Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 10:30 AM EDT

PDB ID	:	2NDH
BMRB ID	:	26061
Title	:	NMR solution structure of MAL/TIRAP TIR domain (C116A)
Authors	:	Lavrencic, P.; Mobli, M.
Deposited on	:	2016-05-27

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

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

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

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

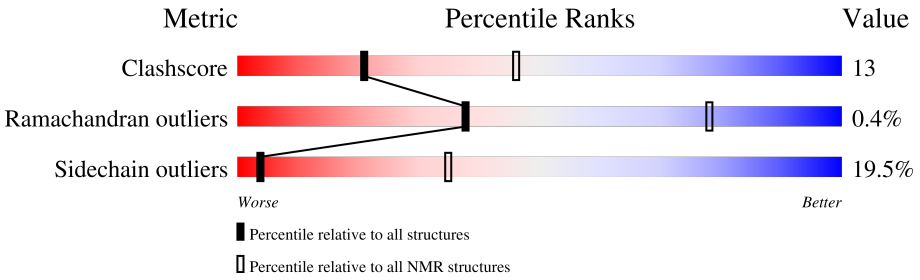
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 68%.

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	143	59% 23% . 14%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 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:84-A:122, A:134-A:192, A:197-A:221 (123)	1.66	3

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2179 atoms, of which 1079 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Toll/interleukin-1 receptor domain-containing adapter protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	143	2179	694	1079	187	210	9	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ALA	CYS	engineered mutation	UNP P58753

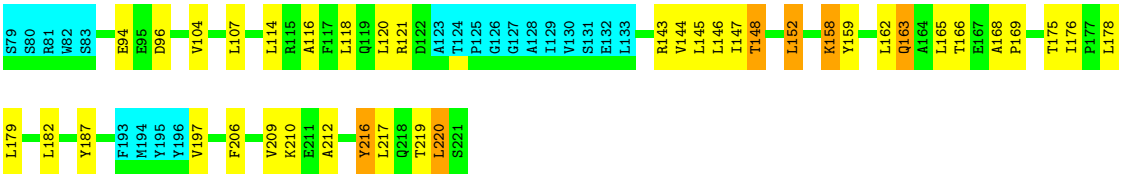
4 Residue-property plots (i)

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: Toll/interleukin-1 receptor domain-containing adapter protein

Chain A:



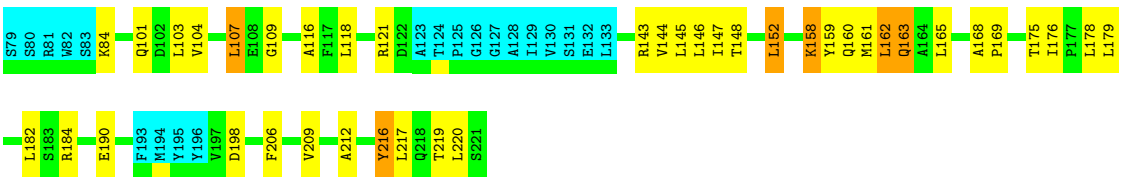
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein

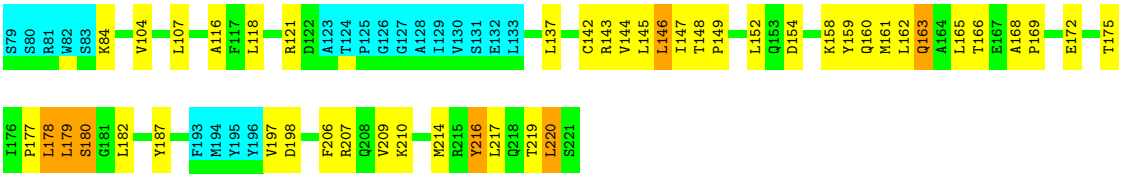
Chain A:



4.2.2 Score per residue for model 2

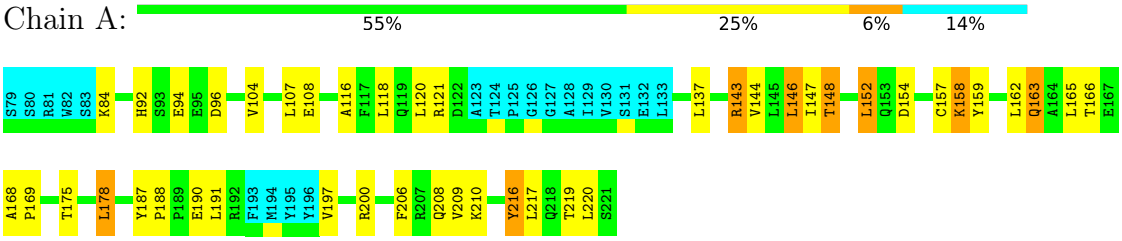
• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein

Chain A:



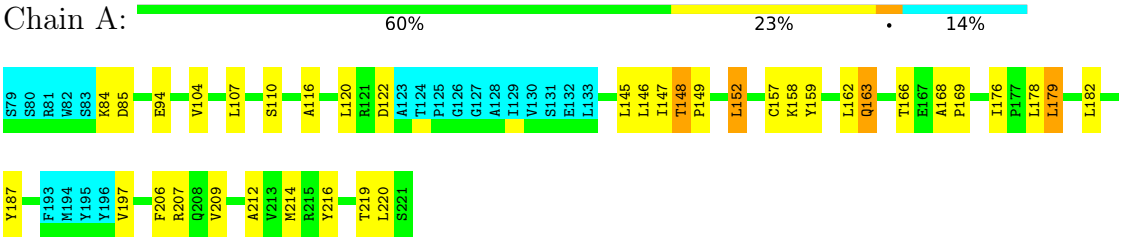
4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



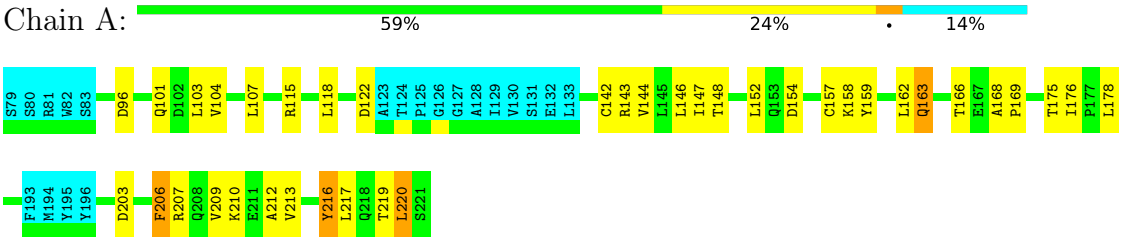
4.2.4 Score per residue for model 4

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



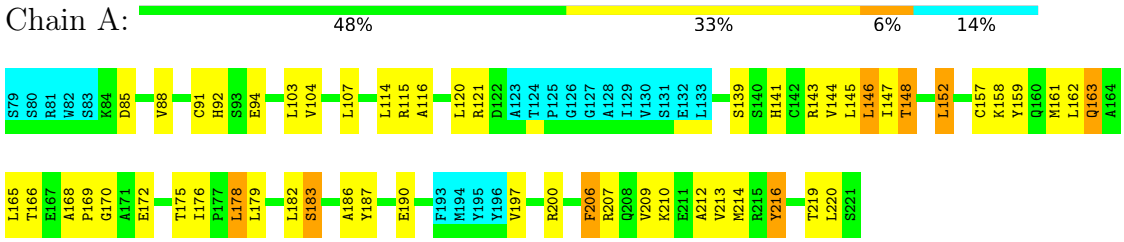
4.2.5 Score per residue for model 5

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



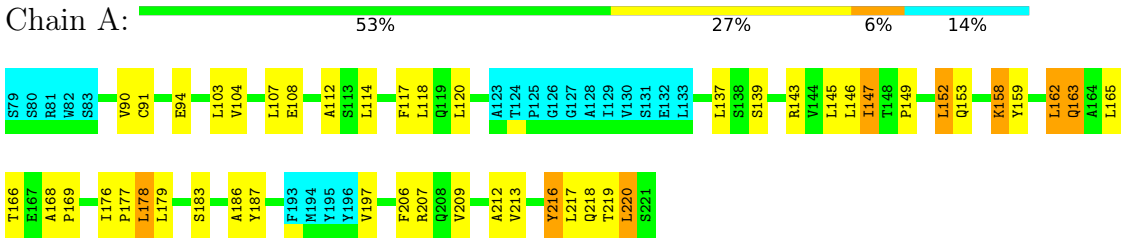
4.2.6 Score per residue for model 6

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



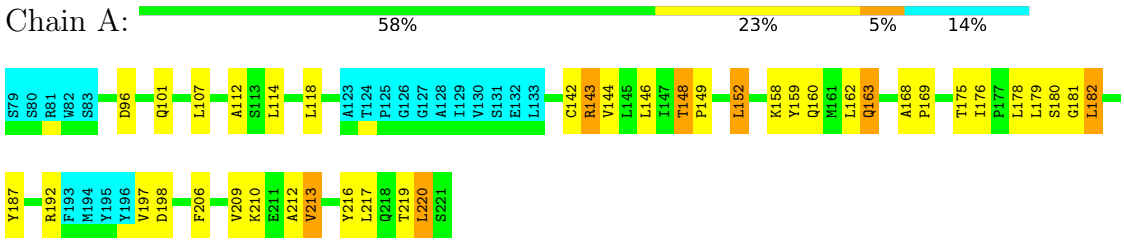
4.2.7 Score per residue for model 7

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



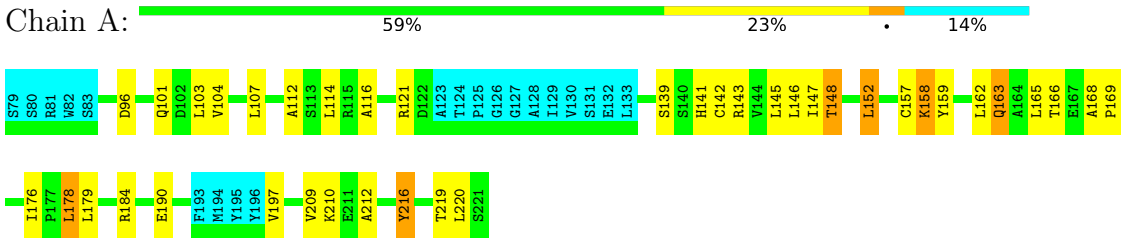
4.2.8 Score per residue for model 8

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.9 Score per residue for model 9

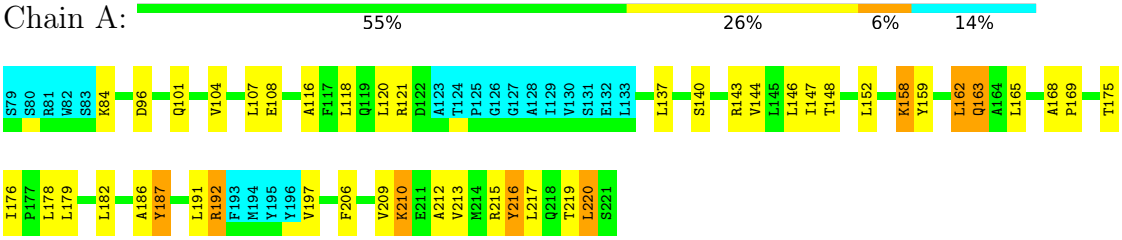
• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.10 Score per residue for model 10

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein

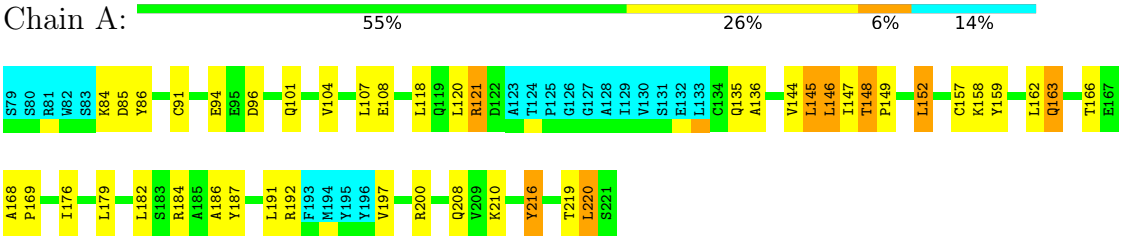
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein

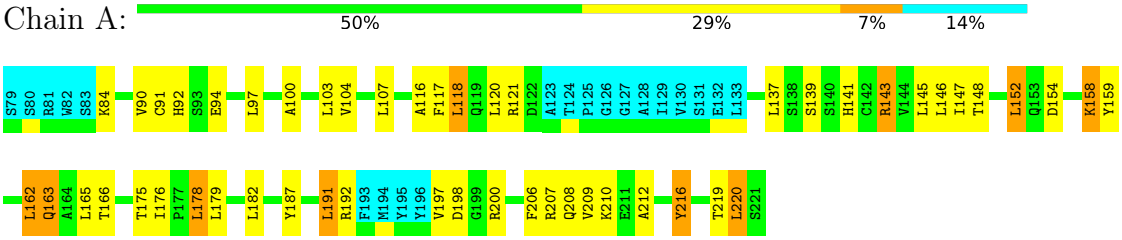
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein

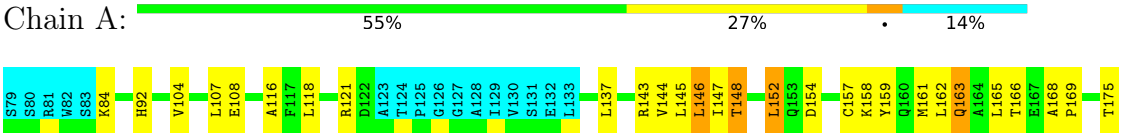
Chain A:

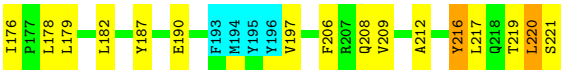


4.2.13 Score per residue for model 13

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein

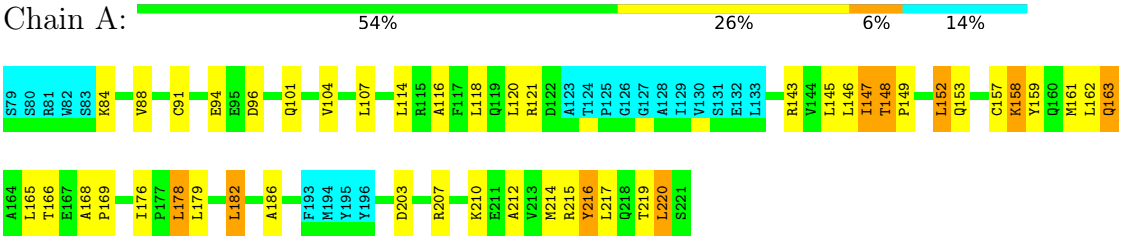
Chain A:





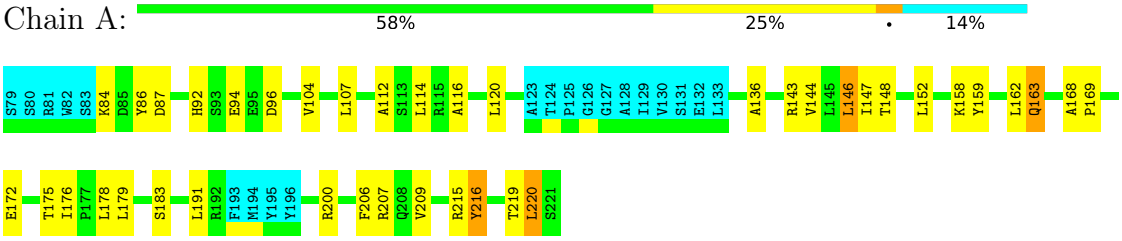
4.2.14 Score per residue for model 14

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



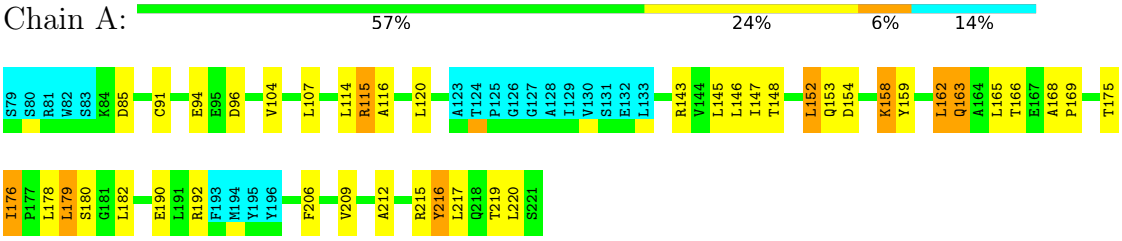
4.2.15 Score per residue for model 15

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



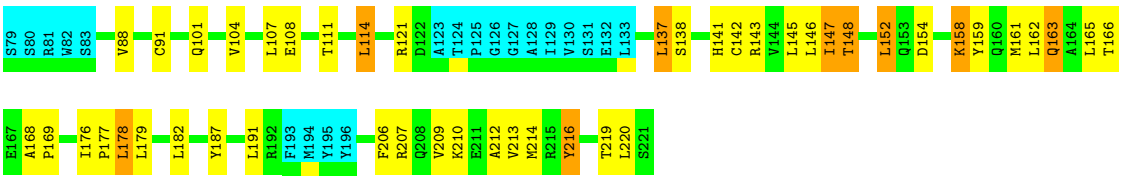
4.2.16 Score per residue for model 16

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



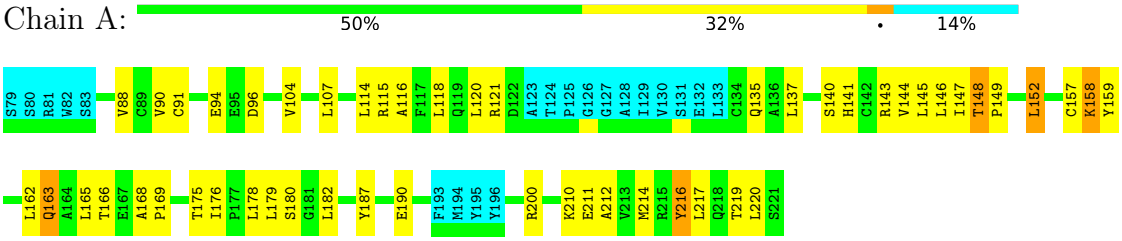
4.2.17 Score per residue for model 17

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



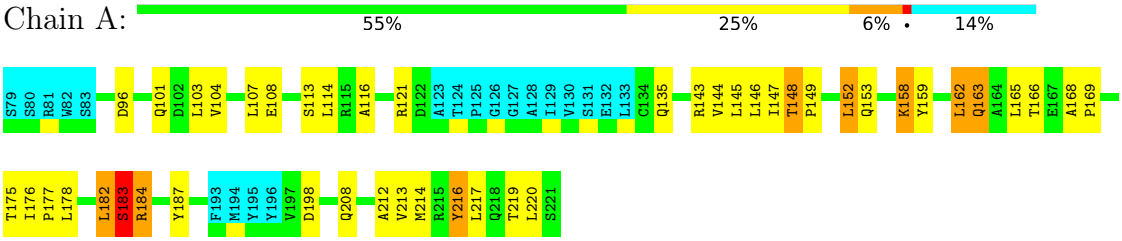
4.2.18 Score per residue for model 18

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



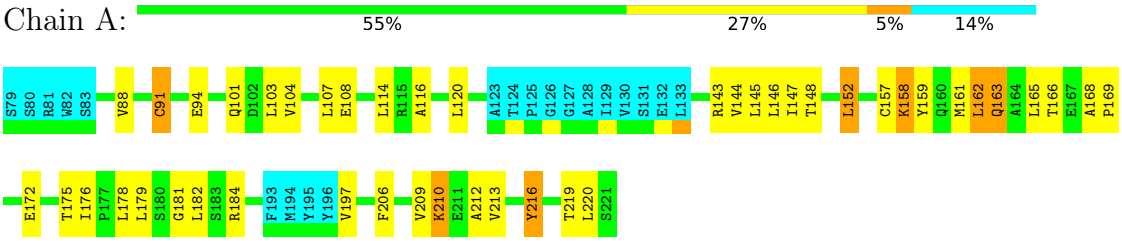
4.2.19 Score per residue for model 19

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.20 Score per residue for model 20

• Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 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	2.1
CYANA	refinement	2.1

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	1185
Number of shifts mapped to atoms	1185
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	68%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	944	933	933	25±5
All	All	18880	18660	18660	501

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:VAL:HG23	1:A:116:ALA:HB3	0.86	1.47	15	11
1:A:112:ALA:HB1	1:A:114:LEU:HD13	0.83	1.49	7	3
1:A:179:LEU:HD12	1:A:182:LEU:HD12	0.80	1.53	12	1
1:A:176:ILE:HD13	1:A:212:ALA:HB3	0.79	1.55	8	9
1:A:144:VAL:HG13	1:A:176:ILE:HD11	0.78	1.54	10	9
1:A:162:LEU:C	1:A:162:LEU:HD22	0.77	1.99	20	1
1:A:145:LEU:HD21	1:A:147:ILE:HD11	0.76	1.56	7	3
1:A:137:LEU:HD22	1:A:137:LEU:C	0.75	2.01	17	1
1:A:219:THR:HG23	1:A:220:LEU:HD23	0.71	1.63	15	5
1:A:182:LEU:HD12	1:A:187:TYR:CE1	0.67	2.25	8	2
1:A:216:TYR:O	1:A:219:THR:HG22	0.66	1.90	14	20
1:A:182:LEU:HD13	1:A:187:TYR:CZ	0.66	2.25	19	1
1:A:94:GLU:O	1:A:97:LEU:HD23	0.65	1.92	12	1
1:A:137:LEU:HD12	1:A:143:ARG:HD3	0.65	1.68	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:ILE:HD13	1:A:212:ALA:HB1	0.64	1.68	12	6
1:A:176:ILE:HD13	1:A:212:ALA:CB	0.64	2.22	18	4
1:A:179:LEU:HD12	1:A:182:LEU:HD13	0.64	1.69	17	1
1:A:94:GLU:CB	1:A:120:LEU:HD21	0.63	2.23	15	7
1:A:88:VAL:CG2	1:A:114:LEU:HD21	0.63	2.24	18	3
1:A:159:TYR:O	1:A:162:LEU:HD22	0.62	1.95	7	15
1:A:88:VAL:CG2	1:A:114:LEU:HD11	0.62	2.25	20	2
1:A:162:LEU:HD13	1:A:163:GLN:N	0.62	2.09	20	1
1:A:187:TYR:CE2	1:A:197:VAL:HG21	0.61	2.30	4	3
1:A:143:ARG:HB2	1:A:175:THR:HG22	0.61	1.73	19	12
1:A:191:LEU:HD23	1:A:197:VAL:CG1	0.61	2.26	11	1
1:A:178:LEU:O	1:A:179:LEU:HD23	0.61	1.95	8	1
1:A:165:LEU:HD13	1:A:190:GLU:CB	0.61	2.26	3	2
1:A:86:TYR:CZ	1:A:136:ALA:HB1	0.61	2.31	15	2
1:A:159:TYR:O	1:A:162:LEU:HD23	0.60	1.96	4	4
1:A:143:ARG:CB	1:A:175:THR:HG22	0.59	2.27	16	7
1:A:104:VAL:HG22	1:A:108:GLU:HG3	0.59	1.75	17	6
1:A:149:PRO:O	1:A:186:ALA:HB1	0.59	1.98	11	1
1:A:182:LEU:HD21	1:A:186:ALA:HB3	0.59	1.74	14	1
1:A:187:TYR:HB2	1:A:191:LEU:HD21	0.59	1.75	12	1
1:A:145:LEU:HD12	1:A:175:THR:CB	0.59	2.28	19	1
1:A:88:VAL:HG23	1:A:114:LEU:HD11	0.59	1.74	20	1
1:A:179:LEU:HB3	1:A:182:LEU:HD11	0.59	1.75	8	1
1:A:182:LEU:HD22	1:A:187:TYR:CE1	0.58	2.33	19	4
1:A:187:TYR:CZ	1:A:197:VAL:HG21	0.58	2.32	7	2
1:A:176:ILE:CD1	1:A:212:ALA:HB1	0.58	2.29	12	6
1:A:91:CYS:O	1:A:145:LEU:HD23	0.57	1.99	18	3
1:A:182:LEU:HD21	1:A:186:ALA:CB	0.57	2.29	14	1
1:A:145:LEU:HD12	1:A:175:THR:OG1	0.57	1.99	18	2
1:A:159:TYR:O	1:A:162:LEU:HD12	0.57	2.00	20	1
1:A:165:LEU:HD13	1:A:190:GLU:HG2	0.57	1.77	18	1
1:A:165:LEU:HD13	1:A:190:GLU:HB3	0.57	1.77	9	4
1:A:147:ILE:HD12	1:A:152:LEU:CB	0.56	2.30	20	3
1:A:149:PRO:HB3	1:A:179:LEU:HD21	0.56	1.77	4	1
1:A:137:LEU:C	1:A:137:LEU:CD2	0.56	2.74	17	1
1:A:149:PRO:HA	1:A:152:LEU:HD22	0.56	1.77	7	1
1:A:181:GLY:O	1:A:182:LEU:HD22	0.56	2.00	20	1
1:A:91:CYS:O	1:A:145:LEU:HD22	0.56	2.00	11	1
1:A:91:CYS:O	1:A:145:LEU:HD12	0.56	2.01	7	3
1:A:182:LEU:HD12	1:A:187:TYR:CD1	0.56	2.35	11	2
1:A:112:ALA:HB1	1:A:114:LEU:CD1	0.56	2.31	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:VAL:HG21	1:A:114:LEU:HD21	0.56	1.78	18	2
1:A:148:THR:O	1:A:152:LEU:HD23	0.56	2.01	17	3
1:A:178:LEU:HD23	1:A:212:ALA:HB2	0.55	1.78	9	1
1:A:216:TYR:CD2	1:A:217:LEU:HD22	0.55	2.36	19	2
1:A:181:GLY:C	1:A:182:LEU:HD23	0.55	2.22	8	1
1:A:114:LEU:HD23	1:A:115:ARG:N	0.55	2.16	6	3
1:A:179:LEU:HD23	1:A:182:LEU:HG	0.55	1.77	20	1
1:A:104:VAL:CG2	1:A:116:ALA:HB3	0.54	2.32	12	6
1:A:216:TYR:CE1	1:A:217:LEU:HD23	0.54	2.36	5	4
1:A:178:LEU:HD11	1:A:208:GLN:OE1	0.54	2.01	3	1
1:A:182:LEU:O	1:A:182:LEU:HD12	0.54	2.01	6	1
1:A:148:THR:O	1:A:152:LEU:HD22	0.54	2.02	14	8
1:A:192:ARG:HB3	1:A:197:VAL:HG13	0.54	1.79	10	1
1:A:86:TYR:CE2	1:A:136:ALA:HB1	0.54	2.36	11	2
1:A:94:GLU:HB3	1:A:120:LEU:HD21	0.54	1.78	15	1
1:A:179:LEU:HD13	1:A:180:SER:N	0.54	2.18	2	1
1:A:162:LEU:C	1:A:162:LEU:HD12	0.54	2.24	4	3
1:A:178:LEU:HD23	1:A:209:VAL:HG23	0.54	1.79	6	1
1:A:94:GLU:HB2	1:A:120:LEU:HD21	0.54	1.80	11	1
1:A:179:LEU:HD22	1:A:197:VAL:HG11	0.54	1.80	20	1
1:A:179:LEU:HD21	1:A:182:LEU:O	0.54	2.03	14	1
1:A:149:PRO:CB	1:A:182:LEU:HD12	0.54	2.33	19	1
1:A:149:PRO:HB3	1:A:179:LEU:HD11	0.53	1.79	2	1
1:A:158:LYS:HE3	1:A:165:LEU:HD12	0.53	1.79	7	12
1:A:182:LEU:HD23	1:A:187:TYR:CE1	0.53	2.39	2	1
1:A:177:PRO:O	1:A:178:LEU:HD22	0.53	2.04	19	1
1:A:162:LEU:HD12	1:A:162:LEU:C	0.53	2.24	5	1
1:A:179:LEU:HD11	1:A:200:ARG:HA	0.53	1.81	6	1
1:A:94:GLU:CG	1:A:120:LEU:HD21	0.53	2.34	3	4
1:A:137:LEU:HD11	1:A:143:ARG:NE	0.53	2.19	12	1
1:A:178:LEU:C	1:A:179:LEU:HD23	0.53	2.24	8	1
1:A:191:LEU:HD23	1:A:197:VAL:HG11	0.52	1.81	11	1
1:A:179:LEU:HD12	1:A:182:LEU:HB2	0.52	1.80	10	1
1:A:103:LEU:HD22	1:A:210:LYS:HB2	0.52	1.79	12	1
1:A:152:LEU:HD12	1:A:152:LEU:O	0.52	2.05	11	4
1:A:179:LEU:HB2	1:A:182:LEU:HD13	0.52	1.81	16	2
1:A:91:CYS:O	1:A:145:LEU:HD13	0.52	2.05	20	2
1:A:144:VAL:HG12	1:A:146:LEU:CD2	0.52	2.35	15	6
1:A:143:ARG:O	1:A:176:ILE:HG22	0.52	2.05	17	5
1:A:152:LEU:HD23	1:A:153:GLN:N	0.51	2.20	7	1
1:A:103:LEU:HD11	1:A:213:VAL:HG11	0.51	1.83	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:LEU:CB	1:A:182:LEU:HD13	0.51	2.35	16	1
1:A:162:LEU:C	1:A:162:LEU:CD2	0.51	2.73	20	1
1:A:178:LEU:O	1:A:179:LEU:HD22	0.51	2.06	9	3
1:A:137:LEU:HD12	1:A:143:ARG:NE	0.51	2.20	18	1
1:A:145:LEU:CD2	1:A:147:ILE:HD11	0.50	2.36	14	1
1:A:206:PHE:O	1:A:209:VAL:HG22	0.50	2.07	3	7
1:A:162:LEU:HD23	1:A:163:GLN:N	0.50	2.22	12	15
1:A:104:VAL:HG22	1:A:108:GLU:CG	0.49	2.36	7	1
1:A:145:LEU:HD23	1:A:177:PRO:HB3	0.49	1.84	2	1
1:A:103:LEU:HD13	1:A:209:VAL:CG1	0.49	2.37	9	1
1:A:188:PRO:HG2	1:A:191:LEU:HD13	0.49	1.85	3	1
1:A:219:THR:CG2	1:A:220:LEU:HD23	0.49	2.37	10	5
1:A:181:GLY:C	1:A:182:LEU:HD22	0.49	2.28	20	1
1:A:149:PRO:HD3	1:A:179:LEU:HD12	0.49	1.83	18	1
1:A:161:MET:HE2	1:A:165:LEU:HD11	0.49	1.83	1	4
1:A:182:LEU:HD23	1:A:187:TYR:CD1	0.49	2.43	2	1
1:A:162:LEU:HD12	1:A:163:GLN:N	0.49	2.23	5	4
1:A:162:LEU:HD13	1:A:163:GLN:H	0.49	1.65	20	1
1:A:178:LEU:HD22	1:A:198:ASP:HB3	0.48	1.84	12	1
1:A:217:LEU:HD13	1:A:220:LEU:HD23	0.48	1.83	19	2
1:A:178:LEU:C	1:A:179:LEU:HD22	0.48	2.28	7	3
1:A:217:LEU:HD12	1:A:218:GLN:N	0.48	2.24	7	1
1:A:178:LEU:CD2	1:A:212:ALA:HB2	0.48	2.39	9	1
1:A:187:TYR:CE2	1:A:197:VAL:HG11	0.47	2.44	6	1
1:A:118:LEU:HD12	1:A:120:LEU:HD13	0.47	1.85	12	1
1:A:103:LEU:HD12	1:A:104:VAL:N	0.47	2.24	1	2
1:A:137:LEU:HD13	1:A:143:ARG:NH1	0.47	2.25	7	1
1:A:145:LEU:HD12	1:A:175:THR:HB	0.47	1.85	19	2
1:A:143:ARG:HB3	1:A:175:THR:HG22	0.47	1.86	18	2
1:A:176:ILE:HG23	1:A:176:ILE:O	0.47	2.10	12	6
1:A:114:LEU:HD22	1:A:216:TYR:OH	0.47	2.09	19	1
1:A:219:THR:CG2	1:A:220:LEU:HD22	0.46	2.40	19	15
1:A:210:LYS:O	1:A:213:VAL:HG12	0.46	2.10	8	5
1:A:137:LEU:HD22	1:A:138:SER:N	0.46	2.24	17	1
1:A:103:LEU:HD13	1:A:209:VAL:HG11	0.46	1.87	9	1
1:A:152:LEU:CD2	1:A:179:LEU:HD11	0.46	2.41	11	1
1:A:177:PRO:HG2	1:A:197:VAL:HG12	0.46	1.88	7	1
1:A:179:LEU:HD23	1:A:197:VAL:HB	0.46	1.87	12	1
1:A:177:PRO:HG3	1:A:191:LEU:HD22	0.46	1.88	17	1
1:A:147:ILE:HD12	1:A:152:LEU:HB2	0.46	1.88	20	2
1:A:187:TYR:CD2	1:A:191:LEU:HD12	0.46	2.45	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:182:LEU:HD22	1:A:187:TYR:CD2	0.45	2.46	10	1
1:A:213:VAL:O	1:A:217:LEU:HD12	0.45	2.11	10	1
1:A:103:LEU:HD13	1:A:103:LEU:O	0.45	2.11	6	1
1:A:187:TYR:OH	1:A:197:VAL:HG21	0.45	2.12	3	1
1:A:206:PHE:O	1:A:209:VAL:HG12	0.45	2.12	10	8
1:A:192:ARG:HG3	1:A:197:VAL:HG22	0.45	1.88	8	1
1:A:178:LEU:HD13	1:A:179:LEU:N	0.45	2.26	14	2
1:A:90:VAL:HG12	1:A:117:PHE:O	0.45	2.11	7	2
1:A:183:SER:OG	1:A:186:ALA:HB2	0.45	2.12	7	1
1:A:178:LEU:HD13	1:A:198:ASP:HB2	0.45	1.88	19	1
1:A:182:LEU:HD11	1:A:186:ALA:HB3	0.45	1.89	14	1
1:A:103:LEU:HD21	1:A:213:VAL:HG11	0.45	1.88	19	1
1:A:137:LEU:HD12	1:A:143:ARG:CD	0.44	2.41	10	1
1:A:161:MET:HE3	1:A:165:LEU:HD11	0.44	1.88	13	1
1:A:149:PRO:CB	1:A:182:LEU:HD23	0.44	2.41	14	1
1:A:179:LEU:HD23	1:A:197:VAL:CG1	0.44	2.43	12	1
1:A:182:LEU:HD13	1:A:187:TYR:OH	0.44	2.12	19	1
1:A:219:THR:HG23	1:A:220:LEU:HD22	0.43	1.90	11	15
1:A:168:ALA:HB1	1:A:169:PRO:HD2	0.43	1.90	17	19
1:A:182:LEU:HD23	1:A:186:ALA:HB1	0.43	1.90	10	1
1:A:94:GLU:HG3	1:A:120:LEU:HD21	0.43	1.90	20	3
1:A:161:MET:HE3	1:A:165:LEU:HD21	0.43	1.91	20	2
1:A:179:LEU:HD12	1:A:182:LEU:CD1	0.43	2.42	17	1
1:A:149:PRO:HB3	1:A:182:LEU:HD12	0.43	1.91	19	1
1:A:162:LEU:HD22	1:A:163:GLN:N	0.43	2.28	20	1
1:A:178:LEU:C	1:A:178:LEU:HD13	0.43	2.34	20	6
1:A:183:SER:CB	1:A:186:ALA:HB2	0.43	2.44	6	1
1:A:179:LEU:CD2	1:A:182:LEU:HD13	0.43	2.44	4	1
1:A:86:TYR:OH	1:A:136:ALA:HB1	0.43	2.14	15	1
1:A:179:LEU:HD12	1:A:182:LEU:HG	0.42	1.91	1	1
1:A:137:LEU:HD21	1:A:143:ARG:NH1	0.42	2.29	2	1
1:A:90:VAL:HG21	1:A:100:ALA:HB1	0.42	1.91	12	1
1:A:182:LEU:HD13	1:A:187:TYR:CE1	0.42	2.50	6	1
1:A:179:LEU:HB3	1:A:182:LEU:HD23	0.42	1.91	20	1
1:A:178:LEU:HD22	1:A:198:ASP:O	0.42	2.14	2	1
1:A:210:LYS:HG2	1:A:211:GLU:N	0.42	2.29	18	1
1:A:104:VAL:HG22	1:A:108:GLU:HG2	0.42	1.90	7	1
1:A:149:PRO:HB3	1:A:182:LEU:HD22	0.42	1.92	8	1
1:A:144:VAL:HG12	1:A:146:LEU:HD22	0.41	1.91	2	1
1:A:162:LEU:HD23	1:A:163:GLN:H	0.41	1.75	6	9
1:A:182:LEU:HD23	1:A:183:SER:H	0.41	1.76	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:162:LEU:HD22	1:A:162:LEU:O	0.41	2.13	20	1
1:A:179:LEU:HD23	1:A:197:VAL:CB	0.41	2.45	12	1
1:A:178:LEU:HG	1:A:209:VAL:HG12	0.41	1.92	8	1
1:A:118:LEU:HD13	1:A:120:LEU:HD13	0.41	1.91	10	1
1:A:176:ILE:HD12	1:A:212:ALA:HB1	0.41	1.91	16	1
1:A:178:LEU:HD21	1:A:208:GLN:OE1	0.41	2.16	19	1
1:A:144:VAL:HG12	1:A:146:LEU:HD23	0.41	1.92	11	1
1:A:216:TYR:CD1	1:A:217:LEU:HD23	0.41	2.51	14	1
1:A:165:LEU:HD13	1:A:190:GLU:CG	0.41	2.44	18	1
1:A:103:LEU:O	1:A:107:LEU:HD22	0.41	2.16	1	1
1:A:112:ALA:O	1:A:114:LEU:HD12	0.40	2.15	9	1
1:A:118:LEU:HD12	1:A:118:LEU:O	0.40	2.16	14	1
1:A:217:LEU:HD22	1:A:217:LEU:H	0.40	1.76	8	1
1:A:176:ILE:CG1	1:A:176:ILE:O	0.40	2.70	13	1
1:A:90:VAL:HG23	1:A:144:VAL:O	0.40	2.16	18	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	122/143 (85%)	106±2 (87±2%)	15±2 (13±2%)	0±1 (0±1%)	38	78
All	All	2440/2860 (85%)	2121 (87%)	309 (13%)	10 (0%)	38	78

All 8 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	206	PHE	2
1	A	184	ARG	2
1	A	109	GLY	1
1	A	170	GLY	1
1	A	197	VAL	1
1	A	121	ARG	1
1	A	192	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	183	SER	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	103/119 (87%)	83±3 (80±3%)	20±3 (20±3%)	4	35
All	All	2060/2380 (87%)	1658 (80%)	402 (20%)	4	35

All 65 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	107	LEU	20
1	A	146	LEU	20
1	A	152	LEU	20
1	A	158	LYS	20
1	A	163	GLN	20
1	A	148	THR	19
1	A	216	TYR	18
1	A	147	ILE	16
1	A	166	THR	16
1	A	121	ARG	13
1	A	178	LEU	12
1	A	96	ASP	11
1	A	84	LYS	10
1	A	101	GLN	10
1	A	118	LEU	10
1	A	220	LEU	10
1	A	157	CYS	10
1	A	207	ARG	9
1	A	210	LYS	8
1	A	162	LEU	7
1	A	154	ASP	7
1	A	214	MET	7
1	A	145	LEU	5
1	A	142	CYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	92	HIS	5
1	A	200	ARG	5
1	A	141	HIS	5
1	A	184	ARG	4
1	A	172	GLU	4
1	A	180	SER	4
1	A	85	ASP	4
1	A	139	SER	4
1	A	215	ARG	4
1	A	160	GLN	3
1	A	179	LEU	3
1	A	143	ARG	3
1	A	183	SER	3
1	A	182	LEU	3
1	A	191	LEU	3
1	A	192	ARG	3
1	A	135	GLN	3
1	A	208	GLN	3
1	A	153	GLN	3
1	A	190	GLU	2
1	A	198	ASP	2
1	A	137	LEU	2
1	A	115	ARG	2
1	A	203	ASP	2
1	A	140	SER	2
1	A	176	ILE	2
1	A	217	LEU	2
1	A	110	SER	1
1	A	122	ASP	1
1	A	213	VAL	1
1	A	108	GLU	1
1	A	187	TYR	1
1	A	221	SER	1
1	A	87	ASP	1
1	A	111	THR	1
1	A	114	LEU	1
1	A	94	GLU	1
1	A	120	LEU	1
1	A	113	SER	1
1	A	91	CYS	1
1	A	103	LEU	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 68% for the well-defined parts and 63% 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	1185
Number of shifts mapped to atoms	1185
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	116	-0.31 ± 0.06	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	109	0.40 ± 0.20	None needed (< 0.5 ppm)
$^{13}C'$	107	0.01 ± 0.14	None needed (< 0.5 ppm)
^{15}N	100	0.19 ± 0.22	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 68%, i.e. 1115 atoms were assigned a chemical shift out of a possible 1633. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	507/610 (83%)	203/248 (82%)	209/246 (85%)	95/116 (82%)
Sidechain	570/922 (62%)	397/603 (66%)	170/284 (60%)	3/35 (9%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	38/101 (38%)	23/49 (47%)	14/49 (29%)	1/3 (33%)
Overall	1115/1633 (68%)	623/900 (69%)	393/579 (68%)	99/154 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 63%, i.e. 1185 atoms were assigned a chemical shift out of a possible 1891. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	538/710 (76%)	215/289 (74%)	223/286 (78%)	100/135 (74%)
Sidechain	609/1040 (59%)	424/682 (62%)	182/320 (57%)	3/38 (8%)
Aromatic	38/141 (27%)	23/68 (34%)	14/69 (20%)	1/4 (25%)
Overall	1185/1891 (63%)	662/1039 (64%)	419/675 (62%)	104/177 (59%)

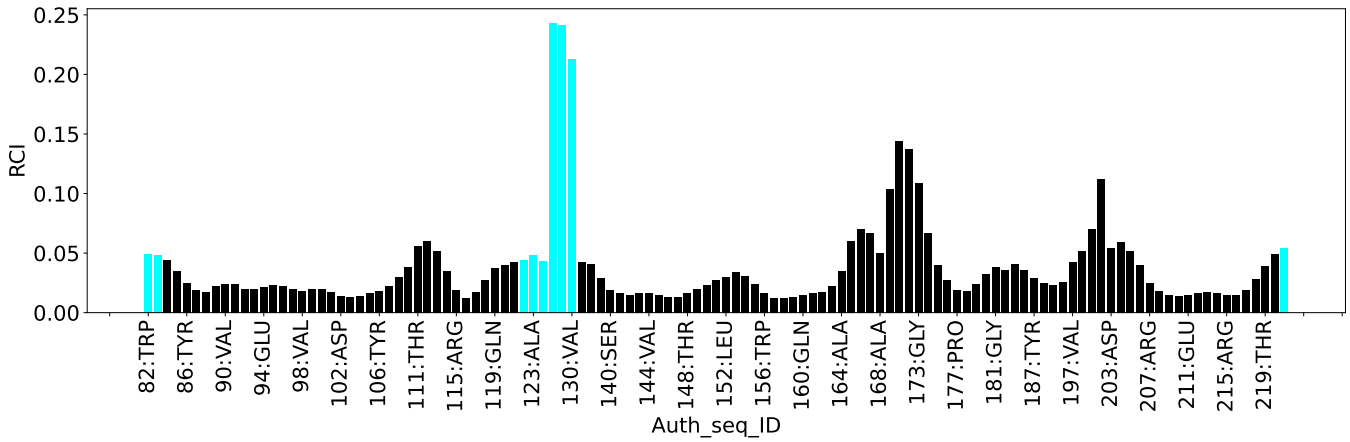
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1268
Intra-residue (|i-j|=0)	313
Sequential (|i-j|=1)	397
Medium range (|i-j|>1 and |i-j|<5)	286
Long range (|i-j|≥5)	272
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	8.9
Number of long range restraints per residue[1]	1.9

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	5.0	0.2
0.2-0.5 (Medium)	2.7	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)

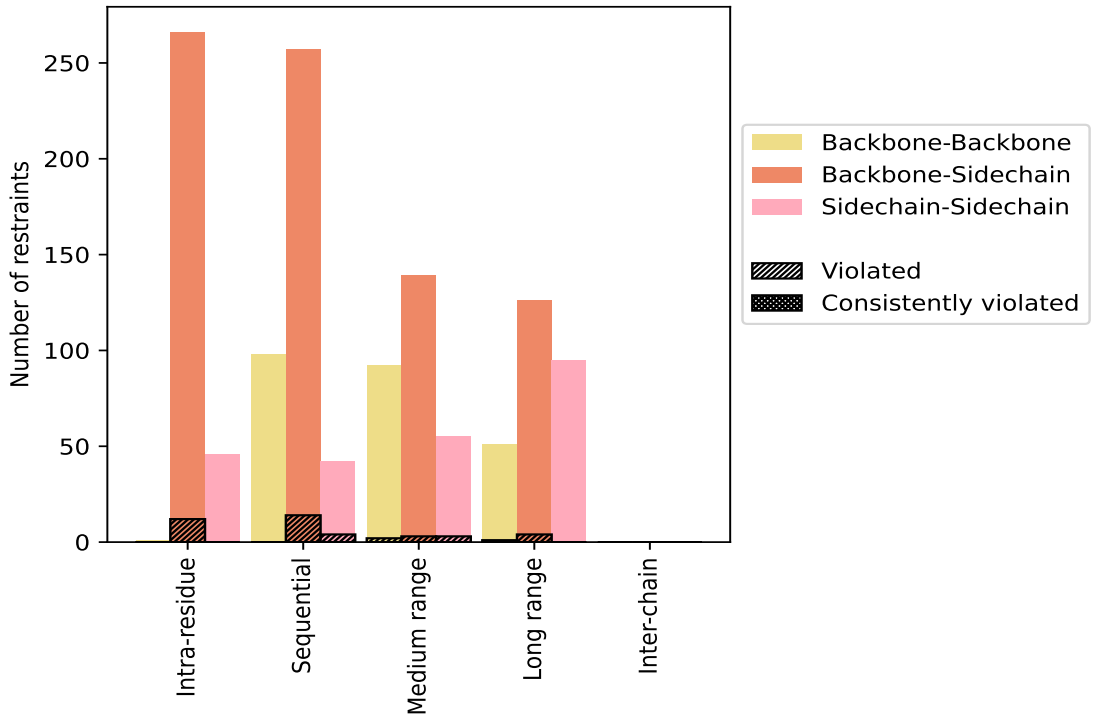
9.1 Summary of distance violations (i)

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)	313	24.7	12	3.8	0.9	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	266	21.0	12	4.5	0.9	0	0.0	0.0
Sidechain-Sidechain	46	3.6	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	397	31.3	18	4.5	1.4	0	0.0	0.0
Backbone-Backbone	98	7.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	257	20.3	14	5.4	1.1	0	0.0	0.0
Sidechain-Sidechain	42	3.3	4	9.5	0.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	286	22.6	8	2.8	0.6	0	0.0	0.0
Backbone-Backbone	92	7.3	2	2.2	0.2	0	0.0	0.0
Backbone-Sidechain	139	11.0	3	2.2	0.2	0	0.0	0.0
Sidechain-Sidechain	55	4.3	3	5.5	0.2	0	0.0	0.0
Long range (|i-j|≥5)	272	21.5	5	1.8	0.4	0	0.0	0.0
Backbone-Backbone	51	4.0	1	2.0	0.1	0	0.0	0.0
Backbone-Sidechain	126	9.9	4	3.2	0.3	0	0.0	0.0
Sidechain-Sidechain	95	7.5	0	0.0	0.0	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	1268	100.0	43	3.4	3.4	0	0.0	0.0
Backbone-Backbone	242	19.1	3	1.2	0.2	0	0.0	0.0
Backbone-Sidechain	788	62.1	33	4.2	2.6	0	0.0	0.0
Sidechain-Sidechain	238	18.8	7	2.9	0.6	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	1	1	0	2	0	4	0.19	0.36	0.1	0.16
2	2	2	0	2	0	6	0.18	0.33	0.08	0.14
3	2	1	0	2	0	5	0.19	0.32	0.08	0.14
4	1	3	0	2	0	6	0.19	0.35	0.08	0.18
5	1	2	0	2	0	5	0.19	0.33	0.08	0.18
6	3	0	0	1	0	4	0.31	0.45	0.11	0.32
7	2	5	0	1	0	8	0.19	0.38	0.09	0.18
8	2	5	0	2	0	9	0.18	0.35	0.08	0.15
9	3	3	3	1	0	10	0.19	0.45	0.11	0.14
10	3	6	1	2	0	12	0.19	0.38	0.09	0.14
11	3	5	2	2	0	12	0.16	0.3	0.05	0.16

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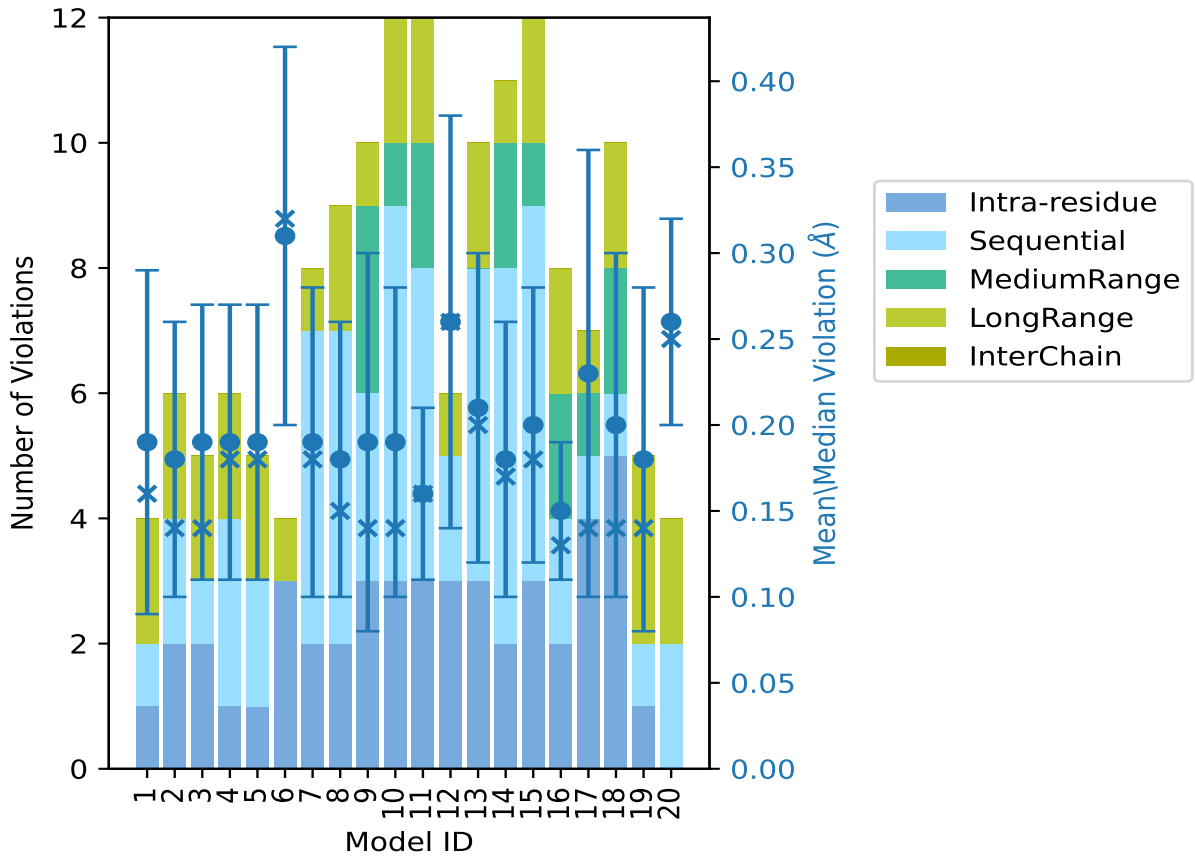
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	3	2	0	1	0	6	0.26	0.46	0.12	0.26
13	3	5	0	2	0	10	0.21	0.38	0.09	0.2
14	2	6	2	1	0	11	0.18	0.38	0.08	0.17
15	3	6	1	2	0	12	0.2	0.38	0.08	0.18
16	2	2	2	2	0	8	0.15	0.21	0.04	0.13
17	4	1	1	1	0	7	0.23	0.45	0.13	0.14
18	5	1	2	2	0	10	0.2	0.45	0.1	0.14
19	1	1	0	3	0	5	0.18	0.38	0.1	0.14
20	0	2	0	2	0	4	0.26	0.35	0.06	0.25

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

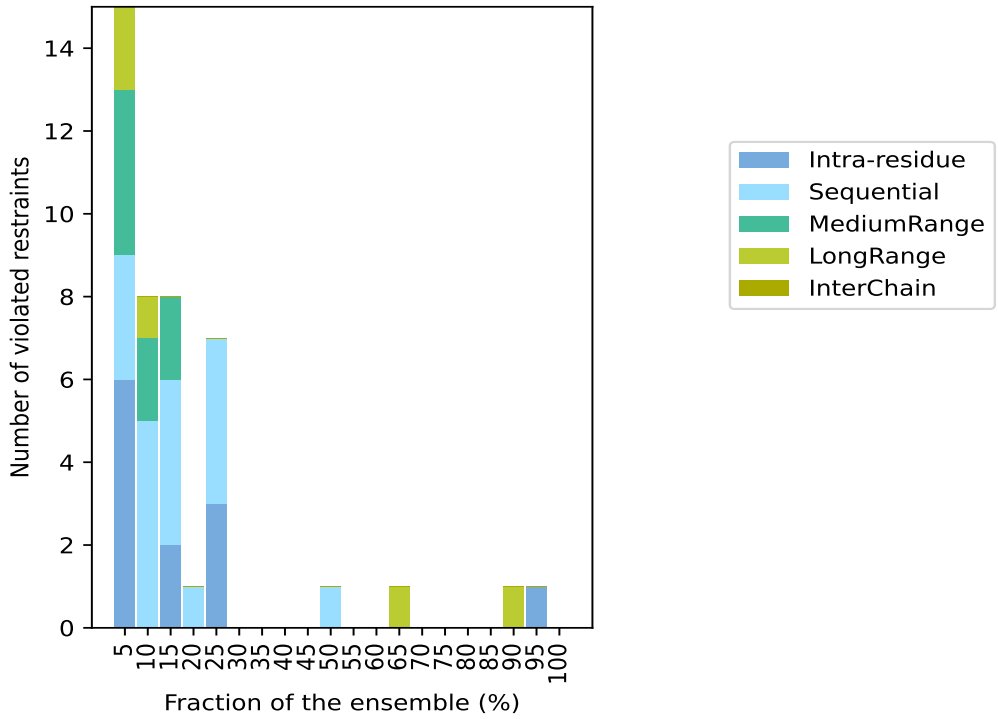
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1225(IR:301, SQ:379, MR:278, LR:267, IC:0) restraints are not violated in the ensemble.

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

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

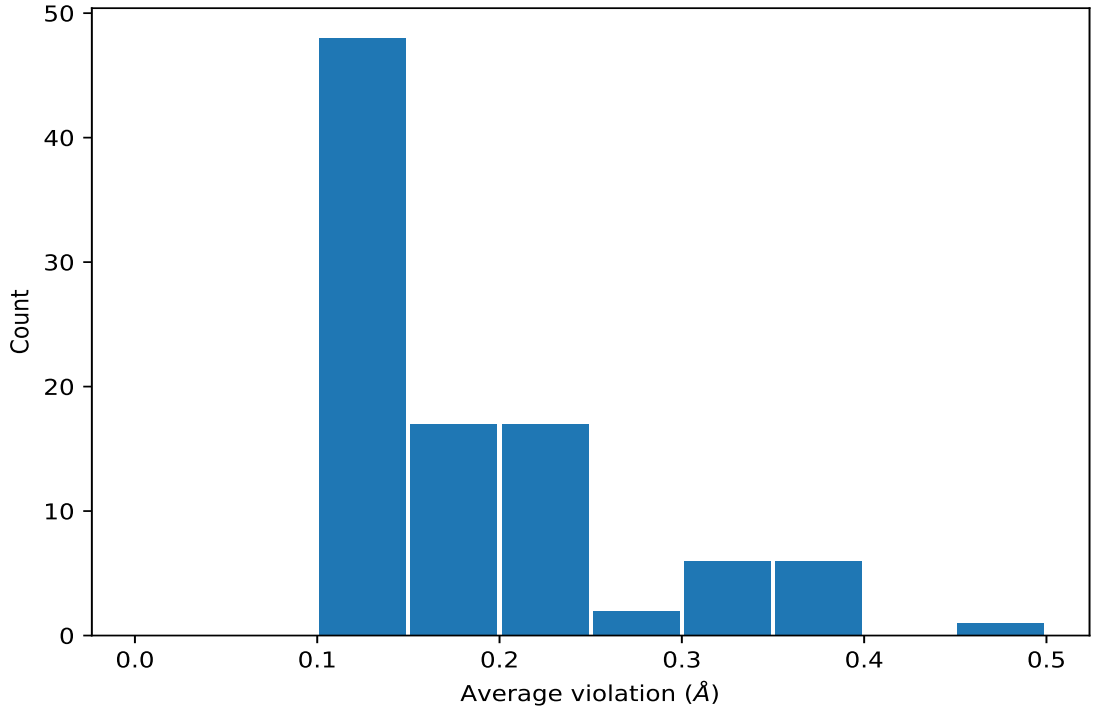
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (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)
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	19	0.13	0.01	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	19	0.13	0.01	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	19	0.13	0.01	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	19	0.13	0.01	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	19	0.13	0.01	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	19	0.13	0.01	0.14
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	18	0.13	0.04	0.11
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	13	0.33	0.04	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	13	0.33	0.04	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	13	0.33	0.04	0.33
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD11	10	0.15	0.03	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD12	10	0.15	0.03	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD13	10	0.15	0.03	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD21	10	0.15	0.03	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD22	10	0.15	0.03	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD23	10	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,814)	1:A:141:HIS:HA	1:A:141:HIS:HE1	5	0.45	0.0	0.45
(1,1267)	1:A:220:LEU:HD11	1:A:221:SER:H	5	0.38	0.0	0.38
(1,1267)	1:A:220:LEU:HD12	1:A:221:SER:H	5	0.38	0.0	0.38
(1,1267)	1:A:220:LEU:HD13	1:A:221:SER:H	5	0.38	0.0	0.38
(1,1267)	1:A:220:LEU:HD21	1:A:221:SER:H	5	0.38	0.0	0.38
(1,1267)	1:A:220:LEU:HD22	1:A:221:SER:H	5	0.38	0.0	0.38
(1,1267)	1:A:220:LEU:HD23	1:A:221:SER:H	5	0.38	0.0	0.38
(1,852)	1:A:141:HIS:H	1:A:141:HIS:HD2	5	0.32	0.0	0.32
(1,256)	1:A:220:LEU:HD21	1:A:221:SER:H	5	0.24	0.0	0.24
(1,256)	1:A:220:LEU:HD22	1:A:221:SER:H	5	0.24	0.0	0.24
(1,256)	1:A:220:LEU:HD23	1:A:221:SER:H	5	0.24	0.0	0.24
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD11	5	0.22	0.01	0.22
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD12	5	0.22	0.01	0.22
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD13	5	0.22	0.01	0.22
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD11	5	0.21	0.0	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD12	5	0.21	0.0	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD13	5	0.21	0.0	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD21	5	0.21	0.0	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD22	5	0.21	0.0	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD23	5	0.21	0.0	0.21
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG21	5	0.13	0.01	0.13
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG22	5	0.13	0.01	0.13
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG23	5	0.13	0.01	0.13
(1,1096)	1:A:162:LEU:HD11	1:A:163:GLN:HG3	4	0.17	0.0	0.17
(1,1096)	1:A:162:LEU:HD12	1:A:163:GLN:HG3	4	0.17	0.0	0.17
(1,1096)	1:A:162:LEU:HD13	1:A:163:GLN:HG3	4	0.17	0.0	0.17
(1,1096)	1:A:162:LEU:HD21	1:A:163:GLN:HG3	4	0.17	0.0	0.17
(1,1096)	1:A:162:LEU:HD22	1:A:163:GLN:HG3	4	0.17	0.0	0.17
(1,1096)	1:A:162:LEU:HD23	1:A:163:GLN:HG3	4	0.17	0.0	0.17
(1,841)	1:A:176:ILE:HA	1:A:176:ILE:HD11	3	0.22	0.01	0.23
(1,841)	1:A:176:ILE:HA	1:A:176:ILE:HD12	3	0.22	0.01	0.23
(1,841)	1:A:176:ILE:HA	1:A:176:ILE:HD13	3	0.22	0.01	0.23
(1,1191)	1:A:209:VAL:HG11	1:A:211:GLU:H	3	0.19	0.02	0.2
(1,1191)	1:A:209:VAL:HG12	1:A:211:GLU:H	3	0.19	0.02	0.2
(1,1191)	1:A:209:VAL:HG13	1:A:211:GLU:H	3	0.19	0.02	0.2
(1,1191)	1:A:209:VAL:HG21	1:A:211:GLU:H	3	0.19	0.02	0.2
(1,1191)	1:A:209:VAL:HG22	1:A:211:GLU:H	3	0.19	0.02	0.2
(1,1191)	1:A:209:VAL:HG23	1:A:211:GLU:H	3	0.19	0.02	0.2
(1,429)	1:A:208:GLN:HA	1:A:210:LYS:H	3	0.16	0.0	0.16
(1,1190)	1:A:209:VAL:HG11	1:A:210:LYS:HE2	3	0.15	0.02	0.14
(1,1190)	1:A:209:VAL:HG11	1:A:210:LYS:HE3	3	0.15	0.02	0.14
(1,1190)	1:A:209:VAL:HG12	1:A:210:LYS:HE2	3	0.15	0.02	0.14

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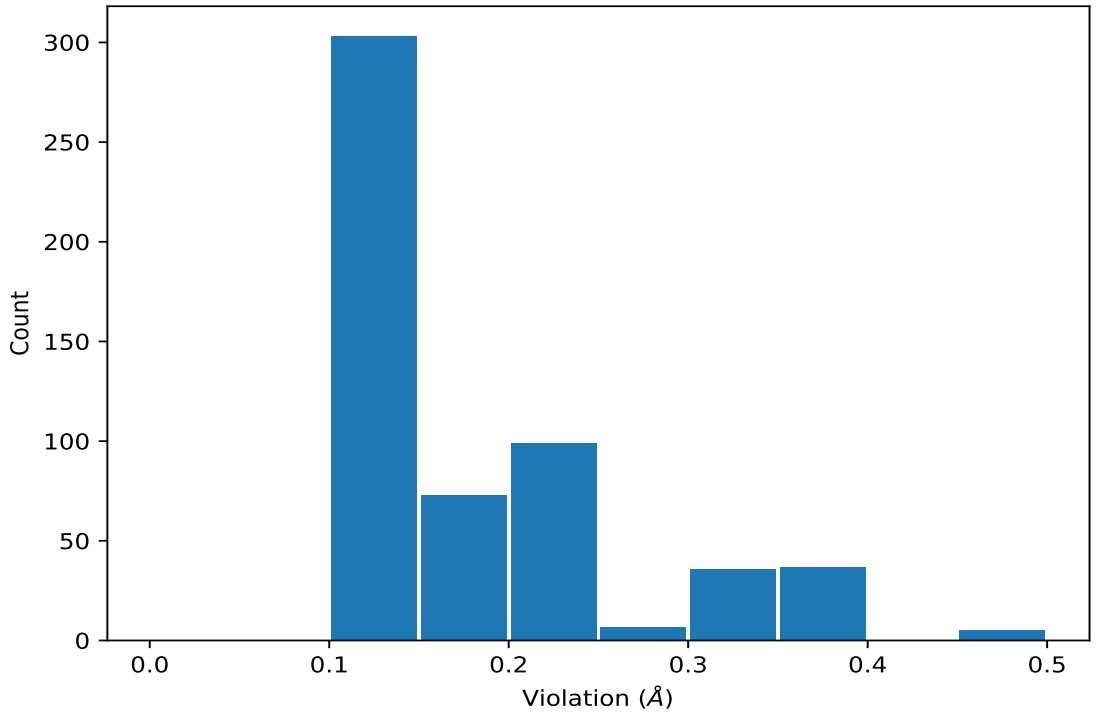
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1190)	1:A:209:VAL:HG12	1:A:210:LYS:HE3	3	0.15	0.02	0.14
(1,1190)	1:A:209:VAL:HG13	1:A:210:LYS:HE2	3	0.15	0.02	0.14
(1,1190)	1:A:209:VAL:HG13	1:A:210:LYS:HE3	3	0.15	0.02	0.14
(1,1190)	1:A:209:VAL:HG21	1:A:210:LYS:HE2	3	0.15	0.02	0.14
(1,1190)	1:A:209:VAL:HG21	1:A:210:LYS:HE3	3	0.15	0.02	0.14
(1,1190)	1:A:209:VAL:HG22	1:A:210:LYS:HE2	3	0.15	0.02	0.14
(1,1190)	1:A:209:VAL:HG22	1:A:210:LYS:HE3	3	0.15	0.02	0.14
(1,1190)	1:A:209:VAL:HG23	1:A:210:LYS:HE2	3	0.15	0.02	0.14
(1,1190)	1:A:209:VAL:HG23	1:A:210:LYS:HE3	3	0.15	0.02	0.14
(1,532)	1:A:215:ARG:HA	1:A:215:ARG:HG2	3	0.13	0.01	0.14
(1,375)	1:A:209:VAL:HG21	1:A:210:LYS:H	3	0.13	0.02	0.13
(1,375)	1:A:209:VAL:HG22	1:A:210:LYS:H	3	0.13	0.02	0.13
(1,375)	1:A:209:VAL:HG23	1:A:210:LYS:H	3	0.13	0.02	0.13
(1,816)	1:A:175:THR:HB	1:A:176:ILE:HG21	3	0.13	0.0	0.13
(1,816)	1:A:175:THR:HB	1:A:176:ILE:HG22	3	0.13	0.0	0.13
(1,816)	1:A:175:THR:HB	1:A:176:ILE:HG23	3	0.13	0.0	0.13
(1,1241)	1:A:215:ARG:HB2	1:A:216:TYR:H	3	0.12	0.0	0.12
(1,1241)	1:A:215:ARG:HB3	1:A:216:TYR:H	3	0.12	0.0	0.12
(1,240)	1:A:216:TYR:HD1	1:A:217:LEU:H	2	0.32	0.03	0.32
(1,240)	1:A:216:TYR:HD2	1:A:217:LEU:H	2	0.32	0.03	0.32
(1,1072)	1:A:153:GLN:HG2	1:A:154:ASP:H	2	0.3	0.04	0.3
(1,1072)	1:A:153:GLN:HG3	1:A:154:ASP:H	2	0.3	0.04	0.3
(1,1201)	1:A:210:LYS:HD2	1:A:211:GLU:H	2	0.2	0.0	0.2
(1,1201)	1:A:210:LYS:HD3	1:A:211:GLU:H	2	0.2	0.0	0.2
(1,339)	1:A:215:ARG:H	1:A:216:TYR:HD1	2	0.18	0.03	0.18
(1,339)	1:A:215:ARG:H	1:A:216:TYR:HD2	2	0.18	0.03	0.18
(1,1212)	1:A:212:ALA:H	1:A:215:ARG:HD2	2	0.16	0.05	0.16
(1,1212)	1:A:212:ALA:H	1:A:215:ARG:HD3	2	0.16	0.05	0.16
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG11	2	0.13	0.0	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG12	2	0.13	0.0	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG13	2	0.13	0.0	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG21	2	0.13	0.0	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG22	2	0.13	0.0	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG23	2	0.13	0.0	0.13
(1,847)	1:A:144:VAL:HA	1:A:176:ILE:HD11	2	0.12	0.01	0.12
(1,847)	1:A:144:VAL:HA	1:A:176:ILE:HD12	2	0.12	0.01	0.12
(1,847)	1:A:144:VAL:HA	1:A:176:ILE:HD13	2	0.12	0.01	0.12
(1,1256)	1:A:217:LEU:HB2	1:A:218:GLN:H	2	0.12	0.01	0.12
(1,1256)	1:A:217:LEU:HB3	1:A:218:GLN:H	2	0.12	0.01	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)
(1,814)	1:A:141:HIS:HA	1:A:141:HIS:HE1	12	0.46
(1,814)	1:A:141:HIS:HA	1:A:141:HIS:HE1	6	0.45
(1,814)	1:A:141:HIS:HA	1:A:141:HIS:HE1	9	0.45
(1,814)	1:A:141:HIS:HA	1:A:141:HIS:HE1	17	0.45
(1,814)	1:A:141:HIS:HA	1:A:141:HIS:HE1	18	0.45
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	19	0.38
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	19	0.38
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	19	0.38
(1,1267)	1:A:220:LEU:HD11	1:A:221:SER:H	7	0.38
(1,1267)	1:A:220:LEU:HD12	1:A:221:SER:H	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1267)	1:A:220:LEU:HD13	1:A:221:SER:H	7	0.38
(1,1267)	1:A:220:LEU:HD21	1:A:221:SER:H	7	0.38
(1,1267)	1:A:220:LEU:HD22	1:A:221:SER:H	7	0.38
(1,1267)	1:A:220:LEU:HD23	1:A:221:SER:H	7	0.38
(1,1267)	1:A:220:LEU:HD11	1:A:221:SER:H	10	0.38
(1,1267)	1:A:220:LEU:HD12	1:A:221:SER:H	10	0.38
(1,1267)	1:A:220:LEU:HD13	1:A:221:SER:H	10	0.38
(1,1267)	1:A:220:LEU:HD21	1:A:221:SER:H	10	0.38
(1,1267)	1:A:220:LEU:HD22	1:A:221:SER:H	10	0.38
(1,1267)	1:A:220:LEU:HD23	1:A:221:SER:H	10	0.38
(1,1267)	1:A:220:LEU:HD11	1:A:221:SER:H	13	0.38
(1,1267)	1:A:220:LEU:HD12	1:A:221:SER:H	13	0.38
(1,1267)	1:A:220:LEU:HD13	1:A:221:SER:H	13	0.38
(1,1267)	1:A:220:LEU:HD21	1:A:221:SER:H	13	0.38
(1,1267)	1:A:220:LEU:HD22	1:A:221:SER:H	13	0.38
(1,1267)	1:A:220:LEU:HD23	1:A:221:SER:H	13	0.38
(1,1267)	1:A:220:LEU:HD11	1:A:221:SER:H	14	0.38
(1,1267)	1:A:220:LEU:HD12	1:A:221:SER:H	14	0.38
(1,1267)	1:A:220:LEU:HD13	1:A:221:SER:H	14	0.38
(1,1267)	1:A:220:LEU:HD21	1:A:221:SER:H	14	0.38
(1,1267)	1:A:220:LEU:HD22	1:A:221:SER:H	14	0.38
(1,1267)	1:A:220:LEU:HD23	1:A:221:SER:H	14	0.38
(1,1267)	1:A:220:LEU:HD11	1:A:221:SER:H	15	0.38
(1,1267)	1:A:220:LEU:HD12	1:A:221:SER:H	15	0.38
(1,1267)	1:A:220:LEU:HD13	1:A:221:SER:H	15	0.38
(1,1267)	1:A:220:LEU:HD21	1:A:221:SER:H	15	0.38
(1,1267)	1:A:220:LEU:HD22	1:A:221:SER:H	15	0.38
(1,1267)	1:A:220:LEU:HD23	1:A:221:SER:H	15	0.38
(1,673)	1:A:114:LEU:HA	1:A:114:LEU:HG	17	0.37
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	1	0.36
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	1	0.36
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	1	0.36
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	8	0.35
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	8	0.35
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	8	0.35
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	20	0.35
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	20	0.35
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	20	0.35
(1,240)	1:A:216:TYR:HD1	1:A:217:LEU:H	4	0.35
(1,240)	1:A:216:TYR:HD2	1:A:217:LEU:H	4	0.35
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	13	0.34
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	13	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	13	0.34
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	15	0.34
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	15	0.34
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	15	0.34
(1,1072)	1:A:153:GLN:HG2	1:A:154:ASP:H	12	0.34
(1,1072)	1:A:153:GLN:HG3	1:A:154:ASP:H	12	0.34
(1,852)	1:A:141:HIS:H	1:A:141:HIS:HD2	17	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	2	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	2	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	2	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	5	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	5	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	5	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	6	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	6	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	6	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	10	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	10	0.33
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	10	0.33
(1,852)	1:A:141:HIS:H	1:A:141:HIS:HD2	6	0.32
(1,852)	1:A:141:HIS:H	1:A:141:HIS:HD2	9	0.32
(1,852)	1:A:141:HIS:H	1:A:141:HIS:HD2	12	0.32
(1,852)	1:A:141:HIS:H	1:A:141:HIS:HD2	18	0.32
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	3	0.32
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	3	0.32
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	3	0.32
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	11	0.3
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	11	0.3
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	11	0.3
(1,240)	1:A:216:TYR:HD1	1:A:217:LEU:H	8	0.28
(1,240)	1:A:216:TYR:HD2	1:A:217:LEU:H	8	0.28
(1,1072)	1:A:153:GLN:HG2	1:A:154:ASP:H	20	0.26
(1,1072)	1:A:153:GLN:HG3	1:A:154:ASP:H	20	0.26
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	20	0.24
(1,256)	1:A:220:LEU:HD21	1:A:221:SER:H	7	0.24
(1,256)	1:A:220:LEU:HD22	1:A:221:SER:H	7	0.24
(1,256)	1:A:220:LEU:HD23	1:A:221:SER:H	7	0.24
(1,256)	1:A:220:LEU:HD21	1:A:221:SER:H	10	0.24
(1,256)	1:A:220:LEU:HD22	1:A:221:SER:H	10	0.24
(1,256)	1:A:220:LEU:HD23	1:A:221:SER:H	10	0.24
(1,256)	1:A:220:LEU:HD21	1:A:221:SER:H	13	0.24
(1,256)	1:A:220:LEU:HD22	1:A:221:SER:H	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,256)	1:A:220:LEU:HD23	1:A:221:SER:H	13	0.24
(1,256)	1:A:220:LEU:HD21	1:A:221:SER:H	14	0.24
(1,256)	1:A:220:LEU:HD22	1:A:221:SER:H	14	0.24
(1,256)	1:A:220:LEU:HD23	1:A:221:SER:H	14	0.24
(1,841)	1:A:176:ILE:HA	1:A:176:ILE:HD11	2	0.23
(1,841)	1:A:176:ILE:HA	1:A:176:ILE:HD12	2	0.23
(1,841)	1:A:176:ILE:HA	1:A:176:ILE:HD13	2	0.23
(1,841)	1:A:176:ILE:HA	1:A:176:ILE:HD11	3	0.23
(1,841)	1:A:176:ILE:HA	1:A:176:ILE:HD12	3	0.23
(1,841)	1:A:176:ILE:HA	1:A:176:ILE:HD13	3	0.23
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD11	15	0.23
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD12	15	0.23
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD13	15	0.23
(1,256)	1:A:220:LEU:HD21	1:A:221:SER:H	15	0.23
(1,256)	1:A:220:LEU:HD22	1:A:221:SER:H	15	0.23
(1,256)	1:A:220:LEU:HD23	1:A:221:SER:H	15	0.23
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD11	7	0.22
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD12	7	0.22
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD13	7	0.22
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD11	10	0.22
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD12	10	0.22
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD13	10	0.22
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD11	14	0.22
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD12	14	0.22
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD13	14	0.22
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG21	18	0.22
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG22	18	0.22
(1,418)	1:A:145:LEU:H	1:A:176:ILE:HG23	18	0.22
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD11	13	0.22
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD12	13	0.22
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD13	13	0.22
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD21	13	0.22
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD22	13	0.22
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD23	13	0.22
(1,841)	1:A:176:ILE:HA	1:A:176:ILE:HD11	11	0.21
(1,841)	1:A:176:ILE:HA	1:A:176:ILE:HD12	11	0.21
(1,841)	1:A:176:ILE:HA	1:A:176:ILE:HD13	11	0.21
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD11	13	0.21
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD12	13	0.21
(1,667)	1:A:219:THR:H	1:A:220:LEU:HD13	13	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD11	7	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD12	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD13	7	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD21	7	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD22	7	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD23	7	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD11	10	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD12	10	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD13	10	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD21	10	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD22	10	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD23	10	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD11	14	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD12	14	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD13	14	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD21	14	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD22	14	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD23	14	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD11	15	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD12	15	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD13	15	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD21	15	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD22	15	0.21
(1,1265)	1:A:220:LEU:HA	1:A:220:LEU:HD23	15	0.21
(1,1212)	1:A:212:ALA:H	1:A:215:ARG:HD2	16	0.21
(1,1212)	1:A:212:ALA:H	1:A:215:ARG:HD3	16	0.21
(1,1201)	1:A:210:LYS:HD2	1:A:211:GLU:H	16	0.21
(1,1201)	1:A:210:LYS:HD3	1:A:211:GLU:H	16	0.21
(1,339)	1:A:215:ARG:H	1:A:216:TYR:HD1	4	0.2
(1,339)	1:A:215:ARG:H	1:A:216:TYR:HD2	4	0.2
(1,1201)	1:A:210:LYS:HD2	1:A:211:GLU:H	18	0.2
(1,1201)	1:A:210:LYS:HD3	1:A:211:GLU:H	18	0.2
(1,1191)	1:A:209:VAL:HG11	1:A:211:GLU:H	9	0.2
(1,1191)	1:A:209:VAL:HG12	1:A:211:GLU:H	9	0.2
(1,1191)	1:A:209:VAL:HG13	1:A:211:GLU:H	9	0.2
(1,1191)	1:A:209:VAL:HG21	1:A:211:GLU:H	9	0.2
(1,1191)	1:A:209:VAL:HG22	1:A:211:GLU:H	9	0.2
(1,1191)	1:A:209:VAL:HG23	1:A:211:GLU:H	9	0.2
(1,1191)	1:A:209:VAL:HG11	1:A:211:GLU:H	14	0.2
(1,1191)	1:A:209:VAL:HG12	1:A:211:GLU:H	14	0.2
(1,1191)	1:A:209:VAL:HG13	1:A:211:GLU:H	14	0.2
(1,1191)	1:A:209:VAL:HG21	1:A:211:GLU:H	14	0.2
(1,1191)	1:A:209:VAL:HG22	1:A:211:GLU:H	14	0.2
(1,1191)	1:A:209:VAL:HG23	1:A:211:GLU:H	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD11	12	0.2
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD12	12	0.2
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD13	12	0.2
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD21	12	0.2
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD22	12	0.2
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD23	12	0.2
(1,988)	1:A:120:LEU:HA	1:A:120:LEU:HD11	13	0.18
(1,988)	1:A:120:LEU:HA	1:A:120:LEU:HD12	13	0.18
(1,988)	1:A:120:LEU:HA	1:A:120:LEU:HD13	13	0.18
(1,988)	1:A:120:LEU:HA	1:A:120:LEU:HD21	13	0.18
(1,988)	1:A:120:LEU:HA	1:A:120:LEU:HD22	13	0.18
(1,988)	1:A:120:LEU:HA	1:A:120:LEU:HD23	13	0.18
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	4	0.18
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	5	0.18
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	8	0.18
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	15	0.18
(1,1190)	1:A:209:VAL:HG11	1:A:210:LYS:HE2	11	0.18
(1,1190)	1:A:209:VAL:HG11	1:A:210:LYS:HE3	11	0.18
(1,1190)	1:A:209:VAL:HG12	1:A:210:LYS:HE2	11	0.18
(1,1190)	1:A:209:VAL:HG12	1:A:210:LYS:HE3	11	0.18
(1,1190)	1:A:209:VAL:HG13	1:A:210:LYS:HE2	11	0.18
(1,1190)	1:A:209:VAL:HG13	1:A:210:LYS:HE3	11	0.18
(1,1190)	1:A:209:VAL:HG21	1:A:210:LYS:HE2	11	0.18
(1,1190)	1:A:209:VAL:HG21	1:A:210:LYS:HE3	11	0.18
(1,1190)	1:A:209:VAL:HG22	1:A:210:LYS:HE2	11	0.18
(1,1190)	1:A:209:VAL:HG22	1:A:210:LYS:HE3	11	0.18
(1,1190)	1:A:209:VAL:HG23	1:A:210:LYS:HE2	11	0.18
(1,1190)	1:A:209:VAL:HG23	1:A:210:LYS:HE3	11	0.18
(1,1096)	1:A:162:LEU:HD11	1:A:163:GLN:HG3	5	0.18
(1,1096)	1:A:162:LEU:HD12	1:A:163:GLN:HG3	5	0.18
(1,1096)	1:A:162:LEU:HD13	1:A:163:GLN:HG3	5	0.18
(1,1096)	1:A:162:LEU:HD21	1:A:163:GLN:HG3	5	0.18
(1,1096)	1:A:162:LEU:HD22	1:A:163:GLN:HG3	5	0.18
(1,1096)	1:A:162:LEU:HD23	1:A:163:GLN:HG3	5	0.18
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD11	1	0.18
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD12	1	0.18
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD13	1	0.18
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD21	1	0.18
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD22	1	0.18
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD23	1	0.18
(1,429)	1:A:208:GLN:HA	1:A:210:LYS:H	14	0.17
(1,1096)	1:A:162:LEU:HD11	1:A:163:GLN:HG3	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1096)	1:A:162:LEU:HD12	1:A:163:GLN:HG3	4	0.17
(1,1096)	1:A:162:LEU:HD13	1:A:163:GLN:HG3	4	0.17
(1,1096)	1:A:162:LEU:HD21	1:A:163:GLN:HG3	4	0.17
(1,1096)	1:A:162:LEU:HD22	1:A:163:GLN:HG3	4	0.17
(1,1096)	1:A:162:LEU:HD23	1:A:163:GLN:HG3	4	0.17
(1,1096)	1:A:162:LEU:HD11	1:A:163:GLN:HG3	8	0.17
(1,1096)	1:A:162:LEU:HD12	1:A:163:GLN:HG3	8	0.17
(1,1096)	1:A:162:LEU:HD13	1:A:163:GLN:HG3	8	0.17
(1,1096)	1:A:162:LEU:HD21	1:A:163:GLN:HG3	8	0.17
(1,1096)	1:A:162:LEU:HD22	1:A:163:GLN:HG3	8	0.17
(1,1096)	1:A:162:LEU:HD23	1:A:163:GLN:HG3	8	0.17
(1,1096)	1:A:162:LEU:HD11	1:A:163:GLN:HG3	15	0.17
(1,1096)	1:A:162:LEU:HD12	1:A:163:GLN:HG3	15	0.17
(1,1096)	1:A:162:LEU:HD13	1:A:163:GLN:HG3	15	0.17
(1,1096)	1:A:162:LEU:HD21	1:A:163:GLN:HG3	15	0.17
(1,1096)	1:A:162:LEU:HD22	1:A:163:GLN:HG3	15	0.17
(1,1096)	1:A:162:LEU:HD23	1:A:163:GLN:HG3	15	0.17
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD11	20	0.17
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD12	20	0.17
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD13	20	0.17
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD21	20	0.17
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD22	20	0.17
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD23	20	0.17
(1,429)	1:A:208:GLN:HA	1:A:210:LYS:H	9	0.16
(1,429)	1:A:208:GLN:HA	1:A:210:LYS:H	11	0.16
(1,1191)	1:A:209:VAL:HG11	1:A:211:GLU:H	11	0.16
(1,1191)	1:A:209:VAL:HG12	1:A:211:GLU:H	11	0.16
(1,1191)	1:A:209:VAL:HG13	1:A:211:GLU:H	11	0.16
(1,1191)	1:A:209:VAL:HG21	1:A:211:GLU:H	11	0.16
(1,1191)	1:A:209:VAL:HG22	1:A:211:GLU:H	11	0.16
(1,1191)	1:A:209:VAL:HG23	1:A:211:GLU:H	11	0.16
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD11	11	0.16
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD12	11	0.16
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD13	11	0.16
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD21	11	0.16
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD22	11	0.16
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD23	11	0.16
(1,375)	1:A:209:VAL:HG21	1:A:210:LYS:H	11	0.15
(1,375)	1:A:209:VAL:HG22	1:A:210:LYS:H	11	0.15
(1,375)	1:A:209:VAL:HG23	1:A:210:LYS:H	11	0.15
(1,339)	1:A:215:ARG:H	1:A:216:TYR:HD1	8	0.15
(1,339)	1:A:215:ARG:H	1:A:216:TYR:HD2	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1125)	1:A:178:LEU:HD11	1:A:199:GLY:HA2	19	0.15
(1,1125)	1:A:178:LEU:HD11	1:A:199:GLY:HA3	19	0.15
(1,1125)	1:A:178:LEU:HD12	1:A:199:GLY:HA2	19	0.15
(1,1125)	1:A:178:LEU:HD12	1:A:199:GLY:HA3	19	0.15
(1,1125)	1:A:178:LEU:HD13	1:A:199:GLY:HA2	19	0.15
(1,1125)	1:A:178:LEU:HD13	1:A:199:GLY:HA3	19	0.15
(1,1125)	1:A:178:LEU:HD21	1:A:199:GLY:HA2	19	0.15
(1,1125)	1:A:178:LEU:HD21	1:A:199:GLY:HA3	19	0.15
(1,1125)	1:A:178:LEU:HD22	1:A:199:GLY:HA2	19	0.15
(1,1125)	1:A:178:LEU:HD22	1:A:199:GLY:HA3	19	0.15
(1,1125)	1:A:178:LEU:HD23	1:A:199:GLY:HA2	19	0.15
(1,1125)	1:A:178:LEU:HD23	1:A:199:GLY:HA3	19	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD11	8	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD12	8	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD13	8	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD21	8	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD22	8	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD23	8	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD11	16	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD12	16	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD13	16	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD21	16	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD22	16	0.15
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD23	16	0.15
(1,858)	1:A:186:ALA:HB1	1:A:187:TYR:HE1	19	0.14
(1,858)	1:A:186:ALA:HB1	1:A:187:TYR:HE2	19	0.14
(1,858)	1:A:186:ALA:HB2	1:A:187:TYR:HE1	19	0.14
(1,858)	1:A:186:ALA:HB2	1:A:187:TYR:HE2	19	0.14
(1,858)	1:A:186:ALA:HB3	1:A:187:TYR:HE1	19	0.14
(1,858)	1:A:186:ALA:HB3	1:A:187:TYR:HE2	19	0.14
(1,532)	1:A:215:ARG:HA	1:A:215:ARG:HG2	10	0.14
(1,532)	1:A:215:ARG:HA	1:A:215:ARG:HG2	15	0.14
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG21	7	0.14
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG22	7	0.14
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG23	7	0.14
(1,235)	1:A:216:TYR:H	1:A:216:TYR:HD1	8	0.14
(1,235)	1:A:216:TYR:H	1:A:216:TYR:HD2	8	0.14
(1,224)	1:A:210:LYS:HG2	1:A:213:VAL:H	18	0.14
(1,216)	1:A:207:ARG:HA	1:A:211:GLU:H	18	0.14
(1,1238)	1:A:215:ARG:HA	1:A:215:ARG:HD2	11	0.14
(1,1238)	1:A:215:ARG:HA	1:A:215:ARG:HD3	11	0.14
(1,1190)	1:A:209:VAL:HG11	1:A:210:LYS:HE2	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1190)	1:A:209:VAL:HG11	1:A:210:LYS:HE3	9	0.14
(1,1190)	1:A:209:VAL:HG12	1:A:210:LYS:HE2	9	0.14
(1,1190)	1:A:209:VAL:HG12	1:A:210:LYS:HE3	9	0.14
(1,1190)	1:A:209:VAL:HG13	1:A:210:LYS:HE2	9	0.14
(1,1190)	1:A:209:VAL:HG13	1:A:210:LYS:HE3	9	0.14
(1,1190)	1:A:209:VAL:HG21	1:A:210:LYS:HE2	9	0.14
(1,1190)	1:A:209:VAL:HG21	1:A:210:LYS:HE3	9	0.14
(1,1190)	1:A:209:VAL:HG22	1:A:210:LYS:HE2	9	0.14
(1,1190)	1:A:209:VAL:HG22	1:A:210:LYS:HE3	9	0.14
(1,1190)	1:A:209:VAL:HG23	1:A:210:LYS:HE2	9	0.14
(1,1190)	1:A:209:VAL:HG23	1:A:210:LYS:HE3	9	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	2	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	2	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	2	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	2	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	2	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	2	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	3	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	3	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	3	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	3	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	3	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	3	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	6	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	6	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	6	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	6	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	6	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	6	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	9	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	9	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	9	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	9	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	9	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	9	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	10	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	10	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	10	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	10	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	10	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	10	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	11	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	11	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	11	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	11	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	11	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	13	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	13	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	13	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	13	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	13	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	13	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	14	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	14	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	14	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	14	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	14	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	14	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	17	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	17	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	17	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	17	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	17	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	17	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	18	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	18	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	18	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	18	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	18	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	18	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	19	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	19	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	19	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	19	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	19	0.14
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	19	0.14
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD11	5	0.14
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD12	5	0.14
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD13	5	0.14
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD21	5	0.14
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD22	5	0.14
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD23	5	0.14
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG11	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG12	9	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG13	9	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG21	9	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG22	9	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG23	9	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG11	10	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG12	10	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG13	10	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG21	10	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG22	10	0.13
(1,929)	1:A:101:GLN:HG3	1:A:104:VAL:HG23	10	0.13
(1,847)	1:A:144:VAL:HA	1:A:176:ILE:HD11	4	0.13
(1,847)	1:A:144:VAL:HA	1:A:176:ILE:HD12	4	0.13
(1,847)	1:A:144:VAL:HA	1:A:176:ILE:HD13	4	0.13
(1,816)	1:A:175:THR:HB	1:A:176:ILE:HG21	2	0.13
(1,816)	1:A:175:THR:HB	1:A:176:ILE:HG22	2	0.13
(1,816)	1:A:175:THR:HB	1:A:176:ILE:HG23	2	0.13
(1,816)	1:A:175:THR:HB	1:A:176:ILE:HG21	3	0.13
(1,816)	1:A:175:THR:HB	1:A:176:ILE:HG22	3	0.13
(1,816)	1:A:175:THR:HB	1:A:176:ILE:HG23	3	0.13
(1,651)	1:A:210:LYS:HG2	1:A:214:MET:HG3	16	0.13
(1,375)	1:A:209:VAL:HG21	1:A:210:LYS:H	9	0.13
(1,375)	1:A:209:VAL:HG22	1:A:210:LYS:H	9	0.13
(1,375)	1:A:209:VAL:HG23	1:A:210:LYS:H	9	0.13
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG21	10	0.13
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG22	10	0.13
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG23	10	0.13
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG21	15	0.13
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG22	15	0.13
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG23	15	0.13
(1,1256)	1:A:217:LEU:HB2	1:A:218:GLN:H	13	0.13
(1,1256)	1:A:217:LEU:HB3	1:A:218:GLN:H	13	0.13
(1,1190)	1:A:209:VAL:HG11	1:A:210:LYS:HE2	14	0.13
(1,1190)	1:A:209:VAL:HG11	1:A:210:LYS:HE3	14	0.13
(1,1190)	1:A:209:VAL:HG12	1:A:210:LYS:HE2	14	0.13
(1,1190)	1:A:209:VAL:HG12	1:A:210:LYS:HE3	14	0.13
(1,1190)	1:A:209:VAL:HG13	1:A:210:LYS:HE2	14	0.13
(1,1190)	1:A:209:VAL:HG13	1:A:210:LYS:HE3	14	0.13
(1,1190)	1:A:209:VAL:HG21	1:A:210:LYS:HE2	14	0.13
(1,1190)	1:A:209:VAL:HG21	1:A:210:LYS:HE3	14	0.13
(1,1190)	1:A:209:VAL:HG22	1:A:210:LYS:HE2	14	0.13
(1,1190)	1:A:209:VAL:HG22	1:A:210:LYS:HE3	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1190)	1:A:209:VAL:HG23	1:A:210:LYS:HE2	14	0.13
(1,1190)	1:A:209:VAL:HG23	1:A:210:LYS:HE3	14	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	1	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	1	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	1	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	1	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	1	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	1	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	7	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	7	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	7	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	7	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	7	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	7	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	12	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	12	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	12	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	12	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	12	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	12	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	16	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	16	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	16	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	16	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	16	0.13
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	16	0.13
(1,816)	1:A:175:THR:HB	1:A:176:ILE:HG21	11	0.12
(1,816)	1:A:175:THR:HB	1:A:176:ILE:HG22	11	0.12
(1,816)	1:A:175:THR:HB	1:A:176:ILE:HG23	11	0.12
(1,768)	1:A:124:THR:H	1:A:124:THR:HG21	18	0.12
(1,768)	1:A:124:THR:H	1:A:124:THR:HG22	18	0.12
(1,768)	1:A:124:THR:H	1:A:124:THR:HG23	18	0.12
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	2	0.12
(1,532)	1:A:215:ARG:HA	1:A:215:ARG:HG2	16	0.12
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG21	13	0.12
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG22	13	0.12
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG23	13	0.12
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG21	14	0.12
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG22	14	0.12
(1,242)	1:A:218:GLN:H	1:A:219:THR:HG23	14	0.12
(1,146)	1:A:152:LEU:HB3	1:A:153:GLN:H	8	0.12
(1,1241)	1:A:215:ARG:HB2	1:A:216:TYR:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1241)	1:A:215:ARG:HB3	1:A:216:TYR:H	11	0.12
(1,1241)	1:A:215:ARG:HB2	1:A:216:TYR:H	15	0.12
(1,1241)	1:A:215:ARG:HB3	1:A:216:TYR:H	15	0.12
(1,1193)	1:A:210:LYS:H	1:A:210:LYS:HE2	18	0.12
(1,1193)	1:A:210:LYS:H	1:A:210:LYS:HE3	18	0.12
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD11	17	0.12
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD12	17	0.12
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD13	17	0.12
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD21	17	0.12
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD22	17	0.12
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD23	17	0.12
(1,946)	1:A:104:VAL:HG11	1:A:107:LEU:HB2	17	0.11
(1,946)	1:A:104:VAL:HG11	1:A:107:LEU:HB3	17	0.11
(1,946)	1:A:104:VAL:HG12	1:A:107:LEU:HB2	17	0.11
(1,946)	1:A:104:VAL:HG12	1:A:107:LEU:HB3	17	0.11
(1,946)	1:A:104:VAL:HG13	1:A:107:LEU:HB2	17	0.11
(1,946)	1:A:104:VAL:HG13	1:A:107:LEU:HB3	17	0.11
(1,946)	1:A:104:VAL:HG21	1:A:107:LEU:HB2	17	0.11
(1,946)	1:A:104:VAL:HG21	1:A:107:LEU:HB3	17	0.11
(1,946)	1:A:104:VAL:HG22	1:A:107:LEU:HB2	17	0.11
(1,946)	1:A:104:VAL:HG22	1:A:107:LEU:HB3	17	0.11
(1,946)	1:A:104:VAL:HG23	1:A:107:LEU:HB2	17	0.11
(1,946)	1:A:104:VAL:HG23	1:A:107:LEU:HB3	17	0.11
(1,847)	1:A:144:VAL:HA	1:A:176:ILE:HD11	12	0.11
(1,847)	1:A:144:VAL:HA	1:A:176:ILE:HD12	12	0.11
(1,847)	1:A:144:VAL:HA	1:A:176:ILE:HD13	12	0.11
(1,696)	1:A:106:TYR:HD1	1:A:107:LEU:HA	9	0.11
(1,696)	1:A:106:TYR:HD2	1:A:107:LEU:HA	9	0.11
(1,644)	1:A:176:ILE:HG21	1:A:212:ALA:HA	16	0.11
(1,644)	1:A:176:ILE:HG22	1:A:212:ALA:HA	16	0.11
(1,644)	1:A:176:ILE:HG23	1:A:212:ALA:HA	16	0.11
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	1	0.11
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	3	0.11
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	7	0.11
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	9	0.11
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	10	0.11
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	11	0.11
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	13	0.11
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	14	0.11
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	16	0.11
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	17	0.11
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,616)	1:A:162:LEU:HA	1:A:167:GLU:H	19	0.11
(1,375)	1:A:209:VAL:HG21	1:A:210:LYS:H	14	0.11
(1,375)	1:A:209:VAL:HG22	1:A:210:LYS:H	14	0.11
(1,375)	1:A:209:VAL:HG23	1:A:210:LYS:H	14	0.11
(1,1256)	1:A:217:LEU:HB2	1:A:218:GLN:H	7	0.11
(1,1256)	1:A:217:LEU:HB3	1:A:218:GLN:H	7	0.11
(1,1241)	1:A:215:ARG:HB2	1:A:216:TYR:H	10	0.11
(1,1241)	1:A:215:ARG:HB3	1:A:216:TYR:H	10	0.11
(1,1212)	1:A:212:ALA:H	1:A:215:ARG:HD2	15	0.11
(1,1212)	1:A:212:ALA:H	1:A:215:ARG:HD3	15	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	4	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	4	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	4	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	4	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	4	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	4	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	5	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	5	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	5	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	5	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	5	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	5	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	8	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	8	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	8	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	8	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	8	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	8	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD11	15	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD12	15	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD13	15	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD21	15	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD22	15	0.11
(1,1093)	1:A:162:LEU:HA	1:A:162:LEU:HD23	15	0.11
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD11	2	0.11
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD12	2	0.11
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD13	2	0.11
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD21	2	0.11
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD22	2	0.11
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD23	2	0.11
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD11	10	0.11
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD12	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD13	10	0.11
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD21	10	0.11
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD22	10	0.11
(1,1057)	1:A:151:PHE:H	1:A:152:LEU:HD23	10	0.11

10 Dihedral-angle violation analysis (i)

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