



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 08:40 PM UTC

PDB ID : 2L9N / pdb_00002l9n
BMRB ID : 17479
Title : Structure of the human Shwachman-Bodian-Diamond syndrome (SBDS) protein
Authors : Hilcenko, C.; Freund, S.M.V.; Warren, A.J.
Deposited on : 2011-02-21

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

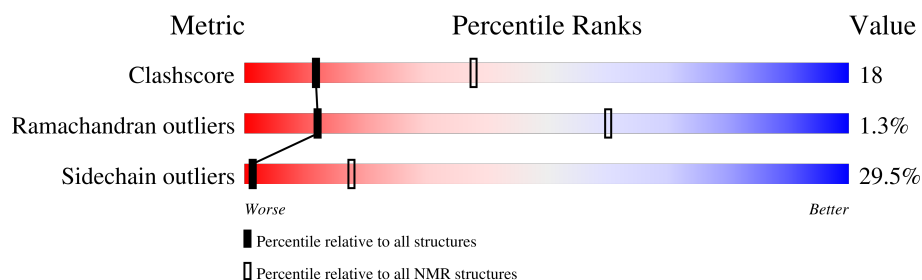
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

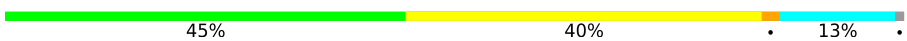
The overall completeness of chemical shifts assignment is 79%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	252	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:15-A:40, A:46-A:94 (75)	0.47	1
2	A:95-A:169 (75)	1.03	16
3	A:171-A:238 (68)	0.86	17

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4129 atoms, of which 2114 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribosome maturation protein SBDS.

Mol	Chain	Residues	Atoms						Trace
1	A	250	Total	C	H	N	O	S	0
			4129	1272	2114	352	380	11	

There are 2 discrepancies between the modelled and reference sequences:

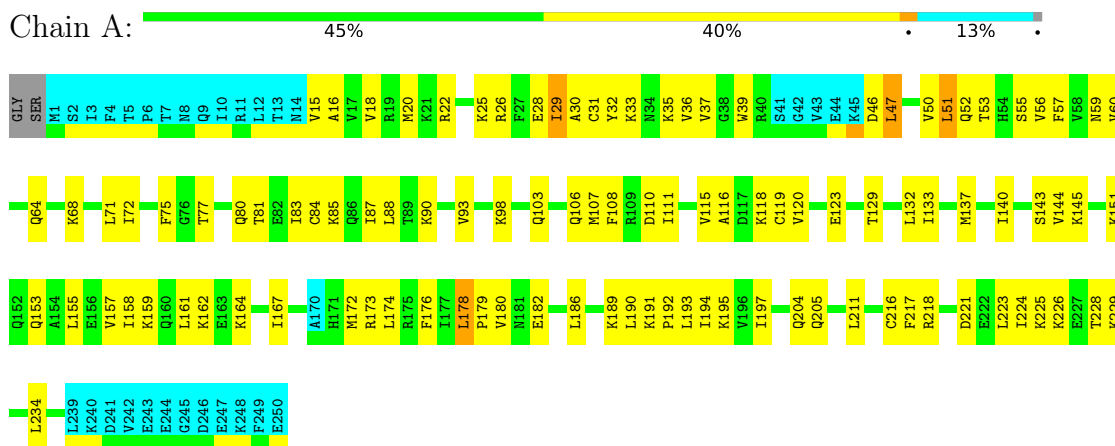
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9Y3A5
A	0	SER	-	expression tag	UNP Q9Y3A5

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Ribosome maturation protein SBDS

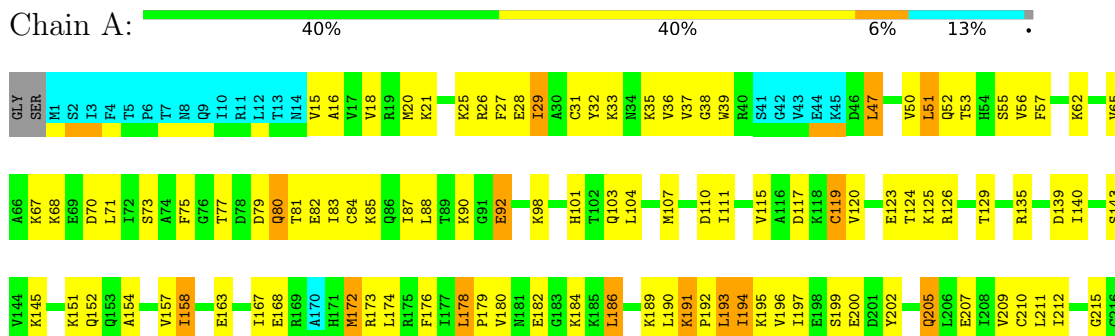


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Ribosome maturation protein SBDS

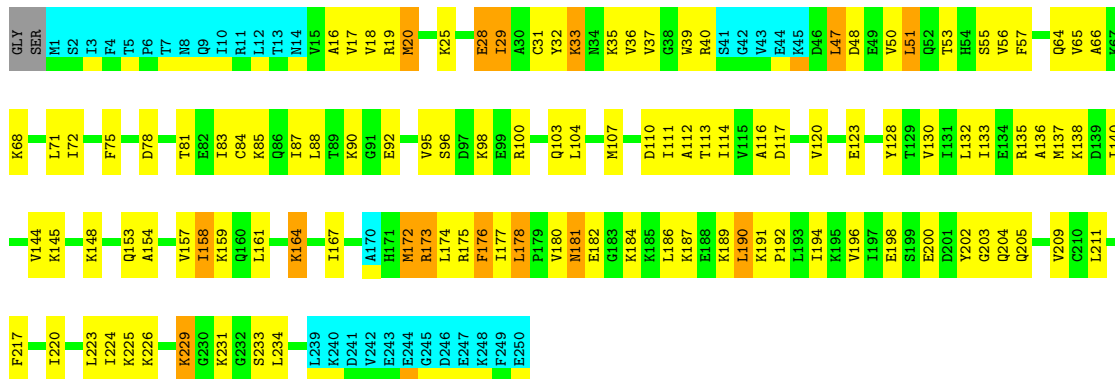




4.2.2 Score per residue for model 2

- Molecule 1: Ribosome maturation protein SBDS

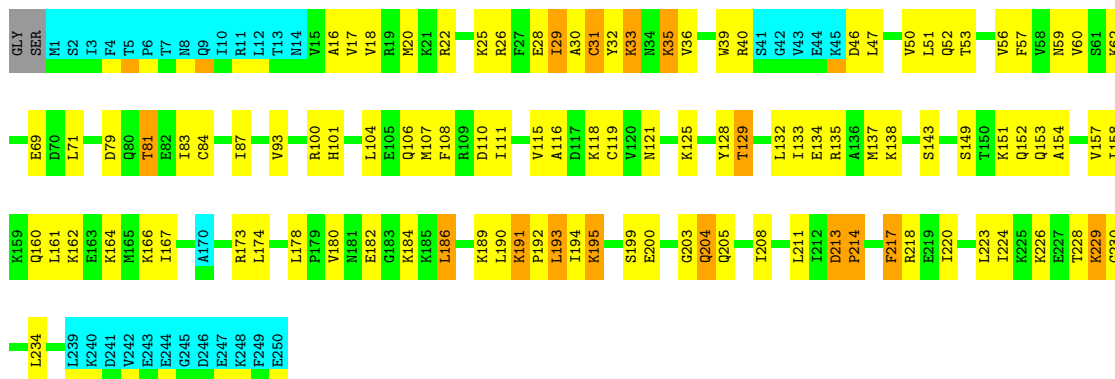
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Ribosome maturation protein SBDS

Chain A:

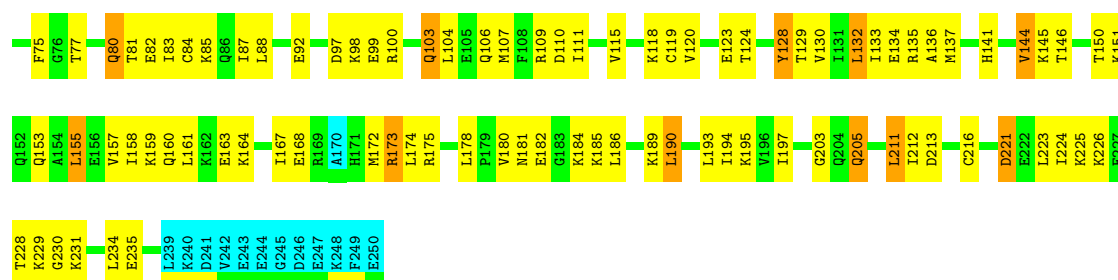


4.2.4 Score per residue for model 4

- Molecule 1: Ribosome maturation protein SBDS

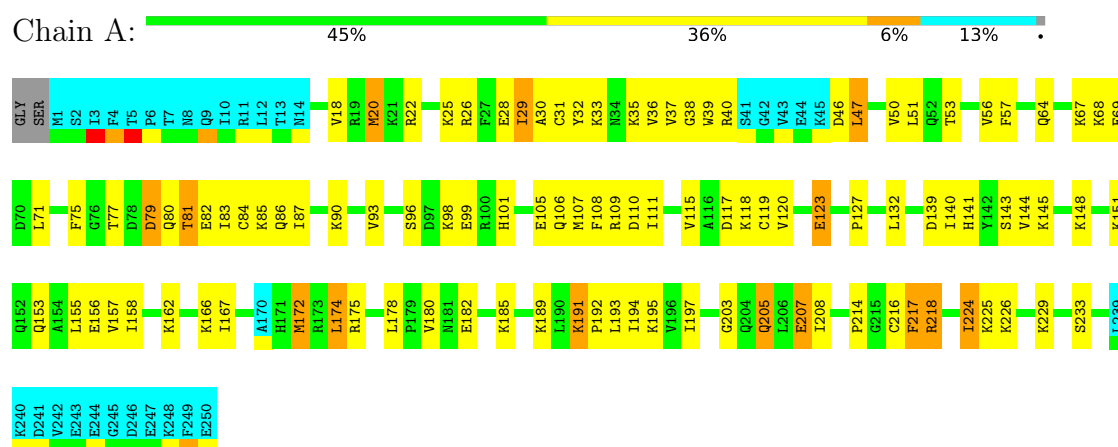
Chain A:





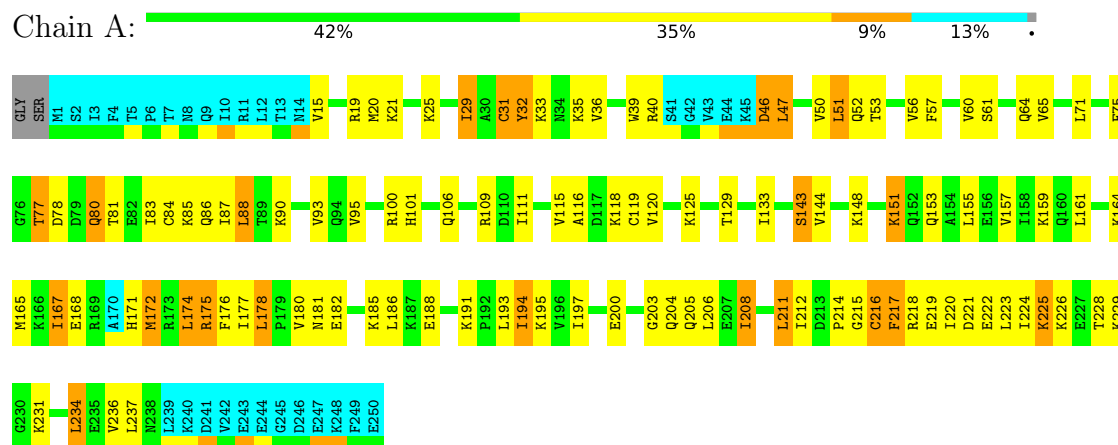
4.2.5 Score per residue for model 5

- Molecule 1: Ribosome maturation protein SBDS



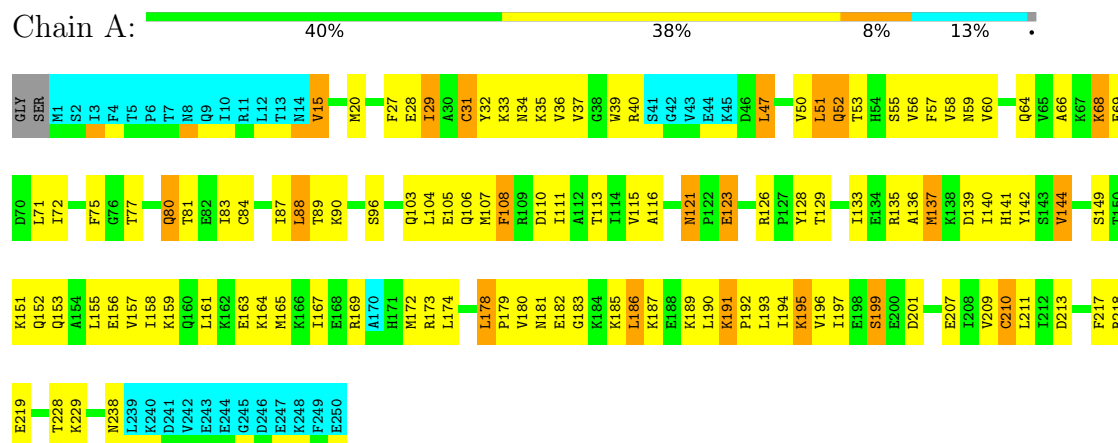
4.2.6 Score per residue for model 6

- Molecule 1: Ribosome maturation protein SBDS



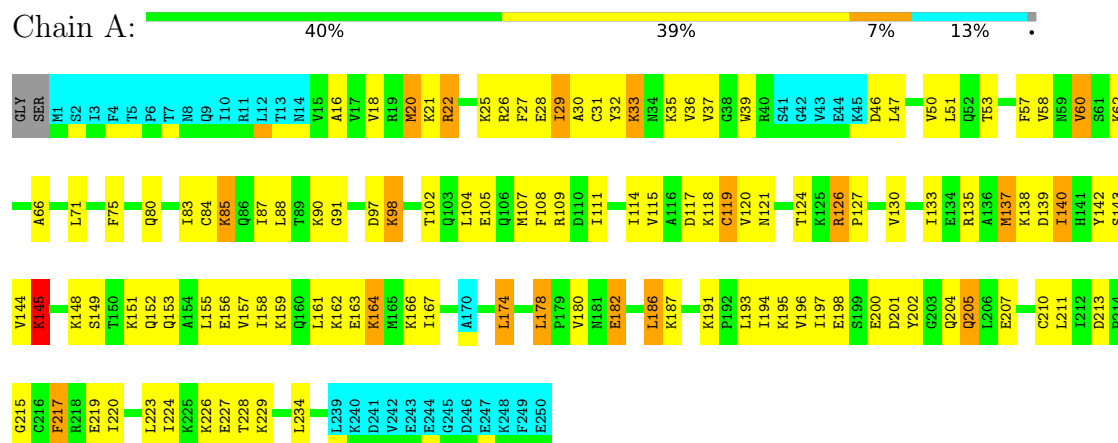
4.2.7 Score per residue for model 7

- Molecule 1: Ribosome maturation protein SBDS



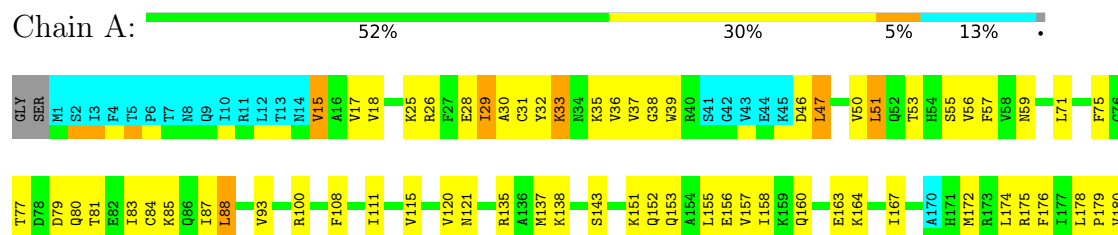
4.2.8 Score per residue for model 8

- Molecule 1: Ribosome maturation protein SBDS



4.2.9 Score per residue for model 9

- Molecule 1: Ribosome maturation protein SBDS

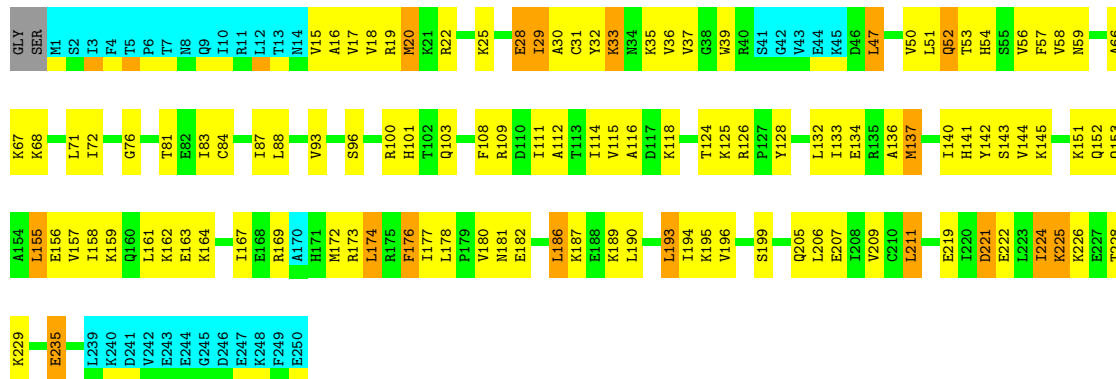




4.2.10 Score per residue for model 10

- Molecule 1: Ribosome maturation protein SBDS

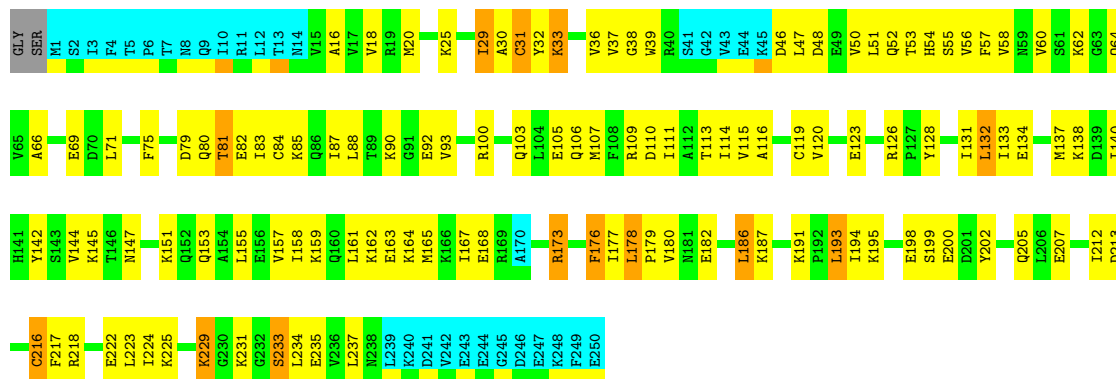
Chain A: 42% 38% 7% 13% .



4.2.11 Score per residue for model 11

- Molecule 1: Ribosome maturation protein SBDS

Chain A: 39% 42% 5% 13% .

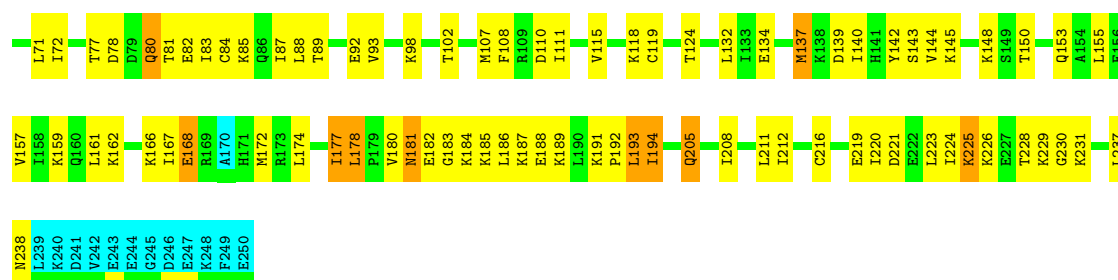


4.2.12 Score per residue for model 12

- Molecule 1: Ribosome maturation protein SBDS

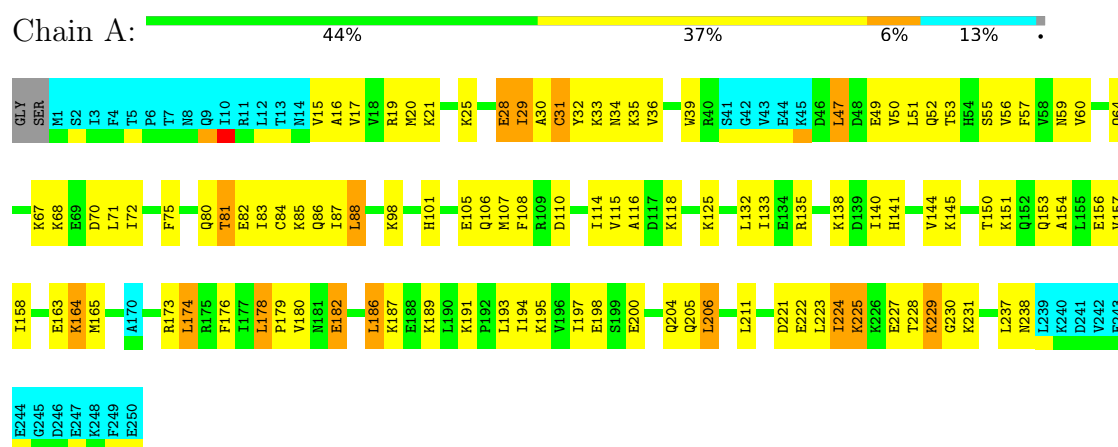
Chain A: 44% 37% 6% 13% .





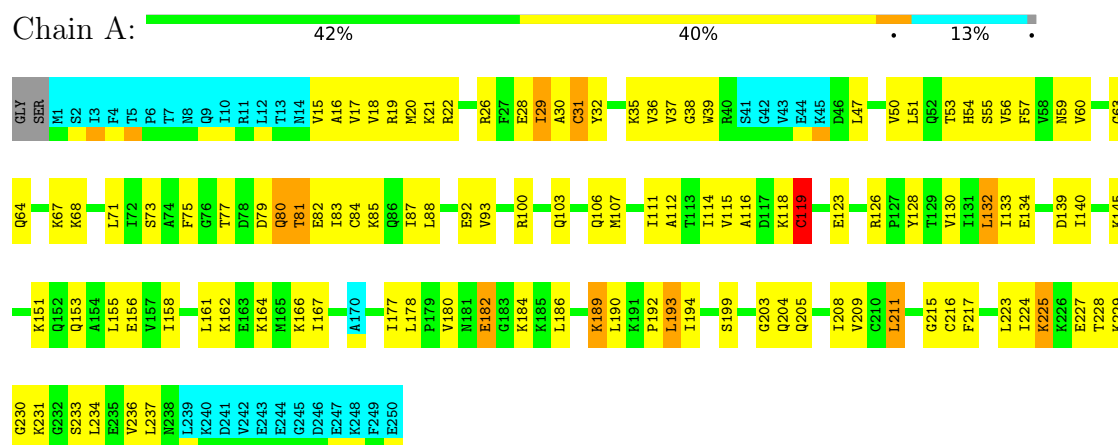
4.2.13 Score per residue for model 13

- Molecule 1: Ribosome maturation protein SBDS



4.2.14 Score per residue for model 14

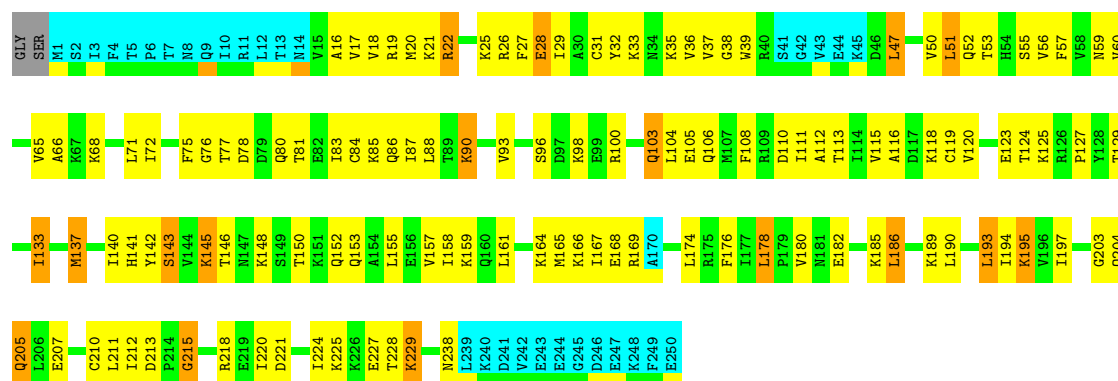
- Molecule 1: Ribosome maturation protein SBDS



4.2.15 Score per residue for model 15

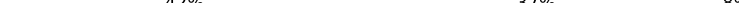
- Molecule 1: Ribosome maturation protein SBDS

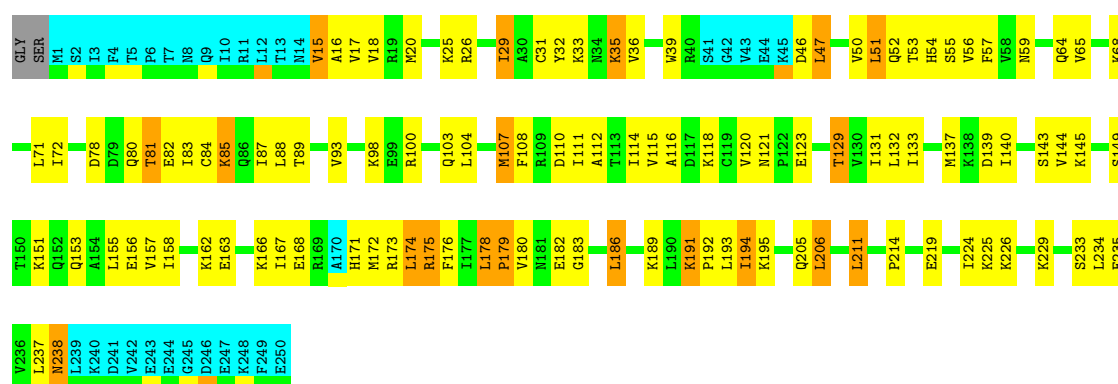
Chain A: 37% 43% 7% 13%



4.2.16 Score per residue for model 16

- Molecule 1: Ribosome maturation protein SBDS

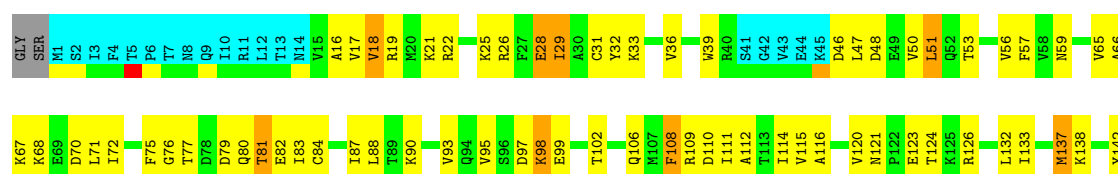
Chain A:  42% 37% 8% 13%

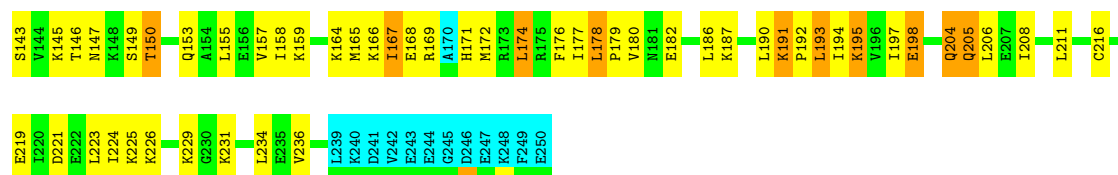


4.2.17 Score per residue for model 17

- Molecule 1: Ribosome maturation protein SBDS

Chain A: 39% 40% 7% 13% .

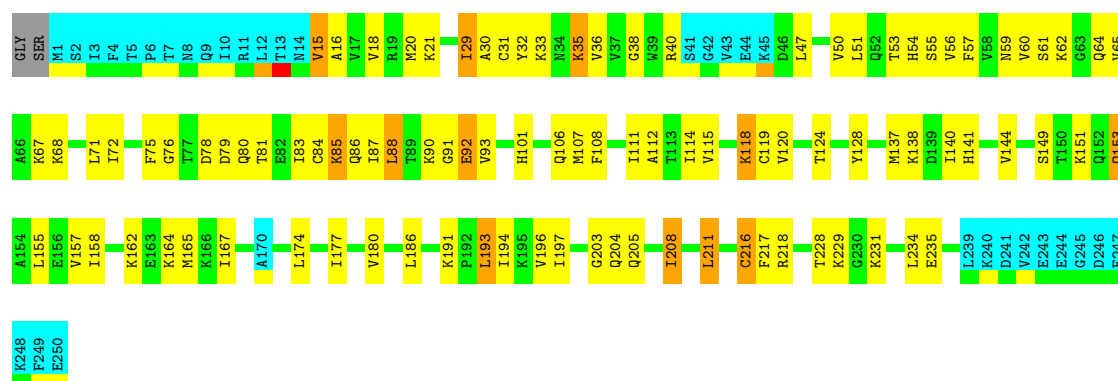




4.2.18 Score per residue for model 18

- Molecule 1: Ribosome maturation protein SBDS

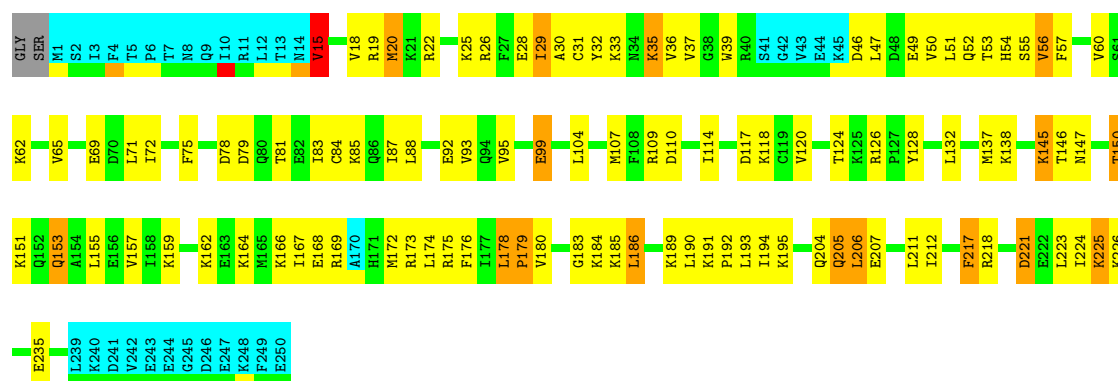
Chain A: 48% 34% 5% 13%



4.2.19 Score per residue for model 19

- Molecule 1: Ribosome maturation protein SBDS

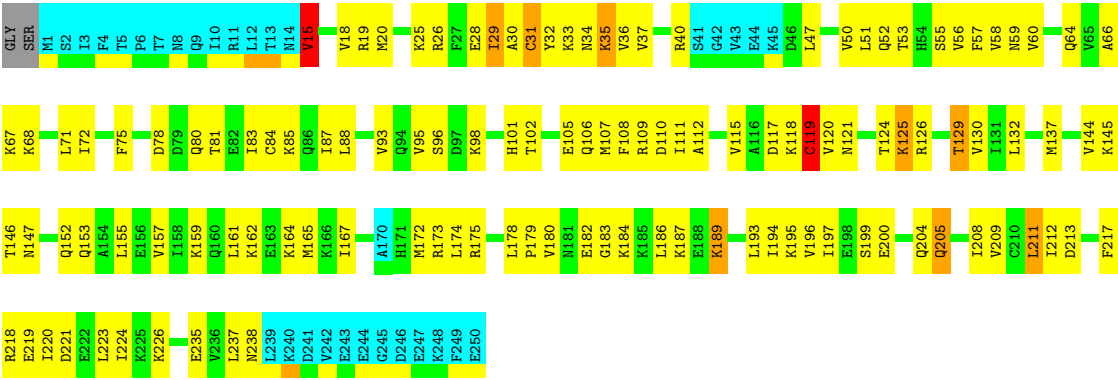
Chain A: 43% 37% 6% 13%



4.2.20 Score per residue for model 20

- Molecule 1: Ribosome maturation protein SBDS

Chain A: 38% 44% 13%



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure calculation	
CNS	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	2846
Number of shifts mapped to atoms	2846
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality [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	1761	1866	1862	64±8
All	All	35220	37320	37240	1271

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:LEU:HD22	1:A:83:ILE:HD13	1.03	1.26	6	20
1:A:136:ALA:HB1	1:A:161:LEU:HD21	1.00	1.29	4	1
1:A:56:VAL:HG21	1:A:71:LEU:HD21	0.96	1.31	3	14
1:A:186:LEU:HD11	1:A:190:LEU:HD23	0.93	1.41	2	1
1:A:193:LEU:HD23	1:A:194:ILE:HG23	0.92	1.41	4	4
1:A:196:VAL:HG12	1:A:211:LEU:HD22	0.89	1.40	18	1
1:A:32:TYR:O	1:A:36:VAL:HG23	0.87	1.70	19	20
1:A:30:ALA:HB3	1:A:53:THR:HG22	0.85	1.45	14	9
1:A:51:LEU:HD11	1:A:84:CYS:CB	0.83	2.02	18	17
1:A:196:VAL:HG12	1:A:211:LEU:CD2	0.83	2.04	18	1
1:A:190:LEU:HD13	1:A:211:LEU:HD21	0.82	1.47	19	2
1:A:177:ILE:HD12	1:A:208:ILE:HG22	0.80	1.53	18	1
1:A:153:GLN:O	1:A:157:VAL:HG23	0.80	1.77	20	14
1:A:158:ILE:HG23	1:A:167:ILE:HG23	0.79	1.53	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:ILE:HD13	1:A:137:MET:HE1	0.79	1.55	8	1
1:A:31:CYS:SG	1:A:50:VAL:HG22	0.78	2.19	20	5
1:A:47:LEU:HD12	1:A:51:LEU:HD12	0.78	1.52	14	4
1:A:33:LYS:O	1:A:37:VAL:HG23	0.78	1.78	15	1
1:A:29:ILE:HG21	1:A:84:CYS:SG	0.77	2.19	13	18
1:A:56:VAL:CG2	1:A:71:LEU:HD21	0.77	2.10	15	10
1:A:107:MET:HE2	1:A:145:LYS:O	0.77	1.80	19	2
1:A:36:VAL:HG11	1:A:93:VAL:HG11	0.76	1.57	17	1
1:A:16:ALA:HB2	1:A:33:LYS:HG3	0.76	1.58	15	6
1:A:107:MET:HE1	1:A:148:LYS:O	0.76	1.80	8	1
1:A:116:ALA:HB2	1:A:133:ILE:CD1	0.76	2.11	17	8
1:A:178:LEU:CD2	1:A:186:LEU:HD13	0.76	2.11	6	1
1:A:194:ILE:HD11	1:A:211:LEU:HB3	0.75	1.59	1	2
1:A:20:MET:HB2	1:A:87:ILE:HG23	0.75	1.59	1	16
1:A:178:LEU:CD2	1:A:186:LEU:HD22	0.74	2.12	8	2
1:A:111:ILE:O	1:A:115:VAL:HG23	0.74	1.83	6	16
1:A:39:TRP:CE3	1:A:50:VAL:HG11	0.73	2.18	16	2
1:A:20:MET:CB	1:A:87:ILE:HG23	0.73	2.13	14	9
1:A:210:CYS:C	1:A:211:LEU:HD12	0.73	2.08	7	2
1:A:177:ILE:C	1:A:178:LEU:HD13	0.73	2.08	11	1
1:A:30:ALA:HB3	1:A:53:THR:CB	0.73	2.13	19	2
1:A:116:ALA:HB2	1:A:133:ILE:HD11	0.73	1.58	2	1
1:A:186:LEU:HD12	1:A:190:LEU:HD11	0.73	1.60	14	1
1:A:18:VAL:HG22	1:A:93:VAL:HG12	0.73	1.61	17	1
1:A:187:LYS:CG	1:A:209:VAL:HG21	0.72	2.13	10	1
1:A:137:MET:HE2	1:A:142:TYR:CD2	0.72	2.19	12	1
1:A:31:CYS:HB3	1:A:51:LEU:HD23	0.72	1.60	14	6
1:A:190:LEU:HD22	1:A:211:LEU:CD2	0.72	2.14	9	1
1:A:31:CYS:SG	1:A:36:VAL:HG21	0.72	2.24	17	10
1:A:114:ILE:HG23	1:A:118:LYS:HD2	0.72	1.59	16	2
1:A:35:LYS:CB	1:A:50:VAL:HG23	0.71	2.15	7	8
1:A:47:LEU:HG	1:A:81:THR:HG22	0.71	1.62	17	6
1:A:51:LEU:HD11	1:A:84:CYS:SG	0.71	2.26	6	13
1:A:107:MET:HE1	1:A:150:THR:HG22	0.71	1.60	13	1
1:A:20:MET:HE3	1:A:87:ILE:HG12	0.71	1.63	3	4
1:A:18:VAL:HG22	1:A:93:VAL:HG23	0.70	1.60	11	3
1:A:112:ALA:HA	1:A:133:ILE:HG21	0.70	1.64	10	2
1:A:56:VAL:HG21	1:A:71:LEU:CD2	0.70	2.16	5	11
1:A:31:CYS:SG	1:A:88:LEU:HD21	0.70	2.27	4	4
1:A:172:MET:HE2	1:A:218:ARG:HB2	0.70	1.63	5	1
1:A:115:VAL:HG13	1:A:167:ILE:HG21	0.69	1.63	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:HD21	1:A:85:LYS:HE3	0.69	1.64	4	4
1:A:30:ALA:HB3	1:A:53:THR:HB	0.69	1.63	19	1
1:A:196:VAL:HG13	1:A:209:VAL:HG23	0.69	1.63	2	1
1:A:119:CYS:SG	1:A:167:ILE:HD13	0.69	2.28	20	2
1:A:51:LEU:HD13	1:A:54:HIS:HA	0.68	1.63	19	4
1:A:186:LEU:CD1	1:A:190:LEU:HD23	0.68	2.17	2	1
1:A:178:LEU:HD11	1:A:186:LEU:CD2	0.68	2.18	4	1
1:A:80:GLN:HA	1:A:83:ILE:HD12	0.68	1.65	12	10
1:A:178:LEU:HD11	1:A:209:VAL:HG12	0.68	1.66	9	1
1:A:39:TRP:CH2	1:A:47:LEU:HD23	0.68	2.24	7	6
1:A:130:VAL:HA	1:A:133:ILE:HD12	0.68	1.65	4	3
1:A:31:CYS:SG	1:A:88:LEU:HD11	0.68	2.28	1	7
1:A:178:LEU:HD22	1:A:186:LEU:HB2	0.67	1.64	10	1
1:A:39:TRP:CZ3	1:A:50:VAL:HG11	0.67	2.24	13	3
1:A:112:ALA:O	1:A:133:ILE:HD13	0.67	1.88	2	2
1:A:158:ILE:HG23	1:A:167:ILE:CG2	0.67	2.20	14	2
1:A:194:ILE:HB	1:A:211:LEU:HD23	0.67	1.65	7	1
1:A:15:VAL:HG23	1:A:32:TYR:CD1	0.67	2.24	19	1
1:A:186:LEU:HD11	1:A:229:LYS:HG3	0.67	1.66	11	1
1:A:177:ILE:CG2	1:A:206:LEU:HD12	0.66	2.19	10	2
1:A:47:LEU:HD12	1:A:51:LEU:CD1	0.66	2.19	14	2
1:A:47:LEU:HD12	1:A:81:THR:HG22	0.66	1.65	16	1
1:A:220:ILE:O	1:A:224:ILE:HG22	0.66	1.90	20	5
1:A:111:ILE:CD1	1:A:144:VAL:HG11	0.66	2.21	6	1
1:A:193:LEU:HD11	1:A:224:ILE:HG21	0.66	1.68	17	4
1:A:178:LEU:HD23	1:A:229:LYS:HD2	0.66	1.67	2	1
1:A:33:LYS:O	1:A:37:VAL:HG22	0.66	1.91	5	2
1:A:51:LEU:HD11	1:A:84:CYS:HB3	0.66	1.66	18	1
1:A:35:LYS:HB2	1:A:50:VAL:HG23	0.65	1.66	7	4
1:A:197:ILE:HG21	1:A:212:ILE:CD1	0.65	2.21	15	1
1:A:180:VAL:HG12	1:A:205:GLN:C	0.65	2.16	11	3
1:A:83:ILE:HG22	1:A:87:ILE:HD11	0.65	1.69	18	8
1:A:140:ILE:O	1:A:140:ILE:HD13	0.65	1.91	8	1
1:A:224:ILE:HD12	1:A:225:LYS:N	0.65	2.06	9	5
1:A:71:LEU:HD22	1:A:83:ILE:CD1	0.65	2.22	16	5
1:A:178:LEU:HD11	1:A:186:LEU:HD22	0.65	1.69	1	3
1:A:189:LYS:HD3	1:A:224:ILE:HD11	0.65	1.67	10	2
1:A:47:LEU:CD1	1:A:81:THR:HG22	0.65	2.22	16	1
1:A:158:ILE:HG23	1:A:167:ILE:HB	0.65	1.69	18	2
1:A:72:ILE:HD11	1:A:78:ASP:OD1	0.65	1.91	20	7
1:A:217:PHE:CD1	1:A:220:ILE:HD13	0.65	2.26	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:PHE:CZ	1:A:65:VAL:HG22	0.64	2.27	1	10
1:A:111:ILE:HA	1:A:114:ILE:HD12	0.64	1.70	2	3
1:A:186:LEU:HD12	1:A:190:LEU:CD1	0.64	2.23	14	1
1:A:178:LEU:HD12	1:A:183:GLY:HA2	0.64	1.68	19	1
1:A:178:LEU:HB3	1:A:186:LEU:HD11	0.64	1.69	20	1
1:A:47:LEU:HD13	1:A:51:LEU:HB2	0.64	1.68	15	5
1:A:29:ILE:HG23	1:A:56:VAL:HA	0.64	1.69	4	6
1:A:193:LEU:HD23	1:A:194:ILE:HD11	0.64	1.70	8	1
1:A:194:ILE:HB	1:A:211:LEU:HD22	0.64	1.68	15	2
1:A:75:PHE:CE2	1:A:83:ILE:HG23	0.64	2.28	11	4
1:A:190:LEU:HD13	1:A:211:LEU:CD2	0.64	2.20	19	2
1:A:176:PHE:HB2	1:A:211:LEU:HD11	0.64	1.69	6	1
1:A:185:LYS:HE2	1:A:228:THR:HG23	0.64	1.67	7	1
1:A:178:LEU:HD12	1:A:207:GLU:O	0.64	1.92	7	1
1:A:16:ALA:HB3	1:A:31:CYS:O	0.63	1.92	8	10
1:A:18:VAL:HG11	1:A:88:LEU:HA	0.63	1.70	18	1
1:A:171:HIS:O	1:A:172:MET:HE3	0.63	1.93	6	1
1:A:187:LYS:HG2	1:A:209:VAL:HG21	0.63	1.71	10	1
1:A:186:LEU:HD12	1:A:187:LYS:N	0.63	2.08	12	1
1:A:186:LEU:HD11	1:A:225:LYS:HA	0.63	1.68	16	1
1:A:35:LYS:HB3	1:A:50:VAL:HG23	0.63	1.70	4	10
1:A:178:LEU:HD12	1:A:178:LEU:N	0.63	2.09	2	2
1:A:133:ILE:HG22	1:A:137:MET:HE2	0.63	1.71	2	2
1:A:158:ILE:HG22	1:A:167:ILE:CG1	0.63	2.24	17	1
1:A:180:VAL:HG22	1:A:205:GLN:HA	0.63	1.71	3	11
1:A:174:LEU:O	1:A:211:LEU:HD12	0.63	1.94	15	2
1:A:186:LEU:HD21	1:A:229:LYS:CD	0.63	2.24	11	1
1:A:15:VAL:HG22	1:A:31:CYS:O	0.63	1.94	20	2
1:A:194:ILE:HG13	1:A:211:LEU:HD22	0.62	1.71	20	1
1:A:173:ARG:C	1:A:174:LEU:HD22	0.62	2.19	2	1
1:A:120:VAL:HG12	1:A:127:PRO:N	0.62	2.10	8	1
1:A:20:MET:HE1	1:A:22:ARG:HG3	0.62	1.69	15	1
1:A:84:CYS:O	1:A:88:LEU:HD13	0.62	1.94	12	5
1:A:211:LEU:HD11	1:A:221:ASP:OD2	0.62	1.94	4	1
1:A:51:LEU:HD21	1:A:84:CYS:HB3	0.62	1.70	9	1
1:A:154:ALA:O	1:A:158:ILE:HG23	0.62	1.94	1	1
1:A:158:ILE:HA	1:A:167:ILE:HG21	0.62	1.71	4	1
1:A:33:LYS:HG3	1:A:95:VAL:HG11	0.62	1.71	6	1
1:A:194:ILE:CD1	1:A:211:LEU:HD13	0.62	2.25	14	1
1:A:178:LEU:HD13	1:A:186:LEU:HB3	0.62	1.70	19	1
1:A:178:LEU:HD13	1:A:186:LEU:CB	0.61	2.25	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:PRO:HA	1:A:206:LEU:HD23	0.61	1.73	16	2
1:A:53:THR:HG21	1:A:57:PHE:CE1	0.61	2.29	14	17
1:A:112:ALA:HB1	1:A:133:ILE:CD1	0.61	2.25	15	1
1:A:37:VAL:HG22	1:A:147:ASN:O	0.61	1.95	19	1
1:A:193:LEU:HD13	1:A:224:ILE:HD13	0.61	1.72	6	2
1:A:36:VAL:HG13	1:A:88:LEU:HG	0.61	1.73	14	3
1:A:112:ALA:HB1	1:A:130:VAL:HG12	0.60	1.70	20	1
1:A:211:LEU:HD11	1:A:225:LYS:HE3	0.60	1.73	10	1
1:A:47:LEU:HD21	1:A:85:LYS:CE	0.60	2.27	14	4
1:A:158:ILE:HG22	1:A:167:ILE:HD12	0.60	1.72	9	1
1:A:128:TYR:CD1	1:A:132:LEU:HD13	0.60	2.32	14	4
1:A:47:LEU:HD13	1:A:51:LEU:CB	0.60	2.26	15	1
1:A:33:LYS:O	1:A:37:VAL:HG13	0.60	1.97	9	3
1:A:158:ILE:HA	1:A:167:ILE:HD13	0.60	1.74	10	1
1:A:190:LEU:HD12	1:A:211:LEU:HD22	0.60	1.73	10	1
1:A:116:ALA:HB2	1:A:133:ILE:HD13	0.60	1.74	13	1
1:A:173:ARG:HG2	1:A:212:ILE:HD12	0.59	1.73	19	2
1:A:211:LEU:O	1:A:212:ILE:HD13	0.59	1.96	4	1
1:A:56:VAL:O	1:A:66:ALA:HB3	0.59	1.97	10	4
1:A:120:VAL:HG12	1:A:127:PRO:HA	0.59	1.72	15	2
1:A:144:VAL:HG13	1:A:153:GLN:HG2	0.59	1.74	12	1
1:A:37:VAL:HG23	1:A:147:ASN:HA	0.59	1.75	20	1
1:A:194:ILE:HD11	1:A:211:LEU:HD22	0.59	1.74	16	1
1:A:71:LEU:CD2	1:A:83:ILE:HD13	0.59	2.16	6	1
1:A:194:ILE:HD13	1:A:211:LEU:HB3	0.59	1.74	18	1
1:A:211:LEU:HD12	1:A:211:LEU:N	0.59	2.13	6	2
1:A:31:CYS:SG	1:A:36:VAL:HG22	0.59	2.38	19	2
1:A:180:VAL:HG12	1:A:205:GLN:CA	0.58	2.28	11	3
1:A:178:LEU:HD22	1:A:183:GLY:HA2	0.58	1.74	7	2
1:A:18:VAL:HG22	1:A:93:VAL:HA	0.58	1.74	18	3
1:A:197:ILE:HG22	1:A:210:CYS:O	0.58	1.98	15	1
1:A:114:ILE:HG23	1:A:118:LYS:HG3	0.58	1.74	19	1
1:A:142:TYR:CD2	1:A:144:VAL:HG22	0.58	2.33	7	1
1:A:18:VAL:CG2	1:A:93:VAL:HG23	0.58	2.28	11	1
1:A:30:ALA:HB3	1:A:53:THR:OG1	0.58	1.98	18	2
1:A:110:ASP:HB3	1:A:150:THR:HG21	0.58	1.76	12	1
1:A:233:SER:O	1:A:234:LEU:HD12	0.58	1.98	2	1
1:A:167:ILE:N	1:A:167:ILE:HD13	0.58	2.13	17	2
1:A:161:LEU:CB	1:A:167:ILE:HD11	0.58	2.28	10	1
1:A:18:VAL:HG13	1:A:92:GLU:C	0.58	2.24	11	4
1:A:157:VAL:HG12	1:A:161:LEU:HD12	0.58	1.75	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ILE:HG22	1:A:56:VAL:HA	0.58	1.76	19	1
1:A:18:VAL:HG21	1:A:88:LEU:HD12	0.58	1.76	20	2
1:A:186:LEU:HD23	1:A:229:LYS:CD	0.58	2.29	3	1
1:A:129:THR:O	1:A:133:ILE:HD12	0.58	1.99	16	1
1:A:173:ARG:HG3	1:A:212:ILE:HG23	0.57	1.75	11	1
1:A:158:ILE:HG22	1:A:167:ILE:HG13	0.57	1.74	17	1
1:A:29:ILE:HG23	1:A:56:VAL:HG13	0.57	1.73	19	1
1:A:186:LEU:HD22	1:A:229:LYS:HG3	0.57	1.75	2	1
1:A:120:VAL:HG21	1:A:216:CYS:HB2	0.57	1.74	4	3
1:A:31:CYS:SG	1:A:51:LEU:HD23	0.57	2.39	20	1
1:A:196:VAL:HG13	1:A:209:VAL:CG1	0.57	2.29	20	1
1:A:137:MET:CE	1:A:161:LEU:HD11	0.57	2.29	15	1
1:A:211:LEU:C	1:A:212:ILE:HD12	0.57	2.24	15	1
1:A:158:ILE:HA	1:A:167:ILE:HD11	0.57	1.76	17	2
1:A:37:VAL:HG21	1:A:146:THR:O	0.57	1.99	19	1
1:A:30:ALA:HB3	1:A:53:THR:CG2	0.57	2.28	11	4
1:A:18:VAL:HG22	1:A:93:VAL:CG2	0.57	2.30	11	1
1:A:186:LEU:HD21	1:A:229:LYS:HD3	0.57	1.77	11	1
1:A:224:ILE:O	1:A:228:THR:HG23	0.57	2.00	8	3
1:A:120:VAL:HG11	1:A:216:CYS:HB2	0.57	1.76	18	2
1:A:178:LEU:HD21	1:A:207:GLU:OE1	0.57	2.00	15	1
1:A:18:VAL:HG11	1:A:87:ILE:O	0.57	2.00	17	1
1:A:178:LEU:HD22	1:A:178:LEU:N	0.57	2.15	1	2
1:A:194:ILE:CD1	1:A:211:LEU:HD23	0.56	2.30	2	1
1:A:114:ILE:HG23	1:A:118:LYS:HD3	0.56	1.76	18	1
1:A:47:LEU:HA	1:A:50:VAL:HG12	0.56	1.78	10	10
1:A:16:ALA:HB2	1:A:33:LYS:CG	0.56	2.30	12	4
1:A:111:ILE:HD11	1:A:153:GLN:OE1	0.56	1.99	11	1
1:A:186:LEU:HD23	1:A:190:LEU:HD11	0.56	1.76	1	2
1:A:118:LYS:O	1:A:120:VAL:HG13	0.56	2.00	15	1
1:A:120:VAL:HG21	1:A:216:CYS:HB3	0.56	1.76	5	1
1:A:47:LEU:HD21	1:A:85:LYS:HD2	0.56	1.78	18	2
1:A:137:MET:HE2	1:A:142:TYR:CD1	0.56	2.36	11	1
1:A:174:LEU:N	1:A:211:LEU:O	0.56	2.39	16	6
1:A:75:PHE:CD1	1:A:83:ILE:HG23	0.56	2.36	19	2
1:A:136:ALA:O	1:A:140:ILE:HG22	0.56	2.00	7	2
1:A:58:VAL:HG23	1:A:66:ALA:N	0.56	2.16	8	1
1:A:120:VAL:HG12	1:A:126:ARG:C	0.56	2.25	8	1
1:A:17:VAL:HG12	1:A:28:GLU:HG2	0.55	1.76	17	4
1:A:110:ASP:OD1	1:A:114:ILE:HD11	0.55	2.01	11	1
1:A:196:VAL:C	1:A:197:ILE:HD12	0.55	2.25	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:LEU:HD21	1:A:225:LYS:HG2	0.55	1.77	15	1
1:A:190:LEU:HD23	1:A:224:ILE:HD11	0.55	1.78	14	1
1:A:180:VAL:HG22	1:A:205:GLN:CA	0.55	2.32	20	10
1:A:56:VAL:CB	1:A:71:LEU:HD21	0.55	2.31	16	5
1:A:18:VAL:HG21	1:A:88:LEU:CD1	0.55	2.32	20	2
1:A:120:VAL:HG21	1:A:125:LYS:HE2	0.55	1.78	20	1
1:A:178:LEU:HD23	1:A:186:LEU:HB3	0.55	1.79	17	2
1:A:178:LEU:HD12	1:A:183:GLY:CA	0.55	2.32	12	1
1:A:107:MET:HB3	1:A:144:VAL:HG11	0.55	1.77	16	1
1:A:196:VAL:HG13	1:A:209:VAL:CG2	0.55	2.29	2	1
1:A:144:VAL:HG13	1:A:153:GLN:OE1	0.55	2.01	4	1
1:A:172:MET:SD	1:A:174:LEU:HD21	0.55	2.42	5	1
1:A:178:LEU:HD13	1:A:178:LEU:N	0.55	2.15	11	1
1:A:177:ILE:N	1:A:177:ILE:HD13	0.55	2.16	12	1
1:A:186:LEU:HD23	1:A:190:LEU:CD1	0.55	2.31	15	1
1:A:110:ASP:OD2	1:A:150:THR:HG21	0.55	2.01	4	1
1:A:75:PHE:CZ	1:A:83:ILE:HG23	0.55	2.37	14	5
1:A:154:ALA:O	1:A:158:ILE:HG22	0.55	2.01	13	2
1:A:47:LEU:HD12	1:A:81:THR:CG2	0.55	2.32	16	1
1:A:75:PHE:CE1	1:A:83:ILE:HG23	0.54	2.37	19	4
1:A:189:LYS:HG3	1:A:228:THR:HG21	0.54	1.79	14	2
1:A:176:PHE:CE2	1:A:190:LEU:HD11	0.54	2.37	17	1
1:A:167:ILE:HD12	1:A:167:ILE:O	0.54	2.02	19	2
1:A:36:VAL:HG11	1:A:93:VAL:HG21	0.54	1.79	20	1
1:A:167:ILE:HD13	1:A:167:ILE:H	0.54	1.61	6	2
1:A:93:VAL:HG13	1:A:93:VAL:O	0.54	2.00	9	8
1:A:178:LEU:N	1:A:178:LEU:HD23	0.54	2.17	19	2
1:A:189:LYS:HD3	1:A:228:THR:HG21	0.54	1.79	12	1
1:A:47:LEU:HD21	1:A:85:LYS:HE2	0.54	1.78	11	4
1:A:119:CYS:HB3	1:A:167:ILE:HD11	0.54	1.79	14	2
1:A:33:LYS:O	1:A:37:VAL:HG12	0.54	2.03	10	2
1:A:51:LEU:HD11	1:A:84:CYS:HB2	0.54	1.79	18	1
1:A:172:MET:HE2	1:A:218:ARG:CB	0.54	2.33	5	1
1:A:29:ILE:HD11	1:A:88:LEU:CD1	0.54	2.33	16	1
1:A:193:LEU:HD21	1:A:220:ILE:HG22	0.54	1.80	12	2
1:A:140:ILE:HG22	1:A:140:ILE:O	0.54	2.03	13	3
1:A:53:THR:CG2	1:A:57:PHE:CE1	0.53	2.91	19	4
1:A:107:MET:HE3	1:A:146:THR:HA	0.53	1.80	20	1
1:A:186:LEU:HD21	1:A:225:LYS:CG	0.53	2.33	15	1
1:A:194:ILE:HD11	1:A:221:ASP:CG	0.53	2.29	15	1
1:A:98:LYS:O	1:A:102:THR:HG23	0.53	2.03	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:193:LEU:HD13	1:A:224:ILE:CD1	0.53	2.34	15	1
1:A:83:ILE:HG22	1:A:87:ILE:CD1	0.53	2.32	3	4
1:A:39:TRP:C	1:A:39:TRP:CD1	0.53	2.87	14	13
1:A:18:VAL:HG23	1:A:31:CYS:SG	0.53	2.44	10	8
1:A:178:LEU:HD12	1:A:183:GLY:HA3	0.53	1.80	20	2
1:A:29:ILE:HD11	1:A:87:ILE:CG2	0.52	2.33	5	1
1:A:18:VAL:HG22	1:A:93:VAL:HG13	0.52	1.81	14	1
1:A:32:TYR:O	1:A:36:VAL:CG2	0.52	2.57	15	14
1:A:217:PHE:CE1	1:A:220:ILE:HD11	0.52	2.39	8	1
1:A:116:ALA:HB2	1:A:133:ILE:CG1	0.52	2.35	10	1
1:A:98:LYS:O	1:A:102:THR:HG22	0.52	2.05	17	3
1:A:20:MET:HE3	1:A:22:ARG:HG3	0.52	1.81	4	1
1:A:174:LEU:HD11	1:A:218:ARG:HD3	0.52	1.81	7	1
1:A:174:LEU:HB3	1:A:211:LEU:HD13	0.52	1.81	17	1
1:A:178:LEU:CD1	1:A:186:LEU:HD22	0.52	2.34	11	2
1:A:180:VAL:HG12	1:A:205:GLN:HA	0.52	1.80	4	1
1:A:34:ASN:O	1:A:37:VAL:HG12	0.52	2.03	20	2
1:A:174:LEU:HD22	1:A:211:LEU:HD22	0.52	1.81	12	1
1:A:15:VAL:HG23	1:A:32:TYR:CE1	0.52	2.39	19	1
1:A:180:VAL:HG13	1:A:204:GLN:C	0.52	2.30	3	7
1:A:217:PHE:CD1	1:A:220:ILE:HD11	0.52	2.40	8	1
1:A:112:ALA:CB	1:A:130:VAL:HG12	0.52	2.34	20	1
1:A:189:LYS:CE	1:A:224:ILE:HD11	0.52	2.34	20	1
1:A:47:LEU:HD21	1:A:85:LYS:HG2	0.52	1.81	12	5
1:A:15:VAL:HG22	1:A:52:GLN:NE2	0.52	2.20	6	2
1:A:190:LEU:HD23	1:A:224:ILE:CD1	0.52	2.34	14	1
1:A:47:LEU:CD1	1:A:51:LEU:HD12	0.52	2.35	5	3
1:A:180:VAL:HG22	1:A:205:GLN:C	0.52	2.30	16	5
1:A:137:MET:CE	1:A:157:VAL:HG13	0.52	2.34	10	1
1:A:32:TYR:C	1:A:36:VAL:HG23	0.51	2.29	4	2
1:A:196:VAL:CG1	1:A:209:VAL:HG11	0.51	2.36	1	1
1:A:186:LEU:HD12	1:A:186:LEU:C	0.51	2.29	12	1
1:A:200:GLU:HB2	1:A:208:ILE:HD11	0.51	1.82	6	1
1:A:71:LEU:HD22	1:A:83:ILE:HD12	0.51	1.81	16	1
1:A:27:PHE:CD2	1:A:75:PHE:CE2	0.51	2.99	15	3
1:A:211:LEU:N	1:A:211:LEU:HD22	0.51	2.21	1	1
1:A:20:MET:HE2	1:A:87:ILE:HA	0.51	1.83	8	1
1:A:103:GLN:HB3	1:A:146:THR:HG21	0.51	1.83	15	2
1:A:155:LEU:HA	1:A:158:ILE:HD12	0.51	1.82	5	3
1:A:158:ILE:HA	1:A:167:ILE:HD12	0.51	1.82	16	2
1:A:180:VAL:HG23	1:A:205:GLN:O	0.51	2.06	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:174:LEU:CG	1:A:237:LEU:HD23	0.51	2.36	6	1
1:A:193:LEU:HD22	1:A:224:ILE:HG21	0.51	1.81	15	4
1:A:111:ILE:O	1:A:115:VAL:HG12	0.51	2.04	15	1
1:A:173:ARG:CG	1:A:212:ILE:HD12	0.51	2.36	1	1
1:A:193:LEU:CD1	1:A:224:ILE:HG21	0.50	2.36	4	3
1:A:211:LEU:HD23	1:A:221:ASP:OD2	0.50	2.05	6	1
1:A:29:ILE:CG2	1:A:56:VAL:HG13	0.50	2.36	19	1
1:A:186:LEU:HD23	1:A:229:LYS:HD2	0.50	1.83	3	1
1:A:84:CYS:O	1:A:88:LEU:HD23	0.50	2.06	18	1
1:A:190:LEU:HD21	1:A:221:ASP:OD1	0.50	2.06	17	2
1:A:111:ILE:HD13	1:A:144:VAL:HG11	0.50	1.83	6	1
1:A:113:THR:HG22	1:A:117:ASP:OD2	0.50	2.07	2	1
1:A:196:VAL:CG1	1:A:209:VAL:HG21	0.50	2.36	9	1
1:A:68:LYS:O	1:A:72:ILE:HD12	0.50	2.06	4	3
1:A:178:LEU:HD22	1:A:178:LEU:H	0.50	1.67	11	2
1:A:199:SER:CB	1:A:209:VAL:HG22	0.50	2.37	14	1
1:A:186:LEU:HD12	1:A:228:THR:HG23	0.50	1.83	6	1
1:A:193:LEU:O	1:A:194:ILE:HG23	0.49	2.07	1	2
1:A:29:ILE:H	1:A:29:ILE:HD13	0.49	1.67	12	1
1:A:137:MET:HE3	1:A:137:MET:HA	0.49	1.83	12	1
1:A:115:VAL:CG1	1:A:167:ILE:HG21	0.49	2.34	18	1
1:A:28:GLU:OE2	1:A:60:VAL:HG23	0.49	2.07	20	5
1:A:175:ARG:HD3	1:A:236:VAL:HG13	0.49	1.85	6	1
1:A:194:ILE:HD13	1:A:221:ASP:OD1	0.49	2.07	12	1
1:A:158:ILE:HG22	1:A:167:ILE:CD1	0.49	2.37	15	1
1:A:158:ILE:HD11	1:A:167:ILE:O	0.49	2.07	2	1
1:A:182:GLU:O	1:A:186:LEU:HD23	0.49	2.07	14	1
1:A:58:VAL:HG23	1:A:66:ALA:HB2	0.49	1.83	10	2
1:A:186:LEU:HD21	1:A:229:LYS:HG3	0.49	1.84	18	1
1:A:20:MET:HE3	1:A:87:ILE:CG1	0.49	2.37	14	3
1:A:133:ILE:CG2	1:A:137:MET:HE2	0.49	2.37	17	1
1:A:39:TRP:CH2	1:A:85:LYS:HD3	0.49	2.42	16	1
1:A:174:LEU:O	1:A:211:LEU:N	0.49	2.46	3	4
1:A:15:VAL:HG21	1:A:52:GLN:HG2	0.49	1.84	16	2
1:A:39:TRP:CH2	1:A:47:LEU:CD2	0.49	2.96	10	10
1:A:178:LEU:N	1:A:178:LEU:HD22	0.49	2.22	11	1
1:A:36:VAL:HG22	1:A:88:LEU:CD1	0.49	2.38	18	1
1:A:20:MET:HE1	1:A:22:ARG:HD2	0.49	1.84	3	1
1:A:178:LEU:HG	1:A:186:LEU:HD13	0.49	1.84	11	1
1:A:72:ILE:HD11	1:A:78:ASP:CG	0.49	2.32	12	1
1:A:186:LEU:HD21	1:A:229:LYS:HB3	0.49	1.84	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:178:LEU:HD11	1:A:207:GLU:HB3	0.49	1.85	5	1
1:A:17:VAL:HG11	1:A:28:GLU:OE2	0.49	2.08	9	1
1:A:108:PHE:CE1	1:A:144:VAL:HG23	0.48	2.43	18	1
1:A:18:VAL:CG2	1:A:93:VAL:HG12	0.48	2.35	17	1
1:A:95:VAL:HG11	1:A:99:GLU:OE2	0.48	2.07	19	1
1:A:196:VAL:O	1:A:197:ILE:HG23	0.48	2.08	8	2
1:A:120:VAL:HG11	1:A:125:LYS:HE2	0.48	1.84	20	1
1:A:157:VAL:HG22	1:A:161:LEU:HD12	0.48	1.84	3	2
1:A:194:ILE:HG22	1:A:217:PHE:CD1	0.48	2.44	5	1
1:A:142:TYR:CE2	1:A:144:VAL:HG22	0.48	2.44	8	1
1:A:47:LEU:CG	1:A:81:THR:HG22	0.48	2.38	17	2
1:A:109:ARG:O	1:A:113:THR:HG23	0.48	2.07	11	1
1:A:115:VAL:HG13	1:A:133:ILE:CD1	0.48	2.39	13	1
1:A:129:THR:OG1	1:A:132:LEU:HD23	0.48	2.08	20	1
1:A:142:TYR:HE2	1:A:144:VAL:HG22	0.48	1.68	8	1
1:A:190:LEU:HD12	1:A:194:ILE:CG2	0.48	2.39	10	1
1:A:18:VAL:HG22	1:A:93:VAL:CB	0.48	2.39	11	1
1:A:177:ILE:HD11	1:A:236:VAL:HG23	0.48	1.85	17	1
1:A:15:VAL:CG2	1:A:32:TYR:CD1	0.47	2.97	19	1
1:A:29:ILE:HD11	1:A:88:LEU:HD12	0.47	1.86	2	5
1:A:107:MET:HE3	1:A:144:VAL:HG23	0.47	1.85	5	1
1:A:178:LEU:O	1:A:178:LEU:HD12	0.47	2.09	5	1
1:A:137:MET:HE1	1:A:157:VAL:HG13	0.47	1.86	10	1
1:A:186:LEU:HD11	1:A:229:LYS:HA	0.47	1.86	13	1
1:A:174:LEU:HD12	1:A:211:LEU:HB2	0.47	1.86	18	1
1:A:178:LEU:HD11	1:A:186:LEU:HD23	0.47	1.86	4	1
1:A:120:VAL:HG11	1:A:216:CYS:CB	0.47	2.39	9	1
1:A:194:ILE:HD11	1:A:211:LEU:HD13	0.47	1.85	20	1
1:A:180:VAL:HG23	1:A:181:ASN:N	0.47	2.24	12	2
1:A:110:ASP:O	1:A:113:THR:HG22	0.47	2.10	7	2
1:A:178:LEU:HD22	1:A:186:LEU:HD22	0.47	1.85	8	1
1:A:137:MET:HE1	1:A:161:LEU:HD11	0.47	1.87	15	1
1:A:16:ALA:HB2	1:A:33:LYS:HB3	0.47	1.87	10	2
1:A:193:LEU:HD13	1:A:224:ILE:HG21	0.47	1.86	13	2
1:A:197:ILE:CD1	1:A:212:ILE:HD11	0.47	2.39	6	1
1:A:115:VAL:CG1	1:A:133:ILE:HD12	0.47	2.40	13	1
1:A:206:LEU:O	1:A:206:LEU:CD2	0.47	2.63	13	1
1:A:197:ILE:HD12	1:A:197:ILE:N	0.47	2.25	20	1
1:A:75:PHE:CE2	1:A:83:ILE:CG2	0.47	2.98	1	5
1:A:176:PHE:CE1	1:A:235:GLU:CB	0.47	2.98	10	1
1:A:189:LYS:CD	1:A:224:ILE:HD11	0.47	2.39	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:GLU:O	1:A:57:PHE:N	0.47	2.47	20	8
1:A:108:PHE:HA	1:A:111:ILE:HD12	0.47	1.85	8	2
1:A:199:SER:OG	1:A:209:VAL:HG22	0.47	2.09	7	1
1:A:178:LEU:HD11	1:A:209:VAL:CG1	0.47	2.40	9	1
1:A:191:LYS:N	1:A:192:PRO:CD	0.46	2.78	9	5
1:A:39:TRP:CZ3	1:A:47:LEU:CD2	0.46	2.98	6	1
1:A:161:LEU:HD12	1:A:167:ILE:HD11	0.46	1.86	7	2
1:A:18:VAL:HG13	1:A:92:GLU:O	0.46	2.10	18	1
1:A:112:ALA:HB1	1:A:130:VAL:CG1	0.46	2.41	20	1
1:A:56:VAL:HG11	1:A:71:LEU:HD21	0.46	1.86	18	3
1:A:57:PHE:CE2	1:A:65:VAL:HG22	0.46	2.45	19	2
1:A:161:LEU:HD23	1:A:164:LYS:NZ	0.46	2.25	8	1
1:A:29:ILE:HD13	1:A:88:LEU:CD1	0.46	2.40	9	1
1:A:161:LEU:HB2	1:A:167:ILE:HD11	0.46	1.86	10	1
1:A:224:ILE:HG23	1:A:225:LYS:N	0.46	2.26	6	3
1:A:194:ILE:HD12	1:A:194:ILE:C	0.46	2.35	18	2
1:A:129:THR:OG1	1:A:132:LEU:HD12	0.46	2.11	3	1
1:A:29:ILE:HD13	1:A:88:LEU:HD13	0.46	1.88	9	1
1:A:85:LYS:CE	1:A:85:LYS:CA	0.46	2.94	16	1
1:A:185:LYS:HD3	1:A:228:THR:HG23	0.46	1.87	4	1
1:A:197:ILE:HG21	1:A:212:ILE:HD11	0.46	1.87	15	1
1:A:36:VAL:HG22	1:A:88:LEU:HD21	0.45	1.88	14	2
1:A:114:ILE:HG23	1:A:118:LYS:CG	0.45	2.40	19	1
1:A:33:LYS:HB2	1:A:95:VAL:HG11	0.45	1.89	20	1
1:A:15:VAL:HG12	1:A:16:ALA:N	0.45	2.26	1	2
1:A:50:VAL:HG13	1:A:51:LEU:N	0.45	2.27	14	9
1:A:178:LEU:HD23	1:A:182:GLU:HB3	0.45	1.89	10	1
1:A:115:VAL:HG13	1:A:133:ILE:HG21	0.45	1.87	15	1
1:A:136:ALA:HB1	1:A:164:LYS:CE	0.45	2.42	2	1
1:A:75:PHE:CE1	1:A:83:ILE:CG2	0.45	3.00	4	2
1:A:137:MET:HE3	1:A:142:TYR:CG	0.45	2.46	10	1
1:A:115:VAL:HG13	1:A:116:ALA:N	0.45	2.27	15	1
1:A:196:VAL:CG1	1:A:209:VAL:CG1	0.45	2.95	1	1
1:A:194:ILE:CG2	1:A:217:PHE:CD1	0.45	3.00	5	3
1:A:100:ARG:O	1:A:104:LEU:HD13	0.45	2.12	15	1
1:A:194:ILE:HG22	1:A:195:LYS:N	0.45	2.27	11	5
1:A:40:ARG:HA	1:A:89:THR:HG22	0.45	1.89	12	1
1:A:174:LEU:HD22	1:A:211:LEU:HD13	0.45	1.89	13	1
1:A:197:ILE:HD12	1:A:198:GLU:HB2	0.45	1.89	17	1
1:A:46:ASP:O	1:A:50:VAL:HG12	0.45	2.11	12	2
1:A:39:TRP:CD1	1:A:39:TRP:C	0.45	2.95	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:189:LYS:HE2	1:A:224:ILE:HD11	0.45	1.87	20	1
1:A:120:VAL:HG22	1:A:215:GLY:HA3	0.45	1.88	15	1
1:A:18:VAL:HB	1:A:29:ILE:HD11	0.45	1.89	19	1
1:A:22:ARG:CD	1:A:75:PHE:CZ	0.45	3.00	8	1
1:A:178:LEU:HD22	1:A:186:LEU:HD13	0.45	1.89	13	1
1:A:194:ILE:HD13	1:A:211:LEU:HD13	0.45	1.89	14	1
1:A:190:LEU:HD22	1:A:211:LEU:HD21	0.44	1.88	9	1
1:A:37:VAL:HG12	1:A:146:THR:O	0.44	2.12	15	1
1:A:36:VAL:HG22	1:A:88:LEU:CD2	0.44	2.42	17	1
1:A:111:ILE:CG2	1:A:112:ALA:N	0.44	2.79	17	2
1:A:180:VAL:HG13	1:A:181:ASN:N	0.44	2.27	7	3
1:A:196:VAL:HG12	1:A:211:LEU:HB3	0.44	1.88	10	1
1:A:18:VAL:HG12	1:A:87:ILE:HG22	0.44	1.90	19	1
1:A:196:VAL:HG13	1:A:209:VAL:HG11	0.44	1.89	20	1
1:A:176:PHE:CD2	1:A:190:LEU:CD1	0.44	3.01	15	1
1:A:191:LYS:CB	1:A:192:PRO:CD	0.44	2.96	3	5
1:A:112:ALA:HB1	1:A:130:VAL:HG13	0.44	1.88	14	1
1:A:128:TYR:CE1	1:A:132:LEU:HD13	0.44	2.47	14	1
1:A:154:ALA:O	1:A:158:ILE:HD12	0.44	2.13	3	1
1:A:18:VAL:HG22	1:A:93:VAL:CA	0.44	2.43	11	3
1:A:53:THR:HG23	1:A:53:THR:O	0.44	2.13	5	2
1:A:108:PHE:CE1	1:A:137:MET:HE2	0.44	2.48	7	1
1:A:18:VAL:HB	1:A:29:ILE:HD12	0.44	1.88	9	1
1:A:190:LEU:CD1	1:A:194:ILE:HG22	0.44	2.43	10	1
1:A:137:MET:HE2	1:A:142:TYR:CE1	0.44	2.47	11	1
1:A:29:ILE:HD13	1:A:29:ILE:N	0.44	2.28	12	1
1:A:177:ILE:CD1	1:A:208:ILE:HG22	0.44	2.36	18	1
1:A:186:LEU:HD22	1:A:228:THR:CG2	0.44	2.42	3	1
1:A:137:MET:HE1	1:A:161:LEU:HG	0.44	1.89	12	1
1:A:158:ILE:HG23	1:A:159:LYS:N	0.43	2.28	2	1
1:A:151:LYS:HG2	1:A:220:ILE:HD11	0.43	1.89	6	1
1:A:182:GLU:O	1:A:186:LEU:HD12	0.43	2.13	8	2
1:A:161:LEU:HB3	1:A:167:ILE:HD11	0.43	1.90	10	1
1:A:194:ILE:HD11	1:A:221:ASP:CB	0.43	2.42	15	1
1:A:225:LYS:HG3	1:A:226:LYS:N	0.43	2.28	17	1
1:A:120:VAL:HG11	1:A:215:GLY:O	0.43	2.13	1	1
1:A:116:ALA:HB2	1:A:133:ILE:HD12	0.43	1.89	3	1
1:A:72:ILE:O	1:A:76:GLY:N	0.43	2.51	10	4
1:A:145:LYS:HD2	1:A:150:THR:HG23	0.43	1.90	17	1
1:A:157:VAL:HG13	1:A:158:ILE:N	0.43	2.29	8	5
1:A:186:LEU:HD13	1:A:228:THR:HB	0.43	1.90	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:211:LEU:HD13	1:A:221:ASP:OD2	0.43	2.13	19	1
1:A:17:VAL:HG13	1:A:60:VAL:HG21	0.43	1.90	14	3
1:A:58:VAL:CG2	1:A:66:ALA:HB2	0.43	2.43	20	2
1:A:196:VAL:CG1	1:A:209:VAL:CG2	0.43	2.96	9	1
1:A:140:ILE:O	1:A:141:HIS:CG	0.43	2.71	13	1
1:A:140:ILE:HD11	1:A:161:LEU:HD23	0.43	1.91	14	1
1:A:191:LYS:HA	1:A:196:VAL:HG21	0.43	1.90	1	1
1:A:196:VAL:CG1	1:A:209:VAL:HG23	0.43	2.41	2	1
1:A:178:LEU:HD12	1:A:233:SER:HB3	0.43	1.90	11	1
1:A:161:LEU:HD22	1:A:164:LYS:HZ1	0.43	1.73	2	1
1:A:47:LEU:CD1	1:A:51:LEU:CD1	0.43	2.96	5	1
1:A:111:ILE:HD11	1:A:144:VAL:HG11	0.43	1.91	12	1
1:A:194:ILE:HD11	1:A:211:LEU:HD23	0.43	1.91	13	1
1:A:31:CYS:CB	1:A:36:VAL:CG2	0.43	2.96	18	1
1:A:213:ASP:CB	1:A:214:PRO:CD	0.43	2.97	3	1
1:A:174:LEU:HD21	1:A:237:LEU:CD2	0.43	2.43	6	1
1:A:116:ALA:HB1	1:A:128:TYR:O	0.43	2.14	10	1
1:A:85:LYS:CE	1:A:85:LYS:HA	0.43	2.42	16	1
1:A:111:ILE:HG23	1:A:112:ALA:N	0.43	2.29	18	2
1:A:53:THR:O	1:A:54:HIS:HB2	0.43	2.14	18	2
1:A:33:LYS:CG	1:A:95:VAL:HG11	0.43	2.41	6	2
1:A:15:VAL:HG22	1:A:32:TYR:HA	0.43	1.91	9	2
1:A:167:ILE:HG22	1:A:168:GLU:N	0.43	2.29	11	2
1:A:137:MET:HE1	1:A:157:VAL:CG1	0.43	2.44	15	1
1:A:33:LYS:HD3	1:A:95:VAL:HG12	0.43	1.89	17	1
1:A:115:VAL:HG13	1:A:167:ILE:HG12	0.42	1.91	1	1
1:A:111:ILE:CG2	1:A:157:VAL:HG11	0.42	2.44	20	2
1:A:178:LEU:HD13	1:A:186:LEU:HD11	0.42	1.91	12	1
1:A:20:MET:HE2	1:A:90:LYS:HE3	0.42	1.89	15	1
1:A:173:ARG:HG2	1:A:212:ILE:HG23	0.42	1.91	20	1
1:A:33:LYS:CB	1:A:95:VAL:HG12	0.42	2.44	2	1
1:A:37:VAL:HG23	1:A:38:GLY:N	0.42	2.28	11	2
1:A:31:CYS:SG	1:A:51:LEU:HD22	0.42	2.54	9	1
1:A:77:THR:O	1:A:78:ASP:CB	0.42	2.67	6	1
1:A:121:ASN:O	1:A:125:LYS:N	0.42	2.52	20	1
1:A:116:ALA:HB2	1:A:133:ILE:HG13	0.42	1.90	10	1
1:A:54:HIS:CD2	1:A:54:HIS:N	0.42	2.86	14	1
1:A:33:LYS:HB2	1:A:95:VAL:HG12	0.42	1.92	2	1
1:A:180:VAL:CG1	1:A:181:ASN:N	0.42	2.82	2	3
1:A:172:MET:HE1	1:A:174:LEU:HD21	0.42	1.92	5	1
1:A:15:VAL:HG22	1:A:52:GLN:CD	0.42	2.39	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:PHE:CD1	1:A:234:LEU:O	0.42	2.72	6	1
1:A:190:LEU:HB3	1:A:211:LEU:HD21	0.42	1.91	7	1
1:A:210:CYS:C	1:A:211:LEU:HD22	0.42	2.39	1	1
1:A:177:ILE:HG23	1:A:177:ILE:O	0.42	2.14	2	1
1:A:158:ILE:HD13	1:A:167:ILE:CD1	0.42	2.45	8	1
1:A:225:LYS:O	1:A:229:LYS:N	0.42	2.53	12	1
1:A:176:PHE:CE1	1:A:225:LYS:CE	0.42	3.02	13	1
1:A:18:VAL:O	1:A:28:GLU:HA	0.42	2.15	17	2
1:A:31:CYS:HB2	1:A:36:VAL:CG2	0.42	2.45	18	1
1:A:114:ILE:HG13	1:A:150:THR:HG22	0.42	1.92	19	1
1:A:16:ALA:HB2	1:A:33:LYS:HG2	0.42	1.92	17	1
1:A:18:VAL:CG2	1:A:31:CYS:SG	0.42	3.08	17	1
1:A:36:VAL:HG22	1:A:88:LEU:HD13	0.42	1.91	18	1
1:A:197:ILE:HD11	1:A:212:ILE:HD11	0.42	1.90	1	1
1:A:133:ILE:HA	1:A:165:MET:HE1	0.42	1.91	17	1
1:A:186:LEU:HD12	1:A:190:LEU:HG	0.42	1.91	3	1
1:A:178:LEU:CD1	1:A:209:VAL:HG12	0.42	2.43	9	1
1:A:140:ILE:HD11	1:A:164:LYS:HB2	0.42	1.91	13	1
1:A:201:ASP:CB	1:A:207:GLU:CG	0.41	2.98	8	2
1:A:87:ILE:O	1:A:91:GLY:N	0.41	2.53	18	2
1:A:178:LEU:CG	1:A:186:LEU:HD22	0.41	2.45	11	1
1:A:108:PHE:HD1	1:A:144:VAL:HG21	0.41	1.75	13	1
1:A:178:LEU:N	1:A:178:LEU:CD2	0.41	2.83	4	1
1:A:83:ILE:O	1:A:86:GLN:HG2	0.41	2.15	15	1
1:A:18:VAL:HG22	1:A:93:VAL:HG22	0.41	1.92	20	1
1:A:189:LYS:HD2	1:A:228:THR:HG21	0.41	1.92	9	1
1:A:75:PHE:CZ	1:A:83:ILE:CG2	0.41	3.03	14	1
1:A:144:VAL:HG12	1:A:145:LYS:N	0.41	2.30	2	1
1:A:174:LEU:HD21	1:A:237:LEU:HD23	0.41	1.91	6	1
1:A:211:LEU:HD22	1:A:221:ASP:OD1	0.41	2.16	13	1
1:A:57:PHE:CE1	1:A:65:VAL:HG22	0.41	2.49	1	1
1:A:15:VAL:HG21	1:A:52:GLN:HG3	0.41	1.92	7	1
1:A:18:VAL:O	1:A:29:ILE:HD13	0.41	2.15	16	1
1:A:37:VAL:HG13	1:A:38:GLY:N	0.41	2.31	14	2
1:A:173:ARG:C	1:A:174:LEU:HD12	0.41	2.40	4	1
1:A:206:LEU:CD2	1:A:206:LEU:C	0.41	2.93	13	1
1:A:233:SER:O	1:A:234:LEU:HD22	0.41	2.15	14	1
1:A:194:ILE:CD1	1:A:211:LEU:HD22	0.41	2.44	16	1
1:A:108:PHE:CE2	1:A:144:VAL:HG21	0.41	2.51	20	1
1:A:193:LEU:O	1:A:217:PHE:CE1	0.41	2.74	6	1
1:A:121:ASN:O	1:A:123:GLU:N	0.41	2.54	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:ILE:HG21	1:A:211:LEU:HD13	0.41	1.93	10	1
1:A:177:ILE:HD11	1:A:236:VAL:CG2	0.41	2.46	14	1
1:A:196:VAL:HG12	1:A:211:LEU:HG	0.41	1.92	7	1
1:A:140:ILE:HD13	1:A:140:ILE:C	0.41	2.40	8	1
1:A:172:MET:HE1	1:A:174:LEU:HD13	0.41	1.91	17	1
1:A:193:LEU:O	1:A:194:ILE:CG2	0.41	2.68	1	1
1:A:26:ARG:O	1:A:27:PHE:CD1	0.41	2.74	8	1
1:A:53:THR:O	1:A:53:THR:HG23	0.41	2.16	8	1
1:A:29:ILE:CD1	1:A:88:LEU:CD1	0.41	2.98	10	1
1:A:108:PHE:CD2	1:A:144:VAL:HG21	0.41	2.51	10	1
1:A:176:PHE:CZ	1:A:229:LYS:HD3	0.41	2.49	11	1
1:A:178:LEU:HG	1:A:186:LEU:HD22	0.41	1.93	11	1
1:A:174:LEU:HD13	1:A:175:ARG:H	0.41	1.75	16	1
1:A:31:CYS:HB3	1:A:36:VAL:HG21	0.41	1.93	7	1
1:A:212:ILE:HG22	1:A:213:ASP:N	0.41	2.31	9	1
1:A:75:PHE:CE2	1:A:83:ILE:HG21	0.40	2.51	1	1
1:A:16:ALA:HB2	1:A:33:LYS:HD2	0.40	1.91	11	1
1:A:177:ILE:HD13	1:A:177:ILE:H	0.40	1.76	12	1
1:A:193:LEU:O	1:A:217:PHE:CZ	0.40	2.75	20	1
1:A:178:LEU:HD21	1:A:186:LEU:HD22	0.40	1.91	6	1
1:A:211:LEU:N	1:A:211:LEU:CD1	0.40	2.84	6	1
1:A:193:LEU:HD23	1:A:194:ILE:CD1	0.40	2.45	8	1
1:A:191:LYS:N	1:A:192:PRO:HD2	0.40	2.30	12	1
1:A:212:ILE:HD12	1:A:212:ILE:N	0.40	2.31	15	1
1:A:108:PHE:CE1	1:A:143:SER:O	0.40	2.74	17	1
1:A:15:VAL:HG12	1:A:31:CYS:O	0.40	2.17	1	1
1:A:176:PHE:HD2	1:A:211:LEU:HD11	0.40	1.77	2	1
1:A:178:LEU:HD22	1:A:186:LEU:CB	0.40	2.45	8	1
1:A:193:LEU:HD23	1:A:221:ASP:OD1	0.40	2.16	10	1
1:A:27:PHE:CD2	1:A:75:PHE:CZ	0.40	3.10	15	1
1:A:120:VAL:HG11	1:A:216:CYS:H	0.40	1.77	17	1
1:A:32:TYR:O	1:A:36:VAL:N	0.40	2.54	4	1
1:A:168:GLU:O	1:A:215:GLY:HA2	0.40	2.16	15	1
1:A:133:ILE:CG2	1:A:137:MET:CE	0.40	2.99	17	1
1:A:167:ILE:N	1:A:167:ILE:CD1	0.40	2.83	17	1
1:A:176:PHE:CZ	1:A:235:GLU:HB3	0.40	2.52	1	1
1:A:128:TYR:CE1	1:A:132:LEU:HD22	0.40	2.52	4	1
1:A:214:PRO:O	1:A:216:CYS:N	0.40	2.54	6	1
1:A:174:LEU:O	1:A:211:LEU:HB2	0.40	2.17	15	1
1:A:171:HIS:HA	1:A:214:PRO:HA	0.40	1.92	16	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/252 (87%)	195±4 (90±2%)	20±4 (9±2%)	3±1 (1±1%)	12	60
All	All	4360/5040 (87%)	3905 (90%)	398 (9%)	57 (1%)	12	60

All 20 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	179	PRO	9
1	A	203	GLY	8
1	A	79	ASP	6
1	A	230	GLY	6
1	A	15	VAL	4
1	A	144	VAL	3
1	A	119	CYS	3
1	A	214	PRO	2
1	A	143	SER	2
1	A	215	GLY	2
1	A	145	LYS	2
1	A	238	ASN	2
1	A	194	ILE	1
1	A	123	GLU	1
1	A	124	THR	1
1	A	54	HIS	1
1	A	231	LYS	1
1	A	166	LYS	1
1	A	192	PRO	1
1	A	229	LYS	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/229 (87%)	140±6 (70±3%)	59±6 (30±3%)	1	18
All	All	3980/4580 (87%)	2805 (70%)	1175 (30%)	1	18

All 158 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	29	ILE	20
1	A	81	THR	19
1	A	25	LYS	17
1	A	182	GLU	17
1	A	164	LYS	16
1	A	151	LYS	15
1	A	229	LYS	15
1	A	155	LEU	15
1	A	193	LEU	14
1	A	195	LYS	14
1	A	55	SER	13
1	A	145	LYS	13
1	A	178	LEU	13
1	A	223	LEU	13
1	A	137	MET	13
1	A	47	LEU	12
1	A	68	LYS	12
1	A	80	GLN	12
1	A	172	MET	12
1	A	189	LYS	12
1	A	205	GLN	12
1	A	64	GLN	12
1	A	59	ASN	12
1	A	106	GLN	12
1	A	33	LYS	11
1	A	119	CYS	11
1	A	191	LYS	11
1	A	225	LYS	11
1	A	226	LYS	11
1	A	162	LYS	11
1	A	159	LYS	11
1	A	21	LYS	10
1	A	26	ARG	10
1	A	51	LEU	10
1	A	77	THR	10
1	A	90	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	107	MET	10
1	A	123	GLU	10
1	A	143	SER	10
1	A	186	LEU	10
1	A	217	PHE	10
1	A	234	LEU	10
1	A	19	ARG	10
1	A	132	LEU	10
1	A	35	LYS	10
1	A	46	ASP	10
1	A	118	LYS	10
1	A	67	LYS	9
1	A	82	GLU	9
1	A	98	LYS	9
1	A	103	GLN	9
1	A	110	ASP	9
1	A	124	THR	9
1	A	126	ARG	9
1	A	163	GLU	9
1	A	218	ARG	9
1	A	219	GLU	9
1	A	100	ARG	9
1	A	138	LYS	9
1	A	231	LYS	9
1	A	52	GLN	8
1	A	101	HIS	8
1	A	104	LEU	8
1	A	129	THR	8
1	A	135	ARG	8
1	A	140	ILE	8
1	A	152	GLN	8
1	A	184	LYS	8
1	A	173	ARG	8
1	A	175	ARG	8
1	A	187	LYS	8
1	A	31	CYS	8
1	A	166	LYS	8
1	A	208	ILE	8
1	A	213	ASP	8
1	A	109	ARG	8
1	A	22	ARG	8
1	A	156	GLU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	174	LEU	8
1	A	28	GLU	7
1	A	125	LYS	7
1	A	139	ASP	7
1	A	168	GLU	7
1	A	200	GLU	7
1	A	40	ARG	7
1	A	153	GLN	7
1	A	204	GLN	7
1	A	108	PHE	7
1	A	211	LEU	7
1	A	235	GLU	7
1	A	105	GLU	7
1	A	60	VAL	7
1	A	165	MET	7
1	A	62	LYS	6
1	A	92	GLU	6
1	A	199	SER	6
1	A	238	ASN	6
1	A	20	MET	6
1	A	96	SER	6
1	A	176	PHE	6
1	A	121	ASN	6
1	A	134	GLU	6
1	A	149	SER	6
1	A	141	HIS	6
1	A	216	CYS	6
1	A	15	VAL	6
1	A	237	LEU	6
1	A	117	ASP	5
1	A	207	GLU	5
1	A	221	ASP	5
1	A	227	GLU	5
1	A	128	TYR	5
1	A	148	LYS	5
1	A	198	GLU	5
1	A	69	GLU	5
1	A	185	LYS	5
1	A	88	LEU	5
1	A	169	ARG	5
1	A	202	TYR	4
1	A	99	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	197	ILE	4
1	A	79	ASP	4
1	A	86	GLN	4
1	A	224	ILE	4
1	A	222	GLU	4
1	A	206	LEU	4
1	A	70	ASP	3
1	A	48	ASP	3
1	A	181	ASN	3
1	A	160	GLN	3
1	A	97	ASP	3
1	A	233	SER	3
1	A	194	ILE	3
1	A	85	LYS	3
1	A	150	THR	3
1	A	73	SER	2
1	A	158	ILE	2
1	A	190	LEU	2
1	A	32	TYR	2
1	A	61	SER	2
1	A	167	ILE	2
1	A	188	GLU	2
1	A	89	THR	2
1	A	210	CYS	2
1	A	114	ILE	2
1	A	228	THR	2
1	A	131	ILE	2
1	A	147	ASN	2
1	A	49	GLU	2
1	A	142	TYR	2
1	A	177	ILE	1
1	A	212	ILE	1
1	A	34	ASN	1
1	A	133	ILE	1
1	A	18	VAL	1
1	A	146	THR	1
1	A	171	HIS	1
1	A	56	VAL	1

6.3.3 RNA ⓘ

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 oligosaccharides 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

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	2846
Number of shifts mapped to atoms	2846
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	18

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	243	-0.01 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	225	0.00 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	214	-0.00 ± 0.15	None needed (< 0.5 ppm)
^{15}N	237	0.03 ± 0.36	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 2478 atoms were assigned a chemical shift out of a possible 3152. 0 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1038/1090 (95%)	432/441 (98%)	399/436 (92%)	207/213 (97%)
Sidechain	1406/1922 (73%)	962/1239 (78%)	436/599 (73%)	8/84 (10%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	34/140 (24%)	33/68 (49%)	0/63 (0%)	1/9 (11%)
Overall	2478/3152 (79%)	1427/1748 (82%)	835/1098 (76%)	216/306 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 2833 atoms were assigned a chemical shift out of a possible 3581. 0 out of 43 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	1189/1250 (95%)	495/506 (98%)	457/500 (91%)	237/244 (97%)
Sidechain	1605/2171 (74%)	1099/1398 (79%)	496/680 (73%)	10/93 (11%)
Aromatic	39/160 (24%)	38/78 (49%)	0/73 (0%)	1/9 (11%)
Overall	2833/3581 (79%)	1632/1982 (82%)	953/1253 (76%)	248/346 (72%)

7.1.4 Statistically unusual chemical shifts ⓘ

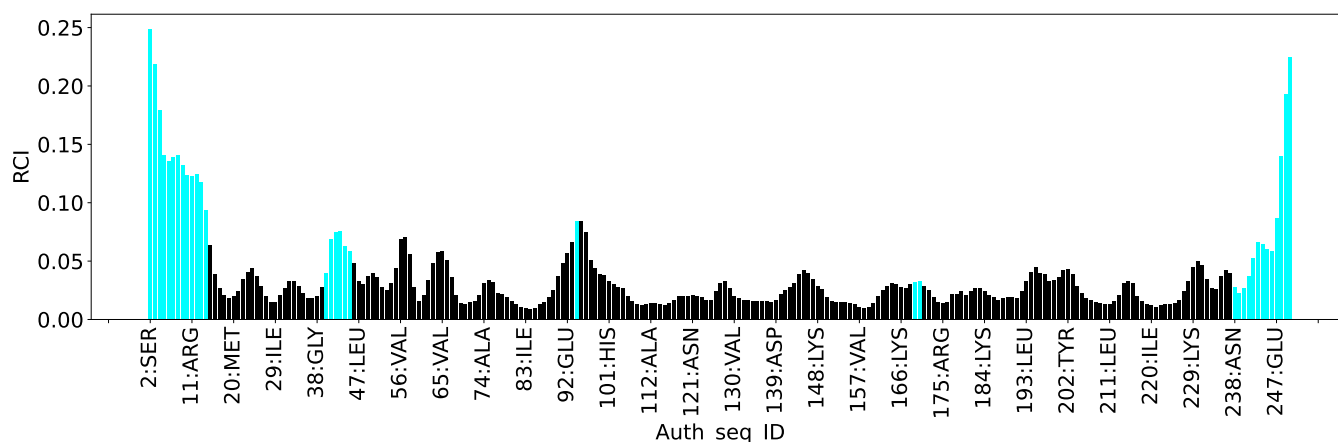
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	124	THR	HG1	4.91	0.08 – 2.19	17.9
1	A	89	THR	HG1	4.65	0.08 – 2.19	16.6
1	A	102	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	228	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	5	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	81	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	53	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	77	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	13	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	146	THR	HG1	4.64	0.08 – 2.19	16.6
1	A	113	THR	HG1	4.63	0.08 – 2.19	16.6
1	A	150	THR	HG1	4.35	0.08 – 2.19	15.2
1	A	72	ILE	CG2	10.27	10.93 – 24.12	-5.5
1	A	52	GLN	HG2	0.93	1.01 – 3.62	-5.3
1	A	77	THR	CG2	15.78	16.06 – 27.03	-5.2
1	A	83	ILE	HG21	-0.61	-0.56 – 2.11	-5.2
1	A	83	ILE	HG22	-0.61	-0.56 – 2.11	-5.2
1	A	83	ILE	HG23	-0.61	-0.56 – 2.11	-5.2

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	4005
Intra-residue ($ i-j =0$)	1476
Sequential ($ i-j =1$)	1117
Medium range ($ i-j >1$ and $ i-j <5$)	592
Long range ($ i-j \geq 5$)	820
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	15.9
Number of long range restraints per residue ¹	3.3

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	2.2	0.2
0.2-0.5 (Medium)	2.8	0.5
>0.5 (Large)	2.9	1.69

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

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

9 Distance violation analysis ⓘ

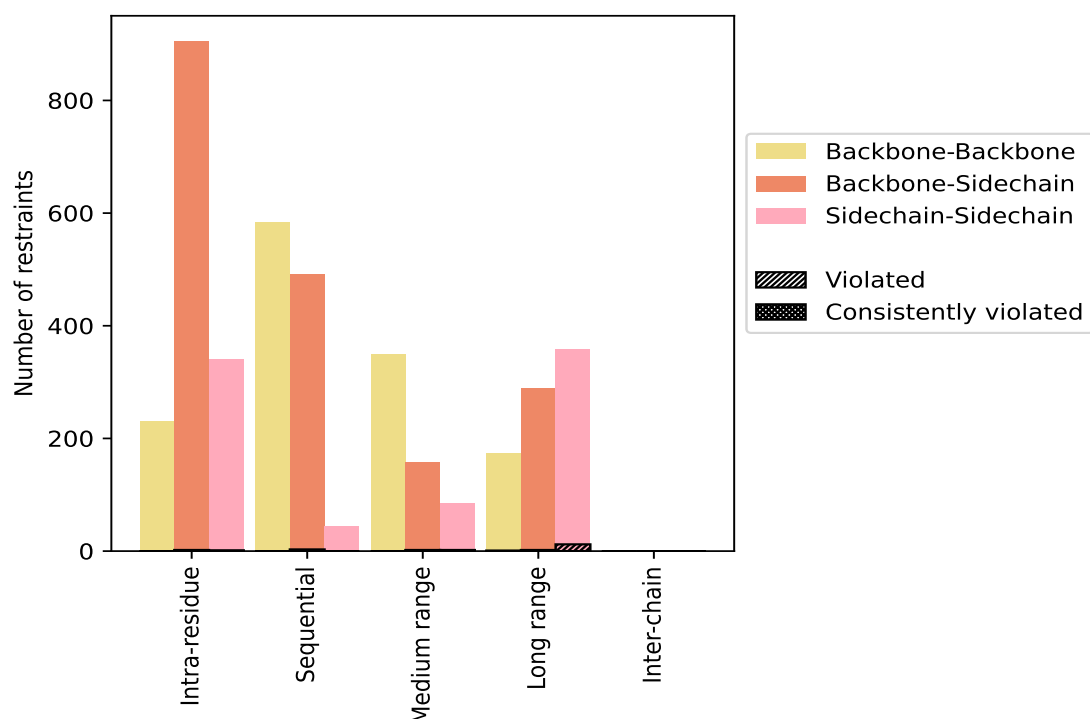
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1476	36.9	3	0.2	0.1	1	0.1	0.0
Backbone-Backbone	230	5.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	905	22.6	2	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	341	8.5	1	0.3	0.0	1	0.3	0.0
Sequential ($i-j =1$)	1117	27.9	3	0.3	0.1	0	0.0	0.0
Backbone-Backbone	583	14.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	491	12.3	3	0.6	0.1	0	0.0	0.0
Sidechain-Sidechain	43	1.1	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	592	14.8	4	0.7	0.1	1	0.2	0.0
Backbone-Backbone	350	8.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	158	3.9	2	1.3	0.0	0	0.0	0.0
Sidechain-Sidechain	84	2.1	2	2.4	0.0	1	1.2	0.0
Long range ($i-j \geq 5$)	820	20.5	15	1.8	0.4	0	0.0	0.0
Backbone-Backbone	174	4.3	1	0.6	0.0	0	0.0	0.0
Backbone-Sidechain	288	7.2	2	0.7	0.0	0	0.0	0.0
Sidechain-Sidechain	358	8.9	12	3.4	0.3	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4005	100.0	25	0.6	0.6	2	0.0	0.0
Backbone-Backbone	1337	33.4	1	0.1	0.0	0	0.0	0.0
Backbone-Sidechain	1842	46.0	9	0.5	0.2	0	0.0	0.0
Sidechain-Sidechain	826	20.6	15	1.8	0.4	2	0.2	0.0

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

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



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

9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	1	2	4	0	8	0.52	1.46	0.39	0.43
2	1	1	2	3	0	7	0.64	1.52	0.55	0.35
3	1	2	2	4	0	9	0.47	1.34	0.35	0.33
4	1	1	2	1	0	5	0.75	1.49	0.45	0.62
5	1	1	2	4	0	8	0.62	1.48	0.43	0.61
6	1	2	1	2	0	6	0.56	1.41	0.42	0.42
7	1	1	3	3	0	8	0.7	1.42	0.42	0.66
8	1	2	1	3	0	7	0.57	1.49	0.41	0.49
9	1	1	2	3	0	7	0.65	1.57	0.57	0.41
10	1	1	1	2	0	5	0.89	1.66	0.62	0.62

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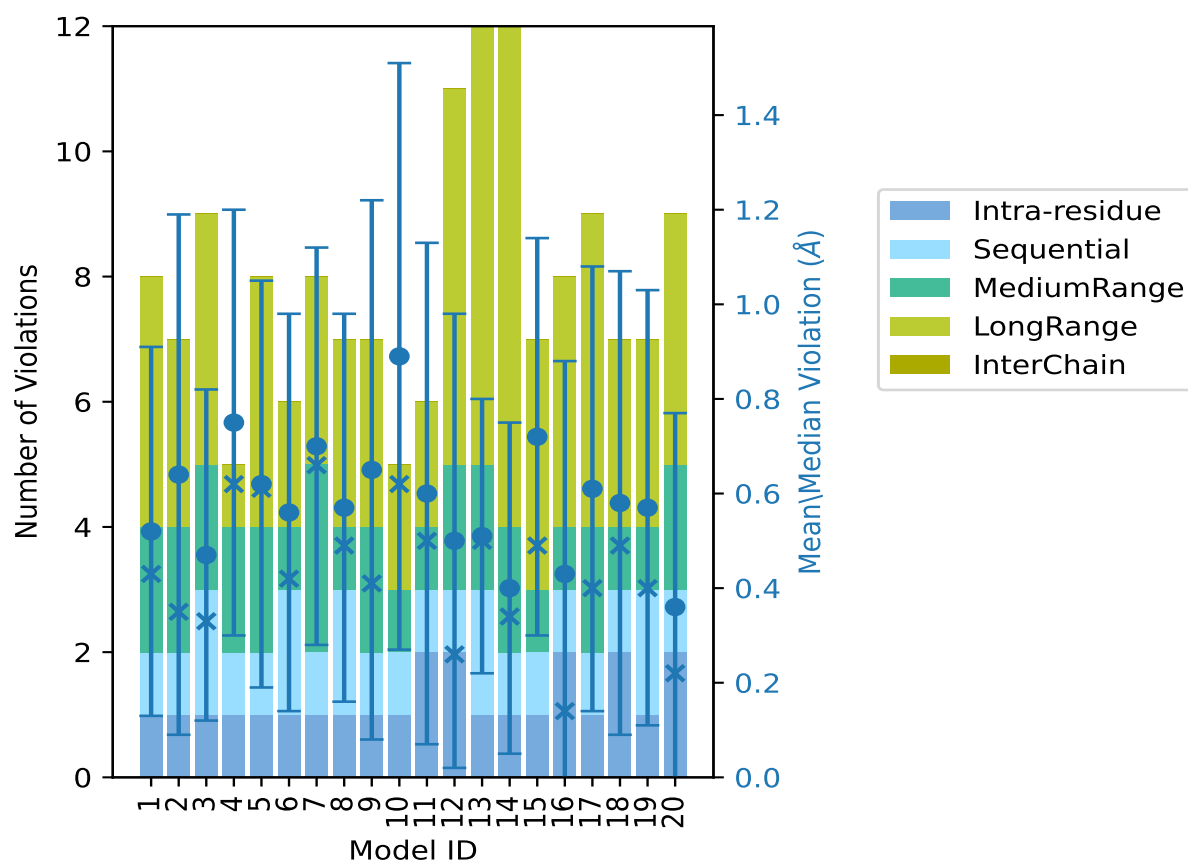
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	2	1	1	2	0	6	0.6	1.69	0.53	0.5
12	2	1	2	6	0	11	0.5	1.49	0.48	0.26
13	1	2	2	7	0	12	0.51	1.22	0.29	0.5
14	1	1	2	8	0	12	0.4	1.44	0.35	0.34
15	1	1	1	4	0	7	0.72	1.43	0.42	0.49
16	2	1	1	4	0	8	0.43	1.35	0.45	0.14
17	1	1	2	5	0	9	0.61	1.41	0.47	0.4
18	2	1	1	3	0	7	0.58	1.38	0.49	0.49
19	1	2	1	3	0	7	0.57	1.64	0.46	0.4
20	2	1	2	4	0	9	0.36	1.46	0.41	0.22

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

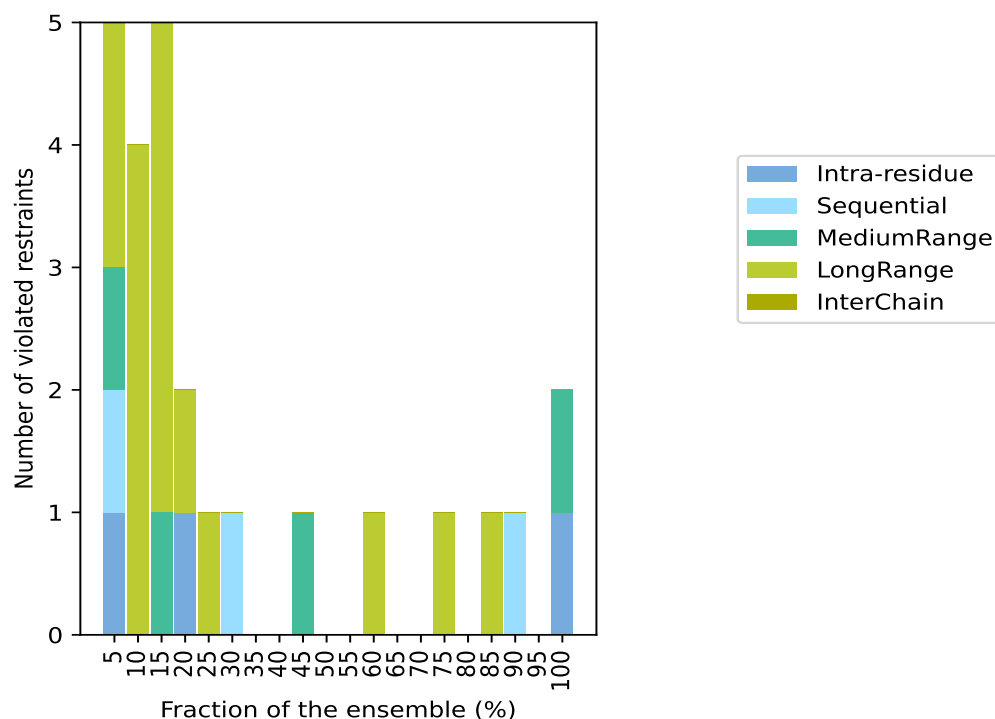
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3980(IR:1473, SQ:1114, MR:588, LR:805, IC:0) restraints are not violated in the ensemble.

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

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

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

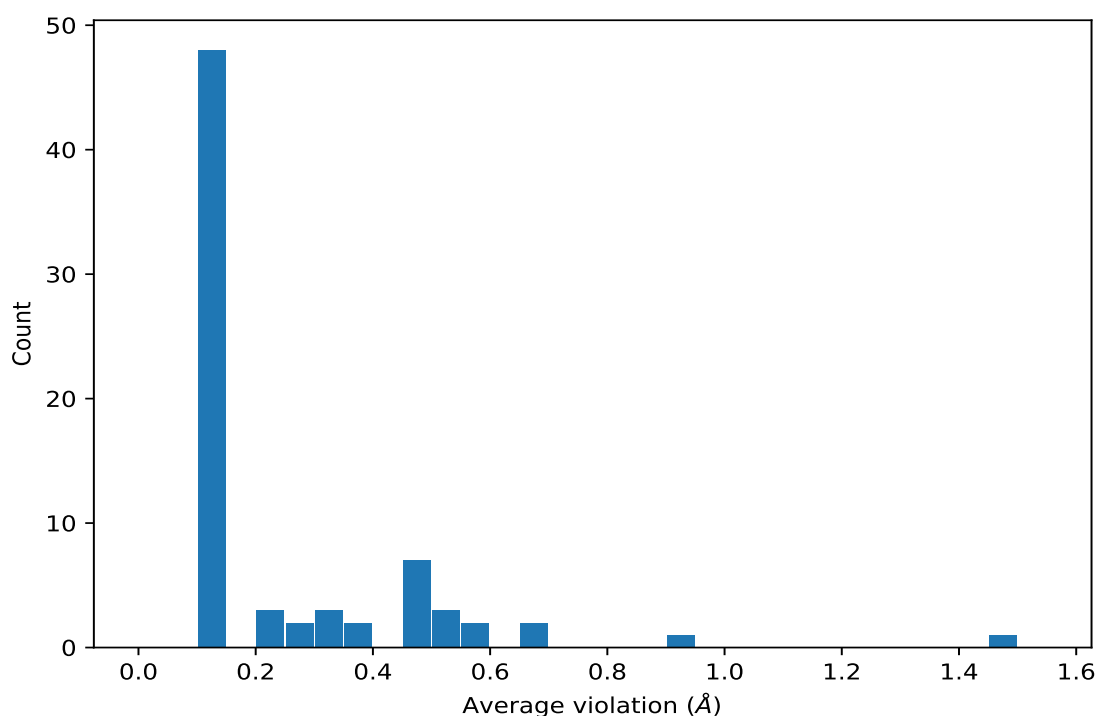
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



9.4.2 Table: Most violated distance restraints [i](#)

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	20	1.46	0.11	1.45
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	20	0.49	0.0	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	20	0.49	0.0	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	20	0.49	0.0	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	20	0.49	0.0	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	20	0.49	0.0	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	20	0.49	0.0	0.49
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	18	0.37	0.16	0.36
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	17	0.92	0.47	0.96
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	15	0.37	0.25	0.25
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD11	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD12	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD13	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD11	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD12	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD13	12	0.15	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD11	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD12	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD13	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD11	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD12	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD13	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD11	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD12	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD13	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD11	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD12	12	0.15	0.03	0.14
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD13	12	0.15	0.03	0.14
(1,2629)	1:239:A:LEU:HB2	1:241:A:ASP:H	9	0.53	0.23	0.6
(1,2575)	1:246:A:ASP:HB3	1:247:A:GLU:H	6	0.68	0.09	0.7
(1,3797)	1:140:A:ILE:HD11	1:160:A:GLN:HG2	5	0.24	0.15	0.17
(1,3797)	1:140:A:ILE:HD12	1:160:A:GLN:HG2	5	0.24	0.15	0.17
(1,3797)	1:140:A:ILE:HD13	1:160:A:GLN:HG2	5	0.24	0.15	0.17
(1,3295)	1:72:A:ILE:HG12	1:78:A:ASP:HB3	4	0.29	0.06	0.3
(1,3295)	1:72:A:ILE:HG13	1:78:A:ASP:HB3	4	0.29	0.06	0.3
(1,1047)	1:75:A:PHE:HB3	1:75:A:PHE:H	4	0.13	0.01	0.13
(1,3838)	1:226:A:LYS:HG2	1:231:A:LYS:HB2	3	0.51	0.19	0.55
(1,3838)	1:226:A:LYS:HG3	1:231:A:LYS:HB2	3	0.51	0.19	0.55
(1,2936)	1:67:A:LYS:HB3	1:70:A:ASP:H	3	0.47	0.41	0.22
(1,3261)	1:55:A:SER:HB3	1:65:A:VAL:HG21	3	0.33	0.06	0.31
(1,3261)	1:55:A:SER:HB3	1:65:A:VAL:HG22	3	0.33	0.06	0.31
(1,3261)	1:55:A:SER:HB3	1:65:A:VAL:HG23	3	0.33	0.06	0.31
(1,3320)	1:85:A:LYS:HE2	1:47:A:LEU:HD21	3	0.13	0.01	0.13
(1,3320)	1:85:A:LYS:HE2	1:47:A:LEU:HD22	3	0.13	0.01	0.13
(1,3320)	1:85:A:LYS:HE2	1:47:A:LEU:HD23	3	0.13	0.01	0.13
(1,3320)	1:85:A:LYS:HE3	1:47:A:LEU:HD21	3	0.13	0.01	0.13
(1,3320)	1:85:A:LYS:HE3	1:47:A:LEU:HD22	3	0.13	0.01	0.13
(1,3320)	1:85:A:LYS:HE3	1:47:A:LEU:HD23	3	0.13	0.01	0.13
(1,3990)	1:211:A:LEU:HA	1:174:A:LEU:HA	3	0.11	0.0	0.11
(1,3798)	1:140:A:ILE:HG12	1:160:A:GLN:HG2	2	0.66	0.26	0.66
(1,3837)	1:226:A:LYS:HE2	1:231:A:LYS:HB2	2	0.56	0.19	0.56
(1,3837)	1:226:A:LYS:HE3	1:231:A:LYS:HB2	2	0.56	0.19	0.56
(1,3806)	1:201:A:ASP:HB2	1:207:A:GLU:HG2	2	0.11	0.0	0.11
(1,3806)	1:201:A:ASP:HB2	1:207:A:GLU:HG3	2	0.11	0.0	0.11
(1,3806)	1:201:A:ASP:HB3	1:207:A:GLU:HG2	2	0.11	0.0	0.11
(1,3806)	1:201:A:ASP:HB3	1:207:A:GLU:HG3	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG11	1:18:A:VAL:HG21	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG11	1:18:A:VAL:HG22	2	0.11	0.0	0.11

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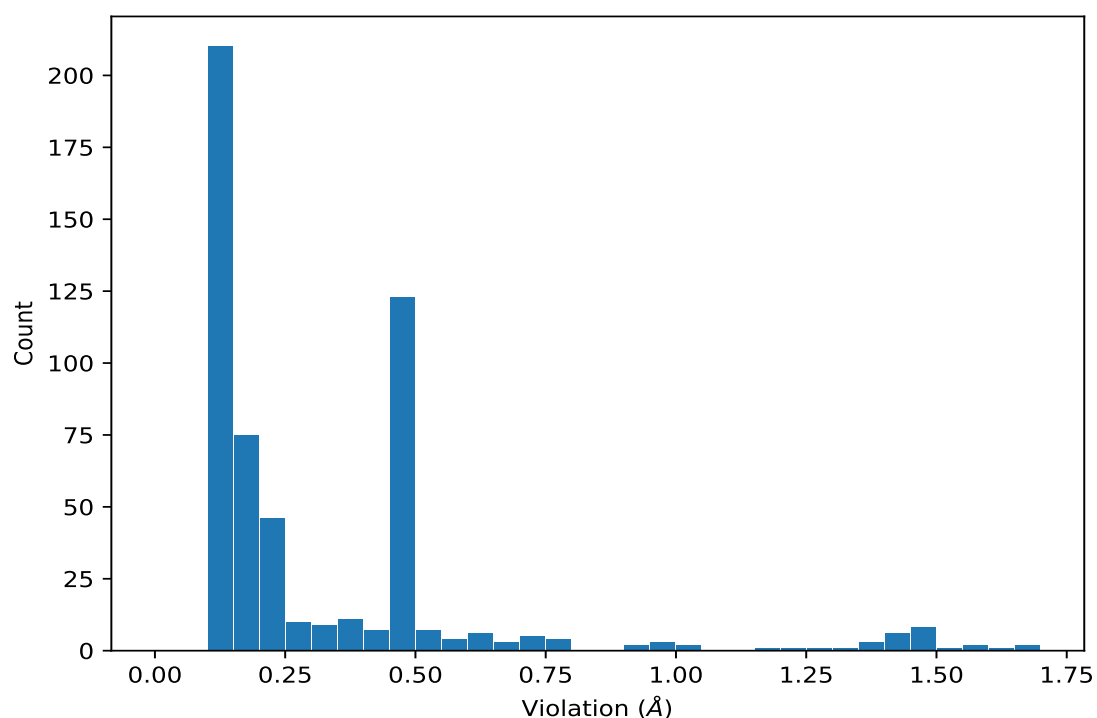
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3340)	1:93:A:VAL:HG11	1:18:A:VAL:HG23	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG12	1:18:A:VAL:HG21	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG12	1:18:A:VAL:HG22	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG12	1:18:A:VAL:HG23	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG13	1:18:A:VAL:HG21	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG13	1:18:A:VAL:HG22	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG13	1:18:A:VAL:HG23	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG21	1:18:A:VAL:HG21	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG21	1:18:A:VAL:HG22	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG21	1:18:A:VAL:HG23	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG22	1:18:A:VAL:HG21	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG22	1:18:A:VAL:HG22	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG22	1:18:A:VAL:HG23	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG23	1:18:A:VAL:HG21	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG23	1:18:A:VAL:HG22	2	0.11	0.0	0.11
(1,3340)	1:93:A:VAL:HG23	1:18:A:VAL:HG23	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

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



9.5.2 Table : All distance violations [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	11	1.69
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	10	1.66
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	19	1.64
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	10	1.58
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	9	1.57
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	2	1.52
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	12	1.49
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	4	1.49
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	8	1.49
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	9	1.48
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	5	1.48
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	2	1.47
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	1	1.46
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	20	1.46
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	14	1.44
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	15	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	7	1.42
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	6	1.41
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	17	1.41
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	17	1.4
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	18	1.38
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	12	1.36
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	16	1.35
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	3	1.34
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	18	1.26
(1,2714)	1:57:A:PHE:HZ	1:55:A:SER:HB3	13	1.22
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	15	1.16
(1,2936)	1:67:A:LYS:HB3	1:70:A:ASP:H	7	1.04
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	7	1.01
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	16	0.99
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	4	0.96
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	5	0.95
(1,3798)	1:140:A:ILE:HG12	1:160:A:GLN:HG2	15	0.91
(1,2629)	1:239:A:LEU:HB2	1:241:A:ASP:H	17	0.9
(1,2575)	1:246:A:ASP:HB3	1:247:A:GLU:H	7	0.79
(1,3837)	1:226:A:LYS:HE2	1:231:A:LYS:HB2	13	0.75
(1,3837)	1:226:A:LYS:HE3	1:231:A:LYS:HB2	13	0.75
(1,2575)	1:246:A:ASP:HB3	1:247:A:GLU:H	5	0.75
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	5	0.73
(1,2575)	1:246:A:ASP:HB3	1:247:A:GLU:H	6	0.73
(1,3838)	1:226:A:LYS:HG2	1:231:A:LYS:HB2	13	0.71
(1,3838)	1:226:A:LYS:HG3	1:231:A:LYS:HB2	13	0.71
(1,2629)	1:239:A:LEU:HB2	1:241:A:ASP:H	12	0.71
(1,2629)	1:239:A:LEU:HB2	1:241:A:ASP:H	13	0.66
(1,2575)	1:246:A:ASP:HB3	1:247:A:GLU:H	3	0.66
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	19	0.65
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	11	0.64
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	8	0.62
(1,2629)	1:239:A:LEU:HB2	1:241:A:ASP:H	4	0.62
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	10	0.62
(1,2575)	1:246:A:ASP:HB3	1:247:A:GLU:H	8	0.61
(1,2629)	1:239:A:LEU:HB2	1:241:A:ASP:H	1	0.6
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	14	0.57
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	3	0.56
(1,3838)	1:226:A:LYS:HG2	1:231:A:LYS:HB2	14	0.55
(1,3838)	1:226:A:LYS:HG3	1:231:A:LYS:HB2	14	0.55
(1,3797)	1:140:A:ILE:HD11	1:160:A:GLN:HG2	13	0.54
(1,3797)	1:140:A:ILE:HD12	1:160:A:GLN:HG2	13	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3797)	1:140:A:ILE:HD13	1:160:A:GLN:HG2	13	0.54
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	1	0.54
(1,2629)	1:239:A:LEU:HB2	1:241:A:ASP:H	7	0.52
(1,2575)	1:246:A:ASP:HB3	1:247:A:GLU:H	13	0.52
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	11	0.5
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	18	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	1	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	1	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	1	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	1	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	1	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	1	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	2	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	2	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	2	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	2	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	2	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	2	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	3	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	3	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	3	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	3	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	3	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	3	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	4	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	4	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	4	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	4	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	4	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	4	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	5	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	5	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	5	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	5	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	5	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	5	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	6	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	6	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	6	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	6	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	6	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	7	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	7	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	7	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	7	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	7	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	7	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	8	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	8	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	8	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	8	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	8	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	8	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	9	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	9	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	9	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	9	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	9	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	9	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	10	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	10	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	10	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	10	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	10	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	10	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	11	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	11	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	11	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	11	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	11	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	11	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	12	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	12	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	12	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	12	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	12	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	12	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	13	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	13	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	13	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	13	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	13	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	13	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	14	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	14	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	14	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	14	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	14	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	14	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	15	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	15	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	15	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	15	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	15	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	15	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	16	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	16	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	16	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	16	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	16	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	16	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	17	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	17	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	17	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	17	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	17	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	17	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	18	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	18	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	18	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	18	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	18	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	18	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	19	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	19	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	19	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	19	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	19	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	19	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG22	20	0.49
(1,375)	1:150:A:THR:HG21	1:150:A:THR:HG23	20	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG21	20	0.49
(1,375)	1:150:A:THR:HG22	1:150:A:THR:HG23	20	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG21	20	0.49
(1,375)	1:150:A:THR:HG23	1:150:A:THR:HG22	20	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	12	0.48
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	15	0.47
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	13	0.42
(1,3261)	1:55:A:SER:HB3	1:65:A:VAL:HG21	9	0.41
(1,3261)	1:55:A:SER:HB3	1:65:A:VAL:HG22	9	0.41
(1,3261)	1:55:A:SER:HB3	1:65:A:VAL:HG23	9	0.41
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	8	0.41
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	19	0.4
(1,3798)	1:140:A:ILE:HG12	1:160:A:GLN:HG2	17	0.4
(1,2629)	1:239:A:LEU:HB2	1:241:A:ASP:H	14	0.38
(1,3837)	1:226:A:LYS:HE2	1:231:A:LYS:HB2	1	0.37
(1,3837)	1:226:A:LYS:HE3	1:231:A:LYS:HB2	1	0.37
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	20	0.37
(1,3295)	1:72:A:ILE:HG12	1:78:A:ASP:HB3	14	0.36
(1,3295)	1:72:A:ILE:HG13	1:78:A:ASP:HB3	14	0.36
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	19	0.36
(1,3853)	1:142:A:TYR:HD1	1:160:A:GLN:HG2	15	0.35
(1,3853)	1:142:A:TYR:HD2	1:160:A:GLN:HG2	15	0.35
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	2	0.35
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	9	0.35
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	1	0.34
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	6	0.34
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	14	0.33
(1,3295)	1:72:A:ILE:HG12	1:78:A:ASP:HB3	3	0.33
(1,3295)	1:72:A:ILE:HG13	1:78:A:ASP:HB3	3	0.33
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	3	0.31
(1,3261)	1:55:A:SER:HB3	1:65:A:VAL:HG21	19	0.31
(1,3261)	1:55:A:SER:HB3	1:65:A:VAL:HG22	19	0.31
(1,3261)	1:55:A:SER:HB3	1:65:A:VAL:HG23	19	0.31
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	17	0.27
(1,3295)	1:72:A:ILE:HG12	1:78:A:ASP:HB3	17	0.27
(1,3295)	1:72:A:ILE:HG13	1:78:A:ASP:HB3	17	0.27
(1,3838)	1:226:A:LYS:HG2	1:231:A:LYS:HB2	12	0.26
(1,3838)	1:226:A:LYS:HG3	1:231:A:LYS:HB2	12	0.26
(1,3261)	1:55:A:SER:HB3	1:65:A:VAL:HG21	13	0.26
(1,3261)	1:55:A:SER:HB3	1:65:A:VAL:HG22	13	0.26
(1,3261)	1:55:A:SER:HB3	1:65:A:VAL:HG23	13	0.26
(1,3856)	1:142:A:TYR:HA	1:137:A:MET:HG2	20	0.25
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	15	0.25
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	8	0.23
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	20	0.22
(1,2936)	1:67:A:LYS:HB3	1:70:A:ASP:H	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2629)	1:239:A:LEU:HB2	1:241:A:ASP:H	2	0.22
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	13	0.22
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD11	2	0.21
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD12	2	0.21
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD13	2	0.21
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD11	2	0.21
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD12	2	0.21
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD13	2	0.21
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD11	2	0.21
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD12	2	0.21
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD13	2	0.21
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD11	2	0.21
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD12	2	0.21
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD13	2	0.21
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD11	2	0.21
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD12	2	0.21
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD13	2	0.21
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD11	2	0.21
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD12	2	0.21
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD13	2	0.21
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	1	0.2
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD11	6	0.2
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD12	6	0.2
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD13	6	0.2
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD11	6	0.2
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD12	6	0.2
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD13	6	0.2
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD11	6	0.2
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD12	6	0.2
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD13	6	0.2
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD11	6	0.2
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD12	6	0.2
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD13	6	0.2
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD11	6	0.2
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD12	6	0.2
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD13	6	0.2
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD11	6	0.2
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD12	6	0.2
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD13	6	0.2
(1,3295)	1:72:A:ILE:HG12	1:78:A:ASP:HB3	5	0.2
(1,3295)	1:72:A:ILE:HG13	1:78:A:ASP:HB3	5	0.2
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	17	0.2
(1,3797)	1:140:A:ILE:HD11	1:160:A:GLN:HG2	17	0.19
(1,3797)	1:140:A:ILE:HD12	1:160:A:GLN:HG2	17	0.19
(1,3797)	1:140:A:ILE:HD13	1:160:A:GLN:HG2	17	0.19
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	2	0.19
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	6	0.19
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD11	12	0.18
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD12	12	0.18
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD13	12	0.18
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD11	12	0.18
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD12	12	0.18
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD13	12	0.18
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD11	12	0.18
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD12	12	0.18
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD13	12	0.18
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD11	12	0.18
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD12	12	0.18
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD13	12	0.18
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD11	12	0.18
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD12	12	0.18
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD13	12	0.18
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD11	12	0.18
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD12	12	0.18
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD13	12	0.18
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	4	0.18
(1,3797)	1:140:A:ILE:HD11	1:160:A:GLN:HG2	7	0.17
(1,3797)	1:140:A:ILE:HD12	1:160:A:GLN:HG2	7	0.17
(1,3797)	1:140:A:ILE:HD13	1:160:A:GLN:HG2	7	0.17
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD11	18	0.17
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD12	18	0.17
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD13	18	0.17
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD11	18	0.17
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD12	18	0.17
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD13	18	0.17
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD11	18	0.17
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD12	18	0.17
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD13	18	0.17
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD11	18	0.17
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD12	18	0.17
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD13	18	0.17
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD11	18	0.17
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD12	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD13	18	0.17
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD11	18	0.17
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD12	18	0.17
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD13	18	0.17
(1,2580)	1:248:A:LYS:H	1:249:A:PHE:HB3	19	0.17
(1,3797)	1:140:A:ILE:HD11	1:160:A:GLN:HG2	3	0.16
(1,3797)	1:140:A:ILE:HD12	1:160:A:GLN:HG2	3	0.16
(1,3797)	1:140:A:ILE:HD13	1:160:A:GLN:HG2	3	0.16
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	13	0.16
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD11	14	0.16
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD12	14	0.16
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD13	14	0.16
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD11	14	0.16
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD12	14	0.16
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD13	14	0.16
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD11	14	0.16
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD12	14	0.16
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD13	14	0.16
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD11	14	0.16
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD12	14	0.16
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD13	14	0.16
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD11	14	0.16
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD12	14	0.16
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD13	14	0.16
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD11	14	0.16
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD12	14	0.16
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD13	14	0.16
(1,3320)	1:85:A:LYS:HE2	1:47:A:LEU:HD21	14	0.15
(1,3320)	1:85:A:LYS:HE2	1:47:A:LEU:HD22	14	0.15
(1,3320)	1:85:A:LYS:HE2	1:47:A:LEU:HD23	14	0.15
(1,3320)	1:85:A:LYS:HE3	1:47:A:LEU:HD21	14	0.15
(1,3320)	1:85:A:LYS:HE3	1:47:A:LEU:HD22	14	0.15
(1,3320)	1:85:A:LYS:HE3	1:47:A:LEU:HD23	14	0.15
(1,1047)	1:75:A:PHE:HB3	1:75:A:PHE:H	18	0.15
(1,3974)	1:190:A:LEU:HD21	1:224:A:ILE:HD11	14	0.14
(1,3974)	1:190:A:LEU:HD21	1:224:A:ILE:HD12	14	0.14
(1,3974)	1:190:A:LEU:HD21	1:224:A:ILE:HD13	14	0.14
(1,3974)	1:190:A:LEU:HD22	1:224:A:ILE:HD11	14	0.14
(1,3974)	1:190:A:LEU:HD22	1:224:A:ILE:HD12	14	0.14
(1,3974)	1:190:A:LEU:HD22	1:224:A:ILE:HD13	14	0.14
(1,3974)	1:190:A:LEU:HD23	1:224:A:ILE:HD11	14	0.14
(1,3974)	1:190:A:LEU:HD23	1:224:A:ILE:HD12	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3974)	1:190:A:LEU:HD23	1:224:A:ILE:HD13	14	0.14
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD11	8	0.14
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD12	8	0.14
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD13	8	0.14
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD11	8	0.14
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD12	8	0.14
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD13	8	0.14
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD11	8	0.14
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD12	8	0.14
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD13	8	0.14
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD11	8	0.14
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD12	8	0.14
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD13	8	0.14
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD11	8	0.14
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD12	8	0.14
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD13	8	0.14
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD11	8	0.14
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD12	8	0.14
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD13	8	0.14
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD11	13	0.14
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD12	13	0.14
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD13	13	0.14
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD11	13	0.14
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD12	13	0.14
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD13	13	0.14
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD11	13	0.14
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD12	13	0.14
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD13	13	0.14
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD11	13	0.14
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD12	13	0.14
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD13	13	0.14
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD11	13	0.14
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD12	13	0.14
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD13	13	0.14
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD11	13	0.14
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD12	13	0.14
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD13	13	0.14
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD11	16	0.14
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD12	16	0.14
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD13	16	0.14
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD11	16	0.14
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD12	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD13	16	0.14
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD11	16	0.14
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD12	16	0.14
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD13	16	0.14
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD11	16	0.14
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD12	16	0.14
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD13	16	0.14
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD11	16	0.14
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD12	16	0.14
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD13	16	0.14
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD11	16	0.14
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD12	16	0.14
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD13	16	0.14
(1,2936)	1:67:A:LYS:HB3	1:70:A:ASP:H	3	0.14
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	16	0.14
(1,3365)	1:178:A:LEU:HB3	1:207:A:GLU:H	18	0.13
(1,3320)	1:85:A:LYS:HE2	1:47:A:LEU:HD21	11	0.13
(1,3320)	1:85:A:LYS:HE2	1:47:A:LEU:HD22	11	0.13
(1,3320)	1:85:A:LYS:HE2	1:47:A:LEU:HD23	11	0.13
(1,3320)	1:85:A:LYS:HE3	1:47:A:LEU:HD21	11	0.13
(1,3320)	1:85:A:LYS:HE3	1:47:A:LEU:HD22	11	0.13
(1,3320)	1:85:A:LYS:HE3	1:47:A:LEU:HD23	11	0.13
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD11	1	0.13
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD12	1	0.13
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD13	1	0.13
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD11	1	0.13
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD12	1	0.13
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD13	1	0.13
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD11	1	0.13
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD12	1	0.13
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD13	1	0.13
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD11	1	0.13
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD12	1	0.13
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD13	1	0.13
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD11	1	0.13
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD12	1	0.13
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD13	1	0.13
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD11	1	0.13
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD12	1	0.13
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD13	1	0.13
(1,2713)	1:55:A:SER:HB3	1:57:A:PHE:HE1	9	0.13
(1,2713)	1:55:A:SER:HB3	1:57:A:PHE:HE2	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2217)	1:67:A:LYS:HB2	1:68:A:LYS:H	12	0.13
(1,1047)	1:75:A:PHE:HB3	1:75:A:PHE:H	12	0.13
(1,1047)	1:75:A:PHE:HB3	1:75:A:PHE:H	16	0.13
(1,3990)	1:211:A:LEU:HA	1:174:A:LEU:HA	10	0.12
(1,3797)	1:140:A:ILE:HD11	1:160:A:GLN:HG2	14	0.12
(1,3797)	1:140:A:ILE:HD12	1:160:A:GLN:HG2	14	0.12
(1,3797)	1:140:A:ILE:HD13	1:160:A:GLN:HG2	14	0.12
(1,3320)	1:85:A:LYS:HE2	1:47:A:LEU:HD21	20	0.12
(1,3320)	1:85:A:LYS:HE2	1:47:A:LEU:HD22	20	0.12
(1,3320)	1:85:A:LYS:HE2	1:47:A:LEU:HD23	20	0.12
(1,3320)	1:85:A:LYS:HE3	1:47:A:LEU:HD21	20	0.12
(1,3320)	1:85:A:LYS:HE3	1:47:A:LEU:HD22	20	0.12
(1,3320)	1:85:A:LYS:HE3	1:47:A:LEU:HD23	20	0.12
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD11	7	0.12
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD12	7	0.12
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD13	7	0.12
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD11	7	0.12
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD12	7	0.12
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD13	7	0.12
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD11	7	0.12
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD12	7	0.12
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD13	7	0.12
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD11	7	0.12
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD12	7	0.12
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD13	7	0.12
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD11	7	0.12
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD12	7	0.12
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD13	7	0.12
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD11	7	0.12
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD12	7	0.12
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD13	7	0.12
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD11	9	0.12
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD12	9	0.12
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD13	9	0.12
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD11	9	0.12
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD12	9	0.12
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD13	9	0.12
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD11	9	0.12
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD12	9	0.12
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD13	9	0.12
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD11	9	0.12
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD12	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD13	9	0.12
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD11	9	0.12
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD12	9	0.12
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD13	9	0.12
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD11	9	0.12
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD12	9	0.12
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD13	9	0.12
(1,2629)	1:239:A:LEU:HB2	1:241:A:ASP:H	20	0.12
(1,1047)	1:75:A:PHE:HB3	1:75:A:PHE:H	11	0.12
(1,3990)	1:211:A:LEU:HA	1:174:A:LEU:HA	12	0.11
(1,3990)	1:211:A:LEU:HA	1:174:A:LEU:HA	16	0.11
(1,3806)	1:201:A:ASP:HB2	1:207:A:GLU:HG2	12	0.11
(1,3806)	1:201:A:ASP:HB2	1:207:A:GLU:HG3	12	0.11
(1,3806)	1:201:A:ASP:HB3	1:207:A:GLU:HG2	12	0.11
(1,3806)	1:201:A:ASP:HB3	1:207:A:GLU:HG3	12	0.11
(1,3806)	1:201:A:ASP:HB2	1:207:A:GLU:HG2	16	0.11
(1,3806)	1:201:A:ASP:HB2	1:207:A:GLU:HG3	16	0.11
(1,3806)	1:201:A:ASP:HB3	1:207:A:GLU:HG2	16	0.11
(1,3806)	1:201:A:ASP:HB3	1:207:A:GLU:HG3	16	0.11
(1,3340)	1:93:A:VAL:HG11	1:18:A:VAL:HG21	20	0.11
(1,3340)	1:93:A:VAL:HG11	1:18:A:VAL:HG22	20	0.11
(1,3340)	1:93:A:VAL:HG11	1:18:A:VAL:HG23	20	0.11
(1,3340)	1:93:A:VAL:HG12	1:18:A:VAL:HG21	20	0.11
(1,3340)	1:93:A:VAL:HG12	1:18:A:VAL:HG22	20	0.11
(1,3340)	1:93:A:VAL:HG12	1:18:A:VAL:HG23	20	0.11
(1,3340)	1:93:A:VAL:HG13	1:18:A:VAL:HG21	20	0.11
(1,3340)	1:93:A:VAL:HG13	1:18:A:VAL:HG22	20	0.11
(1,3340)	1:93:A:VAL:HG13	1:18:A:VAL:HG23	20	0.11
(1,3340)	1:93:A:VAL:HG21	1:18:A:VAL:HG21	20	0.11
(1,3340)	1:93:A:VAL:HG21	1:18:A:VAL:HG22	20	0.11
(1,3340)	1:93:A:VAL:HG21	1:18:A:VAL:HG23	20	0.11
(1,3340)	1:93:A:VAL:HG22	1:18:A:VAL:HG21	20	0.11
(1,3340)	1:93:A:VAL:HG22	1:18:A:VAL:HG22	20	0.11
(1,3340)	1:93:A:VAL:HG22	1:18:A:VAL:HG23	20	0.11
(1,3340)	1:93:A:VAL:HG23	1:18:A:VAL:HG21	20	0.11
(1,3340)	1:93:A:VAL:HG23	1:18:A:VAL:HG22	20	0.11
(1,3340)	1:93:A:VAL:HG23	1:18:A:VAL:HG23	20	0.11
(1,256)	1:51:A:LEU:HA	1:51:A:LEU:HD21	20	0.11
(1,256)	1:51:A:LEU:HA	1:51:A:LEU:HD22	20	0.11
(1,256)	1:51:A:LEU:HA	1:51:A:LEU:HD23	20	0.11
(1,3340)	1:93:A:VAL:HG11	1:18:A:VAL:HG21	14	0.1
(1,3340)	1:93:A:VAL:HG11	1:18:A:VAL:HG22	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3340)	1:93:A:VAL:HG11	1:18:A:VAL:HG23	14	0.1
(1,3340)	1:93:A:VAL:HG12	1:18:A:VAL:HG21	14	0.1
(1,3340)	1:93:A:VAL:HG12	1:18:A:VAL:HG22	14	0.1
(1,3340)	1:93:A:VAL:HG12	1:18:A:VAL:HG23	14	0.1
(1,3340)	1:93:A:VAL:HG13	1:18:A:VAL:HG21	14	0.1
(1,3340)	1:93:A:VAL:HG13	1:18:A:VAL:HG22	14	0.1
(1,3340)	1:93:A:VAL:HG13	1:18:A:VAL:HG23	14	0.1
(1,3340)	1:93:A:VAL:HG21	1:18:A:VAL:HG21	14	0.1
(1,3340)	1:93:A:VAL:HG21	1:18:A:VAL:HG22	14	0.1
(1,3340)	1:93:A:VAL:HG21	1:18:A:VAL:HG23	14	0.1
(1,3340)	1:93:A:VAL:HG22	1:18:A:VAL:HG21	14	0.1
(1,3340)	1:93:A:VAL:HG22	1:18:A:VAL:HG22	14	0.1
(1,3340)	1:93:A:VAL:HG22	1:18:A:VAL:HG23	14	0.1
(1,3340)	1:93:A:VAL:HG23	1:18:A:VAL:HG21	14	0.1
(1,3340)	1:93:A:VAL:HG23	1:18:A:VAL:HG22	14	0.1
(1,3340)	1:93:A:VAL:HG23	1:18:A:VAL:HG23	14	0.1
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD11	5	0.1
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD12	5	0.1
(1,3311)	1:71:A:LEU:HD11	1:83:A:ILE:HD13	5	0.1
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD11	5	0.1
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD12	5	0.1
(1,3311)	1:71:A:LEU:HD12	1:83:A:ILE:HD13	5	0.1
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD11	5	0.1
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD12	5	0.1
(1,3311)	1:71:A:LEU:HD13	1:83:A:ILE:HD13	5	0.1
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD11	5	0.1
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD12	5	0.1
(1,3311)	1:71:A:LEU:HD21	1:83:A:ILE:HD13	5	0.1
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD11	5	0.1
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD12	5	0.1
(1,3311)	1:71:A:LEU:HD22	1:83:A:ILE:HD13	5	0.1
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD11	5	0.1
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD12	5	0.1
(1,3311)	1:71:A:LEU:HD23	1:83:A:ILE:HD13	5	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found