Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 07:29 pm BST

PDB ID	:	7NM2
BMRB ID	:	34603
Title	:	Solution structure of MLKL executioner domain in complex with a fragment
Authors	:	Ruebbelke, M.; Bauer, M.; Hamilton, J.; Binder, F.; Nar, H.; Zeeb, M.
Deposited on	:	2021-02-23

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

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

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

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

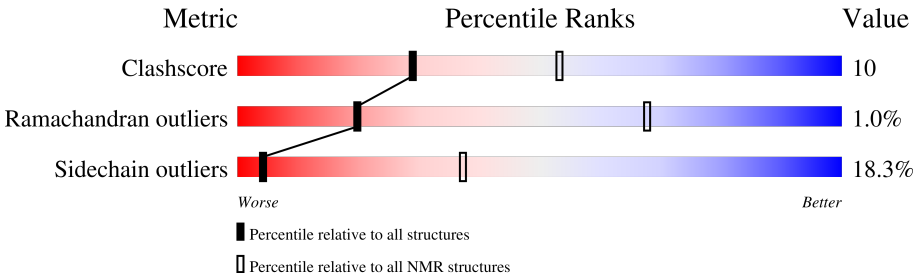
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 78%.

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	157	56% 24% • 18%

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:2-A:47, A:53-A:89, A:96-A:124, A:132-A:148 (129)	0.62	15

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

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

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

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2608 atoms, of which 1315 are hydrogens and 0 are deuteriums.

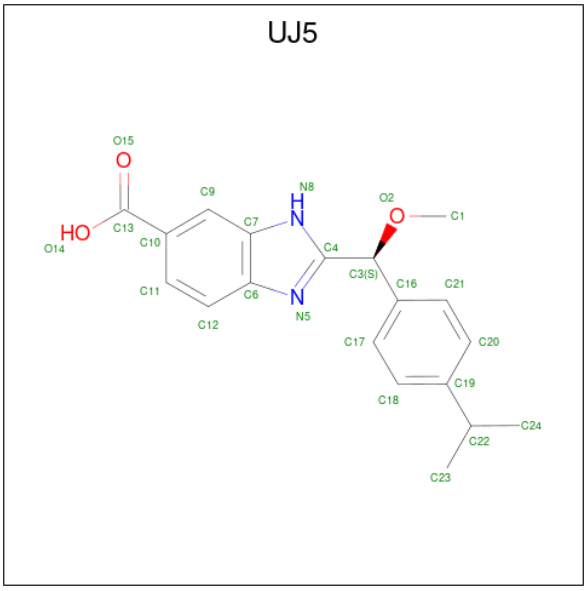
- Molecule 1 is a protein called Mixed lineage kinase domain-like protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	157	2564	786	1295	239	235	9	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8NB16
A	-1	SER	-	expression tag	UNP Q8NB16
A	0	PRO	-	expression tag	UNP Q8NB16
A	1	GLY	-	expression tag	UNP Q8NB16

- Molecule 2 is 2-[({S})-methoxy-(4-propan-2-ylphenyl)methyl]-3 {H}-benzimidazole-5-carb oxylic acid (three-letter code: UJ5) (formula: $C_{19}H_{20}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



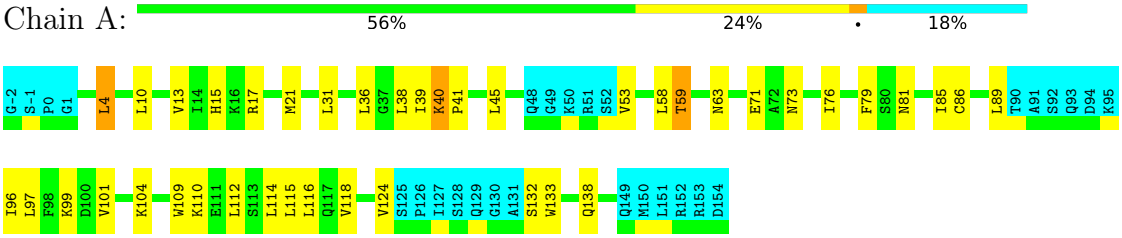
Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
2	A	1	44	19	20	2	3

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: Mixed lineage kinase domain-like protein

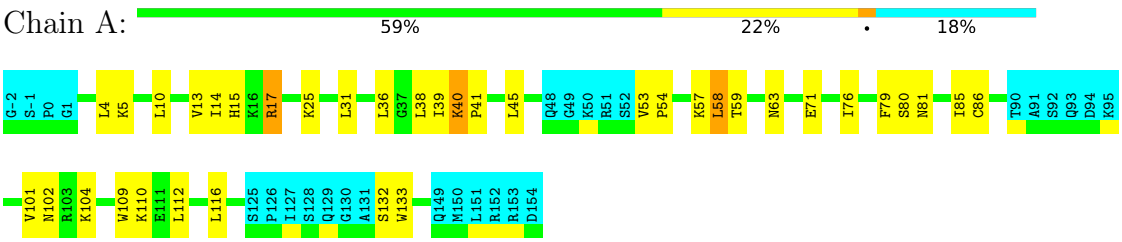


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

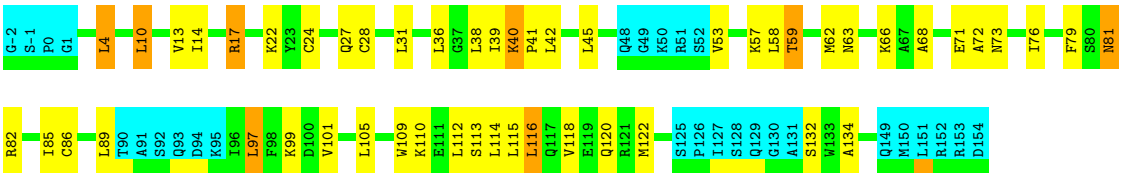
4.2.1 Score per residue for model 1

• Molecule 1: Mixed lineage kinase domain-like protein



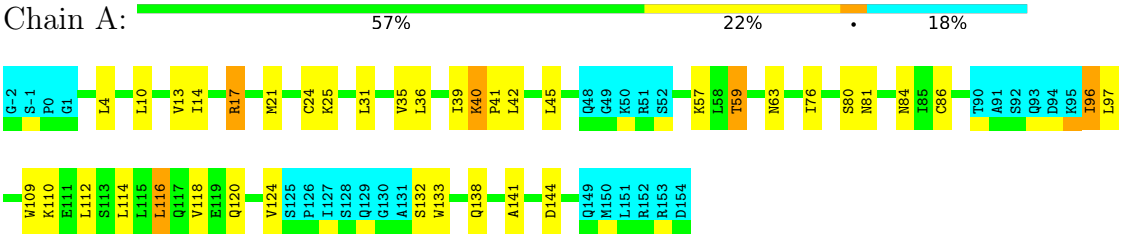
4.2.2 Score per residue for model 2

• Molecule 1: Mixed lineage kinase domain-like protein



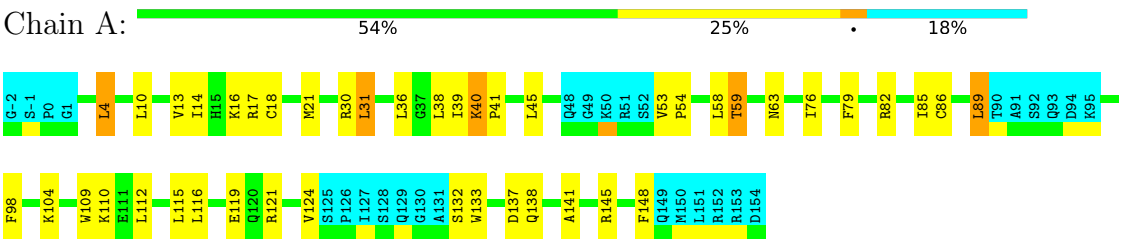
4.2.3 Score per residue for model 3

• Molecule 1: Mixed lineage kinase domain-like protein



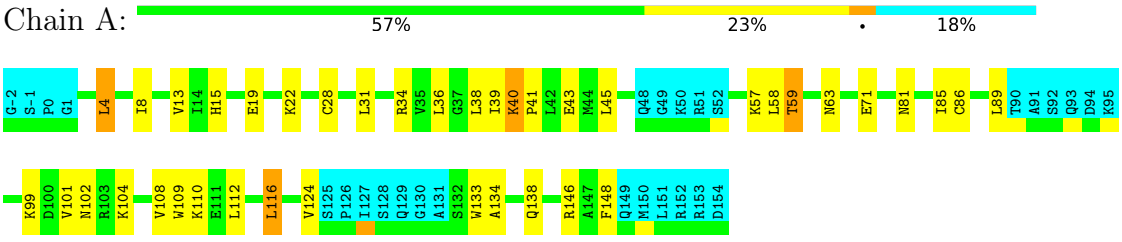
4.2.4 Score per residue for model 4

• Molecule 1: Mixed lineage kinase domain-like protein



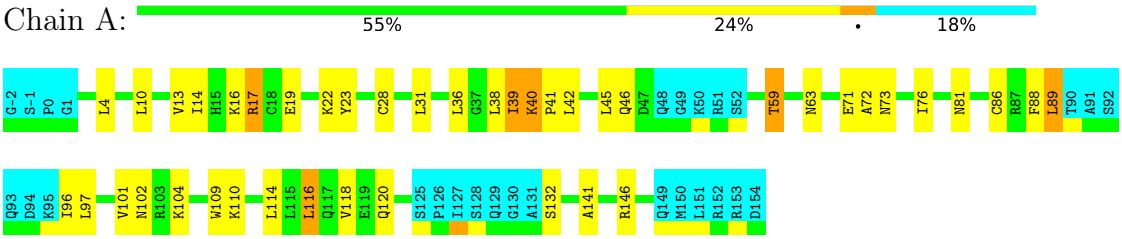
4.2.5 Score per residue for model 5

• Molecule 1: Mixed lineage kinase domain-like protein



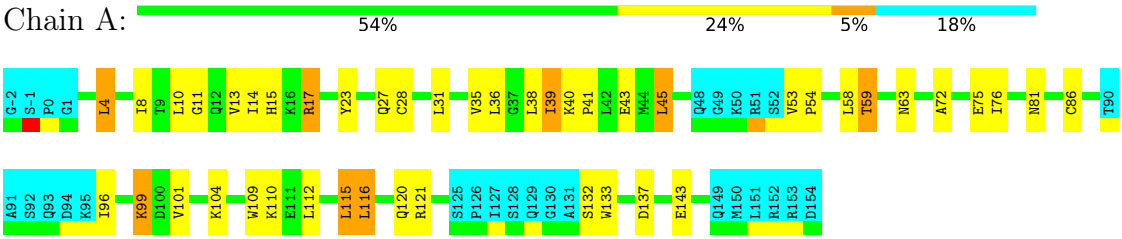
4.2.6 Score per residue for model 6

• Molecule 1: Mixed lineage kinase domain-like protein



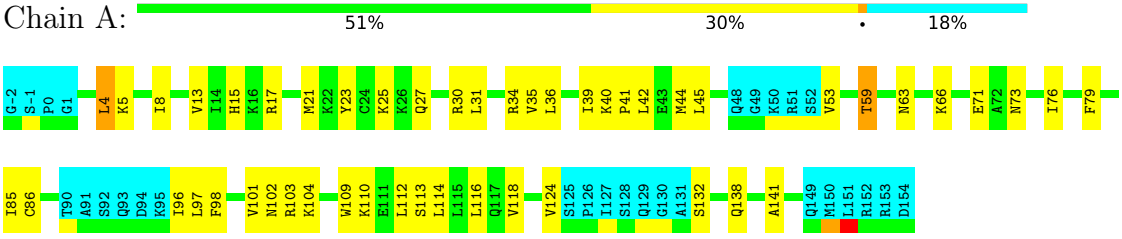
4.2.7 Score per residue for model 7

• Molecule 1: Mixed lineage kinase domain-like protein



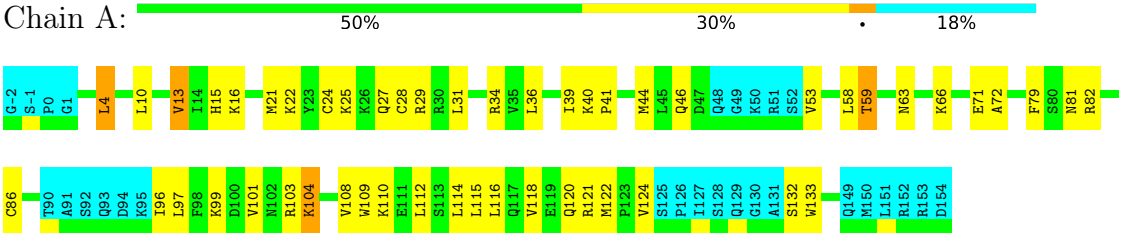
4.2.8 Score per residue for model 8

• Molecule 1: Mixed lineage kinase domain-like protein



4.2.9 Score per residue for model 9

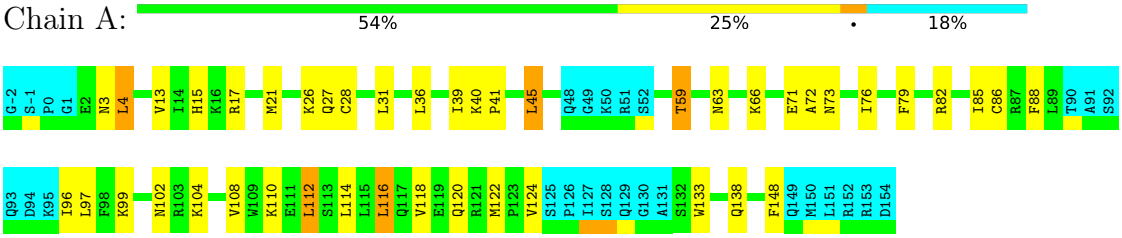
• Molecule 1: Mixed lineage kinase domain-like protein



4.2.10 Score per residue for model 10

• Molecule 1: Mixed lineage kinase domain-like protein

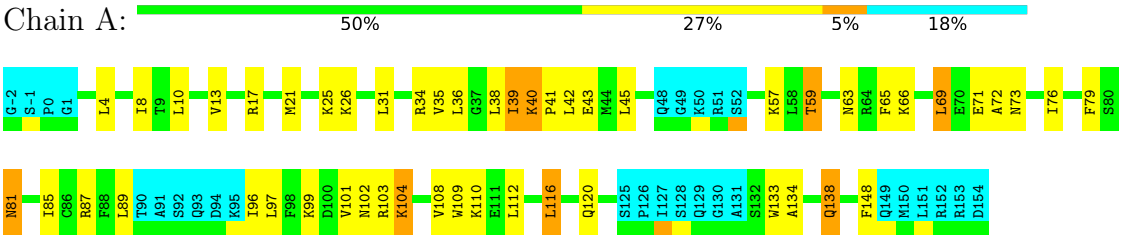
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Mixed lineage kinase domain-like protein

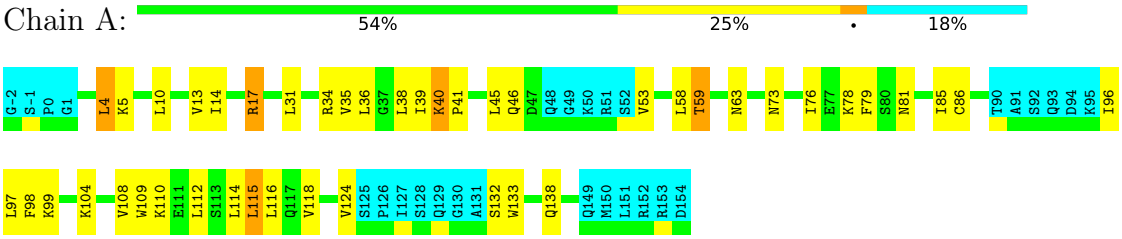
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Mixed lineage kinase domain-like protein

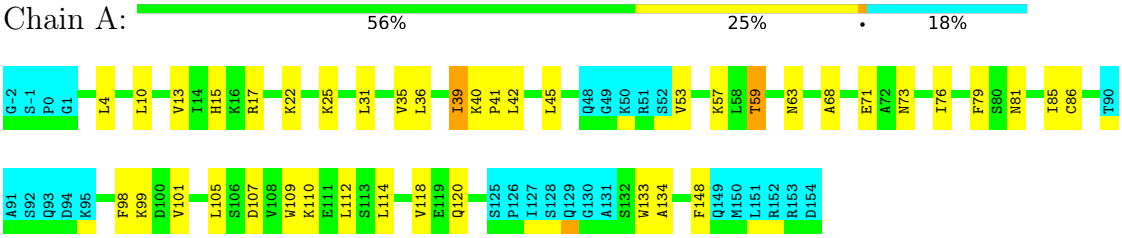
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Mixed lineage kinase domain-like protein

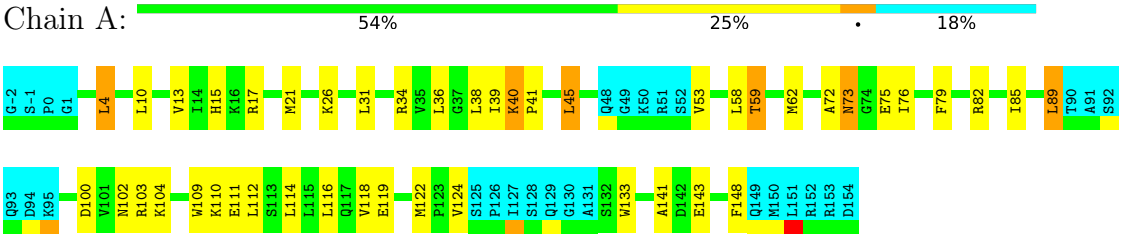
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Mixed lineage kinase domain-like protein

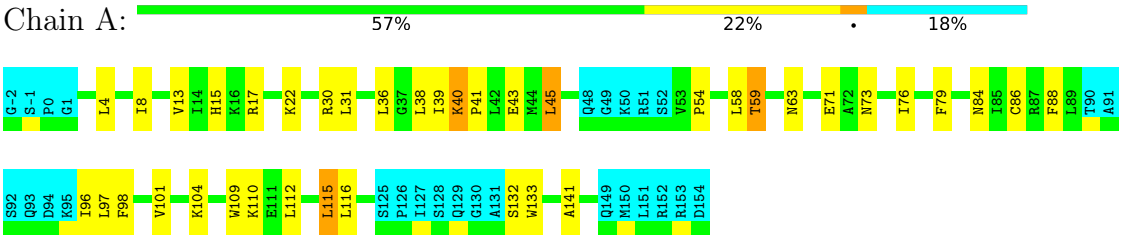
Chain A:



4.2.15 Score per residue for model 15 (medoid)

• Molecule 1: Mixed lineage kinase domain-like protein

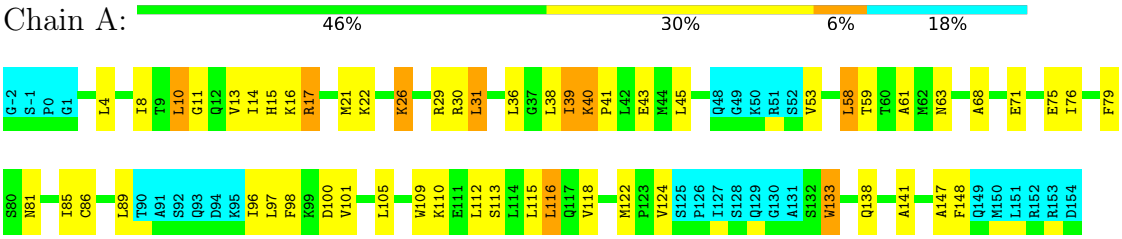
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Mixed lineage kinase domain-like protein

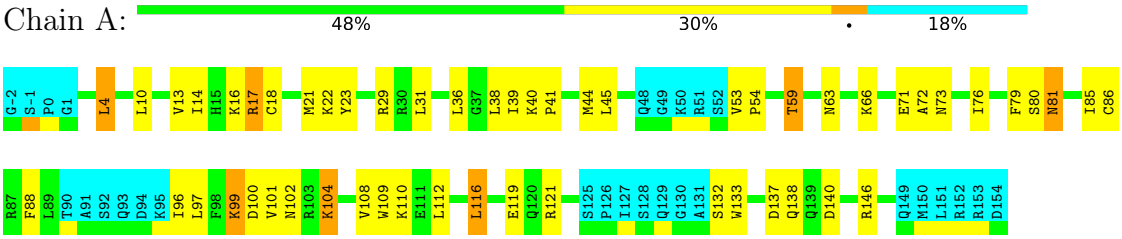
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Mixed lineage kinase domain-like protein

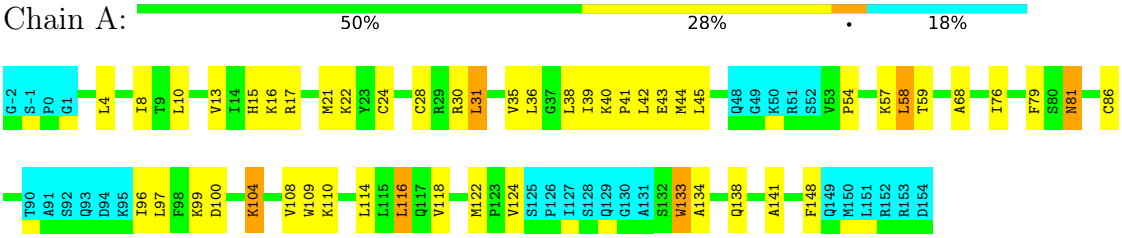
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Mixed lineage kinase domain-like protein

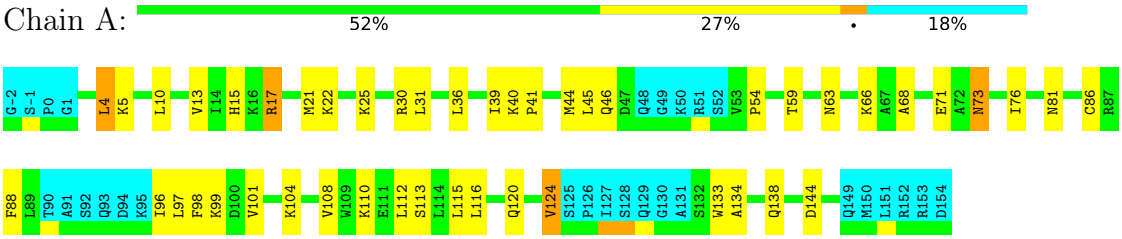
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Mixed lineage kinase domain-like protein

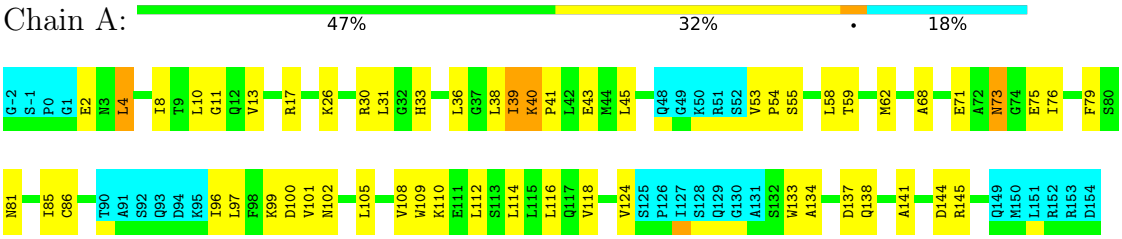
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Mixed lineage kinase domain-like protein

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	3.98.9

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	1730
Number of shifts mapped to atoms	1730
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UJ5

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	1065	1091	1091	22±5
2	A	24	20	0	2±1
All	All	21780	22220	21820	450

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:ILE:HG23	1:A:76:ILE:HD11	0.96	1.36	6	9
1:A:58:LEU:HD13	1:A:115:LEU:HD11	0.95	1.35	7	2
1:A:89:LEU:HD21	1:A:97:LEU:HD11	0.69	1.62	2	2
1:A:53:VAL:HG21	2:A:201:UJ5:C12	0.66	2.20	13	5
1:A:79:PHE:CE2	1:A:97:LEU:HD22	0.66	2.25	15	5
1:A:99:LYS:HE3	1:A:134:ALA:HB1	0.66	1.67	20	6
1:A:114:LEU:O	1:A:118:VAL:HG23	0.64	1.92	9	7
1:A:42:LEU:HD11	1:A:109:TRP:CZ3	0.64	2.28	3	3
1:A:40:LYS:N	1:A:41:PRO:HD2	0.64	2.08	10	20
1:A:31:LEU:HD11	1:A:72:ALA:HB1	0.63	1.71	2	4
1:A:71:GLU:CG	1:A:101:VAL:HG22	0.63	2.23	6	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:TRP:CE3	1:A:112:LEU:HD11	0.63	2.28	16	11
1:A:14:ILE:HG23	1:A:76:ILE:CD1	0.63	2.22	2	7
1:A:31:LEU:HD13	1:A:102:ASN:ND2	0.62	2.09	17	4
1:A:99:LYS:CE	1:A:134:ALA:HB1	0.62	2.24	19	3
1:A:38:LEU:HD22	1:A:109:TRP:CG	0.62	2.30	2	11
1:A:17:ARG:HB3	1:A:76:ILE:HG21	0.61	1.72	1	10
1:A:88:PHE:CD1	1:A:97:LEU:HD23	0.61	2.30	17	4
1:A:58:LEU:HD13	1:A:115:LEU:HD21	0.61	1.73	2	1
1:A:116:LEU:HD23	1:A:120:GLN:CB	0.61	2.26	2	3
1:A:79:PHE:CE2	1:A:97:LEU:HD23	0.60	2.31	8	5
1:A:73:ASN:HA	1:A:76:ILE:HD12	0.60	1.73	2	9
1:A:53:VAL:HG21	2:A:201:UJ5:C6	0.60	2.26	4	6
1:A:31:LEU:HD13	1:A:102:ASN:OD1	0.59	1.96	10	4
1:A:71:GLU:HG2	1:A:101:VAL:HG22	0.59	1.75	5	8
1:A:53:VAL:HG23	1:A:58:LEU:HD23	0.59	1.74	12	1
1:A:17:ARG:HB3	1:A:76:ILE:HD13	0.59	1.75	7	3
1:A:10:LEU:O	1:A:13:VAL:HG12	0.59	1.98	16	12
1:A:54:PRO:HG3	1:A:58:LEU:HD13	0.58	1.76	18	2
1:A:58:LEU:HG	1:A:115:LEU:HD11	0.58	1.75	15	1
1:A:116:LEU:HD23	1:A:120:GLN:HB2	0.58	1.73	2	4
1:A:96:ILE:HD12	1:A:99:LYS:HD3	0.58	1.75	11	5
1:A:53:VAL:HG13	2:A:201:UJ5:C12	0.58	2.29	9	2
1:A:54:PRO:CG	1:A:58:LEU:HD13	0.57	2.29	18	2
1:A:41:PRO:O	1:A:45:LEU:HD23	0.57	2.00	16	6
1:A:113:SER:O	1:A:124:VAL:HG11	0.57	1.98	8	1
1:A:4:LEU:HD11	2:A:201:UJ5:C20	0.57	2.29	5	3
1:A:59:THR:HG23	2:A:201:UJ5:N5	0.57	2.15	5	13
1:A:24:CYS:HB2	1:A:85:ILE:HD12	0.57	1.76	2	1
1:A:79:PHE:O	1:A:85:ILE:HD11	0.57	2.00	2	12
1:A:96:ILE:HD11	1:A:138:GLN:CA	0.57	2.30	11	1
1:A:96:ILE:HD13	1:A:137:ASP:CG	0.57	2.21	7	1
1:A:99:LYS:HE2	1:A:134:ALA:HB1	0.56	1.78	13	2
1:A:27:GLN:CD	1:A:96:ILE:HG23	0.56	2.21	8	1
1:A:62:MET:CE	1:A:112:LEU:HD13	0.56	2.30	20	1
1:A:79:PHE:CD2	1:A:97:LEU:HD23	0.56	2.35	18	3
1:A:109:TRP:CZ3	1:A:112:LEU:HD11	0.55	2.37	1	9
1:A:68:ALA:HB1	1:A:105:LEU:HD23	0.55	1.78	13	4
1:A:96:ILE:HD12	1:A:99:LYS:CD	0.55	2.32	10	2
1:A:53:VAL:HG21	2:A:201:UJ5:C7	0.55	2.31	17	1
1:A:71:GLU:HG3	1:A:101:VAL:HG22	0.54	1.79	13	8
1:A:104:LYS:O	1:A:108:VAL:HG13	0.54	2.01	19	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ILE:HG12	1:A:141:ALA:HB2	0.54	1.78	6	5
1:A:4:LEU:HD21	2:A:201:UJ5:C21	0.54	2.33	20	2
1:A:96:ILE:HD12	1:A:99:LYS:HD2	0.53	1.79	7	2
1:A:40:LYS:N	1:A:41:PRO:CD	0.53	2.71	10	19
1:A:96:ILE:HD11	1:A:138:GLN:HA	0.53	1.81	11	2
1:A:108:VAL:O	1:A:112:LEU:HD23	0.53	2.03	10	2
1:A:8:ILE:HD12	1:A:43:GLU:CD	0.53	2.23	20	3
1:A:39:ILE:HD13	1:A:40:LYS:N	0.53	2.19	11	3
1:A:53:VAL:HG13	2:A:201:UJ5:C9	0.53	2.33	8	2
1:A:114:LEU:O	1:A:118:VAL:HG13	0.53	2.04	18	4
1:A:58:LEU:HD22	2:A:201:UJ5:C17	0.53	2.34	15	1
1:A:59:THR:HG23	2:A:201:UJ5:N8	0.52	2.20	17	1
1:A:59:THR:HG23	2:A:201:UJ5:C7	0.52	2.35	8	1
1:A:112:LEU:HD12	1:A:113:SER:N	0.51	2.21	16	2
1:A:65:PHE:O	1:A:69:LEU:HD22	0.51	2.05	11	1
1:A:68:ALA:CB	1:A:108:VAL:HG21	0.51	2.35	18	1
1:A:85:ILE:HG22	1:A:89:LEU:HD13	0.51	1.81	14	1
1:A:4:LEU:HD11	2:A:201:UJ5:C17	0.51	2.35	9	1
1:A:31:LEU:O	1:A:35:VAL:HG13	0.51	2.06	13	2
1:A:58:LEU:HD12	1:A:115:LEU:CD1	0.51	2.36	16	1
1:A:116:LEU:HD22	1:A:122:MET:HB3	0.50	1.82	2	1
1:A:8:ILE:HD12	1:A:43:GLU:OE1	0.50	2.06	5	2
1:A:59:THR:HG23	2:A:201:UJ5:C4	0.50	2.36	9	2
1:A:31:LEU:HD12	1:A:98:PHE:CG	0.50	2.42	16	2
1:A:59:THR:HG23	2:A:201:UJ5:C6	0.50	2.36	3	2
1:A:122:MET:CE	1:A:124:VAL:HG12	0.50	2.37	14	5
1:A:42:LEU:HD11	1:A:116:LEU:HD11	0.49	1.83	2	1
1:A:24:CYS:SG	1:A:97:LEU:HD11	0.49	2.47	3	1
1:A:85:ILE:HG22	1:A:89:LEU:HD11	0.49	1.83	5	1
1:A:42:LEU:CD2	1:A:116:LEU:HD11	0.49	2.36	6	1
1:A:13:VAL:HG22	1:A:17:ARG:CD	0.49	2.37	1	1
1:A:38:LEU:HD11	1:A:133:TRP:CH2	0.49	2.43	16	1
1:A:24:CYS:SG	1:A:97:LEU:HD13	0.49	2.47	2	3
1:A:13:VAL:HG22	1:A:17:ARG:HD3	0.49	1.83	16	1
1:A:112:LEU:CD1	1:A:116:LEU:HD12	0.49	2.37	19	1
1:A:8:ILE:HD12	1:A:43:GLU:OE2	0.49	2.07	16	4
1:A:4:LEU:HD22	1:A:46:GLN:HB3	0.49	1.83	12	1
1:A:8:ILE:HD12	1:A:43:GLU:HG3	0.49	1.85	18	1
1:A:88:PHE:CD1	1:A:97:LEU:HD12	0.49	2.42	19	1
1:A:54:PRO:HG2	1:A:58:LEU:HD22	0.49	1.84	18	2
1:A:11:GLY:HA3	1:A:39:ILE:HG21	0.49	1.84	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:HD21	1:A:72:ALA:HB1	0.49	1.83	11	4
1:A:4:LEU:HD11	2:A:201:UJ5:C18	0.48	2.37	12	3
1:A:96:ILE:CG1	1:A:141:ALA:HB2	0.48	2.38	20	2
1:A:104:LYS:O	1:A:108:VAL:HG22	0.48	2.08	18	3
1:A:116:LEU:HD23	1:A:120:GLN:HB3	0.48	1.86	3	1
1:A:53:VAL:HG13	2:A:201:UJ5:C10	0.48	2.39	16	1
1:A:58:LEU:HD12	1:A:115:LEU:HD13	0.48	1.84	16	1
1:A:58:LEU:HD13	1:A:115:LEU:CD2	0.48	2.38	2	1
1:A:116:LEU:HD22	1:A:122:MET:CB	0.48	2.39	2	1
1:A:35:VAL:HA	1:A:38:LEU:HD12	0.48	1.85	7	2
1:A:68:ALA:HB2	1:A:108:VAL:HG11	0.48	1.85	19	1
1:A:4:LEU:HD21	2:A:201:UJ5:C17	0.47	2.39	4	2
1:A:89:LEU:CD2	1:A:97:LEU:HD21	0.47	2.38	6	1
1:A:115:LEU:HD12	1:A:115:LEU:O	0.47	2.09	2	1
1:A:45:LEU:HD21	1:A:122:MET:HG3	0.47	1.84	14	1
1:A:45:LEU:CD2	1:A:116:LEU:HD21	0.47	2.40	11	2
1:A:96:ILE:HG22	1:A:98:PHE:H	0.47	1.69	12	3
1:A:58:LEU:HD21	1:A:62:MET:HE2	0.47	1.87	14	1
1:A:58:LEU:HA	1:A:115:LEU:HD13	0.47	1.85	9	1
1:A:115:LEU:HD22	1:A:119:GLU:OE1	0.47	2.10	4	1
1:A:96:ILE:HG13	1:A:141:ALA:HB2	0.47	1.86	18	2
1:A:17:ARG:CG	1:A:76:ILE:HG21	0.46	2.39	19	1
1:A:89:LEU:HD22	1:A:148:PHE:CD2	0.46	2.45	4	1
1:A:115:LEU:HD12	1:A:116:LEU:N	0.46	2.25	19	2
1:A:31:LEU:O	1:A:35:VAL:HG12	0.46	2.10	18	2
1:A:75:GLU:OE1	1:A:101:VAL:HG21	0.46	2.10	7	1
1:A:112:LEU:HA	1:A:115:LEU:HD23	0.46	1.87	15	2
1:A:61:ALA:CB	1:A:115:LEU:HD21	0.46	2.41	16	1
1:A:89:LEU:HD12	1:A:148:PHE:CD2	0.46	2.45	16	1
1:A:85:ILE:HG22	1:A:89:LEU:CD1	0.45	2.41	5	1
1:A:58:LEU:HD21	2:A:201:UJ5:C18	0.45	2.42	7	1
1:A:113:SER:HB2	1:A:124:VAL:HG11	0.45	1.89	19	1
1:A:96:ILE:HD11	1:A:138:GLN:N	0.45	2.26	11	1
1:A:45:LEU:HD21	1:A:120:GLN:HG2	0.45	1.88	6	1
1:A:31:LEU:HD22	1:A:98:PHE:CG	0.45	2.47	15	2
1:A:116:LEU:HD21	2:A:201:UJ5:C24	0.44	2.42	17	1
1:A:4:LEU:HD12	1:A:46:GLN:OE1	0.44	2.13	19	1
1:A:116:LEU:HD23	1:A:120:GLN:HG3	0.44	1.90	9	1
1:A:42:LEU:HD22	1:A:116:LEU:HD11	0.43	1.87	11	2
1:A:79:PHE:CZ	1:A:97:LEU:HD23	0.43	2.48	2	1
1:A:113:SER:HB2	1:A:124:VAL:HG21	0.43	1.89	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:MET:HE1	1:A:112:LEU:HD13	0.43	1.89	20	1
1:A:26:LYS:HE2	1:A:147:ALA:HB2	0.43	1.88	16	1
1:A:24:CYS:SG	1:A:97:LEU:HD22	0.43	2.53	18	1
1:A:31:LEU:HD12	1:A:98:PHE:CD1	0.42	2.49	4	2
1:A:58:LEU:HD12	1:A:58:LEU:O	0.42	2.14	7	1
1:A:31:LEU:HD23	1:A:102:ASN:HB3	0.42	1.92	6	1
1:A:13:VAL:HG22	1:A:16:LYS:HE2	0.41	1.92	9	1
1:A:31:LEU:HD12	1:A:31:LEU:O	0.41	2.15	14	1
1:A:5:LYS:HD3	1:A:8:ILE:HD11	0.41	1.91	8	1
1:A:41:PRO:HG2	1:A:42:LEU:HD12	0.41	1.91	3	1
1:A:17:ARG:HH21	1:A:76:ILE:HG22	0.41	1.75	15	1
1:A:40:LYS:HB3	1:A:41:PRO:HD3	0.41	1.92	19	3
1:A:31:LEU:HD22	1:A:98:PHE:CB	0.41	2.46	8	1
1:A:4:LEU:HD22	1:A:46:GLN:CG	0.41	2.46	12	1
1:A:17:ARG:CB	1:A:76:ILE:HG21	0.41	2.46	7	1
1:A:35:VAL:HG12	1:A:105:LEU:HD13	0.41	1.93	13	1
1:A:31:LEU:O	1:A:31:LEU:HD12	0.41	2.16	20	1
1:A:79:PHE:CZ	1:A:97:LEU:HD22	0.41	2.51	10	1
1:A:38:LEU:HD11	1:A:133:TRP:HH2	0.41	1.76	18	1
1:A:86:CYS:HA	1:A:89:LEU:HD12	0.40	1.93	5	1
1:A:115:LEU:HA	1:A:118:VAL:HG22	0.40	1.93	16	1
1:A:96:ILE:HD13	1:A:137:ASP:OD2	0.40	2.16	17	1
1:A:14:ILE:HG21	1:A:31:LEU:CD1	0.40	2.46	6	1
1:A:88:PHE:CE1	1:A:97:LEU:HD23	0.40	2.51	6	1
1:A:89:LEU:HD13	1:A:148:PHE:CG	0.40	2.52	5	1
1:A:122:MET:HE3	1:A:124:VAL:HG12	0.40	1.93	16	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	129/157 (82%)	120±2 (93±2%)	8±2 (6±2%)	1±1 (1±1%)	20	68
All	All	2580/3140 (82%)	2393 (93%)	162 (6%)	25 (1%)	20	68

All 5 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	21	MET	9
1	A	81	ASN	7
1	A	54	PRO	6
1	A	124	VAL	2
1	A	96	ILE	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	118/140 (84%)	96±2 (82±2%)	22±2 (18±2%)	4	37
All	All	2360/2800 (84%)	1927 (82%)	433 (18%)	4	37

All 72 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	4	LEU	20
1	A	36	LEU	20
1	A	39	ILE	20
1	A	110	LYS	20
1	A	59	THR	18
1	A	63	ASN	17
1	A	116	LEU	17
1	A	133	TRP	17
1	A	17	ARG	14
1	A	45	LEU	13
1	A	15	HIS	12
1	A	40	LYS	12
1	A	104	LYS	12
1	A	81	ASN	12
1	A	132	SER	11
1	A	138	GLN	11
1	A	22	LYS	9
1	A	13	VAL	8
1	A	25	LYS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	57	LYS	7
1	A	28	CYS	7
1	A	66	LYS	7
1	A	30	ARG	7
1	A	58	LEU	6
1	A	10	LEU	6
1	A	31	LEU	6
1	A	34	ARG	6
1	A	73	ASN	6
1	A	82	ARG	5
1	A	16	LYS	5
1	A	44	MET	5
1	A	26	LYS	5
1	A	100	ASP	5
1	A	27	GLN	4
1	A	124	VAL	4
1	A	121	ARG	4
1	A	103	ARG	4
1	A	5	LYS	3
1	A	80	SER	3
1	A	144	ASP	3
1	A	89	LEU	3
1	A	146	ARG	3
1	A	115	LEU	3
1	A	29	ARG	3
1	A	75	GLU	3
1	A	35	VAL	2
1	A	84	ASN	2
1	A	18	CYS	2
1	A	137	ASP	2
1	A	145	ARG	2
1	A	19	GLU	2
1	A	112	LEU	2
1	A	46	GLN	2
1	A	99	LYS	2
1	A	143	GLU	2
1	A	120	GLN	2
1	A	119	GLU	2
1	A	21	MET	2
1	A	62	MET	1
1	A	97	LEU	1
1	A	23	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	3	ASN	1
1	A	71	GLU	1
1	A	69	LEU	1
1	A	87	ARG	1
1	A	78	LYS	1
1	A	107	ASP	1
1	A	111	GLU	1
1	A	140	ASP	1
1	A	2	GLU	1
1	A	33	HIS	1
1	A	55	SER	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

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	UJ5	A	201	-	23,26,26	0.73±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	UJ5	A	201	-	27,37,37	0.95±0.00	0±0 (0±1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UJ5	A	201	-	-	0±0,14,18,18	0±0,3,3,3

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	201	UJ5	O14-C13-C10	2.01	120.06	114.85	10	3

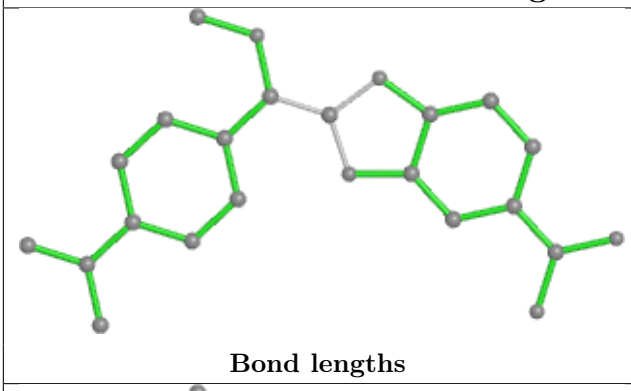
There are no chirality outliers.

There are no torsion outliers.

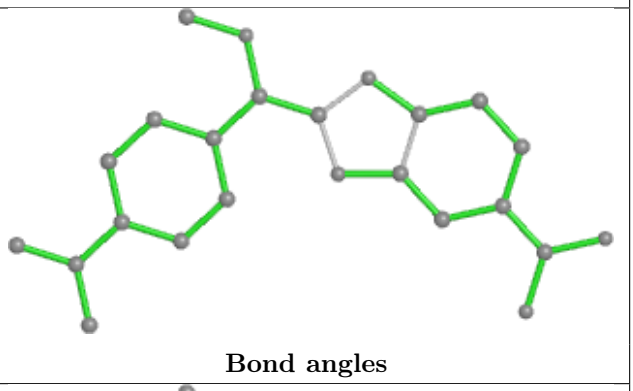
There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

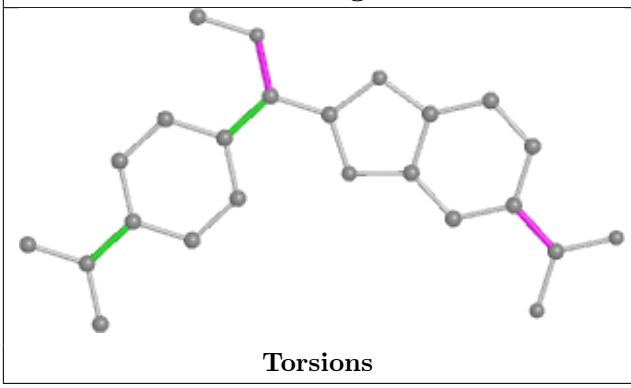
Ligand UJ5 A 201



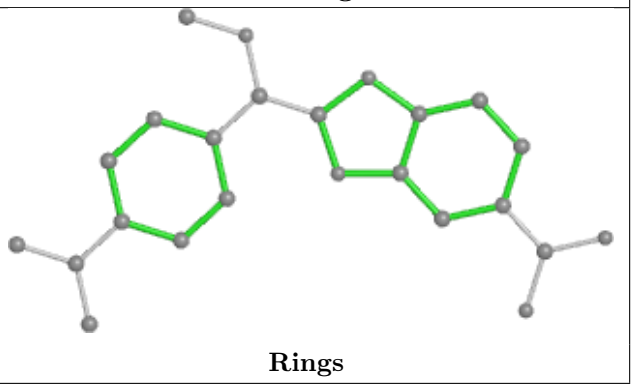
Bond lengths



Bond angles



Torsions



Rings

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 78% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *molecule_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	1730
Number of shifts mapped to atoms	1730
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
$^{13}C_{\alpha}$	154	-0.45 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	139	0.20 ± 0.06	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	141	-0.01 ± 0.24	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 78%, i.e. 1475 atoms were assigned a chemical shift out of a possible 1887. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	498/643 (77%)	251/259 (97%)	127/258 (49%)	120/126 (95%)
Sidechain	911/1140 (80%)	621/732 (85%)	279/349 (80%)	11/59 (19%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	66/104 (63%)	33/53 (62%)	31/46 (67%)	2/5 (40%)
Overall	1475/1887 (78%)	905/1044 (87%)	437/653 (67%)	133/190 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1730 atoms were assigned a chemical shift out of a possible 2238. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	598/783 (76%)	303/317 (96%)	154/314 (49%)	141/152 (93%)
Sidechain	1066/1351 (79%)	726/866 (84%)	325/411 (79%)	15/74 (20%)
Aromatic	66/104 (63%)	33/53 (62%)	31/46 (67%)	2/5 (40%)
Overall	1730/2238 (77%)	1062/1236 (86%)	510/771 (66%)	158/231 (68%)

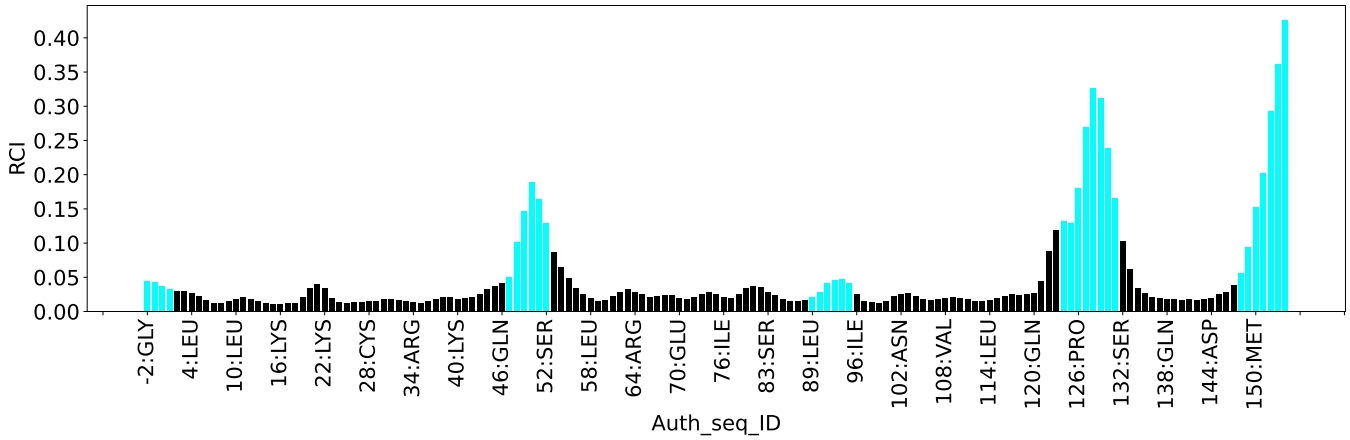
7.1.4 Statistically unusual chemical shifts (i)

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	2580
Intra-residue (|i-j|=0)	609
Sequential (|i-j|=1)	566
Medium range (|i-j|>1 and |i-j|<5)	725
Long range (|i-j|≥5)	680
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	64
Number of restraints per residue	16.4
Number of long range restraints per residue[1]	4.3

[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)	8.2	0.2
0.2-0.5 (Medium)	3.3	0.49
>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)

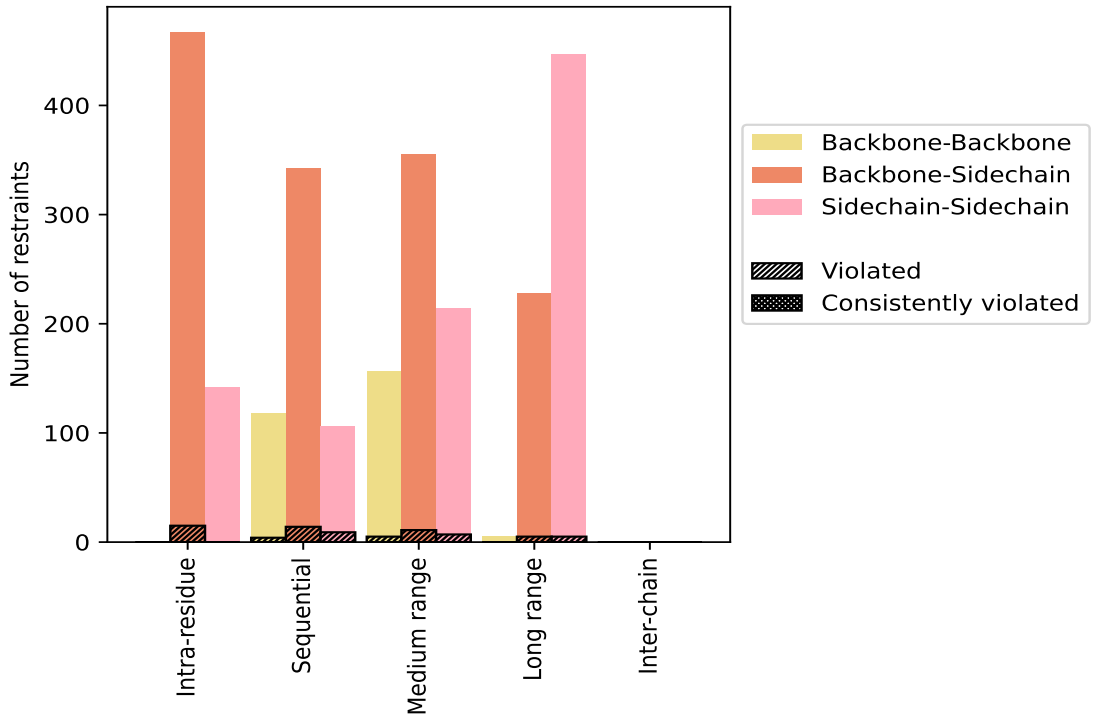
9.1 Summary of distance violations (i)

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)	609	23.6	15	2.5	0.6	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	467	18.1	15	3.2	0.6	0	0.0	0.0
Sidechain-Sidechain	142	5.5	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	566	21.9	27	4.8	1.0	0	0.0	0.0
Backbone-Backbone	118	4.6	4	3.4	0.2	0	0.0	0.0
Backbone-Sidechain	342	13.3	14	4.1	0.5	0	0.0	0.0
Sidechain-Sidechain	106	4.1	9	8.5	0.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	725	28.1	23	3.2	0.9	0	0.0	0.0
Backbone-Backbone	156	6.0	5	3.2	0.2	0	0.0	0.0
Backbone-Sidechain	355	13.8	11	3.1	0.4	0	0.0	0.0
Sidechain-Sidechain	214	8.3	7	3.3	0.3	0	0.0	0.0
Long range (|i-j|≥5)	680	26.4	10	1.5	0.4	0	0.0	0.0
Backbone-Backbone	5	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	228	8.8	5	2.2	0.2	0	0.0	0.0
Sidechain-Sidechain	447	17.3	5	1.1	0.2	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	2580	100.0	75	2.9	2.9	0	0.0	0.0
Backbone-Backbone	279	10.8	9	3.2	0.3	0	0.0	0.0
Backbone-Sidechain	1392	54.0	45	3.2	1.7	0	0.0	0.0
Sidechain-Sidechain	909	35.2	21	2.3	0.8	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	2	1	5	2	0	10	0.19	0.48	0.11	0.15
2	3	5	5	2	0	15	0.19	0.31	0.06	0.17
3	2	2	3	1	0	8	0.16	0.25	0.05	0.15
4	3	1	2	0	0	6	0.19	0.48	0.13	0.14
5	3	3	5	1	0	12	0.2	0.41	0.08	0.18
6	2	4	4	0	0	10	0.18	0.39	0.08	0.15
7	0	3	3	1	0	7	0.18	0.27	0.05	0.14
8	3	4	6	1	0	14	0.18	0.28	0.05	0.16
9	2	5	9	1	0	17	0.19	0.49	0.11	0.14
10	2	6	3	1	0	12	0.17	0.34	0.06	0.16
11	2	4	5	2	0	13	0.18	0.36	0.07	0.16

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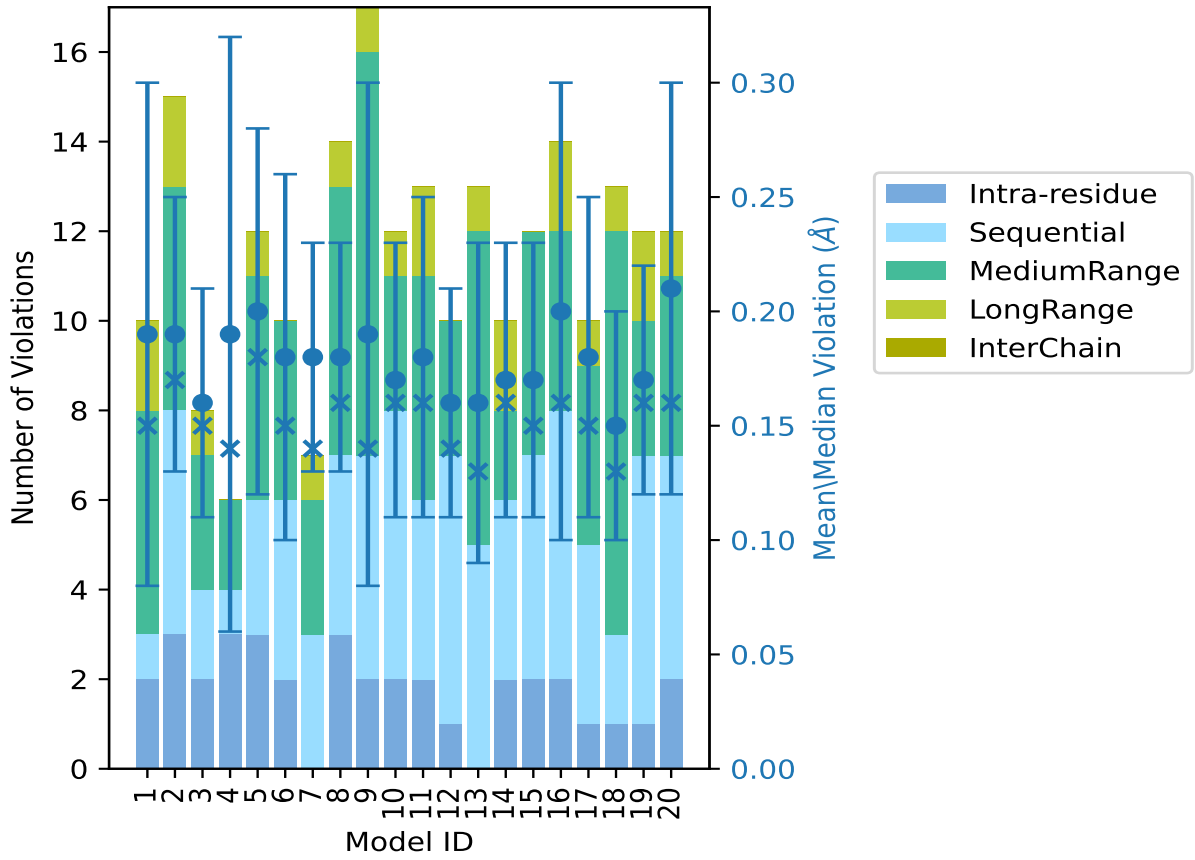
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	6	3	0	0	10	0.16	0.24	0.05	0.14
13	0	5	7	1	0	13	0.16	0.39	0.07	0.13
14	2	4	2	2	0	10	0.17	0.27	0.06	0.16
15	2	5	5	0	0	12	0.17	0.3	0.06	0.15
16	2	6	4	2	0	14	0.2	0.45	0.1	0.16
17	1	4	4	1	0	10	0.18	0.35	0.07	0.15
18	1	2	9	1	0	13	0.15	0.27	0.05	0.13
19	1	6	3	2	0	12	0.17	0.31	0.05	0.16
20	2	5	4	1	0	12	0.21	0.43	0.09	0.16

[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

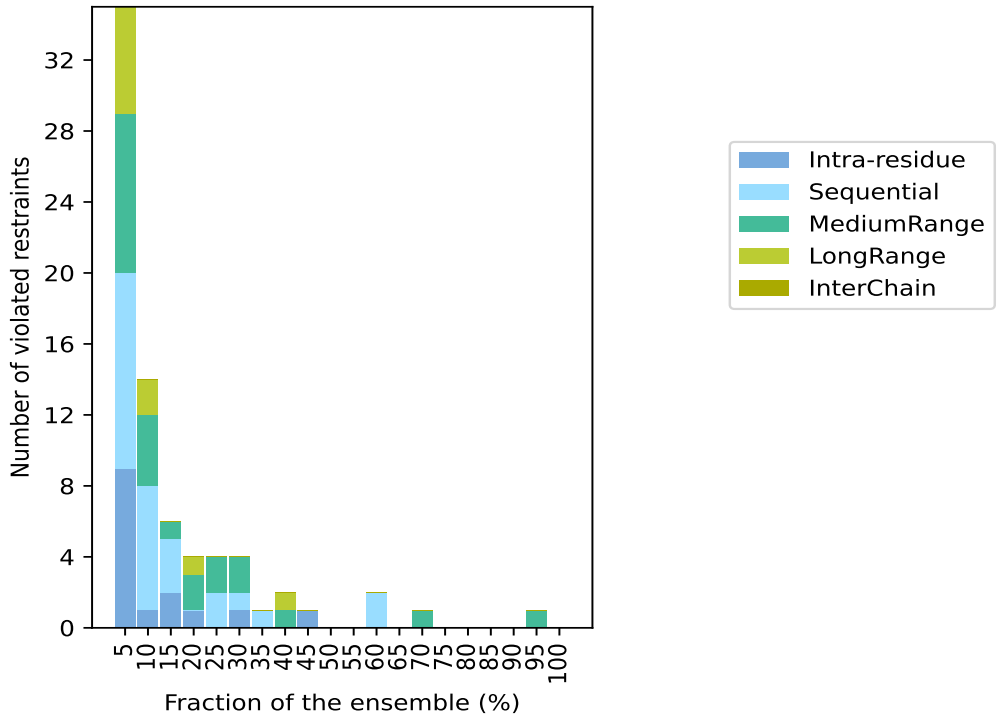
9.3 Distance violation statistics for the ensemble (i)

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, 2505(IR:594, SQ:539, MR:702, LR:670, 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]	%
9	11	9	6	0	35	1	5.0
1	7	4	2	0	14	2	10.0
2	3	1	0	0	6	3	15.0
1	0	2	1	0	4	4	20.0
0	2	2	0	0	4	5	25.0
1	1	2	0	0	4	6	30.0
0	1	0	0	0	1	7	35.0
0	0	1	1	0	2	8	40.0
1	0	0	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	2	0	0	0	2	12	60.0
0	0	0	0	0	0	13	65.0
0	0	1	0	0	1	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	0	0	0	18	90.0
0	0	1	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

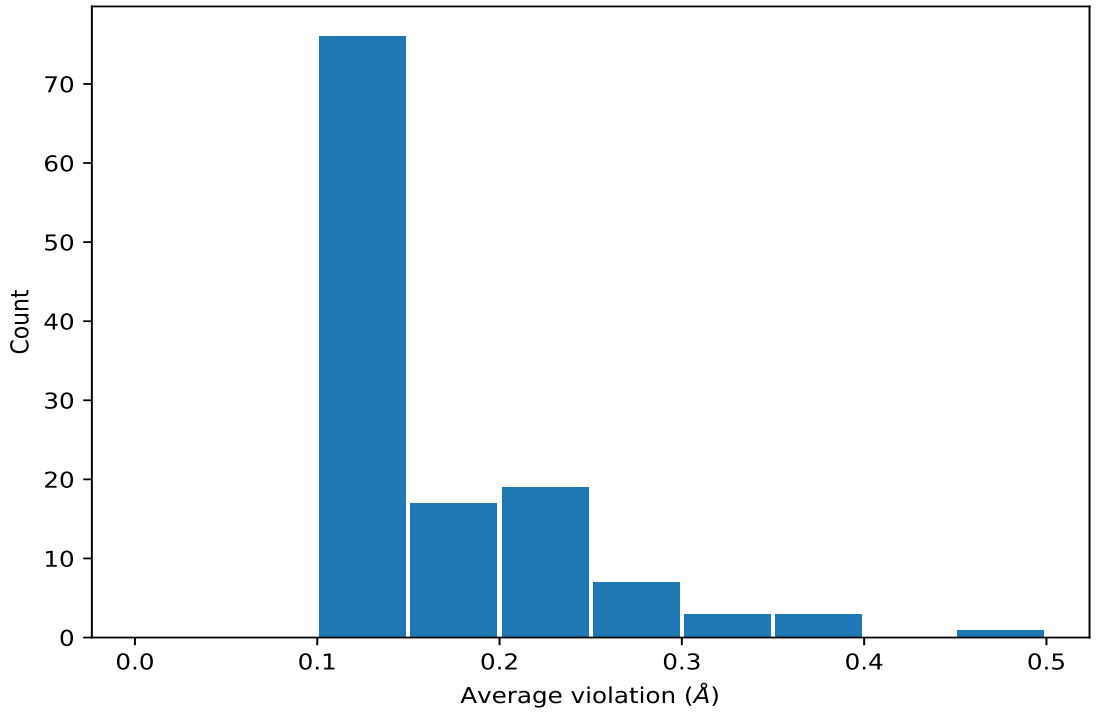
9.3.1 Bar graph : Distance violation statistics for the ensemble



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

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)
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	19	0.17	0.03	0.17
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	19	0.17	0.03	0.17
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	19	0.17	0.03	0.17
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	14	0.14	0.02	0.15
(1,2158)	1:A:52:SER:HB2	1:A:53:VAL:H	12	0.23	0.04	0.22
(1,2158)	1:A:52:SER:HB3	1:A:53:VAL:H	12	0.23	0.04	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB2	12	0.22	0.01	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB3	12	0.22	0.01	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB2	12	0.22	0.01	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB3	12	0.22	0.01	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB2	12	0.22	0.01	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB3	12	0.22	0.01	0.22
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD21	9	0.35	0.1	0.39
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD22	9	0.35	0.1	0.39
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD23	9	0.35	0.1	0.39
(1,1415)	1:A:31:LEU:HG	1:A:98:PHE:HB2	8	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB1	8	0.13	0.02	0.12
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB2	8	0.13	0.02	0.12
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB3	8	0.13	0.02	0.12
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE2	7	0.15	0.05	0.12
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE3	7	0.15	0.05	0.12
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE2	7	0.15	0.05	0.12
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE3	7	0.15	0.05	0.12
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE2	7	0.15	0.05	0.12
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE3	7	0.15	0.05	0.12
(1,811)	1:A:153:ARG:HA	1:A:154:ASP:H	6	0.28	0.03	0.27
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD11	6	0.23	0.05	0.25
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD12	6	0.23	0.05	0.25
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD13	6	0.23	0.05	0.25
(1,285)	1:A:45:LEU:HB3	1:A:48:GLN:HE21	6	0.16	0.03	0.15
(1,1008)	1:A:107:ASP:HA	1:A:110:LYS:HA	6	0.12	0.01	0.12
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG21	5	0.18	0.02	0.19
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG22	5	0.18	0.02	0.19
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG23	5	0.18	0.02	0.19
(1,2046)	1:A:36:LEU:HD11	1:A:40:LYS:HD2	5	0.14	0.02	0.15
(1,2046)	1:A:36:LEU:HD11	1:A:40:LYS:HD3	5	0.14	0.02	0.15
(1,2046)	1:A:36:LEU:HD12	1:A:40:LYS:HD2	5	0.14	0.02	0.15
(1,2046)	1:A:36:LEU:HD12	1:A:40:LYS:HD3	5	0.14	0.02	0.15
(1,2046)	1:A:36:LEU:HD13	1:A:40:LYS:HD2	5	0.14	0.02	0.15
(1,2046)	1:A:36:LEU:HD13	1:A:40:LYS:HD3	5	0.14	0.02	0.15
(1,2046)	1:A:36:LEU:HD21	1:A:40:LYS:HD2	5	0.14	0.02	0.15
(1,2046)	1:A:36:LEU:HD21	1:A:40:LYS:HD3	5	0.14	0.02	0.15
(1,2046)	1:A:36:LEU:HD22	1:A:40:LYS:HD2	5	0.14	0.02	0.15
(1,2046)	1:A:36:LEU:HD22	1:A:40:LYS:HD3	5	0.14	0.02	0.15
(1,2046)	1:A:36:LEU:HD23	1:A:40:LYS:HD2	5	0.14	0.02	0.15
(1,2046)	1:A:36:LEU:HD23	1:A:40:LYS:HD3	5	0.14	0.02	0.15
(1,231)	1:A:40:LYS:HD2	1:A:42:LEU:H	5	0.13	0.01	0.14
(1,231)	1:A:40:LYS:HD3	1:A:42:LEU:H	5	0.13	0.01	0.14
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB1	5	0.11	0.0	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB2	5	0.11	0.0	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB3	5	0.11	0.0	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB1	5	0.11	0.0	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB2	5	0.11	0.0	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB3	5	0.11	0.0	0.11
(1,1163)	1:A:50:LYS:HA	1:A:50:LYS:HG3	4	0.17	0.0	0.17
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG11	4	0.17	0.04	0.16
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG12	4	0.17	0.04	0.16
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG13	4	0.17	0.04	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG21	4	0.17	0.04	0.16
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG22	4	0.17	0.04	0.16
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG23	4	0.17	0.04	0.16
(1,1037)	1:A:31:LEU:HD21	1:A:98:PHE:HA	4	0.14	0.03	0.14
(1,1037)	1:A:31:LEU:HD22	1:A:98:PHE:HA	4	0.14	0.03	0.14
(1,1037)	1:A:31:LEU:HD23	1:A:98:PHE:HA	4	0.14	0.03	0.14
(1,1136)	1:A:40:LYS:HG3	1:A:44:MET:HB2	4	0.12	0.01	0.12
(1,1136)	1:A:40:LYS:HG3	1:A:44:MET:HB3	4	0.12	0.01	0.12
(1,1870)	1:A:13:VAL:HG11	1:A:17:ARG:HD2	3	0.26	0.03	0.27
(1,1870)	1:A:13:VAL:HG11	1:A:17:ARG:HD3	3	0.26	0.03	0.27
(1,1870)	1:A:13:VAL:HG12	1:A:17:ARG:HD2	3	0.26	0.03	0.27
(1,1870)	1:A:13:VAL:HG12	1:A:17:ARG:HD3	3	0.26	0.03	0.27
(1,1870)	1:A:13:VAL:HG13	1:A:17:ARG:HD2	3	0.26	0.03	0.27
(1,1870)	1:A:13:VAL:HG13	1:A:17:ARG:HD3	3	0.26	0.03	0.27
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD11	3	0.2	0.01	0.2
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD12	3	0.2	0.01	0.2
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD13	3	0.2	0.01	0.2
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD21	3	0.2	0.01	0.2
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD22	3	0.2	0.01	0.2
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD23	3	0.2	0.01	0.2
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG11	3	0.14	0.02	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG12	3	0.14	0.02	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG13	3	0.14	0.02	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG21	3	0.14	0.02	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG22	3	0.14	0.02	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG23	3	0.14	0.02	0.16
(1,2190)	1:A:58:LEU:HD11	1:A:59:THR:HB	3	0.13	0.02	0.12
(1,2190)	1:A:58:LEU:HD12	1:A:59:THR:HB	3	0.13	0.02	0.12
(1,2190)	1:A:58:LEU:HD13	1:A:59:THR:HB	3	0.13	0.02	0.12
(1,2190)	1:A:58:LEU:HD21	1:A:59:THR:HB	3	0.13	0.02	0.12
(1,2190)	1:A:58:LEU:HD22	1:A:59:THR:HB	3	0.13	0.02	0.12
(1,2190)	1:A:58:LEU:HD23	1:A:59:THR:HB	3	0.13	0.02	0.12
(1,684)	1:A:124:VAL:HA	1:A:125:SER:H	3	0.13	0.02	0.12
(1,950)	1:A:16:LYS:HA	1:A:16:LYS:HE2	3	0.11	0.0	0.11
(1,950)	1:A:16:LYS:HA	1:A:16:LYS:HE3	3	0.11	0.0	0.11
(1,297)	1:A:52:SER:HA	1:A:53:VAL:H	2	0.45	0.0	0.45
(1,1054)	1:A:35:VAL:HG11	1:A:36:LEU:HA	2	0.38	0.02	0.38
(1,1054)	1:A:35:VAL:HG12	1:A:36:LEU:HA	2	0.38	0.02	0.38
(1,1054)	1:A:35:VAL:HG13	1:A:36:LEU:HA	2	0.38	0.02	0.38
(1,505)	1:A:86:CYS:HB2	1:A:87:ARG:H	2	0.22	0.0	0.22
(1,505)	1:A:86:CYS:HB3	1:A:87:ARG:H	2	0.22	0.0	0.22
(1,402)	1:A:128:SER:HB2	1:A:129:GLN:H	2	0.16	0.01	0.16

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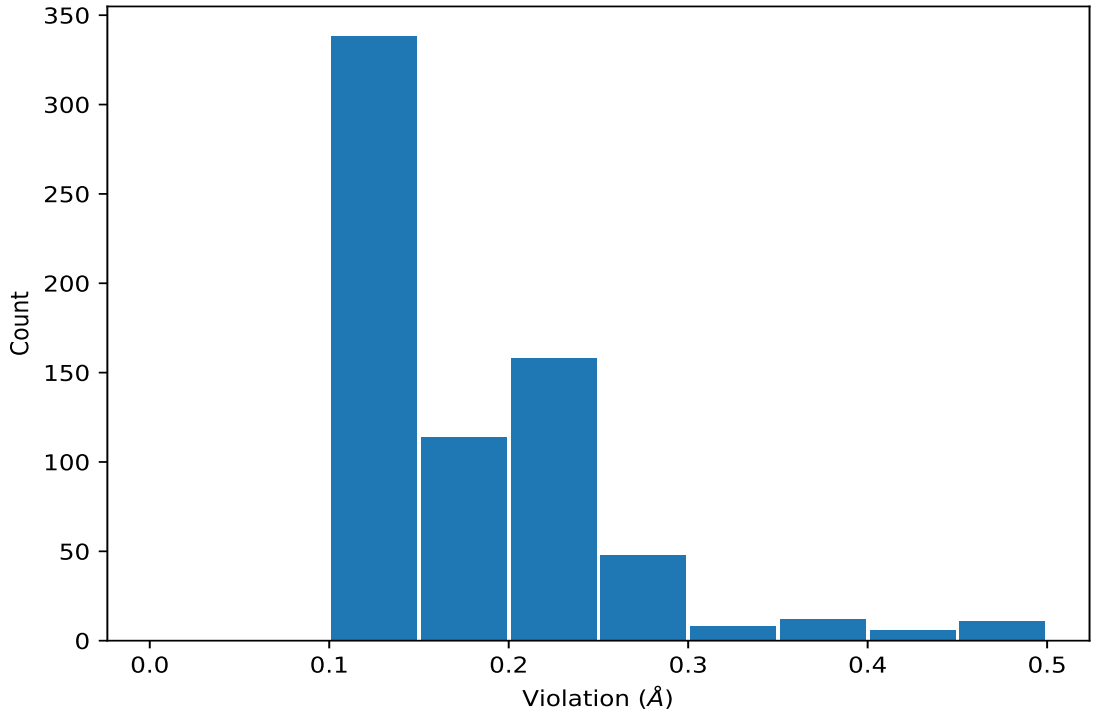
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,402)	1:A:128:SER:HB3	1:A:129:GLN:H	2	0.16	0.01	0.16
(1,1147)	1:A:4:LEU:HG	1:A:46:GLN:HB3	2	0.14	0.02	0.14
(1,1492)	1:A:127:ILE:HG12	1:A:128:SER:HA	2	0.14	0.0	0.14
(1,2513)	1:A:132:SER:HB2	1:A:133:TRP:HD1	2	0.14	0.02	0.14
(1,2513)	1:A:132:SER:HB3	1:A:133:TRP:HD1	2	0.14	0.02	0.14
(1,204)	1:A:36:LEU:HB3	1:A:38:LEU:H	2	0.14	0.02	0.14
(1,859)	1:A:8:ILE:HD11	1:A:44:MET:HA	2	0.14	0.01	0.14
(1,859)	1:A:8:ILE:HD12	1:A:44:MET:HA	2	0.14	0.01	0.14
(1,859)	1:A:8:ILE:HD13	1:A:44:MET:HA	2	0.14	0.01	0.14
(1,1101)	1:A:36:LEU:HA	1:A:39:ILE:HG21	2	0.12	0.02	0.12
(1,1101)	1:A:36:LEU:HA	1:A:39:ILE:HG22	2	0.12	0.02	0.12
(1,1101)	1:A:36:LEU:HA	1:A:39:ILE:HG23	2	0.12	0.02	0.12
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD11	2	0.12	0.01	0.12
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD12	2	0.12	0.01	0.12
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD13	2	0.12	0.01	0.12
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD21	2	0.12	0.01	0.12
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD22	2	0.12	0.01	0.12
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD23	2	0.12	0.01	0.12
(1,1635)	1:A:133:TRP:HA	1:A:133:TRP:HD1	2	0.12	0.0	0.12
(1,320)	1:A:58:LEU:HD11	1:A:59:THR:H	2	0.12	0.0	0.12
(1,320)	1:A:58:LEU:HD12	1:A:59:THR:H	2	0.12	0.0	0.12
(1,320)	1:A:58:LEU:HD13	1:A:59:THR:H	2	0.12	0.0	0.12
(1,2095)	1:A:40:LYS:HE2	1:A:43:GLU:HG2	2	0.12	0.0	0.12
(1,2095)	1:A:40:LYS:HE2	1:A:43:GLU:HG3	2	0.12	0.0	0.12
(1,2095)	1:A:40:LYS:HE3	1:A:43:GLU:HG2	2	0.12	0.0	0.12
(1,2095)	1:A:40:LYS:HE3	1:A:43:GLU:HG3	2	0.12	0.0	0.12

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:A:45:LEU:HA	1:A:45:LEU:HD11	9	0.49
(1,1140)	1:A:45:LEU:HA	1:A:45:LEU:HD12	9	0.49
(1,1140)	1:A:45:LEU:HA	1:A:45:LEU:HD13	9	0.49
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD21	1	0.48
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD22	1	0.48
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD23	1	0.48
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD21	4	0.48
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD22	4	0.48
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD23	4	0.48
(1,297)	1:A:52:SER:HA	1:A:53:VAL:H	9	0.45
(1,297)	1:A:52:SER:HA	1:A:53:VAL:H	16	0.45
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD21	20	0.43
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD22	20	0.43
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD23	20	0.43
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD21	5	0.41
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD22	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD23	5	0.41
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD21	6	0.39
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD22	6	0.39
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD23	6	0.39
(1,1054)	1:A:35:VAL:HG11	1:A:36:LEU:HA	13	0.39
(1,1054)	1:A:35:VAL:HG12	1:A:36:LEU:HA	13	0.39
(1,1054)	1:A:35:VAL:HG13	1:A:36:LEU:HA	13	0.39
(1,1960)	1:A:25:LYS:H	1:A:25:LYS:HG2	16	0.38
(1,1960)	1:A:25:LYS:H	1:A:25:LYS:HG3	16	0.38
(1,1613)	1:A:127:ILE:HG13	1:A:128:SER:HA	20	0.36
(1,1054)	1:A:35:VAL:HG11	1:A:36:LEU:HA	11	0.36
(1,1054)	1:A:35:VAL:HG12	1:A:36:LEU:HA	11	0.36
(1,1054)	1:A:35:VAL:HG13	1:A:36:LEU:HA	11	0.36
(1,811)	1:A:153:ARG:HA	1:A:154:ASP:H	17	0.35
(1,1904)	1:A:16:LYS:HB2	1:A:17:ARG:HD2	10	0.34
(1,1904)	1:A:16:LYS:HB2	1:A:17:ARG:HD3	10	0.34
(1,1904)	1:A:16:LYS:HB3	1:A:17:ARG:HD2	10	0.34
(1,1904)	1:A:16:LYS:HB3	1:A:17:ARG:HD3	10	0.34
(1,2158)	1:A:52:SER:HB2	1:A:53:VAL:H	19	0.31
(1,2158)	1:A:52:SER:HB3	1:A:53:VAL:H	19	0.31
(1,1175)	1:A:52:SER:HB3	1:A:53:VAL:HB	2	0.31
(1,2158)	1:A:52:SER:HB2	1:A:53:VAL:H	15	0.3
(1,2158)	1:A:52:SER:HB3	1:A:53:VAL:H	15	0.3
(1,1870)	1:A:13:VAL:HG11	1:A:17:ARG:HD2	9	0.29
(1,1870)	1:A:13:VAL:HG11	1:A:17:ARG:HD3	9	0.29
(1,1870)	1:A:13:VAL:HG12	1:A:17:ARG:HD2	9	0.29
(1,1870)	1:A:13:VAL:HG12	1:A:17:ARG:HD3	9	0.29
(1,1870)	1:A:13:VAL:HG13	1:A:17:ARG:HD2	9	0.29
(1,1870)	1:A:13:VAL:HG13	1:A:17:ARG:HD3	9	0.29
(1,811)	1:A:153:ARG:HA	1:A:154:ASP:H	8	0.28
(1,811)	1:A:153:ARG:HA	1:A:154:ASP:H	2	0.27
(1,811)	1:A:153:ARG:HA	1:A:154:ASP:H	7	0.27
(1,811)	1:A:153:ARG:HA	1:A:154:ASP:H	14	0.27
(1,1870)	1:A:13:VAL:HG11	1:A:17:ARG:HD2	18	0.27
(1,1870)	1:A:13:VAL:HG11	1:A:17:ARG:HD3	18	0.27
(1,1870)	1:A:13:VAL:HG12	1:A:17:ARG:HD2	18	0.27
(1,1870)	1:A:13:VAL:HG12	1:A:17:ARG:HD3	18	0.27
(1,1870)	1:A:13:VAL:HG13	1:A:17:ARG:HD2	18	0.27
(1,1870)	1:A:13:VAL:HG13	1:A:17:ARG:HD3	18	0.27
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD11	17	0.27
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD12	17	0.27
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD13	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD21	11	0.27
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD22	11	0.27
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD23	11	0.27
(1,811)	1:A:153:ARG:HA	1:A:154:ASP:H	11	0.26
(1,2158)	1:A:52:SER:HB2	1:A:53:VAL:H	20	0.26
(1,2158)	1:A:52:SER:HB3	1:A:53:VAL:H	20	0.26
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE2	16	0.26
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE3	16	0.26
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE2	16	0.26
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE3	16	0.26
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE2	16	0.26
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE3	16	0.26
(1,2156)	1:A:52:SER:H	1:A:53:VAL:HG11	2	0.25
(1,2156)	1:A:52:SER:H	1:A:53:VAL:HG12	2	0.25
(1,2156)	1:A:52:SER:H	1:A:53:VAL:HG13	2	0.25
(1,2156)	1:A:52:SER:H	1:A:53:VAL:HG21	2	0.25
(1,2156)	1:A:52:SER:H	1:A:53:VAL:HG22	2	0.25
(1,2156)	1:A:52:SER:H	1:A:53:VAL:HG23	2	0.25
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD11	3	0.25
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD12	3	0.25
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD13	3	0.25
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD11	5	0.25
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD12	5	0.25
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD13	5	0.25
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD11	15	0.25
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD12	15	0.25
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD13	15	0.25
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB2	5	0.24
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB3	5	0.24
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB2	5	0.24
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB3	5	0.24
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB2	5	0.24
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB3	5	0.24
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD11	12	0.24
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD12	12	0.24
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD13	12	0.24
(1,1415)	1:A:31:LEU:HG	1:A:98:PHE:HB2	14	0.24
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD21	2	0.24
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD22	2	0.24
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD23	2	0.24
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB2	8	0.23
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB3	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB2	8	0.23
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB3	8	0.23
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB2	8	0.23
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB3	8	0.23
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB2	14	0.23
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB3	14	0.23
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB2	14	0.23
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB3	14	0.23
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB2	14	0.23
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB3	14	0.23
(1,2158)	1:A:52:SER:HB2	1:A:53:VAL:H	5	0.23
(1,2158)	1:A:52:SER:HB3	1:A:53:VAL:H	5	0.23
(1,2158)	1:A:52:SER:HB2	1:A:53:VAL:H	6	0.23
(1,2158)	1:A:52:SER:HB3	1:A:53:VAL:H	6	0.23
(1,2158)	1:A:52:SER:HB2	1:A:53:VAL:H	12	0.23
(1,2158)	1:A:52:SER:HB3	1:A:53:VAL:H	12	0.23
(1,1749)	1:A:22:LYS:HD2	1:A:23:TYR:HE1	16	0.23
(1,1749)	1:A:22:LYS:HD2	1:A:23:TYR:HE2	16	0.23
(1,1749)	1:A:22:LYS:HD3	1:A:23:TYR:HE1	16	0.23
(1,1749)	1:A:22:LYS:HD3	1:A:23:TYR:HE2	16	0.23
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD21	8	0.23
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD22	8	0.23
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD23	8	0.23
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB2	1	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB3	1	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB2	1	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB3	1	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB2	1	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB3	1	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB2	7	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB3	7	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB2	7	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB3	7	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB2	7	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB3	7	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB2	9	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB3	9	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB2	9	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB3	9	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB2	9	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB3	9	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB2	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB3	15	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB2	15	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB3	15	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB2	15	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB3	15	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB2	18	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB3	18	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB2	18	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB3	18	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB2	18	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB3	18	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB2	19	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB3	19	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB2	19	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB3	19	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB2	19	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB3	19	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB2	20	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB3	20	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB2	20	0.22
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB3	20	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB2	20	0.22
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB3	20	0.22
(1,505)	1:A:86:CYS:HB2	1:A:87:ARG:H	6	0.22
(1,505)	1:A:86:CYS:HB3	1:A:87:ARG:H	6	0.22
(1,505)	1:A:86:CYS:HB2	1:A:87:ARG:H	8	0.22
(1,505)	1:A:86:CYS:HB3	1:A:87:ARG:H	8	0.22
(1,285)	1:A:45:LEU:HB3	1:A:48:GLN:HE21	2	0.22
(1,2158)	1:A:52:SER:HB2	1:A:53:VAL:H	3	0.22
(1,2158)	1:A:52:SER:HB3	1:A:53:VAL:H	3	0.22
(1,2158)	1:A:52:SER:HB2	1:A:53:VAL:H	7	0.22
(1,2158)	1:A:52:SER:HB3	1:A:53:VAL:H	7	0.22
(1,2158)	1:A:52:SER:HB2	1:A:53:VAL:H	10	0.22
(1,2158)	1:A:52:SER:HB3	1:A:53:VAL:H	10	0.22
(1,2158)	1:A:52:SER:HB2	1:A:53:VAL:H	14	0.22
(1,2158)	1:A:52:SER:HB3	1:A:53:VAL:H	14	0.22
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG11	8	0.22
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG12	8	0.22
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG13	8	0.22
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG21	8	0.22
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG22	8	0.22
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG23	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	18	0.22
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	18	0.22
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	18	0.22
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB2	13	0.21
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB3	13	0.21
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB2	13	0.21
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB3	13	0.21
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB2	13	0.21
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB3	13	0.21
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB2	16	0.21
(1,927)	1:A:14:ILE:HD11	1:A:15:HIS:HB3	16	0.21
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB2	16	0.21
(1,927)	1:A:14:ILE:HD12	1:A:15:HIS:HB3	16	0.21
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB2	16	0.21
(1,927)	1:A:14:ILE:HD13	1:A:15:HIS:HB3	16	0.21
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD11	1	0.21
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD12	1	0.21
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD13	1	0.21
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD21	1	0.21
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD22	1	0.21
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD23	1	0.21
(1,1870)	1:A:13:VAL:HG11	1:A:17:ARG:HD2	8	0.21
(1,1870)	1:A:13:VAL:HG11	1:A:17:ARG:HD3	8	0.21
(1,1870)	1:A:13:VAL:HG12	1:A:17:ARG:HD2	8	0.21
(1,1870)	1:A:13:VAL:HG12	1:A:17:ARG:HD3	8	0.21
(1,1870)	1:A:13:VAL:HG13	1:A:17:ARG:HD2	8	0.21
(1,1870)	1:A:13:VAL:HG13	1:A:17:ARG:HD3	8	0.21
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG21	11	0.21
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG22	11	0.21
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG23	11	0.21
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	9	0.21
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	9	0.21
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	9	0.21
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD21	19	0.21
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD22	19	0.21
(1,1144)	1:A:45:LEU:HA	1:A:45:LEU:HD23	19	0.21
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD11	2	0.2
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD12	2	0.2
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD13	2	0.2
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD21	2	0.2
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD22	2	0.2
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD23	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2158)	1:A:52:SER:HB2	1:A:53:VAL:H	13	0.2
(1,2158)	1:A:52:SER:HB3	1:A:53:VAL:H	13	0.2
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG11	11	0.2
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG12	11	0.2
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG13	11	0.2
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG21	11	0.2
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG22	11	0.2
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG23	11	0.2
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	17	0.2
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	17	0.2
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	17	0.2
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE2	10	0.2
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE3	10	0.2
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE2	10	0.2
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE3	10	0.2
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE2	10	0.2
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE3	10	0.2
(1,805)	1:A:151:LEU:HA	1:A:152:ARG:H	12	0.19
(1,668)	1:A:12:GLN:H	1:A:12:GLN:HE22	5	0.19
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD11	14	0.19
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD12	14	0.19
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD13	14	0.19
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD21	14	0.19
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD22	14	0.19
(1,2573)	1:A:151:LEU:HA	1:A:151:LEU:HD23	14	0.19
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG21	6	0.19
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG22	6	0.19
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG23	6	0.19
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG21	19	0.19
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG22	19	0.19
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG23	19	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	1	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	1	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	1	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	2	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	2	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	2	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	5	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	5	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	5	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	11	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	11	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	15	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	15	0.19
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	15	0.19
(1,1013)	1:A:25:LYS:HA	1:A:28:CYS:HA	9	0.19
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG21	10	0.18
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG22	10	0.18
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG23	10	0.18
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	16	0.18
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	16	0.18
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	16	0.18
(1,1415)	1:A:31:LEU:HG	1:A:98:PHE:HB2	5	0.18
(1,694)	1:A:110:LYS:HA	1:A:129:GLN:HE21	2	0.17
(1,402)	1:A:128:SER:HB2	1:A:129:GLN:H	19	0.17
(1,402)	1:A:128:SER:HB3	1:A:129:GLN:H	19	0.17
(1,285)	1:A:45:LEU:HB3	1:A:48:GLN:HE21	5	0.17
(1,1791)	1:A:4:LEU:HA	1:A:4:LEU:HD11	9	0.17
(1,1791)	1:A:4:LEU:HA	1:A:4:LEU:HD12	9	0.17
(1,1791)	1:A:4:LEU:HA	1:A:4:LEU:HD13	9	0.17
(1,1791)	1:A:4:LEU:HA	1:A:4:LEU:HD21	9	0.17
(1,1791)	1:A:4:LEU:HA	1:A:4:LEU:HD22	9	0.17
(1,1791)	1:A:4:LEU:HA	1:A:4:LEU:HD23	9	0.17
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	20	0.17
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	20	0.17
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	20	0.17
(1,1415)	1:A:31:LEU:HG	1:A:98:PHE:HB2	1	0.17
(1,1415)	1:A:31:LEU:HG	1:A:98:PHE:HB2	17	0.17
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB1	15	0.17
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB2	15	0.17
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB3	15	0.17
(1,1163)	1:A:50:LYS:HA	1:A:50:LYS:HG3	3	0.17
(1,1163)	1:A:50:LYS:HA	1:A:50:LYS:HG3	18	0.17
(1,1163)	1:A:50:LYS:HA	1:A:50:LYS:HG3	20	0.17
(1,1037)	1:A:31:LEU:HD21	1:A:98:PHE:HA	16	0.17
(1,1037)	1:A:31:LEU:HD22	1:A:98:PHE:HA	16	0.17
(1,1037)	1:A:31:LEU:HD23	1:A:98:PHE:HA	16	0.17
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	8	0.17
(1,684)	1:A:124:VAL:HA	1:A:125:SER:H	2	0.16
(1,2513)	1:A:132:SER:HB2	1:A:133:TRP:HD1	10	0.16
(1,2513)	1:A:132:SER:HB3	1:A:133:TRP:HD1	10	0.16
(1,2511)	1:A:127:ILE:HG12	1:A:128:SER:HB2	20	0.16
(1,2511)	1:A:127:ILE:HG12	1:A:128:SER:HB3	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2511)	1:A:127:ILE:HG13	1:A:128:SER:HB2	20	0.16
(1,2511)	1:A:127:ILE:HG13	1:A:128:SER:HB3	20	0.16
(1,2190)	1:A:58:LEU:HD11	1:A:59:THR:HB	12	0.16
(1,2190)	1:A:58:LEU:HD12	1:A:59:THR:HB	12	0.16
(1,2190)	1:A:58:LEU:HD13	1:A:59:THR:HB	12	0.16
(1,2190)	1:A:58:LEU:HD21	1:A:59:THR:HB	12	0.16
(1,2190)	1:A:58:LEU:HD22	1:A:59:THR:HB	12	0.16
(1,2190)	1:A:58:LEU:HD23	1:A:59:THR:HB	12	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG11	19	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG12	19	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG13	19	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG21	19	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG22	19	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG23	19	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG11	20	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG12	20	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG13	20	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG21	20	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG22	20	0.16
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG23	20	0.16
(1,2046)	1:A:36:LEU:HD11	1:A:40:LYS:HD2	2	0.16
(1,2046)	1:A:36:LEU:HD11	1:A:40:LYS:HD3	2	0.16
(1,2046)	1:A:36:LEU:HD12	1:A:40:LYS:HD2	2	0.16
(1,2046)	1:A:36:LEU:HD12	1:A:40:LYS:HD3	2	0.16
(1,2046)	1:A:36:LEU:HD13	1:A:40:LYS:HD2	2	0.16
(1,2046)	1:A:36:LEU:HD13	1:A:40:LYS:HD3	2	0.16
(1,2046)	1:A:36:LEU:HD21	1:A:40:LYS:HD2	2	0.16
(1,2046)	1:A:36:LEU:HD21	1:A:40:LYS:HD3	2	0.16
(1,2046)	1:A:36:LEU:HD22	1:A:40:LYS:HD2	2	0.16
(1,2046)	1:A:36:LEU:HD22	1:A:40:LYS:HD3	2	0.16
(1,2046)	1:A:36:LEU:HD23	1:A:40:LYS:HD2	2	0.16
(1,2046)	1:A:36:LEU:HD23	1:A:40:LYS:HD3	2	0.16
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	3	0.16
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	3	0.16
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	3	0.16
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	13	0.16
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	13	0.16
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	13	0.16
(1,1415)	1:A:31:LEU:HG	1:A:98:PHE:HB2	10	0.16
(1,1163)	1:A:50:LYS:HA	1:A:50:LYS:HG3	8	0.16
(1,1147)	1:A:4:LEU:HG	1:A:46:GLN:HB3	9	0.16
(1,1037)	1:A:31:LEU:HD21	1:A:98:PHE:HA	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	1:A:31:LEU:HD22	1:A:98:PHE:HA	18	0.16
(1,1037)	1:A:31:LEU:HD23	1:A:98:PHE:HA	18	0.16
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	10	0.16
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	11	0.16
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	19	0.16
(1,402)	1:A:128:SER:HB2	1:A:129:GLN:H	10	0.15
(1,402)	1:A:128:SER:HB3	1:A:129:GLN:H	10	0.15
(1,285)	1:A:45:LEU:HB3	1:A:48:GLN:HE21	6	0.15
(1,231)	1:A:40:LYS:HD2	1:A:42:LEU:H	8	0.15
(1,231)	1:A:40:LYS:HD3	1:A:42:LEU:H	8	0.15
(1,2046)	1:A:36:LEU:HD11	1:A:40:LYS:HD2	4	0.15
(1,2046)	1:A:36:LEU:HD11	1:A:40:LYS:HD3	4	0.15
(1,2046)	1:A:36:LEU:HD12	1:A:40:LYS:HD2	4	0.15
(1,2046)	1:A:36:LEU:HD12	1:A:40:LYS:HD3	4	0.15
(1,2046)	1:A:36:LEU:HD13	1:A:40:LYS:HD2	4	0.15
(1,2046)	1:A:36:LEU:HD13	1:A:40:LYS:HD3	4	0.15
(1,2046)	1:A:36:LEU:HD21	1:A:40:LYS:HD2	4	0.15
(1,2046)	1:A:36:LEU:HD21	1:A:40:LYS:HD3	4	0.15
(1,2046)	1:A:36:LEU:HD22	1:A:40:LYS:HD2	4	0.15
(1,2046)	1:A:36:LEU:HD22	1:A:40:LYS:HD3	4	0.15
(1,2046)	1:A:36:LEU:HD23	1:A:40:LYS:HD2	4	0.15
(1,2046)	1:A:36:LEU:HD23	1:A:40:LYS:HD3	4	0.15
(1,2046)	1:A:36:LEU:HD11	1:A:40:LYS:HD2	17	0.15
(1,2046)	1:A:36:LEU:HD11	1:A:40:LYS:HD3	17	0.15
(1,2046)	1:A:36:LEU:HD12	1:A:40:LYS:HD2	17	0.15
(1,2046)	1:A:36:LEU:HD12	1:A:40:LYS:HD3	17	0.15
(1,2046)	1:A:36:LEU:HD13	1:A:40:LYS:HD2	17	0.15
(1,2046)	1:A:36:LEU:HD13	1:A:40:LYS:HD3	17	0.15
(1,2046)	1:A:36:LEU:HD21	1:A:40:LYS:HD2	17	0.15
(1,2046)	1:A:36:LEU:HD21	1:A:40:LYS:HD3	17	0.15
(1,2046)	1:A:36:LEU:HD22	1:A:40:LYS:HD2	17	0.15
(1,2046)	1:A:36:LEU:HD22	1:A:40:LYS:HD3	17	0.15
(1,2046)	1:A:36:LEU:HD23	1:A:40:LYS:HD2	17	0.15
(1,2046)	1:A:36:LEU:HD23	1:A:40:LYS:HD3	17	0.15
(1,204)	1:A:36:LEU:HB3	1:A:38:LEU:H	16	0.15
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG21	5	0.15
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG22	5	0.15
(1,1602)	1:A:126:PRO:HA	1:A:127:ILE:HG23	5	0.15
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	19	0.15
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	19	0.15
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	19	0.15
(1,131)	1:A:22:LYS:HB3	1:A:23:TYR:H	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	6	0.15
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	16	0.15
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	20	0.15
(1,859)	1:A:8:ILE:HD11	1:A:44:MET:HA	7	0.14
(1,859)	1:A:8:ILE:HD12	1:A:44:MET:HA	7	0.14
(1,859)	1:A:8:ILE:HD13	1:A:44:MET:HA	7	0.14
(1,823)	1:A:114:LEU:HA	1:A:114:LEU:HG	4	0.14
(1,653)	1:A:115:LEU:H	1:A:115:LEU:HG	2	0.14
(1,285)	1:A:45:LEU:HB3	1:A:48:GLN:HE21	8	0.14
(1,285)	1:A:45:LEU:HB3	1:A:48:GLN:HE21	20	0.14
(1,231)	1:A:40:LYS:HD2	1:A:42:LEU:H	9	0.14
(1,231)	1:A:40:LYS:HD3	1:A:42:LEU:H	9	0.14
(1,231)	1:A:40:LYS:HD2	1:A:42:LEU:H	19	0.14
(1,231)	1:A:40:LYS:HD3	1:A:42:LEU:H	19	0.14
(1,1621)	1:A:109:TRP:HD1	1:A:125:SER:HB2	11	0.14
(1,1621)	1:A:109:TRP:HD1	1:A:125:SER:HB3	11	0.14
(1,1492)	1:A:127:ILE:HG12	1:A:128:SER:HA	4	0.14
(1,1492)	1:A:127:ILE:HG12	1:A:128:SER:HA	12	0.14
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	7	0.14
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	7	0.14
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	7	0.14
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	8	0.14
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	8	0.14
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	8	0.14
(1,1415)	1:A:31:LEU:HG	1:A:98:PHE:HB2	8	0.14
(1,1415)	1:A:31:LEU:HG	1:A:98:PHE:HB2	20	0.14
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB1	17	0.14
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB2	17	0.14
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB3	17	0.14
(1,1136)	1:A:40:LYS:HG3	1:A:44:MET:HB2	15	0.14
(1,1136)	1:A:40:LYS:HG3	1:A:44:MET:HB3	15	0.14
(1,1101)	1:A:36:LEU:HA	1:A:39:ILE:HG21	15	0.14
(1,1101)	1:A:36:LEU:HA	1:A:39:ILE:HG22	15	0.14
(1,1101)	1:A:36:LEU:HA	1:A:39:ILE:HG23	15	0.14
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	7	0.14
(1,1008)	1:A:107:ASP:HA	1:A:110:LYS:HA	10	0.14
(1,905)	1:A:10:LEU:HA	1:A:13:VAL:HA	13	0.13
(1,859)	1:A:8:ILE:HD11	1:A:44:MET:HA	19	0.13
(1,859)	1:A:8:ILE:HD12	1:A:44:MET:HA	19	0.13
(1,859)	1:A:8:ILE:HD13	1:A:44:MET:HA	19	0.13
(1,704)	1:A:105:LEU:HG	1:A:133:TRP:HE1	16	0.13
(1,293)	1:A:52:SER:H	1:A:53:VAL:HB	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:A:40:LYS:HD2	1:A:42:LEU:H	18	0.13
(1,231)	1:A:40:LYS:HD3	1:A:42:LEU:H	18	0.13
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD11	1	0.13
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD12	1	0.13
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD13	1	0.13
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD21	1	0.13
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD22	1	0.13
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD23	1	0.13
(1,2158)	1:A:52:SER:HB2	1:A:53:VAL:H	17	0.13
(1,2158)	1:A:52:SER:HB3	1:A:53:VAL:H	17	0.13
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG11	2	0.13
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG12	2	0.13
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG13	2	0.13
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG21	2	0.13
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG22	2	0.13
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG23	2	0.13
(1,2046)	1:A:36:LEU:HD11	1:A:40:LYS:HD2	13	0.13
(1,2046)	1:A:36:LEU:HD11	1:A:40:LYS:HD3	13	0.13
(1,2046)	1:A:36:LEU:HD12	1:A:40:LYS:HD2	13	0.13
(1,2046)	1:A:36:LEU:HD12	1:A:40:LYS:HD3	13	0.13
(1,2046)	1:A:36:LEU:HD13	1:A:40:LYS:HD2	13	0.13
(1,2046)	1:A:36:LEU:HD13	1:A:40:LYS:HD3	13	0.13
(1,2046)	1:A:36:LEU:HD21	1:A:40:LYS:HD2	13	0.13
(1,2046)	1:A:36:LEU:HD21	1:A:40:LYS:HD3	13	0.13
(1,2046)	1:A:36:LEU:HD22	1:A:40:LYS:HD2	13	0.13
(1,2046)	1:A:36:LEU:HD22	1:A:40:LYS:HD3	13	0.13
(1,2046)	1:A:36:LEU:HD23	1:A:40:LYS:HD2	13	0.13
(1,2046)	1:A:36:LEU:HD23	1:A:40:LYS:HD3	13	0.13
(1,1924)	1:A:18:CYS:HB2	1:A:29:ARG:H	1	0.13
(1,1924)	1:A:18:CYS:HB3	1:A:29:ARG:H	1	0.13
(1,1795)	1:A:4:LEU:HD11	1:A:5:LYS:H	9	0.13
(1,1795)	1:A:4:LEU:HD12	1:A:5:LYS:H	9	0.13
(1,1795)	1:A:4:LEU:HD13	1:A:5:LYS:H	9	0.13
(1,1795)	1:A:4:LEU:HD21	1:A:5:LYS:H	9	0.13
(1,1795)	1:A:4:LEU:HD22	1:A:5:LYS:H	9	0.13
(1,1795)	1:A:4:LEU:HD23	1:A:5:LYS:H	9	0.13
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	4	0.13
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	4	0.13
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	4	0.13
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	6	0.13
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	6	0.13
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	10	0.13
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	10	0.13
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	10	0.13
(1,1429)	1:A:40:LYS:HE2	1:A:44:MET:HB2	9	0.13
(1,1429)	1:A:40:LYS:HE2	1:A:44:MET:HB3	9	0.13
(1,1429)	1:A:40:LYS:HE3	1:A:44:MET:HB2	9	0.13
(1,1429)	1:A:40:LYS:HE3	1:A:44:MET:HB3	9	0.13
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB1	12	0.13
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB2	12	0.13
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB3	12	0.13
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB1	13	0.13
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB2	13	0.13
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB3	13	0.13
(1,121)	1:A:22:LYS:H	1:A:23:TYR:HE1	16	0.13
(1,121)	1:A:22:LYS:H	1:A:23:TYR:HE2	16	0.13
(1,1136)	1:A:40:LYS:HG3	1:A:44:MET:HB2	6	0.13
(1,1136)	1:A:40:LYS:HG3	1:A:44:MET:HB3	6	0.13
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE2	18	0.13
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE3	18	0.13
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE2	18	0.13
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE3	18	0.13
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE2	18	0.13
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE3	18	0.13
(1,1032)	1:A:31:LEU:HD11	1:A:98:PHE:HA	2	0.13
(1,1032)	1:A:31:LEU:HD12	1:A:98:PHE:HA	2	0.13
(1,1032)	1:A:31:LEU:HD13	1:A:98:PHE:HA	2	0.13
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	3	0.13
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	5	0.13
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	18	0.13
(1,1008)	1:A:107:ASP:HA	1:A:110:LYS:HA	5	0.13
(1,961)	1:A:22:LYS:HA	1:A:22:LYS:HG2	15	0.12
(1,955)	1:A:13:VAL:HA	1:A:16:LYS:HE2	9	0.12
(1,955)	1:A:13:VAL:HA	1:A:16:LYS:HE3	9	0.12
(1,950)	1:A:16:LYS:HA	1:A:16:LYS:HE2	16	0.12
(1,950)	1:A:16:LYS:HA	1:A:16:LYS:HE3	16	0.12
(1,684)	1:A:124:VAL:HA	1:A:125:SER:H	8	0.12
(1,642)	1:A:111:GLU:HA	1:A:113:SER:H	9	0.12
(1,320)	1:A:58:LEU:HD11	1:A:59:THR:H	6	0.12
(1,320)	1:A:58:LEU:HD12	1:A:59:THR:H	6	0.12
(1,320)	1:A:58:LEU:HD13	1:A:59:THR:H	6	0.12
(1,285)	1:A:45:LEU:HB3	1:A:48:GLN:HE21	11	0.12
(1,2513)	1:A:132:SER:HB2	1:A:133:TRP:HD1	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2513)	1:A:132:SER:HB3	1:A:133:TRP:HD1	16	0.12
(1,2337)	1:A:99:LYS:HA	1:A:102:ASN:HD21	18	0.12
(1,2337)	1:A:99:LYS:HA	1:A:102:ASN:HD22	18	0.12
(1,2190)	1:A:58:LEU:HD11	1:A:59:THR:HB	13	0.12
(1,2190)	1:A:58:LEU:HD12	1:A:59:THR:HB	13	0.12
(1,2190)	1:A:58:LEU:HD13	1:A:59:THR:HB	13	0.12
(1,2190)	1:A:58:LEU:HD21	1:A:59:THR:HB	13	0.12
(1,2190)	1:A:58:LEU:HD22	1:A:59:THR:HB	13	0.12
(1,2190)	1:A:58:LEU:HD23	1:A:59:THR:HB	13	0.12
(1,2190)	1:A:58:LEU:HD11	1:A:59:THR:HB	19	0.12
(1,2190)	1:A:58:LEU:HD12	1:A:59:THR:HB	19	0.12
(1,2190)	1:A:58:LEU:HD13	1:A:59:THR:HB	19	0.12
(1,2190)	1:A:58:LEU:HD21	1:A:59:THR:HB	19	0.12
(1,2190)	1:A:58:LEU:HD22	1:A:59:THR:HB	19	0.12
(1,2190)	1:A:58:LEU:HD23	1:A:59:THR:HB	19	0.12
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD11	18	0.12
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD12	18	0.12
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD13	18	0.12
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD21	18	0.12
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD22	18	0.12
(1,2167)	1:A:55:SER:H	1:A:58:LEU:HD23	18	0.12
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG11	17	0.12
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG12	17	0.12
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG13	17	0.12
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG21	17	0.12
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG22	17	0.12
(1,2150)	1:A:51:ARG:HA	1:A:53:VAL:HG23	17	0.12
(1,2095)	1:A:40:LYS:HE2	1:A:43:GLU:HG2	12	0.12
(1,2095)	1:A:40:LYS:HE2	1:A:43:GLU:HG3	12	0.12
(1,2095)	1:A:40:LYS:HE3	1:A:43:GLU:HG2	12	0.12
(1,2095)	1:A:40:LYS:HE3	1:A:43:GLU:HG3	12	0.12
(1,204)	1:A:36:LEU:HB3	1:A:38:LEU:H	5	0.12
(1,1916)	1:A:17:ARG:HD2	1:A:76:ILE:HG21	13	0.12
(1,1916)	1:A:17:ARG:HD2	1:A:76:ILE:HG22	13	0.12
(1,1916)	1:A:17:ARG:HD2	1:A:76:ILE:HG23	13	0.12
(1,1916)	1:A:17:ARG:HD3	1:A:76:ILE:HG21	13	0.12
(1,1916)	1:A:17:ARG:HD3	1:A:76:ILE:HG22	13	0.12
(1,1916)	1:A:17:ARG:HD3	1:A:76:ILE:HG23	13	0.12
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD11	14	0.12
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD12	14	0.12
(1,1692)	1:A:151:LEU:HA	1:A:151:LEU:HD13	14	0.12
(1,1635)	1:A:133:TRP:HA	1:A:133:TRP:HD1	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1635)	1:A:133:TRP:HA	1:A:133:TRP:HD1	8	0.12
(1,1415)	1:A:31:LEU:HG	1:A:98:PHE:HB2	11	0.12
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB1	9	0.12
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB2	9	0.12
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB3	9	0.12
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB1	14	0.12
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB2	14	0.12
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB3	14	0.12
(1,1147)	1:A:4:LEU:HG	1:A:46:GLN:HB3	14	0.12
(1,1136)	1:A:40:LYS:HG3	1:A:44:MET:HB2	20	0.12
(1,1136)	1:A:40:LYS:HG3	1:A:44:MET:HB3	20	0.12
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE2	3	0.12
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE3	3	0.12
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE2	3	0.12
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE3	3	0.12
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE2	3	0.12
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE3	3	0.12
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE2	12	0.12
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE3	12	0.12
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE2	12	0.12
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE3	12	0.12
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE2	12	0.12
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE3	12	0.12
(1,1037)	1:A:31:LEU:HD21	1:A:98:PHE:HA	19	0.12
(1,1037)	1:A:31:LEU:HD22	1:A:98:PHE:HA	19	0.12
(1,1037)	1:A:31:LEU:HD23	1:A:98:PHE:HA	19	0.12
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	1	0.12
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	9	0.12
(1,1008)	1:A:107:ASP:HA	1:A:110:LYS:HA	11	0.12
(1,1008)	1:A:107:ASP:HA	1:A:110:LYS:HA	13	0.12
(1,1008)	1:A:107:ASP:HA	1:A:110:LYS:HA	18	0.12
(1,969)	1:A:17:ARG:H	1:A:17:ARG:HD3	10	0.11
(1,950)	1:A:16:LYS:HA	1:A:16:LYS:HE2	4	0.11
(1,950)	1:A:16:LYS:HA	1:A:16:LYS:HE3	4	0.11
(1,950)	1:A:16:LYS:HA	1:A:16:LYS:HE2	10	0.11
(1,950)	1:A:16:LYS:HA	1:A:16:LYS:HE3	10	0.11
(1,872)	1:A:9:THR:HA	1:A:12:GLN:HB3	16	0.11
(1,684)	1:A:124:VAL:HA	1:A:125:SER:H	17	0.11
(1,320)	1:A:58:LEU:HD11	1:A:59:THR:H	14	0.11
(1,320)	1:A:58:LEU:HD12	1:A:59:THR:H	14	0.11
(1,320)	1:A:58:LEU:HD13	1:A:59:THR:H	14	0.11
(1,231)	1:A:40:LYS:HD2	1:A:42:LEU:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:A:40:LYS:HD3	1:A:42:LEU:H	7	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB1	9	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB2	9	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB3	9	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB1	9	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB2	9	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB3	9	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB1	12	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB2	12	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB3	12	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB1	12	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB2	12	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB3	12	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB1	13	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB2	13	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB3	13	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB1	13	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB2	13	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB3	13	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB1	15	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB2	15	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB3	15	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB1	15	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB2	15	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB3	15	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB1	17	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB2	17	0.11
(1,2234)	1:A:66:LYS:HB2	1:A:67:ALA:HB3	17	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB1	17	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB2	17	0.11
(1,2234)	1:A:66:LYS:HB3	1:A:67:ALA:HB3	17	0.11
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG11	15	0.11
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG12	15	0.11
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG13	15	0.11
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG21	15	0.11
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG22	15	0.11
(1,2157)	1:A:52:SER:HA	1:A:53:VAL:HG23	15	0.11
(1,2095)	1:A:40:LYS:HE2	1:A:43:GLU:HG2	3	0.11
(1,2095)	1:A:40:LYS:HE2	1:A:43:GLU:HG3	3	0.11
(1,2095)	1:A:40:LYS:HE3	1:A:43:GLU:HG2	3	0.11
(1,2095)	1:A:40:LYS:HE3	1:A:43:GLU:HG3	3	0.11
(1,2094)	1:A:40:LYS:HD2	1:A:44:MET:HG2	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2094)	1:A:40:LYS:HD2	1:A:44:MET:HG3	13	0.11
(1,2094)	1:A:40:LYS:HD3	1:A:44:MET:HG2	13	0.11
(1,2094)	1:A:40:LYS:HD3	1:A:44:MET:HG3	13	0.11
(1,2046)	1:A:36:LEU:HD11	1:A:40:LYS:HD2	1	0.11
(1,2046)	1:A:36:LEU:HD11	1:A:40:LYS:HD3	1	0.11
(1,2046)	1:A:36:LEU:HD12	1:A:40:LYS:HD2	1	0.11
(1,2046)	1:A:36:LEU:HD12	1:A:40:LYS:HD3	1	0.11
(1,2046)	1:A:36:LEU:HD13	1:A:40:LYS:HD2	1	0.11
(1,2046)	1:A:36:LEU:HD13	1:A:40:LYS:HD3	1	0.11
(1,2046)	1:A:36:LEU:HD21	1:A:40:LYS:HD2	1	0.11
(1,2046)	1:A:36:LEU:HD21	1:A:40:LYS:HD3	1	0.11
(1,2046)	1:A:36:LEU:HD22	1:A:40:LYS:HD2	1	0.11
(1,2046)	1:A:36:LEU:HD22	1:A:40:LYS:HD3	1	0.11
(1,2046)	1:A:36:LEU:HD23	1:A:40:LYS:HD2	1	0.11
(1,2046)	1:A:36:LEU:HD23	1:A:40:LYS:HD3	1	0.11
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG11	14	0.11
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG12	14	0.11
(1,1433)	1:A:99:LYS:H	1:A:101:VAL:HG13	14	0.11
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB1	1	0.11
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB2	1	0.11
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB3	1	0.11
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB1	18	0.11
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB2	18	0.11
(1,1233)	1:A:65:PHE:H	1:A:68:ALA:HB3	18	0.11
(1,1160)	1:A:138:GLN:HA	1:A:138:GLN:HG3	11	0.11
(1,1136)	1:A:40:LYS:HG3	1:A:44:MET:HB2	13	0.11
(1,1136)	1:A:40:LYS:HG3	1:A:44:MET:HB3	13	0.11
(1,1101)	1:A:36:LEU:HA	1:A:39:ILE:HG21	18	0.11
(1,1101)	1:A:36:LEU:HA	1:A:39:ILE:HG22	18	0.11
(1,1101)	1:A:36:LEU:HA	1:A:39:ILE:HG23	18	0.11
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE2	9	0.11
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE3	9	0.11
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE2	9	0.11
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE3	9	0.11
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE2	9	0.11
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE3	9	0.11
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE2	11	0.11
(1,1086)	1:A:39:ILE:HD11	1:A:40:LYS:HE3	11	0.11
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE2	11	0.11
(1,1086)	1:A:39:ILE:HD12	1:A:40:LYS:HE3	11	0.11
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE2	11	0.11
(1,1086)	1:A:39:ILE:HD13	1:A:40:LYS:HE3	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	1:A:31:LEU:HD21	1:A:98:PHE:HA	3	0.11
(1,1037)	1:A:31:LEU:HD22	1:A:98:PHE:HA	3	0.11
(1,1037)	1:A:31:LEU:HD23	1:A:98:PHE:HA	3	0.11
(1,1020)	1:A:22:LYS:HA	1:A:25:LYS:HE2	12	0.11
(1,1020)	1:A:22:LYS:HA	1:A:25:LYS:HE3	12	0.11
(1,1012)	1:A:63:ASN:HA	1:A:66:LYS:HA	2	0.11
(1,1008)	1:A:107:ASP:HA	1:A:110:LYS:HA	15	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found