82	1.50	17	4
1:B:94:LEU:HD22	1:B:115:VAL:HB	0.82	1.50	6	3
1:B:78:ILE:HD13	1:B:97:LEU:HD13	0.80	1.54	11	1
1:A:52:HIS:HA	1:A:56:LYS:HB3	0.79	1.54	15	1
1:B:91:PRO:HB3	1:B:115:VAL:HG11	0.78	1.55	9	1
1:B:75:ALA:HA	1:B:79:ALA:HB3	0.77	1.56	9	2
1:A:53:GLY:HA3	1:B:91:PRO:HB2	0.74	1.59	14	3
1:A:30:PRO:HB3	1:A:54:VAL:HG13	0.74	1.60	9	1
1:B:74:CYS:HB3	1:B:78:ILE:HD12	0.72	1.60	16	5
1:A:17:ILE:HG12	1:A:46:PHE:CD2	0.70	2.21	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ILE:HD13	1:A:36:LEU:HD13	0.70	1.60	11	1
1:A:30:PRO:HB2	1:B:115:VAL:HG13	0.69	1.65	6	1
1:B:90:LEU:HD11	1:B:116:CYS:SG	0.69	2.27	17	1
1:B:78:ILE:HD13	1:B:107:PHE:HB2	0.68	1.65	17	8
1:A:29:LEU:HD21	1:A:55:CYS:HB2	0.68	1.64	4	3
1:A:29:LEU:HD11	1:A:55:CYS:SG	0.68	2.28	12	2
1:A:13:CYS:HB3	1:A:17:ILE:HD12	0.68	1.64	12	2
1:B:113:HIS:HA	1:B:117:LYS:HG2	0.68	1.65	2	1
1:B:90:LEU:HD11	1:B:116:CYS:HB2	0.67	1.65	12	6
1:A:47:CYS:HB3	1:A:61:CYS:SG	0.67	2.29	9	1
1:A:30:PRO:HA	1:A:54:VAL:HG21	0.67	1.66	3	5
1:A:17:ILE:HD13	1:A:46:PHE:HB2	0.66	1.67	1	7
1:B:91:PRO:HA	1:B:115:VAL:HG21	0.66	1.66	15	4
1:A:30:PRO:HB3	1:B:115:VAL:HG13	0.66	1.67	1	1
1:A:30:PRO:HB2	1:B:91:PRO:HB2	0.65	1.67	9	1
1:B:108:CYS:O	1:B:122:CYS:HB3	0.65	1.92	15	2
1:A:53:GLY:HA2	1:B:91:PRO:HB2	0.64	1.69	8	1
1:B:103:CYS:HB2	1:B:121:LEU:HD21	0.64	1.70	1	1
1:B:81:ALA:HB2	1:B:96:ALA:HB3	0.63	1.68	14	2
1:A:29:LEU:HD21	1:A:55:CYS:HB3	0.63	1.70	9	1
1:A:29:LEU:HD11	1:A:55:CYS:HB2	0.63	1.70	17	5
1:A:20:ALA:HB1	1:A:32:VAL:HG13	0.63	1.70	4	1
1:A:28:ASP:C	1:A:30:PRO:HD2	0.63	2.15	16	1
1:B:90:LEU:HD11	1:B:108:CYS:SG	0.62	2.34	9	1
1:A:17:ILE:CD1	1:A:46:PHE:HB2	0.62	2.24	12	7
1:B:74:CYS:O	1:B:78:ILE:HB	0.62	1.94	12	3
1:B:119:LEU:O	1:B:120:HIS:HB2	0.61	1.94	2	3
1:A:13:CYS:CB	1:A:17:ILE:HD12	0.60	2.26	14	1
1:A:29:LEU:HG	1:A:54:VAL:HG22	0.60	1.71	15	1
1:A:29:LEU:HB3	1:A:30:PRO:HD3	0.60	1.74	10	5
1:A:40:GLU:HG2	1:A:42:CYS:H	0.60	1.56	9	1
1:A:30:PRO:CA	1:A:54:VAL:HG11	0.60	2.26	10	1
1:A:33:LEU:HD13	1:A:54:VAL:HB	0.60	1.73	13	1
1:B:108:CYS:HA	1:B:111:HIS:HB2	0.60	1.71	4	2
1:A:28:ASP:OD2	1:A:31:CYS:HB3	0.60	1.96	1	1
1:B:78:ILE:HD13	1:B:97:LEU:HD12	0.59	1.75	5	1
1:A:28:ASP:O	1:A:29:LEU:HB3	0.59	1.98	16	1
1:A:58:LEU:O	1:A:59:HIS:HB2	0.59	1.96	8	2
1:A:17:ILE:HG12	1:A:46:PHE:CD1	0.59	2.32	7	2
1:A:51:CYS:HB2	1:A:55:CYS:SG	0.59	2.37	4	1
1:B:78:ILE:HG12	1:B:107:PHE:CD2	0.59	2.33	11	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:108:CYS:HB3	1:B:111:HIS:O	0.59	1.95	15	1
1:A:52:HIS:O	1:B:92:CYS:HB3	0.59	1.98	11	1
1:A:20:ALA:HB2	1:A:35:ALA:HB3	0.59	1.75	15	1
1:B:90:LEU:N	1:B:91:PRO:HD2	0.58	2.13	10	9
1:A:30:PRO:HG2	1:B:91:PRO:HB2	0.58	1.75	9	1
1:A:52:HIS:ND1	1:B:92:CYS:HB3	0.58	2.13	14	2
1:B:94:LEU:HD13	1:B:115:VAL:HB	0.58	1.75	13	1
1:B:104:ALA:HB1	1:B:121:LEU:HB3	0.58	1.75	11	1
1:A:13:CYS:HA	1:A:17:ILE:HD12	0.58	1.75	17	1
1:A:33:LEU:HD22	1:A:54:VAL:HB	0.57	1.75	1	1
1:B:94:LEU:HD22	1:B:115:VAL:HG23	0.57	1.75	5	1
1:A:30:PRO:CB	1:B:91:PRO:HB2	0.57	2.28	9	1
1:A:13:CYS:O	1:A:17:ILE:HB	0.57	1.98	1	3
1:B:90:LEU:HD12	1:B:94:LEU:HB2	0.57	1.76	7	1
1:A:33:LEU:HD23	1:A:54:VAL:HB	0.57	1.76	3	1
1:B:90:LEU:HB3	1:B:91:PRO:HD3	0.57	1.77	17	4
1:A:30:PRO:CG	1:B:91:PRO:HB2	0.57	2.29	9	1
1:A:31:CYS:HB3	1:B:114:GLY:HA2	0.57	1.77	6	1
1:A:28:ASP:HB3	1:A:32:VAL:HG23	0.56	1.75	7	3
1:A:29:LEU:HG	1:A:54:VAL:CG2	0.56	2.30	11	5
1:A:53:GLY:HA3	1:B:91:PRO:HG2	0.56	1.77	5	1
1:B:91:PRO:HA	1:B:115:VAL:CG2	0.56	2.30	5	2
1:A:28:ASP:OD1	1:A:30:PRO:HD2	0.56	2.01	1	2
1:B:90:LEU:O	1:B:94:LEU:HB2	0.56	2.01	2	1
1:B:103:CYS:SG	1:B:106:CYS:HB2	0.56	2.40	10	1
1:A:29:LEU:HG	1:A:54:VAL:HG21	0.55	1.79	6	1
1:A:24:CYS:SG	1:B:113:HIS:CD2	0.55	2.99	11	1
1:B:78:ILE:CD1	1:B:107:PHE:HB2	0.55	2.31	4	5
1:A:28:ASP:HB2	1:B:113:HIS:CE1	0.55	2.36	2	2
1:A:51:CYS:CB	1:A:56:LYS:HG2	0.55	2.32	6	1
1:A:30:PRO:HA	1:A:54:VAL:CG2	0.55	2.32	9	1
1:A:51:CYS:HB3	1:A:56:LYS:HG2	0.55	1.78	6	1
1:B:108:CYS:HB3	1:B:122:CYS:SG	0.55	2.41	6	1
1:A:29:LEU:N	1:A:30:PRO:HD2	0.55	2.17	11	4
1:B:113:HIS:HA	1:B:117:LYS:HB3	0.55	1.79	15	1
1:A:30:PRO:HA	1:A:54:VAL:CG1	0.55	2.31	10	2
1:A:30:PRO:HG3	1:B:91:PRO:HD3	0.54	1.79	5	1
1:A:13:CYS:HB2	1:A:17:ILE:CD1	0.54	2.28	6	1
1:A:30:PRO:HB2	1:B:114:GLY:HA3	0.54	1.78	8	1
1:B:113:HIS:HA	1:B:117:LYS:HD2	0.54	1.79	5	1
1:B:90:LEU:HD21	1:B:116:CYS:CB	0.54	2.32	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ILE:HG12	1:A:46:PHE:HD2	0.54	1.63	6	4
1:A:30:PRO:HA	1:A:54:VAL:HG22	0.54	1.78	9	1
1:B:98:LYS:HA	1:B:119:LEU:HD11	0.54	1.78	3	1
1:B:94:LEU:HD12	1:B:95:ALA:N	0.54	2.18	16	2
1:A:28:ASP:OD2	1:B:114:GLY:HA2	0.54	2.02	7	1
1:A:21:VAL:HG13	1:A:26:GLY:HA2	0.54	1.79	1	2
1:B:74:CYS:HB3	1:B:103:CYS:SG	0.54	2.43	5	1
1:A:52:HIS:CE1	1:B:92:CYS:HB3	0.54	2.38	8	2
1:A:52:HIS:HB2	1:B:89:ASP:OD2	0.54	2.03	13	1
1:B:78:ILE:O	1:B:82:VAL:HG23	0.54	2.03	2	3
1:A:52:HIS:O	1:B:91:PRO:HB2	0.54	2.02	6	1
1:B:74:CYS:HB3	1:B:78:ILE:CD1	0.54	2.32	6	1
1:A:43:ALA:CB	1:A:60:LEU:HB3	0.53	2.33	10	2
1:B:94:LEU:HG	1:B:98:LYS:HG3	0.53	1.80	5	1
1:B:105:SER:O	1:B:109:GLU:HG2	0.53	2.04	4	1
1:A:28:ASP:OD1	1:A:31:CYS:HB3	0.53	2.04	9	2
1:A:17:ILE:HD13	1:A:46:PHE:HB3	0.53	1.81	4	1
1:A:47:CYS:SG	1:A:60:LEU:HB2	0.53	2.43	9	1
1:A:30:PRO:HD3	1:B:91:PRO:HG3	0.53	1.80	16	2
1:B:81:ALA:HB3	1:B:93:VAL:HG13	0.52	1.81	9	2
1:A:41:GLY:HA2	1:A:60:LEU:HD22	0.52	1.80	13	1
1:B:104:ALA:HB1	1:B:108:CYS:HB2	0.52	1.80	14	1
1:A:33:LEU:HA	1:A:36:LEU:HB3	0.52	1.79	6	2
1:A:31:CYS:HB3	1:B:113:HIS:CE1	0.52	2.40	8	1
1:A:29:LEU:H	1:A:30:PRO:HD2	0.51	1.65	13	1
1:A:30:PRO:HB2	1:B:91:PRO:CB	0.51	2.35	9	1
1:B:108:CYS:SG	1:B:122:CYS:HB3	0.51	2.45	16	1
1:A:30:PRO:HG3	1:B:91:PRO:HG3	0.51	1.81	17	1
1:A:33:LEU:O	1:A:37:LYS:HD3	0.51	2.06	6	1
1:B:90:LEU:HG	1:B:115:VAL:HB	0.51	1.83	10	1
1:A:21:VAL:HG13	1:A:27:ILE:H	0.51	1.65	1	1
1:A:48:GLU:HA	1:A:48:GLU:OE1	0.51	2.06	1	2
1:A:51:CYS:HB2	1:A:55:CYS:HB3	0.51	1.81	4	1
1:B:78:ILE:HD13	1:B:97:LEU:HD22	0.51	1.82	2	1
1:B:78:ILE:HB	1:B:97:LEU:HD13	0.51	1.82	2	1
1:A:53:GLY:O	1:A:56:LYS:HG3	0.51	2.06	2	3
1:A:27:ILE:HG12	1:A:28:ASP:N	0.50	2.21	7	2
1:B:78:ILE:HG12	1:B:107:PHE:CD1	0.50	2.42	8	1
1:A:20:ALA:HB3	1:A:32:VAL:HG13	0.50	1.83	9	1
1:B:90:LEU:HD21	1:B:116:CYS:HB2	0.50	1.83	1	2
1:B:112:CYS:HB3	1:B:117:LYS:HG2	0.50	1.84	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:CYS:O	1:A:61:CYS:HB3	0.50	2.06	15	2
1:A:52:HIS:CD2	1:B:89:ASP:HB2	0.50	2.42	12	1
1:A:45:CYS:O	1:A:48:GLU:HG2	0.49	2.07	2	1
1:A:29:LEU:HG	1:A:54:VAL:HG23	0.49	1.84	11	3
1:B:90:LEU:HG	1:B:115:VAL:HG22	0.49	1.82	16	1
1:B:89:ASP:CG	1:B:91:PRO:HD2	0.49	2.26	13	3
1:A:17:ILE:HD11	1:A:46:PHE:HB2	0.49	1.84	12	1
1:A:31:CYS:HB2	1:B:113:HIS:O	0.49	2.08	2	2
1:A:31:CYS:HB2	1:B:115:VAL:HG13	0.49	1.84	9	1
1:A:30:PRO:HG2	1:B:114:GLY:HA2	0.49	1.83	7	1
1:A:53:GLY:O	1:A:56:LYS:HD3	0.49	2.07	5	1
1:A:28:ASP:CG	1:A:31:CYS:HB3	0.48	2.28	10	1
1:A:14:ALA:HA	1:A:17:ILE:HG22	0.48	1.84	15	1
1:B:114:GLY:O	1:B:117:LYS:HG3	0.48	2.08	2	2
1:A:28:ASP:OD1	1:A:32:VAL:HG23	0.48	2.08	16	2
1:A:29:LEU:O	1:A:33:LEU:HB2	0.48	2.08	7	1
1:A:53:GLY:O	1:A:55:CYS:N	0.48	2.47	13	3
1:B:94:LEU:HG	1:B:115:VAL:HG12	0.48	1.86	10	1
1:A:14:ALA:HA	1:A:18:ALA:HB3	0.48	1.86	9	2
1:A:24:CYS:SG	1:B:114:GLY:HA3	0.48	2.48	9	1
1:B:121:LEU:N	1:B:121:LEU:HD23	0.48	2.24	5	1
1:B:90:LEU:HD22	1:B:107:PHE:CE1	0.48	2.44	9	1
1:A:50:HIS:HA	1:B:89:ASP:OD2	0.47	2.09	15	1
1:A:47:CYS:O	1:A:51:CYS:HB3	0.47	2.09	4	1
1:B:90:LEU:HG	1:B:115:VAL:HG21	0.47	1.86	17	1
1:A:52:HIS:CE1	1:B:89:ASP:HB2	0.47	2.44	15	3
1:B:78:ILE:HG12	1:B:107:PHE:HD2	0.47	1.70	6	2
1:A:24:CYS:SG	1:B:113:HIS:HB2	0.47	2.49	5	2
1:A:60:LEU:HD23	1:A:60:LEU:N	0.47	2.24	17	1
1:B:104:ALA:CB	1:B:121:LEU:HB3	0.46	2.39	10	1
1:B:90:LEU:HG	1:B:115:VAL:CG2	0.46	2.39	13	2
1:B:119:LEU:HB3	1:B:121:LEU:CD2	0.46	2.40	9	1
1:A:47:CYS:O	1:A:51:CYS:HB2	0.46	2.11	11	1
1:A:51:CYS:HB2	1:A:55:CYS:CB	0.46	2.40	4	1
1:B:114:GLY:O	1:B:117:LYS:HG2	0.46	2.10	7	2
1:A:44:SER:O	1:A:48:GLU:HG2	0.46	2.11	17	1
1:A:43:ALA:CB	1:A:60:LEU:HG	0.46	2.39	4	1
1:A:33:LEU:HD22	1:A:54:VAL:CG2	0.46	2.41	9	1
1:A:30:PRO:CG	1:B:91:PRO:HD3	0.45	2.40	5	1
1:A:30:PRO:HB3	1:A:54:VAL:CG1	0.45	2.36	9	1
1:B:113:HIS:O	1:B:117:LYS:HE2	0.45	2.12	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:97:LEU:HD21	1:B:103:CYS:HB2	0.45	1.88	9	1
1:A:29:LEU:HD13	1:A:46:PHE:CE2	0.45	2.46	7	1
1:A:52:HIS:O	1:B:92:CYS:HB2	0.45	2.12	8	1
1:B:97:LEU:O	1:B:97:LEU:HG	0.45	2.12	15	1
1:A:37:LYS:H	1:A:37:LYS:HD3	0.45	1.71	17	1
1:B:89:ASP:OD2	1:B:91:PRO:HG2	0.45	2.11	3	1
1:B:94:LEU:HD23	1:B:115:VAL:HG11	0.45	1.86	4	1
1:A:28:ASP:HB2	1:B:113:HIS:HE1	0.45	1.70	5	1
1:B:94:LEU:HD23	1:B:115:VAL:HG21	0.45	1.88	16	1
1:B:82:VAL:HG22	1:B:88:ILE:HB	0.45	1.89	6	2
1:A:24:CYS:HB3	1:B:113:HIS:CG	0.44	2.47	2	1
1:A:29:LEU:HD21	1:A:55:CYS:CB	0.44	2.41	9	1
1:B:78:ILE:HG13	1:B:107:PHE:CD2	0.44	2.46	15	1
1:A:47:CYS:HA	1:A:50:HIS:HB2	0.44	1.88	7	2
1:A:47:CYS:HA	1:A:50:HIS:O	0.44	2.12	9	1
1:A:30:PRO:CA	1:A:54:VAL:HG21	0.44	2.41	11	1
1:B:89:ASP:H	1:B:93:VAL:HG21	0.44	1.72	14	1
1:A:56:LYS:C	1:A:58:LEU:H	0.44	2.16	3	1
1:A:30:PRO:CB	1:B:115:VAL:HG13	0.44	2.42	1	1
1:B:107:PHE:O	1:B:111:HIS:HD2	0.44	1.95	2	1
1:A:17:ILE:O	1:A:21:VAL:HG23	0.44	2.13	14	1
1:A:55:CYS:SG	1:A:60:LEU:HB2	0.43	2.52	7	2
1:B:119:LEU:HB2	1:B:121:LEU:HD22	0.43	1.89	5	1
1:A:52:HIS:CE1	1:B:89:ASP:HB3	0.43	2.48	8	1
1:B:89:ASP:CG	1:B:90:LEU:H	0.43	2.14	12	2
1:B:121:LEU:H	1:B:121:LEU:HD13	0.43	1.73	3	1
1:B:107:PHE:C	1:B:109:GLU:H	0.43	2.16	6	1
1:A:13:CYS:HB3	1:A:41:GLY:O	0.43	2.13	6	1
1:B:89:ASP:HB3	1:B:93:VAL:HG23	0.43	1.90	13	1
1:A:16:ALA:HB1	1:A:36:LEU:HA	0.43	1.89	17	1
1:A:47:CYS:CB	1:A:61:CYS:SG	0.43	3.06	2	1
1:A:28:ASP:CG	1:A:29:LEU:H	0.43	2.17	3	1
1:B:88:ILE:HD11	1:B:107:PHE:CE2	0.43	2.48	11	1
1:B:119:LEU:O	1:B:120:HIS:CB	0.43	2.66	6	1
1:B:106:CYS:SG	1:B:107:PHE:N	0.43	2.92	7	1
1:A:46:PHE:O	1:A:47:CYS:HB2	0.43	2.14	9	1
1:B:91:PRO:CA	1:B:115:VAL:HG21	0.43	2.43	13	1
1:B:94:LEU:HG	1:B:115:VAL:HG22	0.43	1.90	12	1
1:B:107:PHE:C	1:B:107:PHE:CD1	0.42	2.92	6	1
1:B:88:ILE:HG12	1:B:89:ASP:N	0.42	2.29	13	1
1:A:28:ASP:CG	1:A:30:PRO:HD2	0.42	2.35	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:PHE:O	1:A:50:HIS:HD2	0.42	1.98	1	1
1:A:28:ASP:O	1:A:29:LEU:HB2	0.42	2.13	4	2
1:A:28:ASP:O	1:A:29:LEU:CB	0.42	2.67	16	1
1:A:20:ALA:CB	1:A:32:VAL:HG13	0.42	2.41	4	1
1:A:28:ASP:OD2	1:A:30:PRO:HD2	0.42	2.14	8	1
1:B:77:ALA:HB1	1:B:96:ALA:O	0.42	2.14	13	1
1:B:81:ALA:CB	1:B:93:VAL:HG13	0.42	2.45	13	1
1:B:117:LYS:C	1:B:117:LYS:HD3	0.42	2.35	2	1
1:A:33:LEU:HD12	1:A:34:ALA:N	0.42	2.30	3	1
1:B:103:CYS:SG	1:B:104:ALA:N	0.42	2.93	5	1
1:A:46:PHE:HD1	1:A:50:HIS:CE1	0.42	2.33	9	1
1:B:98:LYS:HE3	1:B:119:LEU:HD11	0.42	1.91	1	1
1:A:30:PRO:HG3	1:B:91:PRO:CB	0.42	2.44	3	1
1:B:89:ASP:O	1:B:90:LEU:HB2	0.41	2.15	4	2
1:B:82:VAL:CG2	1:B:88:ILE:HB	0.41	2.45	6	1
1:A:33:LEU:HG	1:A:54:VAL:HG22	0.41	1.91	12	1
1:B:89:ASP:OD1	1:B:91:PRO:HD2	0.41	2.15	5	1
1:B:105:SER:O	1:B:109:GLU:HB2	0.41	2.15	9	1
1:A:53:GLY:O	1:A:56:LYS:HB3	0.41	2.16	12	1
1:A:29:LEU:N	1:A:30:PRO:CD	0.41	2.83	3	1
1:B:74:CYS:HA	1:B:78:ILE:HD12	0.41	1.93	17	1
1:B:89:ASP:O	1:B:90:LEU:CB	0.41	2.67	3	1
1:A:53:GLY:CA	1:B:91:PRO:HB2	0.41	2.46	7	1
1:A:58:LEU:HD23	1:A:58:LEU:O	0.41	2.16	12	1
1:A:29:LEU:HD13	1:A:46:PHE:HE1	0.41	1.76	8	1
1:A:58:LEU:O	1:A:58:LEU:HD23	0.41	2.16	9	1
1:A:53:GLY:O	1:A:54:VAL:HG22	0.41	2.16	16	1
1:A:46:PHE:C	1:A:48:GLU:H	0.41	2.19	4	1
1:B:91:PRO:CB	1:B:115:VAL:HG11	0.41	2.36	9	1
1:A:29:LEU:H	1:A:30:PRO:CD	0.41	2.29	1	1
1:B:78:ILE:HD12	1:B:93:VAL:HG12	0.41	1.91	2	1
1:B:82:VAL:HG13	1:B:88:ILE:HB	0.41	1.92	2	1
1:B:94:LEU:HB3	1:B:115:VAL:CG2	0.41	2.46	7	1
1:A:30:PRO:HB2	1:B:114:GLY:HA2	0.40	1.93	5	1
1:B:112:CYS:SG	1:B:117:LYS:HG3	0.40	2.56	10	1
1:A:52:HIS:HB2	1:B:91:PRO:HG2	0.40	1.93	6	1
1:B:94:LEU:HB3	1:B:115:VAL:HG23	0.40	1.93	7	1
1:A:51:CYS:O	1:A:56:LYS:HB3	0.40	2.16	14	1
1:A:54:VAL:HG23	1:A:55:CYS:H	0.40	1.77	1	1
1:B:114:GLY:O	1:B:116:CYS:N	0.40	2.49	13	1
1:B:90:LEU:H	1:B:91:PRO:HD2	0.40	1.76	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:88:ILE:O	1:B:89:ASP:HB2	0.40	2.16	17	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	48/61 (79%)	35±3 (72±6%)	10±3 (22±6%)	3±1 (6±2%)	3	19
1	B	44/61 (72%)	32±2 (73±5%)	8±2 (19±5%)	3±1 (8±3%)	2	14
All	All	1564/2074 (75%)	1137 (73%)	318 (20%)	109 (7%)	2	17

All 35 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	29	LEU	17
1	B	90	LEU	17
1	B	89	ASP	10
1	A	54	VAL	6
1	B	115	VAL	6
1	A	28	ASP	6
1	B	120	HIS	4
1	B	108	CYS	4
1	B	109	GLU	3
1	A	48	GLU	3
1	A	27	ILE	2
1	B	91	PRO	2
1	B	98	LYS	2
1	A	58	LEU	2
1	A	40	GLU	2
1	A	13	CYS	2
1	B	114	GLY	2
1	B	77	ALA	2
1	A	44	SER	1
1	A	31	CYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	16	ALA	1
1	A	47	CYS	1
1	B	103	CYS	1
1	A	52	HIS	1
1	B	76	ALA	1
1	B	80	GLY	1
1	A	14	ALA	1
1	A	37	LYS	1
1	A	59	HIS	1
1	B	74	CYS	1
1	B	86	GLY	1
1	A	42	CYS	1
1	A	38	ALA	1
1	A	60	LEU	1
1	B	88	ILE	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	32/41 (78%)	28±1 (87±4%)	4±1 (13±4%)	7 48
1	B	31/41 (76%)	26±2 (84±6%)	5±2 (16±6%)	5 43
All	All	1071/1394 (77%)	916 (86%)	155 (14%)	6 45

All 53 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	B	107	PHE	14
1	A	46	PHE	12
1	B	122	CYS	8
1	A	56	LYS	8
1	B	121	LEU	7
1	A	27	ILE	7
1	B	116	CYS	6
1	B	88	ILE	6
1	A	61	CYS	5

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Mol	Chain	Res	Type	Models (Total)
1	B	117	LYS	5
1	A	37	LYS	4
1	A	50	HIS	4
1	A	42	CYS	3
1	B	111	HIS	3
1	A	60	LEU	3
1	A	55	CYS	3
1	B	113	HIS	3
1	B	98	LYS	3
1	B	108	CYS	3
1	B	103	CYS	2
1	B	105	SER	2
1	B	112	CYS	2
1	B	93	VAL	2
1	A	17	ILE	2
1	A	33	LEU	2
1	A	47	CYS	2
1	B	94	LEU	2
1	A	13	CYS	2
1	B	85	CYS	2
1	A	31	CYS	2
1	B	115	VAL	2
1	A	58	LEU	2
1	A	24	CYS	2
1	A	51	CYS	1
1	B	118	ASP	1
1	B	91	PRO	1
1	B	92	CYS	1
1	B	74	CYS	1
1	A	54	VAL	1
1	B	120	HIS	1
1	B	90	LEU	1
1	A	32	VAL	1
1	A	49	ASP	1
1	A	52	HIS	1
1	B	106	CYS	1
1	A	45	CYS	1
1	A	30	PRO	1
1	B	78	ILE	1
1	B	89	ASP	1
1	B	97	LEU	1
1	A	36	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	44	SER	1
1	A	48	GLU	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)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 22% for the well-defined parts and 19% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	263
Number of shifts mapped to atoms	262
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	50	HIS	HD1	12.833	.	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	43	0.28 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 22%, i.e. 235 atoms were assigned a chemical shift out of a possible 1066. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	119/475 (25%)	81/195 (42%)	0/188 (0%)	38/92 (41%)
Sidechain	112/529 (21%)	112/358 (31%)	0/167 (0%)	0/4 (0%)
Aromatic	4/62 (6%)	4/34 (12%)	0/22 (0%)	0/6 (0%)
Overall	235/1066 (22%)	197/587 (34%)	0/377 (0%)	38/102 (37%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 19%, i.e. 263 atoms were assigned a chemical shift out of a possible 1416. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	134/618 (22%)	91/254 (36%)	0/244 (0%)	43/120 (36%)
Sidechain	125/736 (17%)	125/496 (25%)	0/230 (0%)	0/10 (0%)
Aromatic	4/62 (6%)	4/34 (12%)	0/22 (0%)	0/6 (0%)
Overall	263/1416 (19%)	220/784 (28%)	0/496 (0%)	43/136 (32%)

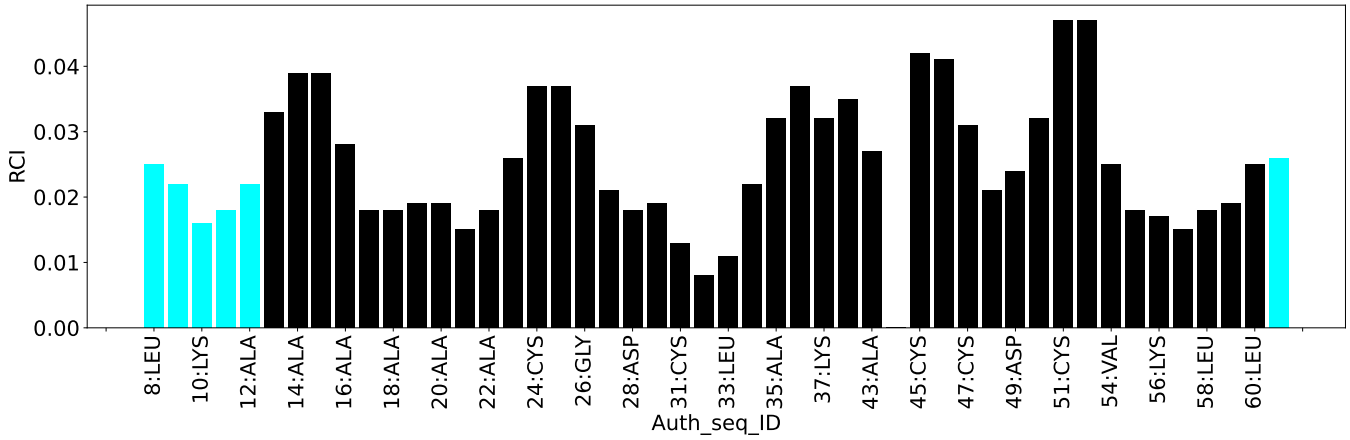
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.00
0.01
0.02
0.03
0.04
8:LEU
10:LYS
12:ALA
14:ALA
16:ALA
18:ALA
20:ALA
22:ALA
24:CYS
26:GLY
28:ASP
31:CYS
33:LEU
35:ALA
37:LYS
43:ALA
45:CYS
47:CYS
49:ASP
51:CYS
54:VAL
56:LYS
58:LEU
60:LEU
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	646
Intra-residue (|i-j|=0)	242
Sequential (|i-j|=1)	222
Medium range (|i-j|>1 and |i-j|<5)	92
Long range (|i-j|≥5)	76
Inter-chain	14
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	5.3
Number of long range restraints per residue[1]	0.6

[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 (i)

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 (i)

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)	22.4	0.2
0.2-0.5 (Medium)	12.2	0.46
>0.5 (Large)	None	None

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

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

9 Distance violation analysis (i)

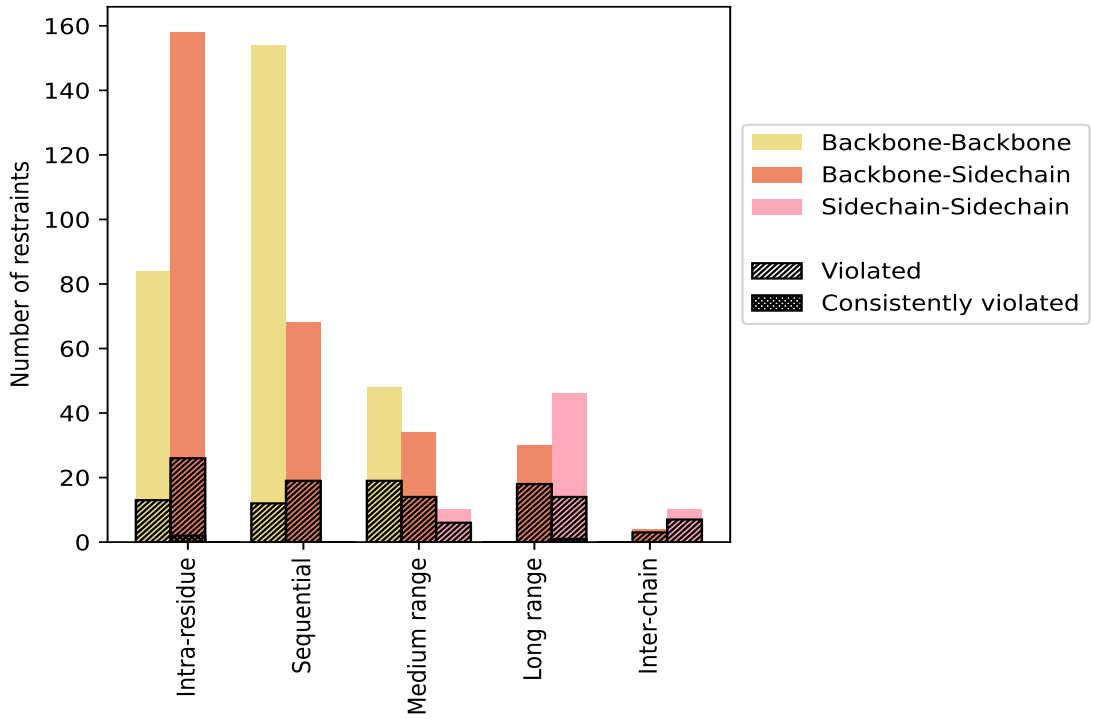
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	242	37.5	39	16.1	6.0	2	0.8	0.3
Backbone-Backbone	84	13.0	13	15.5	2.0	0	0.0	0.0
Backbone-Sidechain	158	24.5	26	16.5	4.0	2	1.3	0.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	222	34.4	31	14.0	4.8	0	0.0	0.0
Backbone-Backbone	154	23.8	12	7.8	1.9	0	0.0	0.0
Backbone-Sidechain	68	10.5	19	27.9	2.9	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	92	14.2	39	42.4	6.0	0	0.0	0.0
Backbone-Backbone	48	7.4	19	39.6	2.9	0	0.0	0.0
Backbone-Sidechain	34	5.3	14	41.2	2.2	0	0.0	0.0
Sidechain-Sidechain	10	1.5	6	60.0	0.9	0	0.0	0.0
Long range (|i-j|≥5)	76	11.8	32	42.1	5.0	1	1.3	0.2
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	30	4.6	18	60.0	2.8	0	0.0	0.0
Sidechain-Sidechain	46	7.1	14	30.4	2.2	1	2.2	0.2
Inter-chain	14	2.2	10	71.4	1.5	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	4	0.6	3	75.0	0.5	0	0.0	0.0
Sidechain-Sidechain	10	1.5	7	70.0	1.1	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	646	100.0	151	23.4	23.4	3	0.5	0.5
Backbone-Backbone	286	44.3	44	15.4	6.8	0	0.0	0.0
Backbone-Sidechain	294	45.5	80	27.2	12.4	2	0.7	0.3
Sidechain-Sidechain	66	10.2	27	40.9	4.2	1	1.5	0.2

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	13	4	11	6	2	36	0.18	0.46	0.07	0.15
2	13	2	6	10	0	31	0.19	0.31	0.06	0.17
3	13	3	7	11	0	34	0.18	0.39	0.07	0.15
4	12	2	13	9	0	36	0.2	0.39	0.06	0.21
5	10	8	10	10	0	38	0.2	0.44	0.09	0.16
6	12	1	14	11	3	41	0.19	0.35	0.07	0.18
7	11	5	11	9	4	40	0.19	0.32	0.07	0.17
8	13	5	8	6	3	35	0.18	0.41	0.08	0.14
9	12	9	10	7	3	41	0.21	0.41	0.08	0.2
10	13	2	7	8	3	33	0.19	0.41	0.08	0.19
11	12	2	4	6	3	27	0.19	0.39	0.08	0.17

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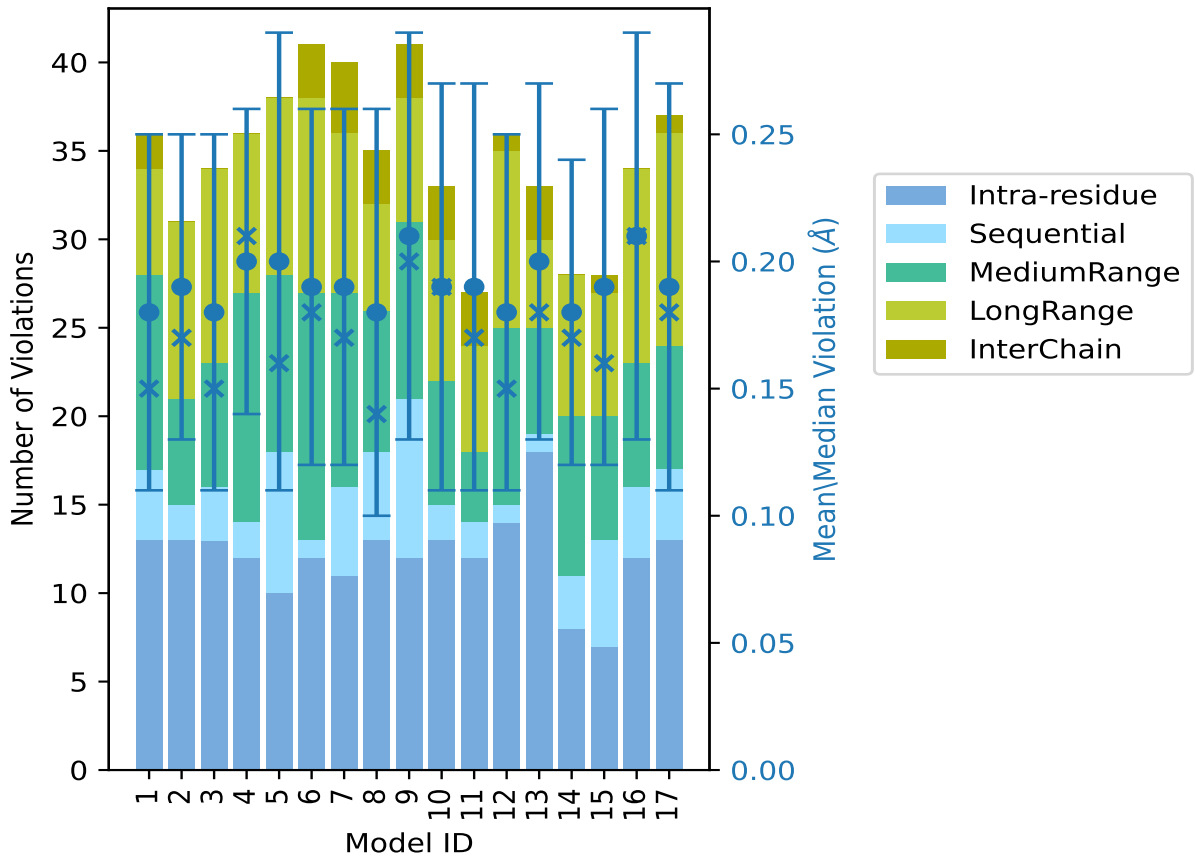
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	14	1	10	10	1	36	0.18	0.34	0.07	0.15
13	18	1	6	5	3	33	0.2	0.46	0.07	0.18
14	8	3	9	8	0	28	0.18	0.3	0.06	0.17
15	7	6	7	7	1	28	0.19	0.35	0.07	0.16
16	12	4	7	11	0	34	0.21	0.38	0.08	0.21
17	13	4	7	12	1	37	0.19	0.39	0.08	0.18

[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 (i)



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

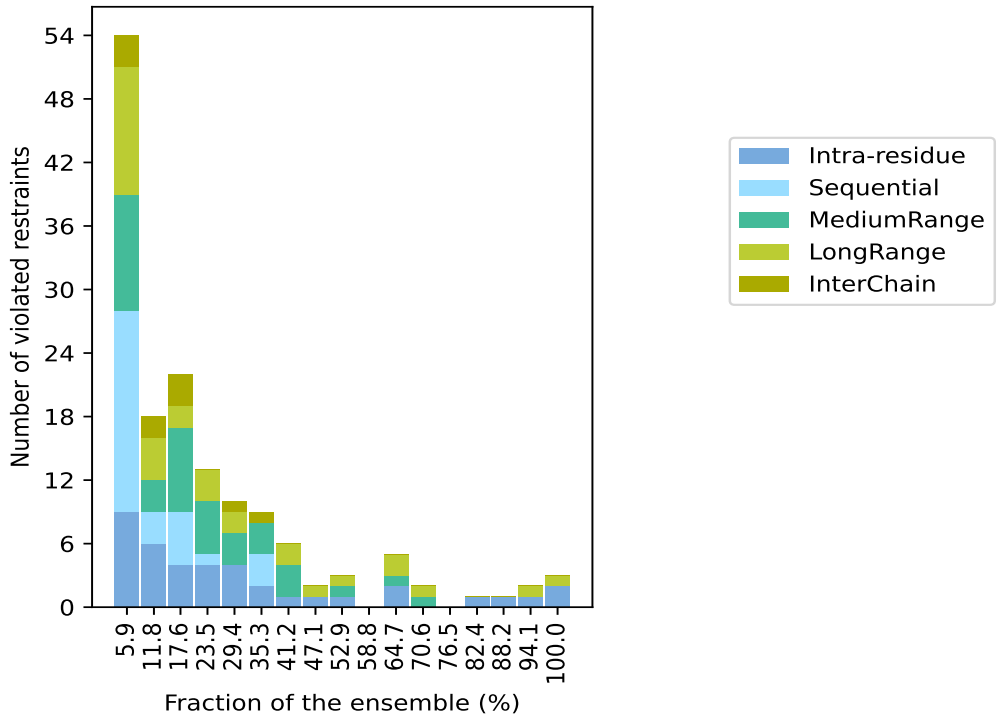
9.3 Distance violation statistics for the ensemble (i)

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, 495(IR:203, SQ:191, MR:53, LR:44, IC:4) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
9	19	11	12	3	54	1	5.9
6	3	3	4	2	18	2	11.8
4	5	8	2	3	22	3	17.6
4	1	5	3	0	13	4	23.5
4	0	3	2	1	10	5	29.4
2	3	3	0	1	9	6	35.3
1	0	3	2	0	6	7	41.2
1	0	0	1	0	2	8	47.1
1	0	1	1	0	3	9	52.9
0	0	0	0	0	0	10	58.8
2	0	1	2	0	5	11	64.7
0	0	1	1	0	2	12	70.6
0	0	0	0	0	0	13	76.5
1	0	0	0	0	1	14	82.4
1	0	0	0	0	1	15	88.2
1	0	0	1	0	2	16	94.1
2	0	0	1	0	3	17	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

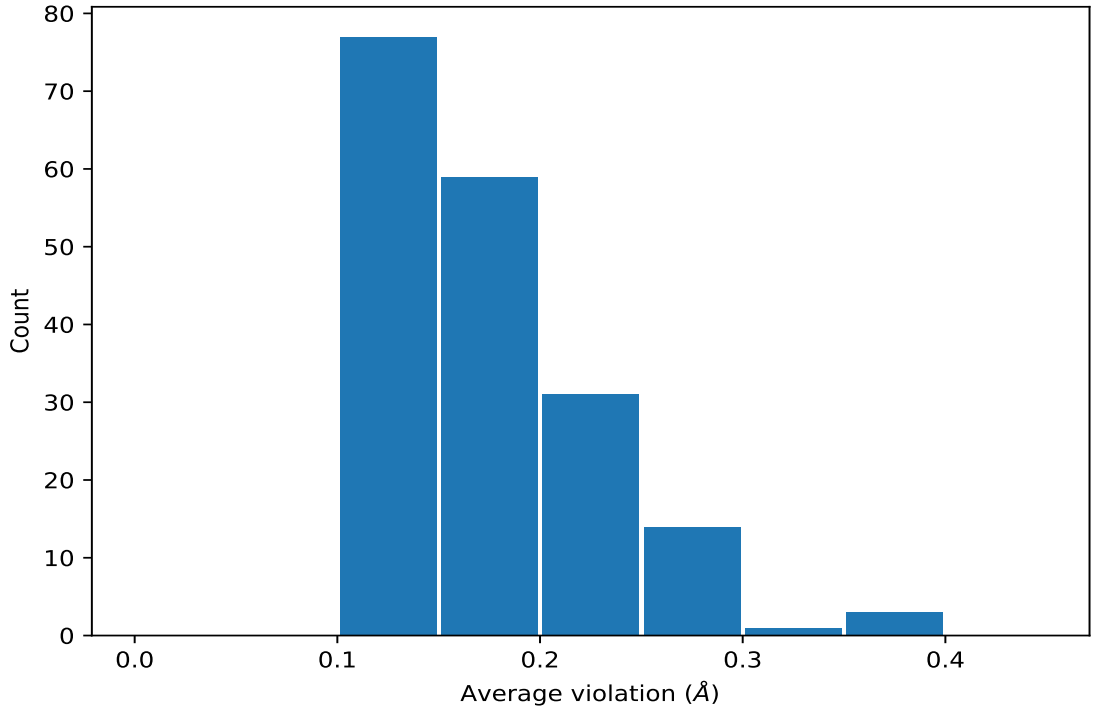
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	17	0.28	0.03	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	17	0.28	0.03	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	17	0.28	0.03	0.3
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	17	0.26	0.04	0.28
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	17	0.26	0.04	0.28
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	17	0.26	0.04	0.28
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	17	0.19	0.04	0.2
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	17	0.19	0.04	0.2
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	16	0.29	0.03	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	16	0.29	0.03	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	16	0.29	0.03	0.3
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	16	0.21	0.05	0.22
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	16	0.21	0.05	0.22
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	15	0.29	0.04	0.3
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	15	0.29	0.04	0.3
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	15	0.29	0.04	0.3

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	14	0.19	0.02	0.18
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG11	12	0.2	0.06	0.18
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG12	12	0.2	0.06	0.18
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG13	12	0.2	0.06	0.18
(1,635)	1:B:109:GLU:HB2	1:B:111:HIS:HD2	12	0.19	0.06	0.17
(1,320)	1:A:48:GLU:HB2	1:A:50:HIS:HD2	11	0.21	0.07	0.2
(1,644)	1:B:109:GLU:HA	1:B:122:CYS:HB3	11	0.2	0.05	0.19
(1,329)	1:A:48:GLU:HA	1:A:61:CYS:HB3	11	0.18	0.06	0.16
(1,234)	1:A:52:HIS:H	1:A:52:HIS:HA	11	0.12	0.01	0.12
(1,587)	1:B:121:LEU:H	1:B:121:LEU:HA	11	0.12	0.01	0.12
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD11	9	0.19	0.08	0.17
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD12	9	0.19	0.08	0.17
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD13	9	0.19	0.08	0.17
(1,293)	1:A:29:LEU:HD11	1:A:33:LEU:HA	9	0.16	0.04	0.15
(1,293)	1:A:29:LEU:HD12	1:A:33:LEU:HA	9	0.16	0.04	0.15
(1,293)	1:A:29:LEU:HD13	1:A:33:LEU:HA	9	0.16	0.04	0.15
(1,272)	1:A:60:LEU:H	1:A:60:LEU:HA	9	0.12	0.01	0.12
(1,21)	1:A:9:LYS:H	1:A:9:LYS:HB3	8	0.19	0.03	0.2
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD11	8	0.19	0.04	0.2
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD12	8	0.19	0.04	0.2
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD13	8	0.19	0.04	0.2
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG21	7	0.19	0.06	0.19
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG22	7	0.19	0.06	0.19
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG23	7	0.19	0.06	0.19
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG21	7	0.19	0.06	0.19
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG22	7	0.19	0.06	0.19
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG23	7	0.19	0.06	0.19
(1,345)	1:B:72:VAL:H	1:B:69:LEU:HA	7	0.19	0.06	0.22
(1,634)	1:B:111:HIS:HD2	1:B:107:PHE:HZ	7	0.17	0.08	0.15
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG11	7	0.16	0.05	0.15
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG12	7	0.16	0.05	0.15
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG13	7	0.16	0.05	0.15
(1,319)	1:A:50:HIS:HD2	1:A:46:PHE:HZ	7	0.13	0.04	0.12
(1,549)	1:B:113:HIS:H	1:B:113:HIS:HA	7	0.12	0.01	0.12
(1,73)	1:A:18:ALA:H	1:A:17:ILE:HB	6	0.35	0.05	0.32
(1,388)	1:B:79:ALA:H	1:B:78:ILE:HB	6	0.3	0.06	0.3
(1,588)	1:B:121:LEU:H	1:B:121:LEU:HB2	6	0.29	0.1	0.33
(1,134)	1:A:29:LEU:H	1:A:27:ILE:HA	6	0.23	0.13	0.17
(1,30)	1:A:11:VAL:H	1:A:8:LEU:HA	6	0.22	0.06	0.22
(1,608)	1:B:90:LEU:HD11	1:B:94:LEU:HA	6	0.18	0.04	0.2
(1,608)	1:B:90:LEU:HD12	1:B:94:LEU:HA	6	0.18	0.04	0.2
(1,608)	1:B:90:LEU:HD13	1:B:94:LEU:HA	6	0.18	0.04	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG12	6	0.16	0.06	0.13
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG13	6	0.16	0.06	0.13
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG12	6	0.16	0.06	0.13
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG13	6	0.16	0.06	0.13
(1,71)	1:A:17:ILE:H	1:A:18:ALA:HA	6	0.13	0.02	0.12
(1,454)	1:B:92:CYS:H	1:B:92:CYS:HA	6	0.12	0.01	0.12
(1,566)	1:B:117:LYS:H	1:B:117:LYS:HG2	5	0.36	0.05	0.38
(1,566)	1:B:117:LYS:H	1:B:117:LYS:HG3	5	0.36	0.05	0.38
(1,350)	1:B:72:VAL:H	1:B:72:VAL:HB	5	0.23	0.01	0.23
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD11	5	0.22	0.12	0.18
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD12	5	0.22	0.12	0.18
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD13	5	0.22	0.12	0.18
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD11	5	0.22	0.12	0.18
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD12	5	0.22	0.12	0.18
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD13	5	0.22	0.12	0.18
(1,35)	1:A:11:VAL:H	1:A:11:VAL:HB	5	0.2	0.01	0.2
(1,187)	1:A:37:LYS:H	1:A:37:LYS:HB2	5	0.19	0.04	0.19
(1,643)	1:B:109:GLU:HA	1:B:122:CYS:HB2	5	0.18	0.07	0.16
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG21	5	0.15	0.02	0.16
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG22	5	0.15	0.02	0.16
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG23	5	0.15	0.02	0.16
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG21	5	0.15	0.02	0.16
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG22	5	0.15	0.02	0.16
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG23	5	0.15	0.02	0.16
(2,2)	1:B:90:LEU:H	1:B:92:CYS:HA	5	0.15	0.04	0.13
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG21	5	0.14	0.02	0.14
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG22	5	0.14	0.02	0.14
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG23	5	0.14	0.02	0.14
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG21	5	0.14	0.02	0.14
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG22	5	0.14	0.02	0.14
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG23	5	0.14	0.02	0.14
(1,639)	1:B:118:ASP:HB3	1:B:115:VAL:HA	5	0.14	0.01	0.14
(1,251)	1:A:56:LYS:H	1:A:56:LYS:HG2	4	0.24	0.1	0.26
(1,251)	1:A:56:LYS:H	1:A:56:LYS:HG3	4	0.24	0.1	0.26
(1,449)	1:B:90:LEU:H	1:B:88:ILE:HA	4	0.2	0.07	0.19
(1,328)	1:A:48:GLU:HA	1:A:61:CYS:HB2	4	0.2	0.05	0.21
(1,20)	1:A:9:LYS:H	1:A:9:LYS:HB2	4	0.19	0.05	0.18
(1,600)	1:B:75:ALA:HA	1:B:78:ILE:HB	4	0.18	0.03	0.18
(2,1)	1:A:29:LEU:H	1:A:31:CYS:HA	4	0.16	0.03	0.17
(1,550)	1:B:113:HIS:H	1:B:113:HIS:HB2	4	0.16	0.02	0.15
(1,285)	1:A:14:ALA:HA	1:A:17:ILE:HB	4	0.15	0.03	0.16
(1,597)	1:B:68:VAL:HA	1:B:71:LYS:HB2	4	0.14	0.04	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,597)	1:B:68:VAL:HA	1:B:71:LYS:HB3	4	0.14	0.04	0.12
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG21	4	0.13	0.02	0.12
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG22	4	0.13	0.02	0.12
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG23	4	0.13	0.02	0.12
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG21	4	0.12	0.01	0.12
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG22	4	0.12	0.01	0.12
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG23	4	0.12	0.01	0.12
(1,139)	1:A:31:CYS:H	1:A:31:CYS:HA	4	0.12	0.01	0.12
(1,460)	1:B:93:VAL:H	1:B:92:CYS:HB2	4	0.12	0.01	0.12
(1,460)	1:B:93:VAL:H	1:B:92:CYS:HB3	4	0.12	0.01	0.12
(1,273)	1:A:60:LEU:H	1:A:60:LEU:HB2	3	0.36	0.07	0.39
(1,47)	1:A:13:CYS:H	1:A:10:LYS:HA	3	0.23	0.02	0.23
(1,539)	1:B:111:HIS:H	1:B:109:GLU:HG2	3	0.21	0.07	0.22
(1,539)	1:B:111:HIS:H	1:B:109:GLU:HG3	3	0.21	0.07	0.22
(1,224)	1:A:50:HIS:H	1:A:48:GLU:HG2	3	0.2	0.06	0.2
(1,224)	1:A:50:HIS:H	1:A:48:GLU:HG3	3	0.2	0.06	0.2
(1,353)	1:B:73:ALA:H	1:B:70:LYS:HA	3	0.2	0.02	0.19
(1,327)	1:A:61:CYS:HB3	1:A:47:CYS:HB3	3	0.19	0.08	0.17
(1,526)	1:B:109:GLU:H	1:B:106:CYS:HA	3	0.18	0.05	0.16
(1,642)	1:B:122:CYS:HB3	1:B:108:CYS:HB3	3	0.18	0.05	0.18
(1,9)	1:B:113:HIS:HE1	1:A:27:ILE:HG12	3	0.17	0.01	0.17
(1,9)	1:B:113:HIS:HE1	1:A:27:ILE:HG13	3	0.17	0.01	0.17
(1,9)	1:B:113:HIS:HE2	1:A:27:ILE:HG12	3	0.17	0.01	0.17
(1,9)	1:B:113:HIS:HE2	1:A:27:ILE:HG13	3	0.17	0.01	0.17
(1,1)	1:B:91:PRO:HD2	1:A:54:VAL:HG11	3	0.17	0.03	0.17
(1,1)	1:B:91:PRO:HD2	1:A:54:VAL:HG12	3	0.17	0.03	0.17
(1,1)	1:B:91:PRO:HD2	1:A:54:VAL:HG13	3	0.17	0.03	0.17
(1,1)	1:B:91:PRO:HD3	1:A:54:VAL:HG11	3	0.17	0.03	0.17
(1,1)	1:B:91:PRO:HD3	1:A:54:VAL:HG12	3	0.17	0.03	0.17
(1,1)	1:B:91:PRO:HD3	1:A:54:VAL:HG13	3	0.17	0.03	0.17
(1,211)	1:A:48:GLU:H	1:A:45:CYS:HA	3	0.17	0.01	0.17
(1,5)	1:B:113:HIS:HD2	1:A:24:CYS:HA	3	0.16	0.02	0.17
(1,358)	1:B:73:ALA:H	1:B:72:VAL:H	3	0.14	0.03	0.12
(1,599)	1:B:74:CYS:HB2	1:B:78:ILE:HG21	3	0.14	0.02	0.15
(1,599)	1:B:74:CYS:HB2	1:B:78:ILE:HG22	3	0.14	0.02	0.15
(1,599)	1:B:74:CYS:HB2	1:B:78:ILE:HG23	3	0.14	0.02	0.15
(1,599)	1:B:74:CYS:HB3	1:B:78:ILE:HG21	3	0.14	0.02	0.15
(1,599)	1:B:74:CYS:HB3	1:B:78:ILE:HG22	3	0.14	0.02	0.15
(1,599)	1:B:74:CYS:HB3	1:B:78:ILE:HG23	3	0.14	0.02	0.15
(1,43)	1:A:12:ALA:H	1:A:11:VAL:H	3	0.13	0.01	0.13
(1,586)	1:B:120:HIS:H	1:B:121:LEU:HD11	3	0.13	0.01	0.13
(1,586)	1:B:120:HIS:H	1:B:121:LEU:HD12	3	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,586)	1:B:120:HIS:H	1:B:121:LEU:HD13	3	0.13	0.01	0.13
(1,74)	1:A:18:ALA:H	1:A:17:ILE:HG12	3	0.13	0.02	0.12
(1,374)	1:B:75:ALA:H	1:B:75:ALA:HA	3	0.13	0.0	0.13
(1,386)	1:B:78:ILE:H	1:B:79:ALA:HA	3	0.13	0.01	0.12
(1,59)	1:A:14:ALA:H	1:A:14:ALA:HA	3	0.12	0.01	0.12
(1,422)	1:B:84:ALA:H	1:B:84:ALA:HA	3	0.12	0.0	0.12
(1,324)	1:A:57:ASP:HB3	1:A:54:VAL:HA	3	0.11	0.0	0.11
(1,335)	1:B:70:LYS:H	1:B:70:LYS:HB2	2	0.24	0.04	0.24
(1,362)	1:B:74:CYS:H	1:B:71:LYS:HA	2	0.24	0.02	0.24
(1,22)	1:A:9:LYS:H	1:A:9:LYS:HG2	2	0.24	0.12	0.24
(1,22)	1:A:9:LYS:H	1:A:9:LYS:HG3	2	0.24	0.12	0.24
(1,617)	1:B:97:LEU:HD11	1:B:98:LYS:HA	2	0.19	0.08	0.19
(1,617)	1:B:97:LEU:HD12	1:B:98:LYS:HA	2	0.19	0.08	0.19
(1,617)	1:B:97:LEU:HD13	1:B:98:LYS:HA	2	0.19	0.08	0.19
(1,548)	1:B:112:CYS:H	1:B:113:HIS:HA	2	0.16	0.01	0.16
(1,6)	1:B:113:HIS:HD2	1:A:24:CYS:HB2	2	0.16	0.04	0.16
(1,13)	1:A:52:HIS:HE1	1:B:88:ILE:HD11	2	0.15	0.04	0.15
(1,13)	1:A:52:HIS:HE1	1:B:88:ILE:HD12	2	0.15	0.04	0.15
(1,13)	1:A:52:HIS:HE1	1:B:88:ILE:HD13	2	0.15	0.04	0.15
(1,13)	1:A:52:HIS:HE2	1:B:88:ILE:HD11	2	0.15	0.04	0.15
(1,13)	1:A:52:HIS:HE2	1:B:88:ILE:HD12	2	0.15	0.04	0.15
(1,13)	1:A:52:HIS:HE2	1:B:88:ILE:HD13	2	0.15	0.04	0.15
(1,314)	1:A:29:LEU:HD11	1:A:46:PHE:HZ	2	0.14	0.02	0.14
(1,314)	1:A:29:LEU:HD12	1:A:46:PHE:HZ	2	0.14	0.02	0.14
(1,314)	1:A:29:LEU:HD13	1:A:46:PHE:HZ	2	0.14	0.02	0.14
(1,524)	1:B:108:CYS:H	1:B:108:CYS:HB2	2	0.14	0.02	0.14
(1,38)	1:A:12:ALA:H	1:A:9:LYS:HA	2	0.14	0.01	0.14
(1,235)	1:A:52:HIS:H	1:A:52:HIS:HB2	2	0.14	0.02	0.14
(1,309)	1:A:27:ILE:HD11	1:A:46:PHE:HD1	2	0.12	0.01	0.12
(1,309)	1:A:27:ILE:HD11	1:A:46:PHE:HD2	2	0.12	0.01	0.12
(1,309)	1:A:27:ILE:HD12	1:A:46:PHE:HD1	2	0.12	0.01	0.12
(1,309)	1:A:27:ILE:HD12	1:A:46:PHE:HD2	2	0.12	0.01	0.12
(1,309)	1:A:27:ILE:HD13	1:A:46:PHE:HD1	2	0.12	0.01	0.12
(1,309)	1:A:27:ILE:HD13	1:A:46:PHE:HD2	2	0.12	0.01	0.12
(1,77)	1:A:18:ALA:H	1:A:18:ALA:HA	2	0.12	0.01	0.12
(1,271)	1:A:59:HIS:H	1:A:60:LEU:HD11	2	0.12	0.01	0.12
(1,271)	1:A:59:HIS:H	1:A:60:LEU:HD12	2	0.12	0.01	0.12
(1,271)	1:A:59:HIS:H	1:A:60:LEU:HD13	2	0.12	0.01	0.12
(1,282)	1:A:7:VAL:HA	1:A:10:LYS:HB2	2	0.12	0.01	0.12
(1,282)	1:A:7:VAL:HA	1:A:10:LYS:HB3	2	0.12	0.01	0.12
(1,308)	1:A:17:ILE:HG12	1:A:46:PHE:HZ	2	0.12	0.01	0.12
(1,584)	1:B:120:HIS:H	1:B:120:HIS:HA	2	0.12	0.0	0.12

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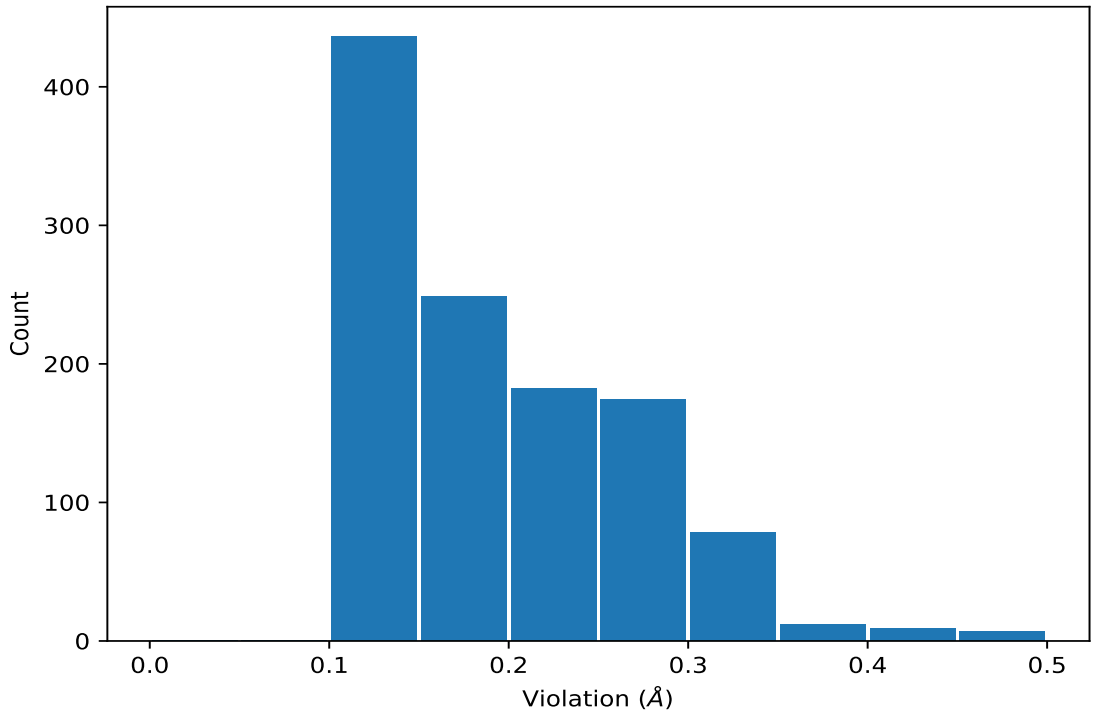
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,623)	1:B:78:ILE:HG12	1:B:107:PHE:HZ	2	0.12	0.0	0.12

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD11	13	0.46
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD12	13	0.46
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD13	13	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD11	13	0.46
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD12	13	0.46
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD13	13	0.46
(1,134)	1:A:29:LEU:H	1:A:27:ILE:HA	1	0.46
(1,73)	1:A:18:ALA:H	1:A:17:ILE:HB	5	0.44
(1,273)	1:A:60:LEU:H	1:A:60:LEU:HB2	5	0.43
(1,566)	1:B:117:LYS:H	1:B:117:LYS:HG2	8	0.41
(1,566)	1:B:117:LYS:H	1:B:117:LYS:HG3	8	0.41
(1,566)	1:B:117:LYS:H	1:B:117:LYS:HG2	9	0.41
(1,566)	1:B:117:LYS:H	1:B:117:LYS:HG3	9	0.41
(1,520)	1:B:108:CYS:H	1:B:107:PHE:HB2	10	0.41
(1,520)	1:B:108:CYS:H	1:B:107:PHE:HB3	10	0.41
(1,320)	1:A:48:GLU:HB2	1:A:50:HIS:HD2	9	0.4
(1,73)	1:A:18:ALA:H	1:A:17:ILE:HB	11	0.39
(1,588)	1:B:121:LEU:H	1:B:121:LEU:HB2	3	0.39
(1,388)	1:B:79:ALA:H	1:B:78:ILE:HB	8	0.39
(1,273)	1:A:60:LEU:H	1:A:60:LEU:HB2	17	0.39
(1,205)	1:A:47:CYS:H	1:A:46:PHE:HB2	4	0.39
(1,205)	1:A:47:CYS:H	1:A:46:PHE:HB3	4	0.39
(1,566)	1:B:117:LYS:H	1:B:117:LYS:HG2	16	0.38
(1,566)	1:B:117:LYS:H	1:B:117:LYS:HG3	16	0.38
(1,588)	1:B:121:LEU:H	1:B:121:LEU:HB2	5	0.37
(1,588)	1:B:121:LEU:H	1:B:121:LEU:HB2	17	0.37
(1,22)	1:A:9:LYS:H	1:A:9:LYS:HG2	5	0.36
(1,22)	1:A:9:LYS:H	1:A:9:LYS:HG3	5	0.36
(1,634)	1:B:111:HIS:HD2	1:B:107:PHE:HZ	6	0.35
(1,388)	1:B:79:ALA:H	1:B:78:ILE:HB	15	0.35
(1,251)	1:A:56:LYS:H	1:A:56:LYS:HG2	16	0.35
(1,251)	1:A:56:LYS:H	1:A:56:LYS:HG3	16	0.35
(1,635)	1:B:109:GLU:HB2	1:B:111:HIS:HD2	6	0.34
(1,566)	1:B:117:LYS:H	1:B:117:LYS:HG2	12	0.34
(1,566)	1:B:117:LYS:H	1:B:117:LYS:HG3	12	0.34
(1,413)	1:B:83:ALA:H	1:B:82:VAL:HB	9	0.33
(1,251)	1:A:56:LYS:H	1:A:56:LYS:HG2	12	0.33
(1,251)	1:A:56:LYS:H	1:A:56:LYS:HG3	12	0.33
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD11	16	0.33
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD12	16	0.33
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD13	16	0.33
(1,134)	1:A:29:LEU:H	1:A:27:ILE:HA	10	0.33
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	7	0.32
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	7	0.32
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	1:A:18:ALA:H	1:A:17:ILE:HB	7	0.32
(1,73)	1:A:18:ALA:H	1:A:17:ILE:HB	15	0.32
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	10	0.32
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	10	0.32
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	10	0.32
(1,388)	1:B:79:ALA:H	1:B:78:ILE:HB	11	0.32
(1,329)	1:A:48:GLU:HA	1:A:61:CYS:HB3	17	0.32
(1,302)	1:A:36:LEU:HD11	1:A:37:LYS:HA	7	0.32
(1,302)	1:A:36:LEU:HD12	1:A:37:LYS:HA	7	0.32
(1,302)	1:A:36:LEU:HD13	1:A:37:LYS:HA	7	0.32
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD11	6	0.32
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD12	6	0.32
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD13	6	0.32
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	10	0.32
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	10	0.32
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	10	0.32
(1,98)	1:A:22:ALA:H	1:A:21:VAL:HB	9	0.31
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	5	0.31
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	5	0.31
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	5	0.31
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	11	0.31
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	11	0.31
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	11	0.31
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	12	0.31
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	12	0.31
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	12	0.31
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	15	0.31
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	15	0.31
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	15	0.31
(1,73)	1:A:18:ALA:H	1:A:17:ILE:HB	2	0.31
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG21	6	0.31
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG22	6	0.31
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG23	6	0.31
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG21	6	0.31
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG22	6	0.31
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG23	6	0.31
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	1	0.31
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	1	0.31
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	1	0.31
(1,449)	1:B:90:LEU:H	1:B:88:ILE:HA	12	0.31
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	2	0.31
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	2	0.31
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	7	0.31
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	7	0.31
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	7	0.31
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	8	0.31
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	8	0.31
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	8	0.31
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG11	10	0.31
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG12	10	0.31
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG13	10	0.31
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	1	0.31
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	1	0.31
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	1	0.31
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	9	0.31
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	9	0.31
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	9	0.31
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	17	0.31
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	17	0.31
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	17	0.31
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	3	0.3
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	3	0.3
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	3	0.3
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	8	0.3
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	8	0.3
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	8	0.3
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	13	0.3
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	13	0.3
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	13	0.3
(1,73)	1:A:18:ALA:H	1:A:17:ILE:HB	8	0.3
(1,644)	1:B:109:GLU:HA	1:B:122:CYS:HB3	16	0.3
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	12	0.3
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	12	0.3
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	12	0.3
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	16	0.3
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	16	0.3
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	16	0.3
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	17	0.3
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	17	0.3
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	17	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	3	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	3	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	11	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	11	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	11	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	13	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	13	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	13	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	14	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	14	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	14	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	15	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	15	0.3
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	15	0.3
(1,327)	1:A:61:CYS:HB3	1:A:47:CYS:HB3	7	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	2	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	2	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	2	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	6	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	6	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	6	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	7	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	7	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	7	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	12	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	12	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	12	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	16	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	16	0.3
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	16	0.3
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	2	0.29
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	2	0.29
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	2	0.29
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	14	0.29
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	14	0.29
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	14	0.29
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	16	0.29
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	16	0.29
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	16	0.29
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	17	0.29
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	17	0.29
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	17	0.29
(1,588)	1:B:121:LEU:H	1:B:121:LEU:HB2	9	0.29
(1,539)	1:B:111:HIS:H	1:B:109:GLU:HG2	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:B:111:HIS:H	1:B:109:GLU:HG3	14	0.29
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	4	0.29
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	4	0.29
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	4	0.29
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	7	0.29
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	7	0.29
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	7	0.29
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	13	0.29
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	13	0.29
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	13	0.29
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	1	0.29
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	1	0.29
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	1	0.29
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	12	0.29
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	12	0.29
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	12	0.29
(1,388)	1:B:79:ALA:H	1:B:78:ILE:HB	2	0.29
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG11	16	0.29
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG12	16	0.29
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG13	16	0.29
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	16	0.29
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	16	0.29
(1,30)	1:A:11:VAL:H	1:A:8:LEU:HA	9	0.29
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	3	0.29
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	3	0.29
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	3	0.29
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	8	0.29
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	8	0.29
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	8	0.29
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	6	0.28
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	6	0.28
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	3	0.28
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	3	0.28
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	3	0.28
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	9	0.28
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	9	0.28
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	9	0.28
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	5	0.28
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	5	0.28
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	5	0.28
(1,335)	1:B:70:LYS:H	1:B:70:LYS:HB2	4	0.28
(1,224)	1:A:50:HIS:H	1:A:48:GLU:HG2	17	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:A:50:HIS:H	1:A:48:GLU:HG3	17	0.28
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	14	0.28
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	14	0.28
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	14	0.28
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	4	0.27
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	4	0.27
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	4	0.27
(1,644)	1:B:109:GLU:HA	1:B:122:CYS:HB3	11	0.27
(1,617)	1:B:97:LEU:HD11	1:B:98:LYS:HA	5	0.27
(1,617)	1:B:97:LEU:HD12	1:B:98:LYS:HA	5	0.27
(1,617)	1:B:97:LEU:HD13	1:B:98:LYS:HA	5	0.27
(1,566)	1:B:117:LYS:H	1:B:117:LYS:HG2	13	0.27
(1,566)	1:B:117:LYS:H	1:B:117:LYS:HG3	13	0.27
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	6	0.27
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	6	0.27
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	6	0.27
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	15	0.27
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	15	0.27
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	15	0.27
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	16	0.27
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	16	0.27
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	16	0.27
(1,345)	1:B:72:VAL:H	1:B:69:LEU:HA	4	0.27
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	10	0.27
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	10	0.27
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	12	0.27
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	12	0.27
(1,273)	1:A:60:LEU:H	1:A:60:LEU:HB2	3	0.27
(1,20)	1:A:9:LYS:H	1:A:9:LYS:HB2	17	0.27
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	5	0.27
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	5	0.27
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	5	0.27
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	15	0.27
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	15	0.27
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	15	0.27
(1,643)	1:B:109:GLU:HA	1:B:122:CYS:HB2	5	0.26
(1,643)	1:B:109:GLU:HA	1:B:122:CYS:HB2	9	0.26
(1,47)	1:A:13:CYS:H	1:A:10:LYS:HA	14	0.26
(1,388)	1:B:79:ALA:H	1:B:78:ILE:HB	5	0.26
(1,362)	1:B:74:CYS:H	1:B:71:LYS:HA	16	0.26
(1,328)	1:A:48:GLU:HA	1:A:61:CYS:HB2	9	0.26
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG11	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG12	3	0.26
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG13	3	0.26
(1,30)	1:A:11:VAL:H	1:A:8:LEU:HA	14	0.26
(1,187)	1:A:37:LYS:H	1:A:37:LYS:HB2	12	0.26
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	4	0.26
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	4	0.26
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	4	0.26
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	13	0.26
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	13	0.26
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	13	0.26
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG12	11	0.26
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG13	11	0.26
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG12	11	0.26
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG13	11	0.26
(1,635)	1:B:109:GLU:HB2	1:B:111:HIS:HD2	5	0.25
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	13	0.25
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	13	0.25
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	17	0.25
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	17	0.25
(1,526)	1:B:109:GLU:H	1:B:106:CYS:HA	1	0.25
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	6	0.25
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	6	0.25
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	6	0.25
(1,350)	1:B:72:VAL:H	1:B:72:VAL:HB	4	0.25
(1,233)	1:A:51:CYS:H	1:A:52:HIS:HA	9	0.25
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	6	0.24
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	6	0.24
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	6	0.24
(1,642)	1:B:122:CYS:HB3	1:B:108:CYS:HB3	16	0.24
(1,608)	1:B:90:LEU:HD11	1:B:94:LEU:HA	9	0.24
(1,608)	1:B:90:LEU:HD12	1:B:94:LEU:HA	9	0.24
(1,608)	1:B:90:LEU:HD13	1:B:94:LEU:HA	9	0.24
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD11	10	0.24
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD12	10	0.24
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD13	10	0.24
(1,519)	1:B:108:CYS:H	1:B:90:LEU:HD11	10	0.24
(1,519)	1:B:108:CYS:H	1:B:90:LEU:HD12	10	0.24
(1,519)	1:B:108:CYS:H	1:B:90:LEU:HD13	10	0.24
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	5	0.24
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	5	0.24
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	5	0.24
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	14	0.24
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	14	0.24
(1,453)	1:B:90:LEU:H	1:B:90:LEU:HG	9	0.24
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	17	0.24
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	17	0.24
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	17	0.24
(1,350)	1:B:72:VAL:H	1:B:72:VAL:HB	3	0.24
(1,345)	1:B:72:VAL:H	1:B:69:LEU:HA	9	0.24
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	7	0.24
(1,329)	1:A:48:GLU:HA	1:A:61:CYS:HB3	13	0.24
(1,329)	1:A:48:GLU:HA	1:A:61:CYS:HB3	16	0.24
(1,320)	1:A:48:GLU:HB2	1:A:50:HIS:HD2	8	0.24
(1,320)	1:A:48:GLU:HB2	1:A:50:HIS:HD2	11	0.24
(1,318)	1:A:36:LEU:HD11	1:A:46:PHE:HB2	4	0.24
(1,318)	1:A:36:LEU:HD12	1:A:46:PHE:HB2	4	0.24
(1,318)	1:A:36:LEU:HD13	1:A:46:PHE:HB2	4	0.24
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	2	0.24
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	2	0.24
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	7	0.24
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	7	0.24
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	17	0.24
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	17	0.24
(1,30)	1:A:11:VAL:H	1:A:8:LEU:HA	4	0.24
(1,21)	1:A:9:LYS:H	1:A:9:LYS:HB3	4	0.24
(2,2)	1:B:90:LEU:H	1:B:92:CYS:HA	10	0.23
(1,644)	1:B:109:GLU:HA	1:B:122:CYS:HB3	17	0.23
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG11	4	0.23
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG12	4	0.23
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG13	4	0.23
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG11	5	0.23
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG12	5	0.23
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG13	5	0.23
(1,635)	1:B:109:GLU:HB2	1:B:111:HIS:HD2	13	0.23
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	4	0.23
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	4	0.23
(1,47)	1:A:13:CYS:H	1:A:10:LYS:HA	16	0.23
(1,362)	1:B:74:CYS:H	1:B:71:LYS:HA	17	0.23
(1,353)	1:B:73:ALA:H	1:B:70:LYS:HA	7	0.23
(1,350)	1:B:72:VAL:H	1:B:72:VAL:HB	13	0.23
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	4	0.23
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	4	0.23
(1,3)	1:A:30:PRO:HD3	1:B:115:VAL:HG11	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:A:30:PRO:HD3	1:B:115:VAL:HG12	9	0.23
(1,3)	1:A:30:PRO:HD3	1:B:115:VAL:HG13	9	0.23
(1,293)	1:A:29:LEU:HD11	1:A:33:LEU:HA	7	0.23
(1,293)	1:A:29:LEU:HD12	1:A:33:LEU:HA	7	0.23
(1,293)	1:A:29:LEU:HD13	1:A:33:LEU:HA	7	0.23
(1,278)	1:A:60:LEU:H	1:A:61:CYS:H	15	0.23
(1,245)	1:A:56:LYS:H	1:A:55:CYS:HB2	9	0.23
(1,644)	1:B:109:GLU:HA	1:B:122:CYS:HB3	13	0.22
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG21	2	0.22
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG22	2	0.22
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG23	2	0.22
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG21	2	0.22
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG22	2	0.22
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG23	2	0.22
(1,608)	1:B:90:LEU:HD11	1:B:94:LEU:HA	17	0.22
(1,608)	1:B:90:LEU:HD12	1:B:94:LEU:HA	17	0.22
(1,608)	1:B:90:LEU:HD13	1:B:94:LEU:HA	17	0.22
(1,560)	1:B:117:LYS:H	1:B:116:CYS:HB2	15	0.22
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD11	16	0.22
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD12	16	0.22
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD13	16	0.22
(1,539)	1:B:111:HIS:H	1:B:109:GLU:HG2	4	0.22
(1,539)	1:B:111:HIS:H	1:B:109:GLU:HG3	4	0.22
(1,506)	1:B:106:CYS:H	1:B:103:CYS:HA	9	0.22
(1,350)	1:B:72:VAL:H	1:B:72:VAL:HB	10	0.22
(1,345)	1:B:72:VAL:H	1:B:69:LEU:HA	12	0.22
(1,345)	1:B:72:VAL:H	1:B:69:LEU:HA	15	0.22
(1,328)	1:A:48:GLU:HA	1:A:61:CYS:HB2	2	0.22
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG11	11	0.22
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG12	11	0.22
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG13	11	0.22
(1,320)	1:A:48:GLU:HB2	1:A:50:HIS:HD2	1	0.22
(1,319)	1:A:50:HIS:HD2	1:A:46:PHE:HZ	4	0.22
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	1	0.22
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	1	0.22
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	3	0.22
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	3	0.22
(1,293)	1:A:29:LEU:HD11	1:A:33:LEU:HA	9	0.22
(1,293)	1:A:29:LEU:HD12	1:A:33:LEU:HA	9	0.22
(1,293)	1:A:29:LEU:HD13	1:A:33:LEU:HA	9	0.22
(1,196)	1:A:46:PHE:H	1:A:36:LEU:HD11	17	0.22
(1,196)	1:A:46:PHE:H	1:A:36:LEU:HD12	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:A:46:PHE:H	1:A:36:LEU:HD13	17	0.22
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG12	15	0.22
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG13	15	0.22
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG12	15	0.22
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG13	15	0.22
(1,644)	1:B:109:GLU:HA	1:B:122:CYS:HB3	6	0.21
(1,635)	1:B:109:GLU:HB2	1:B:111:HIS:HD2	9	0.21
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	1	0.21
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	1	0.21
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	16	0.21
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	16	0.21
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG21	4	0.21
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG22	4	0.21
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG23	4	0.21
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG21	4	0.21
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG22	4	0.21
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG23	4	0.21
(1,600)	1:B:75:ALA:HA	1:B:78:ILE:HB	7	0.21
(1,598)	1:B:75:ALA:HB1	1:B:72:VAL:HA	6	0.21
(1,598)	1:B:75:ALA:HB2	1:B:72:VAL:HA	6	0.21
(1,598)	1:B:75:ALA:HB3	1:B:72:VAL:HA	6	0.21
(1,597)	1:B:68:VAL:HA	1:B:71:LYS:HB2	16	0.21
(1,597)	1:B:68:VAL:HA	1:B:71:LYS:HB3	16	0.21
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD11	15	0.21
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD12	15	0.21
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD13	15	0.21
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD11	17	0.21
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD12	17	0.21
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD13	17	0.21
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	10	0.21
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	10	0.21
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	10	0.21
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	11	0.21
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	11	0.21
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	11	0.21
(1,449)	1:B:90:LEU:H	1:B:88:ILE:HA	4	0.21
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG11	4	0.21
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG12	4	0.21
(1,409)	1:B:82:VAL:H	1:B:82:VAL:HG13	4	0.21
(1,350)	1:B:72:VAL:H	1:B:72:VAL:HB	2	0.21
(1,35)	1:A:11:VAL:H	1:A:11:VAL:HB	2	0.21
(1,35)	1:A:11:VAL:H	1:A:11:VAL:HB	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	6	0.21
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	14	0.21
(1,335)	1:B:70:LYS:H	1:B:70:LYS:HB2	3	0.21
(1,21)	1:A:9:LYS:H	1:A:9:LYS:HB3	16	0.21
(1,204)	1:A:47:CYS:H	1:A:29:LEU:HD11	4	0.21
(1,204)	1:A:47:CYS:H	1:A:29:LEU:HD12	4	0.21
(1,204)	1:A:47:CYS:H	1:A:29:LEU:HD13	4	0.21
(1,197)	1:A:46:PHE:H	1:A:43:ALA:HA	1	0.21
(1,134)	1:A:29:LEU:H	1:A:27:ILE:HA	4	0.21
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	2	0.2
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	2	0.2
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	3	0.2
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	3	0.2
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	9	0.2
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	9	0.2
(1,608)	1:B:90:LEU:HD11	1:B:94:LEU:HA	16	0.2
(1,608)	1:B:90:LEU:HD12	1:B:94:LEU:HA	16	0.2
(1,608)	1:B:90:LEU:HD13	1:B:94:LEU:HA	16	0.2
(1,47)	1:A:13:CYS:H	1:A:10:LYS:HA	7	0.2
(1,388)	1:B:79:ALA:H	1:B:78:ILE:HB	7	0.2
(1,35)	1:A:11:VAL:H	1:A:11:VAL:HB	4	0.2
(1,35)	1:A:11:VAL:H	1:A:11:VAL:HB	10	0.2
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	13	0.2
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	15	0.2
(1,328)	1:A:48:GLU:HA	1:A:61:CYS:HB2	5	0.2
(1,320)	1:A:48:GLU:HB2	1:A:50:HIS:HD2	5	0.2
(1,320)	1:A:48:GLU:HB2	1:A:50:HIS:HD2	10	0.2
(1,224)	1:A:50:HIS:H	1:A:48:GLU:HG2	6	0.2
(1,224)	1:A:50:HIS:H	1:A:48:GLU:HG3	6	0.2
(1,21)	1:A:9:LYS:H	1:A:9:LYS:HB3	6	0.2
(1,21)	1:A:9:LYS:H	1:A:9:LYS:HB3	9	0.2
(1,21)	1:A:9:LYS:H	1:A:9:LYS:HB3	10	0.2
(1,20)	1:A:9:LYS:H	1:A:9:LYS:HB2	1	0.2
(1,1)	1:B:91:PRO:HD2	1:A:54:VAL:HG11	7	0.2
(1,1)	1:B:91:PRO:HD2	1:A:54:VAL:HG12	7	0.2
(1,1)	1:B:91:PRO:HD2	1:A:54:VAL:HG13	7	0.2
(1,1)	1:B:91:PRO:HD3	1:A:54:VAL:HG11	7	0.2
(1,1)	1:B:91:PRO:HD3	1:A:54:VAL:HG12	7	0.2
(1,1)	1:B:91:PRO:HD3	1:A:54:VAL:HG13	7	0.2
(2,1)	1:A:29:LEU:H	1:A:31:CYS:HA	1	0.19
(2,1)	1:A:29:LEU:H	1:A:31:CYS:HA	10	0.19
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD11	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD12	10	0.19
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD13	10	0.19
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD11	10	0.19
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD12	10	0.19
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD13	10	0.19
(1,644)	1:B:109:GLU:HA	1:B:122:CYS:HB3	8	0.19
(1,635)	1:B:109:GLU:HB2	1:B:111:HIS:HD2	1	0.19
(1,633)	1:B:97:LEU:HD11	1:B:107:PHE:HB2	10	0.19
(1,633)	1:B:97:LEU:HD12	1:B:107:PHE:HB2	10	0.19
(1,633)	1:B:97:LEU:HD13	1:B:107:PHE:HB2	10	0.19
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	14	0.19
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	14	0.19
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG21	16	0.19
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG22	16	0.19
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG23	16	0.19
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG21	16	0.19
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG22	16	0.19
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG23	16	0.19
(1,608)	1:B:90:LEU:HD11	1:B:94:LEU:HA	7	0.19
(1,608)	1:B:90:LEU:HD12	1:B:94:LEU:HA	7	0.19
(1,608)	1:B:90:LEU:HD13	1:B:94:LEU:HA	7	0.19
(1,600)	1:B:75:ALA:HA	1:B:78:ILE:HB	6	0.19
(1,6)	1:B:113:HIS:HD2	1:A:24:CYS:HB2	1	0.19
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD11	2	0.19
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD12	2	0.19
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD13	2	0.19
(1,550)	1:B:113:HIS:H	1:B:113:HIS:HB2	14	0.19
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	2	0.19
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	2	0.19
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	2	0.19
(1,358)	1:B:73:ALA:H	1:B:72:VAL:H	8	0.19
(1,353)	1:B:73:ALA:H	1:B:70:LYS:HA	13	0.19
(1,353)	1:B:73:ALA:H	1:B:70:LYS:HA	14	0.19
(1,35)	1:A:11:VAL:H	1:A:11:VAL:HB	13	0.19
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	9	0.19
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	10	0.19
(1,329)	1:A:48:GLU:HA	1:A:61:CYS:HB3	7	0.19
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG11	9	0.19
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG12	9	0.19
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG13	9	0.19
(1,320)	1:A:48:GLU:HB2	1:A:50:HIS:HD2	3	0.19
(1,320)	1:A:48:GLU:HB2	1:A:50:HIS:HD2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:A:48:GLU:HB2	1:A:50:HIS:HD2	13	0.19
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	8	0.19
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	8	0.19
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	14	0.19
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	14	0.19
(1,30)	1:A:11:VAL:H	1:A:8:LEU:HA	7	0.19
(1,30)	1:A:11:VAL:H	1:A:8:LEU:HA	15	0.19
(1,293)	1:A:29:LEU:HD11	1:A:33:LEU:HA	6	0.19
(1,293)	1:A:29:LEU:HD12	1:A:33:LEU:HA	6	0.19
(1,293)	1:A:29:LEU:HD13	1:A:33:LEU:HA	6	0.19
(1,285)	1:A:14:ALA:HA	1:A:17:ILE:HB	7	0.19
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD11	5	0.19
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD12	5	0.19
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD13	5	0.19
(1,187)	1:A:37:LYS:H	1:A:37:LYS:HB2	2	0.19
(1,187)	1:A:37:LYS:H	1:A:37:LYS:HB2	6	0.19
(1,13)	1:A:52:HIS:HE1	1:B:88:ILE:HD11	13	0.19
(1,13)	1:A:52:HIS:HE1	1:B:88:ILE:HD12	13	0.19
(1,13)	1:A:52:HIS:HE1	1:B:88:ILE:HD13	13	0.19
(1,13)	1:A:52:HIS:HE2	1:B:88:ILE:HD11	13	0.19
(1,13)	1:A:52:HIS:HE2	1:B:88:ILE:HD12	13	0.19
(1,13)	1:A:52:HIS:HE2	1:B:88:ILE:HD13	13	0.19
(1,9)	1:B:113:HIS:HE1	1:A:27:ILE:HG12	8	0.18
(1,9)	1:B:113:HIS:HE1	1:A:27:ILE:HG13	8	0.18
(1,9)	1:B:113:HIS:HE2	1:A:27:ILE:HG12	8	0.18
(1,9)	1:B:113:HIS:HE2	1:A:27:ILE:HG13	8	0.18
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD11	6	0.18
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD12	6	0.18
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD13	6	0.18
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD11	6	0.18
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD12	6	0.18
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD13	6	0.18
(1,642)	1:B:122:CYS:HB3	1:B:108:CYS:HB3	17	0.18
(1,634)	1:B:111:HIS:HD2	1:B:107:PHE:HZ	13	0.18
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	5	0.18
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	5	0.18
(1,61)	1:A:16:ALA:H	1:A:13:CYS:HA	6	0.18
(1,5)	1:B:113:HIS:HD2	1:A:24:CYS:HA	8	0.18
(1,464)	1:B:93:VAL:H	1:B:93:VAL:HB	8	0.18
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	8	0.18
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	11	0.18
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG11	6	0.18
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG12	6	0.18
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG13	6	0.18
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG11	15	0.18
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG12	15	0.18
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG13	15	0.18
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	6	0.18
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	6	0.18
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG21	16	0.18
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG22	16	0.18
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG23	16	0.18
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG21	16	0.18
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG22	16	0.18
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG23	16	0.18
(1,293)	1:A:29:LEU:HD11	1:A:33:LEU:HA	16	0.18
(1,293)	1:A:29:LEU:HD12	1:A:33:LEU:HA	16	0.18
(1,293)	1:A:29:LEU:HD13	1:A:33:LEU:HA	16	0.18
(1,285)	1:A:14:ALA:HA	1:A:17:ILE:HB	2	0.18
(1,283)	1:A:14:ALA:HB1	1:A:11:VAL:HA	6	0.18
(1,283)	1:A:14:ALA:HB2	1:A:11:VAL:HA	6	0.18
(1,283)	1:A:14:ALA:HB3	1:A:11:VAL:HA	6	0.18
(1,251)	1:A:56:LYS:H	1:A:56:LYS:HG2	1	0.18
(1,251)	1:A:56:LYS:H	1:A:56:LYS:HG3	1	0.18
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD11	11	0.18
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD12	11	0.18
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD13	11	0.18
(1,211)	1:A:48:GLU:H	1:A:45:CYS:HA	9	0.18
(1,209)	1:A:47:CYS:H	1:A:47:CYS:HB2	9	0.18
(1,187)	1:A:37:LYS:H	1:A:37:LYS:HB2	17	0.18
(1,9)	1:B:113:HIS:HE1	1:A:27:ILE:HG12	11	0.17
(1,9)	1:B:113:HIS:HE1	1:A:27:ILE:HG13	11	0.17
(1,9)	1:B:113:HIS:HE2	1:A:27:ILE:HG12	11	0.17
(1,9)	1:B:113:HIS:HE2	1:A:27:ILE:HG13	11	0.17
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD11	7	0.17
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD12	7	0.17
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD13	7	0.17
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD11	7	0.17
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD12	7	0.17
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD13	7	0.17
(1,644)	1:B:109:GLU:HA	1:B:122:CYS:HB3	2	0.17
(1,644)	1:B:109:GLU:HA	1:B:122:CYS:HB3	14	0.17
(1,635)	1:B:109:GLU:HB2	1:B:111:HIS:HD2	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:B:109:GLU:HB2	1:B:111:HIS:HD2	16	0.17
(1,634)	1:B:111:HIS:HD2	1:B:107:PHE:HZ	9	0.17
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	12	0.17
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	12	0.17
(1,600)	1:B:75:ALA:HA	1:B:78:ILE:HB	2	0.17
(1,548)	1:B:112:CYS:H	1:B:113:HIS:HA	14	0.17
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG21	1	0.17
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG22	1	0.17
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG23	1	0.17
(1,5)	1:B:113:HIS:HD2	1:A:24:CYS:HA	11	0.17
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG11	8	0.17
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG12	8	0.17
(1,465)	1:B:93:VAL:H	1:B:93:VAL:HG13	8	0.17
(1,449)	1:B:90:LEU:H	1:B:88:ILE:HA	13	0.17
(1,361)	1:B:73:ALA:H	1:B:73:ALA:HB1	7	0.17
(1,361)	1:B:73:ALA:H	1:B:73:ALA:HB2	7	0.17
(1,361)	1:B:73:ALA:H	1:B:73:ALA:HB3	7	0.17
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	1	0.17
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	12	0.17
(1,327)	1:A:61:CYS:HB3	1:A:47:CYS:HB3	2	0.17
(1,320)	1:A:48:GLU:HB2	1:A:50:HIS:HD2	12	0.17
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	13	0.17
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	13	0.17
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG21	7	0.17
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG22	7	0.17
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG23	7	0.17
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG21	7	0.17
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG22	7	0.17
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG23	7	0.17
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD11	14	0.17
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD12	14	0.17
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD13	14	0.17
(1,213)	1:A:47:CYS:H	1:A:48:GLU:H	5	0.17
(1,211)	1:A:48:GLU:H	1:A:45:CYS:HA	6	0.17
(1,21)	1:A:9:LYS:H	1:A:9:LYS:HB3	13	0.17
(1,191)	1:A:45:CYS:H	1:A:42:CYS:HA	17	0.17
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG11	11	0.17
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG12	11	0.17
(1,150)	1:A:32:VAL:H	1:A:32:VAL:HG13	11	0.17
(1,1)	1:B:91:PRO:HD2	1:A:54:VAL:HG11	9	0.17
(1,1)	1:B:91:PRO:HD2	1:A:54:VAL:HG12	9	0.17
(1,1)	1:B:91:PRO:HD2	1:A:54:VAL:HG13	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:B:91:PRO:HD3	1:A:54:VAL:HG11	9	0.17
(1,1)	1:B:91:PRO:HD3	1:A:54:VAL:HG12	9	0.17
(1,1)	1:B:91:PRO:HD3	1:A:54:VAL:HG13	9	0.17
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG11	10	0.16
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG12	10	0.16
(1,94)	1:A:21:VAL:H	1:A:21:VAL:HG13	10	0.16
(1,9)	1:B:113:HIS:HE1	1:A:27:ILE:HG12	6	0.16
(1,9)	1:B:113:HIS:HE1	1:A:27:ILE:HG13	6	0.16
(1,9)	1:B:113:HIS:HE2	1:A:27:ILE:HG12	6	0.16
(1,9)	1:B:113:HIS:HE2	1:A:27:ILE:HG13	6	0.16
(1,74)	1:A:18:ALA:H	1:A:17:ILE:HG12	6	0.16
(1,71)	1:A:17:ILE:H	1:A:18:ALA:HA	9	0.16
(1,71)	1:A:17:ILE:H	1:A:18:ALA:HA	13	0.16
(1,643)	1:B:109:GLU:HA	1:B:122:CYS:HB2	6	0.16
(1,639)	1:B:118:ASP:HB3	1:B:115:VAL:HA	5	0.16
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG11	12	0.16
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG12	12	0.16
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG13	12	0.16
(1,635)	1:B:109:GLU:HB2	1:B:111:HIS:HD2	3	0.16
(1,624)	1:B:88:ILE:HD11	1:B:107:PHE:HD1	17	0.16
(1,624)	1:B:88:ILE:HD11	1:B:107:PHE:HD2	17	0.16
(1,624)	1:B:88:ILE:HD12	1:B:107:PHE:HD1	17	0.16
(1,624)	1:B:88:ILE:HD12	1:B:107:PHE:HD2	17	0.16
(1,624)	1:B:88:ILE:HD13	1:B:107:PHE:HD1	17	0.16
(1,624)	1:B:88:ILE:HD13	1:B:107:PHE:HD2	17	0.16
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	7	0.16
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	7	0.16
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	10	0.16
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	10	0.16
(1,599)	1:B:74:CYS:HB2	1:B:78:ILE:HG21	13	0.16
(1,599)	1:B:74:CYS:HB2	1:B:78:ILE:HG22	13	0.16
(1,599)	1:B:74:CYS:HB2	1:B:78:ILE:HG23	13	0.16
(1,599)	1:B:74:CYS:HB3	1:B:78:ILE:HG21	13	0.16
(1,599)	1:B:74:CYS:HB3	1:B:78:ILE:HG22	13	0.16
(1,599)	1:B:74:CYS:HB3	1:B:78:ILE:HG23	13	0.16
(1,588)	1:B:121:LEU:H	1:B:121:LEU:HB2	7	0.16
(1,588)	1:B:121:LEU:H	1:B:121:LEU:HB2	12	0.16
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD11	5	0.16
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD12	5	0.16
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD13	5	0.16
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD11	7	0.16
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD12	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD13	7	0.16
(1,548)	1:B:112:CYS:H	1:B:113:HIS:HA	16	0.16
(1,526)	1:B:109:GLU:H	1:B:106:CYS:HA	10	0.16
(1,524)	1:B:108:CYS:H	1:B:108:CYS:HB2	1	0.16
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	2	0.16
(1,336)	1:B:70:LYS:H	1:B:70:LYS:HB3	5	0.16
(1,329)	1:A:48:GLU:HA	1:A:61:CYS:HB3	10	0.16
(1,329)	1:A:48:GLU:HA	1:A:61:CYS:HB3	11	0.16
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG11	4	0.16
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG12	4	0.16
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG13	4	0.16
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG11	8	0.16
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG12	8	0.16
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG13	8	0.16
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG11	14	0.16
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG12	14	0.16
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG13	14	0.16
(1,314)	1:A:29:LEU:HD11	1:A:46:PHE:HZ	7	0.16
(1,314)	1:A:29:LEU:HD12	1:A:46:PHE:HZ	7	0.16
(1,314)	1:A:29:LEU:HD13	1:A:46:PHE:HZ	7	0.16
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	5	0.16
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	5	0.16
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG21	2	0.16
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG22	2	0.16
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG23	2	0.16
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG21	2	0.16
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG22	2	0.16
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG23	2	0.16
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG21	3	0.16
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG22	3	0.16
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG23	3	0.16
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG21	3	0.16
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG22	3	0.16
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG23	3	0.16
(1,21)	1:A:9:LYS:H	1:A:9:LYS:HB3	8	0.16
(1,10)	1:A:52:HIS:HD2	1:B:85:CYS:HA	7	0.16
(2,2)	1:B:90:LEU:H	1:B:92:CYS:HA	2	0.15
(2,1)	1:A:29:LEU:H	1:A:31:CYS:HA	5	0.15
(1,644)	1:B:109:GLU:HA	1:B:122:CYS:HB3	3	0.15
(1,639)	1:B:118:ASP:HB3	1:B:115:VAL:HA	4	0.15
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG11	3	0.15
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG12	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG13	3	0.15
(1,635)	1:B:109:GLU:HB2	1:B:111:HIS:HD2	7	0.15
(1,635)	1:B:109:GLU:HB2	1:B:111:HIS:HD2	12	0.15
(1,634)	1:B:111:HIS:HD2	1:B:107:PHE:HZ	17	0.15
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	15	0.15
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	15	0.15
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG21	12	0.15
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG22	12	0.15
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG23	12	0.15
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG21	12	0.15
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG22	12	0.15
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG23	12	0.15
(1,599)	1:B:74:CYS:HB2	1:B:78:ILE:HG21	12	0.15
(1,599)	1:B:74:CYS:HB2	1:B:78:ILE:HG22	12	0.15
(1,599)	1:B:74:CYS:HB2	1:B:78:ILE:HG23	12	0.15
(1,599)	1:B:74:CYS:HB3	1:B:78:ILE:HG21	12	0.15
(1,599)	1:B:74:CYS:HB3	1:B:78:ILE:HG22	12	0.15
(1,599)	1:B:74:CYS:HB3	1:B:78:ILE:HG23	12	0.15
(1,586)	1:B:120:HIS:H	1:B:121:LEU:HD11	5	0.15
(1,586)	1:B:120:HIS:H	1:B:121:LEU:HD12	5	0.15
(1,586)	1:B:120:HIS:H	1:B:121:LEU:HD13	5	0.15
(1,550)	1:B:113:HIS:H	1:B:113:HIS:HB2	2	0.15
(1,550)	1:B:113:HIS:H	1:B:113:HIS:HB2	6	0.15
(1,550)	1:B:113:HIS:H	1:B:113:HIS:HB2	13	0.15
(1,512)	1:B:107:PHE:H	1:B:104:ALA:HA	1	0.15
(1,43)	1:A:12:ALA:H	1:A:11:VAL:H	9	0.15
(1,345)	1:B:72:VAL:H	1:B:69:LEU:HA	1	0.15
(1,325)	1:A:55:CYS:HA	1:A:60:LEU:HD11	15	0.15
(1,325)	1:A:55:CYS:HA	1:A:60:LEU:HD12	15	0.15
(1,325)	1:A:55:CYS:HA	1:A:60:LEU:HD13	15	0.15
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG21	12	0.15
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG22	12	0.15
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG23	12	0.15
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG21	12	0.15
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG22	12	0.15
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG23	12	0.15
(1,293)	1:A:29:LEU:HD11	1:A:33:LEU:HA	3	0.15
(1,293)	1:A:29:LEU:HD12	1:A:33:LEU:HA	3	0.15
(1,293)	1:A:29:LEU:HD13	1:A:33:LEU:HA	3	0.15
(1,293)	1:A:29:LEU:HD11	1:A:33:LEU:HA	14	0.15
(1,293)	1:A:29:LEU:HD12	1:A:33:LEU:HA	14	0.15
(1,293)	1:A:29:LEU:HD13	1:A:33:LEU:HA	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG21	2	0.15
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG22	2	0.15
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG23	2	0.15
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG21	2	0.15
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG22	2	0.15
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG23	2	0.15
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD11	12	0.15
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD12	12	0.15
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD13	12	0.15
(1,235)	1:A:52:HIS:H	1:A:52:HIS:HB2	11	0.15
(1,211)	1:A:48:GLU:H	1:A:45:CYS:HA	4	0.15
(1,21)	1:A:9:LYS:H	1:A:9:LYS:HB3	2	0.15
(1,20)	1:A:9:LYS:H	1:A:9:LYS:HB2	3	0.15
(1,644)	1:B:109:GLU:HA	1:B:122:CYS:HB3	5	0.14
(1,644)	1:B:109:GLU:HA	1:B:122:CYS:HB3	12	0.14
(1,639)	1:B:118:ASP:HB3	1:B:115:VAL:HA	1	0.14
(1,639)	1:B:118:ASP:HB3	1:B:115:VAL:HA	2	0.14
(1,635)	1:B:109:GLU:HB2	1:B:111:HIS:HD2	10	0.14
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	8	0.14
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	8	0.14
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG21	13	0.14
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG22	13	0.14
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG23	13	0.14
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG21	13	0.14
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG22	13	0.14
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG23	13	0.14
(1,600)	1:B:75:ALA:HA	1:B:78:ILE:HB	5	0.14
(1,386)	1:B:78:ILE:H	1:B:79:ALA:HA	1	0.14
(1,38)	1:A:12:ALA:H	1:A:9:LYS:HA	4	0.14
(1,329)	1:A:48:GLU:HA	1:A:61:CYS:HB3	3	0.14
(1,329)	1:A:48:GLU:HA	1:A:61:CYS:HB3	9	0.14
(1,329)	1:A:48:GLU:HA	1:A:61:CYS:HB3	14	0.14
(1,293)	1:A:29:LEU:HD11	1:A:33:LEU:HA	15	0.14
(1,293)	1:A:29:LEU:HD12	1:A:33:LEU:HA	15	0.14
(1,293)	1:A:29:LEU:HD13	1:A:33:LEU:HA	15	0.14
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG21	5	0.14
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG22	5	0.14
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG23	5	0.14
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG21	5	0.14
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG22	5	0.14
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG23	5	0.14
(1,272)	1:A:60:LEU:H	1:A:60:LEU:HA	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:A:52:HIS:H	1:A:52:HIS:HA	13	0.14
(1,20)	1:A:9:LYS:H	1:A:9:LYS:HB2	7	0.14
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG21	12	0.14
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG22	12	0.14
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG23	12	0.14
(1,187)	1:A:37:LYS:H	1:A:37:LYS:HB2	1	0.14
(2,2)	1:B:90:LEU:H	1:B:92:CYS:HA	11	0.13
(2,2)	1:B:90:LEU:H	1:B:92:CYS:HA	14	0.13
(1,86)	1:A:20:ALA:H	1:A:20:ALA:HA	17	0.13
(1,77)	1:A:18:ALA:H	1:A:18:ALA:HA	6	0.13
(1,71)	1:A:17:ILE:H	1:A:18:ALA:HA	4	0.13
(1,640)	1:B:116:CYS:HA	1:B:121:LEU:HD11	15	0.13
(1,640)	1:B:116:CYS:HA	1:B:121:LEU:HD12	15	0.13
(1,640)	1:B:116:CYS:HA	1:B:121:LEU:HD13	15	0.13
(1,634)	1:B:111:HIS:HD2	1:B:107:PHE:HZ	16	0.13
(1,608)	1:B:90:LEU:HD11	1:B:94:LEU:HA	1	0.13
(1,608)	1:B:90:LEU:HD12	1:B:94:LEU:HA	1	0.13
(1,608)	1:B:90:LEU:HD13	1:B:94:LEU:HA	1	0.13
(1,608)	1:B:90:LEU:HD11	1:B:94:LEU:HA	5	0.13
(1,608)	1:B:90:LEU:HD12	1:B:94:LEU:HA	5	0.13
(1,608)	1:B:90:LEU:HD13	1:B:94:LEU:HA	5	0.13
(1,602)	1:B:79:ALA:HA	1:B:82:VAL:HB	6	0.13
(1,597)	1:B:68:VAL:HA	1:B:71:LYS:HB2	5	0.13
(1,597)	1:B:68:VAL:HA	1:B:71:LYS:HB3	5	0.13
(1,59)	1:A:14:ALA:H	1:A:14:ALA:HA	13	0.13
(1,587)	1:B:121:LEU:H	1:B:121:LEU:HA	4	0.13
(1,587)	1:B:121:LEU:H	1:B:121:LEU:HA	6	0.13
(1,587)	1:B:121:LEU:H	1:B:121:LEU:HA	13	0.13
(1,586)	1:B:120:HIS:H	1:B:121:LEU:HD11	9	0.13
(1,586)	1:B:120:HIS:H	1:B:121:LEU:HD12	9	0.13
(1,586)	1:B:120:HIS:H	1:B:121:LEU:HD13	9	0.13
(1,549)	1:B:113:HIS:H	1:B:113:HIS:HA	1	0.13
(1,549)	1:B:113:HIS:H	1:B:113:HIS:HA	4	0.13
(1,526)	1:B:109:GLU:H	1:B:106:CYS:HA	5	0.13
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG21	17	0.13
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG22	17	0.13
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG23	17	0.13
(1,502)	1:B:98:LYS:H	1:B:98:LYS:HB2	12	0.13
(1,5)	1:B:113:HIS:HD2	1:A:24:CYS:HA	13	0.13
(1,460)	1:B:93:VAL:H	1:B:92:CYS:HB2	16	0.13
(1,460)	1:B:93:VAL:H	1:B:92:CYS:HB3	16	0.13
(1,454)	1:B:92:CYS:H	1:B:92:CYS:HA	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,454)	1:B:92:CYS:H	1:B:92:CYS:HA	16	0.13
(1,449)	1:B:90:LEU:H	1:B:88:ILE:HA	17	0.13
(1,43)	1:A:12:ALA:H	1:A:11:VAL:H	8	0.13
(1,38)	1:A:12:ALA:H	1:A:9:LYS:HA	6	0.13
(1,374)	1:B:75:ALA:H	1:B:75:ALA:HA	13	0.13
(1,374)	1:B:75:ALA:H	1:B:75:ALA:HA	17	0.13
(1,329)	1:A:48:GLU:HA	1:A:61:CYS:HB3	5	0.13
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG11	12	0.13
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG12	12	0.13
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG13	12	0.13
(1,319)	1:A:50:HIS:HD2	1:A:46:PHE:HZ	3	0.13
(1,319)	1:A:50:HIS:HD2	1:A:46:PHE:HZ	10	0.13
(1,309)	1:A:27:ILE:HD11	1:A:46:PHE:HD1	7	0.13
(1,309)	1:A:27:ILE:HD11	1:A:46:PHE:HD2	7	0.13
(1,309)	1:A:27:ILE:HD12	1:A:46:PHE:HD1	7	0.13
(1,309)	1:A:27:ILE:HD12	1:A:46:PHE:HD2	7	0.13
(1,309)	1:A:27:ILE:HD13	1:A:46:PHE:HD1	7	0.13
(1,309)	1:A:27:ILE:HD13	1:A:46:PHE:HD2	7	0.13
(1,308)	1:A:17:ILE:HG12	1:A:46:PHE:HZ	4	0.13
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	11	0.13
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	11	0.13
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE1	15	0.13
(1,307)	1:A:17:ILE:HG12	1:A:46:PHE:HE2	15	0.13
(1,285)	1:A:14:ALA:HA	1:A:17:ILE:HB	8	0.13
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG21	8	0.13
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG22	8	0.13
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG23	8	0.13
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG21	8	0.13
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG22	8	0.13
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG23	8	0.13
(1,282)	1:A:7:VAL:HA	1:A:10:LYS:HB2	4	0.13
(1,282)	1:A:7:VAL:HA	1:A:10:LYS:HB3	4	0.13
(1,272)	1:A:60:LEU:H	1:A:60:LEU:HA	11	0.13
(1,272)	1:A:60:LEU:H	1:A:60:LEU:HA	16	0.13
(1,271)	1:A:59:HIS:H	1:A:60:LEU:HD11	5	0.13
(1,271)	1:A:59:HIS:H	1:A:60:LEU:HD12	5	0.13
(1,271)	1:A:59:HIS:H	1:A:60:LEU:HD13	5	0.13
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD11	15	0.13
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD12	15	0.13
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD13	15	0.13
(1,234)	1:A:52:HIS:H	1:A:52:HIS:HA	1	0.13
(1,224)	1:A:50:HIS:H	1:A:48:GLU:HG2	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:A:50:HIS:H	1:A:48:GLU:HG3	14	0.13
(1,2)	1:B:91:PRO:HA	1:A:54:VAL:HG11	12	0.13
(1,2)	1:B:91:PRO:HA	1:A:54:VAL:HG12	12	0.13
(1,2)	1:B:91:PRO:HA	1:A:54:VAL:HG13	12	0.13
(1,149)	1:A:32:VAL:H	1:A:32:VAL:HB	11	0.13
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG12	8	0.13
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG13	8	0.13
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG12	8	0.13
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG13	8	0.13
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG12	10	0.13
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG13	10	0.13
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG12	10	0.13
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG13	10	0.13
(1,139)	1:A:31:CYS:H	1:A:31:CYS:HA	13	0.13
(1,134)	1:A:29:LEU:H	1:A:27:ILE:HA	7	0.13
(1,1)	1:B:91:PRO:HD2	1:A:54:VAL:HG11	10	0.13
(1,1)	1:B:91:PRO:HD2	1:A:54:VAL:HG12	10	0.13
(1,1)	1:B:91:PRO:HD2	1:A:54:VAL:HG13	10	0.13
(1,1)	1:B:91:PRO:HD3	1:A:54:VAL:HG11	10	0.13
(1,1)	1:B:91:PRO:HD3	1:A:54:VAL:HG12	10	0.13
(1,1)	1:B:91:PRO:HD3	1:A:54:VAL:HG13	10	0.13
(2,1)	1:A:29:LEU:H	1:A:31:CYS:HA	12	0.12
(1,74)	1:A:18:ALA:H	1:A:17:ILE:HG12	1	0.12
(1,71)	1:A:17:ILE:H	1:A:18:ALA:HA	3	0.12
(1,71)	1:A:17:ILE:H	1:A:18:ALA:HA	14	0.12
(1,639)	1:B:118:ASP:HB3	1:B:115:VAL:HA	3	0.12
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG11	17	0.12
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG12	17	0.12
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG13	17	0.12
(1,635)	1:B:109:GLU:HB2	1:B:111:HIS:HD2	15	0.12
(1,634)	1:B:111:HIS:HD2	1:B:107:PHE:HZ	15	0.12
(1,623)	1:B:78:ILE:HG12	1:B:107:PHE:HZ	6	0.12
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE1	11	0.12
(1,622)	1:B:78:ILE:HG12	1:B:107:PHE:HE2	11	0.12
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG21	3	0.12
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG22	3	0.12
(1,620)	1:B:106:CYS:HB2	1:B:78:ILE:HG23	3	0.12
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG21	3	0.12
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG22	3	0.12
(1,620)	1:B:106:CYS:HB3	1:B:78:ILE:HG23	3	0.12
(1,610)	1:B:97:LEU:HD11	1:B:78:ILE:HA	14	0.12
(1,610)	1:B:97:LEU:HD12	1:B:78:ILE:HA	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:B:97:LEU:HD13	1:B:78:ILE:HA	14	0.12
(1,6)	1:B:113:HIS:HD2	1:A:24:CYS:HB2	9	0.12
(1,59)	1:A:14:ALA:H	1:A:14:ALA:HA	17	0.12
(1,587)	1:B:121:LEU:H	1:B:121:LEU:HA	2	0.12
(1,587)	1:B:121:LEU:H	1:B:121:LEU:HA	10	0.12
(1,587)	1:B:121:LEU:H	1:B:121:LEU:HA	11	0.12
(1,587)	1:B:121:LEU:H	1:B:121:LEU:HA	12	0.12
(1,587)	1:B:121:LEU:H	1:B:121:LEU:HA	16	0.12
(1,586)	1:B:120:HIS:H	1:B:121:LEU:HD11	17	0.12
(1,586)	1:B:120:HIS:H	1:B:121:LEU:HD12	17	0.12
(1,586)	1:B:120:HIS:H	1:B:121:LEU:HD13	17	0.12
(1,584)	1:B:120:HIS:H	1:B:120:HIS:HA	8	0.12
(1,584)	1:B:120:HIS:H	1:B:120:HIS:HA	15	0.12
(1,549)	1:B:113:HIS:H	1:B:113:HIS:HA	8	0.12
(1,549)	1:B:113:HIS:H	1:B:113:HIS:HA	12	0.12
(1,539)	1:B:111:HIS:H	1:B:109:GLU:HG2	6	0.12
(1,539)	1:B:111:HIS:H	1:B:109:GLU:HG3	6	0.12
(1,53)	1:A:14:ALA:H	1:A:12:ALA:HA	14	0.12
(1,524)	1:B:108:CYS:H	1:B:108:CYS:HB2	16	0.12
(1,52)	1:A:14:ALA:H	1:A:12:ALA:HA	14	0.12
(1,514)	1:B:107:PHE:H	1:B:106:CYS:HB2	12	0.12
(1,514)	1:B:107:PHE:H	1:B:106:CYS:HB3	12	0.12
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG21	2	0.12
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG22	2	0.12
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG23	2	0.12
(1,460)	1:B:93:VAL:H	1:B:92:CYS:HB2	10	0.12
(1,460)	1:B:93:VAL:H	1:B:92:CYS:HB3	10	0.12
(1,460)	1:B:93:VAL:H	1:B:92:CYS:HB2	15	0.12
(1,460)	1:B:93:VAL:H	1:B:92:CYS:HB3	15	0.12
(1,46)	1:A:12:ALA:H	1:A:12:ALA:HB1	14	0.12
(1,46)	1:A:12:ALA:H	1:A:12:ALA:HB2	14	0.12
(1,46)	1:A:12:ALA:H	1:A:12:ALA:HB3	14	0.12
(1,454)	1:B:92:CYS:H	1:B:92:CYS:HA	3	0.12
(1,454)	1:B:92:CYS:H	1:B:92:CYS:HA	4	0.12
(1,454)	1:B:92:CYS:H	1:B:92:CYS:HA	13	0.12
(1,43)	1:A:12:ALA:H	1:A:11:VAL:H	16	0.12
(1,422)	1:B:84:ALA:H	1:B:84:ALA:HA	6	0.12
(1,422)	1:B:84:ALA:H	1:B:84:ALA:HA	8	0.12
(1,422)	1:B:84:ALA:H	1:B:84:ALA:HA	13	0.12
(1,386)	1:B:78:ILE:H	1:B:79:ALA:HA	9	0.12
(1,386)	1:B:78:ILE:H	1:B:79:ALA:HA	17	0.12
(1,374)	1:B:75:ALA:H	1:B:75:ALA:HA	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,358)	1:B:73:ALA:H	1:B:72:VAL:H	9	0.12
(1,358)	1:B:73:ALA:H	1:B:72:VAL:H	16	0.12
(1,345)	1:B:72:VAL:H	1:B:69:LEU:HA	8	0.12
(1,329)	1:A:48:GLU:HA	1:A:61:CYS:HB3	2	0.12
(1,328)	1:A:48:GLU:HA	1:A:61:CYS:HB2	16	0.12
(1,324)	1:A:57:ASP:HB3	1:A:54:VAL:HA	4	0.12
(1,319)	1:A:50:HIS:HD2	1:A:46:PHE:HZ	1	0.12
(1,314)	1:A:29:LEU:HD11	1:A:46:PHE:HZ	6	0.12
(1,314)	1:A:29:LEU:HD12	1:A:46:PHE:HZ	6	0.12
(1,314)	1:A:29:LEU:HD13	1:A:46:PHE:HZ	6	0.12
(1,309)	1:A:27:ILE:HD11	1:A:46:PHE:HD1	6	0.12
(1,309)	1:A:27:ILE:HD11	1:A:46:PHE:HD2	6	0.12
(1,309)	1:A:27:ILE:HD12	1:A:46:PHE:HD1	6	0.12
(1,309)	1:A:27:ILE:HD12	1:A:46:PHE:HD2	6	0.12
(1,309)	1:A:27:ILE:HD13	1:A:46:PHE:HD1	6	0.12
(1,309)	1:A:27:ILE:HD13	1:A:46:PHE:HD2	6	0.12
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG21	17	0.12
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG22	17	0.12
(1,305)	1:A:45:CYS:HB2	1:A:17:ILE:HG23	17	0.12
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG21	17	0.12
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG22	17	0.12
(1,305)	1:A:45:CYS:HB3	1:A:17:ILE:HG23	17	0.12
(1,30)	1:A:11:VAL:H	1:A:8:LEU:HA	12	0.12
(1,295)	1:A:36:LEU:HD11	1:A:17:ILE:HA	7	0.12
(1,295)	1:A:36:LEU:HD12	1:A:17:ILE:HA	7	0.12
(1,295)	1:A:36:LEU:HD13	1:A:17:ILE:HA	7	0.12
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG21	4	0.12
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG22	4	0.12
(1,284)	1:A:13:CYS:HB2	1:A:17:ILE:HG23	4	0.12
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG21	4	0.12
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG22	4	0.12
(1,284)	1:A:13:CYS:HB3	1:A:17:ILE:HG23	4	0.12
(1,272)	1:A:60:LEU:H	1:A:60:LEU:HA	1	0.12
(1,272)	1:A:60:LEU:H	1:A:60:LEU:HA	6	0.12
(1,272)	1:A:60:LEU:H	1:A:60:LEU:HA	9	0.12
(1,272)	1:A:60:LEU:H	1:A:60:LEU:HA	13	0.12
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD11	3	0.12
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD12	3	0.12
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD13	3	0.12
(1,235)	1:A:52:HIS:H	1:A:52:HIS:HB2	5	0.12
(1,234)	1:A:52:HIS:H	1:A:52:HIS:HA	2	0.12
(1,234)	1:A:52:HIS:H	1:A:52:HIS:HA	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:A:52:HIS:H	1:A:52:HIS:HA	8	0.12
(1,234)	1:A:52:HIS:H	1:A:52:HIS:HA	10	0.12
(1,234)	1:A:52:HIS:H	1:A:52:HIS:HA	12	0.12
(1,234)	1:A:52:HIS:H	1:A:52:HIS:HA	16	0.12
(1,234)	1:A:52:HIS:H	1:A:52:HIS:HA	17	0.12
(1,199)	1:A:46:PHE:H	1:A:45:CYS:HB2	17	0.12
(1,199)	1:A:46:PHE:H	1:A:45:CYS:HB3	17	0.12
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG21	7	0.12
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG22	7	0.12
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG23	7	0.12
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG21	14	0.12
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG22	14	0.12
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG23	14	0.12
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG12	6	0.12
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG13	6	0.12
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG12	6	0.12
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG13	6	0.12
(1,139)	1:A:31:CYS:H	1:A:31:CYS:HA	4	0.12
(1,139)	1:A:31:CYS:H	1:A:31:CYS:HA	9	0.12
(1,134)	1:A:29:LEU:H	1:A:27:ILE:HA	6	0.12
(1,134)	1:A:29:LEU:H	1:A:27:ILE:HA	17	0.12
(1,124)	1:A:26:GLY:H	1:A:25:GLY:H	1	0.12
(2,2)	1:B:90:LEU:H	1:B:92:CYS:HA	15	0.11
(1,83)	1:A:19:GLY:H	1:A:20:ALA:HA	15	0.11
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD11	1	0.11
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD12	1	0.11
(1,8)	1:B:113:HIS:HE1	1:A:27:ILE:HD13	1	0.11
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD11	1	0.11
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD12	1	0.11
(1,8)	1:B:113:HIS:HE2	1:A:27:ILE:HD13	1	0.11
(1,77)	1:A:18:ALA:H	1:A:18:ALA:HA	9	0.11
(1,74)	1:A:18:ALA:H	1:A:17:ILE:HG12	3	0.11
(1,71)	1:A:17:ILE:H	1:A:18:ALA:HA	1	0.11
(1,643)	1:B:109:GLU:HA	1:B:122:CYS:HB2	4	0.11
(1,643)	1:B:109:GLU:HA	1:B:122:CYS:HB2	8	0.11
(1,642)	1:B:122:CYS:HB3	1:B:108:CYS:HB3	3	0.11
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG11	1	0.11
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG12	1	0.11
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG13	1	0.11
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG11	10	0.11
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG12	10	0.11
(1,636)	1:B:92:CYS:HA	1:B:115:VAL:HG13	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,634)	1:B:111:HIS:HD2	1:B:107:PHE:HZ	3	0.11
(1,629)	1:B:90:LEU:HD11	1:B:107:PHE:HZ	17	0.11
(1,629)	1:B:90:LEU:HD12	1:B:107:PHE:HZ	17	0.11
(1,629)	1:B:90:LEU:HD13	1:B:107:PHE:HZ	17	0.11
(1,623)	1:B:78:ILE:HG12	1:B:107:PHE:HZ	12	0.11
(1,617)	1:B:97:LEU:HD11	1:B:98:LYS:HA	7	0.11
(1,617)	1:B:97:LEU:HD12	1:B:98:LYS:HA	7	0.11
(1,617)	1:B:97:LEU:HD13	1:B:98:LYS:HA	7	0.11
(1,599)	1:B:74:CYS:HB2	1:B:78:ILE:HG21	8	0.11
(1,599)	1:B:74:CYS:HB2	1:B:78:ILE:HG22	8	0.11
(1,599)	1:B:74:CYS:HB2	1:B:78:ILE:HG23	8	0.11
(1,599)	1:B:74:CYS:HB3	1:B:78:ILE:HG21	8	0.11
(1,599)	1:B:74:CYS:HB3	1:B:78:ILE:HG22	8	0.11
(1,599)	1:B:74:CYS:HB3	1:B:78:ILE:HG23	8	0.11
(1,597)	1:B:68:VAL:HA	1:B:71:LYS:HB2	8	0.11
(1,597)	1:B:68:VAL:HA	1:B:71:LYS:HB3	8	0.11
(1,597)	1:B:68:VAL:HA	1:B:71:LYS:HB2	12	0.11
(1,597)	1:B:68:VAL:HA	1:B:71:LYS:HB3	12	0.11
(1,59)	1:A:14:ALA:H	1:A:14:ALA:HA	10	0.11
(1,587)	1:B:121:LEU:H	1:B:121:LEU:HA	1	0.11
(1,587)	1:B:121:LEU:H	1:B:121:LEU:HA	7	0.11
(1,587)	1:B:121:LEU:H	1:B:121:LEU:HA	8	0.11
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD11	3	0.11
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD12	3	0.11
(1,558)	1:B:117:LYS:H	1:B:90:LEU:HD13	3	0.11
(1,549)	1:B:113:HIS:H	1:B:113:HIS:HA	7	0.11
(1,549)	1:B:113:HIS:H	1:B:113:HIS:HA	10	0.11
(1,549)	1:B:113:HIS:H	1:B:113:HIS:HA	11	0.11
(1,528)	1:B:108:CYS:H	1:B:109:GLU:H	5	0.11
(1,511)	1:B:107:PHE:H	1:B:97:LEU:HD11	9	0.11
(1,511)	1:B:107:PHE:H	1:B:97:LEU:HD12	9	0.11
(1,511)	1:B:107:PHE:H	1:B:97:LEU:HD13	9	0.11
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG21	5	0.11
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG22	5	0.11
(1,510)	1:B:107:PHE:H	1:B:78:ILE:HG23	5	0.11
(1,480)	1:B:95:ALA:H	1:B:94:LEU:HG	7	0.11
(1,460)	1:B:93:VAL:H	1:B:92:CYS:HB2	3	0.11
(1,460)	1:B:93:VAL:H	1:B:92:CYS:HB3	3	0.11
(1,454)	1:B:92:CYS:H	1:B:92:CYS:HA	9	0.11
(1,418)	1:B:83:ALA:H	1:B:83:ALA:HA	11	0.11
(1,389)	1:B:79:ALA:H	1:B:78:ILE:HG12	17	0.11
(1,345)	1:B:72:VAL:H	1:B:69:LEU:HA	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:B:71:LYS:H	1:B:69:LEU:HG	5	0.11
(1,327)	1:A:61:CYS:HB3	1:A:47:CYS:HB3	8	0.11
(1,324)	1:A:57:ASP:HB3	1:A:54:VAL:HA	3	0.11
(1,324)	1:A:57:ASP:HB3	1:A:54:VAL:HA	8	0.11
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG11	1	0.11
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG12	1	0.11
(1,321)	1:A:31:CYS:HA	1:A:54:VAL:HG13	1	0.11
(1,320)	1:A:48:GLU:HB2	1:A:50:HIS:HD2	15	0.11
(1,319)	1:A:50:HIS:HD2	1:A:46:PHE:HZ	8	0.11
(1,319)	1:A:50:HIS:HD2	1:A:46:PHE:HZ	9	0.11
(1,319)	1:A:50:HIS:HD2	1:A:46:PHE:HZ	12	0.11
(1,308)	1:A:17:ILE:HG12	1:A:46:PHE:HZ	6	0.11
(1,293)	1:A:29:LEU:HD11	1:A:33:LEU:HA	11	0.11
(1,293)	1:A:29:LEU:HD12	1:A:33:LEU:HA	11	0.11
(1,293)	1:A:29:LEU:HD13	1:A:33:LEU:HA	11	0.11
(1,293)	1:A:29:LEU:HD11	1:A:33:LEU:HA	12	0.11
(1,293)	1:A:29:LEU:HD12	1:A:33:LEU:HA	12	0.11
(1,293)	1:A:29:LEU:HD13	1:A:33:LEU:HA	12	0.11
(1,285)	1:A:14:ALA:HA	1:A:17:ILE:HB	11	0.11
(1,282)	1:A:7:VAL:HA	1:A:10:LYS:HB2	6	0.11
(1,282)	1:A:7:VAL:HA	1:A:10:LYS:HB3	6	0.11
(1,272)	1:A:60:LEU:H	1:A:60:LEU:HA	10	0.11
(1,272)	1:A:60:LEU:H	1:A:60:LEU:HA	12	0.11
(1,271)	1:A:59:HIS:H	1:A:60:LEU:HD11	14	0.11
(1,271)	1:A:59:HIS:H	1:A:60:LEU:HD12	14	0.11
(1,271)	1:A:59:HIS:H	1:A:60:LEU:HD13	14	0.11
(1,268)	1:A:59:HIS:H	1:A:58:LEU:H	8	0.11
(1,251)	1:A:56:LYS:H	1:A:56:LYS:HG2	5	0.11
(1,251)	1:A:56:LYS:H	1:A:56:LYS:HG3	5	0.11
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD11	9	0.11
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD12	9	0.11
(1,243)	1:A:56:LYS:H	1:A:29:LEU:HD13	9	0.11
(1,234)	1:A:52:HIS:H	1:A:52:HIS:HA	14	0.11
(1,234)	1:A:52:HIS:H	1:A:52:HIS:HA	15	0.11
(1,22)	1:A:9:LYS:H	1:A:9:LYS:HG2	11	0.11
(1,22)	1:A:9:LYS:H	1:A:9:LYS:HG3	11	0.11
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG21	1	0.11
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG22	1	0.11
(1,195)	1:A:46:PHE:H	1:A:17:ILE:HG23	1	0.11
(1,145)	1:A:32:VAL:H	1:A:31:CYS:HB2	5	0.11
(1,145)	1:A:32:VAL:H	1:A:31:CYS:HB3	5	0.11
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG12	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:A:52:HIS:HE1	1:B:88:ILE:HG13	7	0.11
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG12	7	0.11
(1,14)	1:A:52:HIS:HE2	1:B:88:ILE:HG13	7	0.11
(1,139)	1:A:31:CYS:H	1:A:31:CYS:HA	3	0.11
(1,13)	1:A:52:HIS:HE1	1:B:88:ILE:HD11	17	0.11
(1,13)	1:A:52:HIS:HE1	1:B:88:ILE:HD12	17	0.11
(1,13)	1:A:52:HIS:HE1	1:B:88:ILE:HD13	17	0.11
(1,13)	1:A:52:HIS:HE2	1:B:88:ILE:HD11	17	0.11
(1,13)	1:A:52:HIS:HE2	1:B:88:ILE:HD12	17	0.11
(1,13)	1:A:52:HIS:HE2	1:B:88:ILE:HD13	17	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found