



Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 06:15 pm BST

PDB ID : 5NWM
BMRB ID : 34131
Title : Insight into the molecular recognition mechanism of the coactivator NCoA1 by STAT6
Authors : Russo, L.; Becker, S.; Griesinger, C.
Deposited on : 2017-05-06

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

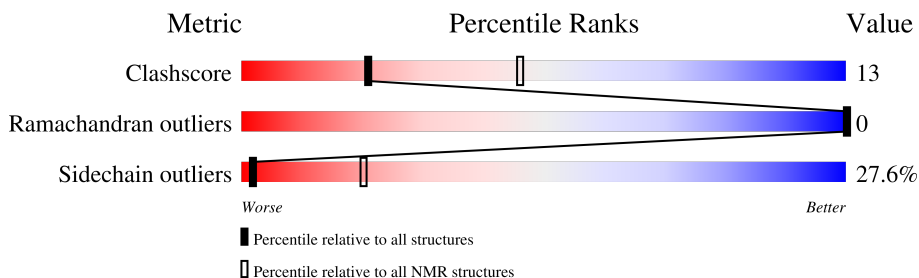
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	132	
2	B	32	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:260-A:303, A:307-A:348, A:356-A:366 (97)	0.32	10

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 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2523 atoms, of which 1247 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	132	2041	641	1008	185	197	10	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	-	expression tag	UNP Q15788
A	255	HIS	-	expression tag	UNP Q15788
A	256	MET	-	expression tag	UNP Q15788
A	343	ARG	LYS	engineered mutation	UNP Q15788

- Molecule 2 is a protein called Signal transducer and activator of transcription 6.

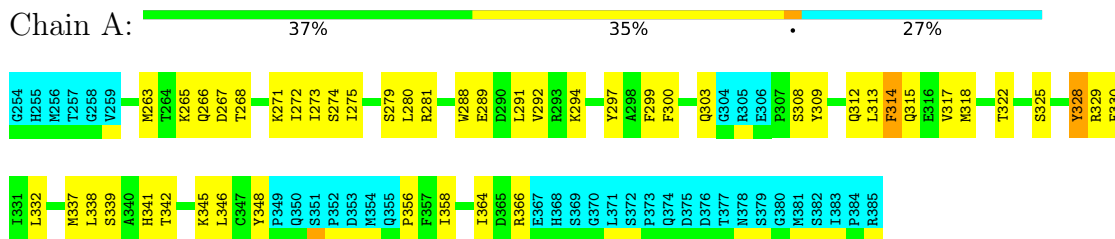
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	32	482	157	239	36	50	0

4 Residue-property plots [i](#)

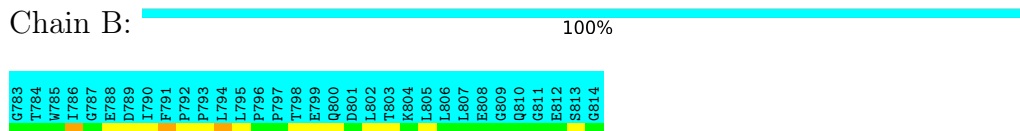
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Nuclear receptor coactivator 1



- Molecule 2: Signal transducer and activator of transcription 6

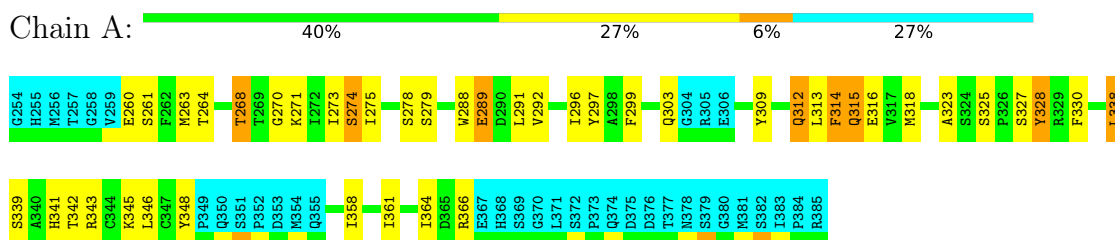


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

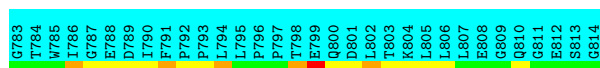
4.2.1 Score per residue for model 1

- Molecule 1: Nuclear receptor coactivator 1




- Molecule 2: Signal transducer and activator of transcription 6

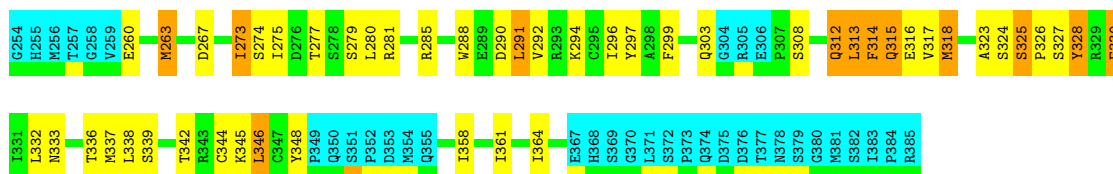
Chain B:  100%



4.2.2 Score per residue for model 2

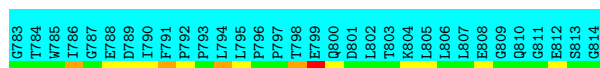
- Molecule 1: Nuclear receptor coactivator 1

Chain A:  36% 28% 9% 27%



- Molecule 2: Signal transducer and activator of transcription 6

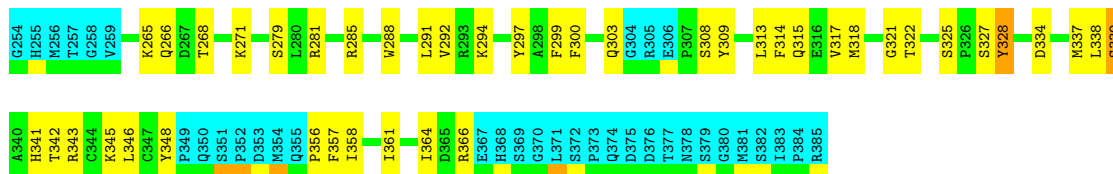
Chain B:  100%



4.2.3 Score per residue for model 3

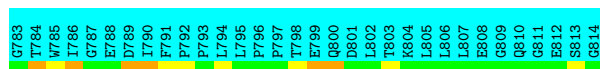
- Molecule 1: Nuclear receptor coactivator 1

Chain A:  41% 31% 27%



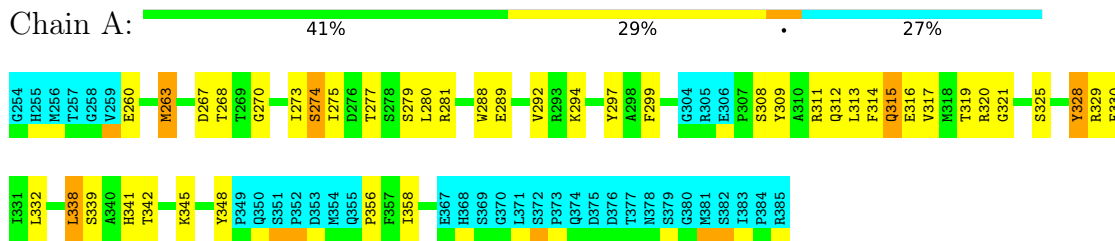
- Molecule 2: Signal transducer and activator of transcription 6

Chain B:  100%

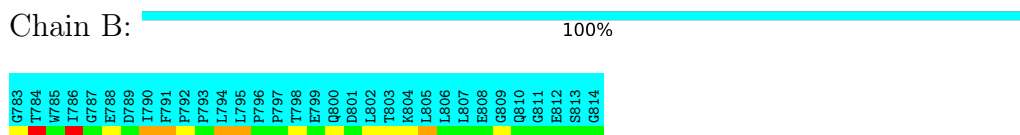


4.2.4 Score per residue for model 4

- Molecule 1: Nuclear receptor coactivator 1

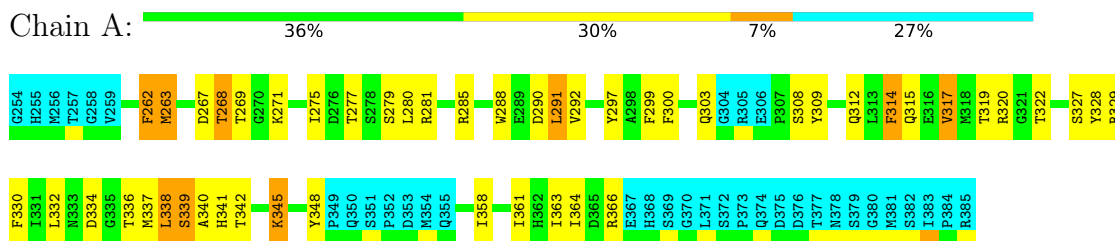


- Molecule 2: Signal transducer and activator of transcription 6

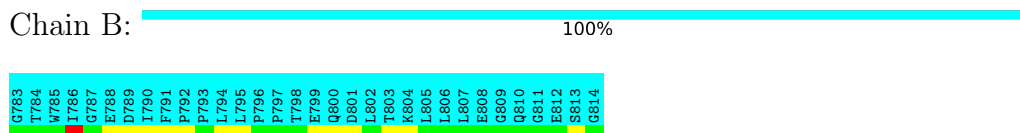


4.2.5 Score per residue for model 5

- Molecule 1: Nuclear receptor coactivator 1

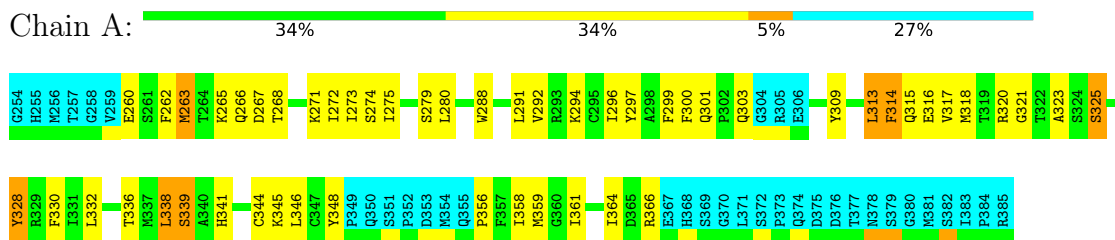


- Molecule 2: Signal transducer and activator of transcription 6



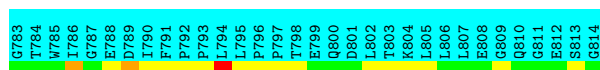
4.2.6 Score per residue for model 6

- Molecule 1: Nuclear receptor coactivator 1



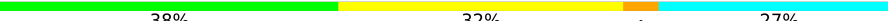
- Molecule 2: Signal transducer and activator of transcription 6

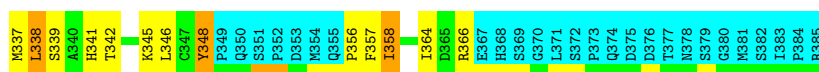
Chain B:  100%



4.2.7 Score per residue for model 7

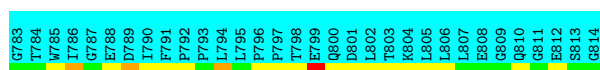
- Molecule 1: Nuclear receptor coactivator 1

Chain A:  38% 32% 27%



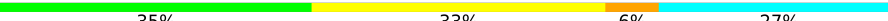
- Molecule 2: Signal transducer and activator of transcription 6

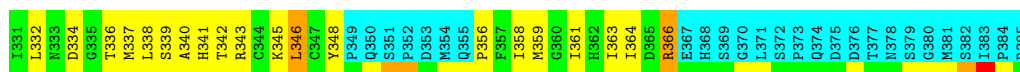
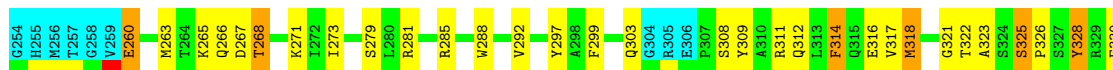
Chain B:  100%



4.2.8 Score per residue for model 8

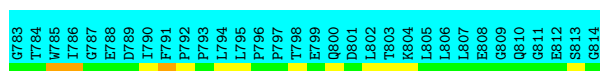
- Molecule 1: Nuclear receptor coactivator 1

Chain A:  35% 33% 6% 27%



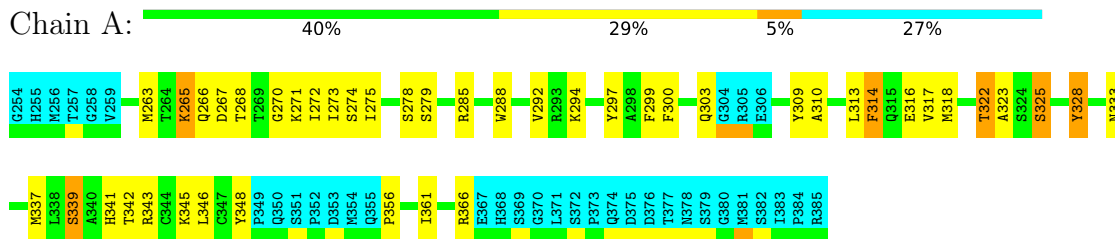
- Molecule 2: Signal transducer and activator of transcription 6

Chain B:  100%

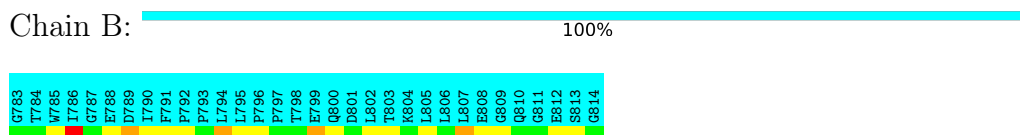


4.2.9 Score per residue for model 9

- Molecule 1: Nuclear receptor coactivator 1

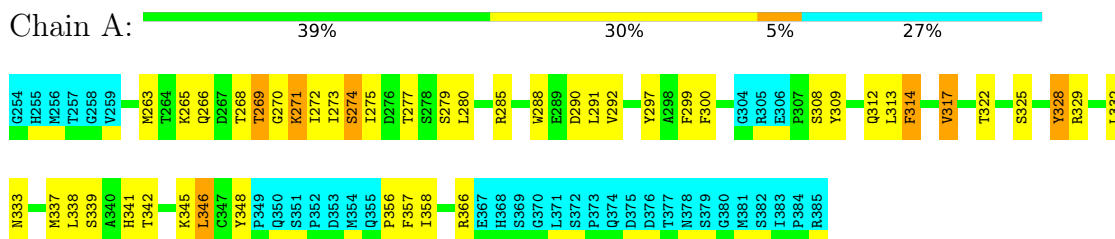


- Molecule 2: Signal transducer and activator of transcription 6

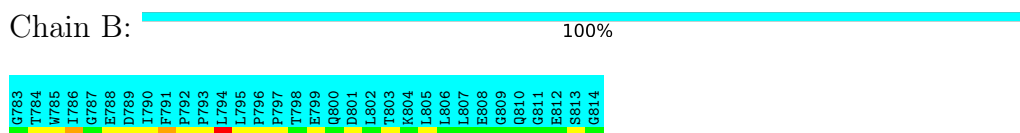


4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Nuclear receptor coactivator 1

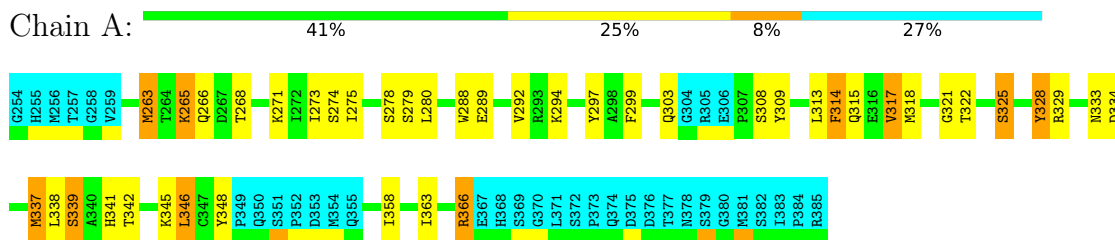


- Molecule 2: Signal transducer and activator of transcription 6



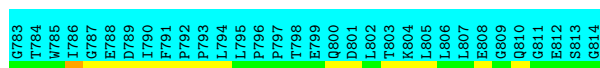
4.2.11 Score per residue for model 11

- Molecule 1: Nuclear receptor coactivator 1




- Molecule 2: Signal transducer and activator of transcription 6

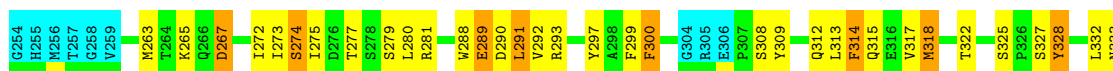
Chain B:  100%



4.2.12 Score per residue for model 12

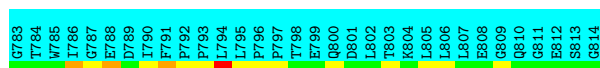
- Molecule 1: Nuclear receptor coactivator 1

Chain A:  39% 28% 7% 27%




- Molecule 2: Signal transducer and activator of transcription 6

Chain B:  100%



4.2.13 Score per residue for model 13

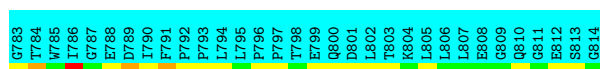
- Molecule 1: Nuclear receptor coactivator 1

Chain A:  37% 32% 5% 27%



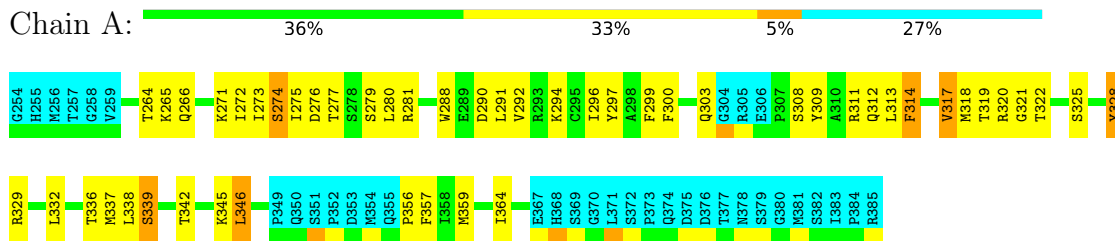
- Molecule 2: Signal transducer and activator of transcription 6

Chain B:  100%

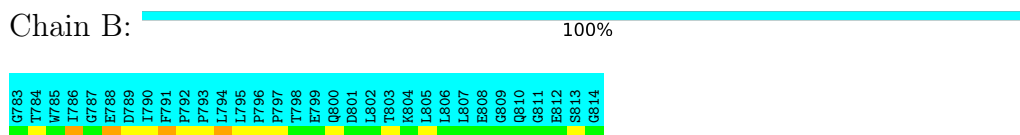


4.2.14 Score per residue for model 14

- Molecule 1: Nuclear receptor coactivator 1

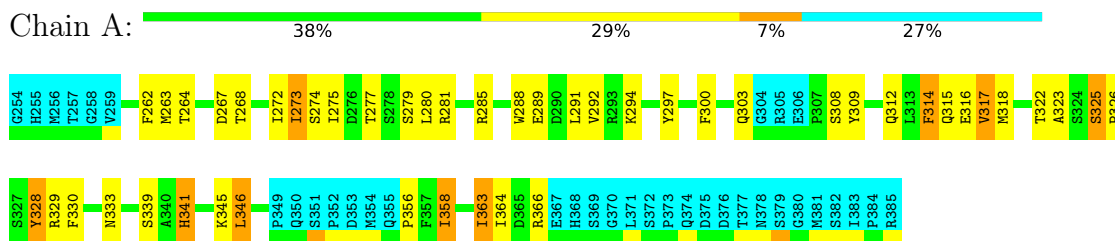


- Molecule 2: Signal transducer and activator of transcription 6

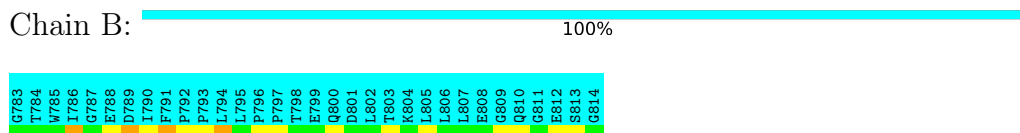


4.2.15 Score per residue for model 15

- Molecule 1: Nuclear receptor coactivator 1

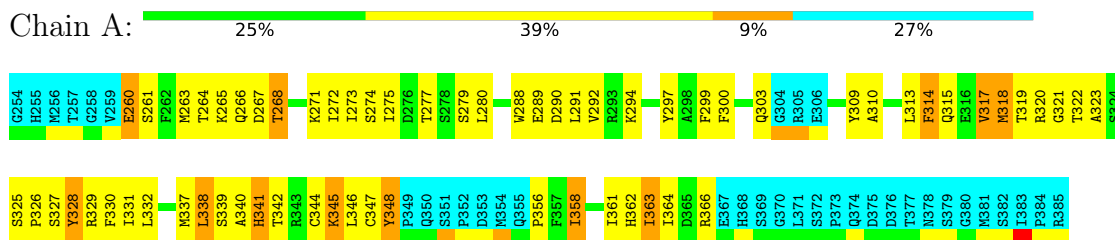


- Molecule 2: Signal transducer and activator of transcription 6



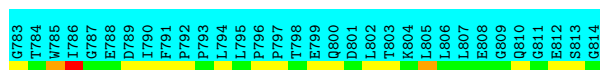
4.2.16 Score per residue for model 16

- Molecule 1: Nuclear receptor coactivator 1



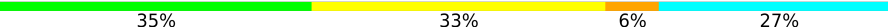
- Molecule 2: Signal transducer and activator of transcription 6

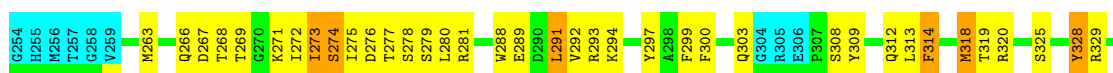
Chain B:  100%



4.2.17 Score per residue for model 17

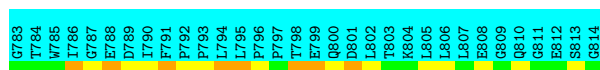
- Molecule 1: Nuclear receptor coactivator 1

Chain A:  35% 33% 6% 27%



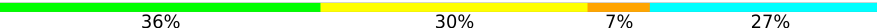
- Molecule 2: Signal transducer and activator of transcription 6

Chain B:  100%



4.2.18 Score per residue for model 18

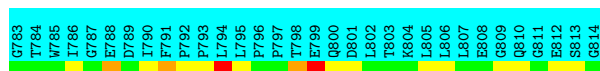
- Molecule 1: Nuclear receptor coactivator 1

Chain A:  36% 30% 7% 27%



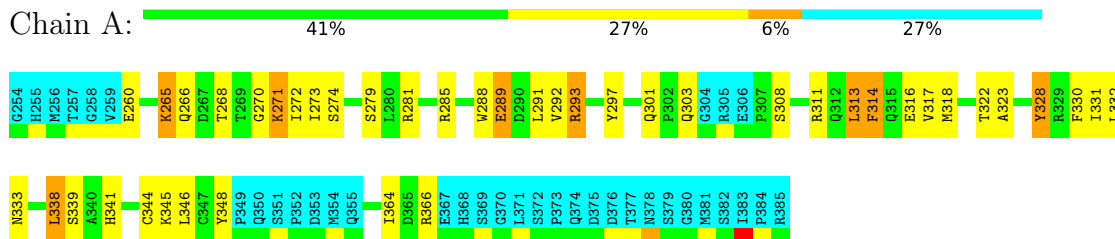
- Molecule 2: Signal transducer and activator of transcription 6

Chain B:  100%

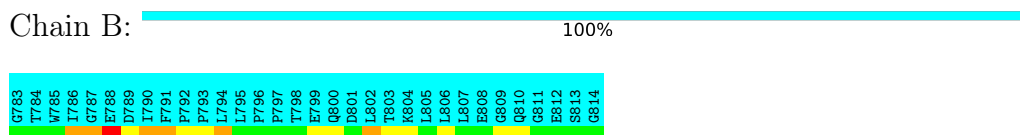


4.2.19 Score per residue for model 19

- Molecule 1: Nuclear receptor coactivator 1

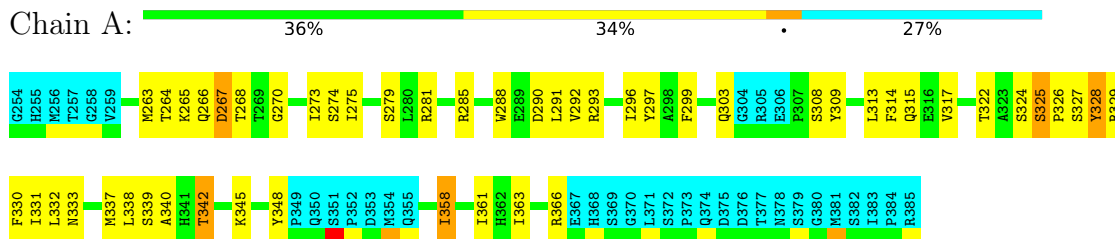


- Molecule 2: Signal transducer and activator of transcription 6

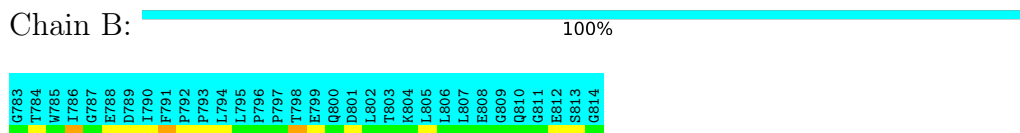


4.2.20 Score per residue for model 20

- Molecule 1: Nuclear receptor coactivator 1



- Molecule 2: Signal transducer and activator of transcription 6



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	refinement	
CYANA	structure calculation	

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	1881
Number of shifts mapped to atoms	1881
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

6 Model quality i

6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	775	772	772	21±6
2	B	0	0	0	0±0
All	All	15500	15440	15440	413

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:332:LEU:HD11	1:A:338:LEU:HD21	0.86	1.44	7	2
1:A:291:LEU:HD21	1:A:364:ILE:HD13	0.81	1.50	19	1
1:A:313:LEU:HD11	1:A:325:SER:N	0.70	2.02	18	2
1:A:299:PHE:CE1	1:A:342:THR:HG21	0.68	2.23	9	5
1:A:299:PHE:CZ	1:A:342:THR:HG21	0.67	2.24	5	5
1:A:263:MET:O	1:A:275:ILE:HG23	0.66	1.91	6	14
1:A:291:LEU:HD22	1:A:332:LEU:HD21	0.66	1.67	2	1
1:A:314:PHE:CE2	1:A:358:ILE:HD13	0.65	2.27	15	2
1:A:332:LEU:CD1	1:A:338:LEU:HD21	0.64	2.21	7	5
1:A:277:THR:HB	1:A:280:LEU:HD23	0.64	1.68	5	1
1:A:313:LEU:HD21	1:A:325:SER:N	0.64	2.07	7	12
1:A:291:LEU:CD2	1:A:332:LEU:HD21	0.64	2.22	2	1
1:A:266:GLN:HG3	1:A:272:ILE:HD13	0.64	1.68	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:291:LEU:HD21	1:A:364:ILE:CD1	0.64	2.23	13	4
1:A:267:ASP:HB2	1:A:273:ILE:HD11	0.64	1.70	4	2
1:A:291:LEU:HD13	1:A:338:LEU:HD21	0.63	1.69	19	1
1:A:291:LEU:HD21	1:A:364:ILE:HD11	0.63	1.68	12	2
1:A:299:PHE:CE2	1:A:342:THR:HG21	0.63	2.29	10	11
1:A:280:LEU:HD13	1:A:288:TRP:CB	0.62	2.25	5	1
1:A:265:LYS:HD2	1:A:273:ILE:HD11	0.62	1.70	20	3
1:A:317:VAL:HG23	1:A:322:THR:HA	0.61	1.71	18	13
1:A:316:GLU:HG2	1:A:323:ALA:HB2	0.61	1.73	18	6
1:A:265:LYS:CD	1:A:273:ILE:HD11	0.61	2.26	10	4
1:A:332:LEU:HD11	1:A:338:LEU:HD12	0.61	1.73	8	5
1:A:272:ILE:HG21	1:A:275:ILE:HD11	0.61	1.72	10	2
1:A:332:LEU:HG	1:A:338:LEU:HD11	0.61	1.72	13	2
1:A:314:PHE:C	1:A:314:PHE:CD1	0.60	2.74	1	1
1:A:291:LEU:HD22	1:A:291:LEU:O	0.60	1.96	5	1
1:A:262:PHE:CE1	1:A:364:ILE:HD11	0.59	2.32	5	2
1:A:265:LYS:HG2	1:A:273:ILE:HD11	0.59	1.74	6	6
1:A:266:GLN:NE2	1:A:358:ILE:HD13	0.59	2.12	20	1
1:A:313:LEU:HD12	1:A:325:SER:OG	0.59	1.98	2	1
1:A:288:TRP:O	1:A:292:VAL:HG23	0.59	1.98	7	20
1:A:332:LEU:HD11	1:A:338:LEU:HD23	0.58	1.75	5	1
1:A:277:THR:HB	1:A:280:LEU:HD12	0.58	1.74	18	7
1:A:313:LEU:HD22	1:A:342:THR:HG23	0.58	1.76	20	1
1:A:313:LEU:HD21	1:A:324:SER:HA	0.58	1.73	20	2
1:A:314:PHE:CZ	1:A:358:ILE:HD13	0.58	2.34	2	3
1:A:319:THR:HG23	1:A:320:ARG:HG2	0.57	1.74	17	6
1:A:291:LEU:HD21	1:A:364:ILE:CG2	0.57	2.29	15	1
1:A:346:LEU:HD23	1:A:346:LEU:O	0.57	1.99	14	8
1:A:346:LEU:HD21	1:A:348:TYR:CD2	0.57	2.35	3	6
1:A:291:LEU:HD13	1:A:291:LEU:C	0.57	2.20	5	3
1:A:291:LEU:HD11	1:A:364:ILE:CD1	0.56	2.29	7	1
1:A:263:MET:HG2	1:A:361:ILE:HG22	0.56	1.77	5	5
1:A:338:LEU:HD22	1:A:366:ARG:HA	0.56	1.76	11	2
1:A:332:LEU:HD11	1:A:338:LEU:HD11	0.56	1.77	16	2
1:A:313:LEU:HD21	1:A:325:SER:H	0.56	1.61	14	6
1:A:264:THR:HG23	1:A:362:HIS:CE1	0.56	2.36	16	1
1:A:265:LYS:CG	1:A:273:ILE:HD11	0.55	2.32	16	2
1:A:322:THR:HG23	1:A:345:LYS:HG3	0.55	1.78	5	2
1:A:336:THR:HG22	1:A:338:LEU:HD21	0.55	1.78	2	1
1:A:343:ARG:CD	1:A:361:ILE:HD11	0.55	2.31	3	2
1:A:280:LEU:HD13	1:A:288:TRP:HB3	0.55	1.76	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:326:PRO:O	1:A:328:TYR:CE1	0.55	2.60	2	2
1:A:346:LEU:HD23	1:A:346:LEU:C	0.55	2.23	10	5
1:A:280:LEU:HD13	1:A:288:TRP:HB2	0.54	1.79	18	8
1:A:273:ILE:HD12	1:A:274:SER:HB3	0.54	1.77	20	2
1:A:267:ASP:CA	1:A:273:ILE:HD11	0.54	2.31	2	4
1:A:332:LEU:HD12	1:A:336:THR:HB	0.54	1.79	5	5
1:A:280:LEU:C	1:A:280:LEU:HD12	0.53	2.24	5	1
1:A:330:PHE:CE2	1:A:338:LEU:HD13	0.53	2.38	13	1
1:A:314:PHE:CE1	1:A:358:ILE:HG21	0.53	2.38	8	1
1:A:260:GLU:HB3	1:A:364:ILE:HD12	0.53	1.78	16	5
1:A:346:LEU:HA	1:A:358:ILE:HD13	0.53	1.79	11	3
1:A:264:THR:HG22	1:A:275:ILE:HG12	0.53	1.79	15	3
1:A:332:LEU:HD11	1:A:338:LEU:CD1	0.53	2.34	12	7
1:A:262:PHE:CD1	1:A:292:VAL:HG22	0.52	2.38	6	1
1:A:346:LEU:C	1:A:346:LEU:HD23	0.52	2.24	13	4
1:A:291:LEU:HD11	1:A:364:ILE:HD12	0.52	1.81	14	2
1:A:336:THR:CG2	1:A:338:LEU:HD21	0.52	2.35	2	2
1:A:291:LEU:O	1:A:291:LEU:HD23	0.52	2.05	16	1
1:A:291:LEU:HD23	1:A:332:LEU:HD21	0.52	1.82	20	1
1:A:291:LEU:HD21	1:A:364:ILE:HG21	0.51	1.81	15	1
1:A:266:GLN:CD	1:A:270:GLY:HA2	0.51	2.26	20	1
1:A:291:LEU:HD23	1:A:338:LEU:HD21	0.51	1.81	5	1
1:A:291:LEU:HD21	1:A:364:ILE:HD12	0.51	1.82	3	1
1:A:328:TYR:O	1:A:339:SER:HA	0.50	2.07	18	20
1:A:291:LEU:HD21	1:A:364:ILE:HG13	0.50	1.83	14	2
1:A:272:ILE:CG2	1:A:275:ILE:HD11	0.50	2.36	10	2
1:A:313:LEU:HD13	1:A:344:CYS:SG	0.50	2.47	2	1
1:A:341:HIS:CD2	1:A:341:HIS:N	0.50	2.80	15	2
1:A:317:VAL:O	1:A:321:GLY:HA2	0.49	2.07	16	8
1:A:313:LEU:HD11	1:A:324:SER:C	0.49	2.28	18	1
1:A:266:GLN:HG2	1:A:267:ASP:O	0.49	2.07	20	1
1:A:260:GLU:CB	1:A:364:ILE:HD12	0.49	2.38	16	1
1:A:313:LEU:HD23	1:A:344:CYS:HB2	0.49	1.85	6	1
1:A:317:VAL:HG23	1:A:322:THR:CA	0.49	2.38	18	4
1:A:291:LEU:CD2	1:A:364:ILE:HD13	0.49	2.32	19	1
1:A:337:MET:O	1:A:338:LEU:HD23	0.48	2.08	20	5
1:A:313:LEU:HD22	1:A:344:CYS:SG	0.48	2.48	19	1
1:A:332:LEU:CG	1:A:338:LEU:HD11	0.48	2.37	13	1
1:A:313:LEU:HD21	1:A:324:SER:CA	0.48	2.39	20	1
1:A:313:LEU:HD22	1:A:344:CYS:HB2	0.48	1.84	2	1
1:A:292:VAL:HG12	1:A:296:ILE:HD12	0.47	1.86	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:314:PHE:HA	1:A:317:VAL:HG12	0.47	1.86	18	3
1:A:325:SER:HB2	1:A:342:THR:HG22	0.47	1.87	20	1
1:A:346:LEU:HD12	1:A:348:TYR:CE1	0.47	2.44	16	1
1:A:313:LEU:HD11	1:A:324:SER:HA	0.46	1.87	2	1
1:A:323:ALA:HB3	1:A:344:CYS:SG	0.46	2.51	16	1
1:A:325:SER:CB	1:A:326:PRO:HD2	0.46	2.41	18	5
1:A:299:PHE:CZ	1:A:313:LEU:HD22	0.46	2.46	12	2
1:A:313:LEU:HD21	1:A:323:ALA:C	0.45	2.31	2	1
1:A:266:GLN:HA	1:A:271:LYS:O	0.45	2.11	11	12
1:A:264:THR:CG2	1:A:362:HIS:CE1	0.45	3.00	16	1
1:A:314:PHE:O	1:A:317:VAL:HG12	0.45	2.12	7	2
1:A:273:ILE:HD12	1:A:274:SER:HB2	0.45	1.88	1	1
1:A:315:GLN:HE21	1:A:316:GLU:N	0.45	2.10	2	1
1:A:346:LEU:HD13	1:A:347:CYS:N	0.45	2.27	16	1
1:A:325:SER:O	1:A:341:HIS:CD2	0.45	2.69	18	1
1:A:316:GLU:CG	1:A:323:ALA:HB2	0.45	2.42	15	3
1:A:291:LEU:HD12	1:A:291:LEU:O	0.44	2.12	19	1
1:A:277:THR:HG22	1:A:280:LEU:HD12	0.44	1.90	16	1
1:A:291:LEU:CD2	1:A:364:ILE:HD12	0.44	2.42	1	1
1:A:280:LEU:HD22	1:A:288:TRP:HB2	0.44	1.89	5	1
1:A:312:GLN:HA	1:A:315:GLN:OE1	0.43	2.13	1	1
1:A:341:HIS:CD2	1:A:342:THR:N	0.43	2.86	18	1
1:A:341:HIS:CD2	1:A:363:ILE:HG23	0.43	2.49	15	1
1:A:332:LEU:HD11	1:A:338:LEU:CD2	0.43	2.43	19	1
1:A:318:MET:HA	1:A:346:LEU:HD23	0.43	1.90	8	1
1:A:336:THR:HG22	1:A:338:LEU:CD2	0.43	2.43	2	2
1:A:325:SER:HB2	1:A:326:PRO:HD2	0.43	1.90	16	2
1:A:340:ALA:HB1	1:A:363:ILE:O	0.43	2.13	8	4
1:A:280:LEU:HD11	1:A:292:VAL:HG21	0.43	1.90	6	1
1:A:265:LYS:HD3	1:A:273:ILE:HD11	0.43	1.88	16	2
1:A:267:ASP:N	1:A:273:ILE:HD11	0.43	2.27	2	3
1:A:315:GLN:O	1:A:319:THR:HG22	0.43	2.13	4	2
1:A:345:LYS:O	1:A:345:LYS:CD	0.42	2.67	16	1
1:A:291:LEU:HG	1:A:364:ILE:HD13	0.42	1.90	2	1
1:A:262:PHE:HE1	1:A:364:ILE:HD11	0.42	1.75	15	1
1:A:291:LEU:HD11	1:A:364:ILE:CG2	0.42	2.44	17	1
1:A:291:LEU:HD21	1:A:338:LEU:HD11	0.42	1.91	1	1
1:A:330:PHE:CD1	1:A:330:PHE:N	0.42	2.88	1	3
1:A:346:LEU:HD21	1:A:348:TYR:CE2	0.42	2.49	3	1
1:A:291:LEU:HD13	1:A:291:LEU:O	0.42	2.15	2	1
1:A:330:PHE:CZ	1:A:338:LEU:HD11	0.41	2.50	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:299:PHE:CE1	1:A:310:ALA:HA	0.41	2.51	9	1
1:A:338:LEU:HD22	1:A:366:ARG:CG	0.41	2.45	18	1
1:A:313:LEU:CD2	1:A:342:THR:HG23	0.41	2.46	9	1
1:A:280:LEU:HD21	1:A:364:ILE:HD11	0.41	1.91	16	1
1:A:313:LEU:HD22	1:A:342:THR:CG2	0.41	2.44	20	1
1:A:312:GLN:O	1:A:315:GLN:HG3	0.41	2.16	2	1
1:A:267:ASP:HB2	1:A:273:ILE:CD1	0.41	2.43	4	1
1:A:346:LEU:HD13	1:A:346:LEU:C	0.40	2.37	16	1
1:A:266:GLN:CG	1:A:272:ILE:HD13	0.40	2.44	19	1
1:A:313:LEU:O	1:A:317:VAL:HG12	0.40	2.17	12	1
1:A:358:ILE:O	1:A:358:ILE:HG22	0.40	2.17	20	1
1:A:343:ARG:HG3	1:A:361:ILE:HD11	0.40	1.92	1	1
1:A:299:PHE:CE1	1:A:313:LEU:HD13	0.40	2.51	6	1
1:A:299:PHE:CE1	1:A:313:LEU:HD22	0.40	2.51	14	1
1:A:313:LEU:HD21	1:A:323:ALA:O	0.40	2.16	19	1
1:A:317:VAL:HG21	1:A:344:CYS:HB3	0.40	1.92	18	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	97/132 (73%)	96±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100 100
2	B	0	-	-	-	-
All	All	1940/3280 (59%)	1912 (99%)	28 (1%)	0 (0%)	100 100

There are no Ramachandran outliers.

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	85/115 (74%)	62±3 (72±3%)	23±3 (28±3%)	2 20
2	B	0	-	-	-
All	All	1700/2840 (60%)	1231 (72%)	469 (28%)	2 20

All 62 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	297	TYR	20
1	A	345	LYS	20
1	A	279	SER	19
1	A	309	TYR	18
1	A	314	PHE	18
1	A	328	TYR	18
1	A	366	ARG	17
1	A	341	HIS	15
1	A	308	SER	15
1	A	303	GLN	14
1	A	315	GLN	12
1	A	281	ARG	12
1	A	312	GLN	11
1	A	348	TYR	11
1	A	294	LYS	11
1	A	329	ARG	11
1	A	274	SER	10
1	A	285	ARG	10
1	A	289	GLU	9
1	A	327	SER	9
1	A	330	PHE	9
1	A	333	ASN	9
1	A	337	MET	9
1	A	338	LEU	8
1	A	317	VAL	8
1	A	325	SER	8
1	A	346	LEU	8
1	A	358	ILE	8
1	A	263	MET	7
1	A	290	ASP	7
1	A	318	MET	7
1	A	334	ASP	7
1	A	339	SER	7
1	A	267	ASP	7
1	A	278	SER	6

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Mol	Chain	Res	Type	Models (Total)
1	A	291	LEU	6
1	A	265	LYS	6
1	A	268	THR	5
1	A	260	GLU	4
1	A	271	LYS	4
1	A	273	ILE	4
1	A	313	LEU	4
1	A	311	ARG	4
1	A	269	THR	4
1	A	359	MET	3
1	A	363	ILE	3
1	A	293	ARG	3
1	A	331	ILE	3
1	A	261	SER	2
1	A	262	PHE	2
1	A	300	PHE	2
1	A	301	GLN	2
1	A	320	ARG	2
1	A	361	ILE	2
1	A	276	ASP	2
1	A	264	THR	1
1	A	316	GLU	1
1	A	322	THR	1
1	A	343	ARG	1
1	A	295	CYS	1
1	A	324	SER	1
1	A	342	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 monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *CS_NCoA1_STAT6_FINAL.str*

7.1.1 Bookkeeping i

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

Total number of shifts	1881
Number of shifts mapped to atoms	1881
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	157	0.01 \pm 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	143	0.32 \pm 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	133	0.13 \pm 0.10	None needed (< 0.5 ppm)
^{15}N	145	-0.06 \pm 0.25	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 88%, i.e. 1188 atoms were assigned a chemical shift out of a possible 1345. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	474/483 (98%)	196/196 (100%)	185/194 (95%)	93/93 (100%)
Sidechain	629/738 (85%)	426/481 (89%)	197/223 (88%)	6/34 (18%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	85/124 (69%)	50/60 (83%)	30/59 (51%)	5/5 (100%)
Overall	1188/1345 (88%)	672/737 (91%)	412/476 (87%)	104/132 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1873 atoms were assigned a chemical shift out of a possible 2181. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	751/812 (92%)	316/332 (95%)	290/328 (88%)	145/152 (95%)
Sidechain	1011/1208 (84%)	686/785 (87%)	314/376 (84%)	11/47 (23%)
Aromatic	111/161 (69%)	62/79 (78%)	41/73 (56%)	8/9 (89%)
Overall	1873/2181 (86%)	1064/1196 (89%)	645/777 (83%)	164/208 (79%)

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.

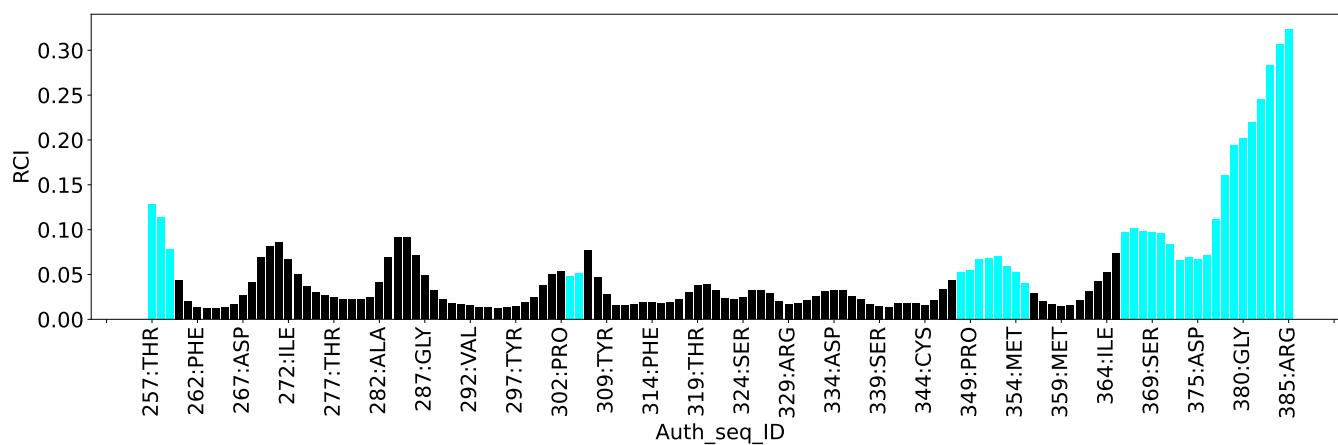
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	319	THR	HG1	-1.78	0.08 – 2.19	-13.8
1	A	377	THR	HG1	-1.71	0.08 – 2.19	-13.5
1	A	269	THR	HG1	-1.64	0.08 – 2.19	-13.2
1	A	264	THR	HG1	-1.60	0.08 – 2.19	-13.0
1	A	286	THR	HG1	-1.43	0.08 – 2.19	-12.2
1	A	271	LYS	CD	39.73	23.50 – 34.42	9.9
1	A	311	ARG	CD	35.84	38.57 – 47.75	-8.0
1	A	310	ALA	HB1	-0.43	0.14 – 2.58	-7.3
1	A	310	ALA	HB2	-0.43	0.14 – 2.58	-7.3
1	A	310	ALA	HB3	-0.43	0.14 – 2.58	-7.3
1	A	289	GLU	HG3	0.78	1.20 – 3.30	-7.0
1	A	288	TRP	CZ2	124.06	107.20 – 121.33	6.9
1	A	313	LEU	CD2	13.17	15.73 – 32.47	-6.5
1	A	288	TRP	CH2	114.99	116.19 – 131.43	-5.8

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

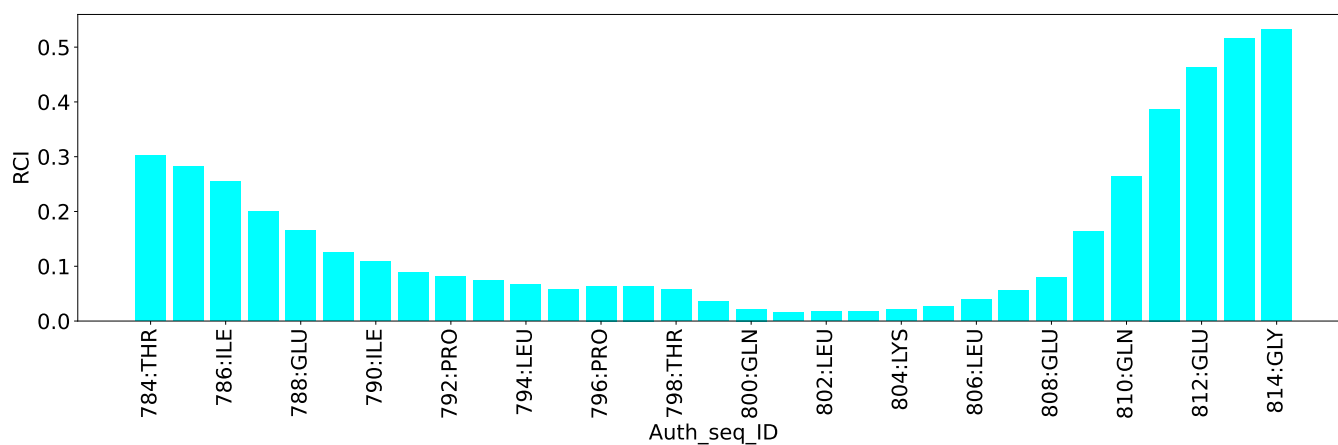
The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted 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:



Random coil index (RCI) for chain B:



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	1307
Intra-residue ($ i-j =0$)	402
Sequential ($ i-j =1$)	385
Medium range ($ i-j >1$ and $ i-j <5$)	200
Long range ($ i-j \geq 5$)	159
Inter-chain	81
Hydrogen bond restraints	80
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	8.0
Number of long range restraints per residue ¹	1.2

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	25.1	0.2
0.2-0.5 (Medium)	24.5	0.5
>0.5 (Large)	40.0	4.19

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis

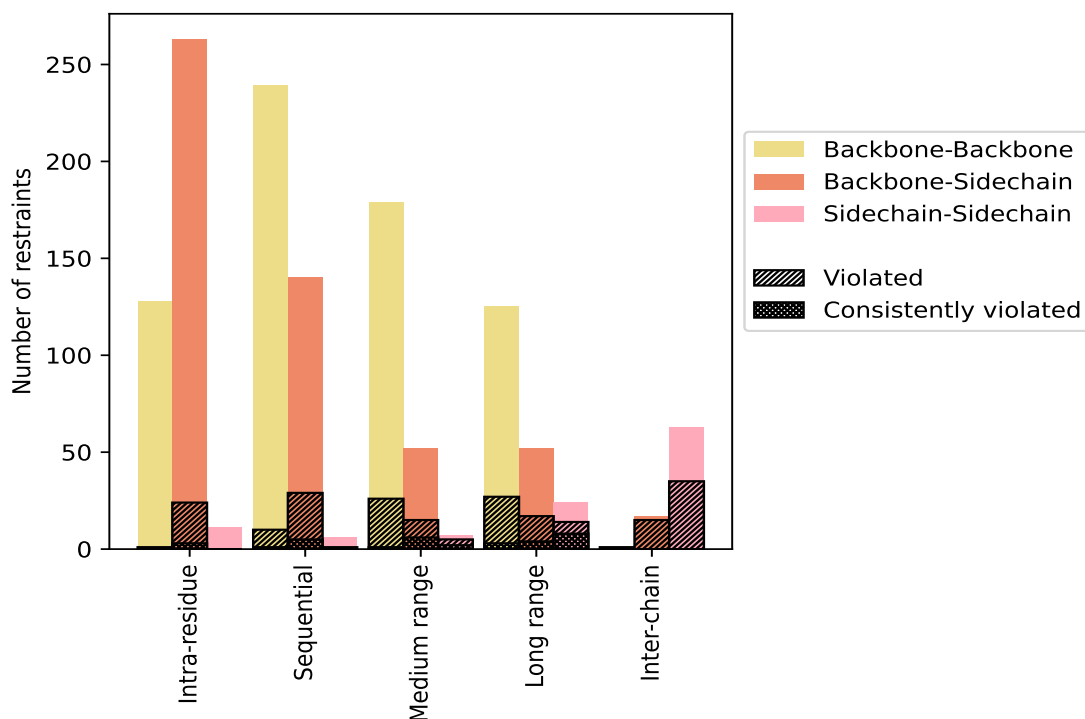
9.1 Summary of distance violations

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	402	30.8	25	6.2	1.9	3	0.7	0.2
Backbone-Backbone	128	9.8	1	0.8	0.1	0	0.0	0.0
Backbone-Sidechain	263	20.1	24	9.1	1.8	3	1.1	0.2
Sidechain-Sidechain	11	0.8	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	385	29.5	40	10.4	3.1	6	1.6	0.5
Backbone-Backbone	239	18.3	10	4.2	0.8	1	0.4	0.1
Backbone-Sidechain	140	10.7	29	20.7	2.2	5	3.6	0.4
Sidechain-Sidechain	6	0.5	1	16.7	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	200	15.3	39	19.5	3.0	8	4.0	0.6
Backbone-Backbone	141	10.8	19	13.5	1.5	0	0.0	0.0
Backbone-Sidechain	52	4.0	15	28.8	1.1	6	11.5	0.5
Sidechain-Sidechain	7	0.5	5	71.4	0.4	2	28.6	0.2
Long range ($i-j \geq 5$)	159	12.2	52	32.7	4.0	13	8.2	1.0
Backbone-Backbone	83	6.4	21	25.3	1.6	1	1.2	0.1
Backbone-Sidechain	52	4.0	17	32.7	1.3	4	7.7	0.3
Sidechain-Sidechain	24	1.8	14	58.3	1.1	8	33.3	0.6
Inter-chain	81	6.2	51	63.0	3.9	0	0.0	0.0
Backbone-Backbone	1	0.1	1	100.0	0.1	0	0.0	0.0
Backbone-Sidechain	17	1.3	15	88.2	1.1	0	0.0	0.0
Sidechain-Sidechain	63	4.8	35	55.6	2.7	0	0.0	0.0
Hydrogen bond	80	6.1	13	16.2	1.0	3	3.8	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1307	100.0	220	16.8	16.8	33	2.5	2.5
Backbone-Backbone	672	51.4	65	9.7	5.0	5	0.7	0.4
Backbone-Sidechain	524	40.1	100	19.1	7.7	18	3.4	1.4
Sidechain-Sidechain	111	8.5	55	49.5	4.2	10	9.0	0.8

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	6	18	19	23	14	80	0.74	3.65	0.8	0.4
2	5	18	18	33	12	86	0.7	3.45	0.76	0.33
3	6	15	22	22	20	85	0.66	3.38	0.68	0.4
4	9	22	18	28	27	104	0.72	3.68	0.74	0.44
5	9	16	24	35	23	107	0.63	3.91	0.75	0.33
6	7	17	18	30	13	85	0.81	3.48	0.74	0.52
7	7	19	19	28	13	86	0.72	3.34	0.74	0.38
8	5	21	19	27	31	103	0.77	3.56	0.74	0.48
9	8	16	18	28	20	90	0.71	3.42	0.7	0.45
10	10	19	19	24	22	94	0.82	3.6	0.81	0.54
11	7	19	18	24	24	92	0.72	3.41	0.7	0.44

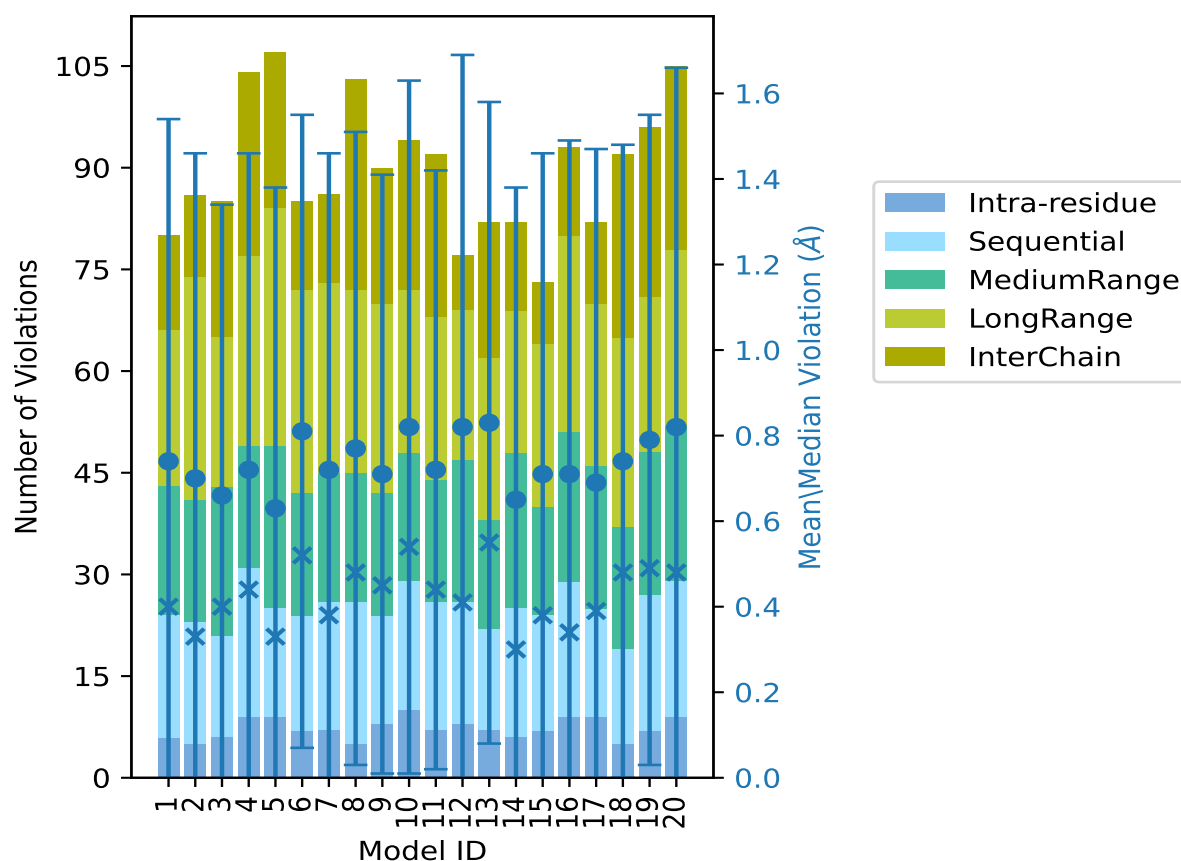
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
12	8	18	21	22	8	77	0.82	3.46	0.87	0.41
13	7	15	16	24	20	82	0.83	3.27	0.75	0.55
14	6	19	23	21	13	82	0.65	3.31	0.73	0.3
15	7	17	16	24	9	73	0.71	3.53	0.75	0.38
16	9	20	22	29	13	93	0.71	3.8	0.78	0.34
17	9	16	21	24	12	82	0.69	3.72	0.78	0.39
18	5	14	18	28	27	92	0.74	4.01	0.74	0.48
19	7	20	21	23	25	96	0.79	3.36	0.76	0.49
20	9	20	23	26	27	105	0.82	4.19	0.84	0.48

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

9.2.1 Bar graph : Distance Violation statistics for each model [\(i\)](#)



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

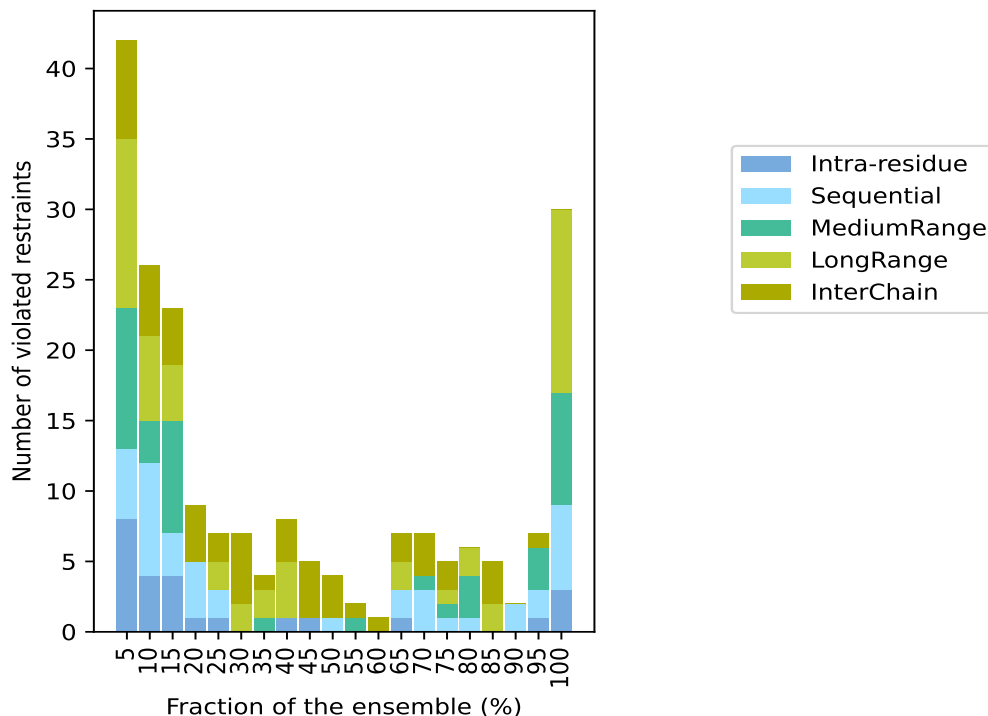
9.3 Distance violation statistics for the ensemble

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, 1020(IR:377, SQ:345, MR:161, LR:107, IC:30) 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	%
8	5	10	12	7	42	1	5.0
4	8	3	6	5	26	2	10.0
4	3	8	4	4	23	3	15.0
1	4	0	0	4	9	4	20.0
1	2	0	2	2	7	5	25.0
0	0	0	2	5	7	6	30.0
0	0	1	2	1	4	7	35.0
1	0	0	4	3	8	8	40.0
1	0	0	0	4	5	9	45.0
0	1	0	0	3	4	10	50.0
0	0	1	0	1	2	11	55.0
0	0	0	0	1	1	12	60.0
1	2	0	2	2	7	13	65.0
0	3	1	0	3	7	14	70.0
0	1	1	1	2	5	15	75.0
0	1	3	2	0	6	16	80.0
0	0	0	2	3	5	17	85.0
0	2	0	0	0	2	18	90.0
1	2	3	0	1	7	19	95.0
3	6	8	13	0	30	20	100.0

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

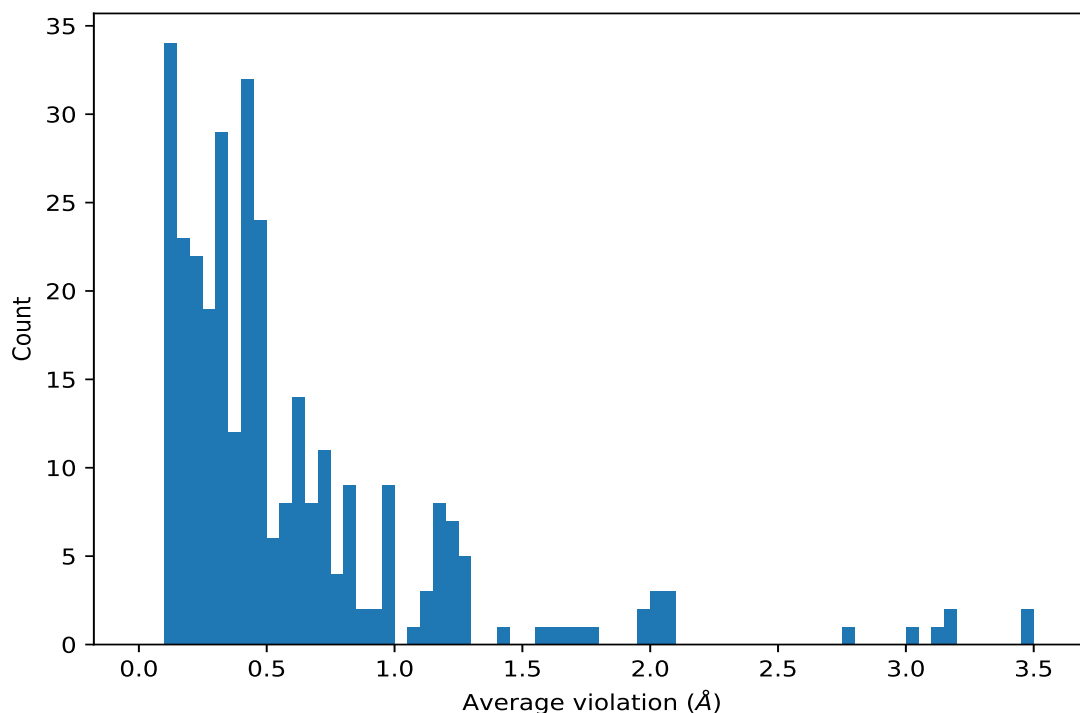
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	20	3.46	0.28	3.38
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	20	3.12	0.24	3.15
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	20	2.78	0.06	2.8
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	20	2.04	0.22	2.02
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	20	2.04	0.22	2.02
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	20	2.04	0.22	2.02
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	20	1.77	0.03	1.78
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	20	1.67	0.39	1.65
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	20	1.6	0.04	1.59
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	20	1.57	0.27	1.57
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	20	1.26	0.49	1.67
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	20	1.26	0.49	1.67
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	20	1.26	0.49	1.67
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	20	1.26	0.25	1.19
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	20	1.23	0.16	1.23
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	20	1.23	0.16	1.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	20	1.22	0.03	1.21
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	20	1.22	0.31	1.23
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	20	1.1	0.28	1.04
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	20	1.06	0.31	1.14
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	20	0.87	0.18	0.9
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	20	0.86	0.29	0.77
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	20	0.69	0.23	0.74
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	20	0.66	0.32	0.68
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	20	0.46	0.03	0.47
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	20	0.45	0.01	0.45
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	20	0.43	0.16	0.48
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	20	0.42	0.02	0.42
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	20	0.37	0.15	0.32
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	20	0.37	0.79	0.18
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	20	0.34	0.06	0.37
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	20	0.31	0.28	0.22
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	20	0.31	0.14	0.24
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	20	0.31	0.14	0.24
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	20	0.29	0.29	0.23
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	20	0.29	0.03	0.29
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	20	0.24	0.04	0.24
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	20	0.15	0.02	0.15
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	20	0.13	0.01	0.13
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	19	3.04	0.38	2.96
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	19	2.07	0.43	2.07
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	19	2.07	0.43	2.07
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	19	2.07	0.43	2.07
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	19	1.44	0.37	1.51
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	19	0.84	0.51	0.65
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	19	0.75	0.08	0.76
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	19	0.4	0.3	0.27
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	19	0.13	0.02	0.12
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	18	0.16	0.02	0.16
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	18	0.14	0.02	0.14
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	17	1.19	0.44	1.19
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	17	1.19	0.44	1.19
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	17	1.19	0.44	1.19
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	17	0.84	0.52	0.83
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	17	0.8	0.49	0.62
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	17	0.17	0.05	0.17
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	17	0.17	0.03	0.17
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	16	1.16	0.02	1.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	16	0.74	0.34	0.76
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	16	0.56	0.23	0.58
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	16	0.3	0.04	0.32
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	16	0.13	0.02	0.13
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	16	0.13	0.02	0.13
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	15	0.8	0.49	0.68
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	15	0.8	0.49	0.68
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	15	0.8	0.49	0.68
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	15	0.55	0.31	0.49
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	15	0.55	0.31	0.49
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	15	0.55	0.31	0.49
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	15	0.38	0.1	0.42
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	15	0.37	0.11	0.33
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	15	0.13	0.03	0.12
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	14	1.18	0.5	1.23
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	14	1.18	0.5	1.23
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	14	1.18	0.5	1.23
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	14	0.93	0.12	0.95
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	14	0.79	0.43	0.78
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	14	0.79	0.43	0.78
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	14	0.79	0.43	0.78
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	14	0.48	0.33	0.31
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	14	0.48	0.33	0.31
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	14	0.48	0.33	0.31
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	14	0.28	0.06	0.3
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	14	0.24	0.08	0.22
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	14	0.24	0.08	0.22
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	14	0.24	0.08	0.22
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	14	0.24	0.08	0.22
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	14	0.24	0.08	0.22
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	14	0.24	0.08	0.22
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	14	0.15	0.03	0.16
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	13	0.98	0.77	0.72
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	13	0.98	0.77	0.72
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	13	0.98	0.77	0.72
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	13	0.98	0.77	0.72
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	13	0.98	0.77	0.72
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	13	0.98	0.77	0.72
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	13	0.98	0.77	0.72
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	13	0.98	0.77	0.72
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	13	0.98	0.77	0.72
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	13	0.92	0.45	0.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	13	0.69	0.37	0.62
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	13	0.69	0.37	0.62
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	13	0.69	0.37	0.62
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	13	0.69	0.37	0.62
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	13	0.69	0.37	0.62
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	13	0.69	0.37	0.62
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	13	0.57	0.17	0.55
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	13	0.31	0.08	0.28
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	13	0.16	0.04	0.15
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	13	0.13	0.01	0.12
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD21	12	0.7	0.37	0.69
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD22	12	0.7	0.37	0.69
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD23	12	0.7	0.37	0.69
(3,39)	1:A:301:GLN:H	1:A:298:ALA:O	12	0.12	0.01	0.12
(1,925)	2:B:800:GLN:HG3	2:B:803:THR:HB	11	1.16	0.34	1.28
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD11	11	0.53	0.21	0.48
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD12	11	0.53	0.21	0.48
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD13	11	0.53	0.21	0.48
(1,1070)	2:B:785:TRP:HB2	2:B:786:ILE:H	10	0.64	0.19	0.7
(1,1139)	1:A:314:PHE:HB3	2:B:794:LEU:HG	10	0.59	0.39	0.51
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD21	10	0.4	0.21	0.36
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD22	10	0.4	0.21	0.36
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD23	10	0.4	0.21	0.36
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD21	10	0.4	0.21	0.36
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD22	10	0.4	0.21	0.36
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD23	10	0.4	0.21	0.36
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD21	10	0.4	0.21	0.36
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD22	10	0.4	0.21	0.36
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD23	10	0.4	0.21	0.36
(1,1063)	1:A:270:GLY:HA3	2:B:794:LEU:HG	10	0.35	0.25	0.26
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG21	9	0.64	0.4	0.5
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG22	9	0.64	0.4	0.5
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG23	9	0.64	0.4	0.5
(1,1043)	1:A:300:PHE:HB3	2:B:796:PRO:HB3	9	0.62	0.38	0.63
(1,1049)	1:A:300:PHE:HA	2:B:796:PRO:HG3	9	0.57	0.32	0.49
(1,1061)	1:A:272:ILE:HB	2:B:797:PRO:HB3	9	0.44	0.4	0.25
(1,1018)	2:B:812:GLU:H	2:B:812:GLU:HB3	9	0.28	0.09	0.29
(1,698)	1:A:316:GLU:HG3	1:A:322:THR:H	8	0.73	0.29	0.73
(1,1056)	1:A:274:SER:HA	2:B:805:LEU:HA	8	0.63	0.27	0.52
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD11	8	0.6	0.38	0.49
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD12	8	0.6	0.38	0.49
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD13	8	0.6	0.38	0.49

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD11	8	0.42	0.18	0.46
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD12	8	0.42	0.18	0.46
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD13	8	0.42	0.18	0.46
(1,828)	1:A:348:TYR:H	1:A:348:TYR:HD1	8	0.3	0.09	0.32
(1,867)	1:A:266:GLN:HA	1:A:272:ILE:HA	8	0.12	0.01	0.12
(1,871)	1:A:266:GLN:HA	1:A:272:ILE:HA	8	0.12	0.01	0.12
(1,887)	1:A:266:GLN:H	1:A:358:ILE:HB	8	0.12	0.01	0.12
(1,560)	1:A:261:SER:H	1:A:364:ILE:HG12	7	1.11	0.21	1.19
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG21	7	0.73	0.49	0.56
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG22	7	0.73	0.49	0.56
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG23	7	0.73	0.49	0.56
(1,1145)	2:B:788:GLU:HA	2:B:791:PHE:H	7	0.22	0.1	0.18
(1,523)	1:A:325:SER:H	1:A:342:THR:H	7	0.15	0.06	0.11
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD11	6	1.24	0.57	0.96
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD12	6	1.24	0.57	0.96
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD13	6	1.24	0.57	0.96
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD11	6	0.82	0.41	0.92
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD12	6	0.82	0.41	0.92
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD13	6	0.82	0.41	0.92
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD11	6	0.74	0.46	0.61
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD12	6	0.74	0.46	0.61
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD13	6	0.74	0.46	0.61
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG21	6	0.48	0.31	0.43
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG22	6	0.48	0.31	0.43
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG23	6	0.48	0.31	0.43
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG21	6	0.48	0.31	0.43
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG22	6	0.48	0.31	0.43
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG23	6	0.48	0.31	0.43
(1,1053)	1:A:296:ILE:HG21	2:B:797:PRO:HD3	6	0.31	0.13	0.32
(1,1053)	1:A:296:ILE:HG22	2:B:797:PRO:HD3	6	0.31	0.13	0.32
(1,1053)	1:A:296:ILE:HG23	2:B:797:PRO:HD3	6	0.31	0.13	0.32
(1,808)	1:A:345:LYS:H	1:A:359:MET:HB2	6	0.14	0.02	0.15
(1,892)	1:A:267:ASP:HA	1:A:357:PHE:HA	6	0.14	0.03	0.13
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD11	5	0.61	0.28	0.71
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD12	5	0.61	0.28	0.71
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD13	5	0.61	0.28	0.71
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD11	5	0.42	0.09	0.44
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD12	5	0.42	0.09	0.44
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD13	5	0.42	0.09	0.44
(1,875)	1:A:266:GLN:HB3	1:A:271:LYS:H	5	0.34	0.45	0.11
(1,639)	1:A:338:LEU:HD21	1:A:339:SER:H	5	0.17	0.03	0.16
(1,639)	1:A:338:LEU:HD22	1:A:339:SER:H	5	0.17	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,639)	1:A:338:LEU:HD23	1:A:339:SER:H	5	0.17	0.03	0.16
(1,1101)	2:B:789:ASP:H	2:B:790:ILE:H	5	0.17	0.09	0.13
(1,412)	1:A:266:GLN:HA	1:A:273:ILE:H	5	0.14	0.02	0.13
(3,11)	1:A:267:ASP:H	1:A:271:LYS:O	5	0.11	0.0	0.11
(1,301)	1:A:375:ASP:H	1:A:375:ASP:HA	5	0.11	0.0	0.11
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG21	4	0.54	0.14	0.52
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG22	4	0.54	0.14	0.52
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG23	4	0.54	0.14	0.52
(1,1036)	2:B:797:PRO:HB3	2:B:798:THR:H	4	0.49	0.17	0.5
(1,1136)	2:B:794:LEU:HD11	1:A:311:ARG:HB2	4	0.43	0.21	0.5
(1,1136)	2:B:794:LEU:HD12	1:A:311:ARG:HB2	4	0.43	0.21	0.5
(1,1136)	2:B:794:LEU:HD13	1:A:311:ARG:HB2	4	0.43	0.21	0.5
(1,1136)	2:B:794:LEU:HD11	1:A:311:ARG:HB3	4	0.43	0.21	0.5
(1,1136)	2:B:794:LEU:HD12	1:A:311:ARG:HB3	4	0.43	0.21	0.5
(1,1136)	2:B:794:LEU:HD13	1:A:311:ARG:HB3	4	0.43	0.21	0.5
(1,1023)	1:A:275:ILE:HD11	2:B:806:LEU:HG	4	0.37	0.22	0.34
(1,1023)	1:A:275:ILE:HD12	2:B:806:LEU:HG	4	0.37	0.22	0.34
(1,1023)	1:A:275:ILE:HD13	2:B:806:LEU:HG	4	0.37	0.22	0.34
(1,913)	2:B:800:GLN:HB2	2:B:801:ASP:H	4	0.37	0.13	0.32
(1,1055)	1:A:274:SER:HA	2:B:805:LEU:HG	4	0.34	0.15	0.32
(1,212)	1:A:261:SER:H	1:A:261:SER:HB3	4	0.22	0.1	0.22
(1,524)	1:A:341:HIS:HB2	1:A:342:THR:H	4	0.21	0.02	0.21
(3,41)	1:A:310:ALA:H	1:A:299:PHE:O	4	0.14	0.01	0.14
(3,55)	1:A:328:TYR:H	1:A:340:ALA:O	4	0.14	0.02	0.14
(1,905)	2:B:798:THR:H	2:B:799:GLU:H	4	0.11	0.0	0.11
(1,825)	1:A:357:PHE:HD1	1:A:359:MET:H	3	3.49	0.08	3.46
(1,824)	1:A:349:PRO:HD2	1:A:357:PHE:HD2	3	3.19	0.11	3.22
(1,824)	1:A:349:PRO:HD3	1:A:357:PHE:HD2	3	3.19	0.11	3.22
(1,827)	1:A:357:PHE:HD1	1:A:359:MET:HG2	3	1.98	0.1	2.01
(1,827)	1:A:357:PHE:HD1	1:A:359:MET:HG3	3	1.98	0.1	2.01
(1,826)	1:A:357:PHE:HD1	1:A:358:ILE:H	3	1.73	0.02	1.73
(1,816)	1:A:357:PHE:H	1:A:357:PHE:HE2	3	0.55	0.02	0.53
(1,1065)	1:A:275:ILE:HB	2:B:806:LEU:HD21	3	0.49	0.15	0.47
(1,1065)	1:A:275:ILE:HB	2:B:806:LEU:HD22	3	0.49	0.15	0.47
(1,1065)	1:A:275:ILE:HB	2:B:806:LEU:HD23	3	0.49	0.15	0.47
(1,1027)	1:A:293:ARG:HD2	2:B:802:LEU:HD11	3	0.42	0.29	0.29
(1,1027)	1:A:293:ARG:HD2	2:B:802:LEU:HD12	3	0.42	0.29	0.29
(1,1027)	1:A:293:ARG:HD2	2:B:802:LEU:HD13	3	0.42	0.29	0.29
(1,1027)	1:A:293:ARG:HD3	2:B:802:LEU:HD11	3	0.42	0.29	0.29
(1,1027)	1:A:293:ARG:HD3	2:B:802:LEU:HD12	3	0.42	0.29	0.29
(1,1027)	1:A:293:ARG:HD3	2:B:802:LEU:HD13	3	0.42	0.29	0.29
(1,109)	1:A:363:ILE:H	1:A:363:ILE:HB	3	0.39	0.02	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1060)	1:A:272:ILE:HB	2:B:797:PRO:HG2	3	0.37	0.16	0.33
(1,1060)	1:A:272:ILE:HB	2:B:797:PRO:HG3	3	0.37	0.16	0.33
(1,1097)	2:B:788:GLU:HA	2:B:790:ILE:H	3	0.32	0.18	0.21
(1,850)	1:A:362:HIS:HA	1:A:363:ILE:HB	3	0.24	0.0	0.24
(1,1071)	2:B:785:TRP:H	2:B:785:TRP:HB3	3	0.21	0.1	0.19
(1,1121)	1:A:310:ALA:HB1	2:B:794:LEU:HD11	3	0.2	0.07	0.2
(1,1121)	1:A:310:ALA:HB1	2:B:794:LEU:HD12	3	0.2	0.07	0.2
(1,1121)	1:A:310:ALA:HB1	2:B:794:LEU:HD13	3	0.2	0.07	0.2
(1,1121)	1:A:310:ALA:HB2	2:B:794:LEU:HD11	3	0.2	0.07	0.2
(1,1121)	1:A:310:ALA:HB2	2:B:794:LEU:HD12	3	0.2	0.07	0.2
(1,1121)	1:A:310:ALA:HB2	2:B:794:LEU:HD13	3	0.2	0.07	0.2
(1,1121)	1:A:310:ALA:HB3	2:B:794:LEU:HD11	3	0.2	0.07	0.2
(1,1121)	1:A:310:ALA:HB3	2:B:794:LEU:HD12	3	0.2	0.07	0.2
(1,1121)	1:A:310:ALA:HB3	2:B:794:LEU:HD13	3	0.2	0.07	0.2
(1,803)	1:A:346:LEU:HA	1:A:358:ILE:HA	3	0.16	0.02	0.16
(1,993)	2:B:805:LEU:H	2:B:805:LEU:HG	3	0.16	0.02	0.17
(1,1154)	2:B:786:ILE:H	2:B:788:GLU:H	3	0.15	0.02	0.16
(1,205)	1:A:327:SER:HA	1:A:341:HIS:H	3	0.14	0.02	0.15
(1,939)	2:B:801:ASP:HA	2:B:804:LYS:H	3	0.13	0.02	0.12
(1,68)	1:A:300:PHE:HA	1:A:311:ARG:H	3	0.13	0.02	0.12
(3,63)	1:A:340:ALA:H	1:A:328:TYR:O	3	0.13	0.01	0.12
(1,877)	1:A:267:ASP:HB2	1:A:269:THR:H	3	0.13	0.01	0.12
(1,344)	1:A:297:TYR:HA	1:A:299:PHE:H	3	0.12	0.02	0.11
(1,421)	1:A:343:ARG:H	1:A:344:CYS:H	3	0.12	0.01	0.12
(1,903)	2:B:799:GLU:H	2:B:801:ASP:H	3	0.12	0.01	0.11
(1,100)	1:A:260:GLU:H	1:A:261:SER:HB3	2	1.26	0.12	1.26
(1,858)	1:A:263:MET:HB2	1:A:276:ASP:H	2	1.13	0.01	1.13
(1,84)	1:A:261:SER:HB2	1:A:262:PHE:H	2	0.64	0.02	0.64
(1,778)	1:A:347:CYS:HG	1:A:359:MET:H	2	0.62	0.4	0.62
(1,1134)	1:A:346:LEU:HD11	2:B:790:ILE:HD11	2	0.48	0.18	0.48
(1,1134)	1:A:346:LEU:HD11	2:B:790:ILE:HD12	2	0.48	0.18	0.48
(1,1134)	1:A:346:LEU:HD11	2:B:790:ILE:HD13	2	0.48	0.18	0.48
(1,1134)	1:A:346:LEU:HD12	2:B:790:ILE:HD11	2	0.48	0.18	0.48
(1,1134)	1:A:346:LEU:HD12	2:B:790:ILE:HD12	2	0.48	0.18	0.48
(1,1134)	1:A:346:LEU:HD12	2:B:790:ILE:HD13	2	0.48	0.18	0.48
(1,1134)	1:A:346:LEU:HD13	2:B:790:ILE:HD11	2	0.48	0.18	0.48
(1,1134)	1:A:346:LEU:HD13	2:B:790:ILE:HD12	2	0.48	0.18	0.48
(1,1134)	1:A:346:LEU:HD13	2:B:790:ILE:HD13	2	0.48	0.18	0.48
(1,1040)	2:B:794:LEU:H	2:B:795:LEU:H	2	0.4	0.29	0.4
(1,1026)	1:A:293:ARG:HG2	2:B:802:LEU:HD11	2	0.34	0.04	0.34
(1,1026)	1:A:293:ARG:HG2	2:B:802:LEU:HD12	2	0.34	0.04	0.34
(1,1026)	1:A:293:ARG:HG2	2:B:802:LEU:HD13	2	0.34	0.04	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1026)	1:A:293:ARG:HG3	2:B:802:LEU:HD11	2	0.34	0.04	0.34
(1,1026)	1:A:293:ARG:HG3	2:B:802:LEU:HD12	2	0.34	0.04	0.34
(1,1026)	1:A:293:ARG:HG3	2:B:802:LEU:HD13	2	0.34	0.04	0.34
(1,1066)	1:A:277:THR:HG21	2:B:806:LEU:HD21	2	0.34	0.14	0.34
(1,1066)	1:A:277:THR:HG21	2:B:806:LEU:HD22	2	0.34	0.14	0.34
(1,1066)	1:A:277:THR:HG21	2:B:806:LEU:HD23	2	0.34	0.14	0.34
(1,1066)	1:A:277:THR:HG22	2:B:806:LEU:HD21	2	0.34	0.14	0.34
(1,1066)	1:A:277:THR:HG22	2:B:806:LEU:HD22	2	0.34	0.14	0.34
(1,1066)	1:A:277:THR:HG22	2:B:806:LEU:HD23	2	0.34	0.14	0.34
(1,1066)	1:A:277:THR:HG23	2:B:806:LEU:HD21	2	0.34	0.14	0.34
(1,1066)	1:A:277:THR:HG23	2:B:806:LEU:HD22	2	0.34	0.14	0.34
(1,1066)	1:A:277:THR:HG23	2:B:806:LEU:HD23	2	0.34	0.14	0.34
(1,1146)	2:B:789:ASP:HA	2:B:791:PHE:H	2	0.33	0.14	0.33
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD11	2	0.28	0.06	0.28
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD12	2	0.28	0.06	0.28
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD13	2	0.28	0.06	0.28
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD21	2	0.28	0.06	0.28
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD22	2	0.28	0.06	0.28
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD23	2	0.28	0.06	0.28
(1,1025)	1:A:275:ILE:HD11	2:B:802:LEU:HD21	2	0.28	0.06	0.28
(1,1025)	1:A:275:ILE:HD11	2:B:802:LEU:HD22	2	0.28	0.06	0.28
(1,1025)	1:A:275:ILE:HD11	2:B:802:LEU:HD23	2	0.28	0.06	0.28
(1,1025)	1:A:275:ILE:HD12	2:B:802:LEU:HD21	2	0.28	0.06	0.28
(1,1025)	1:A:275:ILE:HD12	2:B:802:LEU:HD22	2	0.28	0.06	0.28
(1,1025)	1:A:275:ILE:HD12	2:B:802:LEU:HD23	2	0.28	0.06	0.28
(1,1025)	1:A:275:ILE:HD13	2:B:802:LEU:HD21	2	0.28	0.06	0.28
(1,1025)	1:A:275:ILE:HD13	2:B:802:LEU:HD22	2	0.28	0.06	0.28
(1,1025)	1:A:275:ILE:HD13	2:B:802:LEU:HD23	2	0.28	0.06	0.28
(1,1004)	2:B:807:LEU:H	2:B:807:LEU:HG	2	0.22	0.12	0.22
(1,619)	1:A:273:ILE:HG12	1:A:274:SER:H	2	0.18	0.0	0.18
(1,619)	1:A:273:ILE:HG13	1:A:274:SER:H	2	0.18	0.0	0.18
(1,199)	1:A:268:THR:HA	1:A:270:GLY:H	2	0.18	0.06	0.18
(1,1074)	2:B:785:TRP:HD1	2:B:786:ILE:H	2	0.17	0.01	0.17
(1,382)	1:A:344:CYS:HB3	1:A:345:LYS:H	2	0.16	0.04	0.16
(1,120)	1:A:267:ASP:H	1:A:267:ASP:HB3	2	0.16	0.02	0.16
(1,120)	1:A:267:ASP:H	1:A:267:ASP:HB2	2	0.16	0.02	0.16
(1,764)	1:A:321:GLY:HA2	1:A:346:LEU:H	2	0.15	0.04	0.15
(1,564)	1:A:371:LEU:H	1:A:371:LEU:HG	2	0.15	0.0	0.15
(1,46)	1:A:268:THR:H	1:A:270:GLY:H	2	0.13	0.01	0.13
(1,176)	1:A:328:TYR:H	1:A:340:ALA:H	2	0.12	0.0	0.12
(1,847)	1:A:362:HIS:H	1:A:363:ILE:HA	2	0.12	0.0	0.12
(1,879)	1:A:302:PRO:HA	1:A:307:PRO:HA	2	0.12	0.0	0.12

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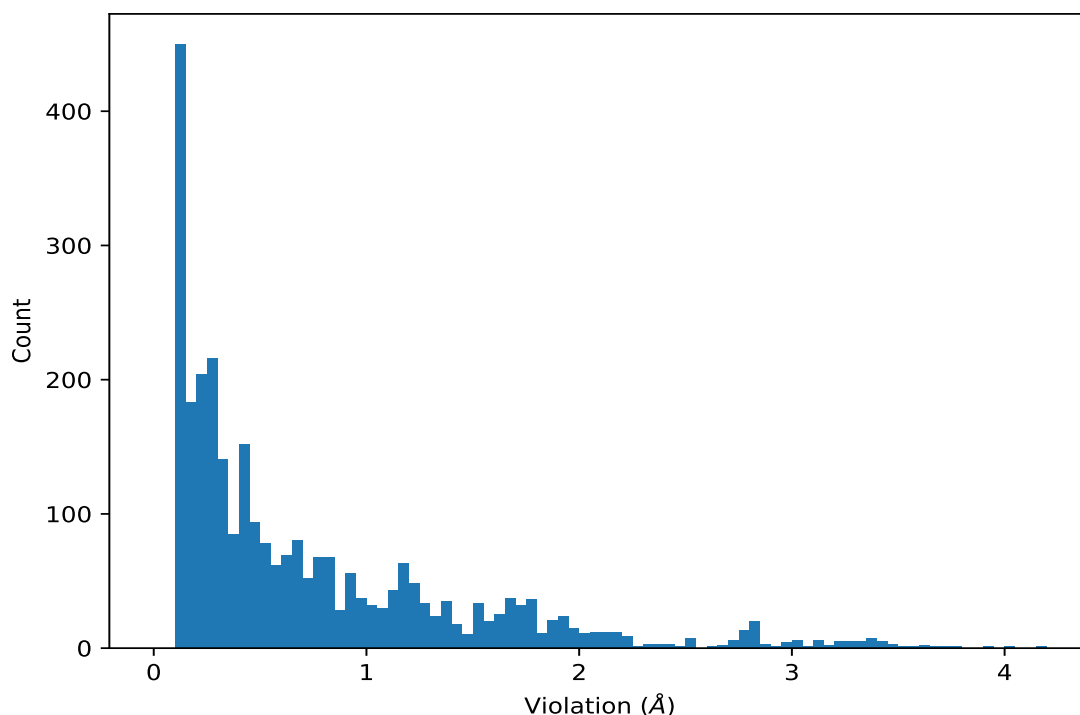
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,420)	1:A:344:CYS:H	1:A:345:LYS:H	2	0.11	0.0	0.11
(1,514)	1:A:264:THR:HA	1:A:274:SER:H	2	0.11	0.0	0.11
(1,1077)	2:B:786:ILE:H	2:B:786:ILE:HB	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	20	4.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	18	4.01
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	5	3.91
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	16	3.8
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	17	3.72
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	4	3.68
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	1	3.65
(1,825)	1:A:357:PHE:HD1	1:A:359:MET:H	10	3.6
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	8	3.56
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	15	3.53
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	6	3.48
(1,825)	1:A:357:PHE:HD1	1:A:359:MET:H	12	3.46
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	2	3.45
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	8	3.43
(1,825)	1:A:357:PHE:HD1	1:A:359:MET:H	20	3.42
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	9	3.42
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	11	3.41
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	12	3.41
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	4	3.4
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	3	3.38
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	12	3.37
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	19	3.36
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	1	3.35
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	19	3.35
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	5	3.35
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	7	3.34
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	10	3.34
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	17	3.32
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	17	3.32
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	14	3.31
(1,824)	1:A:349:PRO:HD2	1:A:357:PHE:HD2	20	3.3
(1,824)	1:A:349:PRO:HD3	1:A:357:PHE:HD2	20	3.3
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	20	3.3
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	13	3.27
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	10	3.27
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	16	3.24
(1,824)	1:A:349:PRO:HD2	1:A:357:PHE:HD2	12	3.22
(1,824)	1:A:349:PRO:HD3	1:A:357:PHE:HD2	12	3.22
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	4	3.22
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	16	3.21
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	18	3.19
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	9	3.18
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	1	3.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	7	3.15
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	13	3.15
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	14	3.14
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	20	3.13
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	11	3.1
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	8	3.08
(1,824)	1:A:349:PRO:HD2	1:A:357:PHE:HD2	10	3.04
(1,824)	1:A:349:PRO:HD3	1:A:357:PHE:HD2	10	3.04
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	13	3.02
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	16	3.02
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	3	3.0
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	6	3.0
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	15	2.98
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	7	2.96
(1,732)	1:A:326:PRO:HD2	1:A:328:TYR:HD2	2	2.95
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	6	2.95
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	19	2.93
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	18	2.86
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	3	2.85
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	8	2.85
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	13	2.84
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	5	2.84
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	5	2.84
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	5	2.84
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	5	2.84
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	5	2.84
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	5	2.84
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	5	2.84
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	5	2.84
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	5	2.84
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	11	2.83
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	16	2.83
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	18	2.83
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	4	2.82
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	1	2.81
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	1	2.81
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	1	2.81
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	5	2.81
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	10	2.81
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	14	2.81
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	20	2.8
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	7	2.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	19	2.78
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	19	2.78
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	19	2.78
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	4	2.77
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	4	2.77
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	4	2.77
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	17	2.77
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	1	2.76
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	9	2.76
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	9	2.75
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	12	2.75
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	11	2.74
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	6	2.73
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	12	2.73
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	15	2.72
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	5	2.72
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	10	2.7
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	19	2.68
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	2	2.68
(1,718)	1:A:309:TYR:HD2	1:A:313:LEU:H	2	2.61
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	18	2.53
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	18	2.53
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	18	2.53
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	15	2.52
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	8	2.5
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	8	2.5
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	8	2.5
(1,1112)	2:B:790:ILE:H	2:B:791:PHE:HD2	14	2.47
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	5	2.43
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	5	2.43
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	5	2.43
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	2	2.36
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	2	2.36
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	2	2.36
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	19	2.33
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	19	2.33
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	19	2.33
(1,724)	1:A:309:TYR:HB3	1:A:328:TYR:HD2	2	2.25
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD11	19	2.23
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD12	19	2.23
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD13	19	2.23
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	16	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	16	2.21
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	16	2.21
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	3	2.2
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	3	2.2
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	3	2.2
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	20	2.19
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	20	2.19
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	20	2.19
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	9	2.16
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	9	2.16
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	9	2.16
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	20	2.15
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	20	2.15
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	20	2.15
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	7	2.15
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	7	2.15
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	7	2.15
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	8	2.14
(1,557)	1:A:266:GLN:HG2	1:A:272:ILE:H	20	2.14
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	9	2.13
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	9	2.13
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	9	2.13
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	14	2.13
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	14	2.13
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	14	2.13
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	17	2.12
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	1	2.1
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	1	2.1
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	1	2.1
(1,827)	1:A:357:PHE:HD1	1:A:359:MET:HG2	10	2.08
(1,827)	1:A:357:PHE:HD1	1:A:359:MET:HG3	10	2.08
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	13	2.08
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	13	2.08
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	13	2.08
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	5	2.07
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	5	2.07
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	5	2.07
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	17	2.07
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	17	2.07
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	17	2.07
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	15	2.07
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	2	2.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	2	2.03
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	2	2.03
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	2	2.03
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	2	2.03
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	2	2.03
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	2	2.03
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	2	2.03
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	2	2.03
(1,827)	1:A:357:PHE:HD1	1:A:359:MET:HG2	12	2.01
(1,827)	1:A:357:PHE:HD1	1:A:359:MET:HG3	12	2.01
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	13	1.99
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	13	1.99
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	13	1.99
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	5	1.97
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	8	1.97
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	6	1.97
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	6	1.97
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	6	1.97
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	20	1.96
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	16	1.96
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	16	1.96
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	16	1.96
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	19	1.96
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	19	1.96
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	19	1.96
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	19	1.95
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	6	1.94
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	6	1.94
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	6	1.94
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	6	1.94
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	7	1.93
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	6	1.93
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	6	1.93
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	6	1.93
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	6	1.93
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	6	1.93
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	6	1.93
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	6	1.93
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	6	1.93
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	6	1.93
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	10	1.92
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	10	1.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	10	1.92
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	10	1.92
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	10	1.92
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	10	1.92
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	12	1.91
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	12	1.91
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	12	1.91
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	18	1.89
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	18	1.89
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	18	1.89
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	19	1.88
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	11	1.88
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	4	1.87
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	4	1.87
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	4	1.87
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	11	1.87
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	11	1.87
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	11	1.87
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	17	1.87
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	17	1.87
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	17	1.87
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	5	1.87
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	5	1.87
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	5	1.87
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	20	1.86
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	4	1.86
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	19	1.85
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	1	1.85
(1,827)	1:A:357:PHE:HD1	1:A:359:MET:HG2	20	1.84
(1,827)	1:A:357:PHE:HD1	1:A:359:MET:HG3	20	1.84
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	15	1.83
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	18	1.83
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	18	1.83
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	18	1.83
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	8	1.83
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	6	1.82
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	6	1.8
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	14	1.8
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	16	1.8
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	18	1.79
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	1	1.79
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	1	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	12	1.79
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	17	1.79
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	20	1.79
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	2	1.79
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	15	1.79
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	15	1.79
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	15	1.79
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	8	1.78
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	9	1.78
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	10	1.77
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	13	1.77
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	16	1.77
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	2	1.77
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	2	1.77
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	2	1.77
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	11	1.77
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	11	1.77
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	11	1.77
(1,826)	1:A:357:PHE:HD1	1:A:358:ILE:H	10	1.76
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	3	1.76
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	7	1.76
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	11	1.76
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	19	1.76
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	6	1.76
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	2	1.75
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	12	1.75
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	12	1.75
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	12	1.75
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	8	1.75
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD11	11	1.75
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD12	11	1.75
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD13	11	1.75
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	10	1.75
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	20	1.74
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	20	1.74
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	20	1.74
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	4	1.74
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	4	1.74
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	10	1.74
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	7	1.73
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	7	1.73
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	7	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,826)	1:A:357:PHE:HD1	1:A:358:ILE:H	20	1.73
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	5	1.73
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	13	1.73
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	13	1.73
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	10	1.72
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	10	1.72
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	10	1.72
(1,717)	1:A:309:TYR:HD2	1:A:311:ARG:H	18	1.72
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	3	1.72
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	3	1.72
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	3	1.72
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	3	1.72
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	6	1.71
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	6	1.71
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	6	1.71
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	12	1.71
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	12	1.71
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	12	1.71
(1,826)	1:A:357:PHE:HD1	1:A:358:ILE:H	12	1.71
(1,707)	1:A:298:ALA:HB1	1:A:328:TYR:HD1	8	1.71
(1,707)	1:A:298:ALA:HB2	1:A:328:TYR:HD1	8	1.71
(1,707)	1:A:298:ALA:HB3	1:A:328:TYR:HD1	8	1.71
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	4	1.71
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	13	1.7
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	13	1.7
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	13	1.7
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	11	1.7
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	11	1.7
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	11	1.7
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	15	1.7
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	15	1.7
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	15	1.7
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	2	1.7
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	7	1.69
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	7	1.69
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	7	1.69
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	14	1.69
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	14	1.69
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	14	1.69
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	16	1.69
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	16	1.69
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	16	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	2	1.69
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	11	1.69
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	11	1.69
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	11	1.69
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	2	1.68
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	2	1.68
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	2	1.68
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	17	1.67
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	17	1.67
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	17	1.67
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	18	1.67
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	18	1.67
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	18	1.67
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	11	1.67
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	13	1.66
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	4	1.66
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	5	1.66
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	18	1.66
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	8	1.65
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	7	1.65
(1,695)	1:A:280:LEU:HD11	1:A:292:VAL:HG21	5	1.65
(1,695)	1:A:280:LEU:HD11	1:A:292:VAL:HG22	5	1.65
(1,695)	1:A:280:LEU:HD11	1:A:292:VAL:HG23	5	1.65
(1,695)	1:A:280:LEU:HD12	1:A:292:VAL:HG21	5	1.65
(1,695)	1:A:280:LEU:HD12	1:A:292:VAL:HG22	5	1.65
(1,695)	1:A:280:LEU:HD12	1:A:292:VAL:HG23	5	1.65
(1,695)	1:A:280:LEU:HD13	1:A:292:VAL:HG21	5	1.65
(1,695)	1:A:280:LEU:HD13	1:A:292:VAL:HG22	5	1.65
(1,695)	1:A:280:LEU:HD13	1:A:292:VAL:HG23	5	1.65
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	4	1.65
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	4	1.65
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	4	1.65
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	20	1.64
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	1	1.63
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	19	1.63
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	3	1.63
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	16	1.62
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	20	1.62
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	15	1.61
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	12	1.61
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	11	1.6
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	13	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	8	1.6
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	8	1.59
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	9	1.59
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	10	1.59
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	12	1.58
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	6	1.58
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	10	1.58
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	10	1.58
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	10	1.58
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG21	8	1.58
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG22	8	1.58
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG23	8	1.58
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	3	1.57
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	17	1.57
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	20	1.56
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	16	1.56
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	9	1.56
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	4	1.56
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	7	1.56
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	15	1.55
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	15	1.55
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	16	1.54
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	16	1.54
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	14	1.54
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	14	1.54
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	15	1.53
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	3	1.53
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	7	1.52
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	7	1.52
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	17	1.52
(1,613)	1:A:301:GLN:H	1:A:309:TYR:HB3	1	1.52
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	15	1.52
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	6	1.52
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	10	1.51
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	10	1.51
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	10	1.51
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	13	1.51
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	13	1.51
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	13	1.51
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	14	1.51
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	10	1.51
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	2	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	20	1.51
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	20	1.51
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	20	1.51
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	1	1.51
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	1	1.51
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	1	1.51
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	14	1.51
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD11	19	1.51
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD12	19	1.51
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD13	19	1.51
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	5	1.5
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	8	1.5
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	9	1.49
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	6	1.48
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	4	1.48
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	4	1.48
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	4	1.48
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	14	1.47
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	14	1.47
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	14	1.47
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	12	1.46
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	1	1.46
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	6	1.45
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	20	1.45
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	6	1.44
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD11	8	1.44
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD12	8	1.44
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD13	8	1.44
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	12	1.43
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	12	1.43
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	12	1.43
(1,560)	1:A:261:SER:H	1:A:364:ILE:HG12	4	1.43
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	11	1.42
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	18	1.42
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	6	1.42
(1,1139)	1:A:314:PHE:HB3	2:B:794:LEU:HG	19	1.41
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	3	1.41
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	3	1.41
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	3	1.41
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	7	1.41
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	15	1.4
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	15	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	15	1.4
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	12	1.4
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	13	1.4
(1,925)	2:B:800:GLN:HG3	2:B:803:THR:HB	10	1.39
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	19	1.39
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	13	1.39
(1,925)	2:B:800:GLN:HG3	2:B:803:THR:HB	20	1.38
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	17	1.38
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	17	1.38
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	9	1.38
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD11	13	1.38
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD12	13	1.38
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD13	13	1.38
(1,100)	1:A:260:GLU:H	1:A:261:SER:HB3	4	1.38
(1,925)	2:B:800:GLN:HG3	2:B:803:THR:HB	13	1.37
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	14	1.37
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	3	1.37
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	20	1.37
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	18	1.37
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	16	1.36
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG21	19	1.36
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG22	19	1.36
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG23	19	1.36
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	13	1.36
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	13	1.36
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	13	1.36
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	13	1.36
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	13	1.36
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	13	1.36
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	4	1.35
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	4	1.35
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	9	1.35
(1,1061)	1:A:272:ILE:HB	2:B:797:PRO:HB3	19	1.35
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	5	1.34
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	5	1.34
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	3	1.34
(1,925)	2:B:800:GLN:HG3	2:B:803:THR:HB	19	1.33
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	9	1.33
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	9	1.33
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	19	1.33
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	13	1.33
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	15	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	19	1.33
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	7	1.32
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	17	1.32
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	4	1.32
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	8	1.31
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	8	1.31
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	8	1.31
(1,925)	2:B:800:GLN:HG3	2:B:803:THR:HB	8	1.31
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	9	1.3
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	9	1.3
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	9	1.3
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	8	1.3
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	7	1.3
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	17	1.3
(1,1043)	1:A:300:PHE:HB3	2:B:796:PRO:HB3	7	1.3
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	3	1.29
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	13	1.29
(1,925)	2:B:800:GLN:HG3	2:B:803:THR:HB	3	1.28
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	14	1.28
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	18	1.28
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	5	1.28
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	18	1.28
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	18	1.28
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	18	1.28
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	18	1.28
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	7	1.28
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	7	1.28
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	7	1.28
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	7	1.28
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	7	1.28
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	7	1.28
(1,698)	1:A:316:GLU:HG3	1:A:322:THR:H	2	1.27
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	11	1.27
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	3	1.27
(1,1056)	1:A:274:SER:HA	2:B:805:LEU:HA	19	1.27
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	16	1.27
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG21	10	1.26
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG22	10	1.26
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG23	10	1.26
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	1	1.26
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	9	1.26
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	2	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	2	1.25
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	2	1.25
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	13	1.25
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	13	1.25
(1,560)	1:A:261:SER:H	1:A:364:ILE:HG12	2	1.25
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	20	1.25
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	19	1.24
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	19	1.24
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	19	1.24
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG21	13	1.24
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG22	13	1.24
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG23	13	1.24
(1,875)	1:A:266:GLN:HB3	1:A:271:LYS:H	20	1.24
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	18	1.24
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD21	13	1.24
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD22	13	1.24
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD23	13	1.24
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	4	1.24
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	7	1.23
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	7	1.23
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	7	1.23
(2,40)	2:B:790:ILE:HD11	2:B:791:PHE:HD2	11	1.23
(2,40)	2:B:790:ILE:HD12	2:B:791:PHE:HD2	11	1.23
(2,40)	2:B:790:ILE:HD13	2:B:791:PHE:HD2	11	1.23
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	10	1.23
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	10	1.23
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	20	1.23
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	20	1.23
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	10	1.23
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	4	1.23
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	2	1.23
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	16	1.23
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD21	8	1.23
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD22	8	1.23
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD23	8	1.23
(1,925)	2:B:800:GLN:HG3	2:B:803:THR:HB	16	1.22
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	7	1.22
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	1	1.22
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	7	1.22
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	4	1.22
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	7	1.22
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	10	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	14	1.22
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	20	1.22
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	13	1.22
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	13	1.22
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	13	1.22
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	12	1.22
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	1	1.22
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	13	1.21
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	1	1.21
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	12	1.21
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	17	1.21
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	10	1.21
(1,925)	2:B:800:GLN:HG3	2:B:803:THR:HB	5	1.2
(1,925)	2:B:800:GLN:HG3	2:B:803:THR:HB	6	1.2
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	8	1.2
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	10	1.2
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	11	1.2
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	4	1.2
(1,560)	1:A:261:SER:H	1:A:364:ILE:HG12	8	1.2
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	6	1.2
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	8	1.2
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	13	1.2
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	5	1.2
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	5	1.2
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	5	1.2
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	16	1.19
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	18	1.19
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	7	1.19
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	7	1.19
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	7	1.19
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	7	1.19
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	7	1.19
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	7	1.19
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	7	1.19
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	7	1.19
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	7	1.19
(1,560)	1:A:261:SER:H	1:A:364:ILE:HG12	6	1.19
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	9	1.19
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	11	1.19
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	19	1.19
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	2	1.19
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	2	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	2	1.19
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	20	1.19
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	20	1.19
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	20	1.19
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	14	1.18
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	14	1.18
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	17	1.18
(1,425)	1:A:287:GLY:H	1:A:288:TRP:HB2	15	1.18
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	8	1.18
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	9	1.18
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	12	1.17
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	9	1.17
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	1	1.17
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	14	1.17
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	15	1.17
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	16	1.17
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	18	1.17
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD11	13	1.17
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD12	13	1.17
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD13	13	1.17
(1,1049)	1:A:300:PHE:HA	2:B:796:PRO:HG3	19	1.17
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	18	1.17
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	14	1.16
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	3	1.16
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	3	1.16
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	1	1.16
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	1	1.16
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	1	1.16
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	2	1.16
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	3	1.16
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	6	1.16
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	9	1.16
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	12	1.16
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	19	1.15
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	19	1.15
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	11	1.15
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	8	1.15
(1,858)	1:A:263:MET:HB2	1:A:276:ASP:H	11	1.14
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	16	1.14
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	4	1.14
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	5	1.14
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	19	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,100)	1:A:260:GLU:H	1:A:261:SER:HB3	7	1.14
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	11	1.13
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	11	1.13
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	16	1.13
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	5	1.13
(1,41)	1:A:267:ASP:HB2	1:A:268:THR:H	11	1.13
(1,858)	1:A:263:MET:HB2	1:A:276:ASP:H	6	1.12
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	14	1.12
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	6	1.12
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	1	1.11
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	1	1.11
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	4	1.11
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	12	1.11
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	8	1.11
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	2	1.11
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	9	1.11
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	9	1.11
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	9	1.11
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	10	1.11
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	10	1.11
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	10	1.11
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	1	1.11
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	20	1.11
(1,729)	1:A:295:CYS:H	1:A:330:PHE:HD1	2	1.1
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	10	1.1
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	17	1.1
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	6	1.1
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG21	19	1.1
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG22	19	1.1
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG23	19	1.1
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG21	19	1.1
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG22	19	1.1
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG23	19	1.1
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	19	1.1
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	18	1.09
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	18	1.09
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	18	1.09
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	15	1.09
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	15	1.09
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	15	1.09
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	2	1.09
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	2	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	2	1.09
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	10	1.08
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	10	1.08
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	10	1.08
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	10	1.08
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	10	1.08
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	10	1.08
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	15	1.07
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	15	1.07
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	16	1.07
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	13	1.07
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	20	1.06
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	16	1.06
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	19	1.06
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	6	1.05
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	17	1.05
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	14	1.05
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	14	1.05
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	14	1.05
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	9	1.05
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	9	1.05
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	9	1.05
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	15	1.04
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	17	1.04
(1,1043)	1:A:300:PHE:HB3	2:B:796:PRO:HB3	13	1.04
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	18	1.03
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	18	1.03
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	6	1.02
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	6	1.02
(1,778)	1:A:347:CYS:HG	1:A:359:MET:H	16	1.02
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	8	1.02
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	13	1.02
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD21	10	1.02
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD22	10	1.02
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD23	10	1.02
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	3	1.01
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	14	1.01
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD11	4	1.01
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD12	4	1.01
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD13	4	1.01
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	13	1.01
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	8	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	8	1.01
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	8	1.01
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	8	1.01
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	8	1.01
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	8	1.01
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	15	1.0
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	17	1.0
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD21	7	1.0
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD22	7	1.0
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD23	7	1.0
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	13	1.0
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	6	1.0
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	8	0.99
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	8	0.99
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	8	0.99
(1,587)	1:A:264:THR:H	1:A:264:THR:HG1	4	0.99
(1,560)	1:A:261:SER:H	1:A:364:ILE:HG12	11	0.99
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	14	0.99
(1,999)	2:B:807:LEU:H	2:B:807:LEU:HB2	9	0.98
(1,731)	1:A:327:SER:HA	1:A:328:TYR:HD2	2	0.98
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	10	0.98
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	12	0.98
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	11	0.98
(1,1063)	1:A:270:GLY:HA3	2:B:794:LEU:HG	19	0.98
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD11	14	0.98
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD12	14	0.98
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD13	14	0.98
(1,1049)	1:A:300:PHE:HA	2:B:796:PRO:HG3	8	0.98
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	9	0.98
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	1	0.97
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	1	0.97
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	1	0.97
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	9	0.97
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	17	0.97
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	17	0.97
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	17	0.97
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	12	0.97
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	12	0.97
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	12	0.97
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	6	0.96
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	6	0.96
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	6	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG2	8	0.96
(1,823)	1:A:347:CYS:HG	1:A:359:MET:HG3	8	0.96
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	4	0.96
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	18	0.96
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	11	0.96
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	20	0.96
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	20	0.96
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	6	0.95
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	6	0.95
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	6	0.95
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	18	0.95
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD11	5	0.95
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD12	5	0.95
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD13	5	0.95
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	13	0.94
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	14	0.94
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	16	0.94
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD11	18	0.94
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD12	18	0.94
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD13	18	0.94
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	18	0.94
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD11	3	0.94
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD12	3	0.94
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD13	3	0.94
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	4	0.94
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	11	0.93
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	10	0.93
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	7	0.93
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	4	0.93
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	15	0.93
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	4	0.92
(1,1139)	1:A:314:PHE:HB3	2:B:794:LEU:HG	5	0.92
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD11	5	0.92
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD12	5	0.92
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD13	5	0.92
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD11	9	0.92
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD12	9	0.92
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD13	9	0.92
(1,925)	2:B:800:GLN:HG3	2:B:803:THR:HB	7	0.91
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD11	18	0.91
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD12	18	0.91
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD13	18	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	12	0.91
(1,1024)	1:A:272:ILE:HD11	2:B:802:LEU:HD21	19	0.91
(1,1024)	1:A:272:ILE:HD11	2:B:802:LEU:HD22	19	0.91
(1,1024)	1:A:272:ILE:HD11	2:B:802:LEU:HD23	19	0.91
(1,1024)	1:A:272:ILE:HD12	2:B:802:LEU:HD21	19	0.91
(1,1024)	1:A:272:ILE:HD12	2:B:802:LEU:HD22	19	0.91
(1,1024)	1:A:272:ILE:HD12	2:B:802:LEU:HD23	19	0.91
(1,1024)	1:A:272:ILE:HD13	2:B:802:LEU:HD21	19	0.91
(1,1024)	1:A:272:ILE:HD13	2:B:802:LEU:HD22	19	0.91
(1,1024)	1:A:272:ILE:HD13	2:B:802:LEU:HD23	19	0.91
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	5	0.9
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	5	0.9
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	5	0.9
(1,560)	1:A:261:SER:H	1:A:364:ILE:HG12	19	0.9
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	4	0.9
(1,1139)	1:A:314:PHE:HB3	2:B:794:LEU:HG	3	0.9
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	6	0.9
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	6	0.9
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	6	0.9
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	9	0.9
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	10	0.9
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	6	0.89
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	7	0.88
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	7	0.88
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	7	0.88
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	3	0.88
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	16	0.87
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	7	0.87
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD21	9	0.87
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD22	9	0.87
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD23	9	0.87
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD21	9	0.87
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD22	9	0.87
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD23	9	0.87
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD21	9	0.87
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD22	9	0.87
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD23	9	0.87
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	6	0.87
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	6	0.87
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	6	0.87
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	6	0.87
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	6	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	6	0.87
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	2	0.86
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	10	0.86
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	6	0.86
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	7	0.86
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	4	0.86
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	8	0.86
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	20	0.85
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	20	0.85
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	20	0.85
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG21	8	0.85
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG22	8	0.85
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG23	8	0.85
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	11	0.85
(1,698)	1:A:316:GLU:HG3	1:A:322:THR:H	19	0.85
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	9	0.85
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	12	0.85
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD11	11	0.85
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD12	11	0.85
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD13	11	0.85
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	18	0.85
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD11	8	0.85
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD12	8	0.85
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD13	8	0.85
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG21	9	0.84
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG22	9	0.84
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG23	9	0.84
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	8	0.84
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	12	0.84
(1,1119)	2:B:791:PHE:H	2:B:791:PHE:HD2	5	0.84
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	16	0.84
(1,1043)	1:A:300:PHE:HB3	2:B:796:PRO:HB3	8	0.84
(1,873)	1:A:266:GLN:HB3	1:A:267:ASP:H	20	0.83
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	11	0.83
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	18	0.83
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	17	0.83
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	12	0.83
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	12	0.83
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	12	0.83
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	13	0.83
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	13	0.83
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	13	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	17	0.83
(1,1070)	2:B:785:TRP:HB2	2:B:786:ILE:H	16	0.83
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	10	0.83
(1,1027)	1:A:293:ARG:HD2	2:B:802:LEU:HD11	13	0.83
(1,1027)	1:A:293:ARG:HD2	2:B:802:LEU:HD12	13	0.83
(1,1027)	1:A:293:ARG:HD2	2:B:802:LEU:HD13	13	0.83
(1,1027)	1:A:293:ARG:HD3	2:B:802:LEU:HD11	13	0.83
(1,1027)	1:A:293:ARG:HD3	2:B:802:LEU:HD12	13	0.83
(1,1027)	1:A:293:ARG:HD3	2:B:802:LEU:HD13	13	0.83
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	3	0.82
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	4	0.82
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	15	0.82
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	18	0.82
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	6	0.82
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	6	0.81
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	20	0.81
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD11	5	0.81
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD12	5	0.81
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD13	5	0.81
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD21	9	0.81
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD22	9	0.81
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD23	9	0.81
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	1	0.8
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	1	0.8
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	1	0.8
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	10	0.8
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	10	0.8
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	10	0.8
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	19	0.8
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	2	0.8
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	3	0.8
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	13	0.8
(1,1070)	2:B:785:TRP:HB2	2:B:786:ILE:H	10	0.8
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	2	0.79
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	7	0.79
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	1	0.78
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	9	0.78
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	8	0.78
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	8	0.78
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	8	0.78
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	8	0.78
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	8	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	8	0.78
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	8	0.78
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	8	0.78
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	8	0.78
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	17	0.78
(1,560)	1:A:261:SER:H	1:A:364:ILE:HG12	16	0.78
(1,1139)	1:A:314:PHE:HB3	2:B:794:LEU:HG	11	0.78
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	5	0.78
(1,1043)	1:A:300:PHE:HB3	2:B:796:PRO:HB3	10	0.78
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	3	0.77
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	3	0.77
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	3	0.77
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	19	0.77
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	19	0.77
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	19	0.77
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	10	0.77
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	5	0.77
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	12	0.77
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	11	0.77
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	8	0.77
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	8	0.77
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	8	0.77
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	9	0.77
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	14	0.77
(1,1070)	2:B:785:TRP:HB2	2:B:786:ILE:H	11	0.77
(1,1061)	1:A:272:ILE:HB	2:B:797:PRO:HB3	5	0.77
(1,1049)	1:A:300:PHE:HA	2:B:796:PRO:HG3	4	0.77
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	18	0.76
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	18	0.76
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	18	0.76
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	8	0.76
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	8	0.76
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	8	0.76
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	3	0.76
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	4	0.76
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	20	0.76
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	13	0.76
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	20	0.76
(1,698)	1:A:316:GLU:HG3	1:A:322:THR:H	17	0.76
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	8	0.76
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	10	0.76
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	9	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	20	0.75
(1,708)	1:A:299:PHE:HB2	1:A:328:TYR:HE1	5	0.75
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	11	0.75
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	11	0.75
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	11	0.75
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	11	0.75
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	11	0.75
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	11	0.75
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	11	0.75
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	11	0.75
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	11	0.75
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	11	0.75
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	6	0.75
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	6	0.75
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	6	0.75
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	18	0.75
(1,1070)	2:B:785:TRP:HB2	2:B:786:ILE:H	14	0.75
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG21	18	0.74
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG22	18	0.74
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG23	18	0.74
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	4	0.73
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	4	0.73
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	4	0.73
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	12	0.73
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	13	0.73
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	17	0.73
(1,698)	1:A:316:GLU:HG3	1:A:322:THR:H	8	0.73
(1,698)	1:A:316:GLU:HG3	1:A:322:THR:H	18	0.73
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	5	0.73
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	9	0.73
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	9	0.73
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	13	0.72
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	13	0.72
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	13	0.72
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	20	0.72
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	4	0.72
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	4	0.72
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	4	0.72
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	4	0.72
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	4	0.72
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	4	0.72
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	4	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	4	0.72
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	4	0.72
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD11	8	0.72
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD12	8	0.72
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD13	8	0.72
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	3	0.72
(1,1070)	2:B:785:TRP:HB2	2:B:786:ILE:H	20	0.72
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD11	3	0.72
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD12	3	0.72
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD13	3	0.72
(1,1056)	1:A:274:SER:HA	2:B:805:LEU:HA	8	0.72
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	4	0.71
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	4	0.71
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	4	0.71
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	4	0.71
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	6	0.71
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	18	0.71
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	10	0.71
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	14	0.71
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD11	20	0.71
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD12	20	0.71
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD13	20	0.71
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	2	0.71
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	12	0.71
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	15	0.71
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	2	0.71
(1,1056)	1:A:274:SER:HA	2:B:805:LEU:HA	3	0.71
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	9	0.7
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	9	0.7
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	9	0.7
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	15	0.7
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	17	0.7
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	20	0.7
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	1	0.7
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	14	0.7
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	19	0.7
(1,1023)	1:A:275:ILE:HD11	2:B:806:LEU:HG	3	0.7
(1,1023)	1:A:275:ILE:HD12	2:B:806:LEU:HG	3	0.7
(1,1023)	1:A:275:ILE:HD13	2:B:806:LEU:HG	3	0.7
(1,698)	1:A:316:GLU:HG3	1:A:322:THR:H	9	0.69
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	8	0.69
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	16	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	16	0.69
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	16	0.69
(1,1065)	1:A:275:ILE:HB	2:B:806:LEU:HD21	3	0.69
(1,1065)	1:A:275:ILE:HB	2:B:806:LEU:HD22	3	0.69
(1,1065)	1:A:275:ILE:HB	2:B:806:LEU:HD23	3	0.69
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD21	4	0.69
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD22	4	0.69
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD23	4	0.69
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD21	6	0.69
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD22	6	0.69
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD23	6	0.69
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	5	0.69
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	11	0.69
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	4	0.68
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	4	0.68
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	4	0.68
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	3	0.68
(1,698)	1:A:316:GLU:HG3	1:A:322:THR:H	1	0.68
(1,1070)	2:B:785:TRP:HB2	2:B:786:ILE:H	17	0.68
(1,1061)	1:A:272:ILE:HB	2:B:797:PRO:HB3	11	0.68
(1,1040)	2:B:794:LEU:H	2:B:795:LEU:H	17	0.68
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	5	0.67
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	7	0.67
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	7	0.67
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	18	0.67
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	18	0.67
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	18	0.67
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	12	0.67
(1,1036)	2:B:797:PRO:HB3	2:B:798:THR:H	6	0.67
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	9	0.67
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	2	0.66
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	2	0.66
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	2	0.66
(1,84)	1:A:261:SER:HB2	1:A:262:PHE:H	4	0.66
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	18	0.66
(1,1134)	1:A:346:LEU:HD11	2:B:790:ILE:HD11	16	0.66
(1,1134)	1:A:346:LEU:HD11	2:B:790:ILE:HD12	16	0.66
(1,1134)	1:A:346:LEU:HD11	2:B:790:ILE:HD13	16	0.66
(1,1134)	1:A:346:LEU:HD12	2:B:790:ILE:HD11	16	0.66
(1,1134)	1:A:346:LEU:HD12	2:B:790:ILE:HD12	16	0.66
(1,1134)	1:A:346:LEU:HD12	2:B:790:ILE:HD13	16	0.66
(1,1134)	1:A:346:LEU:HD13	2:B:790:ILE:HD11	16	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1134)	1:A:346:LEU:HD13	2:B:790:ILE:HD12	16	0.66
(1,1134)	1:A:346:LEU:HD13	2:B:790:ILE:HD13	16	0.66
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD11	5	0.66
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD12	5	0.66
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD13	5	0.66
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	10	0.66
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	19	0.65
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	16	0.65
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	19	0.65
(1,542)	1:A:269:THR:H	1:A:269:THR:HG1	5	0.65
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD11	4	0.65
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD12	4	0.65
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD13	4	0.65
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD11	18	0.65
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD12	18	0.65
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD13	18	0.65
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	11	0.65
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	5	0.65
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD21	20	0.65
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD22	20	0.65
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD23	20	0.65
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	5	0.65
(1,1036)	2:B:797:PRO:HB3	2:B:798:THR:H	20	0.65
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	9	0.64
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	14	0.64
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	20	0.64
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	20	0.64
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	20	0.64
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	20	0.64
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	20	0.64
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	20	0.64
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	20	0.64
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	20	0.64
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	20	0.64
(1,617)	1:A:315:GLN:HE22	1:A:318:MET:H	16	0.64
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	20	0.64
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	20	0.64
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	20	0.64
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	20	0.64
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	18	0.64
(1,1070)	2:B:785:TRP:HB2	2:B:786:ILE:H	2	0.64
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	16	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	16	0.63
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	16	0.63
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	11	0.63
(1,84)	1:A:261:SER:HB2	1:A:262:PHE:H	7	0.63
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	16	0.63
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	16	0.63
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	16	0.63
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	16	0.63
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	16	0.63
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	16	0.63
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	16	0.63
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	16	0.63
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	16	0.63
(1,1070)	2:B:785:TRP:HB2	2:B:786:ILE:H	19	0.63
(1,1043)	1:A:300:PHE:HB3	2:B:796:PRO:HB3	18	0.63
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	17	0.63
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	17	0.63
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	17	0.63
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	17	0.63
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	17	0.63
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	17	0.63
(1,1136)	2:B:794:LEU:HD11	1:A:311:ARG:HB2	10	0.62
(1,1136)	2:B:794:LEU:HD12	1:A:311:ARG:HB2	10	0.62
(1,1136)	2:B:794:LEU:HD13	1:A:311:ARG:HB2	10	0.62
(1,1136)	2:B:794:LEU:HD11	1:A:311:ARG:HB3	10	0.62
(1,1136)	2:B:794:LEU:HD12	1:A:311:ARG:HB3	10	0.62
(1,1136)	2:B:794:LEU:HD13	1:A:311:ARG:HB3	10	0.62
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	16	0.62
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	16	0.62
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	16	0.62
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	16	0.62
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	16	0.62
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	16	0.62
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	16	0.62
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	18	0.62
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	3	0.61
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	4	0.61
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	6	0.61
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	10	0.61
(1,1136)	2:B:794:LEU:HD11	1:A:311:ARG:HB2	13	0.61
(1,1136)	2:B:794:LEU:HD12	1:A:311:ARG:HB2	13	0.61
(1,1136)	2:B:794:LEU:HD13	1:A:311:ARG:HB2	13	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1136)	2:B:794:LEU:HD11	1:A:311:ARG:HB3	13	0.61
(1,1136)	2:B:794:LEU:HD12	1:A:311:ARG:HB3	13	0.61
(1,1136)	2:B:794:LEU:HD13	1:A:311:ARG:HB3	13	0.61
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG21	18	0.61
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG22	18	0.61
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG23	18	0.61
(1,1110)	2:B:790:ILE:H	2:B:791:PHE:HB3	8	0.61
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	7	0.61
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG21	10	0.6
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG22	10	0.6
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG23	10	0.6
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	20	0.6
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	20	0.6
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	20	0.6
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	17	0.6
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	2	0.6
(1,913)	2:B:800:GLN:HB2	2:B:801:ASP:H	10	0.59
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	8	0.59
(1,1100)	2:B:789:ASP:HB2	2:B:791:PHE:H	13	0.59
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	17	0.59
(1,1060)	1:A:272:ILE:HB	2:B:797:PRO:HG2	19	0.59
(1,1060)	1:A:272:ILE:HB	2:B:797:PRO:HG3	19	0.59
(1,816)	1:A:357:PHE:H	1:A:357:PHE:HE2	20	0.58
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	15	0.58
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD11	4	0.58
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD12	4	0.58
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD13	4	0.58
(1,1097)	2:B:788:GLU:HA	2:B:790:ILE:H	19	0.58
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD21	8	0.58
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD22	8	0.58
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD23	8	0.58
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD21	8	0.58
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD22	8	0.58
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD23	8	0.58
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD21	8	0.58
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD22	8	0.58
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD23	8	0.58
(1,1139)	1:A:314:PHE:HB3	2:B:794:LEU:HG	8	0.57
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD11	11	0.57
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD12	11	0.57
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD13	11	0.57
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	16	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	12	0.57
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD11	20	0.57
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD12	20	0.57
(1,1057)	1:A:274:SER:HA	2:B:805:LEU:HD13	20	0.57
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD11	10	0.57
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD12	10	0.57
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD13	10	0.57
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	19	0.57
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	4	0.56
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	4	0.56
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	4	0.56
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	19	0.56
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	19	0.56
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	6	0.56
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	6	0.56
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG21	1	0.56
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG22	1	0.56
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG23	1	0.56
(1,1055)	1:A:274:SER:HA	2:B:805:LEU:HG	19	0.56
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	1	0.55
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	16	0.55
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	18	0.55
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	8	0.55
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD11	8	0.55
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD12	8	0.55
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD13	8	0.55
(1,1063)	1:A:270:GLY:HA3	2:B:794:LEU:HG	1	0.55
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	17	0.55
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	9	0.54
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	9	0.54
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	9	0.54
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	16	0.54
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	16	0.54
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	16	0.54
(1,1156)	2:B:786:ILE:HA	2:B:789:ASP:H	19	0.54
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD11	20	0.54
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD12	20	0.54
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD13	20	0.54
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG21	11	0.54
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG22	11	0.54
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG23	11	0.54
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG21	11	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG22	11	0.54
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG23	11	0.54
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD11	10	0.54
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD12	10	0.54
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD13	10	0.54
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	17	0.53
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	17	0.53
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	17	0.53
(1,816)	1:A:357:PHE:H	1:A:357:PHE:HE2	10	0.53
(1,816)	1:A:357:PHE:H	1:A:357:PHE:HE2	12	0.53
(1,722)	1:A:309:TYR:HE1	1:A:326:PRO:HG2	2	0.53
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	7	0.53
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	9	0.53
(1,1056)	1:A:274:SER:HA	2:B:805:LEU:HA	11	0.53
(1,1049)	1:A:300:PHE:HA	2:B:796:PRO:HG3	5	0.53
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	1	0.52
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	9	0.52
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	10	0.52
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	18	0.52
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	15	0.52
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	15	0.52
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	20	0.52
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	20	0.52
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	6	0.52
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	7	0.52
(1,1056)	1:A:274:SER:HA	2:B:805:LEU:HA	4	0.52
(1,1056)	1:A:274:SER:HA	2:B:805:LEU:HA	13	0.52
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD21	4	0.52
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD22	4	0.52
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD23	4	0.52
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD21	4	0.52
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD22	4	0.52
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD23	4	0.52
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD21	4	0.52
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD22	4	0.52
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD23	4	0.52
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	1	0.51
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	15	0.51
(1,1157)	2:B:786:ILE:HA	2:B:790:ILE:H	19	0.51
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	15	0.51
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	15	0.51
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	15	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	16	0.51
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	3	0.51
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	12	0.5
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	17	0.5
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	18	0.5
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG21	6	0.5
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG22	6	0.5
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG23	6	0.5
(2,30)	2:B:802:LEU:HD11	2:B:804:LYS:HA	5	0.5
(2,30)	2:B:802:LEU:HD12	2:B:804:LYS:HA	5	0.5
(2,30)	2:B:802:LEU:HD13	2:B:804:LYS:HA	5	0.5
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	16	0.5
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	13	0.5
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	7	0.5
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	7	0.5
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	7	0.5
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD11	11	0.5
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD12	11	0.5
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD13	11	0.5
(1,1053)	1:A:296:ILE:HG21	2:B:797:PRO:HD3	6	0.5
(1,1053)	1:A:296:ILE:HG22	2:B:797:PRO:HD3	6	0.5
(1,1053)	1:A:296:ILE:HG23	2:B:797:PRO:HD3	6	0.5
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	15	0.49
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	2	0.49
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	1	0.49
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	7	0.49
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	7	0.49
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	7	0.49
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	10	0.49
(1,1063)	1:A:270:GLY:HA3	2:B:794:LEU:HG	11	0.49
(1,1049)	1:A:300:PHE:HA	2:B:796:PRO:HG3	18	0.49
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	2	0.48
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	8	0.48
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	13	0.48
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	18	0.48
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	18	0.48
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	4	0.48
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD11	1	0.48
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD12	1	0.48
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD13	1	0.48
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD11	10	0.48
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD12	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD13	10	0.48
(1,1066)	1:A:277:THR:HG21	2:B:806:LEU:HD21	20	0.48
(1,1066)	1:A:277:THR:HG21	2:B:806:LEU:HD22	20	0.48
(1,1066)	1:A:277:THR:HG21	2:B:806:LEU:HD23	20	0.48
(1,1066)	1:A:277:THR:HG22	2:B:806:LEU:HD21	20	0.48
(1,1066)	1:A:277:THR:HG22	2:B:806:LEU:HD22	20	0.48
(1,1066)	1:A:277:THR:HG22	2:B:806:LEU:HD23	20	0.48
(1,1066)	1:A:277:THR:HG23	2:B:806:LEU:HD21	20	0.48
(1,1066)	1:A:277:THR:HG23	2:B:806:LEU:HD22	20	0.48
(1,1066)	1:A:277:THR:HG23	2:B:806:LEU:HD23	20	0.48
(1,1056)	1:A:274:SER:HA	2:B:805:LEU:HA	5	0.48
(1,1049)	1:A:300:PHE:HA	2:B:796:PRO:HG3	11	0.48
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	18	0.48
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	9	0.48
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	9	0.48
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	9	0.48
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	9	0.48
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	9	0.48
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	9	0.48
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	5	0.48
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD11	20	0.48
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD12	20	0.48
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD13	20	0.48
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	3	0.47
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	4	0.47
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	9	0.47
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	10	0.47
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	16	0.47
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	7	0.47
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	20	0.47
(1,1146)	2:B:789:ASP:HA	2:B:791:PHE:H	19	0.47
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	5	0.47
(1,1065)	1:A:275:ILE:HB	2:B:806:LEU:HD21	11	0.47
(1,1065)	1:A:275:ILE:HB	2:B:806:LEU:HD22	11	0.47
(1,1065)	1:A:275:ILE:HB	2:B:806:LEU:HD23	11	0.47
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	20	0.47
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	6	0.46
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	5	0.46
(1,828)	1:A:348:TYR:H	1:A:348:TYR:HD1	14	0.46
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	13	0.46
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	19	0.46
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD11	18	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD12	18	0.46
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD13	18	0.46
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	7	0.46
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	1	0.46
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	1	0.45
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	12	0.45
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	17	0.45
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	18	0.45
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	11	0.45
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	8	0.45
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	8	0.45
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	1	0.45
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	3	0.45
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	4	0.45
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	8	0.45
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	9	0.45
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	12	0.45
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	15	0.45
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	17	0.45
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	18	0.45
(1,1139)	1:A:314:PHE:HB3	2:B:794:LEU:HG	20	0.45
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD11	4	0.45
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD12	4	0.45
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD13	4	0.45
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG21	5	0.45
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG22	5	0.45
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG23	5	0.45
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG21	5	0.45
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG22	5	0.45
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG23	5	0.45
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	9	0.45
(1,1045)	1:A:300:PHE:HD2	2:B:796:PRO:HG3	8	0.45
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	15	0.44
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	19	0.44
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	17	0.44
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	17	0.44
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	17	0.44
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	9	0.44
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	9	0.44
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	5	0.44
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	6	0.44
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	7	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	10	0.44
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	11	0.44
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	13	0.44
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	14	0.44
(1,375)	1:A:320:ARG:H	1:A:321:GLY:HA3	16	0.44
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD11	2	0.44
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD12	2	0.44
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD13	2	0.44
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	3	0.44
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	8	0.44
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	19	0.44
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD11	8	0.44
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD12	8	0.44
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD13	8	0.44
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	2	0.43
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	4	0.43
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	8	0.43
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	14	0.43
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	20	0.43
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG21	13	0.43
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG22	13	0.43
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG23	13	0.43
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	15	0.43
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	15	0.43
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	15	0.43
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	15	0.43
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	15	0.43
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	15	0.43
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	15	0.43
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	15	0.43
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	15	0.43
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	4	0.43
(1,1050)	1:A:310:ALA:HB1	2:B:794:LEU:HD21	10	0.43
(1,1050)	1:A:310:ALA:HB1	2:B:794:LEU:HD22	10	0.43
(1,1050)	1:A:310:ALA:HB1	2:B:794:LEU:HD23	10	0.43
(1,1050)	1:A:310:ALA:HB2	2:B:794:LEU:HD21	10	0.43
(1,1050)	1:A:310:ALA:HB2	2:B:794:LEU:HD22	10	0.43
(1,1050)	1:A:310:ALA:HB2	2:B:794:LEU:HD23	10	0.43
(1,1050)	1:A:310:ALA:HB3	2:B:794:LEU:HD21	10	0.43
(1,1050)	1:A:310:ALA:HB3	2:B:794:LEU:HD22	10	0.43
(1,1050)	1:A:310:ALA:HB3	2:B:794:LEU:HD23	10	0.43
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	14	0.43
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	15	0.43
(1,1023)	1:A:275:ILE:HD11	2:B:806:LEU:HG	19	0.43
(1,1023)	1:A:275:ILE:HD12	2:B:806:LEU:HG	19	0.43
(1,1023)	1:A:275:ILE:HD13	2:B:806:LEU:HG	19	0.43
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	3	0.42
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	9	0.42
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	10	0.42
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	11	0.42
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	13	0.42
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	16	0.42
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG21	7	0.42
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG22	7	0.42
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG23	7	0.42
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	15	0.42
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	15	0.42
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	15	0.42
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	19	0.42
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	14	0.42
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	14	0.42
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	14	0.42
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD11	19	0.42
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD12	19	0.42
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD13	19	0.42
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	6	0.42
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	4	0.42
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	18	0.42
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	6	0.41
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	20	0.41
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	5	0.41
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	12	0.41
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	12	0.41
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	12	0.41
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	1	0.41
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	6	0.41
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD11	20	0.41
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD12	20	0.41
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD13	20	0.41
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG21	1	0.41
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG22	1	0.41
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG23	1	0.41
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG21	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG22	1	0.41
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG23	1	0.41
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG21	4	0.41
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG22	4	0.41
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG23	4	0.41
(1,109)	1:A:363:ILE:H	1:A:363:ILE:HB	15	0.41
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	12	0.41
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD11	20	0.41
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD12	20	0.41
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD13	20	0.41
(1,1053)	1:A:296:ILE:HG21	2:B:797:PRO:HD3	20	0.41
(1,1053)	1:A:296:ILE:HG22	2:B:797:PRO:HD3	20	0.41
(1,1053)	1:A:296:ILE:HG23	2:B:797:PRO:HD3	20	0.41
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	17	0.41
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD21	5	0.41
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD22	5	0.41
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD23	5	0.41
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD21	5	0.41
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD22	5	0.41
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD23	5	0.41
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD21	5	0.41
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD22	5	0.41
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD23	5	0.41
(1,1018)	2:B:812:GLU:H	2:B:812:GLU:HB3	9	0.41
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	19	0.4
(1,828)	1:A:348:TYR:H	1:A:348:TYR:HD1	17	0.4
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	11	0.4
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	11	0.4
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	20	0.4
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	3	0.4
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD11	6	0.4
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD12	6	0.4
(1,1129)	1:A:348:TYR:HB2	2:B:786:ILE:HD13	6	0.4
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD11	3	0.4
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD12	3	0.4
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD13	3	0.4
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	4	0.4
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	4	0.4
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	4	0.4
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	20	0.4
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	14	0.4
(1,109)	1:A:363:ILE:H	1:A:363:ILE:HB	16	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1049)	1:A:300:PHE:HA	2:B:796:PRO:HG3	3	0.4
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD21	18	0.4
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD22	18	0.4
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD23	18	0.4
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD21	18	0.4
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD22	18	0.4
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD23	18	0.4
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD21	18	0.4
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD22	18	0.4
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD23	18	0.4
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	3	0.4
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	3	0.4
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	3	0.4
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	3	0.4
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	3	0.4
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	3	0.4
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	5	0.39
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	14	0.39
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG21	20	0.39
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG22	20	0.39
(2,62)	1:A:314:PHE:HA	2:B:790:ILE:HG23	20	0.39
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	8	0.39
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	17	0.39
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	19	0.39
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	19	0.39
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	19	0.39
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	19	0.39
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	19	0.39
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	19	0.39
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	19	0.39
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	19	0.39
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	19	0.39
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	19	0.39
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	17	0.39
(1,1145)	2:B:788:GLU:HA	2:B:791:PHE:H	19	0.39
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	11	0.39
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	13	0.39
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD21	19	0.39
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD22	19	0.39
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD23	19	0.39
(3,17)	1:A:274:SER:H	1:A:265:LYS:O	7	0.38
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	10	0.38
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	14	0.38
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	15	0.38
(1,709)	1:A:299:PHE:HB2	1:A:328:TYR:HD1	5	0.38
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	15	0.38
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	20	0.38
(1,1136)	2:B:794:LEU:HD11	1:A:311:ARG:HB2	8	0.38
(1,1136)	2:B:794:LEU:HD12	1:A:311:ARG:HB2	8	0.38
(1,1136)	2:B:794:LEU:HD13	1:A:311:ARG:HB2	8	0.38
(1,1136)	2:B:794:LEU:HD11	1:A:311:ARG:HB3	8	0.38
(1,1136)	2:B:794:LEU:HD12	1:A:311:ARG:HB3	8	0.38
(1,1136)	2:B:794:LEU:HD13	1:A:311:ARG:HB3	8	0.38
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD11	9	0.38
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD12	9	0.38
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD13	9	0.38
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	11	0.38
(1,1018)	2:B:812:GLU:H	2:B:812:GLU:HB3	20	0.38
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	9	0.37
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	9	0.37
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	9	0.37
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	9	0.37
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	9	0.37
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	9	0.37
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	4	0.37
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	5	0.37
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	11	0.37
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	12	0.37
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	3	0.37
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	13	0.37
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	9	0.37
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	11	0.37
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	5	0.37
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	6	0.37
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	7	0.37
(1,1055)	1:A:274:SER:HA	2:B:805:LEU:HG	18	0.37
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	1	0.37
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	2	0.37
(1,1026)	1:A:293:ARG:HG2	2:B:802:LEU:HD11	5	0.37
(1,1026)	1:A:293:ARG:HG2	2:B:802:LEU:HD12	5	0.37
(1,1026)	1:A:293:ARG:HG2	2:B:802:LEU:HD13	5	0.37
(1,1026)	1:A:293:ARG:HG3	2:B:802:LEU:HD11	5	0.37
(1,1026)	1:A:293:ARG:HG3	2:B:802:LEU:HD12	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1026)	1:A:293:ARG:HG3	2:B:802:LEU:HD13	5	0.37
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	3	0.36
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	7	0.36
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	1	0.36
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD11	8	0.36
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD12	8	0.36
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD13	8	0.36
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	4	0.36
(1,109)	1:A:363:ILE:H	1:A:363:ILE:HB	11	0.36
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	1	0.36
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	5	0.36
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	20	0.36
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	20	0.36
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	20	0.36
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	20	0.36
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	20	0.36
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	20	0.36
(3,18)	1:A:274:SER:N	1:A:265:LYS:O	7	0.35
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	8	0.35
(1,913)	2:B:800:GLN:HB2	2:B:801:ASP:H	7	0.35
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	2	0.35
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	20	0.35
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	18	0.35
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	10	0.35
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	12	0.35
(1,1101)	2:B:789:ASP:H	2:B:790:ILE:H	19	0.35
(1,1063)	1:A:270:GLY:HA3	2:B:794:LEU:HG	2	0.35
(1,1036)	2:B:797:PRO:HB3	2:B:798:THR:H	9	0.35
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD11	8	0.35
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD12	8	0.35
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD13	8	0.35
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD21	8	0.35
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD22	8	0.35
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD23	8	0.35
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	15	0.35
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	14	0.34
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	14	0.34
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	14	0.34
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	8	0.34
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	8	0.34
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	8	0.34
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	8	0.34
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	8	0.34
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	13	0.34
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	20	0.34
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	14	0.34
(1,705)	1:A:313:LEU:HD21	1:A:325:SER:H	2	0.34
(1,705)	1:A:313:LEU:HD22	1:A:325:SER:H	2	0.34
(1,705)	1:A:313:LEU:HD23	1:A:325:SER:H	2	0.34
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	5	0.34
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	13	0.34
(1,212)	1:A:261:SER:H	1:A:261:SER:HB3	7	0.34
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	16	0.34
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	16	0.34
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	16	0.34
(1,1071)	2:B:785:TRP:H	2:B:785:TRP:HB3	4	0.34
(1,1053)	1:A:296:ILE:HG21	2:B:797:PRO:HD3	8	0.34
(1,1053)	1:A:296:ILE:HG22	2:B:797:PRO:HD3	8	0.34
(1,1053)	1:A:296:ILE:HG23	2:B:797:PRO:HD3	8	0.34
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	16	0.34
(1,1043)	1:A:300:PHE:HB3	2:B:796:PRO:HB3	20	0.34
(1,1004)	2:B:807:LEU:H	2:B:807:LEU:HG	9	0.34
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	8	0.33
(1,828)	1:A:348:TYR:H	1:A:348:TYR:HD1	13	0.33
(1,828)	1:A:348:TYR:H	1:A:348:TYR:HD1	16	0.33
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	9	0.33
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	14	0.33
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	16	0.33
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	5	0.33
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	12	0.33
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	3	0.33
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	2	0.33
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	3	0.33
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	2	0.33
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	10	0.33
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	8	0.33
(1,1070)	2:B:785:TRP:HB2	2:B:786:ILE:H	8	0.33
(1,1060)	1:A:272:ILE:HB	2:B:797:PRO:HG2	1	0.33
(1,1060)	1:A:272:ILE:HB	2:B:797:PRO:HG3	1	0.33
(1,1025)	1:A:275:ILE:HD11	2:B:802:LEU:HD21	4	0.33
(1,1025)	1:A:275:ILE:HD11	2:B:802:LEU:HD22	4	0.33
(1,1025)	1:A:275:ILE:HD11	2:B:802:LEU:HD23	4	0.33
(1,1025)	1:A:275:ILE:HD12	2:B:802:LEU:HD21	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1025)	1:A:275:ILE:HD12	2:B:802:LEU:HD22	4	0.33
(1,1025)	1:A:275:ILE:HD12	2:B:802:LEU:HD23	4	0.33
(1,1025)	1:A:275:ILE:HD13	2:B:802:LEU:HD21	4	0.33
(1,1025)	1:A:275:ILE:HD13	2:B:802:LEU:HD22	4	0.33
(1,1025)	1:A:275:ILE:HD13	2:B:802:LEU:HD23	4	0.33
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	11	0.32
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	11	0.32
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	11	0.32
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	4	0.32
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	4	0.32
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	4	0.32
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	4	0.32
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	4	0.32
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	4	0.32
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	17	0.32
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	5	0.32
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	6	0.32
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	7	0.32
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	11	0.32
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	15	0.32
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	19	0.32
(1,777)	1:A:347:CYS:HG	1:A:359:MET:HB2	16	0.32
(1,777)	1:A:347:CYS:HG	1:A:359:MET:HB3	16	0.32
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	2	0.32
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	11	0.32
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	12	0.32
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	11	0.32
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	16	0.32
(1,1145)	2:B:788:GLU:HA	2:B:791:PHE:H	6	0.32
(1,1065)	1:A:275:ILE:HB	2:B:806:LEU:HD21	19	0.32
(1,1065)	1:A:275:ILE:HB	2:B:806:LEU:HD22	19	0.32
(1,1065)	1:A:275:ILE:HB	2:B:806:LEU:HD23	19	0.32
(1,1061)	1:A:272:ILE:HB	2:B:797:PRO:HB3	1	0.32
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	18	0.32
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	18	0.32
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	18	0.32
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	18	0.32
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	18	0.32
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	18	0.32
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD11	4	0.32
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD12	4	0.32
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD13	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD11	11	0.32
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD12	11	0.32
(1,1028)	1:A:289:GLU:HA	2:B:806:LEU:HD13	11	0.32
(1,1018)	2:B:812:GLU:H	2:B:812:GLU:HB3	12	0.32
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	6	0.31
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	15	0.31
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	16	0.31
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	17	0.31
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	5	0.31
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	5	0.31
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	5	0.31
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	5	0.31
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	5	0.31
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	5	0.31
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	15	0.31
(1,828)	1:A:348:TYR:H	1:A:348:TYR:HD1	10	0.31
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	9	0.31
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	7	0.31
(1,212)	1:A:261:SER:H	1:A:261:SER:HB3	4	0.31
(1,1139)	1:A:314:PHE:HB3	2:B:794:LEU:HG	14	0.31
(1,1053)	1:A:296:ILE:HG21	2:B:797:PRO:HD3	10	0.31
(1,1053)	1:A:296:ILE:HG22	2:B:797:PRO:HD3	10	0.31
(1,1053)	1:A:296:ILE:HG23	2:B:797:PRO:HD3	10	0.31
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD21	10	0.31
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD22	10	0.31
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD23	10	0.31
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD21	10	0.31
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD22	10	0.31
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD23	10	0.31
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD21	10	0.31
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD22	10	0.31
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD23	10	0.31
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	3	0.3
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	10	0.3
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	19	0.3
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	18	0.3
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	18	0.3
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	18	0.3
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG21	18	0.3
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG22	18	0.3
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG23	18	0.3
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	3	0.3
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	3	0.3
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	3	0.3
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	3	0.3
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	3	0.3
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	7	0.3
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	7	0.3
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	7	0.3
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	7	0.3
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	7	0.3
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	7	0.3
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	15	0.3
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	15	0.3
(1,1139)	1:A:314:PHE:HB3	2:B:794:LEU:HG	13	0.3
(1,1134)	1:A:346:LEU:HD11	2:B:790:ILE:HD11	11	0.3
(1,1134)	1:A:346:LEU:HD11	2:B:790:ILE:HD12	11	0.3
(1,1134)	1:A:346:LEU:HD11	2:B:790:ILE:HD13	11	0.3
(1,1134)	1:A:346:LEU:HD12	2:B:790:ILE:HD11	11	0.3
(1,1134)	1:A:346:LEU:HD12	2:B:790:ILE:HD12	11	0.3
(1,1134)	1:A:346:LEU:HD12	2:B:790:ILE:HD13	11	0.3
(1,1134)	1:A:346:LEU:HD13	2:B:790:ILE:HD11	11	0.3
(1,1134)	1:A:346:LEU:HD13	2:B:790:ILE:HD12	11	0.3
(1,1134)	1:A:346:LEU:HD13	2:B:790:ILE:HD13	11	0.3
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG21	20	0.3
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG22	20	0.3
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG23	20	0.3
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	7	0.3
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	10	0.3
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	6	0.3
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	8	0.3
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD21	3	0.3
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD22	3	0.3
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD23	3	0.3
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	12	0.3
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	12	0.3
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	12	0.3
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	12	0.3
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	12	0.3
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	12	0.3
(1,1026)	1:A:293:ARG:HG2	2:B:802:LEU:HD11	13	0.3
(1,1026)	1:A:293:ARG:HG2	2:B:802:LEU:HD12	13	0.3
(1,1026)	1:A:293:ARG:HG2	2:B:802:LEU:HD13	13	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1026)	1:A:293:ARG:HG3	2:B:802:LEU:HD11	13	0.3
(1,1026)	1:A:293:ARG:HG3	2:B:802:LEU:HD12	13	0.3
(1,1026)	1:A:293:ARG:HG3	2:B:802:LEU:HD13	13	0.3
(1,1018)	2:B:812:GLU:H	2:B:812:GLU:HB3	6	0.3
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	12	0.29
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	14	0.29
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	18	0.29
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	8	0.29
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	8	0.29
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	8	0.29
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	13	0.29
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	3	0.29
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	8	0.29
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	6	0.29
(1,735)	1:A:291:LEU:HB2	1:A:332:LEU:HD21	6	0.29
(1,735)	1:A:291:LEU:HB2	1:A:332:LEU:HD22	6	0.29
(1,735)	1:A:291:LEU:HB2	1:A:332:LEU:HD23	6	0.29
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	14	0.29
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	15	0.29
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	16	0.29
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	18	0.29
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	15	0.29
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	15	0.29
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	15	0.29
(1,1121)	1:A:310:ALA:HB1	2:B:794:LEU:HD11	8	0.29
(1,1121)	1:A:310:ALA:HB1	2:B:794:LEU:HD12	8	0.29
(1,1121)	1:A:310:ALA:HB1	2:B:794:LEU:HD13	8	0.29
(1,1121)	1:A:310:ALA:HB2	2:B:794:LEU:HD11	8	0.29
(1,1121)	1:A:310:ALA:HB2	2:B:794:LEU:HD12	8	0.29
(1,1121)	1:A:310:ALA:HB2	2:B:794:LEU:HD13	8	0.29
(1,1121)	1:A:310:ALA:HB3	2:B:794:LEU:HD11	8	0.29
(1,1121)	1:A:310:ALA:HB3	2:B:794:LEU:HD12	8	0.29
(1,1121)	1:A:310:ALA:HB3	2:B:794:LEU:HD13	8	0.29
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	1	0.29
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	15	0.29
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	15	0.29
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	20	0.29
(1,1056)	1:A:274:SER:HA	2:B:805:LEU:HA	18	0.29
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	17	0.29
(1,1036)	2:B:797:PRO:HB3	2:B:798:THR:H	7	0.29
(1,1027)	1:A:293:ARG:HD2	2:B:802:LEU:HD11	10	0.29
(1,1027)	1:A:293:ARG:HD2	2:B:802:LEU:HD12	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1027)	1:A:293:ARG:HD2	2:B:802:LEU:HD13	10	0.29
(1,1027)	1:A:293:ARG:HD3	2:B:802:LEU:HD11	10	0.29
(1,1027)	1:A:293:ARG:HD3	2:B:802:LEU:HD12	10	0.29
(1,1027)	1:A:293:ARG:HD3	2:B:802:LEU:HD13	10	0.29
(1,1018)	2:B:812:GLU:H	2:B:812:GLU:HB3	5	0.29
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	5	0.28
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	9	0.28
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	11	0.28
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	13	0.28
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	20	0.28
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	20	0.28
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	20	0.28
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	20	0.28
(1,913)	2:B:800:GLN:HB2	2:B:801:ASP:H	6	0.28
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	16	0.28
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	4	0.28
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	18	0.28
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	6	0.28
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	19	0.28
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	19	0.28
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	10	0.28
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	7	0.28
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG21	5	0.28
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG22	5	0.28
(1,1123)	1:A:346:LEU:HB3	2:B:786:ILE:HG23	5	0.28
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	5	0.28
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	11	0.28
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD11	5	0.28
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD12	5	0.28
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD13	5	0.28
(1,1063)	1:A:270:GLY:HA3	2:B:794:LEU:HG	3	0.28
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	12	0.28
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD21	19	0.28
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD22	19	0.28
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD23	19	0.28
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD21	19	0.28
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD22	19	0.28
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD23	19	0.28
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD21	19	0.28
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD22	19	0.28
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD23	19	0.28
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	1	0.27
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	1	0.27
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	14	0.27
(1,523)	1:A:325:SER:H	1:A:342:THR:H	18	0.27
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG21	8	0.27
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG22	8	0.27
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG23	8	0.27
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG21	8	0.27
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG22	8	0.27
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG23	8	0.27
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	12	0.27
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	12	0.27
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	12	0.27
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	6	0.27
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	14	0.27
(1,1043)	1:A:300:PHE:HB3	2:B:796:PRO:HB3	19	0.27
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	16	0.26
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	16	0.26
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	16	0.26
(1,913)	2:B:800:GLN:HB2	2:B:801:ASP:H	20	0.26
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	18	0.26
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	3	0.26
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	9	0.26
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	19	0.26
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	14	0.26
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	11	0.26
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	20	0.26
(1,591)	1:A:316:GLU:HG2	1:A:324:SER:H	2	0.26
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	20	0.26
(1,550)	1:A:315:GLN:H	1:A:315:GLN:HE22	20	0.26
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	8	0.26
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	20	0.26
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	17	0.26
(1,1055)	1:A:274:SER:HA	2:B:805:LEU:HG	1	0.26
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD21	17	0.26
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD22	17	0.26
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD23	17	0.26
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD21	17	0.26
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD22	17	0.26
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD23	17	0.26
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD21	17	0.26
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD22	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD23	17	0.26
(1,1018)	2:B:812:GLU:H	2:B:812:GLU:HB3	1	0.26
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	2	0.25
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	4	0.25
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	7	0.25
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	14	0.25
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	14	0.25
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	14	0.25
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	3	0.25
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	3	0.25
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	3	0.25
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	2	0.25
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	5	0.25
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	18	0.25
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	2	0.25
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	10	0.25
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	12	0.25
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	18	0.25
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	4	0.25
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	4	0.25
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	5	0.25
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	11	0.25
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	15	0.25
(1,1145)	2:B:788:GLU:HA	2:B:791:PHE:H	5	0.25
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD11	8	0.25
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD12	8	0.25
(1,1132)	1:A:346:LEU:HB3	2:B:786:ILE:HD13	8	0.25
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	18	0.25
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	3	0.25
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	16	0.25
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	9	0.25
(1,1061)	1:A:272:ILE:HB	2:B:797:PRO:HB3	3	0.25
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD11	4	0.25
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD12	4	0.25
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD13	4	0.25
(1,1023)	1:A:275:ILE:HD11	2:B:806:LEU:HG	7	0.25
(1,1023)	1:A:275:ILE:HD12	2:B:806:LEU:HG	7	0.25
(1,1023)	1:A:275:ILE:HD13	2:B:806:LEU:HG	7	0.25
(1,985)	2:B:804:LYS:HD2	2:B:806:LEU:H	7	0.24
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	9	0.24
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	8	0.24
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:A:362:HIS:HA	1:A:363:ILE:HB	15	0.24
(1,850)	1:A:362:HIS:HA	1:A:363:ILE:HB	16	0.24
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	2	0.24
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	13	0.24
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	1	0.24
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	7	0.24
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	20	0.24
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	3	0.24
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	7	0.24
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	9	0.24
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	11	0.24
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	17	0.24
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	6	0.24
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	10	0.24
(1,524)	1:A:341:HIS:HB2	1:A:342:THR:H	5	0.24
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	5	0.24
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	9	0.24
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	1	0.24
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	6	0.24
(1,199)	1:A:268:THR:HA	1:A:270:GLY:H	20	0.24
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	2	0.24
(1,1070)	2:B:785:TRP:HB2	2:B:786:ILE:H	4	0.24
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD11	17	0.24
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD12	17	0.24
(1,1064)	1:A:273:ILE:HA	2:B:805:LEU:HD13	17	0.24
(1,1063)	1:A:270:GLY:HA3	2:B:794:LEU:HG	12	0.24
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	11	0.24
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	2	0.24
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD11	4	0.24
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD12	4	0.24
(1,1033)	1:A:293:ARG:HG2	2:B:806:LEU:HD13	4	0.24
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD11	4	0.24
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD12	4	0.24
(1,1033)	1:A:293:ARG:HG3	2:B:806:LEU:HD13	4	0.24
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	17	0.23
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	17	0.23
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	17	0.23
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	17	0.23
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	17	0.23
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	17	0.23
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	5	0.23
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	1	0.23
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	11	0.23
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	18	0.23
(1,850)	1:A:362:HIS:HA	1:A:363:ILE:HB	11	0.23
(1,841)	1:A:274:SER:HG	1:A:275:ILE:H	14	0.23
(1,828)	1:A:348:TYR:H	1:A:348:TYR:HD1	11	0.23
(1,778)	1:A:347:CYS:HG	1:A:359:MET:H	7	0.23
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	4	0.23
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	8	0.23
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	14	0.23
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	14	0.23
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	1	0.23
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	18	0.23
(1,563)	1:A:280:LEU:H	1:A:280:LEU:HG	5	0.23
(1,526)	1:A:342:THR:H	1:A:342:THR:HB	9	0.23
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	7	0.23
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	17	0.23
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	17	0.23
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	17	0.23
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	1	0.23
(1,1082)	2:B:786:ILE:HG13	2:B:789:ASP:H	16	0.23
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD21	16	0.23
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD22	16	0.23
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD23	16	0.23
(1,1048)	1:A:300:PHE:HB3	2:B:796:PRO:HA	2	0.23
(1,1041)	2:B:795:LEU:H	2:B:795:LEU:HG	17	0.23
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	14	0.23
(1,1018)	2:B:812:GLU:H	2:B:812:GLU:HB3	3	0.23
(3,53)	1:A:319:THR:H	1:A:315:GLN:O	1	0.22
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG21	4	0.22
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG22	4	0.22
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG23	4	0.22
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	6	0.22
(1,885)	1:A:302:PRO:HB3	1:A:303:GLN:H	16	0.22
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	9	0.22
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	5	0.22
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	1	0.22
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	13	0.22
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	2	0.22
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	2	0.22
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	7	0.22
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	16	0.22
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	16	0.22
(1,639)	1:A:338:LEU:HD21	1:A:339:SER:H	13	0.22
(1,639)	1:A:338:LEU:HD22	1:A:339:SER:H	13	0.22
(1,639)	1:A:338:LEU:HD23	1:A:339:SER:H	13	0.22
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	7	0.22
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	8	0.22
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	18	0.22
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	4	0.22
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	10	0.22
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	11	0.22
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	14	0.22
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	20	0.22
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	3	0.22
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	13	0.22
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	20	0.22
(1,1043)	1:A:300:PHE:HB3	2:B:796:PRO:HB3	9	0.22
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD21	16	0.22
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD22	16	0.22
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD23	16	0.22
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD21	16	0.22
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD22	16	0.22
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD23	16	0.22
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD21	16	0.22
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD22	16	0.22
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD23	16	0.22
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD11	10	0.22
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD12	10	0.22
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD13	10	0.22
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD21	10	0.22
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD22	10	0.22
(1,1031)	1:A:292:VAL:HB	2:B:806:LEU:HD23	10	0.22
(1,1025)	1:A:275:ILE:HD11	2:B:802:LEU:HD21	5	0.22
(1,1025)	1:A:275:ILE:HD11	2:B:802:LEU:HD22	5	0.22
(1,1025)	1:A:275:ILE:HD11	2:B:802:LEU:HD23	5	0.22
(1,1025)	1:A:275:ILE:HD12	2:B:802:LEU:HD21	5	0.22
(1,1025)	1:A:275:ILE:HD12	2:B:802:LEU:HD22	5	0.22
(1,1025)	1:A:275:ILE:HD12	2:B:802:LEU:HD23	5	0.22
(1,1025)	1:A:275:ILE:HD13	2:B:802:LEU:HD21	5	0.22
(1,1025)	1:A:275:ILE:HD13	2:B:802:LEU:HD22	5	0.22
(1,1025)	1:A:275:ILE:HD13	2:B:802:LEU:HD23	5	0.22
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	19	0.21
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	1	0.21
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	1	0.21
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	1	0.21
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	1	0.21
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	1	0.21
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	1	0.21
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	1	0.21
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	1	0.21
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	1	0.21
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	4	0.21
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	8	0.21
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	9	0.21
(1,524)	1:A:341:HIS:HB2	1:A:342:THR:H	18	0.21
(1,524)	1:A:341:HIS:HB2	1:A:342:THR:H	20	0.21
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	20	0.21
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	14	0.21
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	3	0.21
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	12	0.21
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	17	0.21
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	19	0.21
(1,1097)	2:B:788:GLU:HA	2:B:790:ILE:H	16	0.21
(1,1063)	1:A:270:GLY:HA3	2:B:794:LEU:HG	5	0.21
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	12	0.2
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	12	0.2
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	12	0.2
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	3	0.2
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	3	0.2
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	3	0.2
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	11	0.2
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	11	0.2
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	11	0.2
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	11	0.2
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	11	0.2
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	11	0.2
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	7	0.2
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	5	0.2
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	6	0.2
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	17	0.2
(1,821)	1:A:347:CYS:HB2	1:A:356:PRO:HA	10	0.2
(1,789)	1:A:280:LEU:HD21	1:A:291:LEU:HD11	18	0.2
(1,789)	1:A:280:LEU:HD21	1:A:291:LEU:HD12	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,789)	1:A:280:LEU:HD21	1:A:291:LEU:HD13	18	0.2
(1,789)	1:A:280:LEU:HD22	1:A:291:LEU:HD11	18	0.2
(1,789)	1:A:280:LEU:HD22	1:A:291:LEU:HD12	18	0.2
(1,789)	1:A:280:LEU:HD22	1:A:291:LEU:HD13	18	0.2
(1,789)	1:A:280:LEU:HD23	1:A:291:LEU:HD11	18	0.2
(1,789)	1:A:280:LEU:HD23	1:A:291:LEU:HD12	18	0.2
(1,789)	1:A:280:LEU:HD23	1:A:291:LEU:HD13	18	0.2
(1,728)	1:A:330:PHE:H	1:A:330:PHE:HE2	19	0.2
(1,639)	1:A:338:LEU:HD21	1:A:339:SER:H	1	0.2
(1,639)	1:A:338:LEU:HD22	1:A:339:SER:H	1	0.2
(1,639)	1:A:338:LEU:HD23	1:A:339:SER:H	1	0.2
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	1	0.2
(1,554)	1:A:265:LYS:HD3	1:A:266:GLN:H	9	0.2
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	8	0.2
(1,523)	1:A:325:SER:H	1:A:342:THR:H	20	0.2
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	1	0.2
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	6	0.2
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	15	0.2
(1,382)	1:A:344:CYS:HB3	1:A:345:LYS:H	16	0.2
(1,324)	1:A:372:SER:HB2	1:A:374:GLN:H	19	0.2
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	16	0.2
(1,1121)	1:A:310:ALA:HB1	2:B:794:LEU:HD11	9	0.2
(1,1121)	1:A:310:ALA:HB1	2:B:794:LEU:HD12	9	0.2
(1,1121)	1:A:310:ALA:HB1	2:B:794:LEU:HD13	9	0.2
(1,1121)	1:A:310:ALA:HB2	2:B:794:LEU:HD11	9	0.2
(1,1121)	1:A:310:ALA:HB2	2:B:794:LEU:HD12	9	0.2
(1,1121)	1:A:310:ALA:HB2	2:B:794:LEU:HD13	9	0.2
(1,1121)	1:A:310:ALA:HB3	2:B:794:LEU:HD11	9	0.2
(1,1121)	1:A:310:ALA:HB3	2:B:794:LEU:HD12	9	0.2
(1,1121)	1:A:310:ALA:HB3	2:B:794:LEU:HD13	9	0.2
(1,1060)	1:A:272:ILE:HB	2:B:797:PRO:HG2	11	0.2
(1,1060)	1:A:272:ILE:HB	2:B:797:PRO:HG3	11	0.2
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	19	0.19
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	19	0.19
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	19	0.19
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	19	0.19
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	19	0.19
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	19	0.19
(1,892)	1:A:267:ASP:HA	1:A:357:PHE:HA	18	0.19
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	7	0.19
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	10	0.19
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	13	0.19
(1,828)	1:A:348:TYR:H	1:A:348:TYR:HD1	2	0.19
(1,764)	1:A:321:GLY:HA2	1:A:346:LEU:H	9	0.19
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	3	0.19
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	3	0.19
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	5	0.19
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	5	0.19
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	12	0.19
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	12	0.19
(1,609)	1:A:303:GLN:H	1:A:308:SER:HB3	17	0.19
(1,606)	1:A:263:MET:H	1:A:276:ASP:HB2	5	0.19
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	16	0.19
(1,1146)	2:B:789:ASP:HA	2:B:791:PHE:H	16	0.19
(1,1131)	1:A:356:PRO:HG2	2:B:786:ILE:HD11	16	0.19
(1,1131)	1:A:356:PRO:HG2	2:B:786:ILE:HD12	16	0.19
(1,1131)	1:A:356:PRO:HG2	2:B:786:ILE:HD13	16	0.19
(1,1131)	1:A:356:PRO:HG3	2:B:786:ILE:HD11	16	0.19
(1,1131)	1:A:356:PRO:HG3	2:B:786:ILE:HD12	16	0.19
(1,1131)	1:A:356:PRO:HG3	2:B:786:ILE:HD13	16	0.19
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	9	0.19
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	11	0.19
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	15	0.19
(1,1071)	2:B:785:TRP:H	2:B:785:TRP:HB3	10	0.19
(1,1066)	1:A:277:THR:HG21	2:B:806:LEU:HD21	11	0.19
(1,1066)	1:A:277:THR:HG21	2:B:806:LEU:HD22	11	0.19
(1,1066)	1:A:277:THR:HG21	2:B:806:LEU:HD23	11	0.19
(1,1066)	1:A:277:THR:HG22	2:B:806:LEU:HD21	11	0.19
(1,1066)	1:A:277:THR:HG22	2:B:806:LEU:HD22	11	0.19
(1,1066)	1:A:277:THR:HG22	2:B:806:LEU:HD23	11	0.19
(1,1066)	1:A:277:THR:HG23	2:B:806:LEU:HD21	11	0.19
(1,1066)	1:A:277:THR:HG23	2:B:806:LEU:HD22	11	0.19
(1,1066)	1:A:277:THR:HG23	2:B:806:LEU:HD23	11	0.19
(1,993)	2:B:805:LEU:H	2:B:805:LEU:HG	4	0.18
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	13	0.18
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	14	0.18
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	2	0.18
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	10	0.18
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	17	0.18
(1,854)	1:A:262:PHE:HA	1:A:280:LEU:H	5	0.18
(1,828)	1:A:348:TYR:H	1:A:348:TYR:HD1	15	0.18
(1,803)	1:A:346:LEU:HA	1:A:358:ILE:HA	9	0.18
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	13	0.18
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	13	0.18
(1,619)	1:A:273:ILE:HG12	1:A:274:SER:H	4	0.18
(1,619)	1:A:273:ILE:HG13	1:A:274:SER:H	4	0.18
(1,619)	1:A:273:ILE:HG12	1:A:274:SER:H	12	0.18
(1,619)	1:A:273:ILE:HG13	1:A:274:SER:H	12	0.18
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	19	0.18
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	1	0.18
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	4	0.18
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	12	0.18
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	15	0.18
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	9	0.18
(1,524)	1:A:341:HIS:HB2	1:A:342:THR:H	2	0.18
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	4	0.18
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	16	0.18
(1,412)	1:A:266:GLN:HA	1:A:273:ILE:H	4	0.18
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	9	0.18
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	18	0.18
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	4	0.18
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	11	0.18
(1,120)	1:A:267:ASP:H	1:A:267:ASP:HB3	10	0.18
(1,120)	1:A:267:ASP:H	1:A:267:ASP:HB2	10	0.18
(1,1145)	2:B:788:GLU:HA	2:B:791:PHE:H	9	0.18
(1,1102)	2:B:789:ASP:HB2	2:B:790:ILE:H	19	0.18
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	4	0.18
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	19	0.18
(1,1074)	2:B:785:TRP:HD1	2:B:786:ILE:H	4	0.18
(1,1049)	1:A:300:PHE:HA	2:B:796:PRO:HG3	20	0.18
(1,1047)	1:A:300:PHE:HD2	2:B:797:PRO:HD3	11	0.18
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	9	0.17
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	9	0.17
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	9	0.17
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	2	0.17
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	2	0.17
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	2	0.17
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	2	0.17
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	2	0.17
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	2	0.17
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	15	0.17
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	15	0.17
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	15	0.17
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	15	0.17
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	15	0.17
(1,993)	2:B:805:LEU:H	2:B:805:LEU:HG	16	0.17
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	8	0.17
(1,925)	2:B:800:GLN:HG3	2:B:803:THR:HB	1	0.17
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	4	0.17
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	12	0.17
(1,874)	1:A:266:GLN:HB3	1:A:270:GLY:H	18	0.17
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	20	0.17
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	4	0.17
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	7	0.17
(1,808)	1:A:345:LYS:H	1:A:359:MET:HB2	20	0.17
(1,768)	1:A:348:TYR:H	1:A:349:PRO:HD3	17	0.17
(1,720)	1:A:309:TYR:HD1	1:A:325:SER:HB3	2	0.17
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	17	0.17
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	17	0.17
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD21	9	0.17
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD22	9	0.17
(1,694)	1:A:280:LEU:HD11	1:A:291:LEU:HD23	9	0.17
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD21	9	0.17
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD22	9	0.17
(1,694)	1:A:280:LEU:HD12	1:A:291:LEU:HD23	9	0.17
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD21	9	0.17
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD22	9	0.17
(1,694)	1:A:280:LEU:HD13	1:A:291:LEU:HD23	9	0.17
(1,608)	1:A:303:GLN:H	1:A:303:GLN:HE21	17	0.17
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	3	0.17
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	12	0.17
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	17	0.17
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	2	0.17
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	3	0.17
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	5	0.17
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	8	0.17
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	18	0.17
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	16	0.17
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	18	0.17
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	3	0.17
(1,205)	1:A:327:SER:HA	1:A:341:HIS:H	18	0.17
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	6	0.17
(1,1154)	2:B:786:ILE:H	2:B:788:GLU:H	17	0.17
(1,1145)	2:B:788:GLU:HA	2:B:791:PHE:H	3	0.17
(1,1125)	1:A:358:ILE:HB	2:B:790:ILE:HG21	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1125)	1:A:358:ILE:HB	2:B:790:ILE:HG22	18	0.17
(1,1125)	1:A:358:ILE:HB	2:B:790:ILE:HG23	18	0.17
(1,1097)	2:B:788:GLU:HA	2:B:790:ILE:H	5	0.17
(1,1080)	2:B:786:ILE:HG12	2:B:788:GLU:H	10	0.17
(1,1061)	1:A:272:ILE:HB	2:B:797:PRO:HB3	2	0.17
(3,55)	1:A:328:TYR:H	1:A:340:ALA:O	18	0.16
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD11	15	0.16
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD12	15	0.16
(2,67)	1:A:314:PHE:HA	2:B:786:ILE:HD13	15	0.16
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	12	0.16
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	12	0.16
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	12	0.16
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	12	0.16
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	12	0.16
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	12	0.16
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	1	0.16
(1,939)	2:B:801:ASP:HA	2:B:804:LYS:H	17	0.16
(1,892)	1:A:267:ASP:HA	1:A:357:PHE:HA	10	0.16
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	14	0.16
(1,803)	1:A:346:LEU:HA	1:A:358:ILE:HA	3	0.16
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	2	0.16
(1,68)	1:A:300:PHE:HA	1:A:311:ARG:H	9	0.16
(1,639)	1:A:338:LEU:HD21	1:A:339:SER:H	7	0.16
(1,639)	1:A:338:LEU:HD22	1:A:339:SER:H	7	0.16
(1,639)	1:A:338:LEU:HD23	1:A:339:SER:H	7	0.16
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	2	0.16
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	11	0.16
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	13	0.16
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	14	0.16
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	15	0.16
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	2	0.16
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	6	0.16
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	10	0.16
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	9	0.16
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	19	0.16
(1,1154)	2:B:786:ILE:H	2:B:788:GLU:H	14	0.16
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	14	0.16
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	14	0.16
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	14	0.16
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	5	0.16
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	8	0.16
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1074)	2:B:785:TRP:HD1	2:B:786:ILE:H	8	0.16
(1,1053)	1:A:296:ILE:HG21	2:B:797:PRO:HD3	18	0.16
(1,1053)	1:A:296:ILE:HG22	2:B:797:PRO:HD3	18	0.16
(1,1053)	1:A:296:ILE:HG23	2:B:797:PRO:HD3	18	0.16
(1,1030)	1:A:289:GLU:HG3	2:B:806:LEU:HB3	17	0.16
(3,63)	1:A:340:ALA:H	1:A:328:TYR:O	15	0.15
(3,55)	1:A:328:TYR:H	1:A:340:ALA:O	5	0.15
(3,41)	1:A:310:ALA:H	1:A:299:PHE:O	5	0.15
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	14	0.15
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	14	0.15
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	14	0.15
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	14	0.15
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	14	0.15
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	14	0.15
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	3	0.15
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	19	0.15
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	19	0.15
(1,904)	2:B:799:GLU:HA	2:B:802:LEU:H	16	0.15
(1,887)	1:A:266:GLN:H	1:A:358:ILE:HB	4	0.15
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	1	0.15
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	5	0.15
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	13	0.15
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	19	0.15
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	3	0.15
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	11	0.15
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	4	0.15
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	8	0.15
(1,809)	1:A:345:LYS:HB3	1:A:359:MET:H	16	0.15
(1,808)	1:A:345:LYS:H	1:A:359:MET:HB2	4	0.15
(1,808)	1:A:345:LYS:H	1:A:359:MET:HB2	5	0.15
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	5	0.15
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	8	0.15
(1,719)	1:A:309:TYR:HD2	1:A:310:ALA:H	5	0.15
(1,639)	1:A:338:LEU:HD21	1:A:339:SER:H	16	0.15
(1,639)	1:A:338:LEU:HD22	1:A:339:SER:H	16	0.15
(1,639)	1:A:338:LEU:HD23	1:A:339:SER:H	16	0.15
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	6	0.15
(1,564)	1:A:371:LEU:H	1:A:371:LEU:HG	3	0.15
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	7	0.15
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	11	0.15
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	13	0.15
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	19	0.15
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	6	0.15
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	11	0.15
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	13	0.15
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	15	0.15
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	16	0.15
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	7	0.15
(1,344)	1:A:297:TYR:HA	1:A:299:PHE:H	5	0.15
(1,205)	1:A:327:SER:HA	1:A:341:HIS:H	5	0.15
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	12	0.15
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	16	0.15
(1,120)	1:A:267:ASP:H	1:A:267:ASP:HB3	13	0.15
(1,120)	1:A:267:ASP:H	1:A:267:ASP:HB2	13	0.15
(1,1139)	1:A:314:PHE:HB3	2:B:794:LEU:HG	1	0.15
(1,1135)	2:B:794:LEU:HD11	1:A:300:PHE:HE1	9	0.15
(1,1135)	2:B:794:LEU:HD11	1:A:300:PHE:HE2	9	0.15
(1,1135)	2:B:794:LEU:HD12	1:A:300:PHE:HE1	9	0.15
(1,1135)	2:B:794:LEU:HD12	1:A:300:PHE:HE2	9	0.15
(1,1135)	2:B:794:LEU:HD13	1:A:300:PHE:HE1	9	0.15
(1,1135)	2:B:794:LEU:HD13	1:A:300:PHE:HE2	9	0.15
(1,1135)	2:B:794:LEU:HD11	1:A:300:PHE:HE1	9	0.15
(1,1135)	2:B:794:LEU:HD11	1:A:300:PHE:HE2	9	0.15
(1,1135)	2:B:794:LEU:HD12	1:A:300:PHE:HE1	9	0.15
(1,1135)	2:B:794:LEU:HD12	1:A:300:PHE:HE2	9	0.15
(1,1135)	2:B:794:LEU:HD13	1:A:300:PHE:HE1	9	0.15
(1,1135)	2:B:794:LEU:HD13	1:A:300:PHE:HE2	9	0.15
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD11	2	0.15
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD12	2	0.15
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD13	2	0.15
(1,1101)	2:B:789:ASP:H	2:B:790:ILE:H	8	0.15
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	7	0.15
(1,1063)	1:A:270:GLY:HA3	2:B:794:LEU:HG	7	0.15
(1,1063)	1:A:270:GLY:HA3	2:B:794:LEU:HG	15	0.15
(1,1062)	1:A:270:GLY:HA2	2:B:794:LEU:HD11	19	0.15
(1,1062)	1:A:270:GLY:HA2	2:B:794:LEU:HD12	19	0.15
(1,1062)	1:A:270:GLY:HA2	2:B:794:LEU:HD13	19	0.15
(1,1062)	1:A:270:GLY:HA3	2:B:794:LEU:HD21	19	0.15
(1,1062)	1:A:270:GLY:HA3	2:B:794:LEU:HD22	19	0.15
(1,1062)	1:A:270:GLY:HA3	2:B:794:LEU:HD23	19	0.15
(1,1061)	1:A:272:ILE:HB	2:B:797:PRO:HB3	18	0.15
(1,1055)	1:A:274:SER:HA	2:B:805:LEU:HG	8	0.15
(1,1049)	1:A:300:PHE:HA	2:B:796:PRO:HG3	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1027)	1:A:293:ARG:HD2	2:B:802:LEU:HD11	9	0.15
(1,1027)	1:A:293:ARG:HD2	2:B:802:LEU:HD12	9	0.15
(1,1027)	1:A:293:ARG:HD2	2:B:802:LEU:HD13	9	0.15
(1,1027)	1:A:293:ARG:HD3	2:B:802:LEU:HD11	9	0.15
(1,1027)	1:A:293:ARG:HD3	2:B:802:LEU:HD12	9	0.15
(1,1027)	1:A:293:ARG:HD3	2:B:802:LEU:HD13	9	0.15
(1,1018)	2:B:812:GLU:H	2:B:812:GLU:HB3	10	0.15
(3,41)	1:A:310:ALA:H	1:A:299:PHE:O	9	0.14
(2,61)	1:A:346:LEU:HA	2:B:790:ILE:HG21	4	0.14
(2,61)	1:A:346:LEU:HA	2:B:790:ILE:HG22	4	0.14
(2,61)	1:A:346:LEU:HA	2:B:790:ILE:HG23	4	0.14
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG21	20	0.14
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG22	20	0.14
(2,58)	1:A:314:PHE:HA	2:B:786:ILE:HG23	20	0.14
(2,38)	2:B:793:PRO:HD2	2:B:795:LEU:H	17	0.14
(2,38)	2:B:793:PRO:HD3	2:B:795:LEU:H	17	0.14
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD21	18	0.14
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD22	18	0.14
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD23	18	0.14
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD11	18	0.14
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD12	18	0.14
(2,26)	2:B:800:GLN:HE22	2:B:802:LEU:HD13	18	0.14
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	14	0.14
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	3	0.14
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	7	0.14
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	8	0.14
(1,921)	2:B:800:GLN:H	2:B:800:GLN:HE21	10	0.14
(1,877)	1:A:267:ASP:HB2	1:A:269:THR:H	14	0.14
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	3	0.14
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	7	0.14
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	1	0.14
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	16	0.14
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	1	0.14
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	2	0.14
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	12	0.14
(1,808)	1:A:345:LYS:H	1:A:359:MET:HB2	10	0.14
(1,803)	1:A:346:LEU:HA	1:A:358:ILE:HA	10	0.14
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	6	0.14
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	14	0.14
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	16	0.14
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	20	0.14
(1,733)	1:A:326:PRO:HG2	1:A:327:SER:H	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,698)	1:A:316:GLU:HG3	1:A:322:THR:H	20	0.14
(1,639)	1:A:338:LEU:HD21	1:A:339:SER:H	19	0.14
(1,639)	1:A:338:LEU:HD22	1:A:339:SER:H	19	0.14
(1,639)	1:A:338:LEU:HD23	1:A:339:SER:H	19	0.14
(1,586)	1:A:264:THR:H	1:A:362:HIS:HD2	10	0.14
(1,564)	1:A:371:LEU:H	1:A:371:LEU:HG	14	0.14
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	3	0.14
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	14	0.14
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	3	0.14
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	7	0.14
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	10	0.14
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	11	0.14
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	13	0.14
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	14	0.14
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	17	0.14
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	10	0.14
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	14	0.14
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	17	0.14
(1,46)	1:A:268:THR:H	1:A:270:GLY:H	20	0.14
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	10	0.14
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	13	0.14
(1,457)	1:A:309:TYR:HB3	1:A:310:ALA:H	2	0.14
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	7	0.14
(1,288)	1:A:329:ARG:HB2	1:A:330:PHE:H	5	0.14
(1,212)	1:A:261:SER:H	1:A:261:SER:HB3	19	0.14
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD11	14	0.14
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD12	14	0.14
(1,1128)	1:A:346:LEU:HB3	2:B:790:ILE:HD13	14	0.14
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG21	5	0.14
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG22	5	0.14
(1,1122)	1:A:358:ILE:HB	2:B:786:ILE:HG23	5	0.14
(1,1063)	1:A:270:GLY:HA3	2:B:794:LEU:HG	14	0.14
(1,1018)	2:B:812:GLU:H	2:B:812:GLU:HB3	17	0.14
(3,55)	1:A:328:TYR:H	1:A:340:ALA:O	2	0.13
(3,41)	1:A:310:ALA:H	1:A:299:PHE:O	18	0.13
(3,41)	1:A:310:ALA:H	1:A:299:PHE:O	20	0.13
(3,39)	1:A:301:GLN:H	1:A:298:ALA:O	4	0.13
(3,39)	1:A:301:GLN:H	1:A:298:ALA:O	14	0.13
(1,993)	2:B:805:LEU:H	2:B:805:LEU:HG	5	0.13
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	10	0.13
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	12	0.13
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	6	0.13
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	18	0.13
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	20	0.13
(1,903)	2:B:799:GLU:H	2:B:801:ASP:H	8	0.13
(1,892)	1:A:267:ASP:HA	1:A:357:PHE:HA	7	0.13
(1,892)	1:A:267:ASP:HA	1:A:357:PHE:HA	17	0.13
(1,884)	1:A:302:PRO:HB2	1:A:304:GLY:H	14	0.13
(1,871)	1:A:266:GLN:HA	1:A:272:ILE:HA	4	0.13
(1,871)	1:A:266:GLN:HA	1:A:272:ILE:HA	7	0.13
(1,871)	1:A:266:GLN:HA	1:A:272:ILE:HA	12	0.13
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	4	0.13
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	10	0.13
(1,867)	1:A:266:GLN:HA	1:A:272:ILE:HA	4	0.13
(1,867)	1:A:266:GLN:HA	1:A:272:ILE:HA	7	0.13
(1,867)	1:A:266:GLN:HA	1:A:272:ILE:HA	12	0.13
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	15	0.13
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	16	0.13
(1,808)	1:A:345:LYS:H	1:A:359:MET:HB2	17	0.13
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	1	0.13
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	2	0.13
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	3	0.13
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	4	0.13
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	7	0.13
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	11	0.13
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	12	0.13
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	13	0.13
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	17	0.13
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	18	0.13
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	19	0.13
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	5	0.13
(1,527)	1:A:341:HIS:HA	1:A:342:THR:H	20	0.13
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	1	0.13
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	6	0.13
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	12	0.13
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	19	0.13
(1,523)	1:A:325:SER:H	1:A:342:THR:H	8	0.13
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	7	0.13
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	19	0.13
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	6	0.13
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	14	0.13
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	20	0.13
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	10	0.13
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	11	0.13
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	12	0.13
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	19	0.13
(1,421)	1:A:343:ARG:H	1:A:344:CYS:H	8	0.13
(1,415)	1:A:310:ALA:HA	1:A:313:LEU:H	2	0.13
(1,412)	1:A:266:GLN:HA	1:A:273:ILE:H	6	0.13
(1,412)	1:A:266:GLN:HA	1:A:273:ILE:H	7	0.13
(1,412)	1:A:266:GLN:HA	1:A:273:ILE:H	11	0.13
(1,382)	1:A:344:CYS:HB3	1:A:345:LYS:H	14	0.13
(1,1154)	2:B:786:ILE:H	2:B:788:GLU:H	12	0.13
(1,1145)	2:B:788:GLU:HA	2:B:791:PHE:H	7	0.13
(1,1139)	1:A:314:PHE:HB3	2:B:794:LEU:HG	15	0.13
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD11	17	0.13
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD12	17	0.13
(1,1120)	1:A:310:ALA:HA	2:B:794:LEU:HD13	17	0.13
(1,1101)	2:B:789:ASP:H	2:B:790:ILE:H	13	0.13
(1,1096)	2:B:788:GLU:HB3	2:B:790:ILE:H	17	0.13
(1,1061)	1:A:272:ILE:HB	2:B:797:PRO:HB3	20	0.13
(3,63)	1:A:340:ALA:H	1:A:328:TYR:O	6	0.12
(3,63)	1:A:340:ALA:H	1:A:328:TYR:O	8	0.12
(3,39)	1:A:301:GLN:H	1:A:298:ALA:O	1	0.12
(3,39)	1:A:301:GLN:H	1:A:298:ALA:O	3	0.12
(3,39)	1:A:301:GLN:H	1:A:298:ALA:O	10	0.12
(3,39)	1:A:301:GLN:H	1:A:298:ALA:O	11	0.12
(3,39)	1:A:301:GLN:H	1:A:298:ALA:O	12	0.12
(3,39)	1:A:301:GLN:H	1:A:298:ALA:O	16	0.12
(3,11)	1:A:267:ASP:H	1:A:271:LYS:O	14	0.12
(3,11)	1:A:267:ASP:H	1:A:271:LYS:O	19	0.12
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG21	2	0.12
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG22	2	0.12
(2,43)	1:A:314:PHE:HA	2:B:786:ILE:HG23	2	0.12
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	1	0.12
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	4	0.12
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	9	0.12
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	10	0.12
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	11	0.12
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	13	0.12
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	14	0.12
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	15	0.12
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	16	0.12
(1,94)	1:A:289:GLU:HA	1:A:292:VAL:H	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	2:B:801:ASP:HA	2:B:804:LYS:H	2	0.12
(1,939)	2:B:801:ASP:HA	2:B:804:LYS:H	18	0.12
(1,892)	1:A:267:ASP:HA	1:A:357:PHE:HA	8	0.12
(1,887)	1:A:266:GLN:H	1:A:358:ILE:HB	1	0.12
(1,887)	1:A:266:GLN:H	1:A:358:ILE:HB	6	0.12
(1,887)	1:A:266:GLN:H	1:A:358:ILE:HB	20	0.12
(1,879)	1:A:302:PRO:HA	1:A:307:PRO:HA	6	0.12
(1,877)	1:A:267:ASP:HB2	1:A:269:THR:H	5	0.12
(1,877)	1:A:267:ASP:HB2	1:A:269:THR:H	20	0.12
(1,875)	1:A:266:GLN:HB3	1:A:271:LYS:H	15	0.12
(1,871)	1:A:266:GLN:HA	1:A:272:ILE:HA	2	0.12
(1,871)	1:A:266:GLN:HA	1:A:272:ILE:HA	13	0.12
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	14	0.12
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	16	0.12
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	17	0.12
(1,867)	1:A:266:GLN:HA	1:A:272:ILE:HA	2	0.12
(1,867)	1:A:266:GLN:HA	1:A:272:ILE:HA	13	0.12
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	6	0.12
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	7	0.12
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	9	0.12
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	11	0.12
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	14	0.12
(1,847)	1:A:362:HIS:H	1:A:363:ILE:HA	8	0.12
(1,808)	1:A:345:LYS:H	1:A:359:MET:HB2	18	0.12
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	9	0.12
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	10	0.12
(1,743)	1:A:332:LEU:HB2	1:A:336:THR:HB	15	0.12
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB2	10	0.12
(1,711)	1:A:309:TYR:HB2	1:A:325:SER:HB3	10	0.12
(1,68)	1:A:300:PHE:HA	1:A:311:ARG:H	2	0.12
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	4	0.12
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	5	0.12
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	15	0.12
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	20	0.12
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	12	0.12
(1,46)	1:A:268:THR:H	1:A:270:GLY:H	14	0.12
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	5	0.12
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	8	0.12
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	11	0.12
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	13	0.12
(1,421)	1:A:343:ARG:H	1:A:344:CYS:H	12	0.12
(1,412)	1:A:266:GLN:HA	1:A:273:ILE:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:A:323:ALA:H	1:A:344:CYS:H	2	0.12
(1,265)	1:A:321:GLY:HA3	1:A:346:LEU:H	8	0.12
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	1	0.12
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	5	0.12
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	7	0.12
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	8	0.12
(1,176)	1:A:328:TYR:H	1:A:340:ALA:H	5	0.12
(1,176)	1:A:328:TYR:H	1:A:340:ALA:H	18	0.12
(1,1160)	2:B:789:ASP:H	2:B:791:PHE:H	3	0.12
(1,1155)	2:B:786:ILE:HA	2:B:788:GLU:H	19	0.12
(1,1147)	2:B:789:ASP:H	2:B:791:PHE:H	3	0.12
(1,1121)	1:A:310:ALA:HB1	2:B:794:LEU:HD11	18	0.12
(1,1121)	1:A:310:ALA:HB1	2:B:794:LEU:HD12	18	0.12
(1,1121)	1:A:310:ALA:HB1	2:B:794:LEU:HD13	18	0.12
(1,1121)	1:A:310:ALA:HB2	2:B:794:LEU:HD11	18	0.12
(1,1121)	1:A:310:ALA:HB2	2:B:794:LEU:HD12	18	0.12
(1,1121)	1:A:310:ALA:HB2	2:B:794:LEU:HD13	18	0.12
(1,1121)	1:A:310:ALA:HB3	2:B:794:LEU:HD11	18	0.12
(1,1121)	1:A:310:ALA:HB3	2:B:794:LEU:HD12	18	0.12
(1,1121)	1:A:310:ALA:HB3	2:B:794:LEU:HD13	18	0.12
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	6	0.12
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	10	0.12
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	11	0.12
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	15	0.12
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	20	0.12
(1,1090)	2:B:788:GLU:H	2:B:788:GLU:HB3	2	0.12
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD11	19	0.12
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD12	19	0.12
(1,1054)	1:A:296:ILE:HB	2:B:802:LEU:HD13	19	0.12
(1,1053)	1:A:296:ILE:HG21	2:B:797:PRO:HD3	4	0.12
(1,1053)	1:A:296:ILE:HG22	2:B:797:PRO:HD3	4	0.12
(1,1053)	1:A:296:ILE:HG23	2:B:797:PRO:HD3	4	0.12
(1,1043)	1:A:300:PHE:HB3	2:B:796:PRO:HB3	4	0.12
(3,73)	1:A:357:PHE:H	1:A:347:CYS:O	16	0.11
(3,55)	1:A:328:TYR:H	1:A:340:ALA:O	16	0.11
(3,54)	1:A:319:THR:N	1:A:315:GLN:O	16	0.11
(3,47)	1:A:315:GLN:H	1:A:311:ARG:O	1	0.11
(3,45)	1:A:314:PHE:H	1:A:310:ALA:O	5	0.11
(3,39)	1:A:301:GLN:H	1:A:298:ALA:O	2	0.11
(3,39)	1:A:301:GLN:H	1:A:298:ALA:O	5	0.11
(3,39)	1:A:301:GLN:H	1:A:298:ALA:O	9	0.11
(3,39)	1:A:301:GLN:H	1:A:298:ALA:O	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,13)	1:A:270:GLY:H	1:A:267:ASP:O	20	0.11
(3,11)	1:A:267:ASP:H	1:A:271:LYS:O	4	0.11
(3,11)	1:A:267:ASP:H	1:A:271:LYS:O	5	0.11
(3,11)	1:A:267:ASP:H	1:A:271:LYS:O	12	0.11
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG21	14	0.11
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG22	14	0.11
(2,60)	1:A:357:PHE:HB3	2:B:790:ILE:HG23	14	0.11
(1,955)	2:B:802:LEU:H	2:B:802:LEU:HG	5	0.11
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	4	0.11
(1,947)	2:B:802:LEU:H	2:B:803:THR:HB	16	0.11
(1,937)	2:B:801:ASP:H	2:B:803:THR:H	17	0.11
(1,905)	2:B:798:THR:H	2:B:799:GLU:H	4	0.11
(1,905)	2:B:798:THR:H	2:B:799:GLU:H	11	0.11
(1,905)	2:B:798:THR:H	2:B:799:GLU:H	15	0.11
(1,905)	2:B:798:THR:H	2:B:799:GLU:H	16	0.11
(1,903)	2:B:799:GLU:H	2:B:801:ASP:H	3	0.11
(1,903)	2:B:799:GLU:H	2:B:801:ASP:H	12	0.11
(1,892)	1:A:267:ASP:HA	1:A:357:PHE:HA	13	0.11
(1,887)	1:A:266:GLN:H	1:A:358:ILE:HB	5	0.11
(1,887)	1:A:266:GLN:H	1:A:358:ILE:HB	8	0.11
(1,887)	1:A:266:GLN:H	1:A:358:ILE:HB	16	0.11
(1,887)	1:A:266:GLN:H	1:A:358:ILE:HB	19	0.11
(1,879)	1:A:302:PRO:HA	1:A:307:PRO:HA	9	0.11
(1,875)	1:A:266:GLN:HB3	1:A:271:LYS:H	1	0.11
(1,875)	1:A:266:GLN:HB3	1:A:271:LYS:H	5	0.11
(1,875)	1:A:266:GLN:HB3	1:A:271:LYS:H	14	0.11
(1,871)	1:A:266:GLN:HA	1:A:272:ILE:HA	5	0.11
(1,871)	1:A:266:GLN:HA	1:A:272:ILE:HA	6	0.11
(1,871)	1:A:266:GLN:HA	1:A:272:ILE:HA	17	0.11
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	2	0.11
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	8	0.11
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	9	0.11
(1,87)	1:A:262:PHE:H	1:A:361:ILE:HA	15	0.11
(1,867)	1:A:266:GLN:HA	1:A:272:ILE:HA	5	0.11
(1,867)	1:A:266:GLN:HA	1:A:272:ILE:HA	6	0.11
(1,867)	1:A:266:GLN:HA	1:A:272:ILE:HA	17	0.11
(1,865)	1:A:265:LYS:HA	1:A:359:MET:HA	5	0.11
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	3	0.11
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	13	0.11
(1,864)	1:A:265:LYS:HA	1:A:358:ILE:H	17	0.11
(1,847)	1:A:362:HIS:H	1:A:363:ILE:HA	16	0.11
(1,764)	1:A:321:GLY:HA2	1:A:346:LEU:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:A:300:PHE:HA	1:A:311:ARG:H	6	0.11
(1,525)	1:A:342:THR:H	1:A:343:ARG:H	8	0.11
(1,523)	1:A:325:SER:H	1:A:342:THR:H	2	0.11
(1,523)	1:A:325:SER:H	1:A:342:THR:H	4	0.11
(1,523)	1:A:325:SER:H	1:A:342:THR:H	12	0.11
(1,523)	1:A:325:SER:H	1:A:342:THR:H	15	0.11
(1,514)	1:A:264:THR:HA	1:A:274:SER:H	5	0.11
(1,514)	1:A:264:THR:HA	1:A:274:SER:H	7	0.11
(1,513)	1:A:265:LYS:H	1:A:274:SER:H	4	0.11
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	1	0.11
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	3	0.11
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	12	0.11
(1,459)	1:A:310:ALA:H	1:A:312:GLN:H	17	0.11
(1,44)	1:A:268:THR:H	1:A:357:PHE:HA	8	0.11
(1,421)	1:A:343:ARG:H	1:A:344:CYS:H	15	0.11
(1,420)	1:A:344:CYS:H	1:A:345:LYS:H	3	0.11
(1,420)	1:A:344:CYS:H	1:A:345:LYS:H	19	0.11
(1,419)	1:A:322:THR:HA	1:A:344:CYS:H	16	0.11
(1,344)	1:A:297:TYR:HA	1:A:299:PHE:H	14	0.11
(1,344)	1:A:297:TYR:HA	1:A:299:PHE:H	18	0.11
(1,301)	1:A:375:ASP:H	1:A:375:ASP:HA	1	0.11
(1,301)	1:A:375:ASP:H	1:A:375:ASP:HA	4	0.11
(1,301)	1:A:375:ASP:H	1:A:375:ASP:HA	5	0.11
(1,301)	1:A:375:ASP:H	1:A:375:ASP:HA	6	0.11
(1,301)	1:A:375:ASP:H	1:A:375:ASP:HA	12	0.11
(1,212)	1:A:261:SER:H	1:A:261:SER:HB3	20	0.11
(1,205)	1:A:327:SER:HA	1:A:341:HIS:H	2	0.11
(1,199)	1:A:268:THR:HA	1:A:270:GLY:H	14	0.11
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	2	0.11
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	3	0.11
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	9	0.11
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	10	0.11
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	13	0.11
(1,190)	1:A:276:ASP:H	1:A:277:THR:HA	14	0.11
(1,1145)	2:B:788:GLU:HA	2:B:791:PHE:H	4	0.11
(1,1136)	2:B:794:LEU:HD11	1:A:311:ARG:HB2	9	0.11
(1,1136)	2:B:794:LEU:HD12	1:A:311:ARG:HB2	9	0.11
(1,1136)	2:B:794:LEU:HD13	1:A:311:ARG:HB2	9	0.11
(1,1136)	2:B:794:LEU:HD11	1:A:311:ARG:HB3	9	0.11
(1,1136)	2:B:794:LEU:HD12	1:A:311:ARG:HB3	9	0.11
(1,1136)	2:B:794:LEU:HD13	1:A:311:ARG:HB3	9	0.11
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD11	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD12	1	0.11
(1,1133)	1:A:346:LEU:HB2	2:B:790:ILE:HD13	1	0.11
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD11	11	0.11
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD12	11	0.11
(1,1130)	1:A:346:LEU:HA	2:B:786:ILE:HD13	11	0.11
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG21	2	0.11
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG22	2	0.11
(1,1126)	1:A:348:TYR:HD1	2:B:786:ILE:HG23	2	0.11
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG21	2	0.11
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG22	2	0.11
(1,1126)	1:A:348:TYR:HD2	2:B:786:ILE:HG23	2	0.11
(1,1101)	2:B:789:ASP:H	2:B:790:ILE:H	2	0.11
(1,1101)	2:B:789:ASP:H	2:B:790:ILE:H	17	0.11
(1,1092)	2:B:788:GLU:HB3	2:B:789:ASP:H	3	0.11
(1,1077)	2:B:786:ILE:H	2:B:786:ILE:HB	16	0.11
(1,1077)	2:B:786:ILE:H	2:B:786:ILE:HB	19	0.11
(1,1071)	2:B:785:TRP:H	2:B:785:TRP:HB3	7	0.11
(1,1061)	1:A:272:ILE:HB	2:B:797:PRO:HB3	8	0.11
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD21	14	0.11
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD22	14	0.11
(1,1052)	1:A:296:ILE:HB	2:B:802:LEU:HD23	14	0.11
(1,1040)	2:B:794:LEU:H	2:B:795:LEU:H	3	0.11
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD21	13	0.11
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD22	13	0.11
(1,1034)	1:A:296:ILE:HD11	2:B:802:LEU:HD23	13	0.11
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD21	13	0.11
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD22	13	0.11
(1,1034)	1:A:296:ILE:HD12	2:B:802:LEU:HD23	13	0.11
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD21	13	0.11
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD22	13	0.11
(1,1034)	1:A:296:ILE:HD13	2:B:802:LEU:HD23	13	0.11
(1,1023)	1:A:275:ILE:HD11	2:B:806:LEU:HG	11	0.11
(1,1023)	1:A:275:ILE:HD12	2:B:806:LEU:HG	11	0.11
(1,1023)	1:A:275:ILE:HD13	2:B:806:LEU:HG	11	0.11
(1,1004)	2:B:807:LEU:H	2:B:807:LEU:HG	20	0.11

10 Dihedral-angle violation analysis

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