Full wwPDB NMR Structure Validation Report

Dec 24, 2024 – 03:41 PM EST

PDB ID	:	2LFV
BMRB ID	:	17783
Title	:	Solution Structure of the SPOR domain from E. coli DamX
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Deposited on	:	2011-07-15

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:

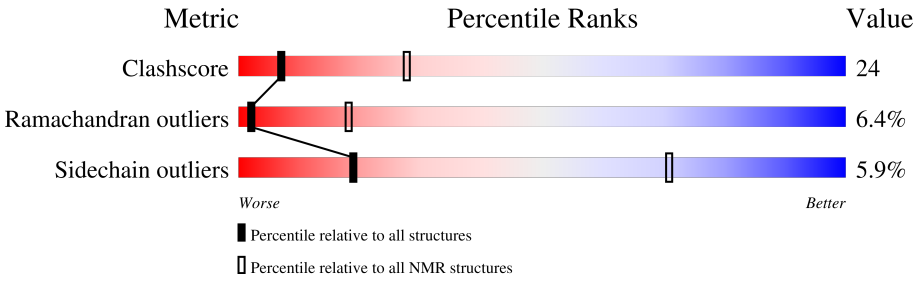
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 96%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	106	43% 30% • 25%

2 Ensemble composition and analysis

This entry contains 25 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:345-A:424 (80)	0.85	1

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 6, 7, 9, 11, 12, 13, 16, 17, 18, 19, 20, 21, 22, 23, 25
2	8, 10, 15
3	5, 14
Single-model clusters	24

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1652 atoms, of which 815 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein damX.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	106	1652	522	815	157	157	1	0

There are 15 discrepancies between the modelled and reference sequences:

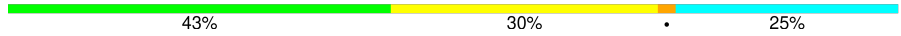
Chain	Residue	Modelled	Actual	Comment	Reference
A	323	MET	-	expression tag	UNP P11557
A	324	ARG	-	expression tag	UNP P11557
A	325	GLY	-	expression tag	UNP P11557
A	326	SER	-	expression tag	UNP P11557
A	327	HIS	-	expression tag	UNP P11557
A	328	HIS	-	expression tag	UNP P11557
A	329	HIS	-	expression tag	UNP P11557
A	330	HIS	-	expression tag	UNP P11557
A	331	HIS	-	expression tag	UNP P11557
A	332	HIS	-	expression tag	UNP P11557
A	333	GLY	-	expression tag	UNP P11557
A	334	SER	-	expression tag	UNP P11557
A	335	ASN	-	expression tag	UNP P11557
A	336	ASN	-	expression tag	UNP P11557
A	337	ASN	-	expression tag	UNP P11557

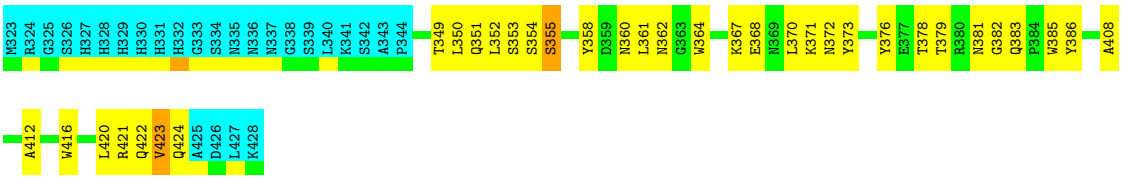
4 Residue-property plots (i)

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: Protein damX

Chain A: 



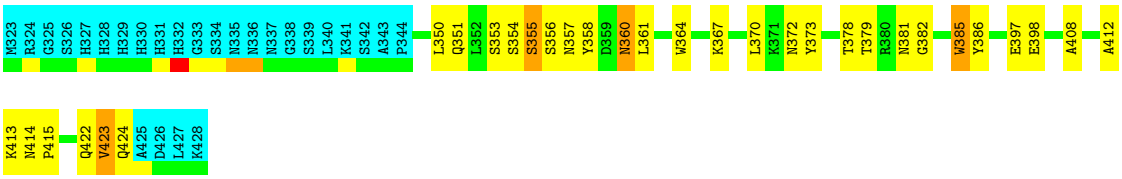
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Protein damX

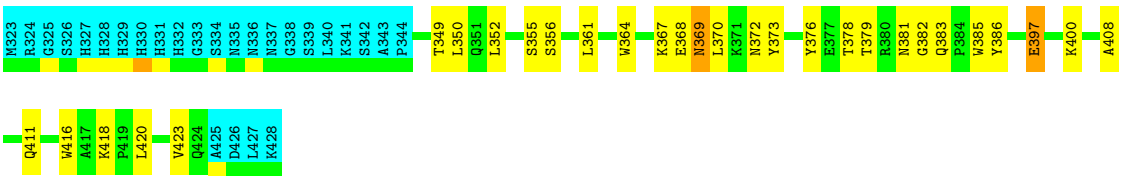
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: Protein damX

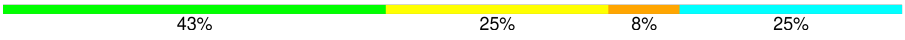
Chain A: 



4.2.3 Score per residue for model 3

• Molecule 1: Protein damX

Chain A:



4.2.4 Score per residue for model 4

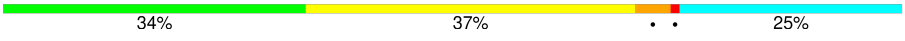
• Molecule 1: Protein damX

Chain A:

4.2.5 Score per residue for model 5

• Molecule 1: Protein damX

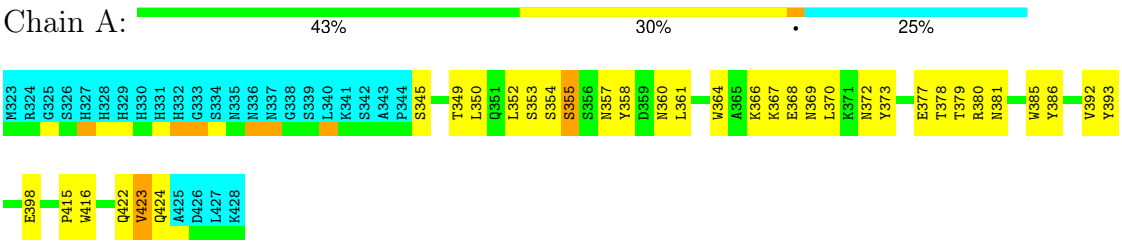
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Protein damX

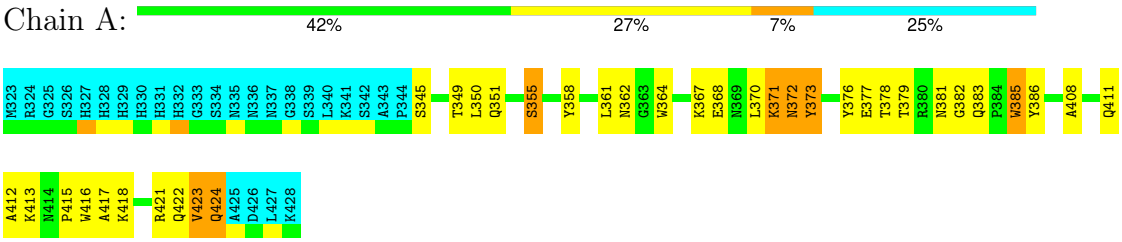
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Protein damX

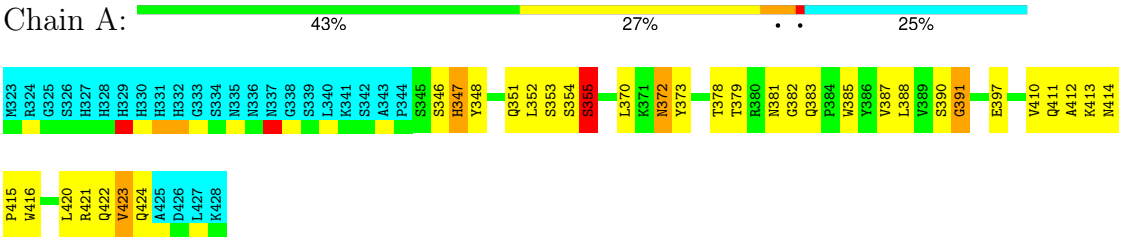
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: Protein damX

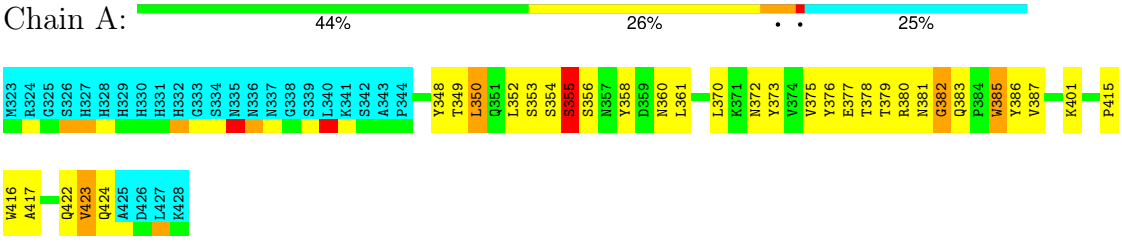
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: Protein damX

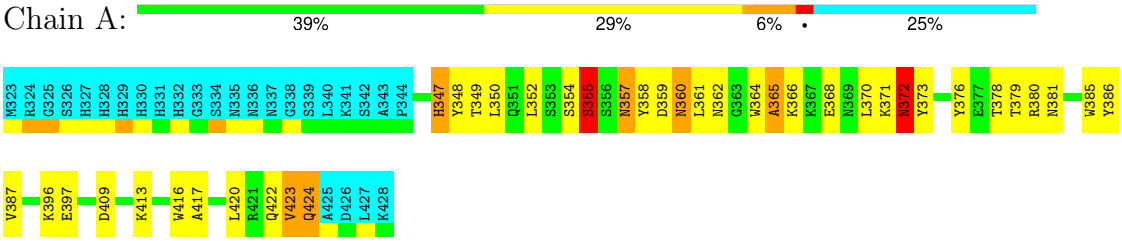
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Protein damX

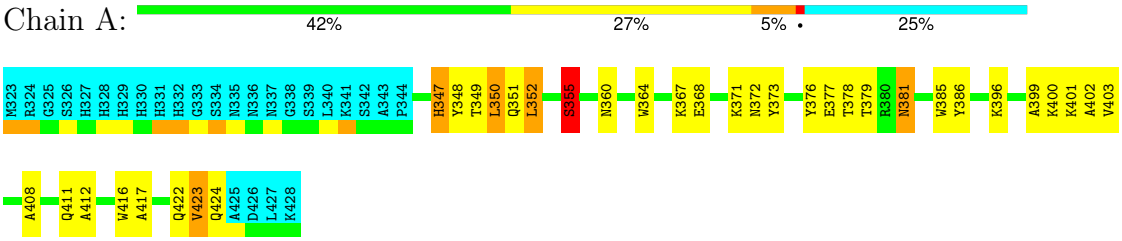
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Protein damX

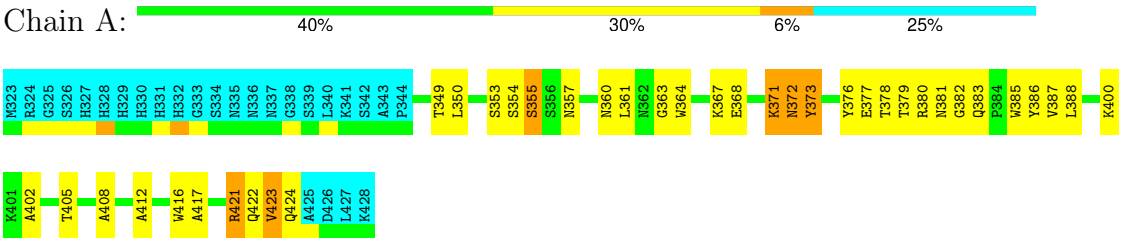
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Protein damX

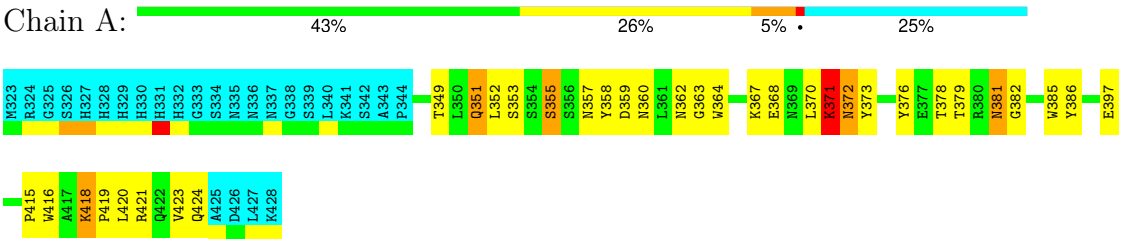
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Protein damX

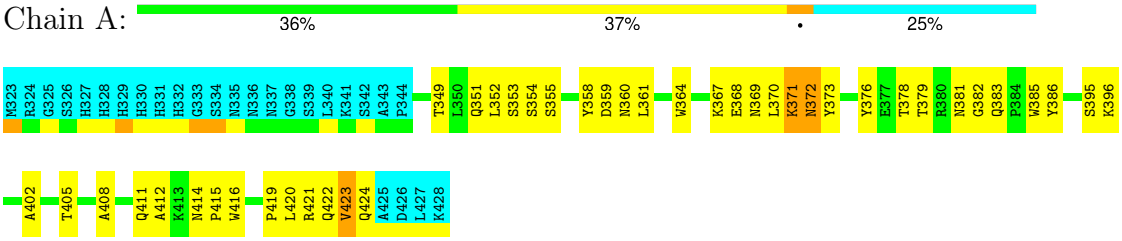
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Protein damX

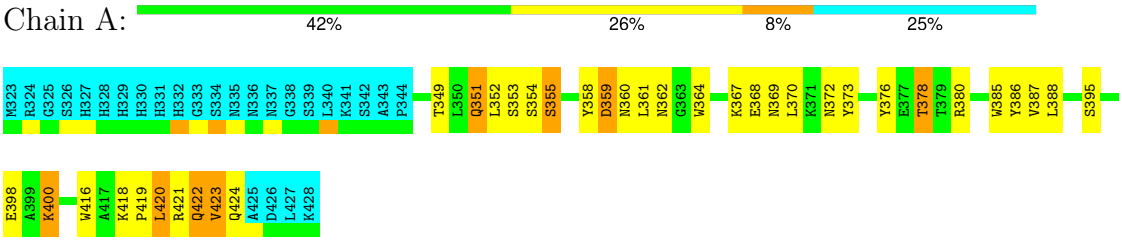
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Protein damX

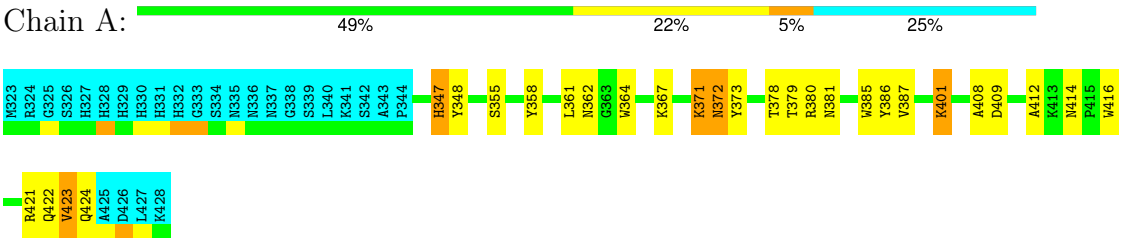
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Protein damX

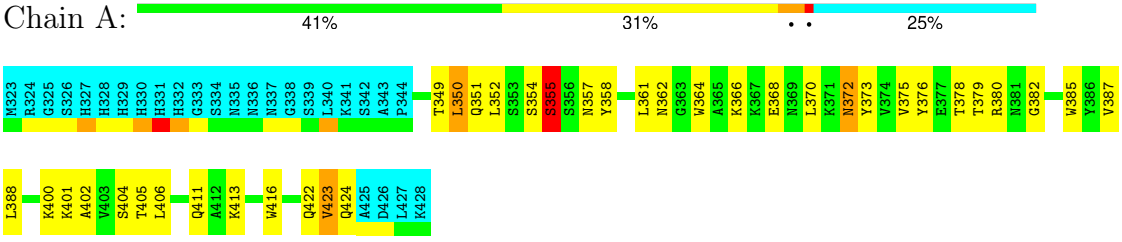
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Protein damX

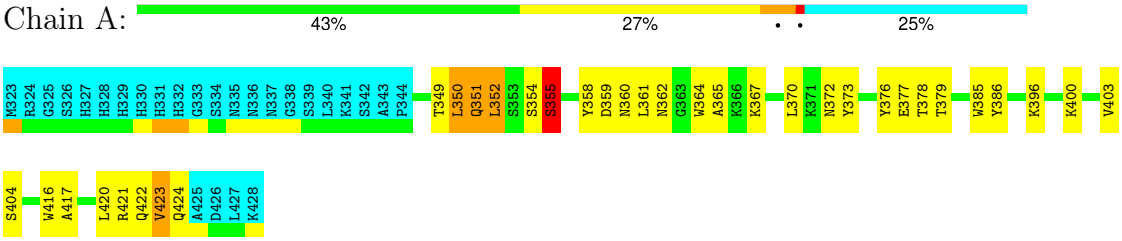
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Protein damX

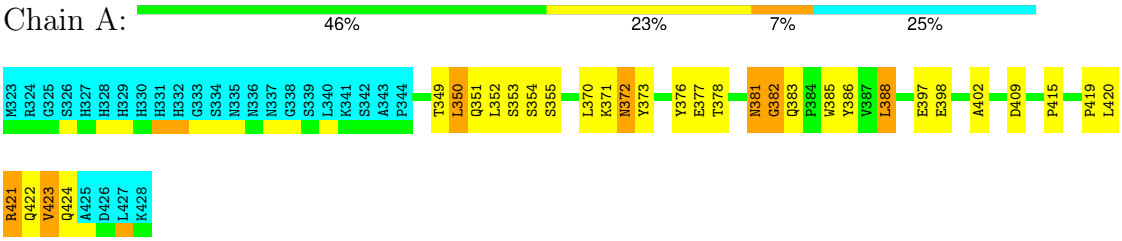
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Protein damX

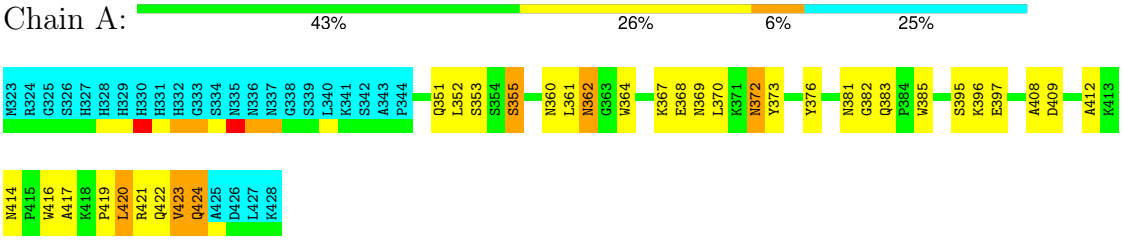
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Protein damX

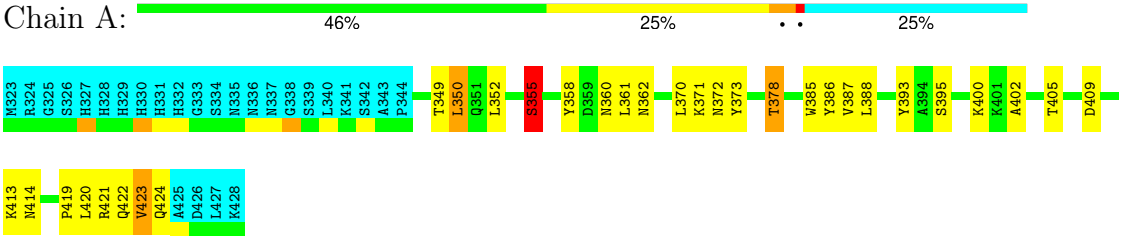
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: Protein damX

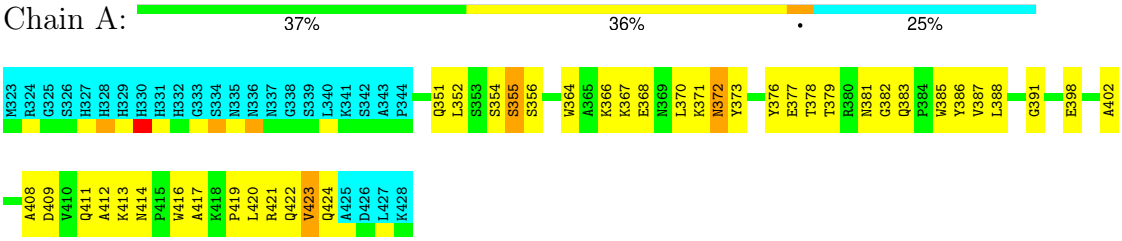
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: Protein damX

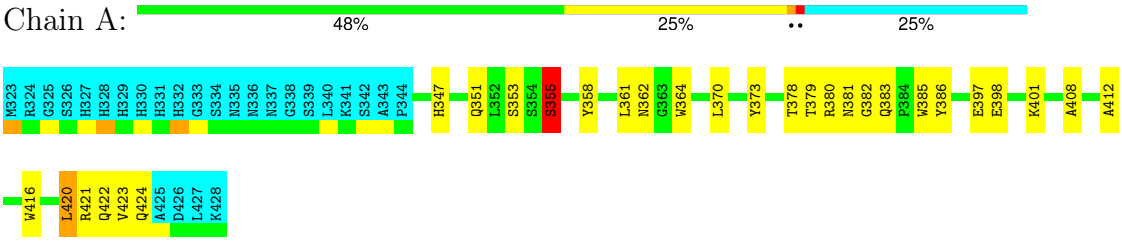
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: Protein damX

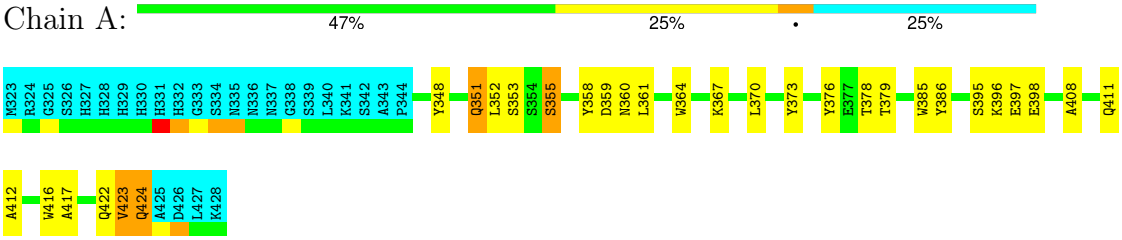
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: Protein damX

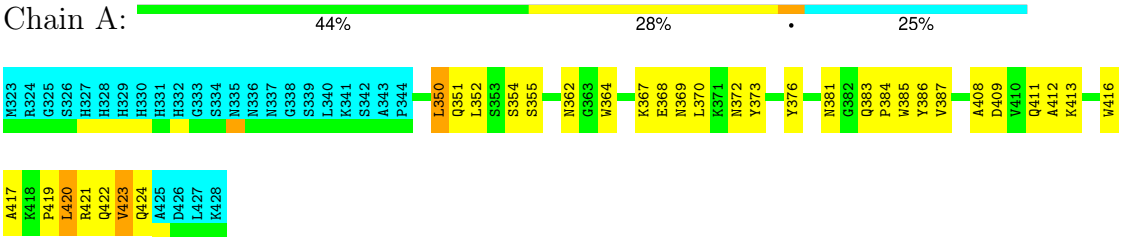
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: Protein damX

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 250 calculated structures, 25 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.23
X-PLOR NIH	refinement	2.23

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	1284
Number of shifts mapped to atoms	1283
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	96%

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	640	630	629	30±5
All	All	16000	15750	15725	749

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:352:LEU:N	1:A:352:LEU:HD13	0.79	1.92	18	1
1:A:388:LEU:HD22	1:A:388:LEU:N	0.77	1.95	19	3
1:A:378:THR:HG22	1:A:379:THR:H	0.69	1.48	2	4
1:A:361:LEU:HD12	1:A:385:TRP:CH2	0.64	2.27	21	5
1:A:361:LEU:C	1:A:361:LEU:HD13	0.63	2.14	16	3
1:A:378:THR:HG22	1:A:379:THR:N	0.63	2.08	14	4
1:A:416:TRP:CE2	1:A:418:LYS:NZ	0.62	2.68	2	1
1:A:385:TRP:CG	1:A:386:TYR:N	0.62	2.68	25	10
1:A:396:LYS:NZ	1:A:400:LYS:NZ	0.61	2.49	18	1
1:A:351:GLN:NE2	1:A:380:ARG:NH1	0.61	2.48	23	1
1:A:386:TYR:CD1	1:A:386:TYR:N	0.60	2.69	21	9
1:A:352:LEU:N	1:A:352:LEU:CD1	0.60	2.65	18	7
1:A:354:SER:H	1:A:413:LYS:HZ2	0.59	1.40	8	1
1:A:386:TYR:N	1:A:386:TYR:CD1	0.59	2.70	25	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:402:ALA:O	1:A:405:THR:HG22	0.59	1.97	4	3
1:A:355:SER:N	1:A:380:ARG:HH12	0.58	1.96	9	1
1:A:352:LEU:HD12	1:A:352:LEU:N	0.57	2.14	24	6
1:A:420:LEU:C	1:A:420:LEU:HD12	0.57	2.20	13	1
1:A:372:ASN:HD22	1:A:372:ASN:N	0.57	1.96	16	1
1:A:388:LEU:N	1:A:388:LEU:CD2	0.57	2.67	19	3
1:A:385:TRP:CD2	1:A:386:TYR:N	0.56	2.73	12	11
1:A:351:GLN:NE2	1:A:380:ARG:HH22	0.56	1.98	17	1
1:A:358:TYR:CE1	1:A:362:ASN:ND2	0.56	2.74	23	3
1:A:352:LEU:HD22	1:A:352:LEU:N	0.55	2.16	19	1
1:A:355:SER:OG	1:A:356:SER:N	0.55	2.40	22	3
1:A:421:ARG:NH2	1:A:422:GLN:NE2	0.55	2.55	12	1
1:A:381:ASN:HD22	1:A:381:ASN:N	0.55	1.98	25	2
1:A:355:SER:O	1:A:385:TRP:CE3	0.55	2.60	12	23
1:A:361:LEU:HD22	1:A:385:TRP:CH2	0.55	2.37	12	7
1:A:396:LYS:HZ2	1:A:400:LYS:NZ	0.54	2.00	18	1
1:A:355:SER:OG	1:A:385:TRP:CH2	0.54	2.60	4	1
1:A:420:LEU:N	1:A:420:LEU:HD12	0.54	2.17	10	1
1:A:422:GLN:O	1:A:424:GLN:N	0.54	2.41	19	22
1:A:416:TRP:CD1	1:A:416:TRP:N	0.54	2.75	4	7
1:A:370:LEU:O	1:A:373:TYR:CE1	0.54	2.61	25	18
1:A:420:LEU:CD2	1:A:420:LEU:N	0.54	2.71	8	2
1:A:388:LEU:N	1:A:388:LEU:CD1	0.54	2.71	15	1
1:A:351:GLN:HE22	1:A:380:ARG:NH1	0.54	2.01	17	1
1:A:351:GLN:OE1	1:A:353:SER:N	0.54	2.41	24	4
1:A:395:SER:O	1:A:397:GLU:N	0.53	2.41	20	1
1:A:370:LEU:O	1:A:373:TYR:CD1	0.53	2.62	24	15
1:A:347:HIS:O	1:A:348:TYR:CD2	0.53	2.61	8	4
1:A:388:LEU:N	1:A:388:LEU:HD12	0.53	2.17	15	1
1:A:420:LEU:N	1:A:420:LEU:HD22	0.53	2.17	8	2
1:A:364:TRP:CD1	1:A:368:GLU:OE1	0.53	2.62	25	8
1:A:352:LEU:N	1:A:352:LEU:CD2	0.53	2.71	19	1
1:A:354:SER:OG	1:A:380:ARG:NH1	0.53	2.42	9	1
1:A:364:TRP:O	1:A:367:LYS:N	0.53	2.42	22	13
1:A:364:TRP:CZ2	1:A:368:GLU:OE1	0.53	2.62	12	4
1:A:381:ASN:O	1:A:383:GLN:N	0.53	2.42	12	12
1:A:352:LEU:CD1	1:A:352:LEU:N	0.53	2.72	6	3
1:A:372:ASN:O	1:A:372:ASN:ND2	0.53	2.42	12	5
1:A:372:ASN:N	1:A:372:ASN:ND2	0.53	2.53	16	1
1:A:416:TRP:CE3	1:A:417:ALA:O	0.53	2.62	9	12
1:A:355:SER:O	1:A:385:TRP:CD2	0.53	2.61	17	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:355:SER:O	1:A:380:ARG:NH1	0.53	2.42	9	1
1:A:351:GLN:OE1	1:A:416:TRP:NE1	0.53	2.42	20	1
1:A:351:GLN:NE2	1:A:353:SER:O	0.52	2.43	1	1
1:A:380:ARG:NH1	1:A:381:ASN:ND2	0.52	2.57	6	2
1:A:360:ASN:N	1:A:360:ASN:OD1	0.52	2.42	10	1
1:A:376:TYR:CE2	1:A:378:THR:OG1	0.52	2.62	2	2
1:A:358:TYR:O	1:A:361:LEU:N	0.52	2.41	10	6
1:A:411:GLN:O	1:A:414:ASN:N	0.52	2.42	14	3
1:A:364:TRP:NE1	1:A:368:GLU:OE1	0.52	2.42	25	3
1:A:385:TRP:CE2	1:A:386:TYR:O	0.52	2.63	23	4
1:A:360:ASN:OD1	1:A:361:LEU:N	0.52	2.42	12	1
1:A:351:GLN:HE22	1:A:353:SER:CA	0.52	2.17	24	1
1:A:350:LEU:N	1:A:350:LEU:CD2	0.52	2.72	2	7
1:A:390:SER:OG	1:A:391:GLY:N	0.52	2.42	8	1
1:A:356:SER:OG	1:A:380:ARG:NH2	0.52	2.42	9	1
1:A:385:TRP:CZ2	1:A:386:TYR:O	0.52	2.63	25	10
1:A:395:SER:OG	1:A:396:LYS:N	0.52	2.41	24	3
1:A:358:TYR:O	1:A:360:ASN:N	0.52	2.43	5	7
1:A:377:GLU:OE1	1:A:377:GLU:N	0.52	2.43	9	1
1:A:402:ALA:O	1:A:405:THR:N	0.52	2.42	21	2
1:A:364:TRP:CH2	1:A:368:GLU:OE1	0.52	2.62	17	1
1:A:408:ALA:O	1:A:412:ALA:N	0.52	2.42	25	12
1:A:359:ASP:O	1:A:362:ASN:ND2	0.52	2.42	5	4
1:A:349:THR:HG23	1:A:349:THR:O	0.52	2.05	2	5
1:A:408:ALA:O	1:A:411:GLN:N	0.52	2.42	22	6
1:A:357:ASN:ND2	1:A:360:ASN:OD1	0.52	2.43	13	2
1:A:378:THR:OG1	1:A:379:THR:N	0.52	2.43	9	8
1:A:351:GLN:NE2	1:A:416:TRP:HE1	0.52	2.03	3	2
1:A:350:LEU:N	1:A:350:LEU:HD22	0.51	2.20	2	7
1:A:350:LEU:HD12	1:A:350:LEU:N	0.51	2.20	9	1
1:A:351:GLN:NE2	1:A:354:SER:OG	0.51	2.44	17	1
1:A:414:ASN:O	1:A:414:ASN:ND2	0.51	2.43	1	2
1:A:385:TRP:CE3	1:A:386:TYR:N	0.51	2.79	14	5
1:A:395:SER:N	1:A:398:GLU:OE2	0.51	2.43	15	1
1:A:353:SER:OG	1:A:354:SER:N	0.51	2.44	3	9
1:A:352:LEU:N	1:A:352:LEU:HD12	0.51	2.21	4	3
1:A:354:SER:H	1:A:413:LYS:NZ	0.51	2.04	8	2
1:A:387:VAL:HG11	1:A:418:LYS:HZ2	0.51	1.65	3	1
1:A:364:TRP:CH2	1:A:368:GLU:OE2	0.51	2.64	6	1
1:A:421:ARG:O	1:A:421:ARG:NE	0.51	2.44	12	1
1:A:378:THR:HG23	1:A:379:THR:N	0.50	2.21	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:420:LEU:O	1:A:422:GLN:N	0.50	2.45	19	4
1:A:364:TRP:CZ2	1:A:368:GLU:OE2	0.50	2.65	6	2
1:A:381:ASN:N	1:A:381:ASN:OD1	0.50	2.43	11	1
1:A:377:GLU:H	1:A:377:GLU:CD	0.50	2.10	19	3
1:A:376:TYR:N	1:A:376:TYR:CD1	0.50	2.79	20	7
1:A:375:VAL:HG23	1:A:375:VAL:O	0.50	2.07	17	3
1:A:352:LEU:HD13	1:A:352:LEU:H	0.50	1.64	18	1
1:A:422:GLN:C	1:A:424:GLN:N	0.50	2.65	20	21
1:A:381:ASN:N	1:A:381:ASN:ND2	0.49	2.60	25	2
1:A:357:ASN:N	1:A:357:ASN:ND2	0.49	2.59	10	1
1:A:355:SER:H	1:A:380:ARG:NH1	0.49	2.05	9	1
1:A:357:ASN:N	1:A:357:ASN:OD1	0.49	2.43	17	1
1:A:398:GLU:CD	1:A:398:GLU:H	0.49	2.10	15	3
1:A:380:ARG:NH2	1:A:416:TRP:CZ2	0.49	2.81	12	1
1:A:387:VAL:HG11	1:A:418:LYS:NZ	0.48	2.23	3	1
1:A:420:LEU:HD23	1:A:420:LEU:O	0.48	2.08	3	4
1:A:353:SER:OG	1:A:364:TRP:CH2	0.48	2.60	23	2
1:A:420:LEU:HD12	1:A:421:ARG:N	0.48	2.22	13	1
1:A:355:SER:N	1:A:380:ARG:NH1	0.48	2.60	9	1
1:A:350:LEU:N	1:A:350:LEU:CD1	0.48	2.76	9	1
1:A:351:GLN:NE2	1:A:353:SER:C	0.48	2.67	3	2
1:A:361:LEU:O	1:A:361:LEU:HD23	0.48	2.09	20	1
1:A:351:GLN:NE2	1:A:380:ARG:CZ	0.48	2.77	23	1
1:A:419:PRO:O	1:A:421:ARG:N	0.48	2.47	22	3
1:A:358:TYR:C	1:A:360:ASN:N	0.48	2.67	13	7
1:A:376:TYR:CE1	1:A:387:VAL:O	0.48	2.67	12	4
1:A:360:ASN:N	1:A:360:ASN:ND2	0.48	2.59	13	1
1:A:347:HIS:O	1:A:420:LEU:CD1	0.48	2.62	23	1
1:A:396:LYS:NZ	1:A:396:LYS:CB	0.48	2.77	5	3
1:A:355:SER:C	1:A:385:TRP:CE3	0.48	2.87	23	7
1:A:388:LEU:CD2	1:A:388:LEU:N	0.47	2.76	3	1
1:A:376:TYR:CD2	1:A:377:GLU:O	0.47	2.67	7	4
1:A:377:GLU:CD	1:A:377:GLU:N	0.47	2.67	12	1
1:A:356:SER:O	1:A:357:ASN:ND2	0.47	2.48	1	1
1:A:364:TRP:CZ2	1:A:368:GLU:CD	0.47	2.87	10	3
1:A:378:THR:CG2	1:A:379:THR:N	0.47	2.78	2	4
1:A:397:GLU:CG	1:A:398:GLU:N	0.47	2.77	1	3
1:A:364:TRP:NE1	1:A:368:GLU:CD	0.47	2.67	13	3
1:A:398:GLU:CD	1:A:398:GLU:N	0.47	2.68	5	2
1:A:351:GLN:NE2	1:A:351:GLN:C	0.47	2.68	11	1
1:A:360:ASN:N	1:A:360:ASN:HD22	0.47	2.06	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:420:LEU:C	1:A:422:GLN:N	0.47	2.67	23	4
1:A:378:THR:N	1:A:385:TRP:O	0.47	2.46	21	4
1:A:362:ASN:OD1	1:A:363:GLY:N	0.47	2.48	5	2
1:A:421:ARG:NE	1:A:421:ARG:C	0.47	2.68	12	1
1:A:368:GLU:CD	1:A:368:GLU:N	0.47	2.67	13	3
1:A:367:LYS:O	1:A:369:ASN:ND2	0.47	2.46	20	2
1:A:398:GLU:N	1:A:398:GLU:OE1	0.47	2.48	5	1
1:A:405:THR:HG23	1:A:406:LEU:N	0.46	2.25	17	1
1:A:398:GLU:O	1:A:402:ALA:N	0.46	2.47	3	2
1:A:396:LYS:HZ2	1:A:400:LYS:HZ2	0.46	1.53	18	1
1:A:388:LEU:N	1:A:388:LEU:HD22	0.46	2.25	3	1
1:A:358:TYR:CE1	1:A:362:ASN:OD1	0.46	2.69	7	1
1:A:351:GLN:CD	1:A:352:LEU:N	0.46	2.68	11	1
1:A:351:GLN:NE2	1:A:380:ARG:HH12	0.46	2.09	17	1
1:A:377:GLU:CG	1:A:378:THR:N	0.46	2.78	18	3
1:A:351:GLN:NE2	1:A:352:LEU:N	0.46	2.63	11	1
1:A:364:TRP:CE2	1:A:368:GLU:OE1	0.46	2.69	13	2
1:A:419:PRO:C	1:A:421:ARG:N	0.46	2.68	22	7
1:A:355:SER:O	1:A:385:TRP:CG	0.46	2.69	10	1
1:A:364:TRP:CE2	1:A:368:GLU:CD	0.46	2.89	10	1
1:A:359:ASP:C	1:A:362:ASN:ND2	0.46	2.69	15	2
1:A:378:THR:CG2	1:A:379:THR:H	0.46	2.22	14	4
1:A:400:LYS:CB	1:A:400:LYS:NZ	0.46	2.77	21	2
1:A:351:GLN:OE1	1:A:416:TRP:CD1	0.46	2.68	20	1
1:A:362:ASN:C	1:A:362:ASN:HD22	0.46	2.14	20	1
1:A:361:LEU:O	1:A:365:ALA:N	0.45	2.48	18	1
1:A:351:GLN:HE22	1:A:380:ARG:NH2	0.45	2.08	23	1
1:A:345:SER:OG	1:A:421:ARG:N	0.45	2.50	7	1
1:A:421:ARG:C	1:A:421:ARG:HE	0.45	2.14	12	1
1:A:357:ASN:O	1:A:357:ASN:ND2	0.45	2.49	4	1
1:A:420:LEU:H	1:A:420:LEU:HD12	0.45	1.72	23	1
1:A:361:LEU:HD12	1:A:385:TRP:CZ2	0.45	2.46	23	3
1:A:351:GLN:HE22	1:A:380:ARG:CZ	0.45	2.24	23	1
1:A:351:GLN:CD	1:A:416:TRP:HE1	0.45	2.15	22	3
1:A:373:TYR:CD1	1:A:373:TYR:C	0.45	2.90	12	1
1:A:362:ASN:C	1:A:362:ASN:ND2	0.45	2.70	20	1
1:A:380:ARG:NH2	1:A:418:LYS:NZ	0.45	2.64	15	2
1:A:401:LYS:CB	1:A:401:LYS:NZ	0.45	2.79	16	1
1:A:368:GLU:N	1:A:368:GLU:CD	0.45	2.70	3	3
1:A:413:LYS:CD	1:A:413:LYS:H	0.45	2.25	4	1
1:A:363:GLY:O	1:A:367:LYS:N	0.45	2.48	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:376:TYR:CD1	1:A:376:TYR:N	0.45	2.85	25	2
1:A:422:GLN:O	1:A:423:VAL:C	0.45	2.56	25	1
1:A:349:THR:O	1:A:350:LEU:HD22	0.44	2.12	10	2
1:A:409:ASP:N	1:A:409:ASP:OD1	0.44	2.50	5	2
1:A:354:SER:N	1:A:413:LYS:HZ2	0.44	2.09	8	1
1:A:418:LYS:NZ	1:A:418:LYS:CB	0.44	2.80	13	1
1:A:351:GLN:OE1	1:A:351:GLN:O	0.44	2.35	15	1
1:A:385:TRP:NE1	1:A:387:VAL:HG22	0.44	2.27	10	1
1:A:381:ASN:C	1:A:383:GLN:N	0.44	2.70	12	7
1:A:372:ASN:C	1:A:372:ASN:ND2	0.44	2.71	10	1
1:A:351:GLN:HE22	1:A:380:ARG:HH12	0.44	1.54	17	1
1:A:372:ASN:ND2	1:A:372:ASN:O	0.44	2.49	16	1
1:A:359:ASP:C	1:A:362:ASN:HD21	0.44	2.16	15	1
1:A:351:GLN:NE2	1:A:380:ARG:NH2	0.44	2.64	17	1
1:A:411:GLN:C	1:A:413:LYS:N	0.44	2.71	17	1
1:A:351:GLN:O	1:A:351:GLN:OE1	0.44	2.36	3	2
1:A:345:SER:CB	1:A:424:GLN:HE22	0.44	2.25	6	1
1:A:390:SER:O	1:A:391:GLY:O	0.44	2.36	8	1
1:A:400:LYS:C	1:A:402:ALA:N	0.44	2.69	5	1
1:A:361:LEU:C	1:A:361:LEU:CD1	0.43	2.86	15	3
1:A:349:THR:O	1:A:350:LEU:O	0.43	2.36	19	2
1:A:357:ASN:O	1:A:360:ASN:OD1	0.43	2.36	12	1
1:A:357:ASN:ND2	1:A:360:ASN:ND2	0.43	2.66	13	1
1:A:371:LYS:O	1:A:372:ASN:O	0.43	2.37	14	2
1:A:351:GLN:CG	1:A:353:SER:O	0.43	2.66	20	1
1:A:387:VAL:C	1:A:388:LEU:HD12	0.43	2.33	21	1
1:A:362:ASN:O	1:A:366:LYS:CG	0.43	2.66	3	2
1:A:371:LYS:O	1:A:373:TYR:N	0.43	2.51	12	1
1:A:401:LYS:O	1:A:404:SER:N	0.43	2.50	17	1
1:A:364:TRP:O	1:A:368:GLU:OE1	0.43	2.37	20	3
1:A:387:VAL:HG22	1:A:388:LEU:N	0.43	2.28	17	2
1:A:368:GLU:CD	1:A:370:LEU:HD21	0.43	2.34	6	1
1:A:380:ARG:NH1	1:A:381:ASN:OD1	0.43	2.51	10	1
1:A:352:LEU:O	1:A:353:SER:OG	0.43	2.36	13	1
1:A:416:TRP:CZ2	1:A:418:LYS:NZ	0.43	2.84	13	1
1:A:405:THR:CG2	1:A:406:LEU:N	0.43	2.81	17	1
1:A:361:LEU:CD1	1:A:386:TYR:O	0.43	2.67	18	1
1:A:395:SER:C	1:A:397:GLU:N	0.43	2.68	20	1
1:A:376:TYR:CE2	1:A:378:THR:CG2	0.43	3.02	24	1
1:A:400:LYS:O	1:A:402:ALA:N	0.43	2.52	5	1
1:A:371:LYS:O	1:A:372:ASN:C	0.43	2.57	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:373:TYR:C	1:A:373:TYR:CD1	0.43	2.90	7	1
1:A:400:LYS:CG	1:A:401:LYS:N	0.43	2.81	11	1
1:A:420:LEU:C	1:A:420:LEU:CD1	0.43	2.87	13	1
1:A:366:LYS:O	1:A:369:ASN:OD1	0.43	2.37	6	1
1:A:361:LEU:C	1:A:361:LEU:HD23	0.43	2.34	10	1
1:A:420:LEU:N	1:A:420:LEU:CD1	0.43	2.82	10	1
1:A:351:GLN:CD	1:A:380:ARG:HH22	0.43	2.18	17	1
1:A:351:GLN:OE1	1:A:353:SER:O	0.43	2.36	24	2
1:A:360:ASN:ND2	1:A:360:ASN:N	0.43	2.66	20	1
1:A:361:LEU:HD23	1:A:361:LEU:C	0.43	2.34	20	1
1:A:358:TYR:O	1:A:362:ASN:OD1	0.43	2.37	7	2
1:A:419:PRO:C	1:A:421:ARG:H	0.43	2.17	15	2
1:A:378:THR:HG22	1:A:385:TRP:O	0.42	2.14	12	1
1:A:367:LYS:C	1:A:369:ASN:N	0.42	2.72	14	2
1:A:421:ARG:O	1:A:424:GLN:OE1	0.42	2.37	16	2
1:A:354:SER:O	1:A:355:SER:OG	0.42	2.36	25	1
1:A:370:LEU:O	1:A:371:LYS:O	0.42	2.37	7	2
1:A:346:SER:O	1:A:347:HIS:O	0.42	2.37	8	1
1:A:410:VAL:C	1:A:412:ALA:N	0.42	2.70	8	1
1:A:422:GLN:C	1:A:424:GLN:H	0.42	2.18	10	2
1:A:416:TRP:NE1	1:A:418:LYS:NZ	0.42	2.67	2	1
1:A:414:ASN:N	1:A:414:ASN:ND2	0.42	2.68	4	1
1:A:364:TRP:CE2	1:A:368:GLU:OE2	0.42	2.72	10	2
1:A:348:TYR:O	1:A:349:THR:OG1	0.42	2.37	9	1
1:A:385:TRP:NE1	1:A:387:VAL:HG12	0.42	2.29	16	1
1:A:351:GLN:C	1:A:352:LEU:HD12	0.42	2.34	14	1
1:A:413:LYS:O	1:A:414:ASN:OD1	0.42	2.37	1	1
1:A:351:GLN:C	1:A:352:LEU:HD22	0.42	2.35	5	1
1:A:368:GLU:CD	1:A:368:GLU:H	0.42	2.17	14	1
1:A:349:THR:OG1	1:A:418:LYS:O	0.42	2.38	13	1
1:A:368:GLU:OE2	1:A:409:ASP:OD2	0.42	2.38	22	1
1:A:358:TYR:CD1	1:A:358:TYR:C	0.41	2.94	1	6
1:A:378:THR:CB	1:A:385:TRP:O	0.41	2.68	3	1
1:A:412:ALA:C	1:A:414:ASN:H	0.41	2.18	16	2
1:A:392:VAL:HG22	1:A:393:TYR:N	0.41	2.29	6	2
1:A:364:TRP:CZ3	1:A:368:GLU:OE2	0.41	2.73	6	1
1:A:420:LEU:C	1:A:422:GLN:H	0.41	2.19	21	1
1:A:354:SER:O	1:A:355:SER:CB	0.41	2.67	10	3
1:A:372:ASN:C	1:A:372:ASN:HD22	0.41	2.19	5	1
1:A:369:ASN:O	1:A:369:ASN:ND2	0.41	2.49	2	1
1:A:396:LYS:O	1:A:400:LYS:N	0.41	2.52	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:347:HIS:O	1:A:348:TYR:CG	0.41	2.73	11	3
1:A:403:VAL:CG1	1:A:404:SER:N	0.41	2.83	18	1
1:A:403:VAL:HG13	1:A:404:SER:N	0.41	2.29	18	1
1:A:381:ASN:O	1:A:382:GLY:C	0.41	2.59	19	4
1:A:387:VAL:HG13	1:A:387:VAL:O	0.41	2.15	25	1
1:A:399:ALA:O	1:A:402:ALA:HB3	0.41	2.16	11	1
1:A:403:VAL:CG1	1:A:411:GLN:CD	0.41	2.89	11	1
1:A:357:ASN:ND2	1:A:360:ASN:CG	0.41	2.74	13	1
1:A:361:LEU:HD13	1:A:362:ASN:N	0.41	2.31	15	1
1:A:373:TYR:CD1	1:A:373:TYR:N	0.41	2.89	21	1
1:A:366:LYS:N	1:A:366:LYS:CD	0.41	2.83	22	1
1:A:378:THR:HG21	1:A:387:VAL:HG12	0.40	1.94	12	1
1:A:393:TYR:C	1:A:395:SER:N	0.40	2.74	21	1
1:A:369:ASN:O	1:A:369:ASN:OD1	0.40	2.40	25	1
1:A:397:GLU:O	1:A:400:LYS:N	0.40	2.52	2	1
1:A:351:GLN:CG	1:A:352:LEU:N	0.40	2.83	5	2
1:A:365:ALA:O	1:A:366:LYS:C	0.40	2.60	10	1
1:A:365:ALA:O	1:A:368:GLU:N	0.40	2.54	10	1
1:A:413:LYS:O	1:A:413:LYS:CG	0.40	2.69	10	1
1:A:360:ASN:HD22	1:A:360:ASN:C	0.40	2.18	1	1
1:A:375:VAL:O	1:A:375:VAL:CG2	0.40	2.68	17	1
1:A:414:ASN:N	1:A:414:ASN:HD22	0.40	2.13	20	1
1:A:383:GLN:NE2	1:A:384:PRO:O	0.40	2.55	25	1
1:A:358:TYR:C	1:A:360:ASN:H	0.40	2.19	14	3
1:A:387:VAL:O	1:A:387:VAL:HG13	0.40	2.16	22	1
1:A:395:SER:OG	1:A:398:GLU:OE2	0.40	2.37	3	1
1:A:398:GLU:O	1:A:402:ALA:CB	0.40	2.70	22	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	80/106 (75%)	60±5 (75±6%)	15±4 (19±5%)	5±2 (6±2%)	2	18
All	All	2000/2650 (75%)	1492 (75%)	380 (19%)	128 (6%)	2	18

All 19 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	423	VAL	22
1	A	372	ASN	21
1	A	382	GLY	14
1	A	350	LEU	13
1	A	355	SER	12
1	A	415	PRO	10
1	A	397	GLU	7
1	A	359	ASP	5
1	A	371	LYS	5
1	A	347	HIS	4
1	A	421	ARG	3
1	A	419	PRO	2
1	A	391	GLY	2
1	A	424	GLN	2
1	A	400	LYS	2
1	A	365	ALA	1
1	A	409	ASP	1
1	A	396	LYS	1
1	A	420	LEU	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	70/91 (77%)	66±1 (94±2%)	4±1 (6±2%)	19 71
All	All	1750/2275 (77%)	1646 (94%)	104 (6%)	19 71

All 31 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	355	SER	16
1	A	352	LEU	7
1	A	372	ASN	6
1	A	360	ASN	5
1	A	351	GLN	5

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Mol	Chain	Res	Type	Models (Total)
1	A	378	THR	5
1	A	420	LEU	5
1	A	409	ASP	5
1	A	373	TYR	5
1	A	371	LYS	5
1	A	413	LYS	4
1	A	349	THR	4
1	A	385	TRP	3
1	A	401	LYS	3
1	A	381	ASN	3
1	A	357	ASN	2
1	A	400	LYS	2
1	A	414	ASN	2
1	A	418	LYS	2
1	A	424	GLN	2
1	A	421	ARG	2
1	A	362	ASN	2
1	A	369	ASN	1
1	A	386	TYR	1
1	A	398	GLU	1
1	A	377	GLU	1
1	A	416	TRP	1
1	A	422	GLN	1
1	A	388	LEU	1
1	A	348	TYR	1
1	A	379	THR	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no oligosaccharides 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 96% for the well-defined parts and 91% 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	1284
Number of shifts mapped to atoms	1283
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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

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

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	323	MET	H	8.453	0.007	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	101	0.02 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	95	0.18 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	101	0.22 ± 0.16	None needed (< 0.5 ppm)
^{15}N	94	0.51 ± 0.49	None needed (imprecise)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 96%, i.e. 1040 atoms were assigned a chemical shift out of a possible 1084. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	393/395 (99%)	158/159 (99%)	160/160 (100%)	75/76 (99%)
Sidechain	559/591 (95%)	374/382 (98%)	171/183 (93%)	14/26 (54%)
Aromatic	88/98 (90%)	44/46 (96%)	41/47 (87%)	3/5 (60%)
Overall	1040/1084 (96%)	576/587 (98%)	372/390 (95%)	92/107 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1283 atoms were assigned a chemical shift out of a possible 1415. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	497/526 (94%)	201/213 (94%)	202/212 (95%)	94/101 (93%)
Sidechain	679/743 (91%)	454/480 (95%)	208/229 (91%)	17/34 (50%)
Aromatic	107/146 (73%)	56/70 (80%)	48/59 (81%)	3/17 (18%)
Overall	1283/1415 (91%)	711/763 (93%)	458/500 (92%)	114/152 (75%)

7.1.4 Statistically unusual chemical shifts (i)

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

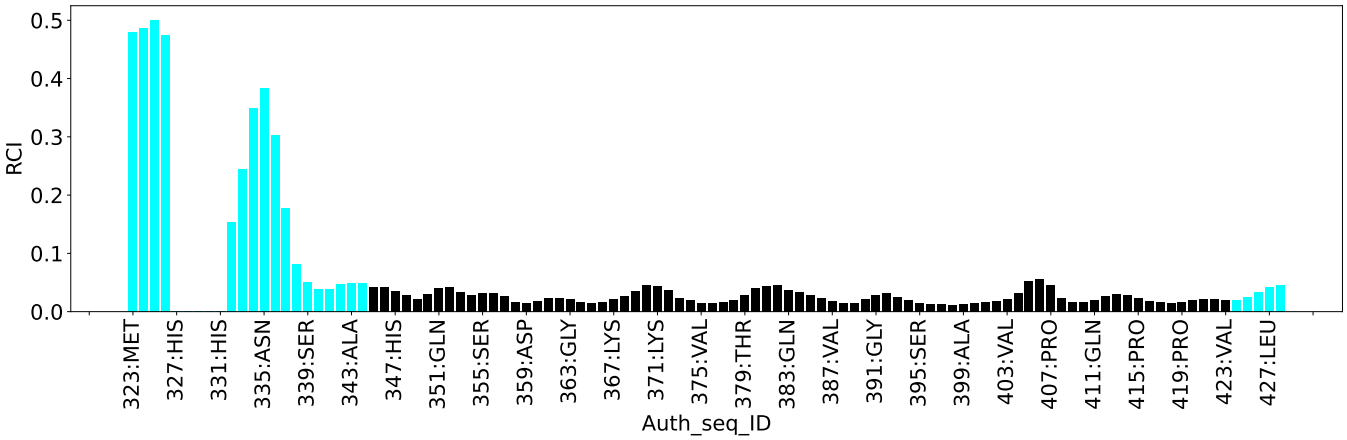
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	405	THR	HG1	4.97	0.08 – 2.19	18.2
1	A	368	GLU	HG3	0.65	1.20 – 3.30	-7.6
1	A	380	ARG	HD2	1.83	1.97 – 4.26	-5.6
1	A	368	GLU	HB3	0.84	0.95 – 3.05	-5.5
1	A	351	GLN	HB3	0.68	0.71 – 3.33	-5.1

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	2804
Intra-residue (|i-j|=0)	997
Sequential (|i-j|=1)	625
Medium range (|i-j|>1 and |i-j|<5)	409
Long range (|i-j|≥5)	773
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	162
Number of unmapped restraints	0
Number of restraints per residue	28.0
Number of long range restraints per residue[1]	7.3

[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)	9.3	0.2
0.2-0.5 (Medium)	4.3	0.5
>0.5 (Large)	2.6	3.35

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.0	2.69
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

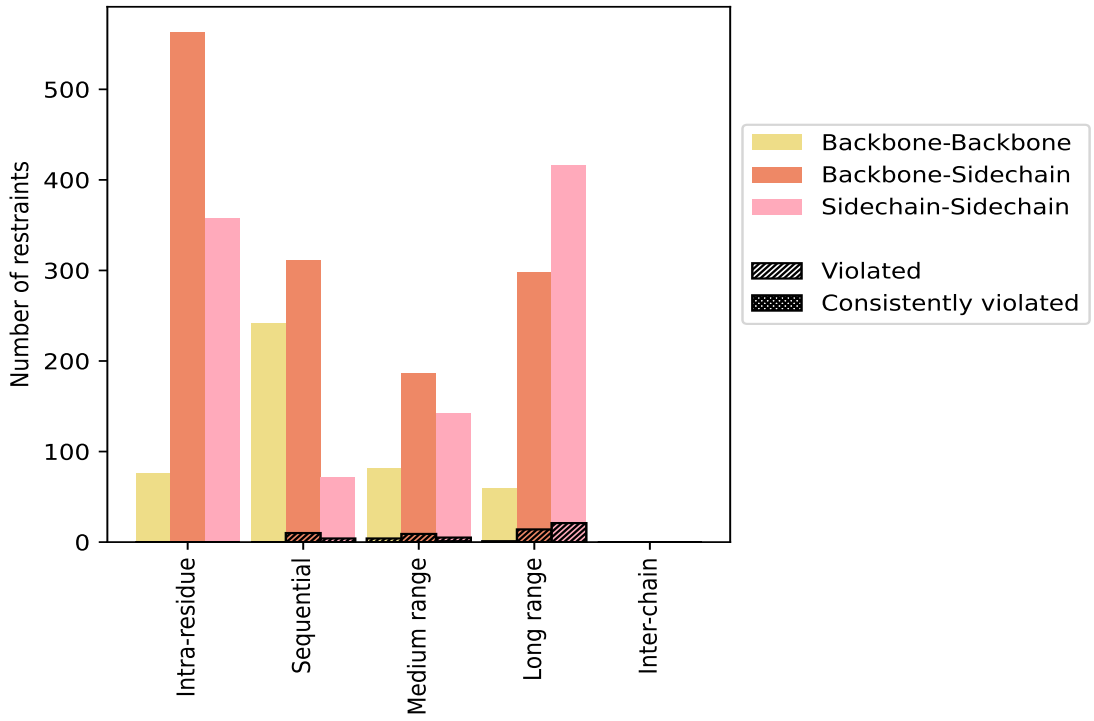
9.1 Summary of distance violations (i)

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)	997	35.6	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	76	2.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	563	20.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	358	12.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	625	22.3	14	2.2	0.5	0	0.0	0.0
Backbone-Backbone	242	8.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	311	11.1	10	3.2	0.4	0	0.0	0.0
Sidechain-Sidechain	72	2.6	4	5.6	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	409	14.6	18	4.4	0.6	1	0.2	0.0
Backbone-Backbone	81	2.9	4	4.9	0.1	0	0.0	0.0
Backbone-Sidechain	186	6.6	9	4.8	0.3	0	0.0	0.0
Sidechain-Sidechain	142	5.1	5	3.5	0.2	1	0.7	0.0
Long range (|i-j|≥5)	773	27.6	36	4.7	1.3	0	0.0	0.0
Backbone-Backbone	59	2.1	1	1.7	0.0	0	0.0	0.0
Backbone-Sidechain	298	10.6	14	4.7	0.5	0	0.0	0.0
Sidechain-Sidechain	416	14.8	21	5.0	0.7	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	2804	100.0	68	2.4	2.4	1	0.0	0.0
Backbone-Backbone	458	16.3	5	1.1	0.2	0	0.0	0.0
Backbone-Sidechain	1358	48.4	33	2.4	1.2	0	0.0	0.0
Sidechain-Sidechain	988	35.2	30	3.0	1.1	1	0.1	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	0	3	5	8	0	16	0.28	1.09	0.27	0.15
2	0	5	4	7	0	16	0.25	0.61	0.12	0.2
3	0	3	4	14	0	21	0.28	1.7	0.34	0.15
4	0	2	6	4	0	12	0.38	1.17	0.37	0.22
5	0	3	7	5	0	15	0.27	1.04	0.23	0.21
6	0	3	7	7	0	17	0.19	0.56	0.12	0.15
7	0	4	7	6	0	17	0.3	0.91	0.26	0.17
8	0	3	8	7	0	18	0.33	1.13	0.31	0.16
9	0	3	5	7	0	15	0.35	1.18	0.32	0.2
10	0	1	4	11	0	16	0.32	1.94	0.44	0.16

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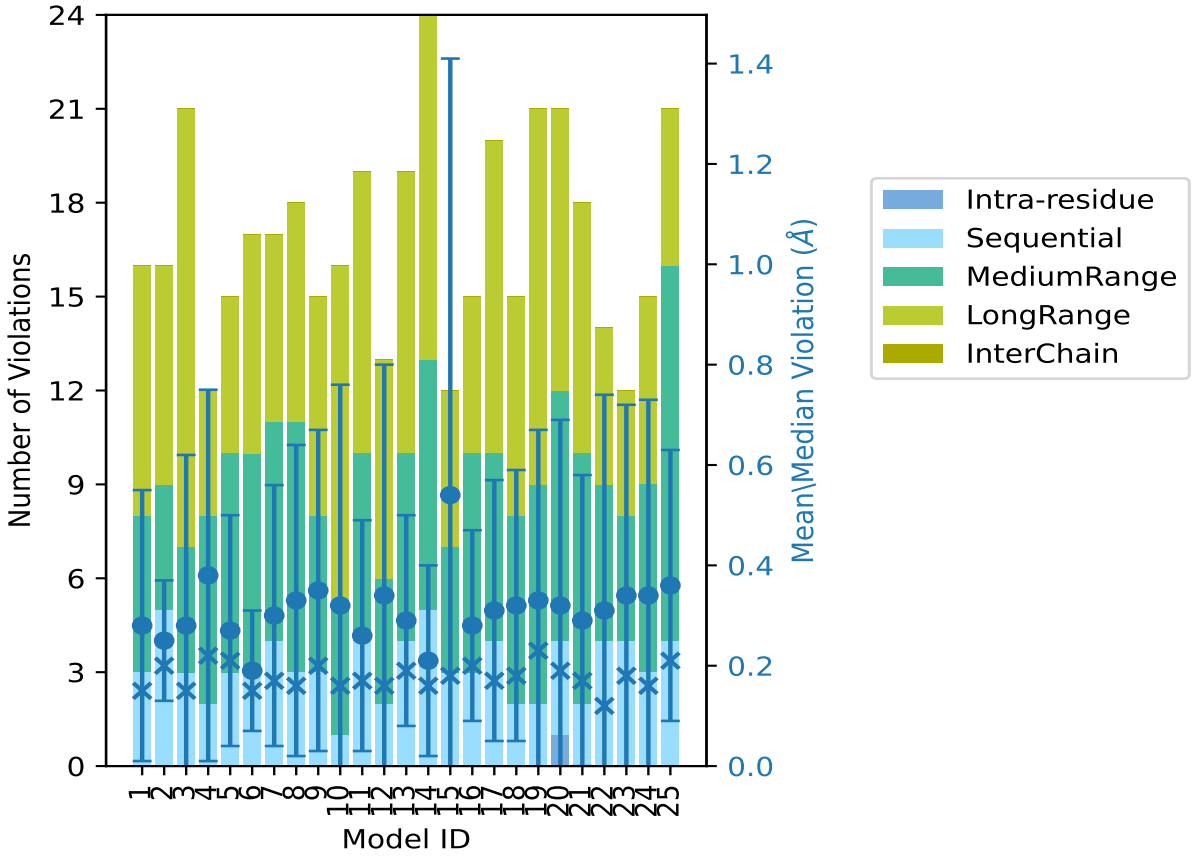
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	4	6	9	0	19	0.26	0.93	0.23	0.17
12	0	2	4	7	0	13	0.34	1.83	0.46	0.16
13	0	4	6	9	0	19	0.29	0.94	0.21	0.19
14	0	5	8	11	0	24	0.21	1.05	0.19	0.16
15	0	3	4	5	0	12	0.54	3.35	0.87	0.18
16	0	3	7	5	0	15	0.28	0.72	0.19	0.2
17	0	4	6	10	0	20	0.31	1.09	0.26	0.17
18	0	2	6	7	0	15	0.32	1.01	0.27	0.18
19	0	2	7	12	0	21	0.33	1.67	0.34	0.23
20	1	3	8	9	0	21	0.32	1.61	0.37	0.19
21	0	2	8	8	0	18	0.29	1.25	0.29	0.17
22	0	4	5	5	0	14	0.31	1.74	0.43	0.12
23	0	4	4	4	0	12	0.34	1.29	0.38	0.18
24	0	3	6	6	0	15	0.34	1.37	0.39	0.16
25	0	4	12	5	0	21	0.36	1.04	0.27	0.21

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

9.2.1 Bar graph : Distance Violation statistics for each model (i)



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

9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2736(IR:997, SQ:611, MR:391, LR:737, 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]	%
0	4	5	10	0	19	1	4.0
0	4	1	5	0	10	2	8.0
0	0	1	0	0	1	3	12.0
0	3	1	8	0	12	4	16.0
0	0	1	1	0	2	5	20.0
0	0	0	1	0	1	6	24.0

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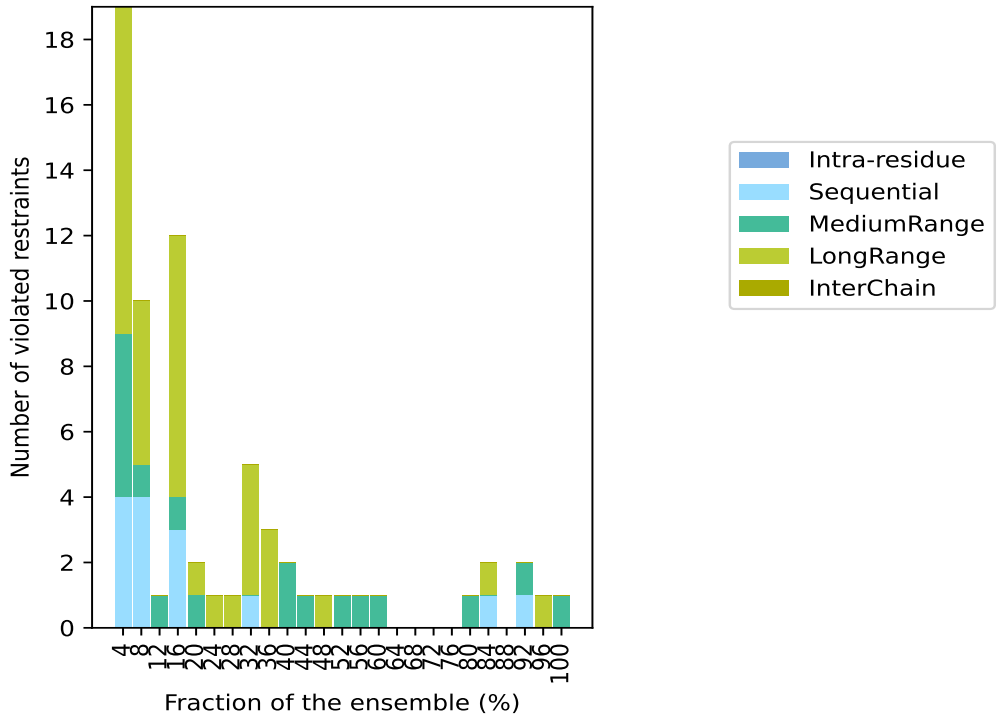
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	1	0	1	7	28.0
0	1	0	4	0	5	8	32.0
0	0	0	3	0	3	9	36.0
0	0	2	0	0	2	10	40.0
0	0	1	0	0	1	11	44.0
0	0	0	1	0	1	12	48.0
0	0	1	0	0	1	13	52.0
0	0	1	0	0	1	14	56.0
0	0	1	0	0	1	15	60.0
0	0	0	0	0	0	16	64.0
0	0	0	0	0	0	17	68.0
0	0	0	0	0	0	18	72.0
0	0	0	0	0	0	19	76.0
0	0	1	0	0	1	20	80.0
0	1	0	1	0	2	21	84.0
0	0	0	0	0	0	22	88.0
0	1	1	0	0	2	23	92.0
0	0	0	1	0	1	24	96.0
0	0	1	0	0	1	25	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

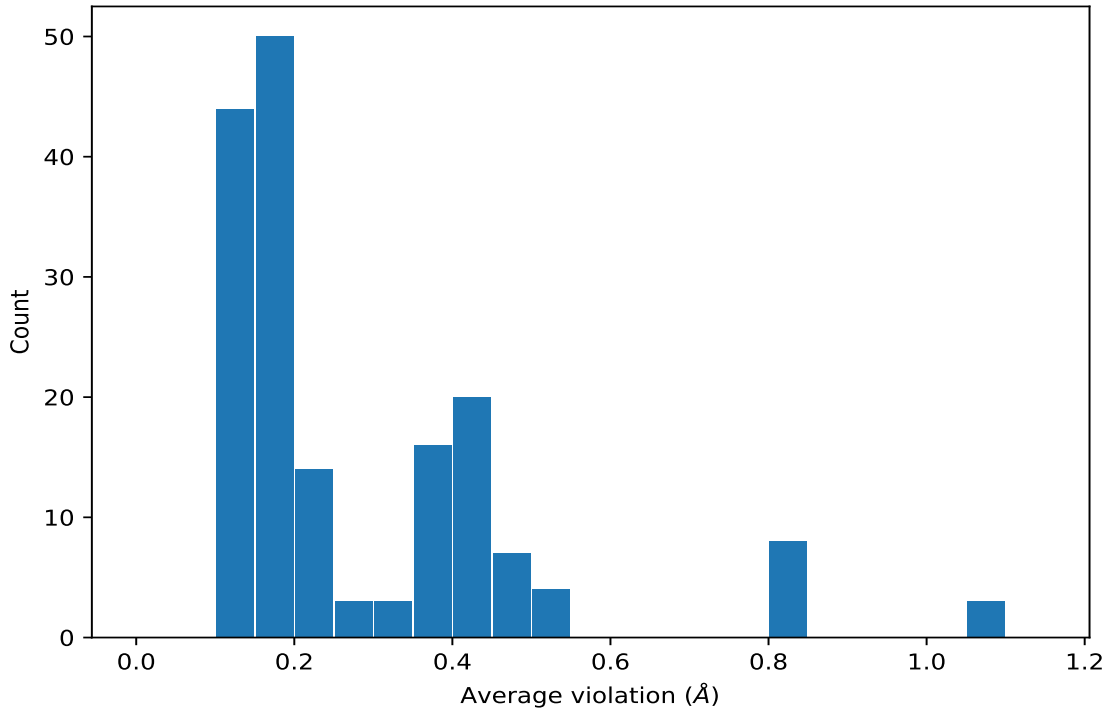
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 theviolation 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)
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	25	1.08	0.71	0.94
(1,115)	1:385:A:TRP:HZ3	1:413:A:LYS:HD2	25	1.08	0.71	0.94
(1,115)	1:385:A:TRP:HZ3	1:413:A:LYS:HD3	25	1.08	0.71	0.94
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD1	24	0.82	0.33	0.92
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD2	24	0.82	0.33	0.92
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD1	24	0.82	0.33	0.92
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD2	24	0.82	0.33	0.92
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE1	24	0.82	0.33	0.92
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE2	24	0.82	0.33	0.92
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HE1	24	0.82	0.33	0.92
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HE2	24	0.82	0.33	0.92
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	23	0.21	0.05	0.22
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	23	0.21	0.05	0.22
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	23	0.18	0.02	0.17
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	23	0.18	0.02	0.17
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	21	0.24	0.1	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	21	0.24	0.1	0.24
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	21	0.18	0.05	0.17
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	21	0.18	0.05	0.17
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	21	0.18	0.05	0.17
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	21	0.18	0.05	0.17
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	21	0.18	0.05	0.17
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	21	0.18	0.05	0.17
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	20	0.53	0.27	0.45
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	20	0.53	0.27	0.45
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HD1	20	0.53	0.27	0.45
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HD2	20	0.53	0.27	0.45
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	15	0.17	0.07	0.16
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	15	0.17	0.07	0.16
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	15	0.17	0.07	0.16
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB2	14	0.37	0.14	0.34
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB3	14	0.37	0.14	0.34
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB2	14	0.37	0.14	0.34
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB3	14	0.37	0.14	0.34
(1,66)	1:352:A:LEU:HB2	1:415:A:PRO:HB2	14	0.37	0.14	0.34
(1,66)	1:352:A:LEU:HB2	1:415:A:PRO:HB3	14	0.37	0.14	0.34
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB2	13	0.16	0.05	0.14
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB3	13	0.16	0.05	0.14
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG21	13	0.16	0.05	0.14
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG22	13	0.16	0.05	0.14
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG23	13	0.16	0.05	0.14
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB2	12	0.15	0.02	0.14
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB3	12	0.15	0.02	0.14
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA2	11	0.37	0.16	0.35
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA3	11	0.37	0.16	0.35
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA2	11	0.37	0.16	0.35
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA3	11	0.37	0.16	0.35
(1,1976)	1:422:A:GLN:HA	1:424:A:GLN:HA	10	0.14	0.04	0.12
(1,2005)	1:424:A:GLN:HA	1:422:A:GLN:HA	10	0.14	0.04	0.12
(1,1305)	1:387:A:VAL:HG11	1:380:A:ARG:HA	9	0.13	0.02	0.13
(1,1305)	1:387:A:VAL:HG12	1:380:A:ARG:HA	9	0.13	0.02	0.13
(1,1305)	1:387:A:VAL:HG13	1:380:A:ARG:HA	9	0.13	0.02	0.13
(1,1305)	1:387:A:VAL:HG21	1:380:A:ARG:HA	9	0.13	0.02	0.13
(1,1305)	1:387:A:VAL:HG22	1:380:A:ARG:HA	9	0.13	0.02	0.13
(1,1305)	1:387:A:VAL:HG23	1:380:A:ARG:HA	9	0.13	0.02	0.13
(1,797)	1:364:A:TRP:HE3	1:385:A:TRP:HZ2	9	0.12	0.01	0.11
(1,1254)	1:385:A:TRP:HZ2	1:364:A:TRP:HE3	9	0.12	0.01	0.11
(1,340)	1:423:A:VAL:HG12	1:427:A:LEU:HG	8	0.47	0.18	0.49

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,340)	1:423:A:VAL:HG13	1:427:A:LEU:HG	8	0.47	0.18	0.49
(1,340)	1:423:A:VAL:HG11	1:427:A:LEU:HG	8	0.47	0.18	0.49
(1,340)	1:423:A:VAL:HG22	1:427:A:LEU:HG	8	0.47	0.18	0.49
(1,340)	1:423:A:VAL:HG21	1:427:A:LEU:HG	8	0.47	0.18	0.49
(1,1124)	1:378:A:THR:HG21	1:385:A:TRP:HA	8	0.19	0.06	0.18
(1,1124)	1:378:A:THR:HG22	1:385:A:TRP:HA	8	0.19	0.06	0.18
(1,1124)	1:378:A:THR:HG23	1:385:A:TRP:HA	8	0.19	0.06	0.18
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG21	8	0.19	0.06	0.18
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG22	8	0.19	0.06	0.18
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG23	8	0.19	0.06	0.18
(1,2189)	1:353:A:SER:H	1:389:A:VAL:HA	8	0.15	0.02	0.16
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG2	8	0.15	0.04	0.14
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG3	8	0.15	0.04	0.14
(1,230)	1:390:A:SER:H	1:352:A:LEU:HB2	7	0.33	0.19	0.23
(1,230)	1:390:A:SER:H	1:352:A:LEU:HB3	7	0.33	0.19	0.23
(1,230)	1:390:A:SER:H	1:352:A:LEU:HG	7	0.33	0.19	0.23
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD1	6	0.15	0.03	0.14
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD2	6	0.15	0.03	0.14
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD1	6	0.15	0.03	0.14
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD2	6	0.15	0.03	0.14
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD1	6	0.15	0.03	0.14
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD2	6	0.15	0.03	0.14
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD1	6	0.15	0.03	0.14
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD2	6	0.15	0.03	0.14
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD1	6	0.15	0.03	0.14
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD2	6	0.15	0.03	0.14
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD1	6	0.15	0.03	0.14
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD2	6	0.15	0.03	0.14
(1,86)	1:358:A:TYR:HE1	1:362:A:ASN:HA	5	0.46	0.16	0.5
(1,86)	1:358:A:TYR:HE2	1:362:A:ASN:HA	5	0.46	0.16	0.5
(1,1224)	1:385:A:TRP:HD1	1:379:A:THR:HA	5	0.11	0.01	0.11
(1,226)	1:389:A:VAL:HG12	1:418:A:LYS:HD2	4	0.43	0.21	0.43
(1,226)	1:389:A:VAL:HG12	1:418:A:LYS:HD3	4	0.43	0.21	0.43
(1,226)	1:389:A:VAL:HG13	1:418:A:LYS:HD2	4	0.43	0.21	0.43
(1,226)	1:389:A:VAL:HG13	1:418:A:LYS:HD3	4	0.43	0.21	0.43
(1,226)	1:389:A:VAL:HG12	1:418:A:LYS:HG2	4	0.43	0.21	0.43
(1,226)	1:389:A:VAL:HG12	1:418:A:LYS:HG3	4	0.43	0.21	0.43
(1,226)	1:389:A:VAL:HG21	1:418:A:LYS:HD2	4	0.43	0.21	0.43
(1,226)	1:389:A:VAL:HG21	1:418:A:LYS:HD3	4	0.43	0.21	0.43
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG11	4	0.35	0.12	0.32
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG12	4	0.35	0.12	0.32
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG13	4	0.35	0.12	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG21	4	0.35	0.12	0.32
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG22	4	0.35	0.12	0.32
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG23	4	0.35	0.12	0.32
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG21	4	0.28	0.04	0.29
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG22	4	0.28	0.04	0.29
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG23	4	0.28	0.04	0.29
(1,4)	1:336:A:ASN:HD21	1:337:A:ASN:HA	4	0.2	0.15	0.12
(1,4)	1:336:A:ASN:HD22	1:337:A:ASN:HA	4	0.2	0.15	0.12
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG21	4	0.18	0.01	0.18
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG22	4	0.18	0.01	0.18
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG23	4	0.18	0.01	0.18
(1,153)	1:375:A:VAL:HB	1:386:A:TYR:HD1	4	0.16	0.04	0.16
(1,153)	1:375:A:VAL:HB	1:386:A:TYR:HD2	4	0.16	0.04	0.16
(1,2158)	1:351:A:GLN:H	1:352:A:LEU:HB2	4	0.14	0.01	0.15
(1,2158)	1:351:A:GLN:H	1:352:A:LEU:HB3	4	0.14	0.01	0.15
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG11	4	0.14	0.03	0.15
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG12	4	0.14	0.03	0.15
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG13	4	0.14	0.03	0.15
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG21	4	0.14	0.03	0.15
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG22	4	0.14	0.03	0.15
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG23	4	0.14	0.03	0.15
(1,195)	1:385:A:TRP:HZ3	1:356:A:SER:HB2	4	0.14	0.0	0.14
(1,195)	1:385:A:TRP:HZ3	1:356:A:SER:HB3	4	0.14	0.0	0.14
(1,196)	1:385:A:TRP:HZ3	1:356:A:SER:HB2	4	0.14	0.0	0.14
(1,196)	1:385:A:TRP:HZ3	1:356:A:SER:HB3	4	0.14	0.0	0.14
(1,694)	1:356:A:SER:HB2	1:385:A:TRP:HZ3	4	0.14	0.0	0.14
(1,694)	1:356:A:SER:HB3	1:385:A:TRP:HZ3	4	0.14	0.0	0.14
(1,857)	1:365:A:ALA:HB1	1:375:A:VAL:HA	4	0.12	0.01	0.11
(1,857)	1:365:A:ALA:HB2	1:375:A:VAL:HA	4	0.12	0.01	0.11
(1,857)	1:365:A:ALA:HB3	1:375:A:VAL:HA	4	0.12	0.01	0.11
(1,1607)	1:405:A:THR:HG21	1:401:A:LYS:HG2	3	0.15	0.03	0.16
(1,1607)	1:405:A:THR:HG21	1:401:A:LYS:HG3	3	0.15	0.03	0.16
(1,1607)	1:405:A:THR:HG22	1:401:A:LYS:HG2	3	0.15	0.03	0.16
(1,1607)	1:405:A:THR:HG22	1:401:A:LYS:HG3	3	0.15	0.03	0.16
(1,1607)	1:405:A:THR:HG23	1:401:A:LYS:HG2	3	0.15	0.03	0.16
(1,1607)	1:405:A:THR:HG23	1:401:A:LYS:HG3	3	0.15	0.03	0.16
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD11	2	0.42	0.15	0.42
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD12	2	0.42	0.15	0.42
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD13	2	0.42	0.15	0.42
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD21	2	0.42	0.15	0.42
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD22	2	0.42	0.15	0.42
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD23	2	0.42	0.15	0.42

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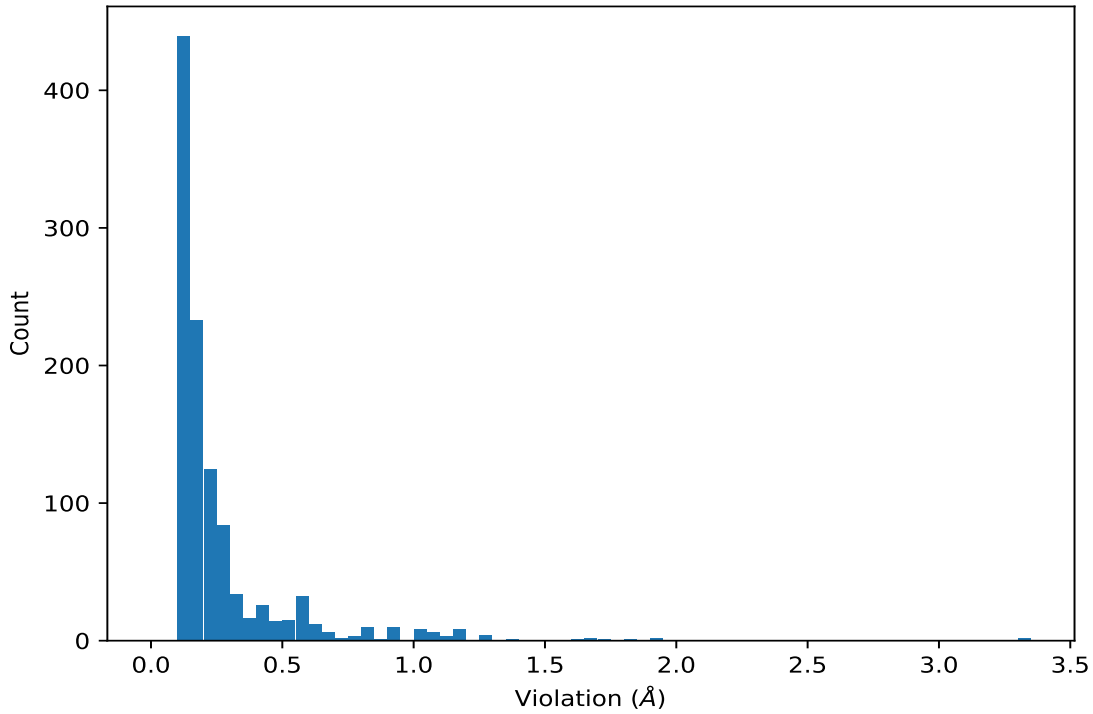
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD11	2	0.42	0.15	0.42
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD12	2	0.42	0.15	0.42
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD13	2	0.42	0.15	0.42
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD21	2	0.42	0.15	0.42
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD22	2	0.42	0.15	0.42
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD23	2	0.42	0.15	0.42
(1,41)	1:349:A:THR:HB	1:420:A:LEU:HG	2	0.24	0.11	0.24
(1,41)	1:349:A:THR:HB	1:418:A:LYS:HG2	2	0.24	0.11	0.24
(1,41)	1:349:A:THR:HB	1:418:A:LYS:HG3	2	0.24	0.11	0.24
(1,190)	1:385:A:TRP:HH2	1:358:A:TYR:HA	2	0.22	0.12	0.22
(1,624)	1:351:A:GLN:HG2	1:350:A:LEU:HB2	2	0.2	0.0	0.2
(1,624)	1:351:A:GLN:HG2	1:350:A:LEU:HB3	2	0.2	0.0	0.2
(1,624)	1:351:A:GLN:HG3	1:350:A:LEU:HB2	2	0.2	0.0	0.2
(1,624)	1:351:A:GLN:HG3	1:350:A:LEU:HB3	2	0.2	0.0	0.2
(1,808)	1:364:A:TRP:HZ2	1:353:A:SER:HB2	2	0.14	0.04	0.14
(1,808)	1:364:A:TRP:HZ2	1:353:A:SER:HB3	2	0.14	0.04	0.14
(1,1593)	1:404:A:SER:HA	1:403:A:VAL:HB	2	0.12	0.01	0.12
(1,706)	1:358:A:TYR:HA	1:362:A:ASN:HB2	2	0.12	0.02	0.12
(1,706)	1:358:A:TYR:HA	1:362:A:ASN:HB3	2	0.12	0.02	0.12
(1,1094)	1:377:A:GLU:HG2	1:376:A:TYR:HE1	2	0.12	0.0	0.12
(1,1094)	1:377:A:GLU:HG2	1:376:A:TYR:HE2	2	0.12	0.0	0.12
(1,1094)	1:377:A:GLU:HG3	1:376:A:TYR:HE1	2	0.12	0.0	0.12
(1,1094)	1:377:A:GLU:HG3	1:376:A:TYR:HE2	2	0.12	0.0	0.12
(1,752)	1:361:A:LEU:HD11	1:353:A:SER:HA	2	0.11	0.0	0.11
(1,752)	1:361:A:LEU:HD12	1:353:A:SER:HA	2	0.11	0.0	0.11
(1,752)	1:361:A:LEU:HD13	1:353:A:SER:HA	2	0.11	0.0	0.11
(1,752)	1:361:A:LEU:HD21	1:353:A:SER:HA	2	0.11	0.0	0.11
(1,752)	1:361:A:LEU:HD22	1:353:A:SER:HA	2	0.11	0.0	0.11
(1,752)	1:361:A:LEU:HD23	1:353:A:SER:HA	2	0.11	0.0	0.11
(1,1018)	1:374:A:VAL:HB	1:373:A:TYR:HA	2	0.11	0.0	0.11

[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)
(1,115)	1:385:A:TRP:HZ3	1:413:A:LYS:HD2	15	3.35
(1,115)	1:385:A:TRP:HZ3	1:413:A:LYS:HD3	15	3.35
(1,115)	1:385:A:TRP:HZ3	1:413:A:LYS:HD2	10	1.94
(1,115)	1:385:A:TRP:HZ3	1:413:A:LYS:HD3	10	1.94
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	12	1.83
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	22	1.74
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	3	1.7
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	19	1.67
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	20	1.61
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	24	1.37
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD1	23	1.29
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD2	23	1.29
(1,115)	1:385:A:TRP:HZ3	1:413:A:LYS:HD2	21	1.25
(1,115)	1:385:A:TRP:HZ3	1:413:A:LYS:HD3	21	1.25
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE1	24	1.2
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE2	24	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD1	9	1.18
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD2	9	1.18
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD1	4	1.17
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD2	4	1.17
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD1	20	1.16
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD2	20	1.16
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	4	1.14
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD1	8	1.13
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD2	8	1.13
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD1	1	1.09
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD2	1	1.09
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD1	17	1.09
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD2	17	1.09
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD1	14	1.05
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD2	14	1.05
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	25	1.04
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	25	1.04
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	23	1.04
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE1	5	1.04
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE2	5	1.04
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	9	1.02
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD1	18	1.01
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD2	18	1.01
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	8	0.95
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	8	0.95
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	18	0.94
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HE1	13	0.94
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HE2	13	0.94
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	11	0.93
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	7	0.91
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	7	0.91
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD1	7	0.9
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD2	7	0.9
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	25	0.87
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	17	0.84
(1,340)	1:423:A:VAL:HG13	1:427:A:LEU:HG	25	0.83
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD1	11	0.82
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HD2	11	0.82
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	21	0.8
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	21	0.8
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HD1	22	0.8
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HD2	22	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE1	12	0.8
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE2	12	0.8
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	8	0.79
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	1	0.78
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	1	0.78
(1,226)	1:389:A:VAL:HG12	1:418:A:LYS:HD2	16	0.72
(1,226)	1:389:A:VAL:HG12	1:418:A:LYS:HD3	16	0.72
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	17	0.7
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	17	0.7
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB2	19	0.69
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB3	19	0.69
(1,44)	1:349:A:THR:HG22	1:418:A:LYS:HD2	19	0.65
(1,44)	1:349:A:THR:HG22	1:418:A:LYS:HD3	19	0.65
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	3	0.64
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	3	0.64
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA2	25	0.62
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA3	25	0.62
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA2	25	0.62
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA3	25	0.62
(1,230)	1:390:A:SER:H	1:352:A:LEU:HB2	25	0.61
(1,230)	1:390:A:SER:H	1:352:A:LEU:HB3	25	0.61
(1,86)	1:358:A:TYR:HE1	1:362:A:ASN:HA	2	0.61
(1,86)	1:358:A:TYR:HE2	1:362:A:ASN:HA	2	0.61
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HE1	10	0.61
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HE2	10	0.61
(1,230)	1:390:A:SER:H	1:352:A:LEU:HB2	4	0.6
(1,230)	1:390:A:SER:H	1:352:A:LEU:HB3	4	0.6
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	16	0.59
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE1	15	0.59
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE2	15	0.59
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE1	19	0.59
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE2	19	0.59
(1,86)	1:358:A:TYR:HE1	1:362:A:ASN:HA	16	0.58
(1,86)	1:358:A:TYR:HE2	1:362:A:ASN:HA	16	0.58
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD11	8	0.57
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD12	8	0.57
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD13	8	0.57
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD21	8	0.57
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD22	8	0.57
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD23	8	0.57
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD11	8	0.57
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD12	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD13	8	0.57
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD21	8	0.57
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD22	8	0.57
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD23	8	0.57
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA2	7	0.56
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA3	7	0.56
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA2	7	0.56
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA3	7	0.56
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD1	6	0.56
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD2	6	0.56
(1,340)	1:423:A:VAL:HG12	1:427:A:LEU:HG	7	0.55
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	9	0.55
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	9	0.55
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB2	13	0.55
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB3	13	0.55
(1,340)	1:423:A:VAL:HG11	1:427:A:LEU:HG	15	0.54
(1,340)	1:423:A:VAL:HG12	1:427:A:LEU:HG	24	0.53
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA2	8	0.53
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA3	8	0.53
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA2	8	0.53
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA3	8	0.53
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG11	13	0.52
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG12	13	0.52
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG13	13	0.52
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG21	13	0.52
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG22	13	0.52
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG23	13	0.52
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	13	0.52
(1,86)	1:358:A:TYR:HE1	1:362:A:ASN:HA	11	0.5
(1,86)	1:358:A:TYR:HE2	1:362:A:ASN:HA	11	0.5
(1,226)	1:389:A:VAL:HG21	1:418:A:LYS:HD2	20	0.49
(1,226)	1:389:A:VAL:HG21	1:418:A:LYS:HD3	20	0.49
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	5	0.49
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB2	15	0.48
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB3	15	0.48
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB2	3	0.47
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB3	3	0.47
(1,4)	1:336:A:ASN:HD21	1:337:A:ASN:HA	9	0.47
(1,4)	1:336:A:ASN:HD22	1:337:A:ASN:HA	9	0.47
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	15	0.46
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	15	0.46
(1,340)	1:423:A:VAL:HG13	1:427:A:LEU:HG	13	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD1	25	0.45
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD2	25	0.45
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	10	0.44
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	10	0.44
(1,86)	1:358:A:TYR:HE1	1:362:A:ASN:HA	25	0.44
(1,86)	1:358:A:TYR:HE2	1:362:A:ASN:HA	25	0.44
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA2	21	0.43
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA3	21	0.43
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA2	21	0.43
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA3	21	0.43
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB2	25	0.43
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB3	25	0.43
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA2	1	0.42
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA3	1	0.42
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA2	1	0.42
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA3	1	0.42
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	20	0.41
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	20	0.41
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG11	17	0.41
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG12	17	0.41
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG13	17	0.41
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG21	17	0.41
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG22	17	0.41
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG23	17	0.41
(1,340)	1:423:A:VAL:HG12	1:427:A:LEU:HG	18	0.4
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	14	0.4
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE1	21	0.4
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE2	21	0.4
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	16	0.39
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	16	0.39
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB2	24	0.39
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB3	24	0.39
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	6	0.38
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	6	0.38
(1,226)	1:389:A:VAL:HG12	1:418:A:LYS:HG2	18	0.37
(1,226)	1:389:A:VAL:HG12	1:418:A:LYS:HG3	18	0.37
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	25	0.36
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	25	0.36
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	25	0.36
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	20	0.36
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	20	0.36
(1,230)	1:390:A:SER:H	1:352:A:LEU:HG	17	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB2	1	0.36
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB3	1	0.36
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	2	0.35
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	2	0.35
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA2	17	0.35
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA3	17	0.35
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA2	17	0.35
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA3	17	0.35
(1,190)	1:385:A:TRP:HH2	1:358:A:TYR:HA	2	0.35
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	9	0.34
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	9	0.34
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	18	0.34
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	18	0.34
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	2	0.34
(1,41)	1:349:A:THR:HB	1:418:A:LYS:HG2	19	0.34
(1,41)	1:349:A:THR:HB	1:418:A:LYS:HG3	19	0.34
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG21	17	0.33
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG22	17	0.33
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG23	17	0.33
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	2	0.33
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	2	0.33
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA2	3	0.32
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA3	3	0.32
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA2	3	0.32
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA3	3	0.32
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB2	4	0.32
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB3	4	0.32
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	5	0.31
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	5	0.31
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	5	0.31
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	20	0.31
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	20	0.31
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	20	0.31
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	20	0.31
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	20	0.31
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	20	0.31
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG21	14	0.3
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG22	14	0.3
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG23	14	0.3
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	13	0.3
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	13	0.3
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG21	19	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG22	19	0.3
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG23	19	0.3
(1,1124)	1:378:A:THR:HG21	1:385:A:TRP:HA	19	0.3
(1,1124)	1:378:A:THR:HG22	1:385:A:TRP:HA	19	0.3
(1,1124)	1:378:A:THR:HG23	1:385:A:TRP:HA	19	0.3
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG21	19	0.3
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG22	19	0.3
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG23	19	0.3
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB2	21	0.3
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB3	21	0.3
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	1	0.29
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	1	0.29
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	21	0.29
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	21	0.29
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB2	11	0.29
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB3	11	0.29
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA2	22	0.28
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA3	22	0.28
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA2	22	0.28
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA3	22	0.28
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	12	0.28
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	12	0.28
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD1	2	0.28
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD2	2	0.28
(1,66)	1:352:A:LEU:HB2	1:415:A:PRO:HB2	6	0.28
(1,66)	1:352:A:LEU:HB2	1:415:A:PRO:HB3	6	0.28
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	16	0.27
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	16	0.27
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	17	0.27
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	17	0.27
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG21	2	0.27
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG22	2	0.27
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG23	2	0.27
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	23	0.27
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	23	0.27
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	18	0.26
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	18	0.26
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	19	0.26
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	19	0.26
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG21	5	0.26
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG22	5	0.26
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG23	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1124)	1:378:A:THR:HG21	1:385:A:TRP:HA	5	0.26
(1,1124)	1:378:A:THR:HG22	1:385:A:TRP:HA	5	0.26
(1,1124)	1:378:A:THR:HG23	1:385:A:TRP:HA	5	0.26
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	10	0.26
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	10	0.26
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	10	0.26
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	10	0.26
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	10	0.26
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	10	0.26
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	16	0.26
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	16	0.26
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	7	0.26
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD11	18	0.26
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD12	18	0.26
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD13	18	0.26
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD21	18	0.26
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD22	18	0.26
(1,24)	1:344:A:PRO:HG2	1:420:A:LEU:HD23	18	0.26
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD11	18	0.26
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD12	18	0.26
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD13	18	0.26
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD21	18	0.26
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD22	18	0.26
(1,24)	1:344:A:PRO:HG3	1:420:A:LEU:HD23	18	0.26
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	1	0.25
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	1	0.25
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	5	0.25
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	5	0.25
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	8	0.25
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	8	0.25
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	22	0.25
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	22	0.25
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	5	0.25
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	5	0.25
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE1	3	0.25
(1,77)	1:357:A:ASN:HB3	1:386:A:TYR:HE2	3	0.25
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	24	0.24
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	24	0.24
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	7	0.24
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	7	0.24
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG11	14	0.24
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG12	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG13	14	0.24
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG21	14	0.24
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG22	14	0.24
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG23	14	0.24
(1,675)	1:354:A:SER:HA	1:387:A:VAL:HB	10	0.24
(1,340)	1:423:A:VAL:HG22	1:427:A:LEU:HG	20	0.24
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA2	9	0.24
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA3	9	0.24
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA2	9	0.24
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA3	9	0.24
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	19	0.24
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	19	0.24
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB2	12	0.24
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB3	12	0.24
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	6	0.23
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	6	0.23
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG21	3	0.23
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG22	3	0.23
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG23	3	0.23
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG2	20	0.23
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG3	20	0.23
(1,1124)	1:378:A:THR:HG21	1:385:A:TRP:HA	3	0.23
(1,1124)	1:378:A:THR:HG22	1:385:A:TRP:HA	3	0.23
(1,1124)	1:378:A:THR:HG23	1:385:A:TRP:HA	3	0.23
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	14	0.23
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	14	0.23
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	14	0.23
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	14	0.23
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	14	0.23
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	14	0.23
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	8	0.23
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	8	0.23
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	19	0.23
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	19	0.23
(1,408)	1:334:A:SER:HA	1:332:A:HIS:HA	14	0.23
(1,340)	1:423:A:VAL:HG21	1:427:A:LEU:HG	21	0.23
(1,331)	1:419:A:PRO:HD2	1:416:A:TRP:HH2	6	0.23
(1,230)	1:390:A:SER:H	1:352:A:LEU:HB2	11	0.23
(1,230)	1:390:A:SER:H	1:352:A:LEU:HB3	11	0.23
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	4	0.22
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	4	0.22
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	7	0.22
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	11	0.22
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	11	0.22
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	13	0.22
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	13	0.22
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	23	0.22
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	23	0.22
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG21	13	0.22
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG22	13	0.22
(1,2384)	1:377:A:GLU:H	1:378:A:THR:HG23	13	0.22
(1,1195)	1:384:A:PRO:HB2	1:379:A:THR:HB	20	0.22
(1,1195)	1:384:A:PRO:HB3	1:379:A:THR:HB	20	0.22
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	4	0.22
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	4	0.22
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	4	0.22
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	4	0.22
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	4	0.22
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	4	0.22
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	11	0.22
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	11	0.22
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	11	0.22
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	11	0.22
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	11	0.22
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	11	0.22
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	25	0.22
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	25	0.22
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	25	0.22
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	25	0.22
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	25	0.22
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	25	0.22
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG11	9	0.22
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG12	9	0.22
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG13	9	0.22
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG21	9	0.22
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG22	9	0.22
(1,727)	1:358:A:TYR:HA	1:375:A:VAL:HG23	9	0.22
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	25	0.21
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	25	0.21
(1,2338)	1:371:A:LYS:H	1:373:A:TYR:HE1	16	0.21
(1,2338)	1:371:A:LYS:H	1:373:A:TYR:HE2	16	0.21
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	4	0.21
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	13	0.21
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	13	0.21
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG21	5	0.21
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG22	5	0.21
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG23	5	0.21
(1,153)	1:375:A:VAL:HB	1:386:A:TYR:HD1	3	0.21
(1,153)	1:375:A:VAL:HB	1:386:A:TYR:HD2	3	0.21
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	2	0.2
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	2	0.2
(1,2005)	1:424:A:GLN:HA	1:422:A:GLN:HA	25	0.2
(1,1976)	1:422:A:GLN:HA	1:424:A:GLN:HA	25	0.2
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG2	21	0.2
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG3	21	0.2
(1,624)	1:351:A:GLN:HG2	1:350:A:LEU:HB2	8	0.2
(1,624)	1:351:A:GLN:HG2	1:350:A:LEU:HB3	8	0.2
(1,624)	1:351:A:GLN:HG3	1:350:A:LEU:HB2	8	0.2
(1,624)	1:351:A:GLN:HG3	1:350:A:LEU:HB3	8	0.2
(1,624)	1:351:A:GLN:HG2	1:350:A:LEU:HB2	10	0.2
(1,624)	1:351:A:GLN:HG2	1:350:A:LEU:HB3	10	0.2
(1,624)	1:351:A:GLN:HG3	1:350:A:LEU:HB2	10	0.2
(1,624)	1:351:A:GLN:HG3	1:350:A:LEU:HB3	10	0.2
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	14	0.2
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	14	0.2
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	22	0.2
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	22	0.2
(1,230)	1:390:A:SER:H	1:352:A:LEU:HG	10	0.2
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG21	2	0.2
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG22	2	0.2
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG23	2	0.2
(1,153)	1:375:A:VAL:HB	1:386:A:TYR:HD1	19	0.2
(1,153)	1:375:A:VAL:HB	1:386:A:TYR:HD2	19	0.2
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD1	16	0.2
(1,77)	1:357:A:ASN:HB2	1:386:A:TYR:HD2	16	0.2
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB2	9	0.2
(1,66)	1:352:A:LEU:HB3	1:415:A:PRO:HB3	9	0.2
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	9	0.19
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	9	0.19
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	15	0.19
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	15	0.19
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG21	2	0.19
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG22	2	0.19
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG23	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2189)	1:353:A:SER:H	1:389:A:VAL:HA	5	0.19
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	11	0.19
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	11	0.19
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	11	0.19
(1,2005)	1:424:A:GLN:HA	1:422:A:GLN:HA	20	0.19
(1,1976)	1:422:A:GLN:HA	1:424:A:GLN:HA	20	0.19
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD1	6	0.19
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD2	6	0.19
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD1	6	0.19
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD2	6	0.19
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD1	6	0.19
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD2	6	0.19
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD1	6	0.19
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD2	6	0.19
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD1	6	0.19
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD2	6	0.19
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD1	6	0.19
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD2	6	0.19
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB2	13	0.19
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB3	13	0.19
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	13	0.19
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	13	0.19
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG21	14	0.18
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG22	14	0.18
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG23	14	0.18
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG11	20	0.18
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG12	20	0.18
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG13	20	0.18
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG21	20	0.18
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG22	20	0.18
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG23	20	0.18
(1,2005)	1:424:A:GLN:HA	1:422:A:GLN:HA	23	0.18
(1,1976)	1:422:A:GLN:HA	1:424:A:GLN:HA	23	0.18
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	5	0.18
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	5	0.18
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG21	14	0.18
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG22	14	0.18
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG23	14	0.18
(1,1124)	1:378:A:THR:HG21	1:385:A:TRP:HA	14	0.18
(1,1124)	1:378:A:THR:HG22	1:385:A:TRP:HA	14	0.18
(1,1124)	1:378:A:THR:HG23	1:385:A:TRP:HA	14	0.18
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	17	0.18
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	17	0.18
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	17	0.18
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	17	0.18
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	17	0.18
(1,808)	1:364:A:TRP:HZ2	1:353:A:SER:HB2	18	0.18
(1,808)	1:364:A:TRP:HZ2	1:353:A:SER:HB3	18	0.18
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD1	16	0.18
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD2	16	0.18
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD1	16	0.18
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD2	16	0.18
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD1	16	0.18
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD2	16	0.18
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD1	16	0.18
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD2	16	0.18
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD1	16	0.18
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD2	16	0.18
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD1	16	0.18
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD2	16	0.18
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	3	0.18
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	3	0.18
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	7	0.18
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	7	0.18
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	9	0.18
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	9	0.18
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	15	0.18
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	15	0.18
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	18	0.18
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	18	0.18
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB2	10	0.18
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB3	10	0.18
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG21	14	0.18
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG22	14	0.18
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG23	14	0.18
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	14	0.17
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	14	0.17
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG21	17	0.17
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG22	17	0.17
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG23	17	0.17
(1,2189)	1:353:A:SER:H	1:389:A:VAL:HA	19	0.17
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	7	0.17
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	7	0.17
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	8	0.17
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	8	0.17
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	8	0.17
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	18	0.17
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	18	0.17
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	18	0.17
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	22	0.17
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	22	0.17
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	22	0.17
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	11	0.17
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	11	0.17
(1,1607)	1:405:A:THR:HG21	1:401:A:LYS:HG2	17	0.17
(1,1607)	1:405:A:THR:HG21	1:401:A:LYS:HG3	17	0.17
(1,1607)	1:405:A:THR:HG22	1:401:A:LYS:HG2	17	0.17
(1,1607)	1:405:A:THR:HG22	1:401:A:LYS:HG3	17	0.17
(1,1607)	1:405:A:THR:HG23	1:401:A:LYS:HG2	17	0.17
(1,1607)	1:405:A:THR:HG23	1:401:A:LYS:HG3	17	0.17
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG21	2	0.17
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG22	2	0.17
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG23	2	0.17
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG21	17	0.17
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG22	17	0.17
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG23	17	0.17
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG2	6	0.17
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG3	6	0.17
(1,1124)	1:378:A:THR:HG21	1:385:A:TRP:HA	2	0.17
(1,1124)	1:378:A:THR:HG22	1:385:A:TRP:HA	2	0.17
(1,1124)	1:378:A:THR:HG23	1:385:A:TRP:HA	2	0.17
(1,1124)	1:378:A:THR:HG21	1:385:A:TRP:HA	17	0.17
(1,1124)	1:378:A:THR:HG22	1:385:A:TRP:HA	17	0.17
(1,1124)	1:378:A:THR:HG23	1:385:A:TRP:HA	17	0.17
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	3	0.17
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	3	0.17
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	3	0.17
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	3	0.17
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	3	0.17
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	3	0.17
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	15	0.17
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	15	0.17
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	15	0.17
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	15	0.17
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	15	0.17
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	16	0.17
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	16	0.17
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	16	0.17
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	16	0.17
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	16	0.17
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	16	0.17
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	21	0.17
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	21	0.17
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	21	0.17
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	21	0.17
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	21	0.17
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	21	0.17
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB2	21	0.17
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB3	21	0.17
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB2	23	0.17
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB3	23	0.17
(1,631)	1:352:A:LEU:HG	1:351:A:GLN:HA	11	0.17
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	16	0.17
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	16	0.17
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	24	0.17
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	24	0.17
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	25	0.17
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	25	0.17
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE1	4	0.17
(1,231)	1:391:A:GLY:HA3	1:393:A:TYR:HE2	4	0.17
(1,88)	1:358:A:TYR:HE1	1:375:A:VAL:HB	20	0.17
(1,88)	1:358:A:TYR:HE2	1:375:A:VAL:HB	20	0.17
(1,2755)	1:422:A:GLN:H	1:423:A:VAL:HB	2	0.16
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG21	13	0.16
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG22	13	0.16
(1,2397)	1:379:A:THR:H	1:378:A:THR:HG23	13	0.16
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG11	25	0.16
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG12	25	0.16
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG13	25	0.16
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG21	25	0.16
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG22	25	0.16
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG23	25	0.16
(1,2189)	1:353:A:SER:H	1:389:A:VAL:HA	20	0.16
(1,2189)	1:353:A:SER:H	1:389:A:VAL:HA	24	0.16
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	14	0.16
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	14	0.16
(1,1951)	1:420:A:LEU:HD11	1:421:A:ARG:HB2	7	0.16
(1,1951)	1:420:A:LEU:HD11	1:421:A:ARG:HB3	7	0.16
(1,1951)	1:420:A:LEU:HD12	1:421:A:ARG:HB2	7	0.16
(1,1951)	1:420:A:LEU:HD12	1:421:A:ARG:HB3	7	0.16
(1,1951)	1:420:A:LEU:HD13	1:421:A:ARG:HB2	7	0.16
(1,1951)	1:420:A:LEU:HD13	1:421:A:ARG:HB3	7	0.16
(1,1951)	1:420:A:LEU:HD21	1:421:A:ARG:HB2	7	0.16
(1,1951)	1:420:A:LEU:HD21	1:421:A:ARG:HB3	7	0.16
(1,1951)	1:420:A:LEU:HD22	1:421:A:ARG:HB2	7	0.16
(1,1951)	1:420:A:LEU:HD22	1:421:A:ARG:HB3	7	0.16
(1,1951)	1:420:A:LEU:HD23	1:421:A:ARG:HB2	7	0.16
(1,1951)	1:420:A:LEU:HD23	1:421:A:ARG:HB3	7	0.16
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	12	0.16
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	12	0.16
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	18	0.16
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	18	0.16
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	24	0.16
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	24	0.16
(1,1607)	1:405:A:THR:HG21	1:401:A:LYS:HG2	12	0.16
(1,1607)	1:405:A:THR:HG21	1:401:A:LYS:HG3	12	0.16
(1,1607)	1:405:A:THR:HG22	1:401:A:LYS:HG2	12	0.16
(1,1607)	1:405:A:THR:HG22	1:401:A:LYS:HG3	12	0.16
(1,1607)	1:405:A:THR:HG23	1:401:A:LYS:HG2	12	0.16
(1,1607)	1:405:A:THR:HG23	1:401:A:LYS:HG3	12	0.16
(1,1305)	1:387:A:VAL:HG11	1:380:A:ARG:HA	19	0.16
(1,1305)	1:387:A:VAL:HG12	1:380:A:ARG:HA	19	0.16
(1,1305)	1:387:A:VAL:HG13	1:380:A:ARG:HA	19	0.16
(1,1305)	1:387:A:VAL:HG21	1:380:A:ARG:HA	19	0.16
(1,1305)	1:387:A:VAL:HG22	1:380:A:ARG:HA	19	0.16
(1,1305)	1:387:A:VAL:HG23	1:380:A:ARG:HA	19	0.16
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	12	0.16
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	12	0.16
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	12	0.16
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	12	0.16
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	12	0.16
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	12	0.16
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	23	0.16
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	23	0.16
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	23	0.16
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	23	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	23	0.16
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	23	0.16
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB2	7	0.16
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB3	7	0.16
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	1	0.16
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	1	0.16
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	6	0.16
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	6	0.16
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	11	0.16
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	11	0.16
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	12	0.16
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	12	0.16
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	21	0.16
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	21	0.16
(1,230)	1:390:A:SER:H	1:352:A:LEU:HG	8	0.16
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	1	0.16
(1,2189)	1:353:A:SER:H	1:389:A:VAL:HA	3	0.15
(1,2158)	1:351:A:GLN:H	1:352:A:LEU:HB2	5	0.15
(1,2158)	1:351:A:GLN:H	1:352:A:LEU:HB3	5	0.15
(1,2158)	1:351:A:GLN:H	1:352:A:LEU:HB2	14	0.15
(1,2158)	1:351:A:GLN:H	1:352:A:LEU:HB3	14	0.15
(1,2158)	1:351:A:GLN:H	1:352:A:LEU:HB2	23	0.15
(1,2158)	1:351:A:GLN:H	1:352:A:LEU:HB3	23	0.15
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	9	0.15
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	9	0.15
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	9	0.15
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	24	0.15
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	24	0.15
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	24	0.15
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	14	0.15
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	14	0.15
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	19	0.15
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	19	0.15
(1,1305)	1:387:A:VAL:HG11	1:380:A:ARG:HA	25	0.15
(1,1305)	1:387:A:VAL:HG12	1:380:A:ARG:HA	25	0.15
(1,1305)	1:387:A:VAL:HG13	1:380:A:ARG:HA	25	0.15
(1,1305)	1:387:A:VAL:HG21	1:380:A:ARG:HA	25	0.15
(1,1305)	1:387:A:VAL:HG22	1:380:A:ARG:HA	25	0.15
(1,1305)	1:387:A:VAL:HG23	1:380:A:ARG:HA	25	0.15
(1,1254)	1:385:A:TRP:HZ2	1:364:A:TRP:HE3	7	0.15
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG2	3	0.15
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG3	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	2	0.15
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	2	0.15
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	2	0.15
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	2	0.15
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	2	0.15
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	2	0.15
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	8	0.15
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	8	0.15
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	8	0.15
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	8	0.15
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	8	0.15
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	8	0.15
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	13	0.15
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	13	0.15
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	13	0.15
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	13	0.15
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	13	0.15
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	13	0.15
(1,797)	1:364:A:TRP:HE3	1:385:A:TRP:HZ2	7	0.15
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB2	24	0.15
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB3	24	0.15
(1,694)	1:356:A:SER:HB2	1:385:A:TRP:HZ3	10	0.15
(1,694)	1:356:A:SER:HB3	1:385:A:TRP:HZ3	10	0.15
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	5	0.15
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	5	0.15
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	10	0.15
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	10	0.15
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	17	0.15
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	17	0.15
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD2	23	0.15
(1,452)	1:342:A:SER:HA	1:344:A:PRO:HD3	23	0.15
(1,196)	1:385:A:TRP:HZ3	1:356:A:SER:HB2	10	0.15
(1,196)	1:385:A:TRP:HZ3	1:356:A:SER:HB3	10	0.15
(1,195)	1:385:A:TRP:HZ3	1:356:A:SER:HB2	10	0.15
(1,195)	1:385:A:TRP:HZ3	1:356:A:SER:HB3	10	0.15
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG21	13	0.15
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG22	13	0.15
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG23	13	0.15
(1,115)	1:385:A:TRP:HZ3	1:388:A:LEU:HG	6	0.15
(1,86)	1:358:A:TYR:HE1	1:362:A:ASN:HA	20	0.15
(1,86)	1:358:A:TYR:HE2	1:362:A:ASN:HA	20	0.15
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB2	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:352:A:LEU:HB2	1:350:A:LEU:HB3	20	0.15
(1,2727)	1:418:A:LYS:H	1:389:A:VAL:HG11	1	0.14
(1,2727)	1:418:A:LYS:H	1:389:A:VAL:HG12	1	0.14
(1,2727)	1:418:A:LYS:H	1:389:A:VAL:HG13	1	0.14
(1,2727)	1:418:A:LYS:H	1:389:A:VAL:HG21	1	0.14
(1,2727)	1:418:A:LYS:H	1:389:A:VAL:HG22	1	0.14
(1,2727)	1:418:A:LYS:H	1:389:A:VAL:HG23	1	0.14
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	3	0.14
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	3	0.14
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	12	0.14
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	12	0.14
(1,2189)	1:353:A:SER:H	1:389:A:VAL:HA	14	0.14
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	19	0.14
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	19	0.14
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	19	0.14
(1,1305)	1:387:A:VAL:HG11	1:380:A:ARG:HA	1	0.14
(1,1305)	1:387:A:VAL:HG12	1:380:A:ARG:HA	1	0.14
(1,1305)	1:387:A:VAL:HG13	1:380:A:ARG:HA	1	0.14
(1,1305)	1:387:A:VAL:HG21	1:380:A:ARG:HA	1	0.14
(1,1305)	1:387:A:VAL:HG22	1:380:A:ARG:HA	1	0.14
(1,1305)	1:387:A:VAL:HG23	1:380:A:ARG:HA	1	0.14
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD1	3	0.14
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD2	3	0.14
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD1	3	0.14
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD2	3	0.14
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD1	3	0.14
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD2	3	0.14
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD1	3	0.14
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD2	3	0.14
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD1	3	0.14
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD2	3	0.14
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD1	3	0.14
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD2	3	0.14
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD1	11	0.14
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD2	11	0.14
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD1	11	0.14
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD2	11	0.14
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD1	11	0.14
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD2	11	0.14
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD1	11	0.14
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD2	11	0.14
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD1	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD2	11	0.14
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD1	11	0.14
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD2	11	0.14
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB2	12	0.14
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB3	12	0.14
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB2	17	0.14
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB3	17	0.14
(1,706)	1:358:A:TYR:HA	1:362:A:ASN:HB2	25	0.14
(1,706)	1:358:A:TYR:HA	1:362:A:ASN:HB3	25	0.14
(1,694)	1:356:A:SER:HB2	1:385:A:TRP:HZ3	3	0.14
(1,694)	1:356:A:SER:HB3	1:385:A:TRP:HZ3	3	0.14
(1,694)	1:356:A:SER:HB2	1:385:A:TRP:HZ3	13	0.14
(1,694)	1:356:A:SER:HB3	1:385:A:TRP:HZ3	13	0.14
(1,694)	1:356:A:SER:HB2	1:385:A:TRP:HZ3	14	0.14
(1,694)	1:356:A:SER:HB3	1:385:A:TRP:HZ3	14	0.14
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA2	15	0.14
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA3	15	0.14
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA2	15	0.14
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA3	15	0.14
(1,226)	1:389:A:VAL:HG13	1:418:A:LYS:HD2	17	0.14
(1,226)	1:389:A:VAL:HG13	1:418:A:LYS:HD3	17	0.14
(1,196)	1:385:A:TRP:HZ3	1:356:A:SER:HB2	3	0.14
(1,196)	1:385:A:TRP:HZ3	1:356:A:SER:HB3	3	0.14
(1,196)	1:385:A:TRP:HZ3	1:356:A:SER:HB2	13	0.14
(1,196)	1:385:A:TRP:HZ3	1:356:A:SER:HB3	13	0.14
(1,196)	1:385:A:TRP:HZ3	1:356:A:SER:HB2	14	0.14
(1,196)	1:385:A:TRP:HZ3	1:356:A:SER:HB3	14	0.14
(1,195)	1:385:A:TRP:HZ3	1:356:A:SER:HB2	3	0.14
(1,195)	1:385:A:TRP:HZ3	1:356:A:SER:HB3	3	0.14
(1,195)	1:385:A:TRP:HZ3	1:356:A:SER:HB2	13	0.14
(1,195)	1:385:A:TRP:HZ3	1:356:A:SER:HB3	13	0.14
(1,195)	1:385:A:TRP:HZ3	1:356:A:SER:HB2	14	0.14
(1,195)	1:385:A:TRP:HZ3	1:356:A:SER:HB3	14	0.14
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB2	1	0.14
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB3	1	0.14
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG21	4	0.14
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG22	4	0.14
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG23	4	0.14
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB2	25	0.14
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB3	25	0.14
(1,2496)	1:392:A:VAL:H	1:390:A:SER:HA	14	0.13
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG11	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG12	17	0.13
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG13	17	0.13
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG21	17	0.13
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG22	17	0.13
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG23	17	0.13
(1,2189)	1:353:A:SER:H	1:389:A:VAL:HA	12	0.13
(1,2158)	1:351:A:GLN:H	1:352:A:LEU:HB2	16	0.13
(1,2158)	1:351:A:GLN:H	1:352:A:LEU:HB3	16	0.13
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	6	0.13
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	6	0.13
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	6	0.13
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	3	0.13
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	3	0.13
(1,1593)	1:404:A:SER:HA	1:403:A:VAL:HB	4	0.13
(1,1305)	1:387:A:VAL:HG11	1:380:A:ARG:HA	4	0.13
(1,1305)	1:387:A:VAL:HG12	1:380:A:ARG:HA	4	0.13
(1,1305)	1:387:A:VAL:HG13	1:380:A:ARG:HA	4	0.13
(1,1305)	1:387:A:VAL:HG21	1:380:A:ARG:HA	4	0.13
(1,1305)	1:387:A:VAL:HG22	1:380:A:ARG:HA	4	0.13
(1,1305)	1:387:A:VAL:HG23	1:380:A:ARG:HA	4	0.13
(1,1305)	1:387:A:VAL:HG11	1:380:A:ARG:HA	11	0.13
(1,1305)	1:387:A:VAL:HG12	1:380:A:ARG:HA	11	0.13
(1,1305)	1:387:A:VAL:HG13	1:380:A:ARG:HA	11	0.13
(1,1305)	1:387:A:VAL:HG21	1:380:A:ARG:HA	11	0.13
(1,1305)	1:387:A:VAL:HG22	1:380:A:ARG:HA	11	0.13
(1,1305)	1:387:A:VAL:HG23	1:380:A:ARG:HA	11	0.13
(1,1254)	1:385:A:TRP:HZ2	1:364:A:TRP:HE3	11	0.13
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG2	25	0.13
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG3	25	0.13
(1,1097)	1:377:A:GLU:HG2	1:386:A:TYR:HA	24	0.13
(1,1097)	1:377:A:GLU:HG3	1:386:A:TYR:HA	24	0.13
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	5	0.13
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	5	0.13
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	5	0.13
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	5	0.13
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	5	0.13
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	5	0.13
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	6	0.13
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	6	0.13
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	6	0.13
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	6	0.13
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	6	0.13
(1,857)	1:365:A:ALA:HB1	1:375:A:VAL:HA	24	0.13
(1,857)	1:365:A:ALA:HB2	1:375:A:VAL:HA	24	0.13
(1,857)	1:365:A:ALA:HB3	1:375:A:VAL:HA	24	0.13
(1,797)	1:364:A:TRP:HE3	1:385:A:TRP:HZ2	11	0.13
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB2	3	0.13
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB3	3	0.13
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB2	9	0.13
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB3	9	0.13
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB2	18	0.13
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB3	18	0.13
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB2	19	0.13
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB3	19	0.13
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA2	10	0.13
(1,236)	1:393:A:TYR:HE1	1:391:A:GLY:HA3	10	0.13
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA2	10	0.13
(1,236)	1:393:A:TYR:HE2	1:391:A:GLY:HA3	10	0.13
(1,230)	1:390:A:SER:H	1:352:A:LEU:HG	18	0.13
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB2	7	0.13
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB3	7	0.13
(1,153)	1:375:A:VAL:HB	1:386:A:TYR:HD1	6	0.13
(1,153)	1:375:A:VAL:HB	1:386:A:TYR:HD2	6	0.13
(1,129)	1:367:A:LYS:H	1:367:A:LYS:HE2	20	0.13
(1,129)	1:367:A:LYS:H	1:367:A:LYS:HE3	20	0.13
(1,41)	1:349:A:THR:HB	1:420:A:LEU:HG	17	0.13
(1,2573)	1:400:A:LYS:H	1:396:A:LYS:HD2	6	0.12
(1,2573)	1:400:A:LYS:H	1:396:A:LYS:HD3	6	0.12
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	20	0.12
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	20	0.12
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB2	22	0.12
(1,2459)	1:387:A:VAL:H	1:388:A:LEU:HB3	22	0.12
(1,2189)	1:353:A:SER:H	1:389:A:VAL:HA	22	0.12
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	17	0.12
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	17	0.12
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	17	0.12
(1,2005)	1:424:A:GLN:HA	1:422:A:GLN:HA	8	0.12
(1,2005)	1:424:A:GLN:HA	1:422:A:GLN:HA	19	0.12
(1,2005)	1:424:A:GLN:HA	1:422:A:GLN:HA	21	0.12
(1,1976)	1:422:A:GLN:HA	1:424:A:GLN:HA	8	0.12
(1,1976)	1:422:A:GLN:HA	1:424:A:GLN:HA	19	0.12
(1,1976)	1:422:A:GLN:HA	1:424:A:GLN:HA	21	0.12
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	15	0.12
(1,1593)	1:404:A:SER:HA	1:403:A:VAL:HB	25	0.12
(1,1305)	1:387:A:VAL:HG11	1:380:A:ARG:HA	8	0.12
(1,1305)	1:387:A:VAL:HG12	1:380:A:ARG:HA	8	0.12
(1,1305)	1:387:A:VAL:HG13	1:380:A:ARG:HA	8	0.12
(1,1305)	1:387:A:VAL:HG21	1:380:A:ARG:HA	8	0.12
(1,1305)	1:387:A:VAL:HG22	1:380:A:ARG:HA	8	0.12
(1,1305)	1:387:A:VAL:HG23	1:380:A:ARG:HA	8	0.12
(1,1254)	1:385:A:TRP:HZ2	1:364:A:TRP:HE3	19	0.12
(1,1254)	1:385:A:TRP:HZ2	1:364:A:TRP:HE3	22	0.12
(1,1224)	1:385:A:TRP:HD1	1:379:A:THR:HA	8	0.12
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG21	13	0.12
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG22	13	0.12
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG23	13	0.12
(1,1161)	1:380:A:ARG:HB2	1:385:A:TRP:HE3	12	0.12
(1,1161)	1:380:A:ARG:HB3	1:385:A:TRP:HE3	12	0.12
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG2	24	0.12
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG3	24	0.12
(1,1124)	1:378:A:THR:HG21	1:385:A:TRP:HA	13	0.12
(1,1124)	1:378:A:THR:HG22	1:385:A:TRP:HA	13	0.12
(1,1124)	1:378:A:THR:HG23	1:385:A:TRP:HA	13	0.12
(1,1094)	1:377:A:GLU:HG2	1:376:A:TYR:HE1	22	0.12
(1,1094)	1:377:A:GLU:HG2	1:376:A:TYR:HE2	22	0.12
(1,1094)	1:377:A:GLU:HG3	1:376:A:TYR:HE1	22	0.12
(1,1094)	1:377:A:GLU:HG3	1:376:A:TYR:HE2	22	0.12
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	9	0.12
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	9	0.12
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	9	0.12
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	9	0.12
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	9	0.12
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	9	0.12
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	24	0.12
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	24	0.12
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	24	0.12
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	24	0.12
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	24	0.12
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	24	0.12
(1,797)	1:364:A:TRP:HE3	1:385:A:TRP:HZ2	19	0.12
(1,797)	1:364:A:TRP:HE3	1:385:A:TRP:HZ2	22	0.12
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD1	2	0.12
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD2	2	0.12
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD1	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD2	2	0.12
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD1	2	0.12
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD2	2	0.12
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD1	2	0.12
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD2	2	0.12
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD1	2	0.12
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD2	2	0.12
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD1	2	0.12
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD2	2	0.12
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB2	1	0.12
(1,742)	1:361:A:LEU:HG	1:355:A:SER:HB3	1	0.12
(1,224)	1:389:A:VAL:HG12	1:423:A:VAL:HG11	10	0.12
(1,224)	1:389:A:VAL:HG12	1:423:A:VAL:HG12	10	0.12
(1,224)	1:389:A:VAL:HG12	1:423:A:VAL:HG13	10	0.12
(1,224)	1:389:A:VAL:HG12	1:423:A:VAL:HG21	10	0.12
(1,224)	1:389:A:VAL:HG12	1:423:A:VAL:HG22	10	0.12
(1,224)	1:389:A:VAL:HG12	1:423:A:VAL:HG23	10	0.12
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG21	18	0.12
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG22	18	0.12
(1,177)	1:382:A:GLY:H	1:379:A:THR:HG23	18	0.12
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB2	24	0.12
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB3	24	0.12
(1,4)	1:336:A:ASN:HD21	1:337:A:ASN:HA	1	0.12
(1,4)	1:336:A:ASN:HD22	1:337:A:ASN:HA	1	0.12
(1,4)	1:336:A:ASN:HD21	1:337:A:ASN:HA	11	0.12
(1,4)	1:336:A:ASN:HD22	1:337:A:ASN:HA	11	0.12
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG11	8	0.11
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG12	8	0.11
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG13	8	0.11
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG21	8	0.11
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG22	8	0.11
(1,2294)	1:366:A:LYS:H	1:375:A:VAL:HG23	8	0.11
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	20	0.11
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	20	0.11
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	20	0.11
(1,2021)	1:425:A:ALA:HB1	1:423:A:VAL:HB	21	0.11
(1,2021)	1:425:A:ALA:HB2	1:423:A:VAL:HB	21	0.11
(1,2021)	1:425:A:ALA:HB3	1:423:A:VAL:HB	21	0.11
(1,2005)	1:424:A:GLN:HA	1:422:A:GLN:HA	5	0.11
(1,2005)	1:424:A:GLN:HA	1:422:A:GLN:HA	6	0.11
(1,2005)	1:424:A:GLN:HA	1:422:A:GLN:HA	14	0.11
(1,1976)	1:422:A:GLN:HA	1:424:A:GLN:HA	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1976)	1:422:A:GLN:HA	1:424:A:GLN:HA	6	0.11
(1,1976)	1:422:A:GLN:HA	1:424:A:GLN:HA	14	0.11
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG2	17	0.11
(1,1754)	1:414:A:ASN:HA	1:413:A:LYS:HG3	17	0.11
(1,1607)	1:405:A:THR:HG21	1:401:A:LYS:HG2	4	0.11
(1,1607)	1:405:A:THR:HG21	1:401:A:LYS:HG3	4	0.11
(1,1607)	1:405:A:THR:HG22	1:401:A:LYS:HG2	4	0.11
(1,1607)	1:405:A:THR:HG22	1:401:A:LYS:HG3	4	0.11
(1,1607)	1:405:A:THR:HG23	1:401:A:LYS:HG2	4	0.11
(1,1607)	1:405:A:THR:HG23	1:401:A:LYS:HG3	4	0.11
(1,1305)	1:387:A:VAL:HG11	1:380:A:ARG:HA	7	0.11
(1,1305)	1:387:A:VAL:HG12	1:380:A:ARG:HA	7	0.11
(1,1305)	1:387:A:VAL:HG13	1:380:A:ARG:HA	7	0.11
(1,1305)	1:387:A:VAL:HG21	1:380:A:ARG:HA	7	0.11
(1,1305)	1:387:A:VAL:HG22	1:380:A:ARG:HA	7	0.11
(1,1305)	1:387:A:VAL:HG23	1:380:A:ARG:HA	7	0.11
(1,1305)	1:387:A:VAL:HG11	1:380:A:ARG:HA	21	0.11
(1,1305)	1:387:A:VAL:HG12	1:380:A:ARG:HA	21	0.11
(1,1305)	1:387:A:VAL:HG13	1:380:A:ARG:HA	21	0.11
(1,1305)	1:387:A:VAL:HG21	1:380:A:ARG:HA	21	0.11
(1,1305)	1:387:A:VAL:HG22	1:380:A:ARG:HA	21	0.11
(1,1305)	1:387:A:VAL:HG23	1:380:A:ARG:HA	21	0.11
(1,1254)	1:385:A:TRP:HZ2	1:364:A:TRP:HE3	1	0.11
(1,1254)	1:385:A:TRP:HZ2	1:364:A:TRP:HE3	6	0.11
(1,1254)	1:385:A:TRP:HZ2	1:364:A:TRP:HE3	20	0.11
(1,1224)	1:385:A:TRP:HD1	1:379:A:THR:HA	11	0.11
(1,1224)	1:385:A:TRP:HD1	1:379:A:THR:HA	18	0.11
(1,1224)	1:385:A:TRP:HD1	1:379:A:THR:HA	22	0.11
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG2	15	0.11
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG3	15	0.11
(1,1094)	1:377:A:GLU:HG2	1:376:A:TYR:HE1	23	0.11
(1,1094)	1:377:A:GLU:HG2	1:376:A:TYR:HE2	23	0.11
(1,1094)	1:377:A:GLU:HG3	1:376:A:TYR:HE1	23	0.11
(1,1094)	1:377:A:GLU:HG3	1:376:A:TYR:HE2	23	0.11
(1,1018)	1:374:A:VAL:HB	1:373:A:TYR:HA	8	0.11
(1,857)	1:365:A:ALA:HB1	1:375:A:VAL:HA	15	0.11
(1,857)	1:365:A:ALA:HB2	1:375:A:VAL:HA	15	0.11
(1,857)	1:365:A:ALA:HB3	1:375:A:VAL:HA	15	0.11
(1,857)	1:365:A:ALA:HB1	1:375:A:VAL:HA	21	0.11
(1,857)	1:365:A:ALA:HB2	1:375:A:VAL:HA	21	0.11
(1,857)	1:365:A:ALA:HB3	1:375:A:VAL:HA	21	0.11
(1,857)	1:365:A:ALA:HB1	1:375:A:VAL:HA	23	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,857)	1:365:A:ALA:HB2	1:375:A:VAL:HA	23	0.11
(1,857)	1:365:A:ALA:HB3	1:375:A:VAL:HA	23	0.11
(1,797)	1:364:A:TRP:HE3	1:385:A:TRP:HZ2	1	0.11
(1,797)	1:364:A:TRP:HE3	1:385:A:TRP:HZ2	6	0.11
(1,797)	1:364:A:TRP:HE3	1:385:A:TRP:HZ2	20	0.11
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD1	12	0.11
(1,762)	1:361:A:LEU:HD11	1:376:A:TYR:HD2	12	0.11
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD1	12	0.11
(1,762)	1:361:A:LEU:HD12	1:376:A:TYR:HD2	12	0.11
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD1	12	0.11
(1,762)	1:361:A:LEU:HD13	1:376:A:TYR:HD2	12	0.11
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD1	12	0.11
(1,762)	1:361:A:LEU:HD21	1:376:A:TYR:HD2	12	0.11
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD1	12	0.11
(1,762)	1:361:A:LEU:HD22	1:376:A:TYR:HD2	12	0.11
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD1	12	0.11
(1,762)	1:361:A:LEU:HD23	1:376:A:TYR:HD2	12	0.11
(1,752)	1:361:A:LEU:HD11	1:353:A:SER:HA	9	0.11
(1,752)	1:361:A:LEU:HD12	1:353:A:SER:HA	9	0.11
(1,752)	1:361:A:LEU:HD13	1:353:A:SER:HA	9	0.11
(1,752)	1:361:A:LEU:HD21	1:353:A:SER:HA	9	0.11
(1,752)	1:361:A:LEU:HD22	1:353:A:SER:HA	9	0.11
(1,752)	1:361:A:LEU:HD23	1:353:A:SER:HA	9	0.11
(1,656)	1:353:A:SER:HA	1:387:A:VAL:HG11	16	0.11
(1,656)	1:353:A:SER:HA	1:387:A:VAL:HG12	16	0.11
(1,656)	1:353:A:SER:HA	1:387:A:VAL:HG13	16	0.11
(1,656)	1:353:A:SER:HA	1:387:A:VAL:HG21	16	0.11
(1,656)	1:353:A:SER:HA	1:387:A:VAL:HG22	16	0.11
(1,656)	1:353:A:SER:HA	1:387:A:VAL:HG23	16	0.11
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB2	8	0.11
(1,177)	1:382:A:GLY:H	1:380:A:ARG:HB3	8	0.11
(1,153)	1:375:A:VAL:HB	1:386:A:TYR:HD1	10	0.11
(1,153)	1:375:A:VAL:HB	1:386:A:TYR:HD2	10	0.11
(1,4)	1:336:A:ASN:HD21	1:337:A:ASN:HA	7	0.11
(1,4)	1:336:A:ASN:HD22	1:337:A:ASN:HA	7	0.11
(1,2005)	1:424:A:GLN:HA	1:422:A:GLN:HA	16	0.1
(1,1976)	1:422:A:GLN:HA	1:424:A:GLN:HA	16	0.1
(1,1847)	1:417:A:ALA:HB1	1:350:A:LEU:HG	10	0.1
(1,1847)	1:417:A:ALA:HB2	1:350:A:LEU:HG	10	0.1
(1,1847)	1:417:A:ALA:HB3	1:350:A:LEU:HG	10	0.1
(1,1305)	1:387:A:VAL:HG11	1:380:A:ARG:HA	9	0.1
(1,1305)	1:387:A:VAL:HG12	1:380:A:ARG:HA	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1305)	1:387:A:VAL:HG13	1:380:A:ARG:HA	9	0.1
(1,1305)	1:387:A:VAL:HG21	1:380:A:ARG:HA	9	0.1
(1,1305)	1:387:A:VAL:HG22	1:380:A:ARG:HA	9	0.1
(1,1305)	1:387:A:VAL:HG23	1:380:A:ARG:HA	9	0.1
(1,1254)	1:385:A:TRP:HZ2	1:364:A:TRP:HE3	3	0.1
(1,1254)	1:385:A:TRP:HZ2	1:364:A:TRP:HE3	14	0.1
(1,1224)	1:385:A:TRP:HD1	1:379:A:THR:HA	7	0.1
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG21	21	0.1
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG22	21	0.1
(1,1210)	1:385:A:TRP:HA	1:378:A:THR:HG23	21	0.1
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG2	22	0.1
(1,1140)	1:379:A:THR:HB	1:380:A:ARG:HG3	22	0.1
(1,1124)	1:378:A:THR:HG21	1:385:A:TRP:HA	21	0.1
(1,1124)	1:378:A:THR:HG22	1:385:A:TRP:HA	21	0.1
(1,1124)	1:378:A:THR:HG23	1:385:A:TRP:HA	21	0.1
(1,1018)	1:374:A:VAL:HB	1:373:A:TYR:HA	25	0.1
(1,950)	1:370:A:LEU:HD11	1:385:A:TRP:HH2	1	0.1
(1,950)	1:370:A:LEU:HD12	1:385:A:TRP:HH2	1	0.1
(1,950)	1:370:A:LEU:HD13	1:385:A:TRP:HH2	1	0.1
(1,950)	1:370:A:LEU:HD21	1:385:A:TRP:HH2	1	0.1
(1,950)	1:370:A:LEU:HD22	1:385:A:TRP:HH2	1	0.1
(1,950)	1:370:A:LEU:HD23	1:385:A:TRP:HH2	1	0.1
(1,808)	1:364:A:TRP:HZ2	1:353:A:SER:HB2	2	0.1
(1,808)	1:364:A:TRP:HZ2	1:353:A:SER:HB3	2	0.1
(1,797)	1:364:A:TRP:HE3	1:385:A:TRP:HZ2	3	0.1
(1,797)	1:364:A:TRP:HE3	1:385:A:TRP:HZ2	14	0.1
(1,752)	1:361:A:LEU:HD11	1:353:A:SER:HA	11	0.1
(1,752)	1:361:A:LEU:HD12	1:353:A:SER:HA	11	0.1
(1,752)	1:361:A:LEU:HD13	1:353:A:SER:HA	11	0.1
(1,752)	1:361:A:LEU:HD21	1:353:A:SER:HA	11	0.1
(1,752)	1:361:A:LEU:HD22	1:353:A:SER:HA	11	0.1
(1,752)	1:361:A:LEU:HD23	1:353:A:SER:HA	11	0.1
(1,706)	1:358:A:TYR:HA	1:362:A:ASN:HB2	11	0.1
(1,706)	1:358:A:TYR:HA	1:362:A:ASN:HB3	11	0.1
(1,190)	1:385:A:TRP:HH2	1:358:A:TYR:HA	22	0.1

10 Dihedral-angle violation analysis

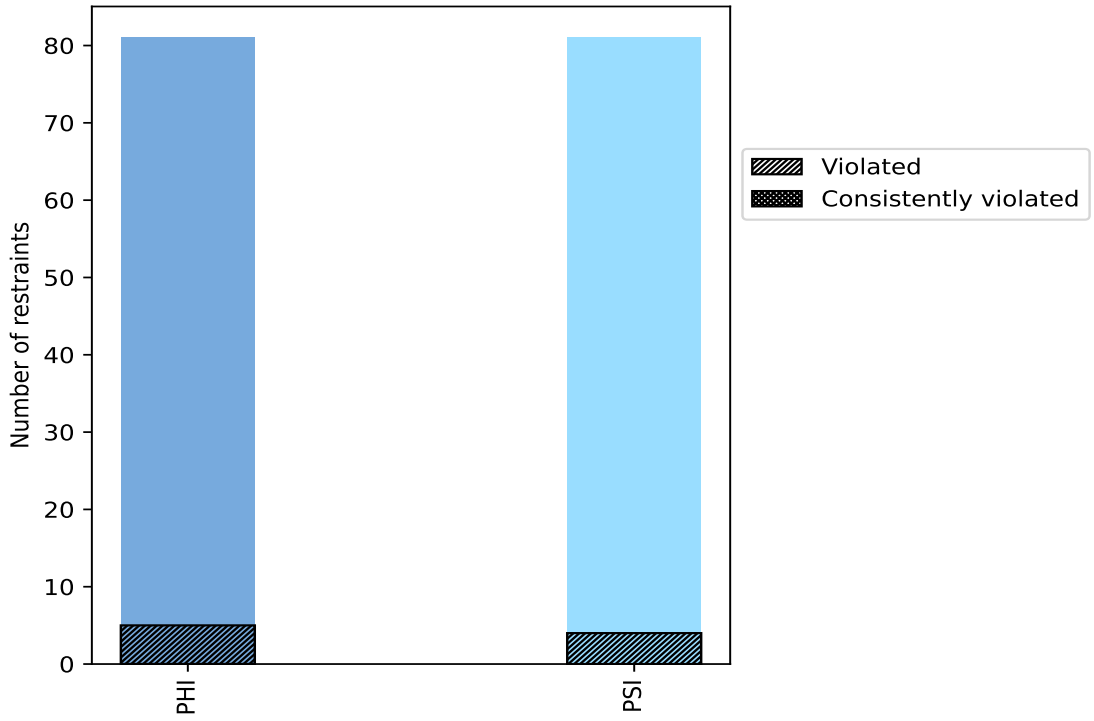
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	81	50.0	5	6.2	3.1	0	0.0	0.0
PSI	81	50.0	4	4.9	2.5	0	0.0	0.0
Total	162	100.0	9	5.6	5.6	0	0.0	0.0

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations



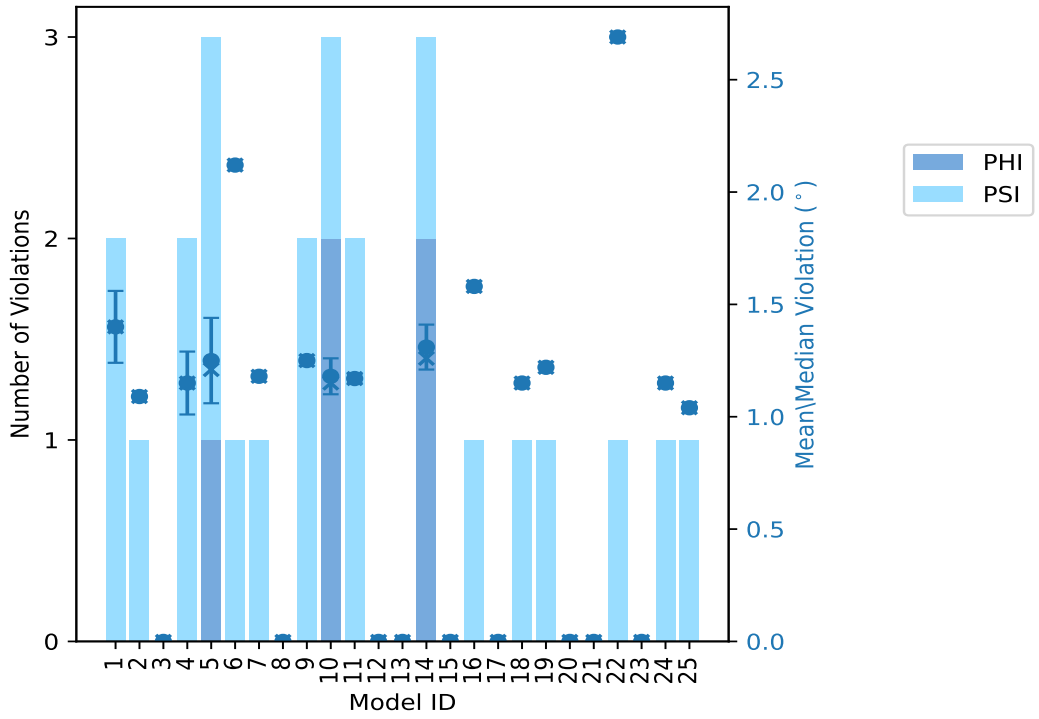
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	2	2	1.4	1.55	0.16	1.4
2	0	1	1	1.09	1.09	0.0	1.09
3	0	0	0	0.0	0.0	0.0	0.0
4	0	2	2	1.15	1.29	0.14	1.15
5	1	2	3	1.25	1.49	0.19	1.21
6	0	1	1	2.12	2.12	0.0	2.12
7	0	1	1	1.18	1.18	0.0	1.18
8	0	0	0	0.0	0.0	0.0	0.0
9	0	2	2	1.25	1.26	0.01	1.25
10	2	1	3	1.18	1.29	0.08	1.15
11	0	2	2	1.17	1.19	0.02	1.17
12	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0.0	0.0	0.0	0.0
14	2	1	3	1.31	1.46	0.1	1.26
15	0	0	0	0.0	0.0	0.0	0.0
16	0	1	1	1.58	1.58	0.0	1.58
17	0	0	0	0.0	0.0	0.0	0.0
18	0	1	1	1.15	1.15	0.0	1.15
19	0	1	1	1.22	1.22	0.0	1.22
20	0	0	0	0.0	0.0	0.0	0.0
21	0	0	0	0.0	0.0	0.0	0.0
22	0	1	1	2.69	2.69	0.0	2.69
23	0	0	0	0.0	0.0	0.0	0.0
24	0	1	1	1.15	1.15	0.0	1.15
25	0	1	1	1.04	1.04	0.0	1.04

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
5	1	6	1	4.0
0	0	0	2	8.0
0	1	1	3	12.0
0	0	0	4	16.0
0	0	0	5	20.0
0	0	0	6	24.0
0	0	0	7	28.0
0	1	1	8	32.0
0	1	1	9	36.0
0	0	0	10	40.0
0	0	0	11	44.0

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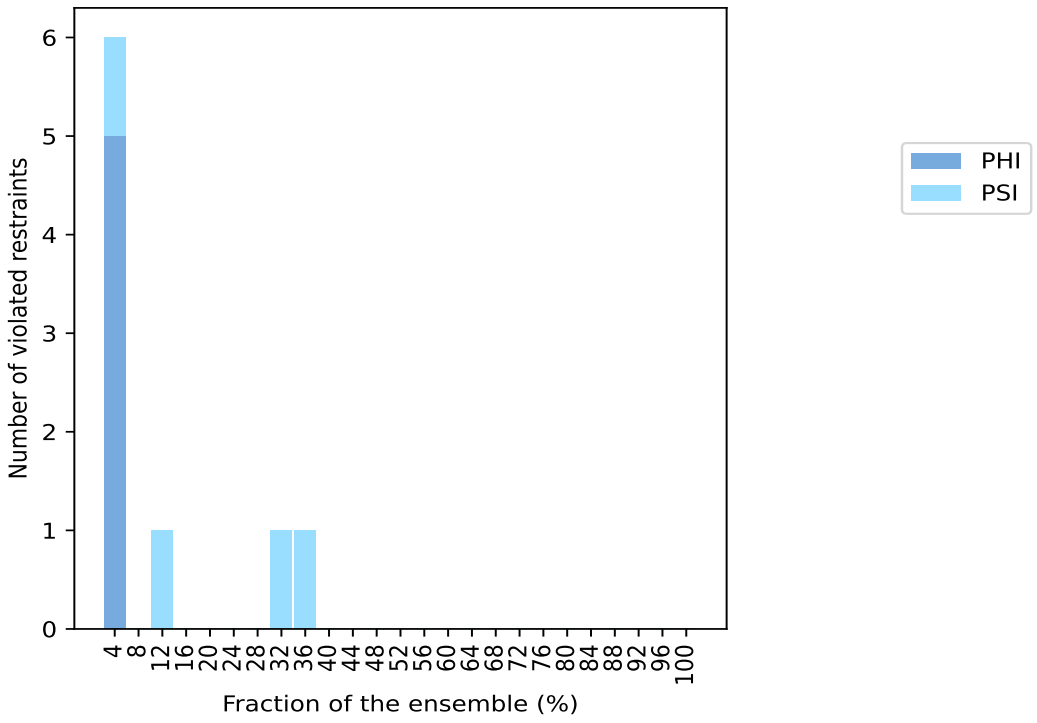
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	48.0
0	0	0	13	52.0
0	0	0	14	56.0
0	0	0	15	60.0
0	0	0	16	64.0
0	0	0	17	68.0
0	0	0	18	72.0
0	0	0	19	76.0
0	0	0	20	80.0
0	0	0	21	84.0
0	0	0	22	88.0
0	0	0	23	92.0
0	0	0	24	96.0
0	0	0	25	100.0

[1] Number of models with violations

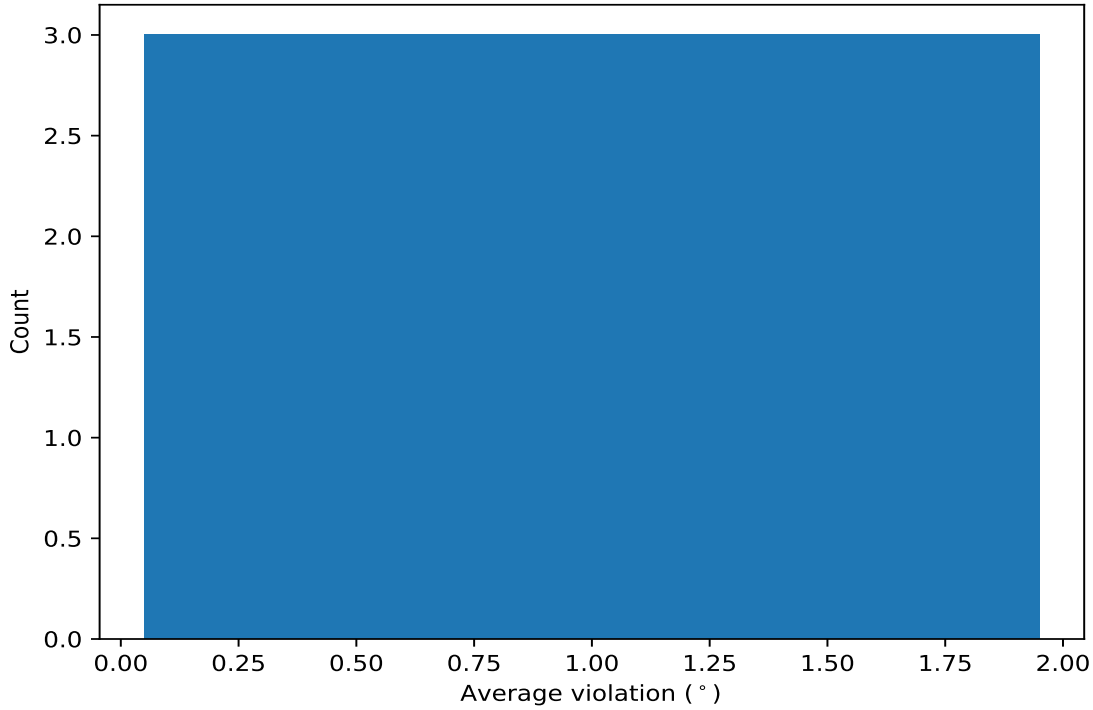
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle 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.

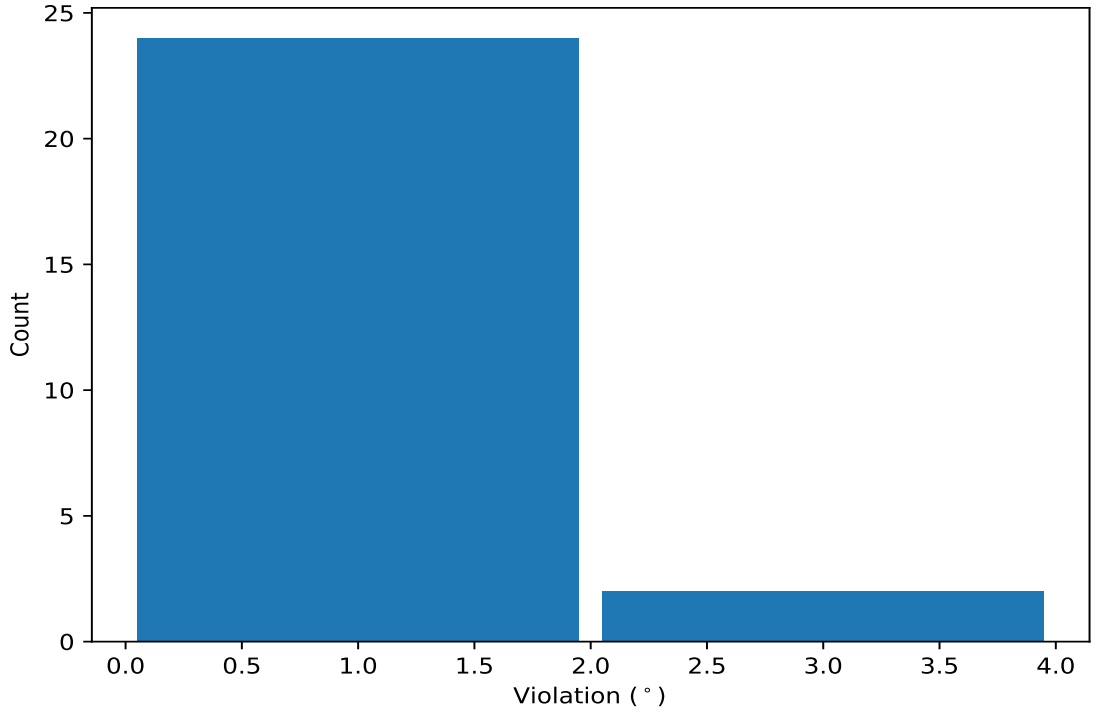
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,70)	1:378:A:THR:N	1:378:A:THR:CA	1:378:A:THR:C	1:379:A:THR:N	9	1.53	0.52	1.29
(1,144)	1:418:A:LYS:N	1:418:A:LYS:CA	1:418:A:LYS:C	1:419:A:PRO:N	8	1.14	0.07	1.15
(1,120)	1:405:A:THR:N	1:405:A:THR:CA	1:405:A:THR:C	1:406:A:LEU:N	3	1.22	0.0	1.22

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints (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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,70)	1:378:A:THR:N	1:378:A:THR:CA	1:378:A:THR:C	1:379:A:THR:N	22	2.69
(1,70)	1:378:A:THR:N	1:378:A:THR:CA	1:378:A:THR:C	1:379:A:THR:N	6	2.12
(1,70)	1:378:A:THR:N	1:378:A:THR:CA	1:378:A:THR:C	1:379:A:THR:N	16	1.58
(1,70)	1:378:A:THR:N	1:378:A:THR:CA	1:378:A:THR:C	1:379:A:THR:N	1	1.55
(1,93)	1:391:A:GLY:C	1:392:A:VAL:N	1:392:A:VAL:CA	1:392:A:VAL:C	5	1.49
(1,23)	1:349:A:THR:C	1:350:A:LEU:N	1:350:A:LEU:CA	1:350:A:LEU:C	14	1.46
(1,70)	1:378:A:THR:N	1:378:A:THR:CA	1:378:A:THR:C	1:379:A:THR:N	4	1.29
(1,19)	1:347:A:HIS:C	1:348:A:TYR:N	1:348:A:TYR:CA	1:348:A:TYR:C	10	1.29
(1,144)	1:418:A:LYS:N	1:418:A:LYS:CA	1:418:A:LYS:C	1:419:A:PRO:N	9	1.26
(1,85)	1:386:A:TYR:C	1:387:A:VAL:N	1:387:A:VAL:CA	1:387:A:VAL:C	14	1.26
(1,70)	1:378:A:THR:N	1:378:A:THR:CA	1:378:A:THR:C	1:379:A:THR:N	9	1.25
(1,138)	1:415:A:PRO:N	1:415:A:PRO:CA	1:415:A:PRO:C	1:416:A:TRP:N	1	1.24
(1,120)	1:405:A:THR:N	1:405:A:THR:CA	1:405:A:THR:C	1:406:A:LEU:N	14	1.22
(1,120)	1:405:A:THR:N	1:405:A:THR:CA	1:405:A:THR:C	1:406:A:LEU:N	19	1.22

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,120)	1:405:A:THR:N	1:405:A:THR:CA	1:405:A:THR:C	1:406:A:LEU:N	5	1.21
(1,70)	1:378:A:THR:N	1:378:A:THR:CA	1:378:A:THR:C	1:379:A:THR:N	11	1.19
(1,144)	1:418:A:LYS:N	1:418:A:LYS:CA	1:418:A:LYS:C	1:419:A:PRO:N	7	1.18
(1,144)	1:418:A:LYS:N	1:418:A:LYS:CA	1:418:A:LYS:C	1:419:A:PRO:N	11	1.16
(1,144)	1:418:A:LYS:N	1:418:A:LYS:CA	1:418:A:LYS:C	1:419:A:PRO:N	10	1.15
(1,144)	1:418:A:LYS:N	1:418:A:LYS:CA	1:418:A:LYS:C	1:419:A:PRO:N	18	1.15
(1,144)	1:418:A:LYS:N	1:418:A:LYS:CA	1:418:A:LYS:C	1:419:A:PRO:N	24	1.15
(1,73)	1:379:A:THR:C	1:380:A:ARG:N	1:380:A:ARG:CA	1:380:A:ARG:C	10	1.1
(1,144)	1:418:A:LYS:N	1:418:A:LYS:CA	1:418:A:LYS:C	1:419:A:PRO:N	2	1.09
(1,70)	1:378:A:THR:N	1:378:A:THR:CA	1:378:A:THR:C	1:379:A:THR:N	5	1.04
(1,70)	1:378:A:THR:N	1:378:A:THR:CA	1:378:A:THR:C	1:379:A:THR:N	25	1.04
(1,144)	1:418:A:LYS:N	1:418:A:LYS:CA	1:418:A:LYS:C	1:419:A:PRO:N	4	1.01