Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2LIR / pdb_00002lir
BMRB ID	:	17903
Title	:	NMR Solution Structure of Yeast Iso-1-cytochrome c Mutant P71H in oxidized states
Authors	:	Lan, W.; Wang, Z.; Yang, Z.; Zhu, J.; Ying, T.; Jiang, X.; Zhang, X.; Wu, H.; Liu, M.; Tan, X.; Cao, C.; Huang, Z.X.
Deposited on	:	2011-08-31

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

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

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

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

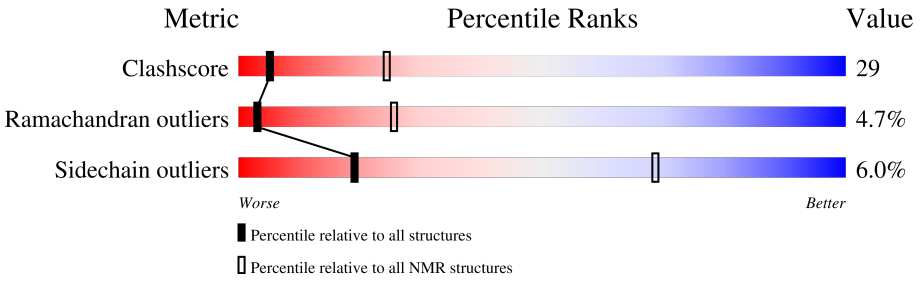
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2.1
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 21%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	108	58% 37%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	A	HEC	104	20	-

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:-3-A:-1, A:1-A:103 (106)	0.78	16

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

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

NmrClust was unable to cluster the ensemble.

Error message: 1 Unexpected character

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1767 atoms, of which 878 are hydrogens and 0 are deuteriums.

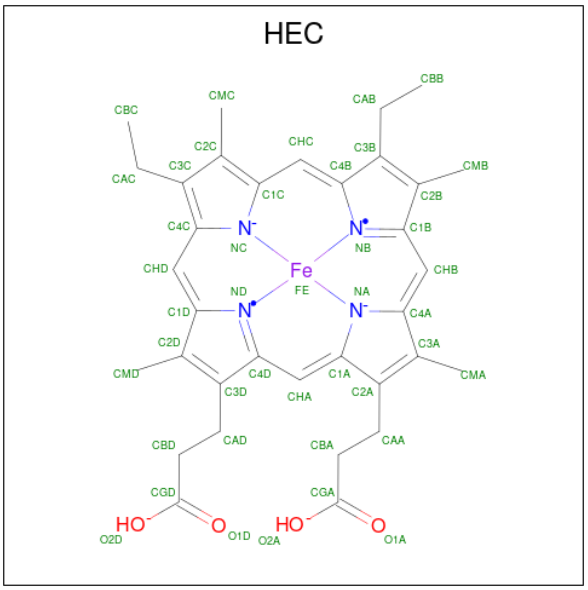
- Molecule 1 is a protein called Cytochrome c iso-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	108	1692	533	846	152	157	4	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	HIS	PRO	engineered mutation	UNP P00044
A	72	ALA	LYS	engineered mutation	UNP P00044
A	102	THR	CYS	engineered mutation	UNP P00044

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					
			Total	C	Fe	H	N	O
2	A	1	75	34	1	32	4	4

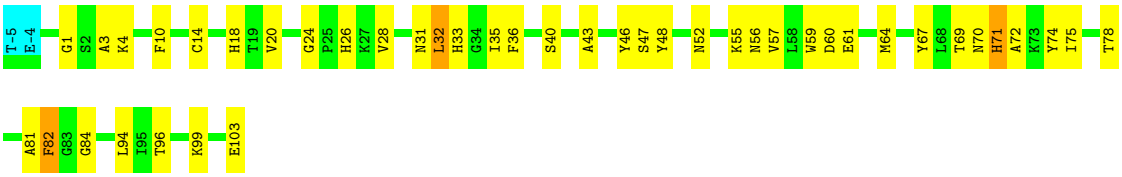
4 Residue-property plots (i)

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: Cytochrome c iso-1

Chain A:



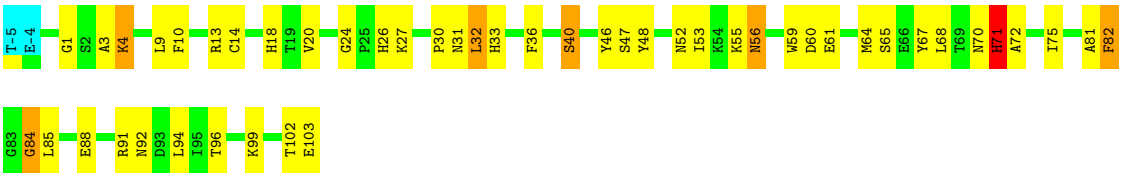
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Cytochrome c iso-1

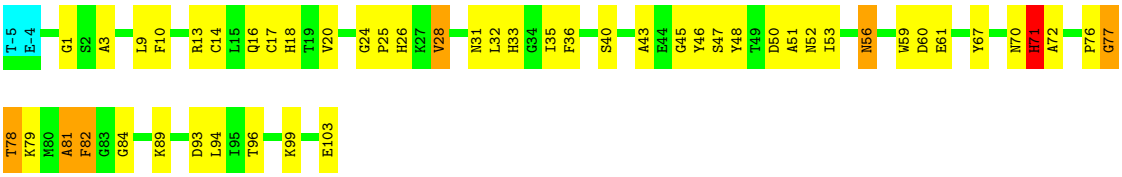
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Cytochrome c iso-1

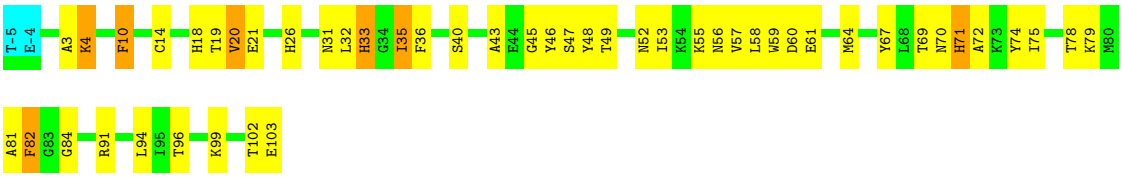
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Cytochrome c iso-1

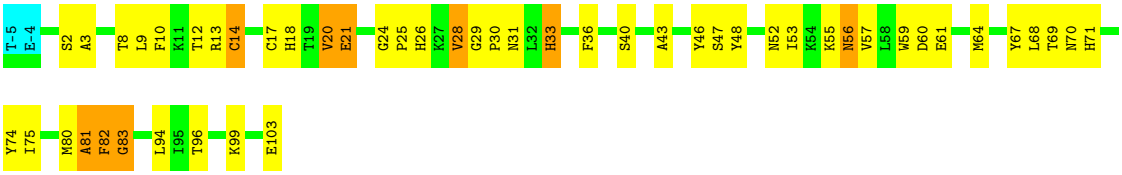
Chain A: 53% 39% 6% •



4.2.4 Score per residue for model 4

- Molecule 1: Cytochrome c iso-1

Chain A: 52% 38% 8% •



4.2.5 Score per residue for model 5

- Molecule 1: Cytochrome c iso-1

Chain A: 61% 32% 5% •

4.2.6 Score per residue for model 6

- Molecule 1: Cytochrome c iso-1

Chain A: 54% 39% 6% •

T-5 E-4 G1 S2 A3 L9 F10 C14 L15 Q16 C17 H18 T19 V20 P25 H26 K27 V28 G29 P30 N31 L32 I35 F36 G37 R38 H39 S40 Y46 S47 Y48 A51 N52 I53 K54 K55 N56 V57 L58 W59 D60 E61 M64 Y67 N70 H71 A72 K73 Y74 I75

P76 G77 T78 K79 M80 A81 L94 I95 T96 K99 T102 E103

4.2.7 Score per residue for model 7

- Molecule 1: Cytochrome c iso-1

Chain A: 55% 40% • • •

T-5 E-4 G1 S2 A3 K4 F10 K11 T12 R13 C14 H18 T19 V20 G24 P25 H26 K27 P30 N31 L32 H33 G34 I35 R38 H39 S40 G41 Q42 A43 E44 G45 Y46 S47 Y48 N52 I53 N56 W59 D60 E61 M64 Y67 N70 H71 A72 K73 Y74

I75 A81 F82 L94 I95 T96 K99 E103

4.2.8 Score per residue for model 8

- Molecule 1: Cytochrome c iso-1

Chain A: 55% 37% 6% •

T-5 E-4 G1 S2 A3 L9 F10 R13 C14 H18 T19 V20 G24 P25 H26 K27 P30 N31 L32 I35 F36 G37 S40 G45 Y46 S47 Y48 N52 K55 N56 V57 L58 W59 D60 E61 M64 Y67 N70 H71 A72 K73 Y74 I75 A81 F82

G83 G84 L85 D90 L94 I95 T96 K99 E103

4.2.9 Score per residue for model 9

- Molecule 1: Cytochrome c iso-1

Chain A: 50% 41% 7% •

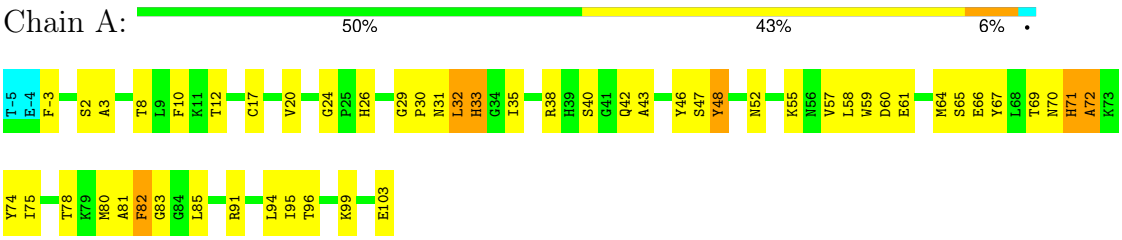
T-5 E-4 A3 K4 K5 G6 A7 F10 C14 C17 H18 T19 V20 H26 N31 L32 H33 G34 I35 F36 G37 S40 A43 E44 G45 Y46 S47 Y48 T49 I53 K54 K55 N56 D60 E61 M64 Y67 L68 T69 N70 H71 A72 I75 T78 K79 M80

A81 F82 G83 G84 L85 E88 R91 N92 D93 L94 I95 T96 Y97 L98 K99 E103

4.2.10 Score per residue for model 10

- Molecule 1: Cytochrome c iso-1

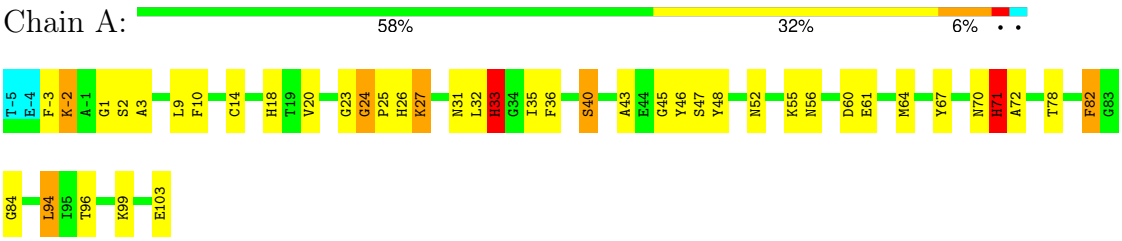
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: Cytochrome c iso-1

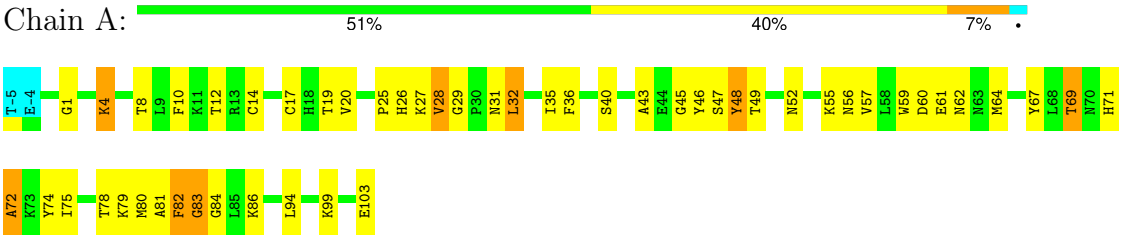
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: Cytochrome c iso-1

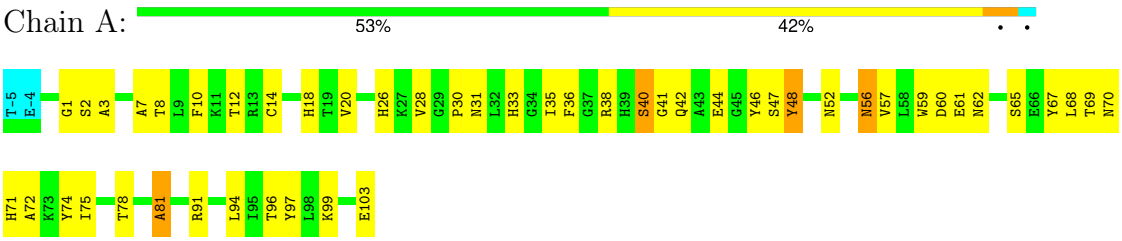
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: Cytochrome c iso-1

Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Cytochrome c iso-1

Chain A: 54% 37% 7% •

T-5 E-4 G1 S2 A3 L9 F10 R13 C14 H18 T19 V20 E21 K22 G23 G24 P25 H26 K27 V28 G29 P30 N31 L32 H33 G34 I35 F36 S40 A43 Y46 S47 Y48 N52 K55 N56 W59 D60 E61 M64 Y67 L68 T69 N70 H71 A72 I75

M80 A81 F82 G83 G84 L85 K86 L94 I95 T96 K99 E103

4.2.15 Score per residue for model 15

• Molecule 1: Cytochrome c iso-1

Chain A: 60% 31% 6% •

T-5 E-4 G1 S2 A3 K4 A7 F10 C14 C17 H18 G24 P25 H26 L32 H33 G34 I35 F36 Y46 S47 Y48 N52 K55 N56 W59 D60 E61 E66 Y67 N70 H71 A72 K73 Y74 I75 T78 K79 M80 A81 F82 L94 I95 T96 Y97

L98 K99 T102 E103

4.2.16 Score per residue for model 16 (medoid)

• Molecule 1: Cytochrome c iso-1

Chain A: 50% 44% 5% •

T-5 E-4 G1 S2 A3 G6 L9 F10 C14 C17 H18 T19 V20 H26 K27 V28 G29 P30 N31 L32 H33 G34 I35 F36 G37 R38 A43 E44 G45 Y46 S47 Y48 T49 N52 K55 N56 V57 L58 W59 D60 E61 Y67 L68 T69 N70 H71 A72 K73 Y74 I75

T78 K79 M80 A81 F82 G83 G84 L85 L94 I95 T96 K99 T102 E103

4.2.17 Score per residue for model 17

• Molecule 1: Cytochrome c iso-1

Chain A: 56% 39% • •

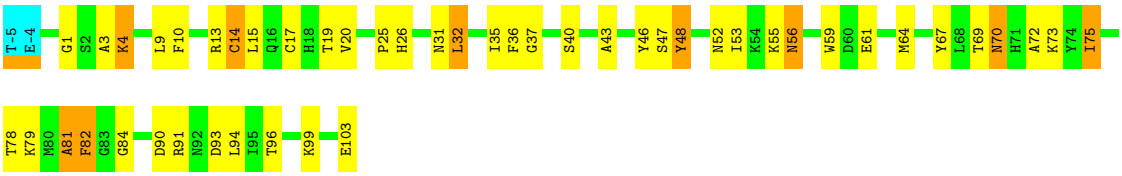
T-5 E-4 F-3 K-2 A-1 G1 S2 A3 K4 F10 C14 C17 H18 T19 V20 H26 N31 L32 H33 G34 I35 F36 S40 A43 E44 G45 Y46 S47 Y48 N52 K55 N56 V57 L58 W59 D60 E61 M64 Y67 L68 T69 N70 H71 A72 I75 T78

A81 F82 G83 G84 L85 K86 R91 L94 I95 T96 K99 E103

4.2.18 Score per residue for model 18

- Molecule 1: Cytochrome c iso-1

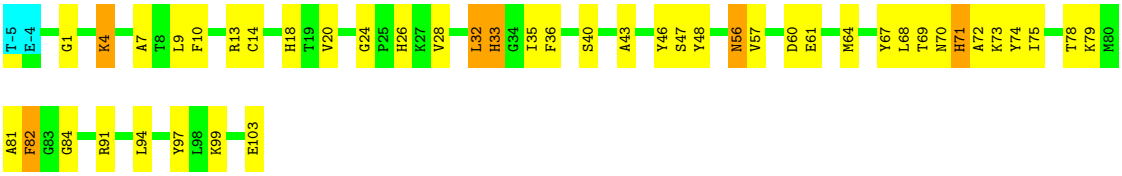
Chain A: 54% 36% 8% •



4.2.19 Score per residue for model 19

- Molecule 1: Cytochrome c iso-1

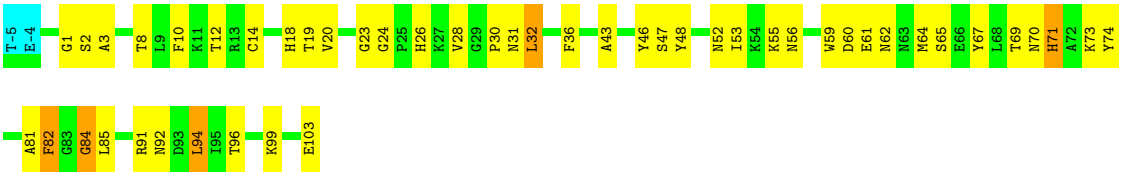
Chain A: 56% 36% 6% •



4.2.20 Score per residue for model 20

- Molecule 1: Cytochrome c iso-1

Chain A: 54% 40% 5% •



5 Refinement protocol and experimental data overview (i)

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
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	616
Number of shifts mapped to atoms	616
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	21%

6 Model quality (i)

6.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.44±0.00	0±0/848 (0.0± 0.0%)	1.21±0.01	1±1/1135 (0.1± 0.1%)
All	All	1.44	0/16960 (0.0%)	1.21	15/22700 (0.1%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	82	PHE	CA-CB-CG	-5.69	108.11	113.80	2	13
1	A	10	PHE	CA-CB-CG	-5.12	108.68	113.80	3	1
1	A	33	HIS	CA-CB-CG	-5.09	108.71	113.80	11	1

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	830	831	828	49±7
2	A	43	32	30	7±3
All	All	17460	17260	17160	998

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ALA:HB1	1:A:78:THR:HG21	0.93	1.37	12	1
1:A:69:THR:HG23	1:A:91:ARG:NH2	0.91	1.80	17	2
1:A:32:LEU:HD11	1:A:35:ILE:HD13	0.85	1.47	19	4
1:A:57:VAL:HG11	1:A:74:TYR:OH	0.83	1.73	16	6
1:A:32:LEU:HD22	1:A:48:TYR:OH	0.83	1.74	5	4
1:A:32:LEU:HD23	1:A:32:LEU:N	0.81	1.90	12	4
1:A:69:THR:HG22	1:A:91:ARG:NH2	0.78	1.92	5	1
1:A:70:ASN:ND2	1:A:80:MET:HE1	0.77	1.94	10	1
1:A:8:THR:O	1:A:12:THR:HG23	0.77	1.80	4	3
1:A:32:LEU:H	1:A:32:LEU:HD22	0.73	1.41	14	1
1:A:4:LYS:H	1:A:4:LYS:HZ3	0.71	1.28	7	1
1:A:4:LYS:HZ3	1:A:4:LYS:N	0.71	1.84	7	1
1:A:43:ALA:HB3	1:A:46:TYR:O	0.71	1.86	10	11
1:A:43:ALA:HB2	1:A:48:TYR:CE1	0.70	2.20	4	10
1:A:81:ALA:HB1	2:A:104:HEC:HBC2	0.70	1.63	7	4
1:A:3:ALA:HB2	1:A:96:THR:HG22	0.69	1.62	20	17
1:A:59:TRP:CE3	1:A:64:MET:SD	0.69	2.85	10	2
1:A:38:ARG:NE	1:A:42:GLN:NE2	0.69	2.41	7	1
1:A:56:ASN:ND2	1:A:56:ASN:N	0.69	2.41	9	1
1:A:46:TYR:CD1	1:A:47:SER:N	0.68	2.62	3	11
1:A:71:HIS:O	1:A:72:ALA:HB3	0.68	1.89	6	3
1:A:71:HIS:O	1:A:72:ALA:HB2	0.68	1.89	12	1
1:A:31:ASN:C	1:A:32:LEU:HD23	0.68	2.14	5	3
1:A:32:LEU:N	1:A:32:LEU:HD22	0.67	2.03	1	2
1:A:36:PHE:CD1	1:A:64:MET:SD	0.67	2.87	11	6
1:A:36:PHE:CE2	1:A:64:MET:SD	0.67	2.87	17	9
1:A:82:PHE:CE2	2:A:104:HEC:HBB2	0.67	2.24	10	1
1:A:36:PHE:CZ	1:A:64:MET:SD	0.66	2.89	17	8
1:A:26:HIS:CE1	1:A:31:ASN:H	0.66	2.09	1	12
1:A:71:HIS:O	1:A:71:HIS:ND1	0.66	2.28	12	1
1:A:82:PHE:CG	1:A:83:GLY:N	0.65	2.61	10	2
1:A:36:PHE:CE1	1:A:64:MET:SD	0.65	2.90	9	10
1:A:80:MET:O	1:A:81:ALA:HB2	0.65	1.92	16	3
1:A:32:LEU:HD12	1:A:35:ILE:HD13	0.65	1.69	14	1
1:A:93:ASP:OD1	1:A:94:LEU:N	0.64	2.30	18	1
1:A:71:HIS:O	1:A:71:HIS:CG	0.64	2.51	12	1
1:A:57:VAL:HG11	1:A:74:TYR:CE1	0.64	2.27	4	1
1:A:20:VAL:O	1:A:33:HIS:CG	0.64	2.51	11	9
1:A:82:PHE:CD1	1:A:83:GLY:N	0.64	2.66	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:PHE:CE1	1:A:20:VAL:HG13	0.63	2.28	14	7
1:A:82:PHE:CD2	1:A:83:GLY:N	0.63	2.66	9	4
1:A:52:ASN:ND2	2:A:104:HEC:CGD	0.63	2.61	15	4
1:A:74:TYR:CZ	1:A:75:ILE:HD11	0.63	2.28	7	1
1:A:46:TYR:CE1	1:A:47:SER:O	0.62	2.52	14	18
1:A:20:VAL:O	1:A:20:VAL:HG12	0.62	1.92	3	2
1:A:4:LYS:H	1:A:4:LYS:NZ	0.62	1.92	7	1
1:A:32:LEU:N	1:A:32:LEU:CD2	0.62	2.63	8	6
1:A:46:TYR:CZ	1:A:47:SER:O	0.62	2.52	10	20
1:A:67:TYR:O	1:A:71:HIS:N	0.62	2.33	12	1
1:A:76:PRO:O	1:A:77:GLY:C	0.62	2.43	2	1
1:A:81:ALA:CB	2:A:104:HEC:HBC2	0.62	2.25	13	1
1:A:7:ALA:HB2	1:A:97:TYR:CD1	0.62	2.30	9	4
1:A:70:ASN:CG	1:A:80:MET:HE1	0.62	2.20	10	1
1:A:10:PHE:CZ	1:A:20:VAL:HG13	0.62	2.30	6	3
1:A:9:LEU:HD11	1:A:13:ARG:HE	0.61	1.55	1	3
1:A:26:HIS:NE2	1:A:46:TYR:N	0.61	2.47	20	5
1:A:48:TYR:CE2	2:A:104:HEC:O1A	0.61	2.53	20	16
1:A:48:TYR:CZ	2:A:104:HEC:O1A	0.61	2.54	14	7
1:A:85:LEU:HD21	1:A:94:LEU:HD12	0.61	1.71	8	3
1:A:18:HIS:CE1	1:A:32:LEU:HD21	0.61	2.31	14	2
1:A:94:LEU:HD21	2:A:104:HEC:CMB	0.61	2.25	9	9
1:A:32:LEU:HD13	1:A:35:ILE:HD13	0.61	1.71	2	2
1:A:19:THR:H	1:A:31:ASN:ND2	0.61	1.94	6	3
1:A:67:TYR:CZ	1:A:71:HIS:O	0.61	2.54	9	7
1:A:70:ASN:HD22	1:A:73:LYS:N	0.60	1.94	20	3
1:A:8:THR:O	1:A:12:THR:HG22	0.60	1.96	13	2
1:A:20:VAL:O	1:A:33:HIS:CD2	0.60	2.54	10	3
1:A:32:LEU:HD11	1:A:48:TYR:OH	0.60	1.96	7	2
1:A:32:LEU:HD22	1:A:32:LEU:H	0.60	1.55	1	1
1:A:52:ASN:HD22	2:A:104:HEC:CGD	0.60	2.09	13	4
1:A:71:HIS:O	1:A:78:THR:HG21	0.60	1.97	11	2
1:A:67:TYR:CE2	2:A:104:HEC:C2A	0.60	2.85	15	9
1:A:67:TYR:CE1	1:A:71:HIS:O	0.60	2.55	1	4
2:A:104:HEC:HBB3	2:A:104:HEC:HMB3	0.60	1.73	1	1
1:A:26:HIS:NE2	1:A:44:GLU:O	0.60	2.35	13	1
1:A:52:ASN:ND2	2:A:104:HEC:O2D	0.59	2.35	2	4
1:A:56:ASN:N	1:A:56:ASN:OD1	0.59	2.36	13	5
1:A:72:ALA:HB3	1:A:80:MET:HE2	0.59	1.73	14	1
1:A:74:TYR:CE2	1:A:75:ILE:CG1	0.59	2.86	7	1
1:A:59:TRP:CE2	2:A:104:HEC:O2A	0.59	2.56	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:HIS:ND1	1:A:81:ALA:C	0.59	2.61	12	1
1:A:26:HIS:HD1	1:A:31:ASN:N	0.59	1.95	7	6
1:A:67:TYR:CE1	2:A:104:HEC:C2A	0.59	2.85	17	5
1:A:50:ASP:OD1	1:A:51:ALA:N	0.59	2.36	2	1
1:A:24:GLY:O	1:A:26:HIS:CD2	0.59	2.56	20	7
1:A:26:HIS:NE2	1:A:45:GLY:C	0.59	2.61	8	10
1:A:33:HIS:CG	1:A:33:HIS:O	0.59	2.54	4	1
1:A:38:ARG:HE	1:A:39:HIS:H	0.59	1.39	7	1
1:A:69:THR:OG1	1:A:91:ARG:NE	0.59	2.36	18	1
1:A:40:SER:OG	1:A:59:TRP:NE1	0.58	2.36	7	2
1:A:26:HIS:ND1	1:A:31:ASN:OD1	0.58	2.36	14	2
1:A:66:GLU:OE1	1:A:74:TYR:CE1	0.58	2.56	15	2
1:A:61:GLU:OE2	1:A:99:LYS:NZ	0.58	2.36	10	6
1:A:40:SER:OG	1:A:59:TRP:CZ2	0.58	2.56	12	2
1:A:69:THR:OG1	1:A:91:ARG:NH1	0.58	2.36	20	4
1:A:40:SER:OG	1:A:59:TRP:CE2	0.58	2.56	12	1
1:A:33:HIS:O	1:A:33:HIS:ND1	0.58	2.37	3	1
1:A:71:HIS:CE1	1:A:81:ALA:O	0.58	2.57	12	1
1:A:32:LEU:HD22	1:A:32:LEU:N	0.58	2.14	14	1
1:A:68:LEU:HD12	1:A:85:LEU:HD23	0.58	1.74	1	1
1:A:72:ALA:HB2	1:A:78:THR:HG22	0.58	1.74	2	1
1:A:53:ILE:O	1:A:56:ASN:ND2	0.58	2.36	9	1
1:A:48:TYR:O	1:A:53:ILE:HD11	0.58	1.99	6	7
1:A:61:GLU:OE1	1:A:99:LYS:NZ	0.58	2.36	4	3
1:A:25:PRO:O	1:A:31:ASN:ND2	0.58	2.37	14	3
1:A:88:GLU:OE1	1:A:91:ARG:NH2	0.57	2.36	1	1
1:A:48:TYR:CE2	2:A:104:HEC:CGA	0.57	2.87	7	1
1:A:10:PHE:CD2	1:A:14:CYS:SG	0.57	2.98	6	5
1:A:43:ALA:CB	1:A:46:TYR:O	0.57	2.53	14	3
1:A:70:ASN:HD22	1:A:73:LYS:H	0.57	1.40	8	3
1:A:4:LYS:CD	1:A:4:LYS:H	0.57	2.13	17	6
1:A:46:TYR:CE2	1:A:47:SER:O	0.57	2.58	2	3
1:A:72:ALA:HB2	1:A:78:THR:OG1	0.57	2.00	13	2
1:A:3:ALA:HB2	1:A:96:THR:CG2	0.57	2.30	11	14
1:A:70:ASN:C	1:A:72:ALA:H	0.57	2.07	14	9
1:A:70:ASN:O	1:A:72:ALA:N	0.56	2.38	1	8
1:A:38:ARG:O	1:A:59:TRP:N	0.56	2.37	16	4
1:A:68:LEU:HD12	1:A:85:LEU:CD2	0.56	2.30	1	1
1:A:26:HIS:HE2	1:A:45:GLY:CA	0.56	2.13	8	1
1:A:79:LYS:O	1:A:80:MET:SD	0.56	2.64	12	1
1:A:18:HIS:ND1	1:A:30:PRO:O	0.56	2.38	20	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:HIS:HD1	1:A:81:ALA:C	0.56	2.07	12	1
1:A:32:LEU:O	1:A:33:HIS:CB	0.56	2.53	19	2
1:A:20:VAL:O	1:A:33:HIS:ND1	0.56	2.38	2	1
1:A:70:ASN:C	1:A:72:ALA:N	0.56	2.64	1	9
1:A:17:CYS:SG	2:A:104:HEC:HMC1	0.56	2.41	4	1
1:A:82:PHE:CD2	1:A:84:GLY:N	0.55	2.75	3	8
1:A:28:VAL:HG13	1:A:29:GLY:N	0.55	2.17	6	2
1:A:9:LEU:HD11	1:A:13:ARG:NE	0.55	2.17	19	3
1:A:71:HIS:O	1:A:72:ALA:CB	0.55	2.55	6	2
1:A:38:ARG:NE	1:A:42:GLN:HE22	0.55	1.99	7	1
1:A:61:GLU:OE2	1:A:99:LYS:CE	0.54	2.55	12	10
1:A:81:ALA:CB	2:A:104:HEC:CHD	0.54	2.86	6	1
1:A:10:PHE:C	1:A:10:PHE:CD1	0.54	2.84	1	15
1:A:29:GLY:C	1:A:31:ASN:H	0.54	2.10	10	2
1:A:75:ILE:CG2	1:A:78:THR:OG1	0.54	2.55	10	3
1:A:67:TYR:CE2	2:A:104:HEC:CAA	0.54	2.90	9	1
1:A:36:PHE:CD2	1:A:64:MET:SD	0.54	3.01	19	4
1:A:38:ARG:NE	1:A:39:HIS:H	0.54	2.01	7	1
1:A:35:ILE:C	1:A:37:GLY:H	0.54	2.10	9	2
1:A:78:THR:CG2	1:A:79:LYS:N	0.54	2.71	16	3
1:A:67:TYR:CZ	2:A:104:HEC:CAA	0.53	2.90	20	3
1:A:19:THR:C	1:A:21:GLU:N	0.53	2.65	3	1
1:A:28:VAL:CG1	1:A:29:GLY:N	0.53	2.71	12	2
1:A:29:GLY:O	1:A:31:ASN:N	0.53	2.41	10	1
1:A:33:HIS:O	1:A:33:HIS:CG	0.53	2.56	3	1
1:A:59:TRP:NE1	2:A:104:HEC:O2A	0.53	2.41	20	2
1:A:59:TRP:CZ2	2:A:104:HEC:O2A	0.53	2.62	20	1
1:A:26:HIS:ND1	1:A:31:ASN:N	0.53	2.56	1	5
1:A:51:ALA:CB	1:A:77:GLY:O	0.53	2.56	6	1
1:A:20:VAL:O	1:A:20:VAL:CG1	0.53	2.57	3	2
1:A:70:ASN:ND2	1:A:73:LYS:CB	0.53	2.72	18	1
1:A:67:TYR:O	1:A:70:ASN:O	0.53	2.27	20	17
1:A:80:MET:O	1:A:81:ALA:CB	0.52	2.58	16	2
1:A:26:HIS:O	1:A:27:LYS:C	0.52	2.52	7	2
1:A:48:TYR:CD2	1:A:52:ASN:ND2	0.52	2.78	20	4
1:A:4:LYS:H	1:A:4:LYS:CE	0.52	2.17	7	2
1:A:76:PRO:O	1:A:78:THR:N	0.52	2.43	2	1
1:A:36:PHE:O	1:A:59:TRP:O	0.52	2.28	13	10
1:A:81:ALA:HB3	2:A:104:HEC:HBC2	0.52	1.80	18	2
1:A:19:THR:O	1:A:21:GLU:N	0.52	2.42	3	1
1:A:85:LEU:HD21	1:A:94:LEU:CD1	0.52	2.35	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:CYS:O	1:A:18:HIS:N	0.52	2.43	16	15
1:A:67:TYR:CE1	2:A:104:HEC:C3A	0.52	2.93	20	4
1:A:19:THR:C	1:A:21:GLU:H	0.52	2.13	3	1
1:A:17:CYS:SG	2:A:104:HEC:CMC	0.51	2.98	18	9
1:A:55:LYS:NZ	1:A:74:TYR:O	0.51	2.43	8	2
1:A:35:ILE:C	1:A:37:GLY:N	0.51	2.66	9	3
1:A:18:HIS:ND1	1:A:32:LEU:CD2	0.51	2.73	1	2
1:A:10:PHE:CE1	1:A:20:VAL:CG1	0.51	2.94	14	2
1:A:68:LEU:HD13	1:A:94:LEU:HD23	0.51	1.83	14	3
1:A:4:LYS:CD	1:A:4:LYS:N	0.51	2.74	18	5
1:A:67:TYR:OH	1:A:71:HIS:O	0.51	2.29	2	7
1:A:71:HIS:CD2	1:A:81:ALA:HB3	0.51	2.41	6	1
1:A:20:VAL:O	1:A:33:HIS:CB	0.51	2.59	11	1
1:A:25:PRO:C	1:A:31:ASN:OD1	0.51	2.54	6	6
1:A:32:LEU:HD12	1:A:48:TYR:OH	0.51	2.06	9	2
1:A:90:ASP:O	1:A:93:ASP:OD1	0.50	2.29	18	1
1:A:65:SER:O	1:A:91:ARG:NH1	0.50	2.43	1	1
1:A:24:GLY:O	1:A:31:ASN:OD1	0.50	2.30	2	4
1:A:24:GLY:C	1:A:31:ASN:OD1	0.50	2.54	11	5
1:A:35:ILE:N	1:A:35:ILE:HD13	0.50	2.20	8	1
1:A:31:ASN:O	1:A:32:LEU:O	0.50	2.29	14	1
1:A:32:LEU:HG	1:A:35:ILE:HD13	0.50	1.83	15	1
1:A:78:THR:HG22	1:A:79:LYS:N	0.50	2.20	16	3
1:A:48:TYR:CD2	2:A:104:HEC:O2D	0.50	2.63	16	2
1:A:52:ASN:O	1:A:55:LYS:O	0.50	2.30	11	14
1:A:25:PRO:O	1:A:31:ASN:OD1	0.50	2.30	6	5
1:A:56:ASN:O	1:A:56:ASN:OD1	0.50	2.30	7	8
1:A:23:GLY:O	1:A:24:GLY:O	0.50	2.30	14	2
1:A:60:ASP:OD1	1:A:61:GLU:OE1	0.50	2.30	8	7
1:A:94:LEU:HD21	2:A:104:HEC:HMB3	0.50	1.83	1	1
1:A:94:LEU:HD21	2:A:104:HEC:HBB3	0.50	1.84	4	1
1:A:69:THR:HG22	1:A:91:ARG:CZ	0.50	2.36	5	1
1:A:30:PRO:O	1:A:31:ASN:O	0.50	2.29	6	1
1:A:61:GLU:CD	1:A:99:LYS:NZ	0.50	2.70	12	4
1:A:35:ILE:HD11	1:A:64:MET:HE3	0.49	1.83	17	2
1:A:48:TYR:OH	2:A:104:HEC:O1A	0.49	2.30	6	5
1:A:12:THR:HG22	1:A:12:THR:O	0.49	2.08	7	1
1:A:53:ILE:O	1:A:56:ASN:OD1	0.49	2.30	18	2
1:A:30:PRO:CG	2:A:104:HEC:O2D	0.49	2.61	8	2
1:A:48:TYR:O	1:A:53:ILE:CD1	0.49	2.61	7	4
1:A:69:THR:O	1:A:70:ASN:OD1	0.49	2.31	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:GLY:O	1:A:31:ASN:OD1	0.49	2.31	11	1
1:A:79:LYS:NZ	2:A:104:HEC:CMD	0.49	2.76	15	1
1:A:78:THR:HG1	2:A:104:HEC:CGD	0.49	2.18	2	1
1:A:20:VAL:O	1:A:21:GLU:O	0.49	2.31	4	1
1:A:26:HIS:O	1:A:27:LYS:O	0.48	2.31	11	1
1:A:52:ASN:CG	2:A:104:HEC:O2D	0.48	2.56	15	1
1:A:67:TYR:O	1:A:70:ASN:C	0.48	2.56	18	1
1:A:60:ASP:OD1	1:A:61:GLU:N	0.48	2.46	7	10
1:A:70:ASN:CG	1:A:71:HIS:H	0.48	2.17	3	3
1:A:41:GLY:N	1:A:48:TYR:CD2	0.48	2.81	7	2
1:A:40:SER:OG	2:A:104:HEC:O2A	0.48	2.32	13	5
1:A:70:ASN:ND2	1:A:72:ALA:O	0.48	2.46	2	1
1:A:38:ARG:NH2	1:A:39:HIS:ND1	0.48	2.61	7	1
1:A:9:LEU:CD1	1:A:13:ARG:HE	0.48	2.21	19	3
1:A:99:LYS:O	1:A:103:GLU:N	0.48	2.44	5	20
1:A:67:TYR:CE2	2:A:104:HEC:C3A	0.48	2.97	7	5
1:A:9:LEU:O	1:A:12:THR:OG1	0.48	2.31	4	1
1:A:78:THR:HG23	2:A:104:HEC:O2D	0.48	2.08	15	1
1:A:40:SER:OG	1:A:75:ILE:CD1	0.48	2.62	1	1
1:A:-3:PHE:O	1:A:-2:LYS:O	0.48	2.32	11	2
1:A:72:ALA:HB1	1:A:79:LYS:O	0.48	2.09	18	1
1:A:10:PHE:CZ	1:A:20:VAL:HG23	0.48	2.44	18	1
1:A:35:ILE:N	1:A:35:ILE:CD1	0.47	2.77	8	1
1:A:35:ILE:O	1:A:37:GLY:N	0.47	2.47	8	3
1:A:22:LYS:O	1:A:24:GLY:N	0.47	2.46	14	1
1:A:9:LEU:HD11	1:A:13:ARG:CZ	0.47	2.40	18	3
1:A:59:TRP:CD2	1:A:64:MET:SD	0.47	3.07	10	2
1:A:3:ALA:O	1:A:4:LYS:C	0.47	2.55	1	1
1:A:92:ASN:O	1:A:96:THR:OG1	0.47	2.31	20	3
1:A:52:ASN:ND2	2:A:104:HEC:O1D	0.47	2.47	2	3
1:A:70:ASN:HD22	1:A:72:ALA:C	0.47	2.17	2	1
1:A:32:LEU:H	1:A:32:LEU:CD2	0.47	2.17	14	1
1:A:52:ASN:OD1	1:A:52:ASN:C	0.47	2.56	20	1
1:A:16:GLN:O	1:A:28:VAL:HG21	0.47	2.10	2	1
1:A:35:ILE:CG2	1:A:59:TRP:CD1	0.47	2.98	5	2
1:A:72:ALA:CB	1:A:78:THR:OG1	0.47	2.62	13	2
1:A:79:LYS:HZ2	2:A:104:HEC:CMD	0.47	2.22	15	1
1:A:36:PHE:HB2	1:A:102:THR:HG21	0.47	1.86	6	3
1:A:32:LEU:CD1	1:A:35:ILE:HD13	0.47	2.33	11	2
1:A:67:TYR:CE2	1:A:71:HIS:O	0.47	2.68	11	2
1:A:71:HIS:HD1	1:A:81:ALA:CA	0.47	2.22	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:VAL:O	1:A:58:LEU:C	0.47	2.56	10	5
1:A:18:HIS:ND1	1:A:32:LEU:HD23	0.47	2.25	8	1
1:A:78:THR:HG23	2:A:104:HEC:CGD	0.47	2.40	15	1
1:A:78:THR:OG1	2:A:104:HEC:CBD	0.47	2.63	18	1
1:A:88:GLU:O	1:A:92:ASN:CG	0.47	2.58	9	2
1:A:82:PHE:CD1	1:A:82:PHE:C	0.46	2.93	4	1
1:A:30:PRO:O	1:A:31:ASN:C	0.46	2.56	6	1
1:A:82:PHE:CE1	1:A:85:LEU:HD13	0.46	2.45	5	1
2:A:104:HEC:HBD1	2:A:104:HEC:HMD3	0.46	1.87	6	1
1:A:18:HIS:CE1	1:A:32:LEU:CD2	0.46	2.98	14	2
1:A:52:ASN:CB	2:A:104:HEC:O1D	0.46	2.64	12	1
1:A:67:TYR:O	1:A:68:LEU:C	0.46	2.57	19	1
1:A:61:GLU:H	1:A:61:GLU:CD	0.46	2.19	3	6
1:A:26:HIS:CD2	1:A:46:TYR:CB	0.46	2.99	2	1
1:A:35:ILE:CD1	1:A:35:ILE:H	0.46	2.24	8	1
2:A:104:HEC:HMC3	2:A:104:HEC:HBC3	0.46	1.88	5	6
1:A:35:ILE:O	1:A:36:PHE:C	0.46	2.59	18	4
1:A:26:HIS:NE2	1:A:45:GLY:CA	0.46	2.78	8	3
1:A:7:ALA:CB	1:A:97:TYR:CD1	0.46	2.99	9	3
1:A:20:VAL:HG23	1:A:21:GLU:N	0.46	2.25	4	1
1:A:48:TYR:CD1	2:A:104:HEC:O2D	0.46	2.69	7	1
1:A:69:THR:HG23	1:A:91:ARG:HH22	0.45	1.69	10	1
1:A:99:LYS:O	1:A:103:GLU:CB	0.45	2.64	10	1
1:A:35:ILE:HD11	1:A:64:MET:CE	0.45	2.42	9	2
1:A:79:LYS:HZ2	2:A:104:HEC:HMD3	0.45	1.72	15	1
2:A:104:HEC:HMA1	2:A:104:HEC:CBA	0.45	2.42	6	1
1:A:6:GLY:HA2	1:A:9:LEU:HD12	0.45	1.87	16	1
1:A:70:ASN:HD22	1:A:72:ALA:H	0.45	1.55	8	1
1:A:47:SER:O	1:A:48:TYR:O	0.45	2.35	13	1
1:A:33:HIS:ND1	1:A:33:HIS:C	0.45	2.71	4	1
1:A:38:ARG:CD	1:A:42:GLN:OE1	0.45	2.65	13	3
1:A:15:LEU:HD12	1:A:19:THR:HG22	0.45	1.89	18	2
1:A:69:THR:OG1	1:A:91:ARG:NH2	0.45	2.50	13	1
1:A:49:THR:N	2:A:104:HEC:O1D	0.45	2.50	16	1
1:A:32:LEU:HD22	1:A:48:TYR:CZ	0.44	2.45	5	1
1:A:9:LEU:HD23	1:A:94:LEU:HG	0.44	1.89	6	3
1:A:38:ARG:CD	1:A:42:GLN:NE2	0.44	2.80	7	1
1:A:64:MET:HE1	2:A:104:HEC:CMA	0.44	2.42	7	2
1:A:20:VAL:HG13	1:A:33:HIS:CD2	0.44	2.47	19	1
1:A:28:VAL:HG12	1:A:29:GLY:N	0.44	2.27	4	1
1:A:26:HIS:CE1	1:A:30:PRO:O	0.44	2.70	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:LYS:C	1:A:56:ASN:HD22	0.44	2.20	9	1
1:A:82:PHE:CZ	1:A:85:LEU:HD13	0.44	2.48	9	1
1:A:24:GLY:CA	1:A:31:ASN:OD1	0.44	2.65	8	1
1:A:29:GLY:C	1:A:31:ASN:N	0.44	2.76	10	1
1:A:31:ASN:O	1:A:32:LEU:C	0.44	2.58	17	1
1:A:49:THR:OG1	1:A:79:LYS:CE	0.44	2.66	3	3
1:A:68:LEU:O	1:A:69:THR:C	0.44	2.59	13	2
1:A:75:ILE:O	1:A:78:THR:HG22	0.44	2.13	18	1
1:A:10:PHE:CE1	1:A:20:VAL:HG23	0.44	2.48	8	1
1:A:84:GLY:O	1:A:86:LYS:N	0.43	2.50	14	3
1:A:35:ILE:CG1	1:A:36:PHE:N	0.43	2.81	9	1
1:A:74:TYR:CE2	1:A:75:ILE:HD11	0.43	2.49	7	1
1:A:68:LEU:CD1	1:A:94:LEU:HD23	0.43	2.43	19	1
1:A:89:LYS:O	1:A:93:ASP:CG	0.43	2.61	2	1
1:A:4:LYS:CG	1:A:5:LYS:N	0.43	2.81	9	1
1:A:44:GLU:O	1:A:46:TYR:N	0.43	2.51	13	1
1:A:78:THR:HG23	1:A:79:LYS:N	0.43	2.28	2	1
2:A:104:HEC:CBD	2:A:104:HEC:CMD	0.43	2.97	6	1
1:A:75:ILE:HG22	1:A:78:THR:OG1	0.43	2.14	10	1
1:A:70:ASN:ND2	1:A:72:ALA:H	0.43	2.12	19	1
1:A:102:THR:O	1:A:103:GLU:C	0.43	2.59	1	1
2:A:104:HEC:HBA1	2:A:104:HEC:HMA3	0.43	1.91	3	1
1:A:48:TYR:N	1:A:48:TYR:CD1	0.42	2.86	13	2
1:A:61:GLU:CD	1:A:99:LYS:HZ2	0.42	2.22	16	1
1:A:26:HIS:CD2	1:A:46:TYR:N	0.42	2.86	1	1
1:A:26:HIS:ND1	1:A:31:ASN:CG	0.42	2.78	16	1
1:A:10:PHE:CD1	1:A:10:PHE:C	0.42	2.97	4	2
1:A:82:PHE:O	1:A:83:GLY:C	0.42	2.61	14	1
1:A:10:PHE:CE1	1:A:20:VAL:HG22	0.42	2.49	6	1
1:A:65:SER:HA	1:A:95:ILE:HD11	0.42	1.92	10	1
1:A:68:LEU:CD2	1:A:94:LEU:HD23	0.42	2.44	13	1
1:A:46:TYR:CG	1:A:47:SER:N	0.42	2.87	10	1
1:A:26:HIS:HD1	1:A:31:ASN:H	0.42	1.51	9	1
1:A:62:ASN:O	1:A:65:SER:OG	0.42	2.32	13	2
1:A:13:ARG:O	1:A:14:CYS:C	0.42	2.62	4	1
1:A:82:PHE:CZ	1:A:85:LEU:HD21	0.42	2.50	10	1
1:A:84:GLY:C	1:A:86:LYS:H	0.42	2.22	14	1
1:A:69:THR:HG23	1:A:91:ARG:CZ	0.42	2.41	17	1
1:A:20:VAL:C	1:A:21:GLU:O	0.41	2.63	4	1
1:A:32:LEU:HD11	2:A:104:HEC:HBA1	0.41	1.91	8	1
1:A:94:LEU:HD11	2:A:104:HEC:HBB3	0.41	1.92	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:-3:PHE:CD1	1:A:-3:PHE:C	0.41	2.98	10	1
1:A:37:GLY:O	1:A:58:LEU:HD11	0.41	2.15	16	1
1:A:72:ALA:O	1:A:75:ILE:C	0.41	2.63	8	1
1:A:102:THR:O	1:A:103:GLU:O	0.41	2.39	15	1
1:A:23:GLY:O	1:A:24:GLY:C	0.41	2.63	20	1
1:A:25:PRO:O	1:A:26:HIS:C	0.41	2.61	15	1
1:A:91:ARG:CB	1:A:91:ARG:NH1	0.41	2.83	18	1
1:A:18:HIS:ND1	1:A:32:LEU:HD21	0.41	2.31	1	1
1:A:32:LEU:CD2	1:A:48:TYR:OH	0.41	2.69	16	1
1:A:55:LYS:C	1:A:56:ASN:ND2	0.41	2.78	9	1
1:A:26:HIS:NE2	1:A:45:GLY:O	0.41	2.54	8	1
1:A:32:LEU:CD1	1:A:48:TYR:OH	0.41	2.68	14	1
1:A:70:ASN:ND2	1:A:71:HIS:H	0.41	2.14	8	1
1:A:19:THR:CG2	1:A:27:LYS:NZ	0.41	2.83	12	1
2:A:104:HEC:HMD3	2:A:104:HEC:CBD	0.41	2.46	14	1
1:A:32:LEU:HD11	1:A:35:ILE:CD1	0.40	2.46	3	1
1:A:64:MET:O	1:A:68:LEU:HD13	0.40	2.16	4	1
1:A:85:LEU:HD11	1:A:90:ASP:HB3	0.40	1.93	8	1
1:A:70:ASN:O	1:A:71:HIS:C	0.40	2.63	9	1
1:A:72:ALA:CB	1:A:78:THR:HG21	0.40	2.28	12	1
1:A:23:GLY:C	1:A:24:GLY:O	0.40	2.64	14	1
1:A:71:HIS:CE1	1:A:82:PHE:CB	0.40	3.03	7	1
2:A:104:HEC:HMA3	2:A:104:HEC:CBA	0.40	2.47	3	1
1:A:18:HIS:ND1	1:A:32:LEU:HD22	0.40	2.31	20	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	105/108 (97%)	91±3 (87±3%)	9±3 (9±2%)	5±2 (5±2%)	3 25
All	All	2100/2160 (97%)	1818 (87%)	184 (9%)	98 (5%)	3 25

All 23 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	1	GLY	15
1	A	81	ALA	15
1	A	72	ALA	9
1	A	71	HIS	7
1	A	33	HIS	7
1	A	48	TYR	7
1	A	32	LEU	6
1	A	27	LYS	4
1	A	84	GLY	3
1	A	28	VAL	3
1	A	83	GLY	3
1	A	82	PHE	3
1	A	24	GLY	3
1	A	20	VAL	2
1	A	31	ASN	2
1	A	-2	LYS	2
1	A	77	GLY	1
1	A	21	GLU	1
1	A	34	GLY	1
1	A	35	ILE	1
1	A	30	PRO	1
1	A	69	THR	1
1	A	-1	ALA	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	86/88 (98%)	81±1 (94±2%)	5±1 (6±2%)	19 68
All	All	1720/1760 (98%)	1616 (94%)	104 (6%)	19 68

All 19 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	71	HIS	16
1	A	40	SER	11
1	A	75	ILE	11

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Mol	Chain	Res	Type	Models (Total)
1	A	56	ASN	9
1	A	94	LEU	9
1	A	2	SER	9
1	A	4	LYS	8
1	A	28	VAL	7
1	A	32	LEU	6
1	A	14	CYS	5
1	A	35	ILE	3
1	A	33	HIS	2
1	A	79	LYS	2
1	A	78	THR	1
1	A	85	LEU	1
1	A	69	THR	1
1	A	70	ASN	1
1	A	19	THR	1
1	A	74	TYR	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	HEC	A	104	1	50,50,50	0.80±0.01	2±0 (4±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	HEC	A	104	1	68,82,82	0.93±0.01	1±0 (1±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	104	1	1±0,1,7,7	0±0,14,54,54	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	104	HEC	O2D-CGD	2.62	1.22	1.30	7	20
2	A	104	HEC	O2A-CGA	2.58	1.22	1.30	3	20

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	104	HEC	CAB-C3B-C4B	2.56	128.13	124.79	18	20
2	A	104	HEC	CAC-C3C-C4C	2.08	127.78	124.91	6	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	104	HEC	NA	20

There are no torsion outliers.

There are no ring outliers.

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

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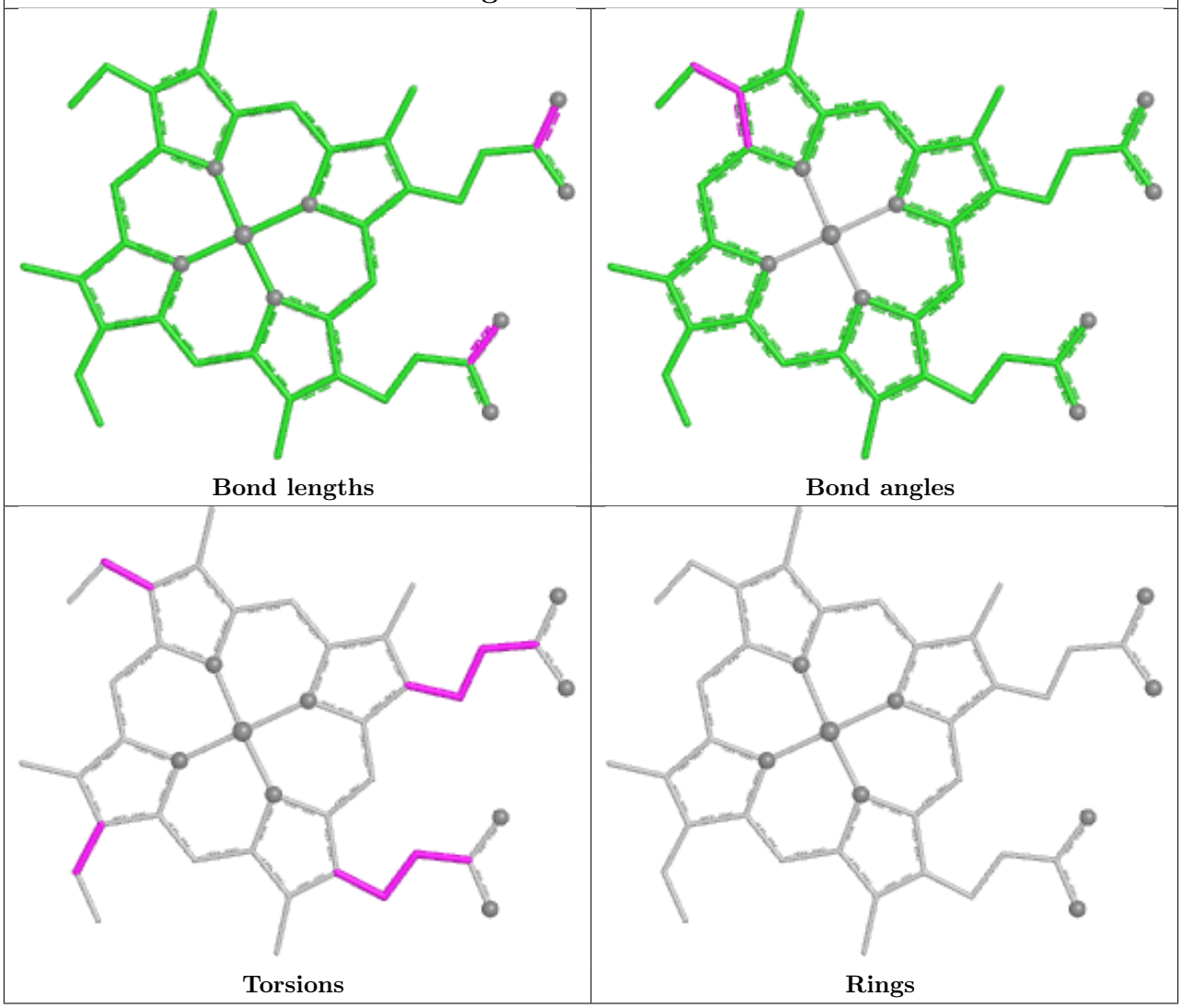

6.7 Other polymers (i)

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 21% for the well-defined parts and 21% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (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	616
Number of shifts mapped to atoms	616
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

- Can not parse the chemical shift value. All 311 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	-3	PHE	HB2	2.615	0.005	.
1	A	-3	PHE	HB3	2.825	0.010	.
1	A	-3	PHE	HD1	7.019	0.010	.
1	A	-3	PHE	HE1	7.197	0.011	.
1	A	-2	LYS	HB2	1.277	0.002	.
1	A	-2	LYS	HD2	1.388	0.002	.
1	A	-2	LYS	HE2	2.811	0.001	.
1	A	-2	LYS	HG2	1.128	0.014	.
1	A	1	GLY	HA2	4.277	0.011	.
1	A	1	GLY	HA3	3.393	0.000	.
1	A	2	SER	HB2	3.378	0.018	.
1	A	2	SER	HB3	3.567	0.002	.
1	A	4	LYS	HB2	1.657	0.000	.
1	A	4	LYS	HE2	2.869	0.015	.
1	A	4	LYS	HE3	2.798	0.000	.
1	A	4	LYS	HG2	1.281	0.000	.
1	A	5	LYS	HB2	1.448	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	LYS	HB3	1.680	0.002	.
1	A	5	LYS	HG2	0.932	0.002	.
1	A	6	GLY	HA2	3.836	0.006	.
1	A	6	GLY	HA3	4.012	0.004	.
1	A	9	LEU	HB3	1.739	0.004	.
1	A	9	LEU	HD11	0.475	0.000	.
1	A	9	LEU	HD12	0.475	0.000	.
1	A	9	LEU	HD13	0.475	0.000	.
1	A	9	LEU	HD21	0.762	0.012	.
1	A	9	LEU	HD22	0.762	0.012	.
1	A	9	LEU	HD23	0.762	0.012	.
1	A	10	PHE	HB2	3.160	0.005	.
1	A	10	PHE	HB3	2.658	0.004	.
1	A	10	PHE	HD2	7.162	0.009	.
1	A	10	PHE	HE2	7.812	0.009	.
1	A	11	LYS	HB2	1.829	0.008	.
1	A	11	LYS	HB3	2.175	0.006	.
1	A	11	LYS	HE2	3.101	0.000	.
1	A	11	LYS	HG2	1.476	0.009	.
1	A	13	ARG	HB2	1.087	0.006	.
1	A	13	ARG	HB3	1.374	0.009	.
1	A	13	ARG	HG2	1.733	0.001	.
1	A	13	ARG	HG3	1.264	0.008	.
1	A	14	CYS	HB2	2.933	0.007	.
1	A	14	CYS	HB3	2.814	0.002	.
1	A	15	LEU	HB2	2.918	0.003	.
1	A	15	LEU	HB3	3.242	0.009	.
1	A	15	LEU	HD11	2.019	0.010	.
1	A	15	LEU	HD12	2.019	0.010	.
1	A	15	LEU	HD13	2.019	0.010	.
1	A	15	LEU	HD21	1.435	0.039	.
1	A	15	LEU	HD22	1.435	0.039	.
1	A	15	LEU	HD23	1.435	0.039	.
1	A	16	GLN	HB2	2.677	0.002	.
1	A	16	GLN	HE21	6.930	0.000	.
1	A	16	GLN	HE22	7.439	0.000	.
1	A	16	GLN	HG2	2.831	0.000	.
1	A	16	GLN	HG3	2.945	0.003	.
1	A	17	CYS	HB2	2.220	0.007	.
1	A	17	CYS	HB3	2.491	0.009	.
1	A	18	HIS	HB2	9.167	0.009	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	18	HIS	HB3	13.912	0.011	.
1	A	20	VAL	HG11	0.445	0.011	.
1	A	20	VAL	HG12	0.445	0.011	.
1	A	20	VAL	HG13	0.445	0.011	.
1	A	20	VAL	HG21	0.753	0.010	.
1	A	20	VAL	HG22	0.753	0.010	.
1	A	20	VAL	HG23	0.753	0.010	.
1	A	21	GLU	HB2	2.193	0.008	.
1	A	21	GLU	HB3	2.400	0.001	.
1	A	21	GLU	HG2	2.646	0.009	.
1	A	21	GLU	HG3	2.800	0.013	.
1	A	22	LYS	HB2	1.792	0.000	.
1	A	22	LYS	HD2	1.545	0.000	.
1	A	22	LYS	HG2	1.125	0.000	.
1	A	22	LYS	HG3	1.297	0.000	.
1	A	23	GLY	HA2	3.803	0.010	.
1	A	23	GLY	HA3	4.093	0.009	.
1	A	24	GLY	HA2	3.776	0.022	.
1	A	24	GLY	HA3	4.374	0.014	.
1	A	25	PRO	HB2	2.191	0.019	.
1	A	25	PRO	HB3	2.336	0.021	.
1	A	25	PRO	HD2	3.466	0.012	.
1	A	25	PRO	HG2	1.919	0.000	.
1	A	25	PRO	HG3	2.054	0.018	.
1	A	26	HIS	HB2	2.815	0.021	.
1	A	26	HIS	HB3	3.020	0.055	.
1	A	27	LYS	HB2	1.805	0.011	.
1	A	27	LYS	HB3	2.367	0.000	.
1	A	27	LYS	HG2	1.231	0.005	.
1	A	28	VAL	HG11	-0.623	0.012	.
1	A	28	VAL	HG12	-0.623	0.012	.
1	A	28	VAL	HG13	-0.623	0.012	.
1	A	28	VAL	HG21	0.808	0.016	.
1	A	28	VAL	HG22	0.808	0.016	.
1	A	28	VAL	HG23	0.808	0.016	.
1	A	29	GLY	HA2	-2.778	0.019	.
1	A	29	GLY	HA3	-0.273	0.016	.
1	A	30	PRO	HB2	-0.244	0.031	.
1	A	30	PRO	HB3	1.340	0.025	.
1	A	30	PRO	HD2	-0.758	0.023	.
1	A	30	PRO	HD3	-3.078	0.008	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	PRO	HG2	-0.634	0.035	.
1	A	31	ASN	HB2	2.477	0.005	.
1	A	31	ASN	HB3	2.954	0.010	.
1	A	31	ASN	HD21	8.029	0.011	.
1	A	31	ASN	HD22	8.337	0.011	.
1	A	32	LEU	HB2	1.992	0.011	.
1	A	32	LEU	HB3	2.379	0.008	.
1	A	32	LEU	HD11	0.991	0.013	.
1	A	32	LEU	HD12	0.991	0.013	.
1	A	32	LEU	HD13	0.991	0.013	.
1	A	32	LEU	HD21	0.595	0.011	.
1	A	32	LEU	HD22	0.595	0.011	.
1	A	32	LEU	HD23	0.595	0.011	.
1	A	33	HIS	HB2	3.209	0.006	.
1	A	33	HIS	HB3	3.337	0.013	.
1	A	34	GLY	HA2	3.718	0.003	.
1	A	34	GLY	HA3	3.750	0.005	.
1	A	35	ILE	HG13	0.462	0.007	.
1	A	36	PHE	HB2	2.772	0.004	.
1	A	36	PHE	HB3	2.847	0.003	.
1	A	36	PHE	HD1	6.928	0.020	.
1	A	36	PHE	HE1	6.173	0.010	.
1	A	37	GLY	HA2	3.618	0.012	.
1	A	37	GLY	HA3	4.185	0.002	.
1	A	38	ARG	HB2	1.715	0.014	.
1	A	38	ARG	HD2	3.151	0.001	.
1	A	38	ARG	HD3	3.324	0.000	.
1	A	38	ARG	HG2	1.984	0.012	.
1	A	39	HIS	HB2	2.737	0.015	.
1	A	39	HIS	HB3	2.957	0.007	.
1	A	40	SER	HB2	3.855	0.013	.
1	A	40	SER	HB3	4.040	0.017	.
1	A	41	GLY	HA2	1.661	0.016	.
1	A	41	GLY	HA3	3.172	0.013	.
1	A	42	GLN	HB2	1.711	0.008	.
1	A	42	GLN	HB3	2.362	0.011	.
1	A	42	GLN	HE21	7.199	0.006	.
1	A	42	GLN	HE22	6.671	0.009	.
1	A	42	GLN	HG2	2.117	0.010	.
1	A	42	GLN	HG3	2.201	0.009	.
1	A	44	GLU	HB2	2.089	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	44	GLU	HB3	2.340	0.000	.
1	A	44	GLU	HG2	2.572	0.004	.
1	A	44	GLU	HG3	2.470	0.003	.
1	A	45	GLY	HA2	3.754	0.014	.
1	A	45	GLY	HA3	4.070	0.017	.
1	A	46	TYR	HB2	0.767	0.005	.
1	A	46	TYR	HB3	1.766	0.018	.
1	A	46	TYR	HD1	4.546	0.002	.
1	A	46	TYR	HD2	5.843	0.023	.
1	A	46	TYR	HE1	3.491	0.032	.
1	A	46	TYR	HE2	5.223	0.009	.
1	A	47	SER	HB2	3.149	0.009	.
1	A	47	SER	HB3	2.960	0.008	.
1	A	48	TYR	HB2	2.587	0.010	.
1	A	48	TYR	HB3	3.294	0.020	.
1	A	48	TYR	HD1	6.932	0.005	.
1	A	50	ASP	HB2	2.575	0.009	.
1	A	50	ASP	HB3	2.632	0.013	.
1	A	52	ASN	HB2	3.152	0.011	.
1	A	52	ASN	HB3	3.075	0.015	.
1	A	52	ASN	HD21	6.846	0.022	.
1	A	52	ASN	HD22	7.471	0.022	.
1	A	53	ILE	HG12	1.096	0.000	.
1	A	53	ILE	HG13	1.239	0.015	.
1	A	54	LYS	HB2	1.761	0.008	.
1	A	54	LYS	HB3	1.538	0.005	.
1	A	54	LYS	HG2	1.373	0.002	.
1	A	55	LYS	HB2	1.837	0.004	.
1	A	55	LYS	HB3	2.123	0.009	.
1	A	55	LYS	HG2	1.313	0.033	.
1	A	56	ASN	HB2	2.270	0.002	.
1	A	56	ASN	HB3	3.326	0.005	.
1	A	56	ASN	HD21	6.404	0.000	.
1	A	56	ASN	HD22	7.190	0.000	.
1	A	57	VAL	HG11	0.468	0.009	.
1	A	57	VAL	HG12	0.468	0.009	.
1	A	57	VAL	HG13	0.468	0.009	.
1	A	57	VAL	HG21	0.585	0.010	.
1	A	57	VAL	HG22	0.585	0.010	.
1	A	57	VAL	HG23	0.585	0.010	.
1	A	58	LEU	HB2	0.680	0.010	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	58	LEU	HB3	1.416	0.008	.
1	A	58	LEU	HD11	0.466	0.008	.
1	A	58	LEU	HD12	0.466	0.008	.
1	A	58	LEU	HD13	0.466	0.008	.
1	A	58	LEU	HD21	0.563	0.011	.
1	A	58	LEU	HD22	0.563	0.011	.
1	A	58	LEU	HD23	0.563	0.011	.
1	A	59	TRP	HB2	2.339	0.016	.
1	A	59	TRP	HB3	3.567	0.025	.
1	A	60	ASP	HB2	2.939	0.003	.
1	A	60	ASP	HB3	2.677	0.002	.
1	A	61	GLU	HB2	1.081	0.013	.
1	A	61	GLU	HB3	1.264	0.012	.
1	A	61	GLU	HG2	0.849	0.018	.
1	A	62	ASN	HB2	2.890	0.010	.
1	A	62	ASN	HB3	2.937	0.016	.
1	A	62	ASN	HD21	7.136	0.010	.
1	A	62	ASN	HD22	7.777	0.006	.
1	A	63	ASN	HB2	2.869	0.021	.
1	A	63	ASN	HB3	3.062	0.014	.
1	A	63	ASN	HD21	7.320	0.001	.
1	A	63	ASN	HD22	7.023	0.014	.
1	A	64	MET	HB2	2.074	0.011	.
1	A	64	MET	HB3	2.341	0.013	.
1	A	64	MET	HG2	1.642	0.007	.
1	A	64	MET	HG3	1.750	0.015	.
1	A	65	SER	HB2	3.921	0.001	.
1	A	65	SER	HB3	3.774	0.000	.
1	A	66	GLU	HB2	2.010	0.016	.
1	A	66	GLU	HG2	2.318	0.014	.
1	A	66	GLU	HG3	2.343	0.009	.
1	A	67	TYR	HB2	2.725	0.020	.
1	A	67	TYR	HB3	2.932	0.012	.
1	A	67	TYR	HD1	7.503	0.024	.
1	A	67	TYR	HE1	7.800	0.021	.
1	A	68	LEU	HB2	0.472	0.005	.
1	A	68	LEU	HB3	0.560	0.028	.
1	A	68	LEU	HD11	-0.989	0.025	.
1	A	68	LEU	HD12	-0.989	0.025	.
1	A	68	LEU	HD13	-0.989	0.025	.
1	A	68	LEU	HD21	-2.768	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	68	LEU	HD22	-2.768	0.020	.
1	A	68	LEU	HD23	-2.768	0.020	.
1	A	70	ASN	HB2	3.349	0.018	.
1	A	70	ASN	HB3	3.469	0.013	.
1	A	70	ASN	HD21	6.671	0.017	.
1	A	70	ASN	HD22	7.437	0.025	.
1	A	71	HIS	HB2	8.683	0.345	.
1	A	71	HIS	HB3	7.799	0.050	.
1	A	73	LYS	HB2	2.030	0.001	.
1	A	74	TYR	HB2	3.963	0.000	.
1	A	74	TYR	HB3	4.138	0.013	.
1	A	74	TYR	HD1	7.782	0.002	.
1	A	74	TYR	HE1	7.169	0.008	.
1	A	75	ILE	HG12	1.568	0.015	.
1	A	76	PRO	HB2	1.805	0.000	.
1	A	76	PRO	HB3	2.226	0.000	.
1	A	76	PRO	HD2	3.49	0.003	.
1	A	76	PRO	HG2	1.805	0.000	.
1	A	76	PRO	HG3	1.908	0.000	.
1	A	77	GLY	HA2	3.947	0.000	.
1	A	79	LYS	HB2	1.380	0.003	.
1	A	79	LYS	HB3	1.654	0.001	.
1	A	79	LYS	HD2	0.742	0.004	.
1	A	79	LYS	HE2	2.114	0.018	.
1	A	79	LYS	HE3	2.332	0.024	.
1	A	79	LYS	HG2	-0.006	0.127	.
1	A	79	LYS	HG3	1.040	0.162	.
1	A	80	MET	HB2	2.083	0.000	.
1	A	80	MET	HB3	1.905	0.000	.
1	A	82	PHE	HB2	2.837	0.024	.
1	A	82	PHE	HB3	3.312	0.009	.
1	A	82	PHE	HD2	6.262	0.005	.
1	A	82	PHE	HE1	6.961	0.014	.
1	A	84	GLY	HA3	4.328	0.008	.
1	A	85	LEU	HB2	0.754	0.010	.
1	A	85	LEU	HB3	1.104	0.010	.
1	A	85	LEU	HD11	-0.049	0.009	.
1	A	85	LEU	HD12	-0.049	0.009	.
1	A	85	LEU	HD13	-0.049	0.009	.
1	A	85	LEU	HD21	0.435	0.015	.
1	A	85	LEU	HD22	0.435	0.015	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	85	LEU	HD23	0.435	0.015	.
1	A	86	LYS	HB2	1.875	0.000	.
1	A	87	LYS	HB2	1.690	0.010	.
1	A	87	LYS	HB3	1.896	0.004	.
1	A	87	LYS	HG2	1.218	0.000	.
1	A	88	GLU	HB2	1.805	0.015	.
1	A	88	GLU	HB3	1.949	0.013	.
1	A	89	LYS	HB2	1.604	0.004	.
1	A	89	LYS	HB3	1.751	0.009	.
1	A	89	LYS	HE3	2.831	0.001	.
1	A	89	LYS	HG2	1.393	0.019	.
1	A	90	ASP	HB2	2.285	0.008	.
1	A	90	ASP	HB3	2.741	0.009	.
1	A	91	ARG	HB2	1.950	0.002	.
1	A	91	ARG	HG2	1.377	0.001	.
1	A	92	ASN	HB2	2.641	0.026	.
1	A	92	ASN	HB3	2.818	0.011	.
1	A	92	ASN	HD21	6.941	0.017	.
1	A	92	ASN	HD22	7.201	0.013	.
1	A	93	ASP	HB2	2.424	0.017	.
1	A	94	LEU	HB2	1.243	0.013	.
1	A	94	LEU	HB3	1.351	0.012	.
1	A	94	LEU	HD11	-0.059	0.032	.
1	A	94	LEU	HD12	-0.059	0.032	.
1	A	94	LEU	HD13	-0.059	0.032	.
1	A	94	LEU	HD21	0.436	0.072	.
1	A	94	LEU	HD22	0.436	0.072	.
1	A	94	LEU	HD23	0.436	0.072	.
1	A	95	ILE	HG12	0.277	0.028	.
1	A	95	ILE	HG13	1.251	0.013	.
1	A	97	TYR	HB2	2.721	0.007	.
1	A	97	TYR	HB3	3.457	0.009	.
1	A	97	TYR	HE2	7.184	0.020	.
1	A	98	LEU	HB2	1.729	0.009	.
1	A	98	LEU	HD11	0.724	0.008	.
1	A	98	LEU	HD12	0.724	0.008	.
1	A	98	LEU	HD13	0.724	0.008	.
1	A	98	LEU	HD21	1.073	0.030	.
1	A	98	LEU	HD22	1.073	0.030	.
1	A	98	LEU	HD23	1.073	0.030	.
1	A	99	LYS	HB2	1.366	0.004	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	LYS	HB3	1.193	0.007	.
1	A	99	LYS	HD2	0.734	0.008	.
1	A	99	LYS	HG2	0.662	0.011	.
1	A	100	LYS	HB2	1.694	0.009	.
1	A	100	LYS	HB3	1.337	0.010	.
1	A	103	GLU	HB2	1.944	0.019	.
1	A	103	GLU	HB3	2.265	0.007	.

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

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 21%, i.e. 305 atoms were assigned a chemical shift out of a possible 1423. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	188/536 (35%)	188/221 (85%)	0/212 (0%)	0/103 (0%)
Sidechain	97/752 (13%)	97/484 (20%)	0/235 (0%)	0/33 (0%)
Aromatic	20/135 (15%)	20/66 (30%)	0/60 (0%)	0/9 (0%)
Overall	305/1423 (21%)	305/771 (40%)	0/507 (0%)	0/145 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 21%, i.e. 305 atoms were assigned a chemical shift out of a possible 1446. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	188/546 (34%)	188/225 (84%)	0/216 (0%)	0/105 (0%)
Sidechain	97/765 (13%)	97/492 (20%)	0/240 (0%)	0/33 (0%)
Aromatic	20/135 (15%)	20/66 (30%)	0/60 (0%)	0/9 (0%)
Overall	305/1446 (21%)	305/783 (39%)	0/516 (0%)	0/147 (0%)

7.1.4 Statistically unusual chemical shifts (i)

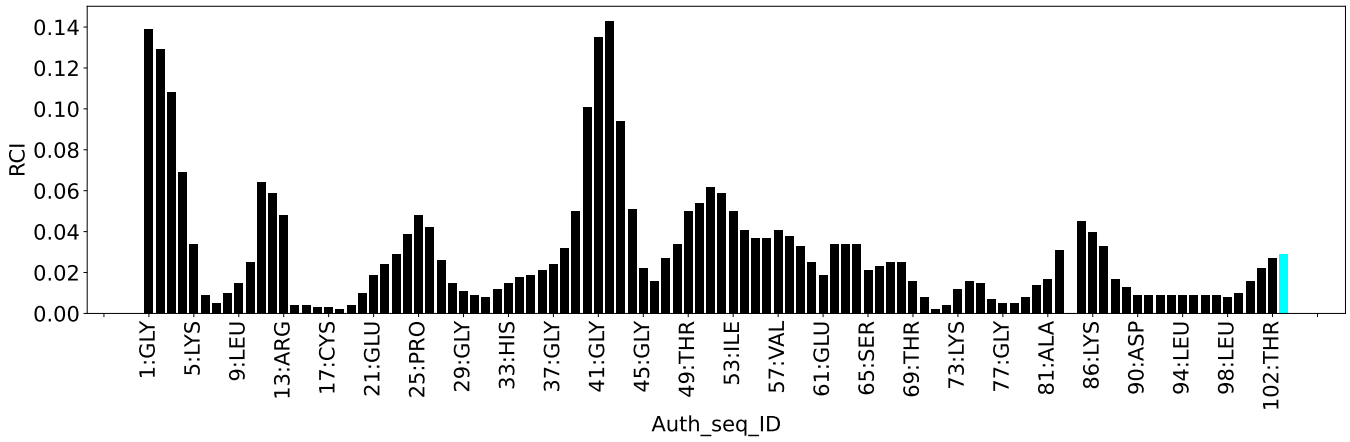
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	71	HIS	HD2	30.24	4.65 – 9.35	49.5
1	A	18	HIS	HE1	-11.98	5.13 – 10.76	-35.4
1	A	18	HIS	HD2	19.30	4.65 – 9.35	26.2
1	A	71	HIS	HA	10.27	2.49 – 6.71	13.4
1	A	18	HIS	HA	8.52	2.49 – 6.71	9.3
1	A	64	MET	HE1	-0.52	-0.03 – 3.80	-6.3
1	A	64	MET	HE2	-0.52	-0.03 – 3.80	-6.3
1	A	64	MET	HE3	-0.52	-0.03 – 3.80	-6.3
1	A	14	CYS	HA	1.47	1.97 – 7.35	-5.9
1	A	75	ILE	HB	3.27	0.35 – 3.22	5.2

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	1399
Intra-residue (|i-j|=0)	497
Sequential (|i-j|=1)	273
Medium range (|i-j|>1 and |i-j|<5)	268
Long range (|i-j|≥5)	312
Inter-chain	49
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	12.8
Number of long range restraints per residue[1]	2.9

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

8.2 Residual restraint violations (i)

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 (i)

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)	27.5	0.2
0.2-0.5 (Medium)	6.2	0.34
>0.5 (Large)	0.1	0.71

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

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

9 Distance violation analysis (i)

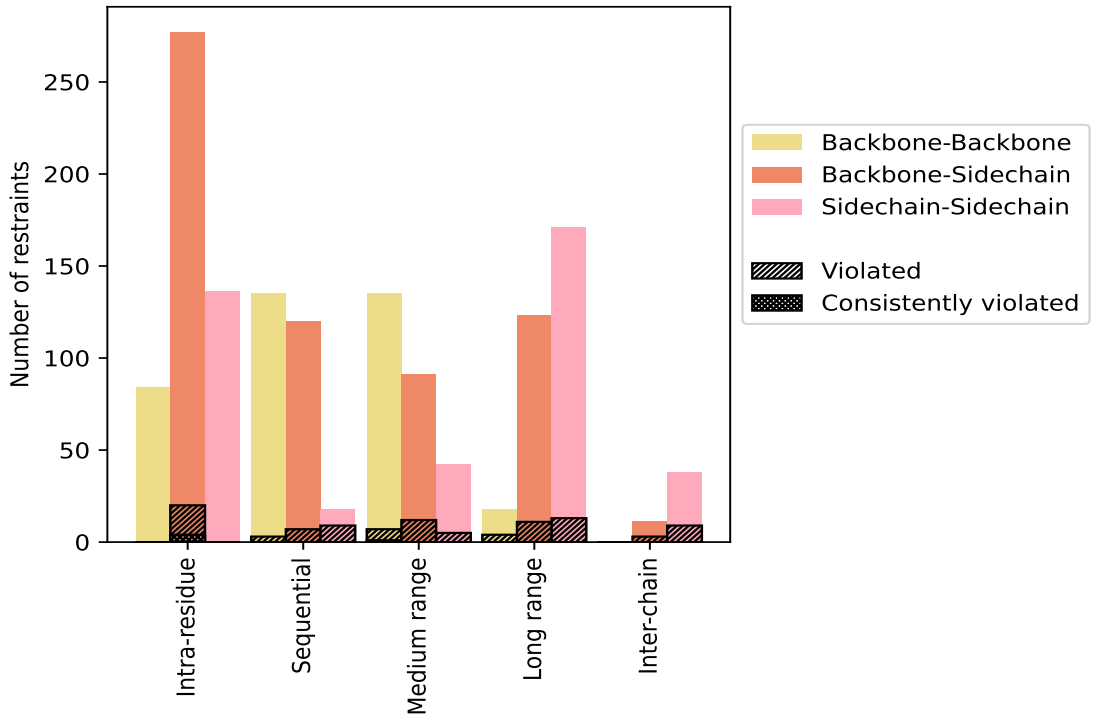
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	497	35.5	20	4.0	1.4	4	0.8	0.3
Backbone-Backbone	84	6.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	277	19.8	20	7.2	1.4	4	1.4	0.3
Sidechain-Sidechain	136	9.7	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	273	19.5	19	7.0	1.4	0	0.0	0.0
Backbone-Backbone	135	9.6	3	2.2	0.2	0	0.0	0.0
Backbone-Sidechain	120	8.6	7	5.8	0.5	0	0.0	0.0
Sidechain-Sidechain	18	1.3	9	50.0	0.6	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	268	19.2	24	9.0	1.7	1	0.4	0.1
Backbone-Backbone	135	9.6	7	5.2	0.5	1	0.7	0.1
Backbone-Sidechain	91	6.5	12	13.2	0.9	0	0.0	0.0
Sidechain-Sidechain	42	3.0	5	11.9	0.4	0	0.0	0.0
Long range (|i-j|≥5)	312	22.3	28	9.0	2.0	0	0.0	0.0
Backbone-Backbone	18	1.3	4	22.2	0.3	0	0.0	0.0
Backbone-Sidechain	123	8.8	11	8.9	0.8	0	0.0	0.0
Sidechain-Sidechain	171	12.2	13	7.6	0.9	0	0.0	0.0
Inter-chain	49	3.5	12	24.5	0.9	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	11	0.8	3	27.3	0.2	0	0.0	0.0
Sidechain-Sidechain	38	2.7	9	23.7	0.6	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1399	100.0	103	7.4	7.4	5	0.4	0.4
Backbone-Backbone	372	26.6	14	3.8	1.0	1	0.3	0.1
Backbone-Sidechain	622	44.5	53	8.5	3.8	4	0.6	0.3
Sidechain-Sidechain	405	28.9	36	8.9	2.6	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	12	10	7	9	1	39	0.15	0.24	0.05	0.13
2	9	7	12	11	4	43	0.16	0.34	0.05	0.14
3	13	5	6	5	5	34	0.16	0.24	0.05	0.15
4	10	4	4	8	0	26	0.16	0.25	0.05	0.13
5	10	6	9	5	5	35	0.16	0.25	0.04	0.14
6	10	7	10	10	2	39	0.16	0.26	0.04	0.15
7	9	7	8	6	4	34	0.15	0.27	0.04	0.14
8	10	5	8	5	3	31	0.15	0.28	0.04	0.14
9	9	4	8	6	2	29	0.15	0.23	0.04	0.14
10	12	8	10	5	5	40	0.15	0.32	0.05	0.13

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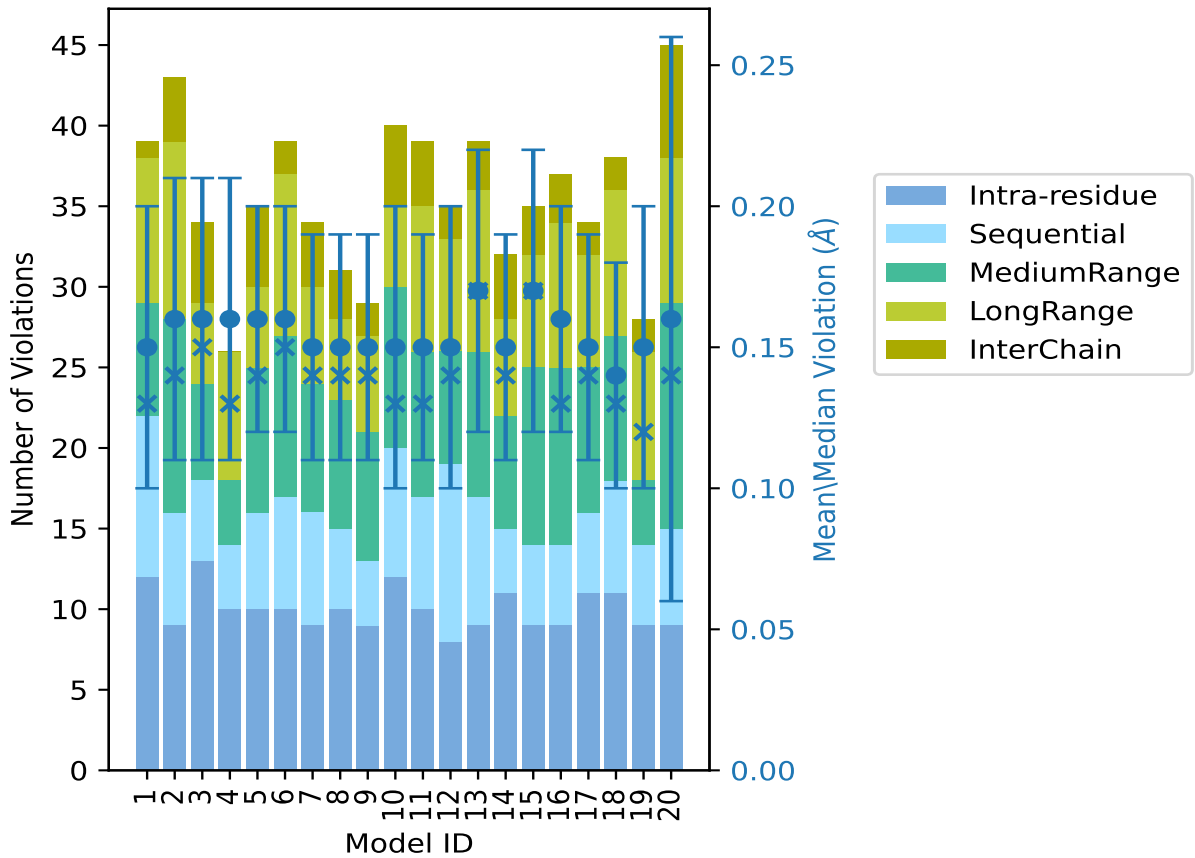
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	10	7	9	9	4	39	0.15	0.24	0.04	0.13
12	8	11	7	7	2	35	0.15	0.29	0.05	0.14
13	9	8	9	10	3	39	0.17	0.31	0.05	0.17
14	11	4	7	6	4	32	0.15	0.24	0.04	0.14
15	9	5	11	7	3	35	0.17	0.34	0.05	0.17
16	9	5	11	9	3	37	0.16	0.29	0.04	0.13
17	11	5	9	7	2	34	0.15	0.24	0.04	0.14
18	11	7	9	9	2	38	0.14	0.24	0.04	0.13
19	9	5	4	8	2	28	0.15	0.25	0.05	0.12
20	9	6	14	9	7	45	0.16	0.71	0.1	0.14

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

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



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

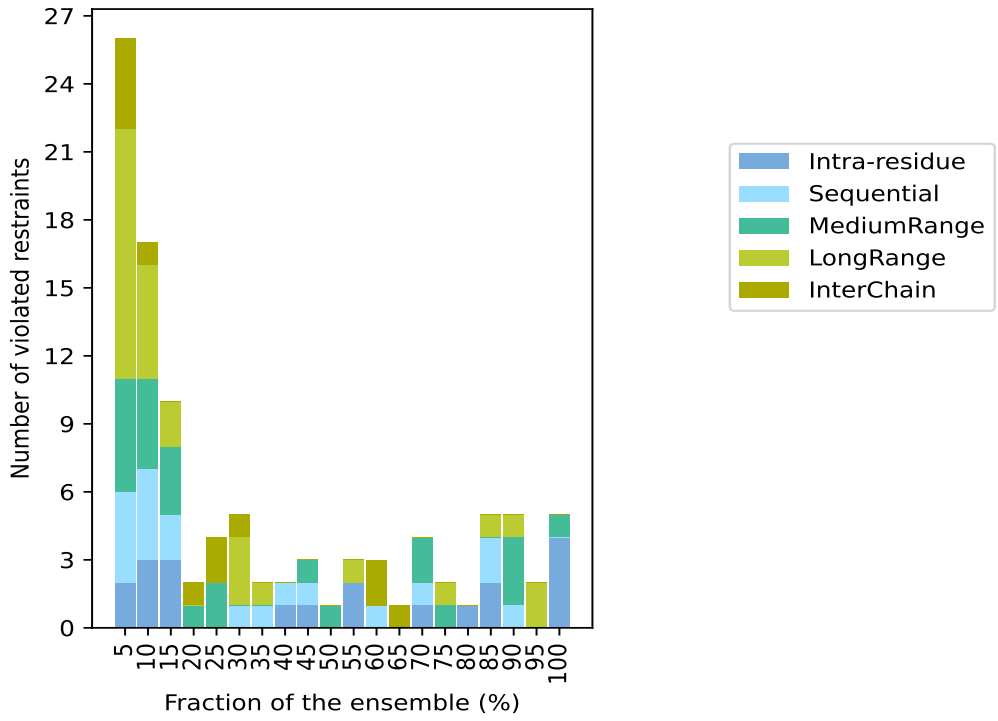
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1296(IR:477, SQ:254, MR:244, LR:284, IC:37) 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]	%
2	4	5	11	4	26	1	5.0
3	4	4	5	1	17	2	10.0
3	2	3	2	0	10	3	15.0
0	0	1	0	1	2	4	20.0
0	0	2	0	2	4	5	25.0
0	1	0	3	1	5	6	30.0
0	1	0	1	0	2	7	35.0
1	1	0	0	0	2	8	40.0
1	1	1	0	0	3	9	45.0
0	0	1	0	0	1	10	50.0
2	0	0	1	0	3	11	55.0
0	1	0	0	2	3	12	60.0
0	0	0	0	1	1	13	65.0
1	1	2	0	0	4	14	70.0
0	0	1	1	0	2	15	75.0
1	0	0	0	0	1	16	80.0
2	2	0	1	0	5	17	85.0
0	1	3	1	0	5	18	90.0
0	0	0	2	0	2	19	95.0
4	0	1	0	0	5	20	100.0

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

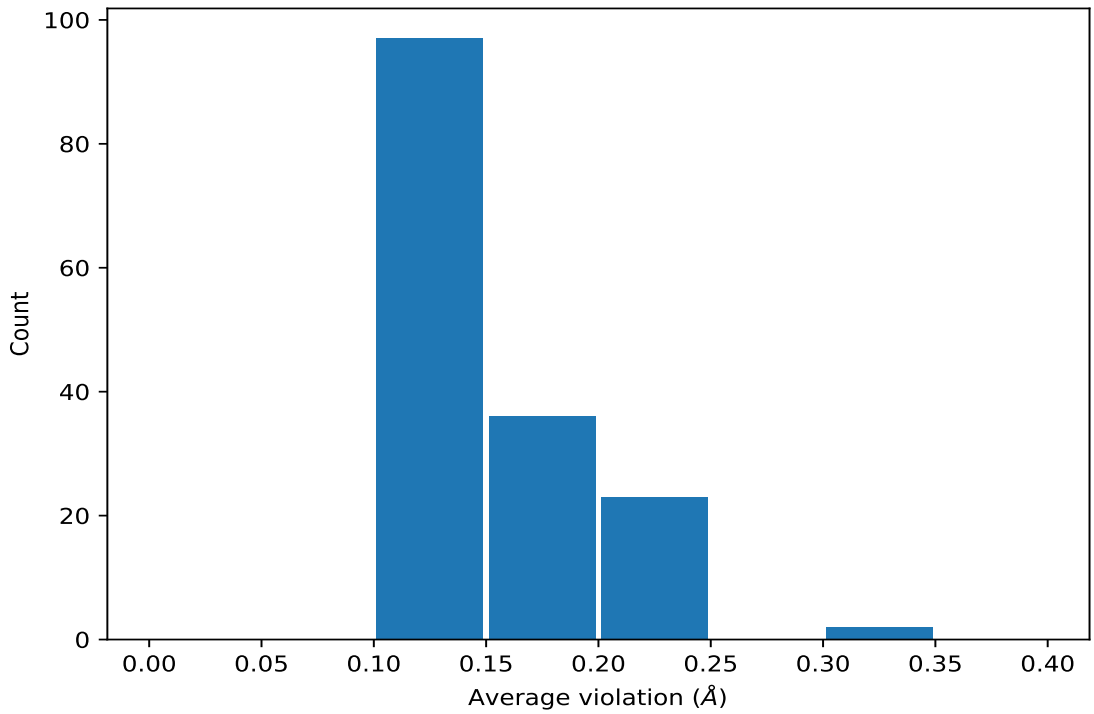
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	20	0.23	0.01	0.23
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	20	0.23	0.01	0.23
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	20	0.23	0.01	0.23
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	20	0.23	0.01	0.23
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	20	0.23	0.01	0.23
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	20	0.23	0.01	0.23
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	20	0.19	0.01	0.19
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	20	0.12	0.0	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	20	0.12	0.0	0.12
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	19	0.16	0.04	0.15
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	19	0.16	0.04	0.15
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	19	0.15	0.04	0.14
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	18	0.19	0.04	0.19
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	18	0.18	0.06	0.16
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	18	0.16	0.03	0.16
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	18	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	18	0.16	0.03	0.16
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	18	0.16	0.03	0.16
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	18	0.16	0.03	0.16
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	18	0.16	0.03	0.16
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	18	0.14	0.02	0.14
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	18	0.13	0.02	0.14
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	18	0.13	0.02	0.14
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	17	0.24	0.0	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	17	0.24	0.0	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	17	0.24	0.0	0.24
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	17	0.14	0.02	0.15
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	17	0.14	0.02	0.13
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	17	0.14	0.02	0.13
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	17	0.14	0.02	0.13
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	17	0.13	0.02	0.13
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	17	0.13	0.02	0.13
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	17	0.12	0.0	0.12
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	16	0.14	0.02	0.15
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	15	0.18	0.04	0.18
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	15	0.15	0.03	0.14
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	14	0.15	0.04	0.15
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	14	0.12	0.01	0.12
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	14	0.12	0.01	0.12
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	14	0.11	0.01	0.12
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	13	0.14	0.02	0.14
(1,803)	1:58:A:LEU:HD12	1:59:A:TRP:HD1	12	0.19	0.07	0.15
(1,803)	1:58:A:LEU:HD11	1:59:A:TRP:HD1	12	0.19	0.07	0.15
(1,803)	1:58:A:LEU:HD13	1:59:A:TRP:HD1	12	0.19	0.07	0.15
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD2	12	0.17	0.06	0.16
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD1	12	0.17	0.06	0.16
(1,1032)	1:72:A:ALA:HB1	2:104:A:HEC:HAA2	12	0.16	0.03	0.17
(1,1032)	1:72:A:ALA:HB2	2:104:A:HEC:HAA2	12	0.16	0.03	0.17
(1,1032)	1:72:A:ALA:HB3	2:104:A:HEC:HAA2	12	0.16	0.03	0.17
(1,342)	1:20:A:VAL:HA	1:33:A:HIS:H	11	0.17	0.03	0.17
(1,143)	1:9:A:LEU:HD11	1:9:A:LEU:H	11	0.12	0.01	0.11
(1,143)	1:9:A:LEU:HD12	1:9:A:LEU:H	11	0.12	0.01	0.11
(1,143)	1:9:A:LEU:HD13	1:9:A:LEU:H	11	0.12	0.01	0.11
(1,143)	1:9:A:LEU:HD21	1:9:A:LEU:H	11	0.12	0.01	0.11
(1,143)	1:9:A:LEU:HD22	1:9:A:LEU:H	11	0.12	0.01	0.11
(1,143)	1:9:A:LEU:HD23	1:9:A:LEU:H	11	0.12	0.01	0.11
(1,394)	1:28:A:VAL:HA	1:28:A:VAL:HB	11	0.12	0.01	0.12
(1,923)	1:64:A:MET:HE1	1:68:A:LEU:H	10	0.14	0.03	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,923)	1:64:A:MET:HE2	1:68:A:LEU:H	10	0.14	0.03	0.13
(1,923)	1:64:A:MET:HE3	1:68:A:LEU:H	10	0.14	0.03	0.13
(1,502)	1:36:A:PHE:HD1	1:33:A:HIS:HA	9	0.18	0.04	0.17
(1,502)	1:36:A:PHE:HD2	1:33:A:HIS:HA	9	0.18	0.04	0.17
(1,1029)	1:72:A:ALA:HB1	1:73:A:LYS:H	9	0.15	0.03	0.14
(1,1029)	1:72:A:ALA:HB2	1:73:A:LYS:H	9	0.15	0.03	0.14
(1,1029)	1:72:A:ALA:HB3	1:73:A:LYS:H	9	0.15	0.03	0.14
(1,745)	1:55:A:LYS:HB3	1:55:A:LYS:H	9	0.14	0.01	0.14
(1,445)	1:32:A:LEU:HB2	1:33:A:HIS:HB3	8	0.17	0.03	0.17
(1,445)	1:32:A:LEU:HB3	1:33:A:HIS:HB3	8	0.17	0.03	0.17
(1,1111)	1:85:A:LEU:HD11	1:85:A:LEU:H	8	0.12	0.02	0.12
(1,1111)	1:85:A:LEU:HD12	1:85:A:LEU:H	8	0.12	0.02	0.12
(1,1111)	1:85:A:LEU:HD13	1:85:A:LEU:H	8	0.12	0.02	0.12
(1,488)	1:35:A:ILE:HG23	1:59:A:TRP:HD1	7	0.24	0.06	0.23
(1,488)	1:35:A:ILE:HG21	1:59:A:TRP:HD1	7	0.24	0.06	0.23
(1,488)	1:35:A:ILE:HG22	1:59:A:TRP:HD1	7	0.24	0.06	0.23
(1,389)	1:27:A:LYS:HG2	1:28:A:VAL:H	7	0.23	0.06	0.24
(1,389)	1:27:A:LYS:HG3	1:28:A:VAL:H	7	0.23	0.06	0.24
(1,1384)	2:104:A:HEC:HAD1	1:79:A:LYS:HG3	6	0.19	0.05	0.2
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG21	6	0.18	0.04	0.18
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG22	6	0.18	0.04	0.18
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG23	6	0.18	0.04	0.18
(1,446)	1:32:A:LEU:HD11	1:42:A:GLN:H	6	0.17	0.03	0.16
(1,446)	1:32:A:LEU:HD12	1:42:A:GLN:H	6	0.17	0.03	0.16
(1,446)	1:32:A:LEU:HD13	1:42:A:GLN:H	6	0.17	0.03	0.16
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD21	6	0.14	0.04	0.14
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD22	6	0.14	0.04	0.14
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB2	6	0.14	0.02	0.14
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB3	6	0.14	0.02	0.14
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB2	6	0.14	0.02	0.14
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB3	6	0.14	0.02	0.14
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB2	6	0.14	0.02	0.14
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB3	6	0.14	0.02	0.14
(1,403)	1:28:A:VAL:HG11	2:104:A:HEC:HHD	5	0.34	0.2	0.34
(1,403)	1:28:A:VAL:HG12	2:104:A:HEC:HHD	5	0.34	0.2	0.34
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC1	5	0.13	0.03	0.12
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC2	5	0.13	0.03	0.12
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC3	5	0.13	0.03	0.12
(1,224)	1:11:A:LYS:HA	1:14:A:CYS:HB2	5	0.12	0.01	0.11
(1,224)	1:11:A:LYS:HA	1:14:A:CYS:HB3	5	0.12	0.01	0.11
(1,62)	1:2:A:SER:H	1:4:A:LYS:HE2	5	0.11	0.0	0.11
(1,62)	1:2:A:SER:H	1:4:A:LYS:HE3	5	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1053)	1:75:A:ILE:HD11	1:78:A:THR:H	4	0.21	0.02	0.21
(1,1053)	1:75:A:ILE:HD12	1:78:A:THR:H	4	0.21	0.02	0.21
(1,1053)	1:75:A:ILE:HD13	1:78:A:THR:H	4	0.21	0.02	0.21
(1,1383)	2:104:A:HEC:HAD1	1:46:A:TYR:HD1	4	0.13	0.03	0.12
(1,1383)	2:104:A:HEC:HAD1	1:46:A:TYR:HD2	4	0.13	0.03	0.12
(1,1383)	2:104:A:HEC:HAD2	1:46:A:TYR:HD1	4	0.13	0.03	0.12
(1,1383)	2:104:A:HEC:HAD2	1:46:A:TYR:HD2	4	0.13	0.03	0.12
(1,121)	1:8:A:THR:HG21	1:8:A:THR:H	3	0.24	0.0	0.24
(1,121)	1:8:A:THR:HG22	1:8:A:THR:H	3	0.24	0.0	0.24
(1,121)	1:8:A:THR:HG23	1:8:A:THR:H	3	0.24	0.0	0.24
(1,299)	1:18:A:HIS:HB2	1:18:A:HIS:H	3	0.22	0.01	0.22
(1,621)	1:45:A:GLY:HA2	1:26:A:HIS:HD1	3	0.18	0.01	0.19
(1,621)	1:45:A:GLY:HA3	1:26:A:HIS:HD1	3	0.18	0.01	0.19
(1,419)	1:30:A:PRO:HA	1:31:A:ASN:HA	3	0.15	0.02	0.16
(1,1105)	1:82:A:PHE:HZ	1:85:A:LEU:HG	3	0.14	0.02	0.15
(1,413)	1:29:A:GLY:HA2	1:31:A:ASN:HD21	3	0.13	0.02	0.13
(1,413)	1:29:A:GLY:HA3	1:31:A:ASN:HD21	3	0.13	0.02	0.13
(1,122)	1:8:A:THR:HB	1:8:A:THR:HA	3	0.12	0.0	0.12
(1,547)	1:38:A:ARG:HD2	1:39:A:HIS:HE1	3	0.12	0.01	0.11
(1,547)	1:38:A:ARG:HD3	1:39:A:HIS:HE1	3	0.12	0.01	0.11
(1,1227)	1:94:A:LEU:HG	1:98:A:LEU:HG	3	0.12	0.0	0.12
(1,208)	1:10:A:PHE:HZ	1:19:A:THR:HB	3	0.11	0.0	0.11
(1,420)	1:30:A:PRO:HB2	1:32:A:LEU:H	2	0.2	0.09	0.2
(1,420)	1:30:A:PRO:HB3	1:32:A:LEU:H	2	0.2	0.09	0.2
(1,401)	1:28:A:VAL:HB	1:29:A:GLY:H	2	0.18	0.02	0.18
(1,636)	1:46:A:TYR:HD2	1:48:A:TYR:H	2	0.17	0.03	0.17
(1,1102)	1:82:A:PHE:HZ	2:104:A:HEC:HHC	2	0.15	0.01	0.15
(1,430)	1:30:A:PRO:HB2	1:46:A:TYR:HA	2	0.15	0.0	0.15
(1,430)	1:30:A:PRO:HB3	1:46:A:TYR:HA	2	0.15	0.0	0.15
(1,440)	1:32:A:LEU:HD11	1:32:A:LEU:H	2	0.14	0.03	0.14
(1,440)	1:32:A:LEU:HD12	1:32:A:LEU:H	2	0.14	0.03	0.14
(1,440)	1:32:A:LEU:HD13	1:32:A:LEU:H	2	0.14	0.03	0.14
(1,440)	1:32:A:LEU:HD21	1:32:A:LEU:H	2	0.14	0.03	0.14
(1,440)	1:32:A:LEU:HD22	1:32:A:LEU:H	2	0.14	0.03	0.14
(1,440)	1:32:A:LEU:HD23	1:32:A:LEU:H	2	0.14	0.03	0.14
(1,467)	1:35:A:ILE:HA	1:35:A:ILE:HB	2	0.12	0.01	0.12
(1,987)	1:68:A:LEU:HG	1:69:A:THR:H	2	0.12	0.01	0.12
(1,210)	1:10:A:PHE:HZ	1:20:A:VAL:HB	2	0.12	0.02	0.12
(1,134)	1:8:A:THR:HB	1:11:A:LYS:HG2	2	0.12	0.01	0.12
(1,134)	1:8:A:THR:HB	1:11:A:LYS:HG3	2	0.12	0.01	0.12
(1,359)	1:23:A:GLY:H	1:33:A:HIS:HB2	2	0.12	0.0	0.12
(1,359)	1:23:A:GLY:H	1:33:A:HIS:HB3	2	0.12	0.0	0.12

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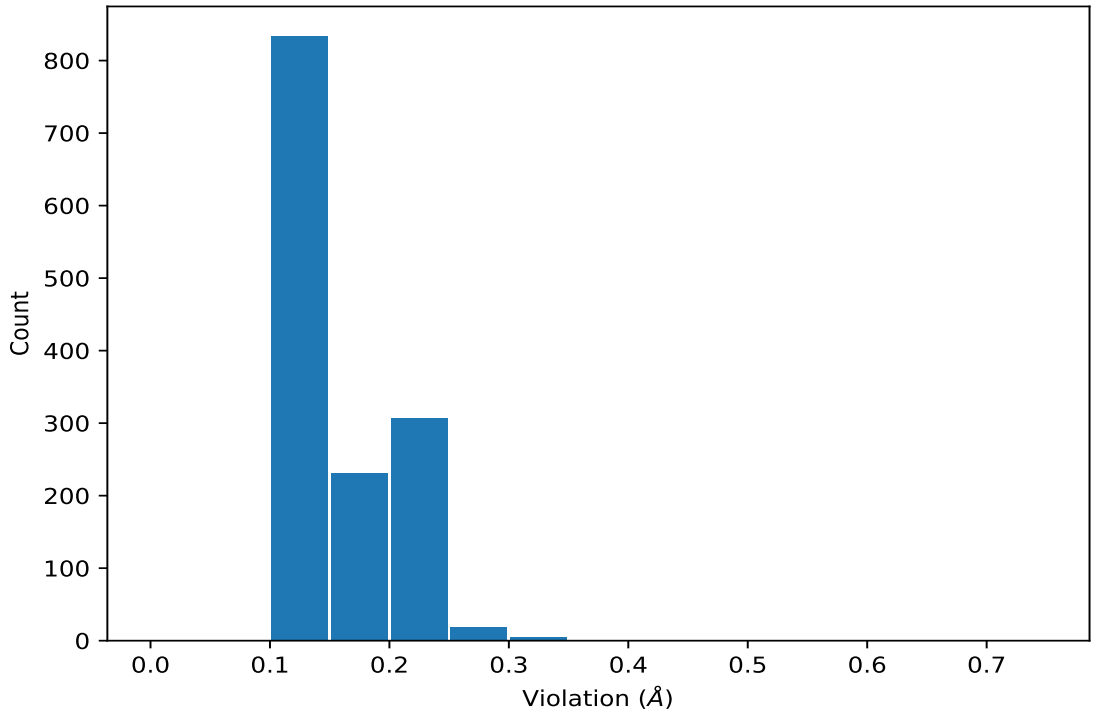
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,444)	1:32:A:LEU:HD11	1:35:A:ILE:H	2	0.12	0.0	0.12
(1,444)	1:32:A:LEU:HD12	1:35:A:ILE:H	2	0.12	0.0	0.12
(1,444)	1:32:A:LEU:HD13	1:35:A:ILE:H	2	0.12	0.0	0.12
(1,453)	1:34:A:GLY:HA2	1:33:A:HIS:H	2	0.12	0.0	0.12
(1,453)	1:34:A:GLY:HA3	1:33:A:HIS:H	2	0.12	0.0	0.12
(1,1263)	1:95:A:ILE:HG21	1:94:A:LEU:H	2	0.12	0.0	0.12
(1,1263)	1:95:A:ILE:HG22	1:94:A:LEU:H	2	0.12	0.0	0.12
(1,1263)	1:95:A:ILE:HG23	1:94:A:LEU:H	2	0.12	0.0	0.12
(1,996)	1:69:A:THR:HB	1:69:A:THR:H	2	0.11	0.0	0.11
(1,1030)	1:72:A:ALA:H	1:78:A:THR:HB	2	0.11	0.01	0.11
(1,200)	1:10:A:PHE:HE1	1:19:A:THR:HG21	2	0.1	0.0	0.1
(1,200)	1:10:A:PHE:HE1	1:19:A:THR:HG22	2	0.1	0.0	0.1
(1,200)	1:10:A:PHE:HE1	1:19:A:THR:HG23	2	0.1	0.0	0.1
(1,200)	1:10:A:PHE:HE2	1:19:A:THR:HG21	2	0.1	0.0	0.1
(1,200)	1:10:A:PHE:HE2	1:19:A:THR:HG22	2	0.1	0.0	0.1
(1,200)	1:10:A:PHE:HE2	1:19:A:THR:HG23	2	0.1	0.0	0.1

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,403)	1:28:A:VAL:HG12	2:104:A:HEC:HHD	20	0.71
(1,488)	1:35:A:ILE:HG21	1:59:A:TRP:HD1	20	0.34
(1,403)	1:28:A:VAL:HG11	2:104:A:HEC:HHD	2	0.34
(1,403)	1:28:A:VAL:HG12	2:104:A:HEC:HHD	15	0.34
(1,803)	1:58:A:LEU:HD11	1:59:A:TRP:HD1	10	0.32
(1,803)	1:58:A:LEU:HD11	1:59:A:TRP:HD1	13	0.31
(1,488)	1:35:A:ILE:HG21	1:59:A:TRP:HD1	16	0.29
(1,420)	1:30:A:PRO:HB2	1:32:A:LEU:H	10	0.29
(1,420)	1:30:A:PRO:HB3	1:32:A:LEU:H	10	0.29
(1,389)	1:27:A:LYS:HG2	1:28:A:VAL:H	12	0.29
(1,389)	1:27:A:LYS:HG3	1:28:A:VAL:H	12	0.29
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD2	13	0.28
(1,803)	1:58:A:LEU:HD11	1:59:A:TRP:HD1	8	0.28
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	2	0.28
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD1	7	0.27
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	13	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	6	0.26
(1,389)	1:27:A:LYS:HG2	1:28:A:VAL:H	13	0.26
(1,389)	1:27:A:LYS:HG3	1:28:A:VAL:H	13	0.26
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	4	0.25
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	4	0.25
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	4	0.25
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	19	0.25
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	5	0.25
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	1	0.24
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	1	0.24
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	1	0.24
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	3	0.24
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	3	0.24
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	3	0.24
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	12	0.24
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	12	0.24
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	12	0.24
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	13	0.24
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	13	0.24
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	13	0.24
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	5	0.24
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	5	0.24
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	5	0.24
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	7	0.24
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	7	0.24
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	7	0.24
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	14	0.24
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	14	0.24
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	14	0.24
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	15	0.24
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	15	0.24
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	15	0.24
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	18	0.24
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	18	0.24
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	18	0.24
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	19	0.24
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	19	0.24
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	19	0.24
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	3	0.24
(1,1053)	1:75:A:ILE:HD11	1:78:A:THR:H	10	0.24
(1,1053)	1:75:A:ILE:HD12	1:78:A:THR:H	10	0.24
(1,1053)	1:75:A:ILE:HD13	1:78:A:THR:H	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	1	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	1	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	1	0.24
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	2	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	2	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	2	0.24
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	4	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	4	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	4	0.24
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	7	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	7	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	7	0.24
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	10	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	10	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	10	0.24
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	11	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	11	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	11	0.24
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	13	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	13	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	13	0.24
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	14	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	14	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	14	0.24
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	15	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	15	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	15	0.24
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	16	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	16	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	16	0.24
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	17	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	17	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	17	0.24
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	18	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	18	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	18	0.24
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	20	0.24
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	20	0.24
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	20	0.24
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	2	0.24
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	20	0.24
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	1	0.24
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	1	0.24
(1,502)	1:36:A:PHE:HD1	1:33:A:HIS:HA	5	0.24
(1,502)	1:36:A:PHE:HD2	1:33:A:HIS:HA	5	0.24
(1,389)	1:27:A:LYS:HG2	1:28:A:VAL:H	1	0.24
(1,389)	1:27:A:LYS:HG3	1:28:A:VAL:H	1	0.24
(1,389)	1:27:A:LYS:HG2	1:28:A:VAL:H	5	0.24
(1,389)	1:27:A:LYS:HG3	1:28:A:VAL:H	5	0.24
(1,389)	1:27:A:LYS:HG2	1:28:A:VAL:H	11	0.24
(1,389)	1:27:A:LYS:HG3	1:28:A:VAL:H	11	0.24
(1,121)	1:8:A:THR:HG21	1:8:A:THR:H	3	0.24
(1,121)	1:8:A:THR:HG22	1:8:A:THR:H	3	0.24
(1,121)	1:8:A:THR:HG23	1:8:A:THR:H	3	0.24
(1,121)	1:8:A:THR:HG21	1:8:A:THR:H	4	0.24
(1,121)	1:8:A:THR:HG22	1:8:A:THR:H	4	0.24
(1,121)	1:8:A:THR:HG23	1:8:A:THR:H	4	0.24
(1,121)	1:8:A:THR:HG21	1:8:A:THR:H	13	0.24
(1,121)	1:8:A:THR:HG22	1:8:A:THR:H	13	0.24
(1,121)	1:8:A:THR:HG23	1:8:A:THR:H	13	0.24
(1,1384)	2:104:A:HEC:HAD1	1:79:A:LYS:HG3	3	0.23
(1,1384)	2:104:A:HEC:HAD1	1:79:A:LYS:HG3	11	0.23
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	4	0.23
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	4	0.23
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	4	0.23
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	5	0.23
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	5	0.23
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	5	0.23
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	6	0.23
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	6	0.23
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	6	0.23
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	8	0.23
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	8	0.23
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	8	0.23
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	9	0.23
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	9	0.23
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	9	0.23
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	10	0.23
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	10	0.23
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	10	0.23
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	11	0.23
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	11	0.23
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	14	0.23
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	14	0.23
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	14	0.23
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	16	0.23
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	16	0.23
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	16	0.23
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	17	0.23
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	17	0.23
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	17	0.23
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	18	0.23
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	18	0.23
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	18	0.23
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	19	0.23
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	19	0.23
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	19	0.23
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	1	0.23
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	1	0.23
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	1	0.23
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	6	0.23
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	6	0.23
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	6	0.23
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	9	0.23
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	9	0.23
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	9	0.23
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	11	0.23
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	11	0.23
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	11	0.23
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	13	0.23
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	13	0.23
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	13	0.23
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	3	0.23
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	3	0.23
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	3	0.23
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	6	0.23
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	6	0.23
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	6	0.23
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	9	0.23
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	9	0.23
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	9	0.23
(1,997)	1:69:A:THR:HG21	1:69:A:THR:H	19	0.23
(1,997)	1:69:A:THR:HG22	1:69:A:THR:H	19	0.23
(1,997)	1:69:A:THR:HG23	1:69:A:THR:H	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	14	0.23
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	16	0.23
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	16	0.23
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	3	0.23
(1,488)	1:35:A:ILE:HG23	1:59:A:TRP:HD1	1	0.23
(1,488)	1:35:A:ILE:HG22	1:59:A:TRP:HD1	13	0.23
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG21	10	0.23
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG22	10	0.23
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG23	10	0.23
(1,299)	1:18:A:HIS:HB2	1:18:A:HIS:H	12	0.23
(1,1384)	2:104:A:HEC:HAD1	1:79:A:LYS:HG3	5	0.22
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	2	0.22
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	2	0.22
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	2	0.22
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	7	0.22
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	7	0.22
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	7	0.22
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	15	0.22
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	15	0.22
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	15	0.22
(1,1269)	1:96:A:THR:HG21	1:96:A:THR:H	20	0.22
(1,1269)	1:96:A:THR:HG22	1:96:A:THR:H	20	0.22
(1,1269)	1:96:A:THR:HG23	1:96:A:THR:H	20	0.22
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	2	0.22
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	2	0.22
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	2	0.22
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	3	0.22
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	3	0.22
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	3	0.22
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	8	0.22
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	8	0.22
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	8	0.22
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	10	0.22
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	10	0.22
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	10	0.22
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	12	0.22
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	12	0.22
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	12	0.22
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	20	0.22
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	20	0.22
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	20	0.22
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	15	0.22
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	18	0.22
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	15	0.22
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	19	0.22
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	3	0.22
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	15	0.22
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	6	0.22
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	6	0.22
(1,502)	1:36:A:PHE:HD1	1:33:A:HIS:HA	15	0.22
(1,502)	1:36:A:PHE:HD2	1:33:A:HIS:HA	15	0.22
(1,488)	1:35:A:ILE:HG21	1:59:A:TRP:HD1	2	0.22
(1,446)	1:32:A:LEU:HD11	1:42:A:GLN:H	2	0.22
(1,446)	1:32:A:LEU:HD12	1:42:A:GLN:H	2	0.22
(1,446)	1:32:A:LEU:HD13	1:42:A:GLN:H	2	0.22
(1,445)	1:32:A:LEU:HB2	1:33:A:HIS:HB3	6	0.22
(1,445)	1:32:A:LEU:HB3	1:33:A:HIS:HB3	6	0.22
(1,389)	1:27:A:LYS:HG2	1:28:A:VAL:H	8	0.22
(1,389)	1:27:A:LYS:HG3	1:28:A:VAL:H	8	0.22
(1,342)	1:20:A:VAL:HA	1:33:A:HIS:H	5	0.22
(1,299)	1:18:A:HIS:HB2	1:18:A:HIS:H	6	0.22
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	16	0.21
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	16	0.21
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	16	0.21
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	16	0.21
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	16	0.21
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	16	0.21
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	17	0.21
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	17	0.21
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	17	0.21
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	17	0.21
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	17	0.21
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	17	0.21
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	16	0.21
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	16	0.21
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	16	0.21
(1,1241)	1:95:A:ILE:HG21	1:95:A:ILE:H	17	0.21
(1,1241)	1:95:A:ILE:HG22	1:95:A:ILE:H	17	0.21
(1,1241)	1:95:A:ILE:HG23	1:95:A:ILE:H	17	0.21
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	6	0.21
(1,1097)	1:82:A:PHE:H	1:81:A:ALA:H	12	0.21
(1,1053)	1:75:A:ILE:HD11	1:78:A:THR:H	9	0.21
(1,1053)	1:75:A:ILE:HD12	1:78:A:THR:H	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1053)	1:75:A:ILE:HD13	1:78:A:THR:H	9	0.21
(1,1053)	1:75:A:ILE:HD11	1:78:A:THR:H	15	0.21
(1,1053)	1:75:A:ILE:HD12	1:78:A:THR:H	15	0.21
(1,1053)	1:75:A:ILE:HD13	1:78:A:THR:H	15	0.21
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	3	0.21
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	16	0.21
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	15	0.21
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	20	0.21
(1,342)	1:20:A:VAL:HA	1:33:A:HIS:H	2	0.21
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD2	10	0.2
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD2	17	0.2
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	1	0.2
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	3	0.2
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	12	0.2
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	17	0.2
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	18	0.2
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	20	0.2
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	2	0.2
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	2	0.2
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	2	0.2
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	2	0.2
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	2	0.2
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	2	0.2
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	20	0.2
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	20	0.2
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	20	0.2
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	20	0.2
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	20	0.2
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	20	0.2
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	15	0.2
(1,1032)	1:72:A:ALA:HB1	2:104:A:HEC:HAA2	3	0.2
(1,1032)	1:72:A:ALA:HB2	2:104:A:HEC:HAA2	3	0.2
(1,1032)	1:72:A:ALA:HB3	2:104:A:HEC:HAA2	3	0.2
(1,1032)	1:72:A:ALA:HB1	2:104:A:HEC:HAA2	6	0.2
(1,1032)	1:72:A:ALA:HB2	2:104:A:HEC:HAA2	6	0.2
(1,1032)	1:72:A:ALA:HB3	2:104:A:HEC:HAA2	6	0.2
(1,1032)	1:72:A:ALA:HB1	2:104:A:HEC:HAA2	12	0.2
(1,1032)	1:72:A:ALA:HB2	2:104:A:HEC:HAA2	12	0.2
(1,1032)	1:72:A:ALA:HB3	2:104:A:HEC:HAA2	12	0.2
(1,1029)	1:72:A:ALA:HB1	1:73:A:LYS:H	7	0.2
(1,1029)	1:72:A:ALA:HB2	1:73:A:LYS:H	7	0.2
(1,1029)	1:72:A:ALA:HB3	1:73:A:LYS:H	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	1:64:A:MET:HE1	1:68:A:LEU:H	5	0.2
(1,923)	1:64:A:MET:HE2	1:68:A:LEU:H	5	0.2
(1,923)	1:64:A:MET:HE3	1:68:A:LEU:H	5	0.2
(1,636)	1:46:A:TYR:HD2	1:48:A:TYR:H	20	0.2
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	12	0.2
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	1	0.2
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	7	0.2
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	4	0.2
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	4	0.2
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	13	0.2
(1,502)	1:36:A:PHE:HD1	1:33:A:HIS:HA	2	0.2
(1,502)	1:36:A:PHE:HD2	1:33:A:HIS:HA	2	0.2
(1,502)	1:36:A:PHE:HD1	1:33:A:HIS:HA	6	0.2
(1,502)	1:36:A:PHE:HD2	1:33:A:HIS:HA	6	0.2
(1,401)	1:28:A:VAL:HB	1:29:A:GLY:H	6	0.2
(1,342)	1:20:A:VAL:HA	1:33:A:HIS:H	15	0.2
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG21	11	0.2
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG22	11	0.2
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG23	11	0.2
(1,299)	1:18:A:HIS:HB2	1:18:A:HIS:H	18	0.2
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	6	0.2
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD2	2	0.19
(1,1384)	2:104:A:HEC:HAD1	1:79:A:LYS:HG3	10	0.19
(1,1383)	2:104:A:HEC:HAD1	1:46:A:TYR:HD1	6	0.19
(1,1383)	2:104:A:HEC:HAD1	1:46:A:TYR:HD2	6	0.19
(1,1383)	2:104:A:HEC:HAD2	1:46:A:TYR:HD1	6	0.19
(1,1383)	2:104:A:HEC:HAD2	1:46:A:TYR:HD2	6	0.19
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	2	0.19
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	4	0.19
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	6	0.19
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	7	0.19
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	8	0.19
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	9	0.19
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	14	0.19
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	15	0.19
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	19	0.19
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	5	0.19
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	5	0.19
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	5	0.19
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	5	0.19
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	5	0.19
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	20	0.19
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC1	5	0.19
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC2	5	0.19
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC3	5	0.19
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	9	0.19
(1,1032)	1:72:A:ALA:HB1	2:104:A:HEC:HAA2	18	0.19
(1,1032)	1:72:A:ALA:HB2	2:104:A:HEC:HAA2	18	0.19
(1,1032)	1:72:A:ALA:HB3	2:104:A:HEC:HAA2	18	0.19
(1,1029)	1:72:A:ALA:HB1	1:73:A:LYS:H	5	0.19
(1,1029)	1:72:A:ALA:HB2	1:73:A:LYS:H	5	0.19
(1,1029)	1:72:A:ALA:HB3	1:73:A:LYS:H	5	0.19
(1,803)	1:58:A:LEU:HD12	1:59:A:TRP:HD1	12	0.19
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	15	0.19
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	8	0.19
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	9	0.19
(1,621)	1:45:A:GLY:HA2	1:26:A:HIS:HD1	1	0.19
(1,621)	1:45:A:GLY:HA3	1:26:A:HIS:HD1	1	0.19
(1,621)	1:45:A:GLY:HA2	1:26:A:HIS:HD1	13	0.19
(1,621)	1:45:A:GLY:HA3	1:26:A:HIS:HD1	13	0.19
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	9	0.19
(1,488)	1:35:A:ILE:HG21	1:59:A:TRP:HD1	18	0.19
(1,446)	1:32:A:LEU:HD11	1:42:A:GLN:H	13	0.19
(1,446)	1:32:A:LEU:HD12	1:42:A:GLN:H	13	0.19
(1,446)	1:32:A:LEU:HD13	1:42:A:GLN:H	13	0.19
(1,445)	1:32:A:LEU:HB2	1:33:A:HIS:HB3	16	0.19
(1,445)	1:32:A:LEU:HB3	1:33:A:HIS:HB3	16	0.19
(1,445)	1:32:A:LEU:HB2	1:33:A:HIS:HB3	18	0.19
(1,445)	1:32:A:LEU:HB3	1:33:A:HIS:HB3	18	0.19
(1,403)	1:28:A:VAL:HG12	2:104:A:HEC:HHD	16	0.19
(1,342)	1:20:A:VAL:HA	1:33:A:HIS:H	4	0.19
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD21	11	0.19
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD22	11	0.19
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD21	17	0.19
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD22	17	0.19
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	5	0.18
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	10	0.18
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	11	0.18
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	13	0.18
(1,1340)	1:101:A:ALA:H	1:103:A:GLU:H	16	0.18
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	12	0.18
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	12	0.18
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	12	0.18
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	12	0.18
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	12	0.18
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	13	0.18
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	13	0.18
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	13	0.18
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	13	0.18
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	13	0.18
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	13	0.18
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	11	0.18
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	10	0.18
(1,1053)	1:75:A:ILE:HD11	1:78:A:THR:H	13	0.18
(1,1053)	1:75:A:ILE:HD12	1:78:A:THR:H	13	0.18
(1,1053)	1:75:A:ILE:HD13	1:78:A:THR:H	13	0.18
(1,923)	1:64:A:MET:HE1	1:68:A:LEU:H	15	0.18
(1,923)	1:64:A:MET:HE2	1:68:A:LEU:H	15	0.18
(1,923)	1:64:A:MET:HE3	1:68:A:LEU:H	15	0.18
(1,803)	1:58:A:LEU:HD12	1:59:A:TRP:HD1	3	0.18
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	20	0.18
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	4	0.18
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	6	0.18
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	7	0.18
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	17	0.18
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	15	0.18
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	15	0.18
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	14	0.18
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG21	1	0.18
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG22	1	0.18
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG23	1	0.18
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG21	19	0.18
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG22	19	0.18
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG23	19	0.18
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD2	14	0.17
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	3	0.17
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	3	0.17
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	3	0.17
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	3	0.17
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	3	0.17
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	3	0.17
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	2	0.17
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	7	0.17
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	2	0.17
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	13	0.17
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	20	0.17
(1,1032)	1:72:A:ALA:HB1	2:104:A:HEC:HAA2	2	0.17
(1,1032)	1:72:A:ALA:HB2	2:104:A:HEC:HAA2	2	0.17
(1,1032)	1:72:A:ALA:HB3	2:104:A:HEC:HAA2	2	0.17
(1,1032)	1:72:A:ALA:HB1	2:104:A:HEC:HAA2	8	0.17
(1,1032)	1:72:A:ALA:HB2	2:104:A:HEC:HAA2	8	0.17
(1,1032)	1:72:A:ALA:HB3	2:104:A:HEC:HAA2	8	0.17
(1,1032)	1:72:A:ALA:HB1	2:104:A:HEC:HAA2	10	0.17
(1,1032)	1:72:A:ALA:HB2	2:104:A:HEC:HAA2	10	0.17
(1,1032)	1:72:A:ALA:HB3	2:104:A:HEC:HAA2	10	0.17
(1,1029)	1:72:A:ALA:HB1	1:73:A:LYS:H	11	0.17
(1,1029)	1:72:A:ALA:HB2	1:73:A:LYS:H	11	0.17
(1,1029)	1:72:A:ALA:HB3	1:73:A:LYS:H	11	0.17
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	8	0.17
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	8	0.17
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	8	0.17
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	15	0.17
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	15	0.17
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	15	0.17
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	17	0.17
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	17	0.17
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	17	0.17
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	14	0.17
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	16	0.17
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	16	0.17
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	3	0.17
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	3	0.17
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	9	0.17
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	9	0.17
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	13	0.17
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	13	0.17
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	18	0.17
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	18	0.17
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	7	0.17
(1,502)	1:36:A:PHE:HD1	1:33:A:HIS:HA	16	0.17
(1,502)	1:36:A:PHE:HD2	1:33:A:HIS:HA	16	0.17
(1,445)	1:32:A:LEU:HB2	1:33:A:HIS:HB3	12	0.17
(1,445)	1:32:A:LEU:HB3	1:33:A:HIS:HB3	12	0.17
(1,445)	1:32:A:LEU:HB2	1:33:A:HIS:HB3	15	0.17
(1,445)	1:32:A:LEU:HB3	1:33:A:HIS:HB3	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:32:A:LEU:HD11	1:32:A:LEU:H	14	0.17
(1,440)	1:32:A:LEU:HD12	1:32:A:LEU:H	14	0.17
(1,440)	1:32:A:LEU:HD13	1:32:A:LEU:H	14	0.17
(1,440)	1:32:A:LEU:HD21	1:32:A:LEU:H	14	0.17
(1,440)	1:32:A:LEU:HD22	1:32:A:LEU:H	14	0.17
(1,440)	1:32:A:LEU:HD23	1:32:A:LEU:H	14	0.17
(1,419)	1:30:A:PRO:HA	1:31:A:ASN:HA	13	0.17
(1,401)	1:28:A:VAL:HB	1:29:A:GLY:H	12	0.17
(1,342)	1:20:A:VAL:HA	1:33:A:HIS:H	11	0.17
(1,342)	1:20:A:VAL:HA	1:33:A:HIS:H	13	0.17
(1,342)	1:20:A:VAL:HA	1:33:A:HIS:H	20	0.17
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD2	15	0.16
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	7	0.16
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	14	0.16
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	17	0.16
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	8	0.16
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	8	0.16
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	8	0.16
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	8	0.16
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	8	0.16
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	8	0.16
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	9	0.16
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	9	0.16
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	9	0.16
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	9	0.16
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	9	0.16
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	9	0.16
(1,1102)	1:82:A:PHE:HZ	2:104:A:HEC:HHC	7	0.16
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	5	0.16
(1,1032)	1:72:A:ALA:HB1	2:104:A:HEC:HAA2	5	0.16
(1,1032)	1:72:A:ALA:HB2	2:104:A:HEC:HAA2	5	0.16
(1,1032)	1:72:A:ALA:HB3	2:104:A:HEC:HAA2	5	0.16
(1,1032)	1:72:A:ALA:HB1	2:104:A:HEC:HAA2	9	0.16
(1,1032)	1:72:A:ALA:HB2	2:104:A:HEC:HAA2	9	0.16
(1,1032)	1:72:A:ALA:HB3	2:104:A:HEC:HAA2	9	0.16
(1,1029)	1:72:A:ALA:HB1	1:73:A:LYS:H	1	0.16
(1,1029)	1:72:A:ALA:HB2	1:73:A:LYS:H	1	0.16
(1,1029)	1:72:A:ALA:HB3	1:73:A:LYS:H	1	0.16
(1,923)	1:64:A:MET:HE1	1:68:A:LEU:H	6	0.16
(1,923)	1:64:A:MET:HE2	1:68:A:LEU:H	6	0.16
(1,923)	1:64:A:MET:HE3	1:68:A:LEU:H	6	0.16
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	16	0.16
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	16	0.16
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	1	0.16
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	10	0.16
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	10	0.16
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	1	0.16
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	7	0.16
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	12	0.16
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	15	0.16
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	13	0.16
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	13	0.16
(1,621)	1:45:A:GLY:HA2	1:26:A:HIS:HD1	14	0.16
(1,621)	1:45:A:GLY:HA3	1:26:A:HIS:HD1	14	0.16
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	1	0.16
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB2	1	0.16
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB3	1	0.16
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB2	1	0.16
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB3	1	0.16
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB2	1	0.16
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB3	1	0.16
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB2	20	0.16
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB3	20	0.16
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB2	20	0.16
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB3	20	0.16
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB2	20	0.16
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB3	20	0.16
(1,446)	1:32:A:LEU:HD11	1:42:A:GLN:H	19	0.16
(1,446)	1:32:A:LEU:HD12	1:42:A:GLN:H	19	0.16
(1,446)	1:32:A:LEU:HD13	1:42:A:GLN:H	19	0.16
(1,445)	1:32:A:LEU:HB2	1:33:A:HIS:HB3	13	0.16
(1,445)	1:32:A:LEU:HB3	1:33:A:HIS:HB3	13	0.16
(1,419)	1:30:A:PRO:HA	1:31:A:ASN:HA	6	0.16
(1,413)	1:29:A:GLY:HA2	1:31:A:ASN:HD21	11	0.16
(1,413)	1:29:A:GLY:HA3	1:31:A:ASN:HD21	11	0.16
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	1	0.16
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	12	0.16
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	14	0.16
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	11	0.16
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	15	0.16
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	16	0.16
(1,76)	1:4:A:LYS:HE3	1:4:A:LYS:H	3	0.16
(1,76)	1:4:A:LYS:HE2	1:4:A:LYS:H	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	2	0.15
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	11	0.15
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	11	0.15
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	11	0.15
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	11	0.15
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	11	0.15
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	11	0.15
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	18	0.15
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	18	0.15
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	18	0.15
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	18	0.15
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	18	0.15
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	18	0.15
(1,1105)	1:82:A:PHE:HZ	1:85:A:LEU:HG	8	0.15
(1,1105)	1:82:A:PHE:HZ	1:85:A:LEU:HG	20	0.15
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	11	0.15
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	11	0.15
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	11	0.15
(1,803)	1:58:A:LEU:HD12	1:59:A:TRP:HD1	5	0.15
(1,803)	1:58:A:LEU:HD12	1:59:A:TRP:HD1	6	0.15
(1,803)	1:58:A:LEU:HD13	1:59:A:TRP:HD1	20	0.15
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	2	0.15
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	3	0.15
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	7	0.15
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	12	0.15
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	16	0.15
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	13	0.15
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	13	0.15
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	5	0.15
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	9	0.15
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	6	0.15
(1,745)	1:55:A:LYS:HB3	1:55:A:LYS:H	10	0.15
(1,745)	1:55:A:LYS:HB3	1:55:A:LYS:H	20	0.15
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	4	0.15
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	4	0.15
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	6	0.15
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	6	0.15
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	8	0.15
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	8	0.15
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	14	0.15
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	14	0.15
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	19	0.15
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	4	0.15
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	14	0.15
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	14	0.15
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	17	0.15
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	17	0.15
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	17	0.15
(1,502)	1:36:A:PHE:HD1	1:33:A:HIS:HA	7	0.15
(1,502)	1:36:A:PHE:HD2	1:33:A:HIS:HA	7	0.15
(1,502)	1:36:A:PHE:HD1	1:33:A:HIS:HA	20	0.15
(1,502)	1:36:A:PHE:HD2	1:33:A:HIS:HA	20	0.15
(1,488)	1:35:A:ILE:HG23	1:59:A:TRP:HD1	12	0.15
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB2	19	0.15
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB3	19	0.15
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB2	19	0.15
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB3	19	0.15
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB2	19	0.15
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB3	19	0.15
(1,455)	1:34:A:GLY:H	1:35:A:ILE:HG12	7	0.15
(1,446)	1:32:A:LEU:HD11	1:42:A:GLN:H	6	0.15
(1,446)	1:32:A:LEU:HD12	1:42:A:GLN:H	6	0.15
(1,446)	1:32:A:LEU:HD13	1:42:A:GLN:H	6	0.15
(1,445)	1:32:A:LEU:HB2	1:33:A:HIS:HB3	20	0.15
(1,445)	1:32:A:LEU:HB3	1:33:A:HIS:HB3	20	0.15
(1,430)	1:30:A:PRO:HB2	1:46:A:TYR:HA	1	0.15
(1,430)	1:30:A:PRO:HB3	1:46:A:TYR:HA	1	0.15
(1,430)	1:30:A:PRO:HB2	1:46:A:TYR:HA	17	0.15
(1,430)	1:30:A:PRO:HB3	1:46:A:TYR:HA	17	0.15
(1,342)	1:20:A:VAL:HA	1:33:A:HIS:H	10	0.15
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG21	3	0.15
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG22	3	0.15
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG23	3	0.15
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD21	2	0.15
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD22	2	0.15
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	2	0.15
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	18	0.15
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	1	0.15
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	2	0.15
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	5	0.15
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	8	0.15
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	18	0.15
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD2	3	0.14
(1,1384)	2:104:A:HEC:HAD1	1:79:A:LYS:HG3	9	0.14
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	10	0.14
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	13	0.14
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	20	0.14
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	6	0.14
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	6	0.14
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	6	0.14
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	6	0.14
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	6	0.14
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	6	0.14
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	9	0.14
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	16	0.14
(1,1111)	1:85:A:LEU:HD11	1:85:A:LEU:H	10	0.14
(1,1111)	1:85:A:LEU:HD12	1:85:A:LEU:H	10	0.14
(1,1111)	1:85:A:LEU:HD13	1:85:A:LEU:H	10	0.14
(1,1111)	1:85:A:LEU:HD11	1:85:A:LEU:H	12	0.14
(1,1111)	1:85:A:LEU:HD12	1:85:A:LEU:H	12	0.14
(1,1111)	1:85:A:LEU:HD13	1:85:A:LEU:H	12	0.14
(1,1102)	1:82:A:PHE:HZ	2:104:A:HEC:HHC	14	0.14
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	8	0.14
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	11	0.14
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	17	0.14
(1,1066)	1:78:A:THR:HA	2:104:A:HEC:HAD1	3	0.14
(1,1066)	1:78:A:THR:HA	2:104:A:HEC:HAD2	3	0.14
(1,1029)	1:72:A:ALA:HB1	1:73:A:LYS:H	2	0.14
(1,1029)	1:72:A:ALA:HB2	1:73:A:LYS:H	2	0.14
(1,1029)	1:72:A:ALA:HB3	1:73:A:LYS:H	2	0.14
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	5	0.14
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	5	0.14
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	5	0.14
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	14	0.14
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	14	0.14
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	14	0.14
(1,803)	1:58:A:LEU:HD12	1:59:A:TRP:HD1	18	0.14
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	6	0.14
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	8	0.14
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	8	0.14
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	3	0.14
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	5	0.14
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	14	0.14
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	20	0.14
(1,745)	1:55:A:LYS:HB3	1:55:A:LYS:H	1	0.14
(1,745)	1:55:A:LYS:HB3	1:55:A:LYS:H	6	0.14
(1,745)	1:55:A:LYS:HB3	1:55:A:LYS:H	11	0.14
(1,745)	1:55:A:LYS:HB3	1:55:A:LYS:H	17	0.14
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	7	0.14
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	7	0.14
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	17	0.14
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	17	0.14
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	18	0.14
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	18	0.14
(1,636)	1:46:A:TYR:HD2	1:48:A:TYR:H	2	0.14
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	5	0.14
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	10	0.14
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	5	0.14
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	12	0.14
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	14	0.14
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	2	0.14
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	2	0.14
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	8	0.14
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	8	0.14
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	12	0.14
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	12	0.14
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	2	0.14
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	4	0.14
(1,502)	1:36:A:PHE:HD1	1:33:A:HIS:HA	13	0.14
(1,502)	1:36:A:PHE:HD2	1:33:A:HIS:HA	13	0.14
(1,463)	1:35:A:ILE:HD11	1:35:A:ILE:H	8	0.14
(1,463)	1:35:A:ILE:HD12	1:35:A:ILE:H	8	0.14
(1,463)	1:35:A:ILE:HD13	1:35:A:ILE:H	8	0.14
(1,446)	1:32:A:LEU:HD11	1:42:A:GLN:H	7	0.14
(1,446)	1:32:A:LEU:HD12	1:42:A:GLN:H	7	0.14
(1,446)	1:32:A:LEU:HD13	1:42:A:GLN:H	7	0.14
(1,446)	1:32:A:LEU:HD11	1:42:A:GLN:H	16	0.14
(1,446)	1:32:A:LEU:HD12	1:42:A:GLN:H	16	0.14
(1,446)	1:32:A:LEU:HD13	1:42:A:GLN:H	16	0.14
(1,428)	1:30:A:PRO:HB2	1:46:A:TYR:HE1	6	0.14
(1,428)	1:30:A:PRO:HB2	1:46:A:TYR:HE2	6	0.14
(1,403)	1:28:A:VAL:HG12	2:104:A:HEC:HHD	19	0.14
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	8	0.14
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	11	0.14
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	6	0.14
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	9	0.14
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	14	0.14
(1,210)	1:10:A:PHE:HZ	1:20:A:VAL:HB	14	0.14
(1,143)	1:9:A:LEU:HD11	1:9:A:LEU:H	3	0.14
(1,143)	1:9:A:LEU:HD12	1:9:A:LEU:H	3	0.14
(1,143)	1:9:A:LEU:HD13	1:9:A:LEU:H	3	0.14
(1,143)	1:9:A:LEU:HD21	1:9:A:LEU:H	3	0.14
(1,143)	1:9:A:LEU:HD22	1:9:A:LEU:H	3	0.14
(1,143)	1:9:A:LEU:HD23	1:9:A:LEU:H	3	0.14
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD2	5	0.13
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD2	8	0.13
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	5	0.13
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	8	0.13
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	11	0.13
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	15	0.13
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	7	0.13
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	7	0.13
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	7	0.13
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	7	0.13
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	7	0.13
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	7	0.13
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	14	0.13
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	14	0.13
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	14	0.13
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	14	0.13
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	14	0.13
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	14	0.13
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	8	0.13
(1,1111)	1:85:A:LEU:HD11	1:85:A:LEU:H	8	0.13
(1,1111)	1:85:A:LEU:HD12	1:85:A:LEU:H	8	0.13
(1,1111)	1:85:A:LEU:HD13	1:85:A:LEU:H	8	0.13
(1,1111)	1:85:A:LEU:HD11	1:85:A:LEU:H	14	0.13
(1,1111)	1:85:A:LEU:HD12	1:85:A:LEU:H	14	0.13
(1,1111)	1:85:A:LEU:HD13	1:85:A:LEU:H	14	0.13
(1,1029)	1:72:A:ALA:HB1	1:73:A:LYS:H	14	0.13
(1,1029)	1:72:A:ALA:HB2	1:73:A:LYS:H	14	0.13
(1,1029)	1:72:A:ALA:HB3	1:73:A:LYS:H	14	0.13
(1,1029)	1:72:A:ALA:HB1	1:73:A:LYS:H	18	0.13
(1,1029)	1:72:A:ALA:HB2	1:73:A:LYS:H	18	0.13
(1,1029)	1:72:A:ALA:HB3	1:73:A:LYS:H	18	0.13
(1,987)	1:68:A:LEU:HG	1:69:A:THR:H	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	1:64:A:MET:HE1	1:68:A:LEU:H	2	0.13
(1,923)	1:64:A:MET:HE2	1:68:A:LEU:H	2	0.13
(1,923)	1:64:A:MET:HE3	1:68:A:LEU:H	2	0.13
(1,923)	1:64:A:MET:HE1	1:68:A:LEU:H	9	0.13
(1,923)	1:64:A:MET:HE2	1:68:A:LEU:H	9	0.13
(1,923)	1:64:A:MET:HE3	1:68:A:LEU:H	9	0.13
(1,923)	1:64:A:MET:HE1	1:68:A:LEU:H	16	0.13
(1,923)	1:64:A:MET:HE2	1:68:A:LEU:H	16	0.13
(1,923)	1:64:A:MET:HE3	1:68:A:LEU:H	16	0.13
(1,923)	1:64:A:MET:HE1	1:68:A:LEU:H	20	0.13
(1,923)	1:64:A:MET:HE2	1:68:A:LEU:H	20	0.13
(1,923)	1:64:A:MET:HE3	1:68:A:LEU:H	20	0.13
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	2	0.13
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	2	0.13
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	2	0.13
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	4	0.13
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	4	0.13
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	4	0.13
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	13	0.13
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	13	0.13
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	13	0.13
(1,819)	1:59:A:TRP:HD1	1:38:A:ARG:H	13	0.13
(1,803)	1:58:A:LEU:HD12	1:59:A:TRP:HD1	2	0.13
(1,803)	1:58:A:LEU:HD11	1:59:A:TRP:HD1	7	0.13
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	4	0.13
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	8	0.13
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	18	0.13
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	5	0.13
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	5	0.13
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	7	0.13
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	7	0.13
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	11	0.13
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	11	0.13
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	12	0.13
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	12	0.13
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	16	0.13
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	16	0.13
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	17	0.13
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	17	0.13
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	6	0.13
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	10	0.13
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	2	0.13
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	9	0.13
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	18	0.13
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	1	0.13
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	5	0.13
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	10	0.13
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	11	0.13
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	15	0.13
(1,745)	1:55:A:LYS:HB3	1:55:A:LYS:H	3	0.13
(1,745)	1:55:A:LYS:HB3	1:55:A:LYS:H	14	0.13
(1,745)	1:55:A:LYS:HB3	1:55:A:LYS:H	16	0.13
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	10	0.13
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	10	0.13
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	16	0.13
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	16	0.13
(1,704)	1:52:A:ASN:HA	1:78:A:THR:HB	20	0.13
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	11	0.13
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	18	0.13
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	7	0.13
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	7	0.13
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	10	0.13
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	10	0.13
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	11	0.13
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	11	0.13
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	8	0.13
(1,549)	1:38:A:ARG:HG2	1:42:A:GLN:H	16	0.13
(1,549)	1:38:A:ARG:HG3	1:42:A:GLN:H	16	0.13
(1,547)	1:38:A:ARG:HD2	1:39:A:HIS:HE1	12	0.13
(1,547)	1:38:A:ARG:HD3	1:39:A:HIS:HE1	12	0.13
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB2	12	0.13
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB3	12	0.13
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB2	12	0.13
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB3	12	0.13
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB2	12	0.13
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB3	12	0.13
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB2	18	0.13
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB3	18	0.13
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB2	18	0.13
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB3	18	0.13
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB2	18	0.13
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB3	18	0.13
(1,467)	1:35:A:ILE:HA	1:35:A:ILE:HB	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:30:A:PRO:HA	1:31:A:ASN:HA	14	0.13
(1,413)	1:29:A:GLY:HA2	1:31:A:ASN:HD21	8	0.13
(1,413)	1:29:A:GLY:HA3	1:31:A:ASN:HD21	8	0.13
(1,375)	1:26:A:HIS:HA	1:31:A:ASN:HA	6	0.13
(1,342)	1:20:A:VAL:HA	1:33:A:HIS:H	16	0.13
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	10	0.13
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	20	0.13
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	10	0.13
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	17	0.13
(1,224)	1:11:A:LYS:HA	1:14:A:CYS:HB2	16	0.13
(1,224)	1:11:A:LYS:HA	1:14:A:CYS:HB3	16	0.13
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	5	0.13
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	7	0.13
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	17	0.13
(1,143)	1:9:A:LEU:HD11	1:9:A:LEU:H	4	0.13
(1,143)	1:9:A:LEU:HD12	1:9:A:LEU:H	4	0.13
(1,143)	1:9:A:LEU:HD13	1:9:A:LEU:H	4	0.13
(1,143)	1:9:A:LEU:HD21	1:9:A:LEU:H	4	0.13
(1,143)	1:9:A:LEU:HD22	1:9:A:LEU:H	4	0.13
(1,143)	1:9:A:LEU:HD23	1:9:A:LEU:H	4	0.13
(1,143)	1:9:A:LEU:HD11	1:9:A:LEU:H	13	0.13
(1,143)	1:9:A:LEU:HD12	1:9:A:LEU:H	13	0.13
(1,143)	1:9:A:LEU:HD13	1:9:A:LEU:H	13	0.13
(1,143)	1:9:A:LEU:HD21	1:9:A:LEU:H	13	0.13
(1,143)	1:9:A:LEU:HD22	1:9:A:LEU:H	13	0.13
(1,143)	1:9:A:LEU:HD23	1:9:A:LEU:H	13	0.13
(1,143)	1:9:A:LEU:HD11	1:9:A:LEU:H	14	0.13
(1,143)	1:9:A:LEU:HD12	1:9:A:LEU:H	14	0.13
(1,143)	1:9:A:LEU:HD13	1:9:A:LEU:H	14	0.13
(1,143)	1:9:A:LEU:HD21	1:9:A:LEU:H	14	0.13
(1,143)	1:9:A:LEU:HD22	1:9:A:LEU:H	14	0.13
(1,143)	1:9:A:LEU:HD23	1:9:A:LEU:H	14	0.13
(1,134)	1:8:A:THR:HB	1:11:A:LYS:HG2	16	0.13
(1,134)	1:8:A:THR:HB	1:11:A:LYS:HG3	16	0.13
(1,1383)	2:104:A:HEC:HAD1	1:46:A:TYR:HD1	16	0.12
(1,1383)	2:104:A:HEC:HAD1	1:46:A:TYR:HD2	16	0.12
(1,1383)	2:104:A:HEC:HAD2	1:46:A:TYR:HD1	16	0.12
(1,1383)	2:104:A:HEC:HAD2	1:46:A:TYR:HD2	16	0.12
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	3	0.12
(1,1263)	1:95:A:ILE:HG21	1:94:A:LEU:H	1	0.12
(1,1263)	1:95:A:ILE:HG22	1:94:A:LEU:H	1	0.12
(1,1263)	1:95:A:ILE:HG23	1:94:A:LEU:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	1	0.12
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	1	0.12
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	1	0.12
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	1	0.12
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	1	0.12
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	1	0.12
(1,1227)	1:94:A:LEU:HG	1:98:A:LEU:HG	2	0.12
(1,1227)	1:94:A:LEU:HG	1:98:A:LEU:HG	12	0.12
(1,1123)	1:85:A:LEU:HA	1:91:A:ARG:H	1	0.12
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC1	11	0.12
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC2	11	0.12
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC3	11	0.12
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC1	12	0.12
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC2	12	0.12
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC3	12	0.12
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	6	0.12
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	7	0.12
(1,1032)	1:72:A:ALA:HB1	2:104:A:HEC:HAA2	11	0.12
(1,1032)	1:72:A:ALA:HB2	2:104:A:HEC:HAA2	11	0.12
(1,1032)	1:72:A:ALA:HB3	2:104:A:HEC:HAA2	11	0.12
(1,1032)	1:72:A:ALA:HB1	2:104:A:HEC:HAA2	13	0.12
(1,1032)	1:72:A:ALA:HB2	2:104:A:HEC:HAA2	13	0.12
(1,1032)	1:72:A:ALA:HB3	2:104:A:HEC:HAA2	13	0.12
(1,1032)	1:72:A:ALA:HB1	2:104:A:HEC:HAA2	20	0.12
(1,1032)	1:72:A:ALA:HB2	2:104:A:HEC:HAA2	20	0.12
(1,1032)	1:72:A:ALA:HB3	2:104:A:HEC:HAA2	20	0.12
(1,1030)	1:72:A:ALA:H	1:78:A:THR:HB	12	0.12
(1,1029)	1:72:A:ALA:HB1	1:73:A:LYS:H	10	0.12
(1,1029)	1:72:A:ALA:HB2	1:73:A:LYS:H	10	0.12
(1,1029)	1:72:A:ALA:HB3	1:73:A:LYS:H	10	0.12
(1,1029)	1:72:A:ALA:HB1	1:73:A:LYS:H	15	0.12
(1,1029)	1:72:A:ALA:HB2	1:73:A:LYS:H	15	0.12
(1,1029)	1:72:A:ALA:HB3	1:73:A:LYS:H	15	0.12
(1,987)	1:68:A:LEU:HG	1:69:A:THR:H	1	0.12
(1,923)	1:64:A:MET:HE1	1:68:A:LEU:H	14	0.12
(1,923)	1:64:A:MET:HE2	1:68:A:LEU:H	14	0.12
(1,923)	1:64:A:MET:HE3	1:68:A:LEU:H	14	0.12
(1,923)	1:64:A:MET:HE1	1:68:A:LEU:H	18	0.12
(1,923)	1:64:A:MET:HE2	1:68:A:LEU:H	18	0.12
(1,923)	1:64:A:MET:HE3	1:68:A:LEU:H	18	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	1	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	1	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	3	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	3	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	3	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	6	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	6	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	6	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	7	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	7	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	7	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	9	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	9	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	9	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	19	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	19	0.12
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	19	0.12
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	13	0.12
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	1	0.12
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	1	0.12
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	3	0.12
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	3	0.12
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	4	0.12
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	4	0.12
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	9	0.12
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	9	0.12
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	4	0.12
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	7	0.12
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	16	0.12
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	17	0.12
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	19	0.12
(1,773)	1:57:A:VAL:HG11	1:75:A:ILE:HD11	12	0.12
(1,773)	1:57:A:VAL:HG11	1:75:A:ILE:HD12	12	0.12
(1,773)	1:57:A:VAL:HG11	1:75:A:ILE:HD13	12	0.12
(1,773)	1:57:A:VAL:HG12	1:75:A:ILE:HD11	12	0.12
(1,773)	1:57:A:VAL:HG12	1:75:A:ILE:HD12	12	0.12
(1,773)	1:57:A:VAL:HG12	1:75:A:ILE:HD13	12	0.12
(1,773)	1:57:A:VAL:HG13	1:75:A:ILE:HD11	12	0.12
(1,773)	1:57:A:VAL:HG13	1:75:A:ILE:HD12	12	0.12
(1,773)	1:57:A:VAL:HG13	1:75:A:ILE:HD13	12	0.12
(1,773)	1:57:A:VAL:HG21	1:75:A:ILE:HD11	12	0.12
(1,773)	1:57:A:VAL:HG21	1:75:A:ILE:HD12	12	0.12
(1,773)	1:57:A:VAL:HG21	1:75:A:ILE:HD13	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,773)	1:57:A:VAL:HG22	1:75:A:ILE:HD11	12	0.12
(1,773)	1:57:A:VAL:HG22	1:75:A:ILE:HD12	12	0.12
(1,773)	1:57:A:VAL:HG22	1:75:A:ILE:HD13	12	0.12
(1,773)	1:57:A:VAL:HG23	1:75:A:ILE:HD11	12	0.12
(1,773)	1:57:A:VAL:HG23	1:75:A:ILE:HD12	12	0.12
(1,773)	1:57:A:VAL:HG23	1:75:A:ILE:HD13	12	0.12
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	4	0.12
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	10	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	2	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	3	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	4	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	6	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	7	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	8	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	9	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	12	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	13	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	14	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	16	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	17	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	18	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	19	0.12
(1,759)	1:57:A:VAL:HA	1:57:A:VAL:HB	20	0.12
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	11	0.12
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	11	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	1	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	2	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	3	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	4	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	5	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	6	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	7	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	8	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	9	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	10	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	11	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	12	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	13	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	14	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	15	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	16	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	18	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	19	0.12
(1,717)	1:53:A:ILE:HB	1:53:A:ILE:HA	20	0.12
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	11	0.12
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	8	0.12
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	9	0.12
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	19	0.12
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	19	0.12
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	10	0.12
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	12	0.12
(1,502)	1:36:A:PHE:HD1	1:33:A:HIS:HA	18	0.12
(1,502)	1:36:A:PHE:HD2	1:33:A:HIS:HA	18	0.12
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB2	13	0.12
(1,487)	1:35:A:ILE:HG21	1:59:A:TRP:HB3	13	0.12
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB2	13	0.12
(1,487)	1:35:A:ILE:HG22	1:59:A:TRP:HB3	13	0.12
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB2	13	0.12
(1,487)	1:35:A:ILE:HG23	1:59:A:TRP:HB3	13	0.12
(1,478)	1:35:A:ILE:HD11	2:104:A:HEC:HMA1	7	0.12
(1,478)	1:35:A:ILE:HD11	2:104:A:HEC:HMA2	7	0.12
(1,478)	1:35:A:ILE:HD11	2:104:A:HEC:HMA3	7	0.12
(1,478)	1:35:A:ILE:HD12	2:104:A:HEC:HMA1	7	0.12
(1,478)	1:35:A:ILE:HD12	2:104:A:HEC:HMA2	7	0.12
(1,478)	1:35:A:ILE:HD12	2:104:A:HEC:HMA3	7	0.12
(1,478)	1:35:A:ILE:HD13	2:104:A:HEC:HMA1	7	0.12
(1,478)	1:35:A:ILE:HD13	2:104:A:HEC:HMA2	7	0.12
(1,478)	1:35:A:ILE:HD13	2:104:A:HEC:HMA3	7	0.12
(1,467)	1:35:A:ILE:HA	1:35:A:ILE:HB	6	0.12
(1,453)	1:34:A:GLY:HA2	1:33:A:HIS:H	10	0.12
(1,453)	1:34:A:GLY:HA3	1:33:A:HIS:H	10	0.12
(1,444)	1:32:A:LEU:HD11	1:35:A:ILE:H	15	0.12
(1,444)	1:32:A:LEU:HD12	1:35:A:ILE:H	15	0.12
(1,444)	1:32:A:LEU:HD13	1:35:A:ILE:H	15	0.12
(1,442)	1:32:A:LEU:H	1:19:A:THR:H	6	0.12
(1,394)	1:28:A:VAL:HA	1:28:A:VAL:HB	1	0.12
(1,394)	1:28:A:VAL:HA	1:28:A:VAL:HB	3	0.12
(1,394)	1:28:A:VAL:HA	1:28:A:VAL:HB	4	0.12
(1,394)	1:28:A:VAL:HA	1:28:A:VAL:HB	7	0.12
(1,394)	1:28:A:VAL:HA	1:28:A:VAL:HB	9	0.12
(1,394)	1:28:A:VAL:HA	1:28:A:VAL:HB	10	0.12
(1,394)	1:28:A:VAL:HA	1:28:A:VAL:HB	17	0.12
(1,359)	1:23:A:GLY:H	1:33:A:HIS:HB2	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:23:A:GLY:H	1:33:A:HIS:HB3	2	0.12
(1,359)	1:23:A:GLY:H	1:33:A:HIS:HB2	11	0.12
(1,359)	1:23:A:GLY:H	1:33:A:HIS:HB3	11	0.12
(1,342)	1:20:A:VAL:HA	1:33:A:HIS:H	19	0.12
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	2	0.12
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	5	0.12
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	9	0.12
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	13	0.12
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	14	0.12
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	16	0.12
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	17	0.12
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD21	10	0.12
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD22	10	0.12
(1,224)	1:11:A:LYS:HA	1:14:A:CYS:HB2	11	0.12
(1,224)	1:11:A:LYS:HA	1:14:A:CYS:HB3	11	0.12
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	2	0.12
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	11	0.12
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	15	0.12
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	18	0.12
(1,208)	1:10:A:PHE:HZ	1:19:A:THR:HB	15	0.12
(1,206)	1:10:A:PHE:HZ	1:18:A:HIS:HB2	6	0.12
(1,206)	1:10:A:PHE:HZ	1:18:A:HIS:HB3	6	0.12
(1,122)	1:8:A:THR:HB	1:8:A:THR:HA	3	0.12
(1,122)	1:8:A:THR:HB	1:8:A:THR:HA	4	0.12
(1,122)	1:8:A:THR:HB	1:8:A:THR:HA	13	0.12
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	1	0.12
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	2	0.12
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	5	0.12
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	6	0.12
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	7	0.12
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	8	0.12
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	10	0.12
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	11	0.12
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	12	0.12
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	14	0.12
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	16	0.12
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	20	0.12
(1,62)	1:2:A:SER:H	1:4:A:LYS:HE2	6	0.12
(1,62)	1:2:A:SER:H	1:4:A:LYS:HE3	6	0.12
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD2	16	0.11
(1,1398)	2:104:A:HEC:HBD1	1:80:A:MET:H	20	0.11
(1,1398)	2:104:A:HEC:HBD2	1:80:A:MET:H	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1384)	2:104:A:HEC:HAD1	1:79:A:LYS:HG3	18	0.11
(1,1383)	2:104:A:HEC:HAD1	1:46:A:TYR:HD1	19	0.11
(1,1383)	2:104:A:HEC:HAD1	1:46:A:TYR:HD2	19	0.11
(1,1383)	2:104:A:HEC:HAD2	1:46:A:TYR:HD1	19	0.11
(1,1383)	2:104:A:HEC:HAD2	1:46:A:TYR:HD2	19	0.11
(1,1383)	2:104:A:HEC:HAD1	1:46:A:TYR:HD1	20	0.11
(1,1383)	2:104:A:HEC:HAD1	1:46:A:TYR:HD2	20	0.11
(1,1383)	2:104:A:HEC:HAD2	1:46:A:TYR:HD1	20	0.11
(1,1383)	2:104:A:HEC:HAD2	1:46:A:TYR:HD2	20	0.11
(1,1308)	1:98:A:LEU:HG	1:97:A:TYR:HE1	5	0.11
(1,1308)	1:98:A:LEU:HG	1:97:A:TYR:HE2	5	0.11
(1,1263)	1:95:A:ILE:HG21	1:94:A:LEU:H	9	0.11
(1,1263)	1:95:A:ILE:HG22	1:94:A:LEU:H	9	0.11
(1,1263)	1:95:A:ILE:HG23	1:94:A:LEU:H	9	0.11
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	15	0.11
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	15	0.11
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	15	0.11
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	15	0.11
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	15	0.11
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	15	0.11
(1,1260)	1:95:A:ILE:HG12	1:99:A:LYS:H	10	0.11
(1,1260)	1:95:A:ILE:HG13	1:99:A:LYS:H	10	0.11
(1,1227)	1:94:A:LEU:HG	1:98:A:LEU:HG	17	0.11
(1,1111)	1:85:A:LEU:HD11	1:85:A:LEU:H	1	0.11
(1,1111)	1:85:A:LEU:HD12	1:85:A:LEU:H	1	0.11
(1,1111)	1:85:A:LEU:HD13	1:85:A:LEU:H	1	0.11
(1,1111)	1:85:A:LEU:HD11	1:85:A:LEU:H	18	0.11
(1,1111)	1:85:A:LEU:HD12	1:85:A:LEU:H	18	0.11
(1,1111)	1:85:A:LEU:HD13	1:85:A:LEU:H	18	0.11
(1,1105)	1:82:A:PHE:HZ	1:85:A:LEU:HG	18	0.11
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC1	10	0.11
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC2	10	0.11
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC3	10	0.11
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	3	0.11
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	16	0.11
(1,996)	1:69:A:THR:HB	1:69:A:THR:H	5	0.11
(1,996)	1:69:A:THR:HB	1:69:A:THR:H	8	0.11
(1,923)	1:64:A:MET:HE1	1:68:A:LEU:H	17	0.11
(1,923)	1:64:A:MET:HE2	1:68:A:LEU:H	17	0.11
(1,923)	1:64:A:MET:HE3	1:68:A:LEU:H	17	0.11
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	20	0.11
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	20	0.11
(1,803)	1:58:A:LEU:HD13	1:59:A:TRP:HD1	11	0.11
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	10	0.11
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	11	0.11
(1,802)	1:58:A:LEU:HG	1:59:A:TRP:HD1	17	0.11
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	19	0.11
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	19	0.11
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	20	0.11
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	20	0.11
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	2	0.11
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	18	0.11
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	2	0.11
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	2	0.11
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	3	0.11
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	3	0.11
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	9	0.11
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	9	0.11
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	20	0.11
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	20	0.11
(1,633)	1:46:A:TYR:HA	1:44:A:GLU:H	13	0.11
(1,632)	1:46:A:TYR:HA	1:48:A:TYR:H	17	0.11
(1,605)	1:42:A:GLN:HG2	1:48:A:TYR:H	20	0.11
(1,605)	1:42:A:GLN:HG3	1:48:A:TYR:H	20	0.11
(1,591)	1:41:A:GLY:HA2	1:43:A:ALA:H	20	0.11
(1,591)	1:41:A:GLY:HA3	1:43:A:ALA:H	20	0.11
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	5	0.11
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	11	0.11
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	19	0.11
(1,550)	1:38:A:ARG:HG2	1:59:A:TRP:HD1	11	0.11
(1,550)	1:38:A:ARG:HG3	1:59:A:TRP:HD1	11	0.11
(1,547)	1:38:A:ARG:HD2	1:39:A:HIS:HE1	1	0.11
(1,547)	1:38:A:ARG:HD3	1:39:A:HIS:HE1	1	0.11
(1,547)	1:38:A:ARG:HD2	1:39:A:HIS:HE1	15	0.11
(1,547)	1:38:A:ARG:HD3	1:39:A:HIS:HE1	15	0.11
(1,453)	1:34:A:GLY:HA2	1:33:A:HIS:H	17	0.11
(1,453)	1:34:A:GLY:HA3	1:33:A:HIS:H	17	0.11
(1,445)	1:32:A:LEU:HB2	1:33:A:HIS:HB3	2	0.11
(1,445)	1:32:A:LEU:HB3	1:33:A:HIS:HB3	2	0.11
(1,444)	1:32:A:LEU:HD11	1:35:A:ILE:H	6	0.11
(1,444)	1:32:A:LEU:HD12	1:35:A:ILE:H	6	0.11
(1,444)	1:32:A:LEU:HD13	1:35:A:ILE:H	6	0.11
(1,440)	1:32:A:LEU:HD11	1:32:A:LEU:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:32:A:LEU:HD12	1:32:A:LEU:H	1	0.11
(1,440)	1:32:A:LEU:HD13	1:32:A:LEU:H	1	0.11
(1,440)	1:32:A:LEU:HD21	1:32:A:LEU:H	1	0.11
(1,440)	1:32:A:LEU:HD22	1:32:A:LEU:H	1	0.11
(1,440)	1:32:A:LEU:HD23	1:32:A:LEU:H	1	0.11
(1,436)	1:31:A:ASN:HB2	1:43:A:ALA:HB1	16	0.11
(1,436)	1:31:A:ASN:HB2	1:43:A:ALA:HB2	16	0.11
(1,436)	1:31:A:ASN:HB2	1:43:A:ALA:HB3	16	0.11
(1,436)	1:31:A:ASN:HB3	1:43:A:ALA:HB1	16	0.11
(1,436)	1:31:A:ASN:HB3	1:43:A:ALA:HB2	16	0.11
(1,436)	1:31:A:ASN:HB3	1:43:A:ALA:HB3	16	0.11
(1,420)	1:30:A:PRO:HB2	1:32:A:LEU:H	1	0.11
(1,420)	1:30:A:PRO:HB3	1:32:A:LEU:H	1	0.11
(1,413)	1:29:A:GLY:HA2	1:31:A:ASN:HD21	18	0.11
(1,413)	1:29:A:GLY:HA3	1:31:A:ASN:HD21	18	0.11
(1,402)	1:28:A:VAL:HG11	1:29:A:GLY:H	12	0.11
(1,402)	1:28:A:VAL:HG12	1:29:A:GLY:H	12	0.11
(1,402)	1:28:A:VAL:HG13	1:29:A:GLY:H	12	0.11
(1,402)	1:28:A:VAL:HG21	1:29:A:GLY:H	12	0.11
(1,402)	1:28:A:VAL:HG22	1:29:A:GLY:H	12	0.11
(1,402)	1:28:A:VAL:HG23	1:29:A:GLY:H	12	0.11
(1,394)	1:28:A:VAL:HA	1:28:A:VAL:HB	8	0.11
(1,394)	1:28:A:VAL:HA	1:28:A:VAL:HB	11	0.11
(1,394)	1:28:A:VAL:HA	1:28:A:VAL:HB	15	0.11
(1,342)	1:20:A:VAL:HA	1:33:A:HIS:H	18	0.11
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG21	15	0.11
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG22	15	0.11
(1,327)	1:19:A:THR:HB	1:20:A:VAL:HG23	15	0.11
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	7	0.11
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	10	0.11
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	15	0.11
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD21	4	0.11
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD22	4	0.11
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	7	0.11
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	19	0.11
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	4	0.11
(1,230)	1:12:A:THR:HB	1:12:A:THR:H	12	0.11
(1,224)	1:11:A:LYS:HA	1:14:A:CYS:HB2	10	0.11
(1,224)	1:11:A:LYS:HA	1:14:A:CYS:HB3	10	0.11
(1,224)	1:11:A:LYS:HA	1:14:A:CYS:HB2	15	0.11
(1,224)	1:11:A:LYS:HA	1:14:A:CYS:HB3	15	0.11
(1,224)	1:11:A:LYS:HA	1:14:A:CYS:HB2	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:11:A:LYS:HA	1:14:A:CYS:HB3	20	0.11
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	12	0.11
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	13	0.11
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	16	0.11
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	20	0.11
(1,208)	1:10:A:PHE:HZ	1:19:A:THR:HB	5	0.11
(1,208)	1:10:A:PHE:HZ	1:19:A:THR:HB	9	0.11
(1,143)	1:9:A:LEU:HD11	1:9:A:LEU:H	2	0.11
(1,143)	1:9:A:LEU:HD12	1:9:A:LEU:H	2	0.11
(1,143)	1:9:A:LEU:HD13	1:9:A:LEU:H	2	0.11
(1,143)	1:9:A:LEU:HD21	1:9:A:LEU:H	2	0.11
(1,143)	1:9:A:LEU:HD22	1:9:A:LEU:H	2	0.11
(1,143)	1:9:A:LEU:HD23	1:9:A:LEU:H	2	0.11
(1,143)	1:9:A:LEU:HD11	1:9:A:LEU:H	10	0.11
(1,143)	1:9:A:LEU:HD12	1:9:A:LEU:H	10	0.11
(1,143)	1:9:A:LEU:HD13	1:9:A:LEU:H	10	0.11
(1,143)	1:9:A:LEU:HD21	1:9:A:LEU:H	10	0.11
(1,143)	1:9:A:LEU:HD22	1:9:A:LEU:H	10	0.11
(1,143)	1:9:A:LEU:HD23	1:9:A:LEU:H	10	0.11
(1,143)	1:9:A:LEU:HD11	1:9:A:LEU:H	18	0.11
(1,143)	1:9:A:LEU:HD12	1:9:A:LEU:H	18	0.11
(1,143)	1:9:A:LEU:HD13	1:9:A:LEU:H	18	0.11
(1,143)	1:9:A:LEU:HD21	1:9:A:LEU:H	18	0.11
(1,143)	1:9:A:LEU:HD22	1:9:A:LEU:H	18	0.11
(1,143)	1:9:A:LEU:HD23	1:9:A:LEU:H	18	0.11
(1,143)	1:9:A:LEU:HD11	1:9:A:LEU:H	19	0.11
(1,143)	1:9:A:LEU:HD12	1:9:A:LEU:H	19	0.11
(1,143)	1:9:A:LEU:HD13	1:9:A:LEU:H	19	0.11
(1,143)	1:9:A:LEU:HD21	1:9:A:LEU:H	19	0.11
(1,143)	1:9:A:LEU:HD22	1:9:A:LEU:H	19	0.11
(1,143)	1:9:A:LEU:HD23	1:9:A:LEU:H	19	0.11
(1,143)	1:9:A:LEU:HD11	1:9:A:LEU:H	20	0.11
(1,143)	1:9:A:LEU:HD12	1:9:A:LEU:H	20	0.11
(1,143)	1:9:A:LEU:HD13	1:9:A:LEU:H	20	0.11
(1,143)	1:9:A:LEU:HD21	1:9:A:LEU:H	20	0.11
(1,143)	1:9:A:LEU:HD22	1:9:A:LEU:H	20	0.11
(1,143)	1:9:A:LEU:HD23	1:9:A:LEU:H	20	0.11
(1,134)	1:8:A:THR:HB	1:11:A:LYS:HG2	17	0.11
(1,134)	1:8:A:THR:HB	1:11:A:LYS:HG3	17	0.11
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	9	0.11
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	15	0.11
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	18	0.11
(1,119)	1:8:A:THR:HB	1:8:A:THR:H	19	0.11
(1,62)	1:2:A:SER:H	1:4:A:LYS:HE2	2	0.11
(1,62)	1:2:A:SER:H	1:4:A:LYS:HE3	2	0.11
(1,62)	1:2:A:SER:H	1:4:A:LYS:HE2	4	0.11
(1,62)	1:2:A:SER:H	1:4:A:LYS:HE3	4	0.11
(1,62)	1:2:A:SER:H	1:4:A:LYS:HE2	13	0.11
(1,62)	1:2:A:SER:H	1:4:A:LYS:HE3	13	0.11
(1,62)	1:2:A:SER:H	1:4:A:LYS:HE2	20	0.11
(1,62)	1:2:A:SER:H	1:4:A:LYS:HE3	20	0.11
(1,1399)	2:104:A:HEC:HHB	1:71:A:HIS:HD2	20	0.1
(1,1385)	2:104:A:HEC:HMA1	1:32:A:LEU:HD11	14	0.1
(1,1385)	2:104:A:HEC:HMA1	1:32:A:LEU:HD12	14	0.1
(1,1385)	2:104:A:HEC:HMA1	1:32:A:LEU:HD13	14	0.1
(1,1385)	2:104:A:HEC:HMA1	1:32:A:LEU:HD21	14	0.1
(1,1385)	2:104:A:HEC:HMA1	1:32:A:LEU:HD22	14	0.1
(1,1385)	2:104:A:HEC:HMA1	1:32:A:LEU:HD23	14	0.1
(1,1385)	2:104:A:HEC:HMA2	1:32:A:LEU:HD11	14	0.1
(1,1385)	2:104:A:HEC:HMA2	1:32:A:LEU:HD12	14	0.1
(1,1385)	2:104:A:HEC:HMA2	1:32:A:LEU:HD13	14	0.1
(1,1385)	2:104:A:HEC:HMA2	1:32:A:LEU:HD21	14	0.1
(1,1385)	2:104:A:HEC:HMA2	1:32:A:LEU:HD22	14	0.1
(1,1385)	2:104:A:HEC:HMA2	1:32:A:LEU:HD23	14	0.1
(1,1385)	2:104:A:HEC:HMA3	1:32:A:LEU:HD11	14	0.1
(1,1385)	2:104:A:HEC:HMA3	1:32:A:LEU:HD12	14	0.1
(1,1385)	2:104:A:HEC:HMA3	1:32:A:LEU:HD13	14	0.1
(1,1385)	2:104:A:HEC:HMA3	1:32:A:LEU:HD21	14	0.1
(1,1385)	2:104:A:HEC:HMA3	1:32:A:LEU:HD22	14	0.1
(1,1385)	2:104:A:HEC:HMA3	1:32:A:LEU:HD23	14	0.1
(1,1380)	2:104:A:HEC:HAC	1:18:A:HIS:HD2	1	0.1
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD21	10	0.1
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD22	10	0.1
(1,1262)	1:95:A:ILE:HG12	1:98:A:LEU:HD23	10	0.1
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD21	10	0.1
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD22	10	0.1
(1,1262)	1:95:A:ILE:HG13	1:98:A:LEU:HD23	10	0.1
(1,1111)	1:85:A:LEU:HD11	1:85:A:LEU:H	17	0.1
(1,1111)	1:85:A:LEU:HD12	1:85:A:LEU:H	17	0.1
(1,1111)	1:85:A:LEU:HD13	1:85:A:LEU:H	17	0.1
(1,1111)	1:85:A:LEU:HD11	1:85:A:LEU:H	20	0.1
(1,1111)	1:85:A:LEU:HD12	1:85:A:LEU:H	20	0.1
(1,1111)	1:85:A:LEU:HD13	1:85:A:LEU:H	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC1	20	0.1
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC2	20	0.1
(1,1096)	1:82:A:PHE:HA	2:104:A:HEC:HMC3	20	0.1
(1,1067)	1:78:A:THR:HA	1:76:A:PRO:HA	19	0.1
(1,1030)	1:72:A:ALA:H	1:78:A:THR:HB	18	0.1
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	2	0.1
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	2	0.1
(1,793)	1:58:A:LEU:HB2	1:59:A:TRP:HD1	18	0.1
(1,793)	1:58:A:LEU:HB3	1:59:A:TRP:HD1	18	0.1
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	1	0.1
(1,792)	1:58:A:LEU:HG	1:59:A:TRP:HE3	12	0.1
(1,768)	1:57:A:VAL:HB	1:59:A:TRP:HZ2	3	0.1
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	11	0.1
(1,765)	1:57:A:VAL:HA	1:39:A:HIS:HD1	19	0.1
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	1	0.1
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	1	0.1
(1,728)	1:53:A:ILE:HG12	1:52:A:ASN:HD22	12	0.1
(1,728)	1:53:A:ILE:HG13	1:52:A:ASN:HD22	12	0.1
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	16	0.1
(1,589)	1:41:A:GLY:H	1:59:A:TRP:HD1	18	0.1
(1,412)	1:29:A:GLY:HA2	1:26:A:HIS:HD1	1	0.1
(1,412)	1:29:A:GLY:HA3	1:26:A:HIS:HD1	1	0.1
(1,394)	1:28:A:VAL:HA	1:28:A:VAL:HB	18	0.1
(1,389)	1:27:A:LYS:HG2	1:28:A:VAL:H	20	0.1
(1,389)	1:27:A:LYS:HG3	1:28:A:VAL:H	20	0.1
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	1	0.1
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	3	0.1
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	11	0.1
(1,312)	1:19:A:THR:HA	1:19:A:THR:HB	19	0.1
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD21	18	0.1
(1,305)	1:18:A:HIS:HD1	1:31:A:ASN:HD22	18	0.1
(1,297)	1:17:A:CYS:HA	1:19:A:THR:H	9	0.1
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	1	0.1
(1,223)	1:11:A:LYS:HA	1:14:A:CYS:H	10	0.1
(1,210)	1:10:A:PHE:HZ	1:20:A:VAL:HB	17	0.1
(1,202)	1:10:A:PHE:HE1	1:32:A:LEU:HD11	2	0.1
(1,202)	1:10:A:PHE:HE1	1:32:A:LEU:HD12	2	0.1
(1,202)	1:10:A:PHE:HE1	1:32:A:LEU:HD13	2	0.1
(1,202)	1:10:A:PHE:HE1	1:32:A:LEU:HD21	2	0.1
(1,202)	1:10:A:PHE:HE1	1:32:A:LEU:HD22	2	0.1
(1,202)	1:10:A:PHE:HE1	1:32:A:LEU:HD23	2	0.1
(1,202)	1:10:A:PHE:HE2	1:32:A:LEU:HD11	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:10:A:PHE:HE2	1:32:A:LEU:HD12	2	0.1
(1,202)	1:10:A:PHE:HE2	1:32:A:LEU:HD13	2	0.1
(1,202)	1:10:A:PHE:HE2	1:32:A:LEU:HD21	2	0.1
(1,202)	1:10:A:PHE:HE2	1:32:A:LEU:HD22	2	0.1
(1,202)	1:10:A:PHE:HE2	1:32:A:LEU:HD23	2	0.1
(1,200)	1:10:A:PHE:HE1	1:19:A:THR:HG21	4	0.1
(1,200)	1:10:A:PHE:HE1	1:19:A:THR:HG22	4	0.1
(1,200)	1:10:A:PHE:HE1	1:19:A:THR:HG23	4	0.1
(1,200)	1:10:A:PHE:HE2	1:19:A:THR:HG21	4	0.1
(1,200)	1:10:A:PHE:HE2	1:19:A:THR:HG22	4	0.1
(1,200)	1:10:A:PHE:HE2	1:19:A:THR:HG23	4	0.1
(1,200)	1:10:A:PHE:HE1	1:19:A:THR:HG21	8	0.1
(1,200)	1:10:A:PHE:HE1	1:19:A:THR:HG22	8	0.1
(1,200)	1:10:A:PHE:HE1	1:19:A:THR:HG23	8	0.1
(1,200)	1:10:A:PHE:HE2	1:19:A:THR:HG21	8	0.1
(1,200)	1:10:A:PHE:HE2	1:19:A:THR:HG22	8	0.1
(1,200)	1:10:A:PHE:HE2	1:19:A:THR:HG23	8	0.1
(1,153)	1:9:A:LEU:HA	1:94:A:LEU:HD11	6	0.1
(1,153)	1:9:A:LEU:HA	1:94:A:LEU:HD12	6	0.1
(1,153)	1:9:A:LEU:HA	1:94:A:LEU:HD13	6	0.1
(1,153)	1:9:A:LEU:HA	1:94:A:LEU:HD21	6	0.1
(1,153)	1:9:A:LEU:HA	1:94:A:LEU:HD22	6	0.1
(1,153)	1:9:A:LEU:HA	1:94:A:LEU:HD23	6	0.1
(1,143)	1:9:A:LEU:HD11	1:9:A:LEU:H	5	0.1
(1,143)	1:9:A:LEU:HD12	1:9:A:LEU:H	5	0.1
(1,143)	1:9:A:LEU:HD13	1:9:A:LEU:H	5	0.1
(1,143)	1:9:A:LEU:HD21	1:9:A:LEU:H	5	0.1
(1,143)	1:9:A:LEU:HD22	1:9:A:LEU:H	5	0.1
(1,143)	1:9:A:LEU:HD23	1:9:A:LEU:H	5	0.1
(1,143)	1:9:A:LEU:HD11	1:9:A:LEU:H	7	0.1
(1,143)	1:9:A:LEU:HD12	1:9:A:LEU:H	7	0.1
(1,143)	1:9:A:LEU:HD13	1:9:A:LEU:H	7	0.1
(1,143)	1:9:A:LEU:HD21	1:9:A:LEU:H	7	0.1
(1,143)	1:9:A:LEU:HD22	1:9:A:LEU:H	7	0.1
(1,143)	1:9:A:LEU:HD23	1:9:A:LEU:H	7	0.1

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found