



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 02:53 PM UTC

PDB ID : 2LIT / pdb_00002lit
BMRB ID : 17904
Title : NMR Solution Structure of Yeast Iso-1-cytochrome c Mutant P71H in reduced 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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

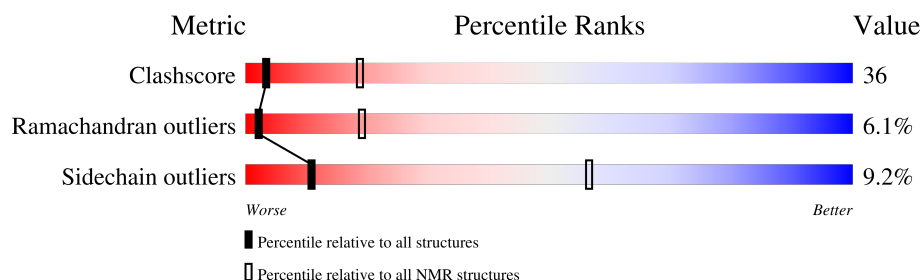
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 43%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	108	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:-3-A:-1, A:1-A:103 (106)	0.77	15

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 1768 atoms, of which 879 are hydrogens and 0 are deuteriums.

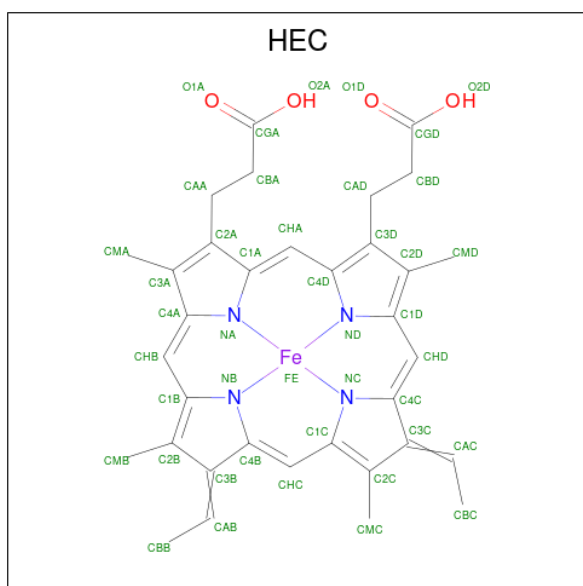
- Molecule 1 is a protein called Cytochrome c iso-1.

Mol	Chain	Residues	Atoms						Trace
1	A	108	Total	C	H	N	O	S	0
			1693	533	847	152	157	4	

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: $C_{34}H_{34}FeN_4O_4$).



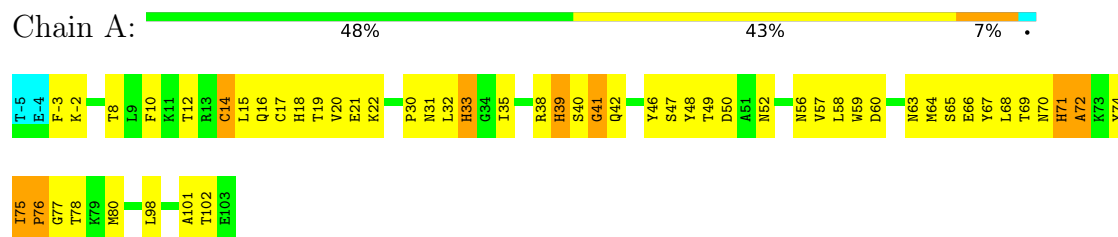
Mol	Chain	Residues	Atoms					
2	A	1	Total	C	Fe	H	N	O
			75	34	1	32	4	4

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

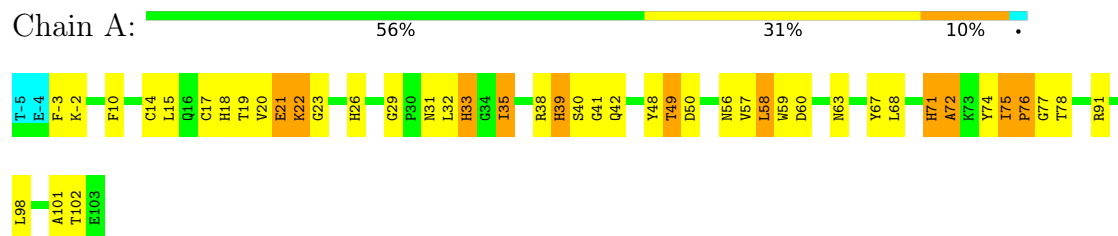


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Cytochrome c iso-1



4.2.2 Score per residue for model 2

- Molecule 1: Cytochrome c iso-1

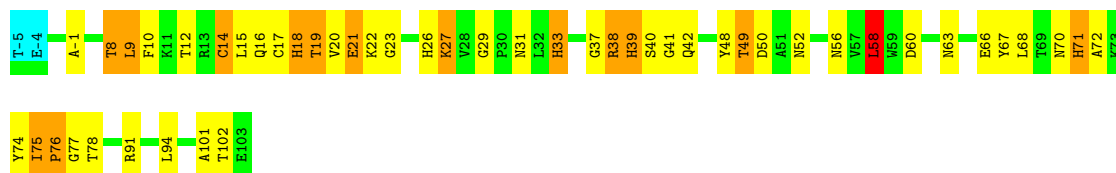




4.2.3 Score per residue for model 3

- Molecule 1: Cytochrome c iso-1

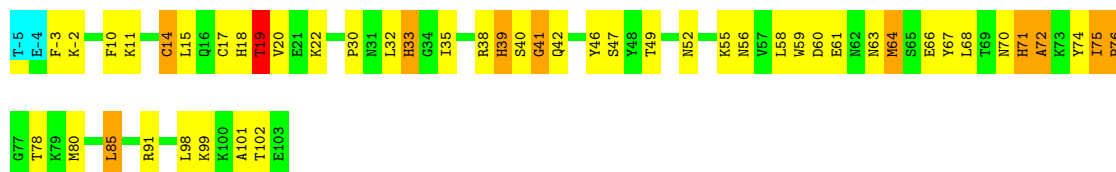
Chain A: 53% 31% 13% ..



4.2.4 Score per residue for model 4

- Molecule 1: Cytochrome c iso-1

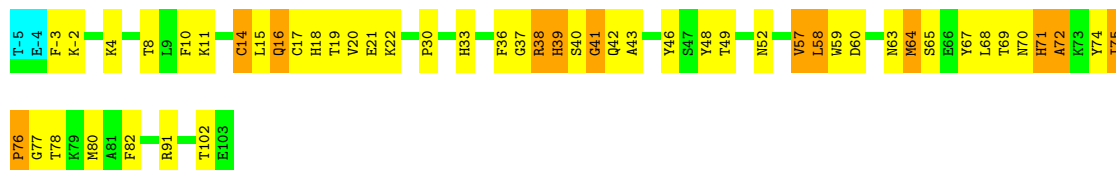
Chain A: 53% 35% 9% ..



4.2.5 Score per residue for model 5

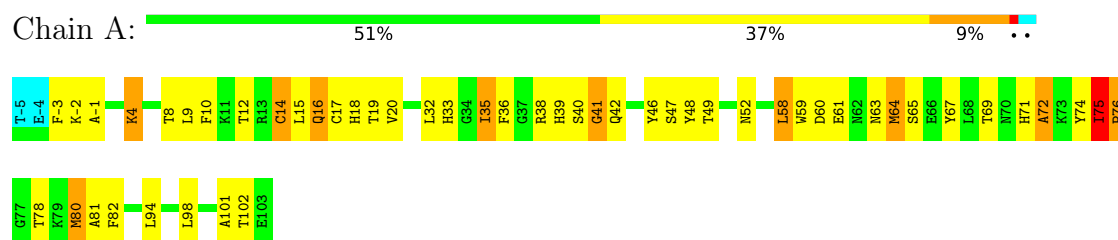
- Molecule 1: Cytochrome c iso-1

Chain A: 51% 36% 11% .



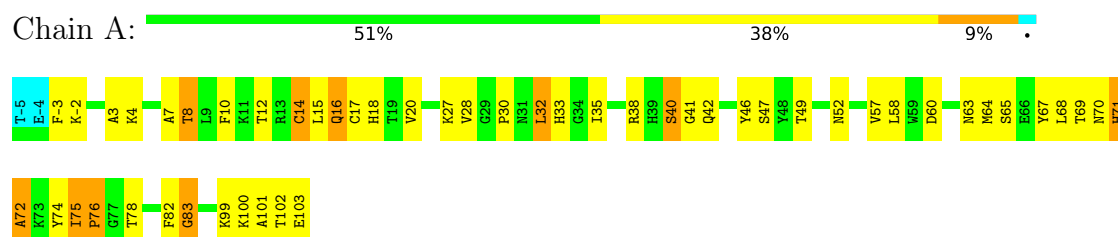
4.2.6 Score per residue for model 6

- Molecule 1: Cytochrome c iso-1



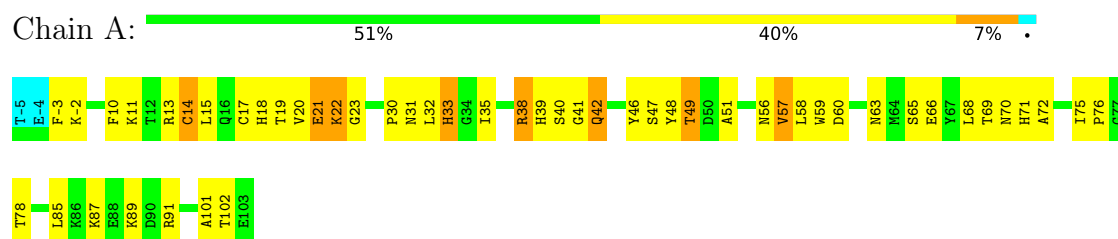
4.2.7 Score per residue for model 7

- Molecule 1: Cytochrome c iso-1



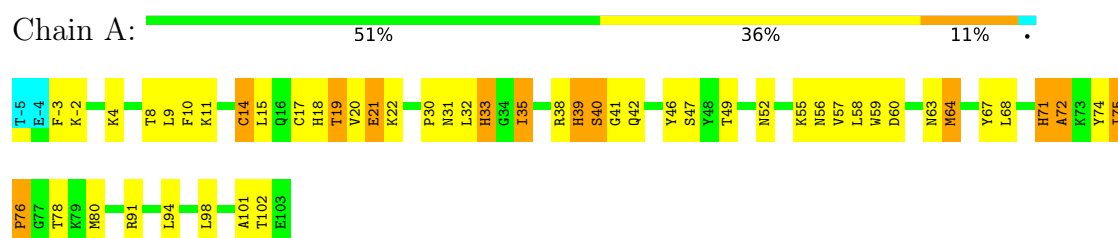
4.2.8 Score per residue for model 8

- Molecule 1: Cytochrome c iso-1



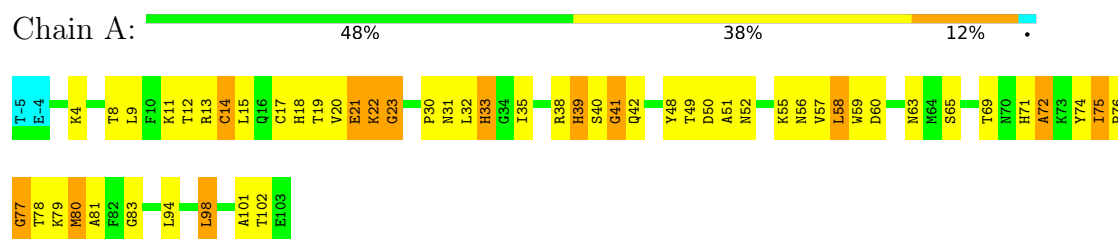
4.2.9 Score per residue for model 9

- Molecule 1: Cytochrome c iso-1



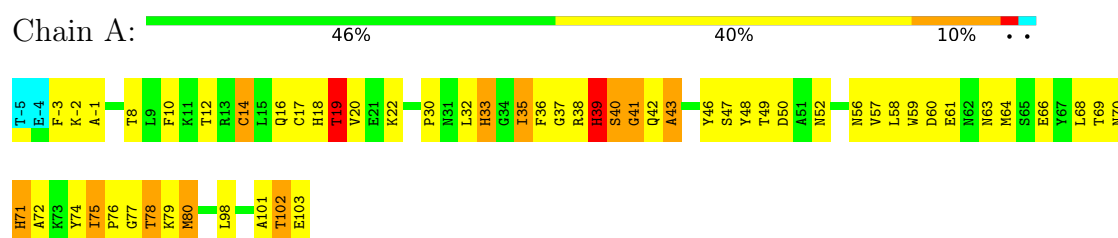
4.2.10 Score per residue for model 10

- Molecule 1: Cytochrome c iso-1



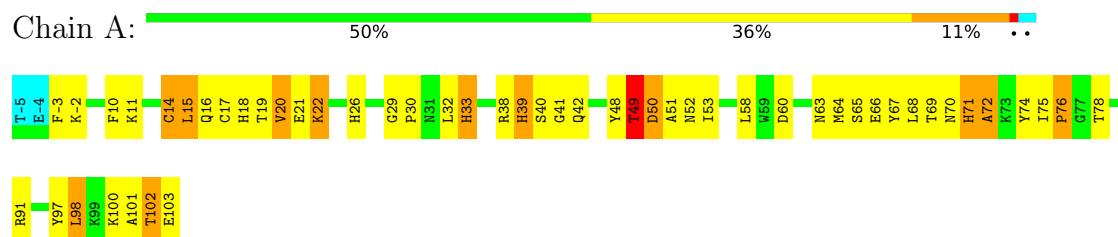
4.2.11 Score per residue for model 11

- Molecule 1: Cytochrome c iso-1



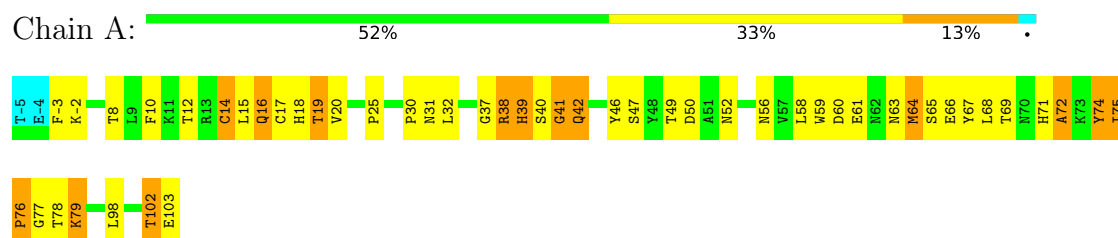
4.2.12 Score per residue for model 12

- Molecule 1: Cytochrome c iso-1



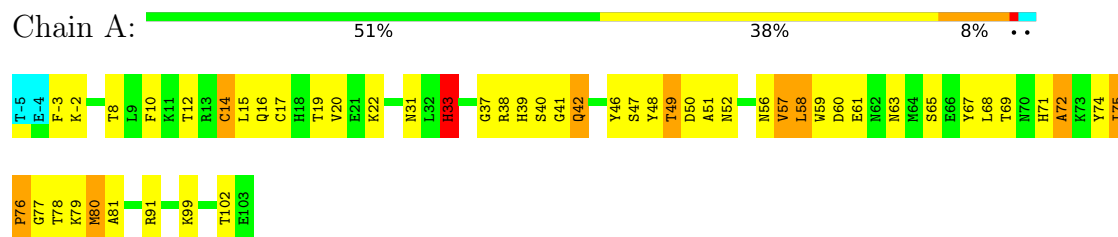
4.2.13 Score per residue for model 13

- Molecule 1: Cytochrome c iso-1



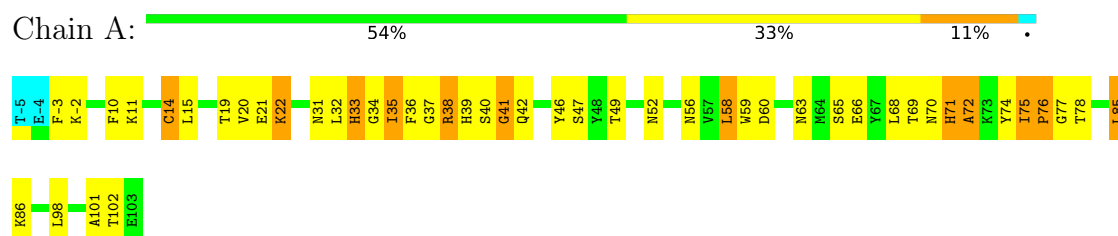
4.2.14 Score per residue for model 14

- Molecule 1: Cytochrome c iso-1



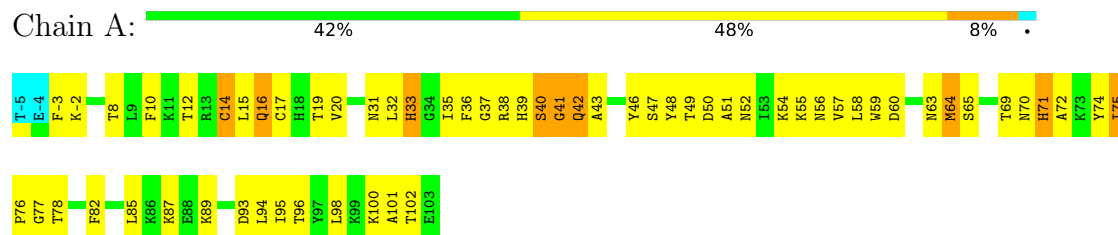
4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Cytochrome c iso-1



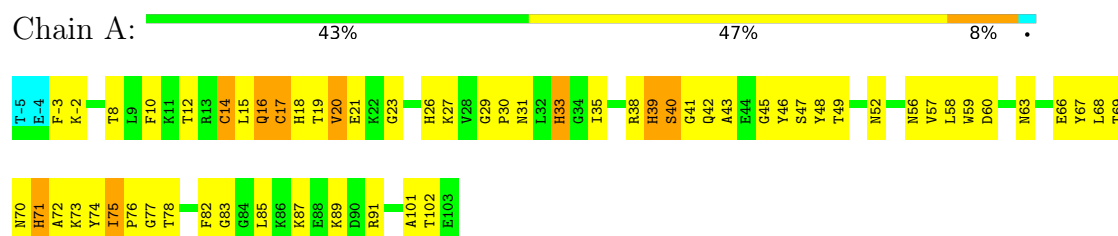
4.2.16 Score per residue for model 16

- Molecule 1: Cytochrome c iso-1



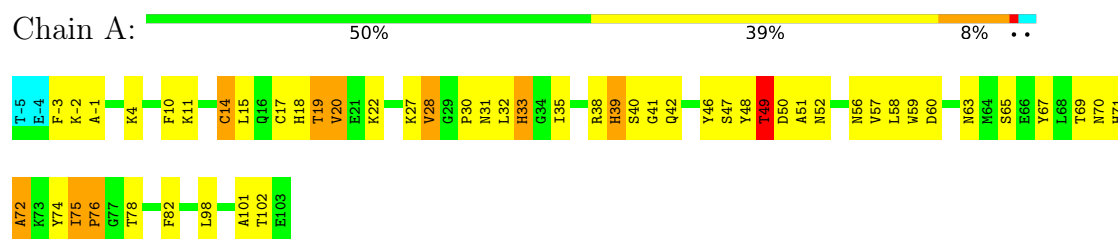
4.2.17 Score per residue for model 17

- Molecule 1: Cytochrome c iso-1



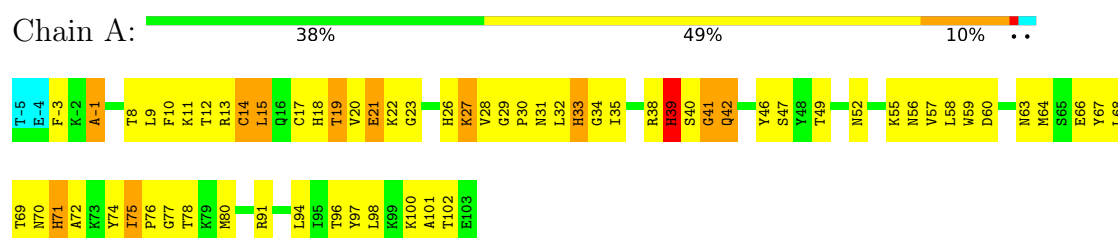
4.2.18 Score per residue for model 18

- Molecule 1: Cytochrome c iso-1



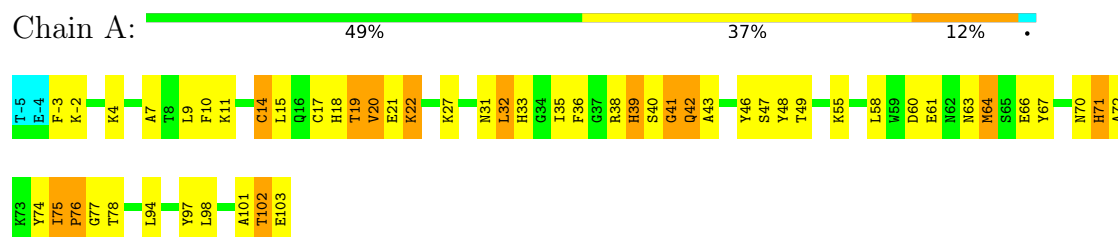
4.2.19 Score per residue for model 19

- Molecule 1: Cytochrome c iso-1



4.2.20 Score per residue for model 20

- Molecule 1: Cytochrome c iso-1



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
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)	43%

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	1.45±0.01	0±0/848 (0.0± 0.0%)	1.21±0.02	0±1/1135 (0.0± 0.1%)
All	All	1.45	0/16960 (0.0%)	1.21	10/22700 (0.0%)

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	27	LYS	CB-CA-C	-5.83	109.84	116.54	19	3
1	A	75	ILE	N-CA-CB	-5.42	108.09	111.83	6	1
1	A	27	LYS	CA-C-O	5.39	121.07	117.94	20	1
1	A	77	GLY	N-CA-C	-5.33	107.91	115.43	10	1
1	A	36	PHE	CA-CB-CG	-5.28	108.52	113.80	6	3
1	A	33	HIS	CA-CB-CG	-5.03	108.77	113.80	14	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	832	828	61±7
2	A	43	32	30	6±3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	17460	17280	17160	1263

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:LEU:HD23	1:A:85:LEU:N	0.86	1.86	4	1
1:A:11:LYS:O	1:A:15:LEU:HD21	0.81	1.76	12	1
1:A:15:LEU:N	1:A:15:LEU:HD23	0.81	1.91	19	7
1:A:20:VAL:O	1:A:20:VAL:HG12	0.76	1.80	15	12
1:A:8:THR:O	1:A:12:THR:HG23	0.75	1.82	17	10
1:A:78:THR:HG21	2:A:104:HEC:O2A	0.74	1.82	10	2
1:A:19:THR:HG22	1:A:19:THR:O	0.73	1.83	1	2
1:A:33:HIS:CE1	1:A:101:ALA:HB1	0.73	2.18	7	2
1:A:15:LEU:H	1:A:15:LEU:HD12	0.73	1.42	12	1
1:A:11:LYS:O	1:A:15:LEU:HD11	0.71	1.85	12	1
1:A:9:LEU:HD23	1:A:94:LEU:HD13	0.71	1.62	19	1
1:A:15:LEU:HD23	1:A:15:LEU:H	0.70	1.46	9	7
1:A:11:LYS:C	1:A:15:LEU:HD11	0.69	2.11	10	1
1:A:10:PHE:CE2	1:A:14:CYS:SG	0.69	2.86	1	13
1:A:39:HIS:CG	1:A:56:ASN:ND2	0.69	2.61	16	12
1:A:78:THR:HG23	1:A:78:THR:O	0.69	1.87	11	5
1:A:11:LYS:O	1:A:15:LEU:HD22	0.68	1.88	4	7
1:A:10:PHE:CE1	1:A:20:VAL:HG12	0.68	2.23	12	1
1:A:78:THR:HG21	2:A:104:HEC:CBD	0.68	2.18	17	1
1:A:10:PHE:CE1	1:A:14:CYS:SG	0.68	2.87	11	1
1:A:58:LEU:HD23	1:A:59:TRP:N	0.68	2.03	8	3
1:A:20:VAL:HG22	1:A:31:ASN:O	0.68	1.88	19	5
1:A:64:MET:SD	1:A:64:MET:N	0.68	2.67	20	5
1:A:11:LYS:O	1:A:15:LEU:HD13	0.68	1.88	9	7
1:A:32:LEU:HD21	1:A:98:LEU:HD11	0.68	1.66	16	4
1:A:20:VAL:HG13	1:A:33:HIS:ND1	0.68	2.03	9	5
1:A:71:HIS:ND1	1:A:71:HIS:N	0.67	2.43	20	5
1:A:71:HIS:CD2	1:A:71:HIS:N	0.67	2.62	17	13
1:A:41:GLY:N	1:A:52:ASN:HD21	0.67	1.88	9	6
1:A:20:VAL:O	1:A:22:LYS:N	0.67	2.27	8	6
1:A:71:HIS:O	1:A:72:ALA:HB3	0.66	1.90	8	5
1:A:20:VAL:HG12	1:A:22:LYS:H	0.66	1.49	10	5
1:A:8:THR:O	1:A:12:THR:HG22	0.66	1.90	19	1
1:A:71:HIS:O	1:A:72:ALA:HB2	0.66	1.90	12	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:ILE:O	1:A:77:GLY:N	0.66	2.29	10	3
1:A:39:HIS:N	1:A:39:HIS:CD2	0.66	2.62	5	2
1:A:85:LEU:N	1:A:85:LEU:CD2	0.65	2.60	4	1
1:A:41:GLY:N	1:A:42:GLN:HE21	0.65	1.89	2	10
1:A:75:ILE:O	1:A:75:ILE:HD12	0.65	1.91	12	1
1:A:39:HIS:CD2	1:A:56:ASN:HD21	0.65	2.09	14	8
1:A:41:GLY:N	1:A:52:ASN:ND2	0.64	2.46	9	7
1:A:55:LYS:CE	1:A:74:TYR:CE1	0.64	2.80	9	1
1:A:39:HIS:CD2	1:A:39:HIS:H	0.64	2.09	5	2
1:A:4:LYS:O	1:A:8:THR:HG23	0.64	1.91	5	4
1:A:41:GLY:C	1:A:42:GLN:NE2	0.64	2.56	8	4
1:A:67:TYR:CE1	2:A:104:HEC:CGA	0.64	2.81	13	1
1:A:39:HIS:CG	1:A:56:ASN:HD21	0.63	2.12	17	8
2:A:104:HEC:HMB1	2:A:104:HEC:HBB3	0.63	1.70	4	3
1:A:65:SER:O	1:A:69:THR:HG23	0.63	1.93	6	11
1:A:15:LEU:HD12	1:A:15:LEU:N	0.63	2.09	12	2
1:A:39:HIS:CD2	1:A:56:ASN:ND2	0.63	2.66	14	2
1:A:39:HIS:CE1	1:A:56:ASN:HD21	0.63	2.11	13	8
1:A:85:LEU:H	1:A:91:ARG:HE	0.63	1.37	8	1
1:A:50:ASP:OD1	1:A:51:ALA:N	0.62	2.32	16	2
1:A:39:HIS:O	1:A:42:GLN:NE2	0.62	2.32	12	15
1:A:46:TYR:CE1	1:A:47:SER:O	0.62	2.53	9	8
1:A:10:PHE:CE1	1:A:14:CYS:O	0.62	2.52	4	5
1:A:10:PHE:CE2	1:A:14:CYS:O	0.62	2.53	8	2
1:A:58:LEU:O	1:A:63:ASN:ND2	0.62	2.32	12	20
1:A:85:LEU:N	1:A:91:ARG:HH21	0.62	1.92	8	2
1:A:41:GLY:O	1:A:42:GLN:NE2	0.61	2.33	13	4
1:A:67:TYR:CZ	2:A:104:HEC:CGA	0.61	2.84	12	2
1:A:15:LEU:N	1:A:15:LEU:CD2	0.61	2.62	19	7
1:A:77:GLY:O	1:A:79:LYS:N	0.61	2.34	11	1
1:A:67:TYR:CD1	2:A:104:HEC:CGA	0.61	2.84	13	1
1:A:15:LEU:O	1:A:17:CYS:N	0.61	2.34	5	6
1:A:33:HIS:CD2	1:A:101:ALA:O	0.60	2.54	7	14
1:A:46:TYR:CE2	1:A:47:SER:O	0.60	2.54	8	7
1:A:32:LEU:N	1:A:32:LEU:CD2	0.60	2.65	7	1
1:A:79:LYS:O	1:A:81:ALA:N	0.60	2.35	14	1
1:A:40:SER:C	1:A:42:GLN:NE2	0.59	2.60	11	3
1:A:55:LYS:NZ	1:A:74:TYR:CD1	0.59	2.70	9	1
1:A:67:TYR:CD1	2:A:104:HEC:O2A	0.59	2.55	13	1
1:A:67:TYR:O	1:A:71:HIS:CD2	0.59	2.55	4	6
1:A:-3:PHE:CD1	1:A:-2:LYS:N	0.59	2.70	2	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:HIS:NE2	1:A:101:ALA:O	0.59	2.35	18	4
1:A:33:HIS:CE1	1:A:101:ALA:O	0.59	2.55	18	2
1:A:26:HIS:O	1:A:29:GLY:O	0.59	2.21	12	6
1:A:85:LEU:H	1:A:91:ARG:NE	0.59	1.95	8	1
1:A:-3:PHE:CE1	1:A:-2:LYS:O	0.59	2.56	5	3
1:A:67:TYR:CG	2:A:104:HEC:O1A	0.59	2.55	13	1
1:A:59:TRP:CZ2	2:A:104:HEC:O2A	0.59	2.56	6	3
1:A:69:THR:O	1:A:70:ASN:ND2	0.59	2.36	12	2
1:A:55:LYS:NZ	1:A:74:TYR:O	0.59	2.36	20	6
1:A:85:LEU:HD23	1:A:85:LEU:H	0.59	1.58	4	1
1:A:67:TYR:CZ	2:A:104:HEC:O2A	0.59	2.55	5	1
1:A:15:LEU:H	1:A:15:LEU:CD1	0.59	2.05	12	1
1:A:38:ARG:NE	1:A:42:GLN:OE1	0.59	2.36	20	1
1:A:68:LEU:HD13	1:A:91:ARG:CD	0.58	2.27	3	2
1:A:-3:PHE:C	1:A:-3:PHE:CD1	0.58	2.80	11	6
1:A:67:TYR:CD2	2:A:104:HEC:O1A	0.58	2.56	13	1
1:A:67:TYR:O	1:A:71:HIS:ND1	0.58	2.36	20	1
1:A:32:LEU:CD1	1:A:35:ILE:HD12	0.58	2.28	9	7
1:A:42:GLN:N	1:A:42:GLN:NE2	0.58	2.51	7	3
1:A:68:LEU:CD1	1:A:68:LEU:N	0.58	2.66	8	3
1:A:67:TYR:CZ	2:A:104:HEC:O1A	0.58	2.56	12	1
1:A:43:ALA:HB3	1:A:46:TYR:O	0.58	1.99	17	1
1:A:82:PHE:CD1	1:A:83:GLY:O	0.58	2.56	17	1
1:A:72:ALA:H	1:A:75:ILE:CD1	0.58	2.12	3	2
1:A:16:GLN:O	1:A:17:CYS:SG	0.58	2.62	7	6
1:A:58:LEU:H	1:A:58:LEU:HD23	0.58	1.59	15	1
1:A:37:GLY:N	1:A:42:GLN:OE1	0.58	2.36	2	1
1:A:99:LYS:O	1:A:103:GLU:N	0.58	2.36	7	1
1:A:60:ASP:O	1:A:64:MET:SD	0.57	2.62	6	5
1:A:46:TYR:CZ	1:A:47:SER:O	0.57	2.57	18	3
1:A:68:LEU:HD13	1:A:91:ARG:HD2	0.57	1.76	3	6
1:A:21:GLU:C	1:A:23:GLY:H	0.57	2.07	1	2
1:A:33:HIS:ND1	1:A:101:ALA:O	0.57	2.37	20	2
1:A:21:GLU:O	1:A:23:GLY:N	0.57	2.38	1	2
1:A:18:HIS:O	1:A:20:VAL:N	0.57	2.37	3	1
1:A:67:TYR:OH	1:A:80:MET:SD	0.57	2.62	9	2
1:A:37:GLY:O	1:A:58:LEU:CD1	0.57	2.52	2	2
1:A:40:SER:N	1:A:57:VAL:O	0.56	2.37	1	9
1:A:31:ASN:O	1:A:32:LEU:CB	0.56	2.52	20	3
1:A:19:THR:OG1	1:A:27:LYS:NZ	0.56	2.36	2	1
1:A:17:CYS:O	1:A:19:THR:N	0.56	2.38	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:LEU:HD12	1:A:68:LEU:N	0.56	2.15	13	2
1:A:42:GLN:N	1:A:48:TYR:CE1	0.56	2.74	11	2
1:A:39:HIS:ND1	1:A:56:ASN:ND2	0.56	2.52	13	7
1:A:78:THR:HG21	2:A:104:HEC:HBD1	0.56	1.75	17	1
1:A:20:VAL:C	1:A:22:LYS:N	0.56	2.63	10	6
1:A:10:PHE:CZ	1:A:14:CYS:SG	0.56	2.99	2	6
1:A:72:ALA:O	1:A:75:ILE:O	0.56	2.24	12	14
1:A:60:ASP:OD1	1:A:63:ASN:ND2	0.56	2.39	12	2
1:A:40:SER:C	1:A:42:GLN:HE22	0.56	2.09	13	3
1:A:16:GLN:HE21	2:A:104:HEC:CMC	0.56	2.13	3	3
1:A:68:LEU:N	1:A:68:LEU:CD1	0.56	2.69	13	4
1:A:67:TYR:CE2	1:A:75:ILE:CD1	0.56	2.89	6	1
1:A:82:PHE:CE1	2:A:104:HEC:HBB2	0.56	2.36	2	4
1:A:85:LEU:H	1:A:91:ARG:HH21	0.56	1.44	17	3
1:A:20:VAL:HG13	1:A:33:HIS:CE1	0.56	2.35	2	3
1:A:9:LEU:HD22	1:A:94:LEU:HD11	0.56	1.78	9	2
1:A:49:THR:O	1:A:50:ASP:CB	0.55	2.54	1	3
1:A:21:GLU:O	1:A:22:LYS:CB	0.55	2.54	20	3
1:A:-3:PHE:CD1	1:A:-3:PHE:C	0.55	2.83	6	7
1:A:77:GLY:O	1:A:78:THR:C	0.55	2.49	10	12
1:A:56:ASN:C	1:A:56:ASN:HD22	0.55	2.08	1	4
1:A:87:LYS:O	1:A:89:LYS:N	0.55	2.39	17	3
1:A:20:VAL:O	1:A:20:VAL:CG1	0.55	2.55	18	9
1:A:20:VAL:O	1:A:23:GLY:N	0.55	2.38	3	2
1:A:32:LEU:HD21	1:A:98:LEU:HD22	0.55	1.78	13	5
1:A:19:THR:HG21	1:A:27:LYS:HZ1	0.55	1.60	17	1
1:A:20:VAL:O	1:A:21:GLU:C	0.55	2.47	3	6
1:A:10:PHE:CZ	1:A:20:VAL:HG21	0.55	2.37	13	3
1:A:67:TYR:OH	1:A:80:MET:CE	0.55	2.55	5	1
1:A:55:LYS:CE	1:A:74:TYR:O	0.55	2.54	19	4
1:A:42:GLN:N	1:A:42:GLN:CD	0.55	2.63	17	3
1:A:48:TYR:CD2	2:A:104:HEC:O1D	0.55	2.60	18	1
1:A:67:TYR:C	1:A:67:TYR:CD1	0.55	2.83	20	3
1:A:40:SER:C	1:A:42:GLN:HE21	0.55	2.10	3	10
1:A:8:THR:O	1:A:12:THR:CG2	0.54	2.55	6	9
1:A:74:TYR:C	1:A:74:TYR:CD1	0.54	2.81	13	6
1:A:71:HIS:O	1:A:72:ALA:CB	0.54	2.54	14	15
1:A:76:PRO:C	1:A:78:THR:H	0.54	2.09	14	16
1:A:38:ARG:O	1:A:39:HIS:O	0.54	2.25	18	12
1:A:9:LEU:HD23	1:A:94:LEU:HD11	0.54	1.80	3	2
1:A:58:LEU:HD23	1:A:58:LEU:C	0.54	2.28	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:PHE:CD2	1:A:83:GLY:O	0.54	2.60	2	2
1:A:33:HIS:ND1	1:A:101:ALA:HB1	0.54	2.17	8	4
1:A:59:TRP:CE3	1:A:64:MET:HE1	0.54	2.38	9	3
2:A:104:HEC:CGA	2:A:104:HEC:O2D	0.54	2.56	7	1
1:A:15:LEU:N	1:A:15:LEU:CD1	0.54	2.70	1	1
1:A:18:HIS:ND1	1:A:30:PRO:O	0.54	2.39	7	11
1:A:82:PHE:CE1	1:A:83:GLY:O	0.54	2.60	17	1
1:A:56:ASN:ND2	1:A:56:ASN:O	0.53	2.41	10	2
1:A:21:GLU:O	1:A:22:LYS:O	0.53	2.26	8	2
1:A:49:THR:C	1:A:51:ALA:H	0.53	2.11	18	2
1:A:79:LYS:O	1:A:80:MET:C	0.53	2.51	10	2
1:A:43:ALA:HB2	1:A:48:TYR:OH	0.53	2.04	17	3
1:A:18:HIS:CE1	1:A:32:LEU:HD13	0.53	2.39	2	1
2:A:104:HEC:CGA	2:A:104:HEC:CHA	0.53	2.86	12	1
1:A:48:TYR:C	1:A:50:ASP:H	0.53	2.11	12	5
1:A:85:LEU:H	1:A:91:ARG:NH2	0.53	2.01	8	1
1:A:82:PHE:CD1	1:A:82:PHE:O	0.53	2.62	6	1
1:A:20:VAL:HG13	1:A:20:VAL:O	0.52	2.03	12	1
1:A:59:TRP:CZ3	1:A:74:TYR:OH	0.52	2.62	17	1
1:A:19:THR:C	1:A:21:GLU:H	0.52	2.13	12	1
1:A:66:GLU:O	1:A:71:HIS:CD2	0.52	2.62	13	1
1:A:59:TRP:CZ2	2:A:104:HEC:O1A	0.52	2.61	11	2
1:A:32:LEU:HD11	1:A:35:ILE:HD12	0.52	1.82	9	1
1:A:37:GLY:O	1:A:38:ARG:O	0.52	2.28	3	4
1:A:68:LEU:N	1:A:68:LEU:HD12	0.52	2.18	8	4
1:A:20:VAL:C	1:A:22:LYS:H	0.52	2.11	12	3
1:A:87:LYS:C	1:A:89:LYS:H	0.52	2.12	17	1
1:A:19:THR:O	1:A:19:THR:CG2	0.52	2.56	1	1
1:A:26:HIS:ND1	1:A:31:ASN:N	0.52	2.57	3	1
1:A:48:TYR:N	1:A:48:TYR:CD1	0.52	2.78	16	6
2:A:104:HEC:CGA	2:A:104:HEC:C1A	0.52	2.88	12	1
1:A:40:SER:OG	1:A:52:ASN:C	0.51	2.53	12	2
1:A:68:LEU:HD23	1:A:91:ARG:HD2	0.51	1.83	5	1
1:A:15:LEU:C	1:A:17:CYS:N	0.51	2.68	12	9
1:A:60:ASP:OD1	1:A:63:ASN:CG	0.51	2.54	3	4
1:A:32:LEU:HD13	1:A:35:ILE:HD12	0.51	1.82	7	1
1:A:15:LEU:C	1:A:17:CYS:H	0.51	2.14	12	9
1:A:42:GLN:O	1:A:43:ALA:C	0.51	2.53	11	2
1:A:18:HIS:O	1:A:19:THR:C	0.51	2.54	8	12
1:A:43:ALA:O	1:A:46:TYR:O	0.51	2.28	20	4
1:A:68:LEU:HD23	1:A:91:ARG:CD	0.51	2.35	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:TRP:O	1:A:60:ASP:OD1	0.51	2.29	9	11
1:A:75:ILE:O	1:A:76:PRO:C	0.51	2.52	12	13
1:A:19:THR:HG21	1:A:25:PRO:O	0.51	2.06	13	1
1:A:11:LYS:O	1:A:15:LEU:CD2	0.51	2.53	12	5
1:A:46:TYR:C	1:A:46:TYR:CD1	0.51	2.89	11	2
1:A:19:THR:O	1:A:31:ASN:OD1	0.51	2.29	16	2
1:A:10:PHE:CD1	1:A:14:CYS:O	0.51	2.63	19	1
1:A:19:THR:O	1:A:21:GLU:N	0.50	2.44	12	5
1:A:35:ILE:O	1:A:42:GLN:OE1	0.50	2.30	11	3
1:A:39:HIS:O	1:A:42:GLN:CG	0.50	2.59	14	1
1:A:76:PRO:C	1:A:78:THR:N	0.50	2.69	11	13
1:A:34:GLY:O	1:A:42:GLN:OE1	0.50	2.30	2	2
1:A:82:PHE:CD1	1:A:82:PHE:C	0.50	2.89	6	1
1:A:39:HIS:CE1	1:A:56:ASN:ND2	0.50	2.79	13	2
1:A:82:PHE:CZ	1:A:85:LEU:HD21	0.50	2.41	16	1
1:A:38:ARG:O	1:A:42:GLN:CD	0.50	2.55	1	2
1:A:40:SER:OG	1:A:52:ASN:O	0.50	2.29	14	12
1:A:85:LEU:N	1:A:91:ARG:NH2	0.50	2.59	8	1
1:A:58:LEU:CD2	1:A:58:LEU:C	0.50	2.84	3	1
1:A:37:GLY:O	1:A:38:ARG:C	0.50	2.53	15	2
1:A:75:ILE:HD13	2:A:104:HEC:O2A	0.50	2.07	13	1
1:A:38:ARG:O	1:A:39:HIS:C	0.50	2.54	12	7
1:A:66:GLU:O	1:A:70:ASN:O	0.50	2.30	2	9
1:A:72:ALA:H	1:A:75:ILE:HD11	0.50	1.65	3	1
1:A:40:SER:O	1:A:42:GLN:NE2	0.50	2.42	7	4
1:A:49:THR:O	1:A:49:THR:OG1	0.50	2.30	18	2
1:A:30:PRO:C	1:A:32:LEU:N	0.50	2.68	8	3
1:A:76:PRO:O	1:A:78:THR:N	0.50	2.45	14	5
1:A:39:HIS:O	1:A:42:GLN:CD	0.50	2.55	2	2
1:A:78:THR:O	1:A:78:THR:CG2	0.50	2.59	15	8
1:A:67:TYR:CD2	1:A:75:ILE:CD1	0.50	2.95	6	1
2:A:104:HEC:HMB3	2:A:104:HEC:HBB2	0.50	1.84	9	2
1:A:19:THR:O	1:A:31:ASN:CG	0.50	2.55	16	1
1:A:14:CYS:SG	2:A:104:HEC:CHC	0.50	2.99	10	6
1:A:71:HIS:HB2	1:A:75:ILE:HD11	0.50	1.82	9	1
1:A:41:GLY:C	1:A:42:GLN:CD	0.50	2.79	11	1
1:A:17:CYS:SG	2:A:104:HEC:CMC	0.49	2.99	8	18
1:A:78:THR:OG1	2:A:104:HEC:HMD3	0.49	2.07	16	1
1:A:79:LYS:O	1:A:80:MET:O	0.49	2.30	10	2
1:A:49:THR:O	1:A:51:ALA:N	0.49	2.42	18	2
1:A:75:ILE:HD12	1:A:75:ILE:C	0.49	2.33	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:THR:O	1:A:70:ASN:OD1	0.49	2.30	19	8
1:A:80:MET:O	1:A:81:ALA:HB3	0.49	2.07	6	1
1:A:49:THR:C	1:A:51:ALA:N	0.49	2.70	12	2
1:A:41:GLY:O	1:A:42:GLN:CD	0.49	2.55	20	2
1:A:38:ARG:CG	1:A:39:HIS:N	0.49	2.74	14	1
1:A:28:VAL:CG1	1:A:29:GLY:N	0.49	2.76	19	1
1:A:46:TYR:CD1	1:A:46:TYR:C	0.49	2.91	16	4
1:A:60:ASP:CG	1:A:61:GLU:N	0.49	2.70	13	5
1:A:10:PHE:O	1:A:14:CYS:N	0.49	2.45	4	6
1:A:56:ASN:ND2	1:A:56:ASN:C	0.49	2.71	1	2
1:A:72:ALA:H	1:A:75:ILE:CG1	0.49	2.21	3	1
1:A:19:THR:O	1:A:20:VAL:C	0.49	2.55	5	3
1:A:81:ALA:O	1:A:83:GLY:N	0.49	2.45	10	1
1:A:41:GLY:N	1:A:42:GLN:HE22	0.49	2.05	11	1
1:A:67:TYR:CE1	2:A:104:HEC:O2A	0.49	2.65	5	2
1:A:8:THR:O	1:A:12:THR:OG1	0.49	2.31	6	3
1:A:58:LEU:HD23	1:A:58:LEU:N	0.49	2.23	16	2
1:A:57:VAL:HG11	1:A:74:TYR:OH	0.49	2.08	1	2
1:A:78:THR:OG1	2:A:104:HEC:HMD2	0.49	2.08	1	1
1:A:102:THR:O	1:A:103:GLU:C	0.49	2.55	11	4
1:A:58:LEU:HD23	1:A:58:LEU:H	0.49	1.67	16	1
1:A:10:PHE:CE1	1:A:20:VAL:HG21	0.49	2.43	13	1
1:A:32:LEU:CD2	1:A:98:LEU:HD22	0.48	2.38	9	5
2:A:104:HEC:CMB	2:A:104:HEC:HBB2	0.48	2.38	8	4
1:A:93:ASP:O	1:A:96:THR:OG1	0.48	2.31	16	1
1:A:41:GLY:N	1:A:42:GLN:NE2	0.48	2.59	2	2
1:A:22:LYS:O	1:A:23:GLY:C	0.48	2.54	8	1
1:A:75:ILE:C	1:A:77:GLY:H	0.48	2.16	10	1
1:A:75:ILE:C	1:A:77:GLY:N	0.48	2.70	10	1
1:A:34:GLY:O	1:A:42:GLN:CB	0.48	2.61	19	1
1:A:15:LEU:O	1:A:16:GLN:C	0.48	2.56	5	3
1:A:11:LYS:O	1:A:15:LEU:CD1	0.48	2.60	12	8
1:A:12:THR:HG23	1:A:13:ARG:HG3	0.48	1.84	19	1
1:A:39:HIS:CD2	1:A:39:HIS:N	0.48	2.81	3	1
1:A:57:VAL:O	1:A:58:LEU:CB	0.48	2.62	5	1
1:A:57:VAL:O	1:A:58:LEU:O	0.48	2.31	14	1
1:A:50:ASP:OD2	1:A:54:LYS:NZ	0.48	2.47	16	1
1:A:26:HIS:O	1:A:27:LYS:C	0.48	2.55	19	1
1:A:18:HIS:O	1:A:19:THR:O	0.48	2.32	4	2
1:A:48:TYR:C	1:A:50:ASP:N	0.48	2.69	14	4
1:A:41:GLY:CA	1:A:52:ASN:HD21	0.48	2.22	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:104:HEC:HBB2	2:A:104:HEC:HMB3	0.48	1.85	19	4
1:A:-1:ALA:O	1:A:96:THR:OG1	0.48	2.30	19	1
1:A:51:ALA:HB3	1:A:76:PRO:HG3	0.48	1.85	8	2
1:A:67:TYR:O	1:A:71:HIS:CG	0.48	2.67	20	3
1:A:40:SER:OG	1:A:57:VAL:N	0.48	2.43	11	3
2:A:104:HEC:O1A	2:A:104:HEC:C1A	0.48	2.62	12	1
1:A:21:GLU:C	1:A:23:GLY:N	0.47	2.72	10	2
2:A:104:HEC:HBB2	2:A:104:HEC:CMB	0.47	2.39	20	2
1:A:15:LEU:N	1:A:15:LEU:HD12	0.47	2.23	1	1
1:A:38:ARG:O	1:A:58:LEU:CD1	0.47	2.62	19	1
1:A:38:ARG:O	1:A:58:LEU:HD12	0.47	2.09	20	2
1:A:67:TYR:CE2	2:A:104:HEC:CBA	0.47	2.97	19	1
1:A:20:VAL:CG1	1:A:33:HIS:CE1	0.47	2.98	14	4
1:A:74:TYR:CD1	1:A:74:TYR:C	0.47	2.92	1	5
1:A:78:THR:HG21	2:A:104:HEC:HBD2	0.47	1.83	17	3
2:A:104:HEC:O2D	2:A:104:HEC:O1A	0.47	2.32	7	1
1:A:78:THR:CG2	1:A:79:LYS:N	0.47	2.77	13	1
1:A:57:VAL:O	1:A:57:VAL:CG2	0.47	2.63	14	1
1:A:58:LEU:H	1:A:58:LEU:CD2	0.47	2.23	16	1
2:A:104:HEC:O2A	2:A:104:HEC:O1D	0.47	2.33	16	1
1:A:74:TYR:CD1	1:A:74:TYR:O	0.47	2.68	13	6
1:A:85:LEU:HD23	1:A:86:LYS:H	0.47	1.70	15	1
1:A:19:THR:HG21	1:A:27:LYS:NZ	0.47	2.24	17	1
1:A:57:VAL:HG21	1:A:74:TYR:OH	0.46	2.10	5	1
2:A:104:HEC:O1A	2:A:104:HEC:CGD	0.46	2.63	7	1
1:A:58:LEU:HD22	1:A:60:ASP:OD1	0.46	2.11	8	1
1:A:71:HIS:HB3	1:A:75:ILE:HD11	0.46	1.87	13	1
1:A:78:THR:O	1:A:78:THR:HG23	0.46	2.10	18	4
1:A:55:LYS:NZ	1:A:74:TYR:CE1	0.46	2.83	9	1
1:A:40:SER:O	1:A:41:GLY:O	0.46	2.34	2	3
1:A:71:HIS:CB	1:A:75:ILE:HD11	0.46	2.40	20	1
1:A:71:HIS:CD2	1:A:71:HIS:H	0.45	2.29	3	1
1:A:33:HIS:CG	1:A:101:ALA:O	0.45	2.69	16	1
1:A:38:ARG:HE	1:A:39:HIS:CE1	0.45	2.30	1	1
1:A:60:ASP:CG	1:A:61:GLU:H	0.45	2.20	13	3
2:A:104:HEC:HMB3	2:A:104:HEC:CBB	0.45	2.41	16	11
1:A:35:ILE:HG21	1:A:64:MET:HE1	0.45	1.89	7	1
1:A:60:ASP:CG	1:A:63:ASN:ND2	0.45	2.75	12	1
1:A:71:HIS:C	1:A:73:LYS:H	0.45	2.20	17	1
1:A:20:VAL:CG1	1:A:33:HIS:ND1	0.45	2.78	9	1
1:A:67:TYR:CD1	1:A:67:TYR:C	0.45	2.94	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:LYS:C	1:A:89:LYS:N	0.45	2.75	17	1
1:A:48:TYR:CE2	2:A:104:HEC:O1D	0.45	2.69	18	1
1:A:67:TYR:CD2	2:A:104:HEC:CBA	0.45	2.99	6	1
1:A:23:GLY:H	1:A:31:ASN:HD21	0.45	1.53	17	1
1:A:13:ARG:HH22	1:A:87:LYS:NZ	0.45	2.10	8	1
2:A:104:HEC:HBB3	2:A:104:HEC:CMB	0.44	2.42	18	3
1:A:75:ILE:O	1:A:76:PRO:O	0.44	2.34	9	4
1:A:41:GLY:H	1:A:52:ASN:HD21	0.44	1.56	11	1
1:A:40:SER:CB	1:A:59:TRP:CD1	0.44	3.00	8	1
1:A:58:LEU:CD2	1:A:60:ASP:OD1	0.44	2.65	8	1
1:A:64:MET:HE1	2:A:104:HEC:HMA1	0.44	1.88	19	1
1:A:16:GLN:O	1:A:27:LYS:NZ	0.44	2.50	7	2
1:A:40:SER:OG	1:A:52:ASN:CG	0.44	2.60	10	1
1:A:32:LEU:CD2	1:A:98:LEU:HD11	0.44	2.41	16	2
1:A:55:LYS:CD	1:A:74:TYR:O	0.44	2.66	19	1
1:A:102:THR:O	1:A:103:GLU:O	0.44	2.36	11	2
1:A:78:THR:OG1	2:A:104:HEC:O1D	0.44	2.32	20	1
1:A:15:LEU:O	1:A:16:GLN:CG	0.44	2.66	5	1
1:A:-3:PHE:CE2	1:A:95:ILE:HG21	0.44	2.47	16	1
1:A:19:THR:C	1:A:21:GLU:N	0.44	2.76	12	2
1:A:35:ILE:HG23	1:A:59:TRP:CD1	0.44	2.47	8	1
1:A:94:LEU:HD21	2:A:104:HEC:HBB2	0.44	1.90	19	1
1:A:14:CYS:H	1:A:15:LEU:HD12	0.44	1.72	10	1
1:A:64:MET:SD	2:A:104:HEC:HMA2	0.44	2.53	12	2
1:A:51:ALA:HB3	1:A:76:PRO:HB3	0.44	1.90	14	1
1:A:61:GLU:OE2	1:A:99:LYS:NZ	0.44	2.50	14	1
1:A:15:LEU:O	1:A:19:THR:OG1	0.43	2.31	20	2
1:A:61:GLU:OE2	1:A:99:LYS:CE	0.43	2.67	4	1
1:A:85:LEU:H	1:A:91:ARG:CZ	0.43	2.26	8	1
1:A:15:LEU:O	1:A:19:THR:CA	0.43	2.66	9	1
1:A:43:ALA:CB	1:A:48:TYR:OH	0.43	2.66	16	1
1:A:32:LEU:N	1:A:32:LEU:HD22	0.43	2.27	7	1
1:A:40:SER:C	1:A:52:ASN:ND2	0.43	2.77	9	1
1:A:67:TYR:CZ	2:A:104:HEC:CBA	0.43	3.01	7	2
1:A:66:GLU:O	1:A:69:THR:OG1	0.43	2.34	13	1
1:A:27:LYS:O	1:A:28:VAL:HG23	0.43	2.13	18	1
1:A:82:PHE:CD1	2:A:104:HEC:HBB2	0.43	2.47	18	1
1:A:33:HIS:HD1	1:A:101:ALA:C	0.43	2.21	6	1
1:A:97:TYR:CE1	1:A:100:LYS:CE	0.43	3.02	12	2
1:A:28:VAL:HG13	1:A:29:GLY:N	0.43	2.28	19	1
1:A:30:PRO:C	1:A:32:LEU:H	0.43	2.22	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:CYS:CB	2:A:104:HEC:C2C	0.43	2.97	16	1
1:A:60:ASP:OD1	1:A:61:GLU:N	0.43	2.50	20	4
1:A:40:SER:OG	1:A:57:VAL:HG12	0.43	2.14	9	1
1:A:32:LEU:HD12	1:A:35:ILE:HD12	0.42	1.89	1	1
1:A:58:LEU:C	1:A:58:LEU:HD23	0.42	2.38	3	1
1:A:3:ALA:O	1:A:7:ALA:N	0.42	2.47	7	1
1:A:66:GLU:O	1:A:70:ASN:N	0.42	2.47	20	1
1:A:30:PRO:O	1:A:32:LEU:N	0.42	2.52	8	1
2:A:104:HEC:CMB	2:A:104:HEC:CBB	0.42	2.98	10	6
1:A:38:ARG:C	1:A:39:HIS:O	0.42	2.63	18	7
1:A:10:PHE:CD2	1:A:14:CYS:O	0.42	2.71	8	1
1:A:50:ASP:OD1	1:A:50:ASP:C	0.42	2.62	2	1
1:A:58:LEU:C	1:A:58:LEU:CD2	0.42	2.93	10	4
1:A:-3:PHE:CE2	1:A:95:ILE:CG2	0.42	3.02	16	1
1:A:12:THR:O	1:A:13:ARG:CG	0.42	2.67	10	1
1:A:9:LEU:HB2	1:A:94:LEU:HD21	0.42	1.92	6	1
1:A:58:LEU:O	1:A:58:LEU:HD12	0.42	2.14	6	1
1:A:52:ASN:OD1	1:A:53:ILE:N	0.41	2.52	12	1
1:A:60:ASP:CG	1:A:61:GLU:OE1	0.41	2.63	13	1
1:A:74:TYR:CE2	1:A:75:ILE:HG23	0.41	2.50	13	2
1:A:31:ASN:O	1:A:33:HIS:N	0.41	2.47	9	1
1:A:71:HIS:O	1:A:71:HIS:CG	0.41	2.71	11	1
1:A:36:PHE:CZ	1:A:64:MET:HE2	0.41	2.51	20	2
1:A:49:THR:O	1:A:50:ASP:C	0.41	2.64	13	2
1:A:30:PRO:O	1:A:31:ASN:C	0.41	2.64	18	1
1:A:94:LEU:N	1:A:94:LEU:CD2	0.41	2.84	16	1
1:A:14:CYS:C	1:A:15:LEU:HD12	0.41	2.40	1	1
1:A:16:GLN:O	1:A:27:LYS:CE	0.41	2.69	7	1
1:A:49:THR:CG2	2:A:104:HEC:O1D	0.41	2.69	8	1
1:A:9:LEU:CD2	1:A:94:LEU:HD11	0.41	2.45	9	1
1:A:48:TYR:CD1	1:A:48:TYR:N	0.41	2.89	20	2
1:A:7:ALA:HB2	1:A:97:TYR:CE1	0.41	2.51	20	1
1:A:94:LEU:HD21	2:A:104:HEC:HMB3	0.41	1.92	2	1
1:A:74:TYR:CD1	1:A:74:TYR:N	0.41	2.89	3	1
1:A:36:PHE:CE1	1:A:64:MET:SD	0.41	3.13	5	1
1:A:50:ASP:O	1:A:51:ALA:C	0.41	2.61	10	1
1:A:10:PHE:CZ	1:A:20:VAL:HG23	0.41	2.50	11	1
1:A:-3:PHE:CD1	1:A:95:ILE:HD12	0.40	2.51	16	1
1:A:59:TRP:CH2	1:A:74:TYR:OH	0.40	2.59	17	1
1:A:72:ALA:H	1:A:75:ILE:HG13	0.40	1.77	3	1
1:A:19:THR:HG22	1:A:21:GLU:HB2	0.40	1.93	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:LEU:HD23	1:A:91:ARG:CG	0.40	2.45	5	1
1:A:40:SER:CB	1:A:52:ASN:OD1	0.40	2.70	10	1
1:A:67:TYR:OH	2:A:104:HEC:O1A	0.40	2.37	12	1
1:A:64:MET:N	1:A:64:MET:SD	0.40	2.94	16	1
1:A:39:HIS:CB	1:A:56:ASN:ND2	0.40	2.84	19	1
1:A:16:GLN:C	1:A:17:CYS:SG	0.40	3.05	5	1
1:A:32:LEU:HD21	1:A:98:LEU:CD2	0.40	2.46	6	1
1:A:41:GLY:CA	1:A:48:TYR:CE1	0.40	3.04	17	1
1:A:38:ARG:O	1:A:39:HIS:CD2	0.40	2.75	8	1
1:A:40:SER:OG	1:A:52:ASN:OD1	0.40	2.39	10	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%)	86±2 (82±2%)	13±2 (12±2%)	6±2 (6±2%)	2	19
All	All	2100/2160 (97%)	1720 (82%)	252 (12%)	128 (6%)	2	19

All 28 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	14	CYS	18
1	A	76	PRO	15
1	A	39	HIS	12
1	A	72	ALA	12
1	A	41	GLY	12
1	A	16	GLN	8
1	A	21	GLU	6
1	A	22	LYS	5
1	A	20	VAL	5
1	A	-1	ALA	5
1	A	38	ARG	4
1	A	19	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	80	MET	3
1	A	18	HIS	2
1	A	58	LEU	2
1	A	28	VAL	2
1	A	71	HIS	2
1	A	49	THR	2
1	A	83	GLY	1
1	A	23	GLY	1
1	A	37	GLY	1
1	A	43	ALA	1
1	A	78	THR	1
1	A	50	ASP	1
1	A	79	LYS	1
1	A	17	CYS	1
1	A	45	GLY	1
1	A	32	LEU	1

6.3.2 Protein sidechains ⓘ

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%)	78±1 (91±2%)	8±1 (9±2%)	11	56
All	All	1720/1760 (98%)	1562 (91%)	158 (9%)	11	56

All 27 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	75	ILE	19
1	A	102	THR	19
1	A	49	THR	18
1	A	33	HIS	15
1	A	71	HIS	12
1	A	35	ILE	9
1	A	19	THR	7
1	A	64	MET	7
1	A	58	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	42	GLN	6
1	A	4	LYS	5
1	A	40	SER	5
1	A	22	LYS	3
1	A	39	HIS	3
1	A	57	VAL	3
1	A	38	ARG	3
1	A	98	LEU	3
1	A	8	THR	2
1	A	85	LEU	2
1	A	80	MET	2
1	A	100	LYS	2
1	A	15	LEU	2
1	A	9	LEU	1
1	A	32	LEU	1
1	A	14	CYS	1
1	A	56	ASN	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	46,50,50	1.33±0.01	4±0 (8±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	58,82,82	1.52±0.04	2±0 (3±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	-	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	CAB-C3B	5.04	1.51	1.35	3	20
2	A	104	HEC	CAC-C3C	4.59	1.49	1.35	9	20
2	A	104	HEC	O2A-CGA	2.58	1.22	1.30	13	20
2	A	104	HEC	O2D-CGD	2.56	1.22	1.30	5	20

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

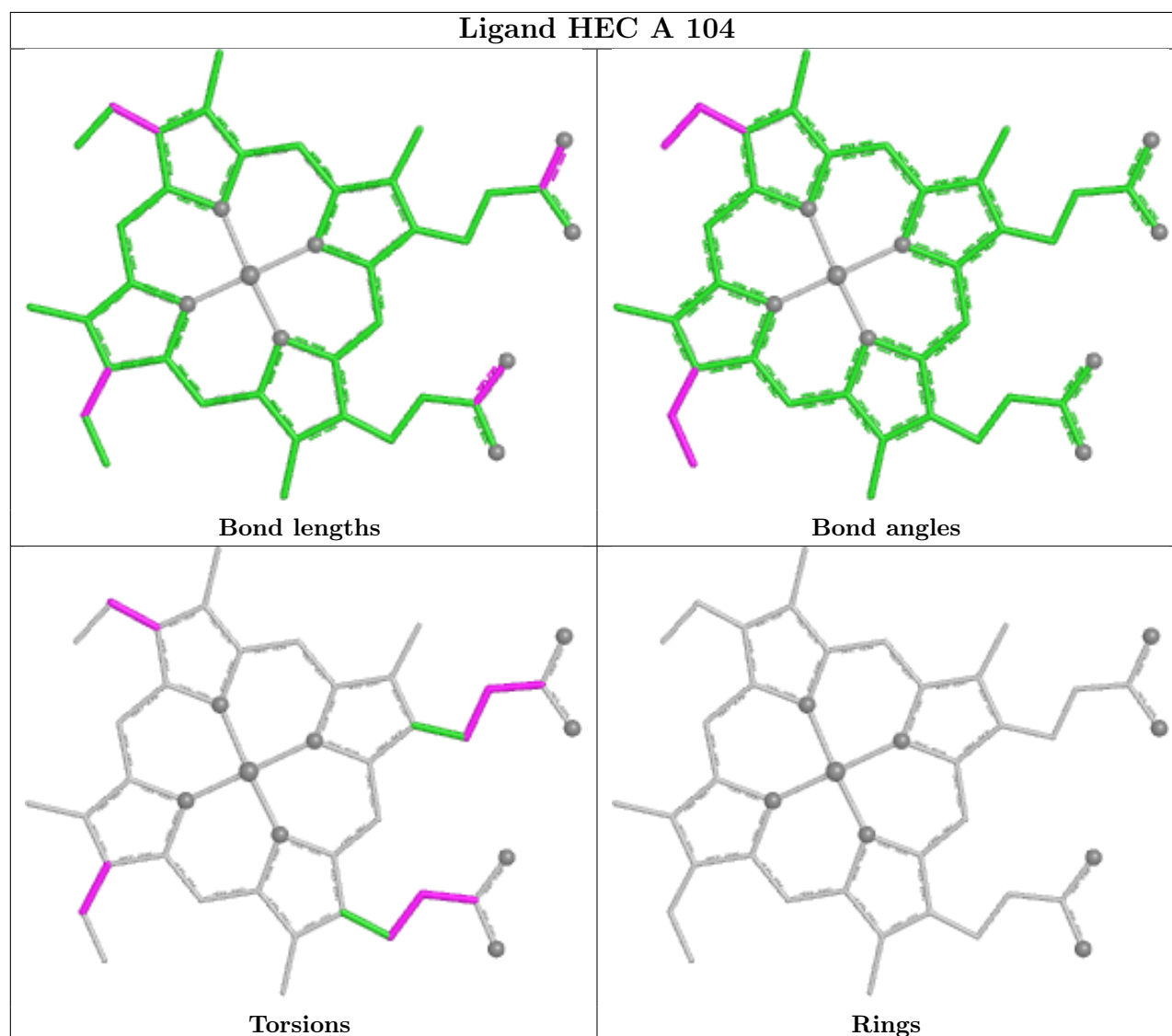
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	104	HEC	CBB-CAB-C3B	7.78	111.89	127.43	10	20
2	A	104	HEC	CBC-CAC-C3C	7.24	112.97	127.43	17	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 43% for the well-defined parts and 43% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	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)	23

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 43%, i.e. 615 atoms were assigned a chemical shift out of a possible 1424. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	211/536 (39%)	211/221 (95%)	0/212 (0%)	0/103 (0%)
Sidechain	361/752 (48%)	361/484 (75%)	0/235 (0%)	0/33 (0%)
Aromatic	43/136 (32%)	43/66 (65%)	0/60 (0%)	0/10 (0%)
Overall	615/1424 (43%)	615/771 (80%)	0/507 (0%)	0/146 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 43%, i.e. 615 atoms were assigned a chemical shift out of a possible 1447. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	211/546 (39%)	211/225 (94%)	0/216 (0%)	0/105 (0%)
Sidechain	361/765 (47%)	361/492 (73%)	0/240 (0%)	0/33 (0%)
Aromatic	43/136 (32%)	43/66 (65%)	0/60 (0%)	0/10 (0%)
Overall	615/1447 (43%)	615/783 (79%)	0/516 (0%)	0/148 (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.

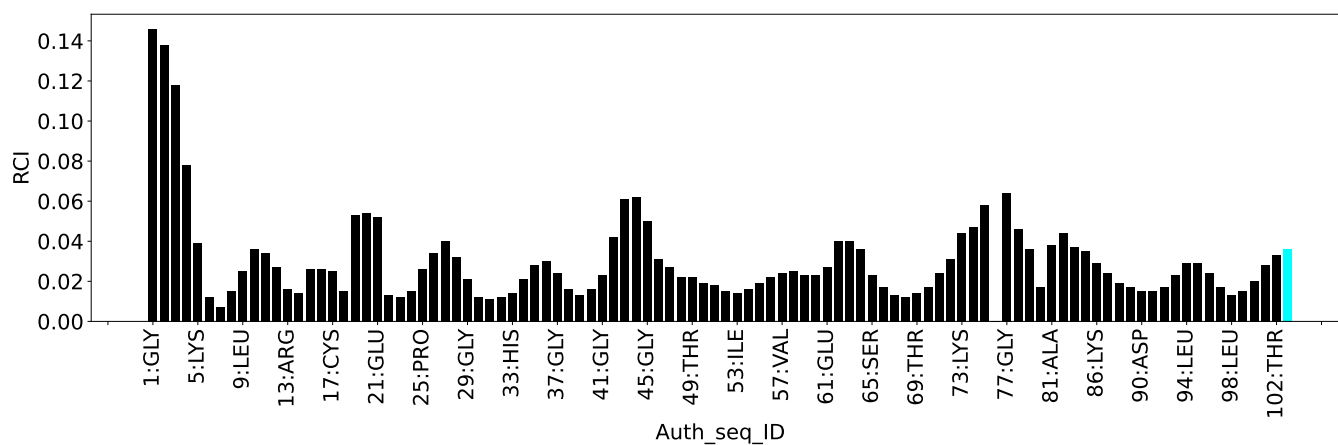
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	80	MET	HG2	-3.76	0.65 – 4.19	-17.5
1	A	18	HIS	HD2	-0.06	4.65 – 9.35	-15.0
1	A	80	MET	HE1	-3.75	-0.03 – 3.80	-14.7
1	A	80	MET	HE2	-3.75	-0.03 – 3.80	-14.7
1	A	80	MET	HE3	-3.75	-0.03 – 3.80	-14.7
1	A	80	MET	HB2	-2.40	0.42 – 3.63	-13.8
1	A	80	MET	HG3	-2.53	0.54 – 4.26	-13.2
1	A	29	GLY	HA2	-0.03	2.15 – 5.77	-11.0
1	A	80	MET	HB3	-0.48	0.33 – 3.66	-7.4
1	A	41	GLY	HA3	1.35	2.08 – 5.71	-7.0
1	A	30	PRO	HD2	1.34	1.93 – 5.38	-6.7
1	A	18	HIS	HB2	0.77	1.36 – 4.85	-6.7
1	A	82	PHE	HB2	0.63	1.20 – 4.80	-6.6
1	A	32	LEU	HD11	-0.89	-0.61 – 2.12	-6.0
1	A	32	LEU	HD12	-0.89	-0.61 – 2.12	-6.0
1	A	32	LEU	HD13	-0.89	-0.61 – 2.12	-6.0
1	A	22	LYS	HB2	0.42	0.58 – 2.97	-5.7
1	A	46	TYR	HB2	0.88	1.09 – 4.72	-5.6
1	A	18	HIS	HB3	1.03	1.18 – 4.91	-5.4
1	A	32	LEU	HD21	-0.69	-0.65 – 2.13	-5.1
1	A	32	LEU	HD22	-0.69	-0.65 – 2.13	-5.1
1	A	32	LEU	HD23	-0.69	-0.65 – 2.13	-5.1
1	A	30	PRO	HB2	0.37	0.37 – 3.78	-5.0

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble

composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1792
Intra-residue ($ i-j =0$)	635
Sequential ($ i-j =1$)	373
Medium range ($ i-j >1$ and $ i-j <5$)	319
Long range ($ i-j \geq 5$)	372
Inter-chain	93
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	16.4
Number of long range restraints per residue ¹	3.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	19.5	0.2
0.2-0.5 (Medium)	5.5	0.5
>0.5 (Large)	1.5	1.34

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 ⓘ

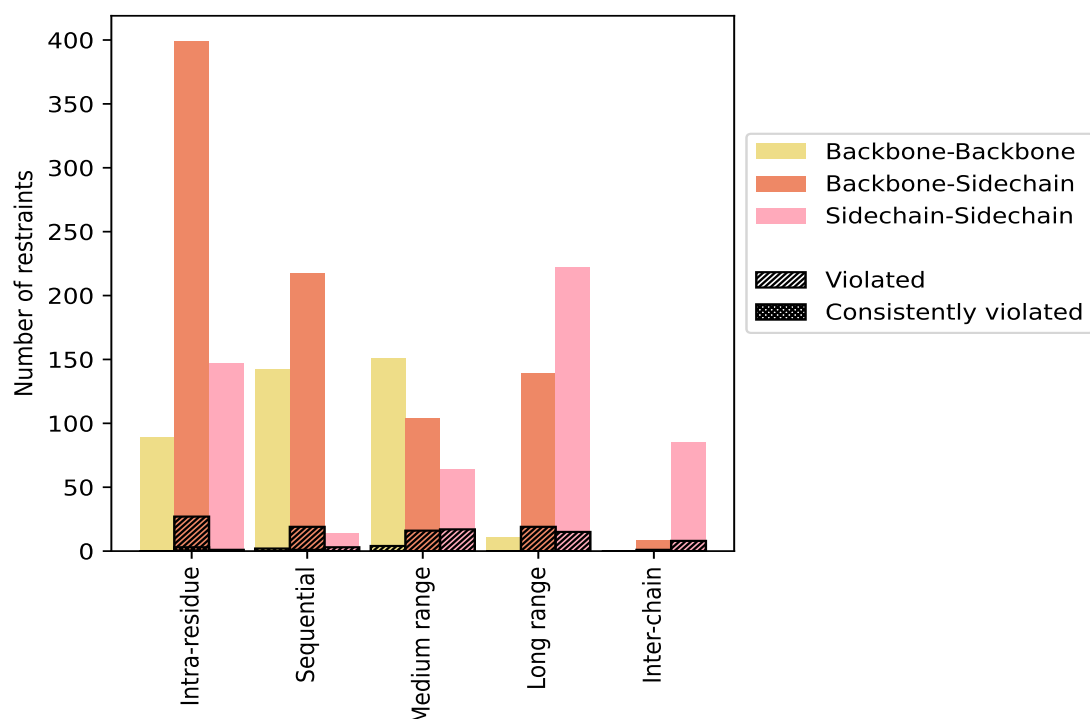
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	635	35.4	28	4.4	1.6	3	0.5	0.2
Backbone-Backbone	89	5.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	399	22.3	27	6.8	1.5	3	0.8	0.2
Sidechain-Sidechain	147	8.2	1	0.7	0.1	0	0.0	0.0
Sequential ($i-j =1$)	373	20.8	24	6.4	1.3	1	0.3	0.1
Backbone-Backbone	142	7.9	2	1.4	0.1	0	0.0	0.0
Backbone-Sidechain	217	12.1	19	8.8	1.1	1	0.5	0.1
Sidechain-Sidechain	14	0.8	3	21.4	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	319	17.8	37	11.6	2.1	0	0.0	0.0
Backbone-Backbone	151	8.4	4	2.6	0.2	0	0.0	0.0
Backbone-Sidechain	104	5.8	16	15.4	0.9	0	0.0	0.0
Sidechain-Sidechain	64	3.6	17	26.6	0.9	0	0.0	0.0
Long range ($i-j \geq 5$)	372	20.8	34	9.1	1.9	0	0.0	0.0
Backbone-Backbone	11	0.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	139	7.8	19	13.7	1.1	0	0.0	0.0
Sidechain-Sidechain	222	12.4	15	6.8	0.8	0	0.0	0.0
Inter-chain	93	5.2	9	9.7	0.5	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	8	0.4	1	12.5	0.1	0	0.0	0.0
Sidechain-Sidechain	85	4.7	8	9.4	0.4	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	1792	100.0	132	7.4	7.4	4	0.2	0.2
Backbone-Backbone	393	21.9	6	1.5	0.3	0	0.0	0.0
Backbone-Sidechain	867	48.4	82	9.5	4.6	4	0.5	0.2
Sidechain-Sidechain	532	29.7	44	8.3	2.5	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	11	4	9	7	3	34	0.2	1.31	0.24	0.13
2	13	5	6	4	2	30	0.2	0.83	0.16	0.14
3	17	4	4	10	4	39	0.18	0.9	0.15	0.13
4	10	6	6	4	2	28	0.19	0.85	0.17	0.13
5	11	5	2	8	4	30	0.2	0.83	0.19	0.13
6	9	5	10	5	2	31	0.19	0.7	0.14	0.14
7	15	6	11	8	2	42	0.16	0.66	0.09	0.12
8	12	7	8	6	2	35	0.17	0.78	0.14	0.12
9	11	5	6	7	1	30	0.17	0.78	0.13	0.13
10	12	3	4	8	2	29	0.18	0.86	0.17	0.12

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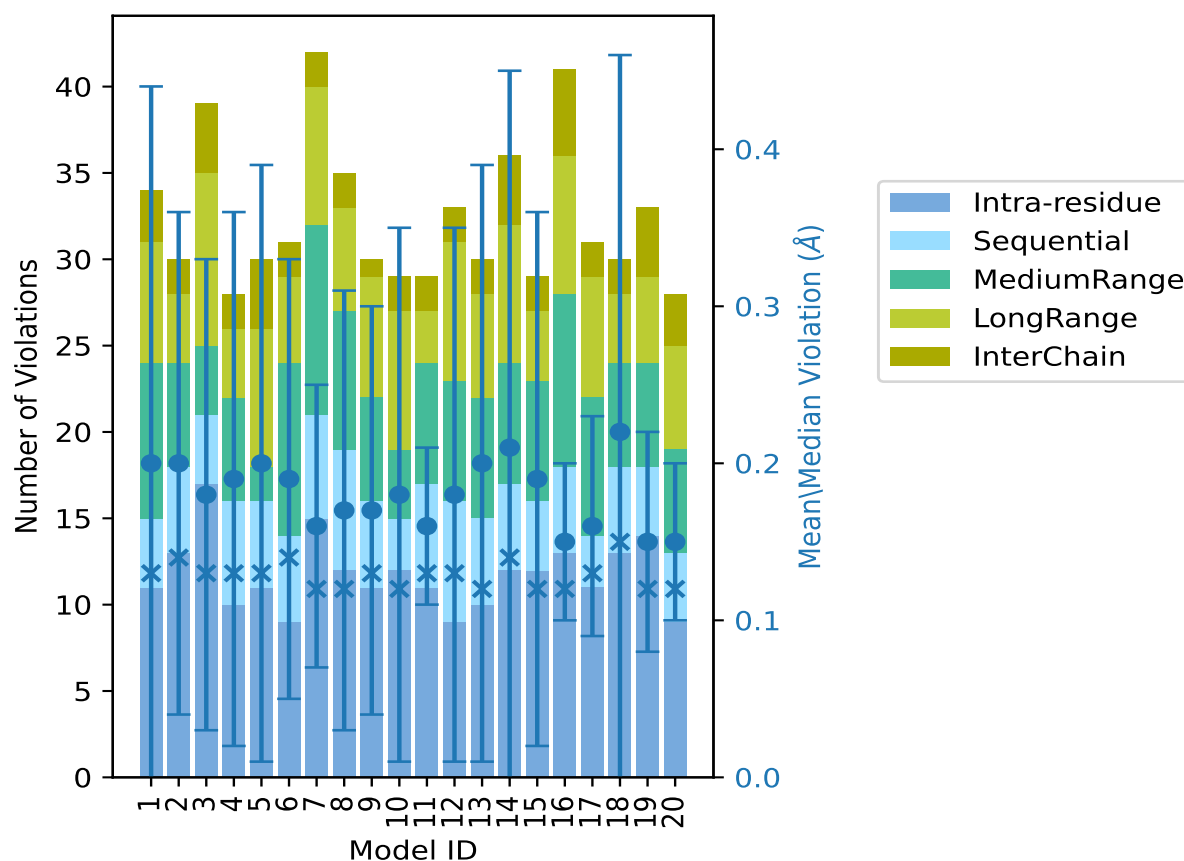
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	11	6	7	3	2	29	0.16	0.26	0.05	0.13
12	9	7	7	8	2	33	0.18	0.84	0.17	0.13
13	10	5	7	6	2	30	0.2	0.94	0.19	0.12
14	12	5	7	8	4	36	0.21	1.34	0.24	0.14
15	12	4	7	4	2	29	0.19	0.88	0.17	0.12
16	13	5	10	8	5	41	0.15	0.3	0.05	0.12
17	11	3	8	7	2	31	0.16	0.41	0.07	0.13
18	13	5	6	4	2	30	0.22	1.28	0.24	0.15
19	14	4	6	5	4	33	0.15	0.42	0.07	0.12
20	9	4	6	6	3	28	0.15	0.27	0.05	0.12

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

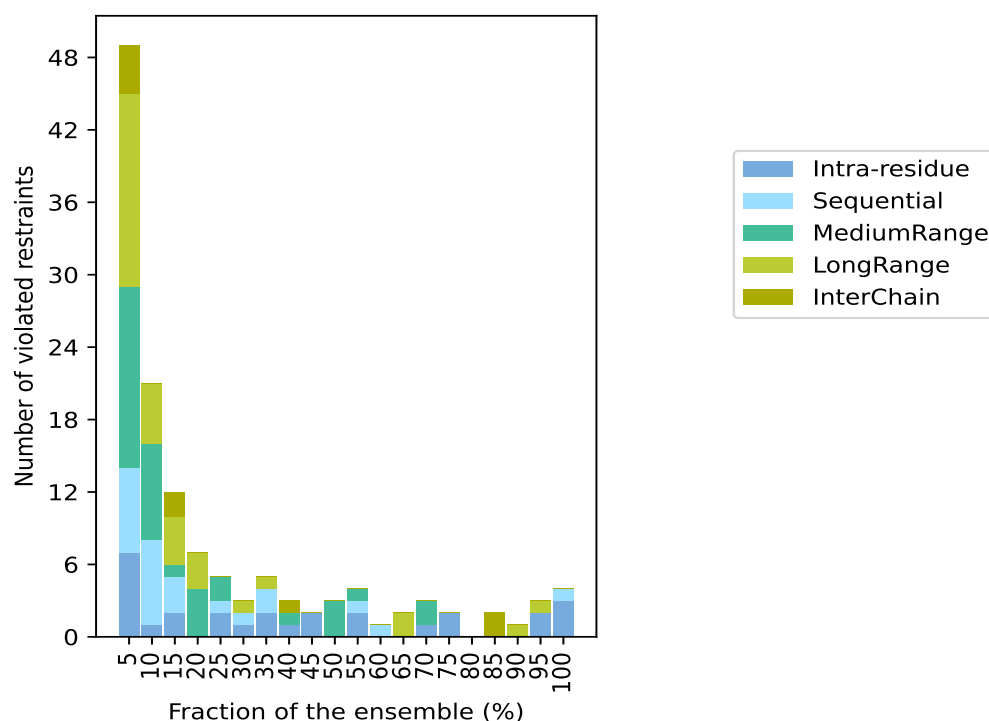
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1660(IR:607, SQ:349, MR:282, LR:338, IC:84) restraints are 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	%
7	7	15	16	4	49	1	5.0
1	7	8	5	0	21	2	10.0
2	3	1	4	2	12	3	15.0
0	0	4	3	0	7	4	20.0
2	1	2	0	0	5	5	25.0
1	1	0	1	0	3	6	30.0
2	2	0	1	0	5	7	35.0
1	0	1	0	1	3	8	40.0
2	0	0	0	0	2	9	45.0
0	0	3	0	0	3	10	50.0
2	1	1	0	0	4	11	55.0
0	1	0	0	0	1	12	60.0
0	0	0	2	0	2	13	65.0
1	0	2	0	0	3	14	70.0
2	0	0	0	0	2	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	2	2	17	85.0
0	0	0	1	0	1	18	90.0
2	0	0	1	0	3	19	95.0
3	1	0	0	0	4	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

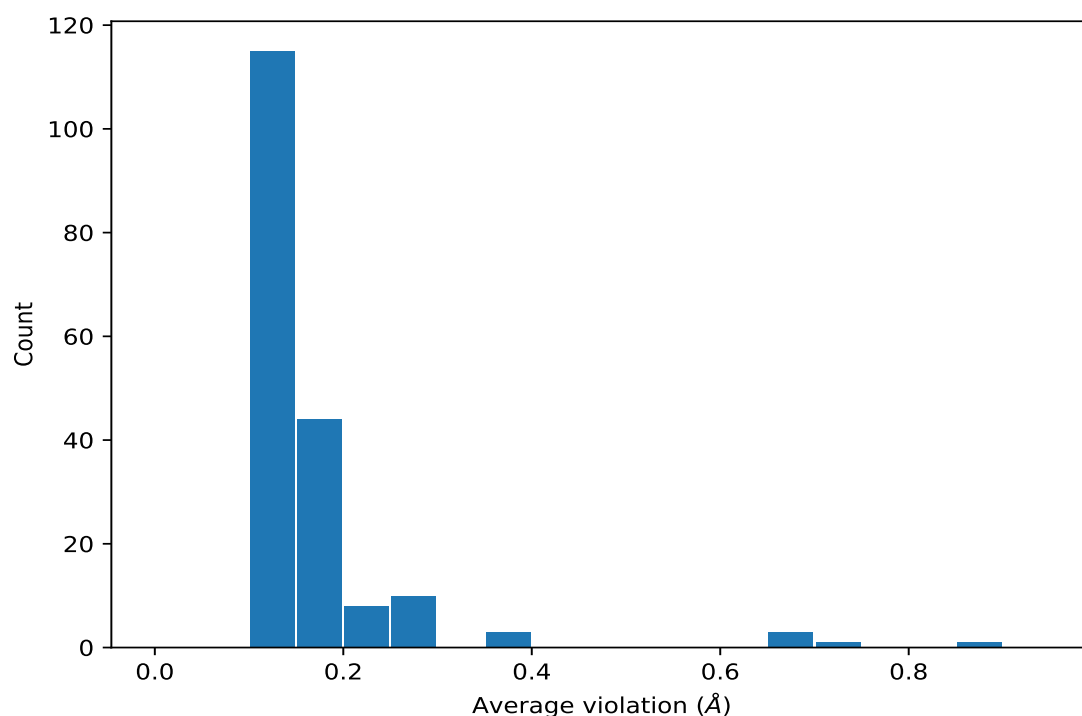
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	20	0.25	0.01	0.25
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	20	0.25	0.01	0.25
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	20	0.25	0.01	0.25
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	20	0.22	0.01	0.22
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	20	0.22	0.01	0.22
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	20	0.11	0.0	0.11
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	20	0.1	0.0	0.1
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	19	0.66	0.27	0.78
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	19	0.66	0.27	0.78
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	19	0.66	0.27	0.78
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	19	0.14	0.02	0.14
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	19	0.12	0.0	0.12
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	18	0.15	0.04	0.13
(1,1779)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	17	0.38	0.18	0.36
(1,1779)	2:104:A:HEC:HMA1	1:59:A:TRP:HE3	17	0.38	0.18	0.36
(1,1779)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	17	0.38	0.18	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	17	0.16	0.03	0.16
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	17	0.16	0.03	0.16
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	17	0.16	0.03	0.16
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	15	0.1	0.0	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	15	0.1	0.0	0.1
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	14	0.73	0.35	0.68
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	14	0.14	0.02	0.15
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	14	0.14	0.02	0.15
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	14	0.1	0.0	0.1
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	13	0.14	0.02	0.13
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	13	0.14	0.03	0.12
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	13	0.14	0.03	0.12
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	13	0.14	0.03	0.12
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	13	0.14	0.03	0.12
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	13	0.14	0.03	0.12
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	13	0.14	0.03	0.12
(1,1308)	1:74:A:TYR:HD1	1:75:A:ILE:H	12	0.14	0.04	0.13
(1,1308)	1:74:A:TYR:HD2	1:75:A:ILE:H	12	0.14	0.04	0.13
(1,171)	1:9:A:LEU:HD11	1:9:A:LEU:HA	11	0.25	0.01	0.26
(1,171)	1:9:A:LEU:HD12	1:9:A:LEU:HA	11	0.25	0.01	0.26
(1,171)	1:9:A:LEU:HD13	1:9:A:LEU:HA	11	0.25	0.01	0.26
(1,120)	1:6:A:GLY:HA3	1:9:A:LEU:HB3	11	0.19	0.02	0.2
(1,160)	1:8:A:THR:HB	1:9:A:LEU:H	11	0.11	0.01	0.11
(1,1648)	1:98:A:LEU:HB3	1:98:A:LEU:H	11	0.11	0.0	0.11
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG21	10	0.15	0.02	0.15
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG22	10	0.15	0.02	0.15
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG23	10	0.15	0.02	0.15
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG21	10	0.15	0.02	0.15
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG22	10	0.15	0.02	0.15
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG23	10	0.15	0.02	0.15
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG21	10	0.15	0.02	0.15
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG22	10	0.15	0.02	0.15
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG23	10	0.15	0.02	0.15
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD21	10	0.15	0.02	0.15
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD22	10	0.15	0.02	0.15
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD23	10	0.15	0.02	0.15
(1,202)	1:10:A:PHE:HA	1:13:A:ARG:HB3	10	0.12	0.02	0.12
(1,413)	1:22:A:LYS:HG3	1:22:A:LYS:HA	9	0.24	0.01	0.24
(1,1474)	1:89:A:LYS:HB3	1:89:A:LYS:H	9	0.1	0.0	0.1
(1,846)	1:49:A:THR:HG21	1:49:A:THR:H	8	0.13	0.03	0.13
(1,846)	1:49:A:THR:HG22	1:49:A:THR:H	8	0.13	0.03	0.13
(1,846)	1:49:A:THR:HG23	1:49:A:THR:H	8	0.13	0.03	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,512)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	8	0.12	0.02	0.12
(1,512)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	8	0.12	0.02	0.12
(1,854)	1:49:A:THR:HG21	1:52:A:ASN:H	8	0.12	0.03	0.12
(1,854)	1:49:A:THR:HG22	1:52:A:ASN:H	8	0.12	0.03	0.12
(1,854)	1:49:A:THR:HG23	1:52:A:ASN:H	8	0.12	0.03	0.12
(1,738)	1:40:A:SER:HB2	1:40:A:SER:H	7	0.13	0.03	0.12
(1,579)	1:32:A:LEU:HD11	1:18:A:HIS:HB2	7	0.12	0.02	0.11
(1,579)	1:32:A:LEU:HD12	1:18:A:HIS:HB2	7	0.12	0.02	0.11
(1,579)	1:32:A:LEU:HD13	1:18:A:HIS:HB2	7	0.12	0.02	0.11
(1,184)	1:9:A:LEU:HB2	1:10:A:PHE:H	7	0.12	0.01	0.12
(1,871)	1:51:A:ALA:HA	1:52:A:ASN:H	7	0.1	0.0	0.1
(1,1490)	1:90:A:ASP:HB3	1:90:A:ASP:H	7	0.1	0.0	0.1
(1,172)	1:9:A:LEU:HD21	1:9:A:LEU:HA	6	0.26	0.02	0.26
(1,172)	1:9:A:LEU:HD22	1:9:A:LEU:HA	6	0.26	0.02	0.26
(1,172)	1:9:A:LEU:HD23	1:9:A:LEU:HA	6	0.26	0.02	0.26
(1,1569)	1:94:A:LEU:HB2	1:95:A:ILE:H	6	0.2	0.02	0.2
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	6	0.11	0.01	0.11
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	6	0.11	0.01	0.11
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	6	0.11	0.01	0.11
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	6	0.11	0.01	0.11
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	6	0.11	0.01	0.11
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	6	0.11	0.01	0.11
(1,412)	1:22:A:LYS:HG2	1:22:A:LYS:H	5	0.2	0.05	0.18
(1,1087)	1:60:A:ASP:HB2	1:61:A:GLU:H	5	0.19	0.02	0.19
(1,1302)	1:74:A:TYR:HA	1:74:A:TYR:HD1	5	0.17	0.01	0.17
(1,1302)	1:74:A:TYR:HA	1:74:A:TYR:HD2	5	0.17	0.01	0.17
(1,1434)	1:85:A:LEU:HD21	1:88:A:GLU:H	5	0.14	0.01	0.14
(1,1434)	1:85:A:LEU:HD22	1:88:A:GLU:H	5	0.14	0.01	0.14
(1,1434)	1:85:A:LEU:HD23	1:88:A:GLU:H	5	0.14	0.01	0.14
(1,1166)	1:64:A:MET:HB2	1:60:A:ASP:H	5	0.14	0.03	0.14
(1,1166)	1:64:A:MET:HB3	1:60:A:ASP:H	5	0.14	0.03	0.14
(1,990)	1:57:A:VAL:HG21	1:40:A:SER:H	4	0.15	0.01	0.16
(1,990)	1:57:A:VAL:HG22	1:40:A:SER:H	4	0.15	0.01	0.16
(1,990)	1:57:A:VAL:HG23	1:40:A:SER:H	4	0.15	0.01	0.16
(1,792)	1:43:A:ALA:HB1	1:46:A:TYR:HD2	4	0.15	0.04	0.12
(1,792)	1:43:A:ALA:HB2	1:46:A:TYR:HD2	4	0.15	0.04	0.12
(1,792)	1:43:A:ALA:HB3	1:46:A:TYR:HD2	4	0.15	0.04	0.12
(1,779)	1:42:A:GLN:HE21	1:39:A:HIS:H	4	0.14	0.03	0.12
(1,779)	1:42:A:GLN:HE22	1:39:A:HIS:H	4	0.14	0.03	0.12
(1,368)	1:19:A:THR:HA	1:17:A:CYS:H	4	0.12	0.02	0.12
(1,733)	1:39:A:HIS:HA	1:59:A:TRP:HD1	4	0.12	0.02	0.12
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD11	4	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD12	4	0.12	0.01	0.12
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD13	4	0.12	0.01	0.12
(1,279)	1:14:A:CYS:HA	1:18:A:HIS:HB2	4	0.12	0.03	0.1
(1,279)	1:14:A:CYS:HA	1:18:A:HIS:HB3	4	0.12	0.03	0.1
(1,769)	1:42:A:GLN:HB2	1:42:A:GLN:H	3	0.27	0.01	0.27
(1,667)	1:35:A:ILE:HG21	2:104:A:HEC:HAA1	3	0.23	0.02	0.22
(1,667)	1:35:A:ILE:HG22	2:104:A:HEC:HAA1	3	0.23	0.02	0.22
(1,667)	1:35:A:ILE:HG23	2:104:A:HEC:HAA1	3	0.23	0.02	0.22
(1,1733)	1:101:A:ALA:HB1	1:20:A:VAL:H	3	0.15	0.03	0.16
(1,1733)	1:101:A:ALA:HB2	1:20:A:VAL:H	3	0.15	0.03	0.16
(1,1733)	1:101:A:ALA:HB3	1:20:A:VAL:H	3	0.15	0.03	0.16
(1,882)	1:51:A:ALA:HB1	1:78:A:THR:H	3	0.14	0.03	0.13
(1,882)	1:51:A:ALA:HB2	1:78:A:THR:H	3	0.14	0.03	0.13
(1,882)	1:51:A:ALA:HB3	1:78:A:THR:H	3	0.14	0.03	0.13
(1,1086)	1:60:A:ASP:HB3	1:61:A:GLU:H	3	0.14	0.0	0.14
(1,634)	1:33:A:HIS:HD2	1:34:A:GLY:H	3	0.13	0.03	0.12
(1,762)	1:41:A:GLY:HA2	1:42:A:GLN:HE21	3	0.13	0.01	0.13
(1,762)	1:41:A:GLY:HA2	1:42:A:GLN:HE22	3	0.13	0.01	0.13
(1,1265)	1:71:A:HIS:HB3	1:71:A:HIS:H	3	0.12	0.01	0.11
(1,396)	1:20:A:VAL:HG21	1:24:A:GLY:H	3	0.12	0.01	0.12
(1,396)	1:20:A:VAL:HG22	1:24:A:GLY:H	3	0.12	0.01	0.12
(1,396)	1:20:A:VAL:HG23	1:24:A:GLY:H	3	0.12	0.01	0.12
(1,657)	1:35:A:ILE:HD11	1:59:A:TRP:HH2	3	0.12	0.01	0.11
(1,657)	1:35:A:ILE:HD12	1:59:A:TRP:HH2	3	0.12	0.01	0.11
(1,657)	1:35:A:ILE:HD13	1:59:A:TRP:HH2	3	0.12	0.01	0.11
(1,1234)	1:68:A:LEU:HD11	2:104:A:HEC:HMA1	3	0.11	0.0	0.11
(1,1234)	1:68:A:LEU:HD11	2:104:A:HEC:HMA2	3	0.11	0.0	0.11
(1,1234)	1:68:A:LEU:HD11	2:104:A:HEC:HMA3	3	0.11	0.0	0.11
(1,1234)	1:68:A:LEU:HD12	2:104:A:HEC:HMA1	3	0.11	0.0	0.11
(1,1234)	1:68:A:LEU:HD12	2:104:A:HEC:HMA2	3	0.11	0.0	0.11
(1,1234)	1:68:A:LEU:HD12	2:104:A:HEC:HMA3	3	0.11	0.0	0.11
(1,1234)	1:68:A:LEU:HD13	2:104:A:HEC:HMA1	3	0.11	0.0	0.11
(1,1234)	1:68:A:LEU:HD13	2:104:A:HEC:HMA2	3	0.11	0.0	0.11
(1,1234)	1:68:A:LEU:HD13	2:104:A:HEC:HMA3	3	0.11	0.0	0.11
(1,504)	1:28:A:VAL:HA	1:46:A:TYR:HD1	3	0.1	0.0	0.1
(1,504)	1:28:A:VAL:HA	1:46:A:TYR:HD2	3	0.1	0.0	0.1
(1,841)	1:48:A:TYR:HD1	1:52:A:ASN:HD21	2	0.87	0.03	0.87
(1,569)	1:32:A:LEU:HA	1:34:A:GLY:H	2	0.19	0.04	0.19
(1,431)	1:22:A:LYS:HD2	1:23:A:GLY:H	2	0.18	0.02	0.18
(1,431)	1:22:A:LYS:HD3	1:23:A:GLY:H	2	0.18	0.02	0.18
(1,147)	1:8:A:THR:HG21	1:8:A:THR:HA	2	0.17	0.01	0.17
(1,147)	1:8:A:THR:HG22	1:8:A:THR:HA	2	0.17	0.01	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,147)	1:8:A:THR:HG23	1:8:A:THR:HA	2	0.17	0.01	0.17
(1,1037)	1:58:A:LEU:HB3	1:63:A:ASN:HD21	2	0.16	0.0	0.16
(1,1037)	1:58:A:LEU:HB3	1:63:A:ASN:HD22	2	0.16	0.0	0.16
(1,367)	1:19:A:THR:HG21	1:21:A:GLU:H	2	0.15	0.02	0.15
(1,367)	1:19:A:THR:HG22	1:21:A:GLU:H	2	0.15	0.02	0.15
(1,367)	1:19:A:THR:HG23	1:21:A:GLU:H	2	0.15	0.02	0.15
(1,881)	1:51:A:ALA:HB1	1:77:A:GLY:HA2	2	0.15	0.03	0.15
(1,881)	1:51:A:ALA:HB2	1:77:A:GLY:HA2	2	0.15	0.03	0.15
(1,881)	1:51:A:ALA:HB3	1:77:A:GLY:HA2	2	0.15	0.03	0.15
(1,1079)	1:59:A:TRP:HE1	1:52:A:ASN:HD22	2	0.15	0.0	0.15
(1,1280)	1:71:A:HIS:HB2	1:74:A:TYR:HE1	2	0.13	0.0	0.13
(1,1280)	1:71:A:HIS:HB2	1:74:A:TYR:HE2	2	0.13	0.0	0.13
(1,1280)	1:71:A:HIS:HB3	1:74:A:TYR:HE1	2	0.13	0.0	0.13
(1,1280)	1:71:A:HIS:HB3	1:74:A:TYR:HE2	2	0.13	0.0	0.13
(1,1405)	1:82:A:PHE:HE1	1:85:A:LEU:HD11	2	0.12	0.02	0.12
(1,1405)	1:82:A:PHE:HE1	1:85:A:LEU:HD12	2	0.12	0.02	0.12
(1,1405)	1:82:A:PHE:HE1	1:85:A:LEU:HD13	2	0.12	0.02	0.12
(1,1405)	1:82:A:PHE:HE2	1:85:A:LEU:HD11	2	0.12	0.02	0.12
(1,1405)	1:82:A:PHE:HE2	1:85:A:LEU:HD12	2	0.12	0.02	0.12
(1,1405)	1:82:A:PHE:HE2	1:85:A:LEU:HD13	2	0.12	0.02	0.12
(1,1724)	1:100:A:LYS:HE2	1:101:A:ALA:H	2	0.12	0.01	0.12
(1,1230)	1:68:A:LEU:HB3	1:69:A:THR:H	2	0.12	0.01	0.12
(1,401)	1:21:A:GLU:H	1:20:A:VAL:H	2	0.12	0.02	0.12
(1,1289)	1:72:A:ALA:HA	1:78:A:THR:HG21	2	0.12	0.0	0.12
(1,1289)	1:72:A:ALA:HA	1:78:A:THR:HG22	2	0.12	0.0	0.12
(1,1289)	1:72:A:ALA:HA	1:78:A:THR:HG23	2	0.12	0.0	0.12
(1,323)	1:16:A:GLN:HG3	1:18:A:HIS:H	2	0.11	0.01	0.11
(1,972)	1:56:A:ASN:HD21	1:39:A:HIS:HD2	2	0.11	0.0	0.11
(1,1397)	1:82:A:PHE:HD1	1:84:A:GLY:HA3	2	0.11	0.0	0.11
(1,1397)	1:82:A:PHE:HD2	1:84:A:GLY:HA3	2	0.11	0.0	0.11
(1,161)	1:8:A:THR:HG21	1:9:A:LEU:H	2	0.11	0.0	0.11
(1,161)	1:8:A:THR:HG22	1:9:A:LEU:H	2	0.11	0.0	0.11
(1,161)	1:8:A:THR:HG23	1:9:A:LEU:H	2	0.11	0.0	0.11
(1,658)	1:35:A:ILE:HD11	1:36:A:PHE:HZ	2	0.11	0.0	0.11
(1,658)	1:35:A:ILE:HD12	1:36:A:PHE:HZ	2	0.11	0.0	0.11
(1,658)	1:35:A:ILE:HD13	1:36:A:PHE:HZ	2	0.11	0.0	0.11
(1,1406)	1:82:A:PHE:HE1	1:85:A:LEU:HD21	2	0.11	0.0	0.11
(1,1406)	1:82:A:PHE:HE1	1:85:A:LEU:HD22	2	0.11	0.0	0.11
(1,1406)	1:82:A:PHE:HE1	1:85:A:LEU:HD23	2	0.11	0.0	0.11
(1,1406)	1:82:A:PHE:HE2	1:85:A:LEU:HD21	2	0.11	0.0	0.11
(1,1406)	1:82:A:PHE:HE2	1:85:A:LEU:HD22	2	0.11	0.0	0.11
(1,1406)	1:82:A:PHE:HE2	1:85:A:LEU:HD23	2	0.11	0.0	0.11

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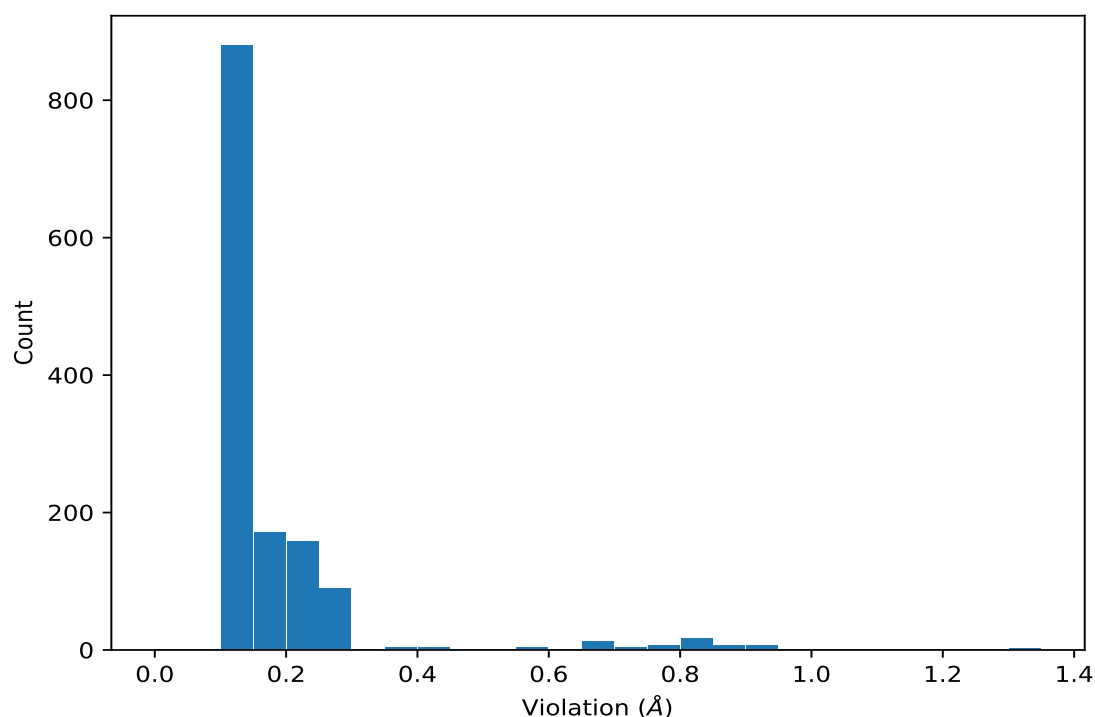
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1568)	1:94:A:LEU:HB3	1:95:A:ILE:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	14	1.34
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	1	1.31
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	18	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	13	0.94
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	13	0.94
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	13	0.94
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	1	0.91
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	1	0.91
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	1	0.91
(1,841)	1:48:A:TYR:HD1	1:52:A:ASN:HD21	3	0.9
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	15	0.88
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	15	0.88
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	15	0.88
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	10	0.86
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	10	0.86
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	10	0.86
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	4	0.85
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	4	0.85
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	4	0.85
(1,841)	1:48:A:TYR:HD1	1:52:A:ASN:HD21	12	0.84
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	12	0.84
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	12	0.84
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	12	0.84
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	18	0.84
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	18	0.84
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	18	0.84
(1,1779)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	5	0.83
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	2	0.83
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	2	0.83
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	2	0.83
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	5	0.82
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	5	0.82
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	5	0.82
(1,1779)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	14	0.79
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	8	0.78
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	9	0.78
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	9	0.78
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	9	0.78
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	13	0.76
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	14	0.72
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	14	0.72
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	14	0.72
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	4	0.7
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	6	0.7
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	6	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	6	0.7
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	10	0.69
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	6	0.67
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	2	0.66
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	3	0.66
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	3	0.66
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	3	0.66
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	7	0.66
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	7	0.66
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	7	0.66
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	15	0.63
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	8	0.59
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	8	0.59
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	8	0.59
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	5	0.57
(1,1779)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	13	0.5
(1,1779)	2:104:A:HEC:HMA1	1:59:A:TRP:HE3	2	0.42
(1,1779)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	19	0.42
(1,1779)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	17	0.41
(1,1779)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	3	0.39
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	9	0.39
(1,1779)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	18	0.37
(1,1779)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	15	0.36
(1,1779)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	1	0.35
(1,1779)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	16	0.3
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	7	0.3
(1,1779)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	12	0.29
(1,172)	1:9:A:LEU:HD21	1:9:A:LEU:HA	19	0.29
(1,172)	1:9:A:LEU:HD22	1:9:A:LEU:HA	19	0.29
(1,172)	1:9:A:LEU:HD23	1:9:A:LEU:HA	19	0.29
(1,1779)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	10	0.28
(1,769)	1:42:A:GLN:HB2	1:42:A:GLN:H	17	0.28
(1,172)	1:9:A:LEU:HD21	1:9:A:LEU:HA	2	0.28
(1,172)	1:9:A:LEU:HD22	1:9:A:LEU:HA	2	0.28
(1,172)	1:9:A:LEU:HD23	1:9:A:LEU:HA	2	0.28
(1,769)	1:42:A:GLN:HB2	1:42:A:GLN:H	9	0.27
(1,412)	1:22:A:LYS:HG2	1:22:A:LYS:H	20	0.27
(1,172)	1:9:A:LEU:HD21	1:9:A:LEU:HA	14	0.27
(1,172)	1:9:A:LEU:HD22	1:9:A:LEU:HA	14	0.27
(1,172)	1:9:A:LEU:HD23	1:9:A:LEU:HA	14	0.27
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	11	0.26
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	11	0.26
(1,769)	1:42:A:GLN:HB2	1:42:A:GLN:H	7	0.26
(1,667)	1:35:A:ILE:HG21	2:104:A:HEC:HAA1	14	0.26
(1,667)	1:35:A:ILE:HG22	2:104:A:HEC:HAA1	14	0.26
(1,667)	1:35:A:ILE:HG23	2:104:A:HEC:HAA1	14	0.26
(1,172)	1:9:A:LEU:HD21	1:9:A:LEU:HA	5	0.26
(1,172)	1:9:A:LEU:HD22	1:9:A:LEU:HA	5	0.26
(1,172)	1:9:A:LEU:HD23	1:9:A:LEU:HA	5	0.26
(1,172)	1:9:A:LEU:HD21	1:9:A:LEU:HA	20	0.26
(1,172)	1:9:A:LEU:HD22	1:9:A:LEU:HA	20	0.26
(1,172)	1:9:A:LEU:HD23	1:9:A:LEU:HA	20	0.26
(1,171)	1:9:A:LEU:HD11	1:9:A:LEU:HA	6	0.26
(1,171)	1:9:A:LEU:HD12	1:9:A:LEU:HA	6	0.26
(1,171)	1:9:A:LEU:HD13	1:9:A:LEU:HA	6	0.26
(1,171)	1:9:A:LEU:HD11	1:9:A:LEU:HA	7	0.26
(1,171)	1:9:A:LEU:HD12	1:9:A:LEU:HA	7	0.26
(1,171)	1:9:A:LEU:HD13	1:9:A:LEU:HA	7	0.26
(1,171)	1:9:A:LEU:HD11	1:9:A:LEU:HA	8	0.26
(1,171)	1:9:A:LEU:HD12	1:9:A:LEU:HA	8	0.26
(1,171)	1:9:A:LEU:HD13	1:9:A:LEU:HA	8	0.26
(1,171)	1:9:A:LEU:HD11	1:9:A:LEU:HA	11	0.26
(1,171)	1:9:A:LEU:HD12	1:9:A:LEU:HA	11	0.26
(1,171)	1:9:A:LEU:HD13	1:9:A:LEU:HA	11	0.26
(1,171)	1:9:A:LEU:HD11	1:9:A:LEU:HA	15	0.26
(1,171)	1:9:A:LEU:HD12	1:9:A:LEU:HA	15	0.26
(1,171)	1:9:A:LEU:HD13	1:9:A:LEU:HA	15	0.26
(1,171)	1:9:A:LEU:HD11	1:9:A:LEU:HA	17	0.26
(1,171)	1:9:A:LEU:HD12	1:9:A:LEU:HA	17	0.26
(1,171)	1:9:A:LEU:HD13	1:9:A:LEU:HA	17	0.26
(1,1779)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	4	0.25
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	2	0.25
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	2	0.25
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	2	0.25
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	4	0.25
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	4	0.25
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	4	0.25
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	6	0.25
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	6	0.25
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	6	0.25
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	7	0.25
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	7	0.25
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	9	0.25
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	9	0.25
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	9	0.25
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	13	0.25
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	13	0.25
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	13	0.25
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	14	0.25
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	14	0.25
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	14	0.25
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	16	0.25
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	16	0.25
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	16	0.25
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	18	0.25
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	18	0.25
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	18	0.25
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	19	0.25
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	19	0.25
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	19	0.25
(1,413)	1:22:A:LYS:HG3	1:22:A:LYS:HA	2	0.25
(1,413)	1:22:A:LYS:HG3	1:22:A:LYS:HA	18	0.25
(1,171)	1:9:A:LEU:HD11	1:9:A:LEU:HA	1	0.25
(1,171)	1:9:A:LEU:HD12	1:9:A:LEU:HA	1	0.25
(1,171)	1:9:A:LEU:HD13	1:9:A:LEU:HA	1	0.25
(1,171)	1:9:A:LEU:HD11	1:9:A:LEU:HA	4	0.25
(1,171)	1:9:A:LEU:HD12	1:9:A:LEU:HA	4	0.25
(1,171)	1:9:A:LEU:HD13	1:9:A:LEU:HA	4	0.25
(1,171)	1:9:A:LEU:HD11	1:9:A:LEU:HA	18	0.25
(1,171)	1:9:A:LEU:HD12	1:9:A:LEU:HA	18	0.25
(1,171)	1:9:A:LEU:HD13	1:9:A:LEU:HA	18	0.25
(1,1687)	1:98:A:LEU:HD11	1:32:A:LEU:H	13	0.24
(1,1687)	1:98:A:LEU:HD12	1:32:A:LEU:H	13	0.24
(1,1687)	1:98:A:LEU:HD13	1:32:A:LEU:H	13	0.24
(1,1687)	1:98:A:LEU:HD21	1:32:A:LEU:H	13	0.24
(1,1687)	1:98:A:LEU:HD22	1:32:A:LEU:H	13	0.24
(1,1687)	1:98:A:LEU:HD23	1:32:A:LEU:H	13	0.24
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	1	0.24
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	1	0.24
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	1	0.24
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	3	0.24
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	3	0.24
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	3	0.24
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	5	0.24
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	5	0.24
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	8	0.24
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	8	0.24
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	8	0.24
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	10	0.24
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	10	0.24
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	10	0.24
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	12	0.24
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	12	0.24
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	12	0.24
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	17	0.24
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	17	0.24
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	17	0.24
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	20	0.24
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	20	0.24
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	20	0.24
(1,1308)	1:74:A:TYR:HD1	1:75:A:ILE:H	11	0.24
(1,1308)	1:74:A:TYR:HD2	1:75:A:ILE:H	11	0.24
(1,413)	1:22:A:LYS:HG3	1:22:A:LYS:HA	6	0.24
(1,413)	1:22:A:LYS:HG3	1:22:A:LYS:HA	7	0.24
(1,413)	1:22:A:LYS:HG3	1:22:A:LYS:HA	11	0.24
(1,413)	1:22:A:LYS:HG3	1:22:A:LYS:HA	16	0.24
(1,413)	1:22:A:LYS:HG3	1:22:A:LYS:HA	17	0.24
(1,412)	1:22:A:LYS:HG2	1:22:A:LYS:H	15	0.24
(1,171)	1:9:A:LEU:HD11	1:9:A:LEU:HA	16	0.24
(1,171)	1:9:A:LEU:HD12	1:9:A:LEU:HA	16	0.24
(1,171)	1:9:A:LEU:HD13	1:9:A:LEU:HA	16	0.24
(1,1581)	1:95:A:ILE:HG21	1:95:A:ILE:H	15	0.23
(1,1581)	1:95:A:ILE:HG22	1:95:A:ILE:H	15	0.23
(1,1581)	1:95:A:ILE:HG23	1:95:A:ILE:H	15	0.23
(1,1569)	1:94:A:LEU:HB2	1:95:A:ILE:H	13	0.23
(1,1410)	1:82:A:PHE:HZ	1:85:A:LEU:HD21	15	0.23
(1,1410)	1:82:A:PHE:HZ	1:85:A:LEU:HD22	15	0.23
(1,1410)	1:82:A:PHE:HZ	1:85:A:LEU:HD23	15	0.23
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	9	0.23
(1,569)	1:32:A:LEU:HA	1:34:A:GLY:H	7	0.23
(1,413)	1:22:A:LYS:HG3	1:22:A:LYS:HA	3	0.23
(1,413)	1:22:A:LYS:HG3	1:22:A:LYS:HA	19	0.23
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	1	0.23
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	1	0.23
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	4	0.23
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	6	0.23
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	6	0.23
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	7	0.23
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	7	0.23
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	10	0.23
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	10	0.23
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	12	0.23
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	12	0.23
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	18	0.23
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	18	0.23
(1,1308)	1:74:A:TYR:HD1	1:75:A:ILE:H	16	0.22
(1,1308)	1:74:A:TYR:HD2	1:75:A:ILE:H	16	0.22
(1,1087)	1:60:A:ASP:HB2	1:61:A:GLU:H	20	0.22
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	4	0.22
(1,792)	1:43:A:ALA:HB1	1:46:A:TYR:HD2	20	0.22
(1,792)	1:43:A:ALA:HB2	1:46:A:TYR:HD2	20	0.22
(1,792)	1:43:A:ALA:HB3	1:46:A:TYR:HD2	20	0.22
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	19	0.22
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	19	0.22
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	19	0.22
(1,667)	1:35:A:ILE:HG21	2:104:A:HEC:HAA1	3	0.22
(1,667)	1:35:A:ILE:HG22	2:104:A:HEC:HAA1	3	0.22
(1,667)	1:35:A:ILE:HG23	2:104:A:HEC:HAA1	3	0.22
(1,667)	1:35:A:ILE:HG21	2:104:A:HEC:HAA1	5	0.22
(1,667)	1:35:A:ILE:HG22	2:104:A:HEC:HAA1	5	0.22
(1,667)	1:35:A:ILE:HG23	2:104:A:HEC:HAA1	5	0.22
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	8	0.22
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	8	0.22
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	8	0.22
(1,172)	1:9:A:LEU:HD21	1:9:A:LEU:HA	3	0.22
(1,172)	1:9:A:LEU:HD22	1:9:A:LEU:HA	3	0.22
(1,172)	1:9:A:LEU:HD23	1:9:A:LEU:HA	3	0.22
(1,120)	1:6:A:GLY:HA3	1:9:A:LEU:HB3	6	0.22
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	2	0.22
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	2	0.22
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	8	0.22
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	8	0.22
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	9	0.22
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	9	0.22
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	14	0.22
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	15	0.22
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	15	0.22
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	16	0.22
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	16	0.22
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	17	0.22
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	17	0.22
(1,1569)	1:94:A:LEU:HB2	1:95:A:ILE:H	2	0.21
(1,1569)	1:94:A:LEU:HB2	1:95:A:ILE:H	4	0.21
(1,1087)	1:60:A:ASP:HB2	1:61:A:GLU:H	2	0.21
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	1	0.21
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	4	0.21
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	4	0.21
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	4	0.21
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	11	0.21
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	11	0.21
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	11	0.21
(1,171)	1:9:A:LEU:HD11	1:9:A:LEU:HA	12	0.21
(1,171)	1:9:A:LEU:HD12	1:9:A:LEU:HA	12	0.21
(1,171)	1:9:A:LEU:HD13	1:9:A:LEU:HA	12	0.21
(1,120)	1:6:A:GLY:HA3	1:9:A:LEU:HB3	1	0.21
(1,120)	1:6:A:GLY:HA3	1:9:A:LEU:HB3	8	0.21
(1,120)	1:6:A:GLY:HA3	1:9:A:LEU:HB3	18	0.21
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	3	0.21
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	3	0.21
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	5	0.21
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	5	0.21
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	11	0.21
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	11	0.21
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	13	0.21
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	13	0.21
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	20	0.21
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	20	0.21
(1,1779)	2:104:A:HEC:HMA1	1:59:A:TRP:HE3	6	0.2
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	14	0.2
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	14	0.2
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	14	0.2
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	14	0.2
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	14	0.2
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	14	0.2
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	16	0.2
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	16	0.2
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	16	0.2
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	16	0.2
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	16	0.2
(1,1569)	1:94:A:LEU:HB2	1:95:A:ILE:H	14	0.2
(1,1569)	1:94:A:LEU:HB2	1:95:A:ILE:H	19	0.2
(1,1039)	1:58:A:LEU:HG	1:37:A:GLY:H	6	0.2
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	17	0.2
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	17	0.2
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	17	0.2
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	20	0.2
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	20	0.2
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	20	0.2
(1,431)	1:22:A:LYS:HD2	1:23:A:GLY:H	12	0.2
(1,431)	1:22:A:LYS:HD3	1:23:A:GLY:H	12	0.2
(1,120)	1:6:A:GLY:HA3	1:9:A:LEU:HB3	12	0.2
(1,120)	1:6:A:GLY:HA3	1:9:A:LEU:HB3	15	0.2
(1,120)	1:6:A:GLY:HA3	1:9:A:LEU:HB3	16	0.2
(1,86)	1:4:A:LYS:HG2	1:5:A:LYS:H	19	0.2
(1,86)	1:4:A:LYS:HG3	1:5:A:LYS:H	19	0.2
(1,1087)	1:60:A:ASP:HB2	1:61:A:GLU:H	11	0.19
(1,854)	1:49:A:THR:HG21	1:52:A:ASN:H	3	0.19
(1,854)	1:49:A:THR:HG22	1:52:A:ASN:H	3	0.19
(1,854)	1:49:A:THR:HG23	1:52:A:ASN:H	3	0.19
(1,779)	1:42:A:GLN:HE21	1:39:A:HIS:H	9	0.19
(1,779)	1:42:A:GLN:HE22	1:39:A:HIS:H	9	0.19
(1,738)	1:40:A:SER:HB2	1:40:A:SER:H	18	0.19
(1,714)	1:38:A:ARG:HG2	1:39:A:HIS:H	18	0.19
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG21	16	0.19
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG22	16	0.19
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG23	16	0.19
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG21	16	0.19
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG22	16	0.19
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG23	16	0.19
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG21	16	0.19
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG22	16	0.19
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG23	16	0.19
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD21	3	0.19
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD22	3	0.19
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD23	3	0.19
(1,120)	1:6:A:GLY:HA3	1:9:A:LEU:HB3	17	0.19
(1,1779)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	11	0.18
(1,1733)	1:101:A:ALA:HB1	1:20:A:VAL:H	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1733)	1:101:A:ALA:HB2	1:20:A:VAL:H	14	0.18
(1,1733)	1:101:A:ALA:HB3	1:20:A:VAL:H	14	0.18
(1,1569)	1:94:A:LEU:HB2	1:95:A:ILE:H	11	0.18
(1,1308)	1:74:A:TYR:HD1	1:75:A:ILE:H	20	0.18
(1,1308)	1:74:A:TYR:HD2	1:75:A:ILE:H	20	0.18
(1,1302)	1:74:A:TYR:HA	1:74:A:TYR:HD1	2	0.18
(1,1302)	1:74:A:TYR:HA	1:74:A:TYR:HD2	2	0.18
(1,1302)	1:74:A:TYR:HA	1:74:A:TYR:HD1	8	0.18
(1,1302)	1:74:A:TYR:HA	1:74:A:TYR:HD2	8	0.18
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	6	0.18
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	11	0.18
(1,882)	1:51:A:ALA:HB1	1:78:A:THR:H	10	0.18
(1,882)	1:51:A:ALA:HB2	1:78:A:THR:H	10	0.18
(1,882)	1:51:A:ALA:HB3	1:78:A:THR:H	10	0.18
(1,881)	1:51:A:ALA:HB1	1:77:A:GLY:HA2	3	0.18
(1,881)	1:51:A:ALA:HB2	1:77:A:GLY:HA2	3	0.18
(1,881)	1:51:A:ALA:HB3	1:77:A:GLY:HA2	3	0.18
(1,738)	1:40:A:SER:HB2	1:40:A:SER:H	1	0.18
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	5	0.18
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	12	0.18
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	12	0.18
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	12	0.18
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	18	0.18
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	18	0.18
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	18	0.18
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	19	0.18
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	19	0.18
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	19	0.18
(1,412)	1:22:A:LYS:HG2	1:22:A:LYS:H	5	0.18
(1,412)	1:22:A:LYS:HG2	1:22:A:LYS:H	13	0.18
(1,279)	1:14:A:CYS:HA	1:18:A:HIS:HB2	10	0.18
(1,279)	1:14:A:CYS:HA	1:18:A:HIS:HB3	10	0.18
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD21	11	0.18
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD22	11	0.18
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD23	11	0.18
(1,147)	1:8:A:THR:HG21	1:8:A:THR:HA	3	0.18
(1,147)	1:8:A:THR:HG22	1:8:A:THR:HA	3	0.18
(1,147)	1:8:A:THR:HG23	1:8:A:THR:HA	3	0.18
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	4	0.17
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	4	0.17
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	4	0.17
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	4	0.17
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	4	0.17
(1,1434)	1:85:A:LEU:HD21	1:88:A:GLU:H	11	0.17
(1,1434)	1:85:A:LEU:HD22	1:88:A:GLU:H	11	0.17
(1,1434)	1:85:A:LEU:HD23	1:88:A:GLU:H	11	0.17
(1,1416)	1:85:A:LEU:HB3	1:85:A:LEU:H	16	0.17
(1,1302)	1:74:A:TYR:HA	1:74:A:TYR:HD1	19	0.17
(1,1302)	1:74:A:TYR:HA	1:74:A:TYR:HD2	19	0.17
(1,1166)	1:64:A:MET:HB2	1:60:A:ASP:H	9	0.17
(1,1166)	1:64:A:MET:HB3	1:60:A:ASP:H	9	0.17
(1,1087)	1:60:A:ASP:HB2	1:61:A:GLU:H	13	0.17
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	16	0.17
(1,990)	1:57:A:VAL:HG21	1:40:A:SER:H	14	0.17
(1,990)	1:57:A:VAL:HG22	1:40:A:SER:H	14	0.17
(1,990)	1:57:A:VAL:HG23	1:40:A:SER:H	14	0.17
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	12	0.17
(1,846)	1:49:A:THR:HG21	1:49:A:THR:H	3	0.17
(1,846)	1:49:A:THR:HG22	1:49:A:THR:H	3	0.17
(1,846)	1:49:A:THR:HG23	1:49:A:THR:H	3	0.17
(1,634)	1:33:A:HIS:HD2	1:34:A:GLY:H	18	0.17
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	9	0.17
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	14	0.17
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG21	11	0.17
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG22	11	0.17
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG23	11	0.17
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG21	11	0.17
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG22	11	0.17
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG23	11	0.17
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG21	11	0.17
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG22	11	0.17
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG23	11	0.17
(1,431)	1:22:A:LYS:HD2	1:23:A:GLY:H	8	0.17
(1,431)	1:22:A:LYS:HD3	1:23:A:GLY:H	8	0.17
(1,367)	1:19:A:THR:HG21	1:21:A:GLU:H	8	0.17
(1,367)	1:19:A:THR:HG22	1:21:A:GLU:H	8	0.17
(1,367)	1:19:A:THR:HG23	1:21:A:GLU:H	8	0.17
(1,120)	1:6:A:GLY:HA3	1:9:A:LEU:HB3	4	0.17
(1,120)	1:6:A:GLY:HA3	1:9:A:LEU:HB3	11	0.17
(1,1733)	1:101:A:ALA:HB1	1:20:A:VAL:H	16	0.16
(1,1733)	1:101:A:ALA:HB2	1:20:A:VAL:H	16	0.16
(1,1733)	1:101:A:ALA:HB3	1:20:A:VAL:H	16	0.16
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	9	0.16
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	9	0.16
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	9	0.16
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	9	0.16
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	9	0.16
(1,1685)	1:98:A:LEU:HD11	2:104:A:HEC:HMB1	16	0.16
(1,1685)	1:98:A:LEU:HD11	2:104:A:HEC:HMB2	16	0.16
(1,1685)	1:98:A:LEU:HD11	2:104:A:HEC:HMB3	16	0.16
(1,1685)	1:98:A:LEU:HD12	2:104:A:HEC:HMB1	16	0.16
(1,1685)	1:98:A:LEU:HD12	2:104:A:HEC:HMB2	16	0.16
(1,1685)	1:98:A:LEU:HD12	2:104:A:HEC:HMB3	16	0.16
(1,1685)	1:98:A:LEU:HD13	2:104:A:HEC:HMB1	16	0.16
(1,1685)	1:98:A:LEU:HD13	2:104:A:HEC:HMB2	16	0.16
(1,1685)	1:98:A:LEU:HD13	2:104:A:HEC:HMB3	16	0.16
(1,1302)	1:74:A:TYR:HA	1:74:A:TYR:HD1	17	0.16
(1,1302)	1:74:A:TYR:HA	1:74:A:TYR:HD2	17	0.16
(1,1166)	1:64:A:MET:HB2	1:60:A:ASP:H	20	0.16
(1,1166)	1:64:A:MET:HB3	1:60:A:ASP:H	20	0.16
(1,1087)	1:60:A:ASP:HB2	1:61:A:GLU:H	6	0.16
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	2	0.16
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	14	0.16
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	15	0.16
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	18	0.16
(1,1037)	1:58:A:LEU:HB3	1:63:A:ASN:HD21	6	0.16
(1,1037)	1:58:A:LEU:HB3	1:63:A:ASN:HD22	6	0.16
(1,1037)	1:58:A:LEU:HB3	1:63:A:ASN:HD21	15	0.16
(1,1037)	1:58:A:LEU:HB3	1:63:A:ASN:HD22	15	0.16
(1,990)	1:57:A:VAL:HG21	1:40:A:SER:H	18	0.16
(1,990)	1:57:A:VAL:HG22	1:40:A:SER:H	18	0.16
(1,990)	1:57:A:VAL:HG23	1:40:A:SER:H	18	0.16
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	14	0.16
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	6	0.16
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	6	0.16
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	10	0.16
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	10	0.16
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	14	0.16
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	14	0.16
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	7	0.16
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	2	0.16
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	2	0.16
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	2	0.16
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	10	0.16
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	10	0.16
(1,599)	1:32:A:LEU:HD21	1:36:A:PHE:HZ	7	0.16
(1,599)	1:32:A:LEU:HD22	1:36:A:PHE:HZ	7	0.16
(1,599)	1:32:A:LEU:HD23	1:36:A:PHE:HZ	7	0.16
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG21	12	0.16
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG22	12	0.16
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG23	12	0.16
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG21	12	0.16
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG22	12	0.16
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG23	12	0.16
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG21	12	0.16
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG22	12	0.16
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG23	12	0.16
(1,579)	1:32:A:LEU:HD11	1:18:A:HIS:HB2	8	0.16
(1,579)	1:32:A:LEU:HD12	1:18:A:HIS:HB2	8	0.16
(1,579)	1:32:A:LEU:HD13	1:18:A:HIS:HB2	8	0.16
(1,512)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	16	0.16
(1,512)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	16	0.16
(1,147)	1:8:A:THR:HG21	1:8:A:THR:HA	7	0.16
(1,147)	1:8:A:THR:HG22	1:8:A:THR:HA	7	0.16
(1,147)	1:8:A:THR:HG23	1:8:A:THR:HA	7	0.16
(1,1434)	1:85:A:LEU:HD21	1:88:A:GLU:H	19	0.15
(1,1434)	1:85:A:LEU:HD22	1:88:A:GLU:H	19	0.15
(1,1434)	1:85:A:LEU:HD23	1:88:A:GLU:H	19	0.15
(1,1302)	1:74:A:TYR:HA	1:74:A:TYR:HD1	3	0.15
(1,1302)	1:74:A:TYR:HA	1:74:A:TYR:HD2	3	0.15
(1,1079)	1:59:A:TRP:HE1	1:52:A:ASN:HD22	12	0.15
(1,1078)	1:59:A:TRP:HE1	1:52:A:ASN:HD21	20	0.15
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	19	0.15
(1,990)	1:57:A:VAL:HG21	1:40:A:SER:H	5	0.15
(1,990)	1:57:A:VAL:HG22	1:40:A:SER:H	5	0.15
(1,990)	1:57:A:VAL:HG23	1:40:A:SER:H	5	0.15
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	2	0.15
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	8	0.15
(1,854)	1:49:A:THR:HG21	1:52:A:ASN:H	16	0.15
(1,854)	1:49:A:THR:HG22	1:52:A:ASN:H	16	0.15
(1,854)	1:49:A:THR:HG23	1:52:A:ASN:H	16	0.15
(1,846)	1:49:A:THR:HG21	1:49:A:THR:H	1	0.15
(1,846)	1:49:A:THR:HG22	1:49:A:THR:H	1	0.15
(1,846)	1:49:A:THR:HG23	1:49:A:THR:H	1	0.15
(1,846)	1:49:A:THR:HG21	1:49:A:THR:H	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:49:A:THR:HG22	1:49:A:THR:H	14	0.15
(1,846)	1:49:A:THR:HG23	1:49:A:THR:H	14	0.15
(1,846)	1:49:A:THR:HG21	1:49:A:THR:H	18	0.15
(1,846)	1:49:A:THR:HG22	1:49:A:THR:H	18	0.15
(1,846)	1:49:A:THR:HG23	1:49:A:THR:H	18	0.15
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	16	0.15
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	16	0.15
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	16	0.15
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	1	0.15
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	1	0.15
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	4	0.15
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	4	0.15
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	12	0.15
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	12	0.15
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	15	0.15
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	15	0.15
(1,762)	1:41:A:GLY:HA2	1:42:A:GLN:HE21	9	0.15
(1,762)	1:41:A:GLY:HA2	1:42:A:GLN:HE22	9	0.15
(1,733)	1:39:A:HIS:HA	1:59:A:TRP:HD1	5	0.15
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	3	0.15
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	19	0.15
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	16	0.15
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	16	0.15
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	16	0.15
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG21	13	0.15
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG22	13	0.15
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG23	13	0.15
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG21	13	0.15
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG22	13	0.15
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG23	13	0.15
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG21	13	0.15
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG22	13	0.15
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG23	13	0.15
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG21	17	0.15
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG22	17	0.15
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG23	17	0.15
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG21	17	0.15
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG22	17	0.15
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG23	17	0.15
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG21	17	0.15
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG22	17	0.15
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG23	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG21	19	0.15
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG22	19	0.15
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG23	19	0.15
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG21	19	0.15
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG22	19	0.15
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG23	19	0.15
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG21	19	0.15
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG22	19	0.15
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG23	19	0.15
(1,569)	1:32:A:LEU:HA	1:34:A:GLY:H	18	0.15
(1,395)	1:20:A:VAL:HG11	1:24:A:GLY:H	12	0.15
(1,395)	1:20:A:VAL:HG12	1:24:A:GLY:H	12	0.15
(1,395)	1:20:A:VAL:HG13	1:24:A:GLY:H	12	0.15
(1,368)	1:19:A:THR:HA	1:17:A:CYS:H	7	0.15
(1,277)	1:14:A:CYS:HA	1:15:A:LEU:HG	1	0.15
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD21	7	0.15
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD22	7	0.15
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD23	7	0.15
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD21	13	0.15
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD22	13	0.15
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD23	13	0.15
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD21	17	0.15
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD22	17	0.15
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD23	17	0.15
(1,120)	1:6:A:GLY:HA3	1:9:A:LEU:HB3	7	0.15
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	10	0.14
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	10	0.14
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	10	0.14
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	10	0.14
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	10	0.14
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	10	0.14
(1,1450)	1:87:A:LYS:HB2	1:90:A:ASP:HB2	6	0.14
(1,1450)	1:87:A:LYS:HB2	1:90:A:ASP:HB3	6	0.14
(1,1450)	1:87:A:LYS:HB3	1:90:A:ASP:HB2	6	0.14
(1,1450)	1:87:A:LYS:HB3	1:90:A:ASP:HB3	6	0.14
(1,1434)	1:85:A:LEU:HD21	1:88:A:GLU:H	2	0.14
(1,1434)	1:85:A:LEU:HD22	1:88:A:GLU:H	2	0.14
(1,1434)	1:85:A:LEU:HD23	1:88:A:GLU:H	2	0.14
(1,1405)	1:82:A:PHE:HE1	1:85:A:LEU:HD11	15	0.14
(1,1405)	1:82:A:PHE:HE1	1:85:A:LEU:HD12	15	0.14
(1,1405)	1:82:A:PHE:HE1	1:85:A:LEU:HD13	15	0.14
(1,1405)	1:82:A:PHE:HE2	1:85:A:LEU:HD11	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1405)	1:82:A:PHE:HE2	1:85:A:LEU:HD12	15	0.14
(1,1405)	1:82:A:PHE:HE2	1:85:A:LEU:HD13	15	0.14
(1,1308)	1:74:A:TYR:HD1	1:75:A:ILE:H	10	0.14
(1,1308)	1:74:A:TYR:HD2	1:75:A:ILE:H	10	0.14
(1,1265)	1:71:A:HIS:HB3	1:71:A:HIS:H	16	0.14
(1,1166)	1:64:A:MET:HB2	1:60:A:ASP:H	14	0.14
(1,1166)	1:64:A:MET:HB3	1:60:A:ASP:H	14	0.14
(1,1086)	1:60:A:ASP:HB3	1:61:A:GLU:H	3	0.14
(1,1086)	1:60:A:ASP:HB3	1:61:A:GLU:H	7	0.14
(1,1079)	1:59:A:TRP:HE1	1:52:A:ASN:HD22	3	0.14
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	7	0.14
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	12	0.14
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	17	0.14
(1,987)	1:57:A:VAL:HG11	1:39:A:HIS:HA	3	0.14
(1,987)	1:57:A:VAL:HG12	1:39:A:HIS:HA	3	0.14
(1,987)	1:57:A:VAL:HG13	1:39:A:HIS:HA	3	0.14
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	18	0.14
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD11	5	0.14
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD12	5	0.14
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD13	5	0.14
(1,842)	1:48:A:TYR:HD1	1:52:A:ASN:HD22	20	0.14
(1,779)	1:42:A:GLN:HE21	1:39:A:HIS:H	17	0.14
(1,779)	1:42:A:GLN:HE22	1:39:A:HIS:H	17	0.14
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	8	0.14
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	8	0.14
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	13	0.14
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	13	0.14
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	6	0.14
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	6	0.14
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	6	0.14
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	13	0.14
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	13	0.14
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	13	0.14
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG21	6	0.14
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG22	6	0.14
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG23	6	0.14
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG21	6	0.14
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG22	6	0.14
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG23	6	0.14
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG21	6	0.14
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG22	6	0.14
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG23	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:32:A:LEU:HD11	1:18:A:HIS:HB2	10	0.14
(1,579)	1:32:A:LEU:HD12	1:18:A:HIS:HB2	10	0.14
(1,579)	1:32:A:LEU:HD13	1:18:A:HIS:HB2	10	0.14
(1,512)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	5	0.14
(1,512)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	5	0.14
(1,512)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	7	0.14
(1,512)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	7	0.14
(1,368)	1:19:A:THR:HA	1:17:A:CYS:H	16	0.14
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD21	2	0.14
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD22	2	0.14
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD23	2	0.14
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD21	14	0.14
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD22	14	0.14
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD23	14	0.14
(1,202)	1:10:A:PHE:HA	1:13:A:ARG:HB3	6	0.14
(1,202)	1:10:A:PHE:HA	1:13:A:ARG:HB3	14	0.14
(1,1724)	1:100:A:LYS:HE2	1:101:A:ALA:H	7	0.13
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	5	0.13
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	5	0.13
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	5	0.13
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	5	0.13
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	5	0.13
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	5	0.13
(1,1434)	1:85:A:LEU:HD21	1:88:A:GLU:H	7	0.13
(1,1434)	1:85:A:LEU:HD22	1:88:A:GLU:H	7	0.13
(1,1434)	1:85:A:LEU:HD23	1:88:A:GLU:H	7	0.13
(1,1434)	1:85:A:LEU:HD21	1:88:A:GLU:H	20	0.13
(1,1434)	1:85:A:LEU:HD22	1:88:A:GLU:H	20	0.13
(1,1434)	1:85:A:LEU:HD23	1:88:A:GLU:H	20	0.13
(1,1308)	1:74:A:TYR:HD1	1:75:A:ILE:H	1	0.13
(1,1308)	1:74:A:TYR:HD2	1:75:A:ILE:H	1	0.13
(1,1308)	1:74:A:TYR:HD1	1:75:A:ILE:H	9	0.13
(1,1308)	1:74:A:TYR:HD2	1:75:A:ILE:H	9	0.13
(1,1308)	1:74:A:TYR:HD1	1:75:A:ILE:H	18	0.13
(1,1308)	1:74:A:TYR:HD2	1:75:A:ILE:H	18	0.13
(1,1308)	1:74:A:TYR:HD1	1:75:A:ILE:H	19	0.13
(1,1308)	1:74:A:TYR:HD2	1:75:A:ILE:H	19	0.13
(1,1280)	1:71:A:HIS:HB2	1:74:A:TYR:HE1	9	0.13
(1,1280)	1:71:A:HIS:HB2	1:74:A:TYR:HE2	9	0.13
(1,1280)	1:71:A:HIS:HB3	1:74:A:TYR:HE1	9	0.13
(1,1280)	1:71:A:HIS:HB3	1:74:A:TYR:HE2	9	0.13
(1,1280)	1:71:A:HIS:HB2	1:74:A:TYR:HE1	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1280)	1:71:A:HIS:HB2	1:74:A:TYR:HE2	16	0.13
(1,1280)	1:71:A:HIS:HB3	1:74:A:TYR:HE1	16	0.13
(1,1280)	1:71:A:HIS:HB3	1:74:A:TYR:HE2	16	0.13
(1,1230)	1:68:A:LEU:HB3	1:69:A:THR:H	14	0.13
(1,1137)	1:63:A:ASN:HD22	1:60:A:ASP:H	3	0.13
(1,1086)	1:60:A:ASP:HB3	1:61:A:GLU:H	12	0.13
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	1	0.13
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	4	0.13
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	9	0.13
(1,990)	1:57:A:VAL:HG21	1:40:A:SER:H	1	0.13
(1,990)	1:57:A:VAL:HG22	1:40:A:SER:H	1	0.13
(1,990)	1:57:A:VAL:HG23	1:40:A:SER:H	1	0.13
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	5	0.13
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	7	0.13
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	17	0.13
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	1	0.13
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	1	0.13
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	1	0.13
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	1	0.13
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	1	0.13
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	1	0.13
(1,882)	1:51:A:ALA:HB1	1:78:A:THR:H	14	0.13
(1,882)	1:51:A:ALA:HB2	1:78:A:THR:H	14	0.13
(1,882)	1:51:A:ALA:HB3	1:78:A:THR:H	14	0.13
(1,792)	1:43:A:ALA:HB1	1:46:A:TYR:HD2	11	0.13
(1,792)	1:43:A:ALA:HB2	1:46:A:TYR:HD2	11	0.13
(1,792)	1:43:A:ALA:HB3	1:46:A:TYR:HD2	11	0.13
(1,791)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	20	0.13
(1,791)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	20	0.13
(1,791)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	20	0.13
(1,762)	1:41:A:GLY:HA2	1:42:A:GLN:HE21	8	0.13
(1,762)	1:41:A:GLY:HA2	1:42:A:GLN:HE22	8	0.13
(1,733)	1:39:A:HIS:HA	1:59:A:TRP:HD1	6	0.13
(1,657)	1:35:A:ILE:HD11	1:59:A:TRP:HH2	9	0.13
(1,657)	1:35:A:ILE:HD12	1:59:A:TRP:HH2	9	0.13
(1,657)	1:35:A:ILE:HD13	1:59:A:TRP:HH2	9	0.13
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	11	0.13
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	12	0.13
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	15	0.13
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	1	0.13
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	1	0.13
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	17	0.13
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	17	0.13
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	17	0.13
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG21	1	0.13
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG22	1	0.13
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG23	1	0.13
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG21	1	0.13
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG22	1	0.13
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG23	1	0.13
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG21	1	0.13
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG22	1	0.13
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG23	1	0.13
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG21	8	0.13
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG22	8	0.13
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG23	8	0.13
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG21	8	0.13
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG22	8	0.13
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG23	8	0.13
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG21	8	0.13
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG22	8	0.13
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG23	8	0.13
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG21	18	0.13
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG22	18	0.13
(1,597)	1:32:A:LEU:HD21	1:35:A:ILE:HG23	18	0.13
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG21	18	0.13
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG22	18	0.13
(1,597)	1:32:A:LEU:HD22	1:35:A:ILE:HG23	18	0.13
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG21	18	0.13
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG22	18	0.13
(1,597)	1:32:A:LEU:HD23	1:35:A:ILE:HG23	18	0.13
(1,563)	1:32:A:LEU:HD21	1:32:A:LEU:H	7	0.13
(1,563)	1:32:A:LEU:HD22	1:32:A:LEU:H	7	0.13
(1,563)	1:32:A:LEU:HD23	1:32:A:LEU:H	7	0.13
(1,468)	1:27:A:LYS:H	1:27:A:LYS:HE2	3	0.13
(1,468)	1:27:A:LYS:H	1:27:A:LYS:HE3	3	0.13
(1,412)	1:22:A:LYS:HG2	1:22:A:LYS:H	9	0.13
(1,401)	1:21:A:GLU:H	1:20:A:VAL:H	4	0.13
(1,396)	1:20:A:VAL:HG21	1:24:A:GLY:H	20	0.13
(1,396)	1:20:A:VAL:HG22	1:24:A:GLY:H	20	0.13
(1,396)	1:20:A:VAL:HG23	1:24:A:GLY:H	20	0.13
(1,367)	1:19:A:THR:HG21	1:21:A:GLU:H	1	0.13
(1,367)	1:19:A:THR:HG22	1:21:A:GLU:H	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:19:A:THR:HG23	1:21:A:GLU:H	1	0.13
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD21	1	0.13
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD22	1	0.13
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD23	1	0.13
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD21	6	0.13
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD22	6	0.13
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD23	6	0.13
(1,202)	1:10:A:PHE:HA	1:13:A:ARG:HB3	10	0.13
(1,202)	1:10:A:PHE:HA	1:13:A:ARG:HB3	17	0.13
(1,184)	1:9:A:LEU:HB2	1:10:A:PHE:H	2	0.13
(1,184)	1:9:A:LEU:HB2	1:10:A:PHE:H	5	0.13
(1,160)	1:8:A:THR:HB	1:9:A:LEU:H	4	0.13
(1,160)	1:8:A:THR:HB	1:9:A:LEU:H	11	0.13
(1,1744)	1:102:A:THR:HG21	1:36:A:PHE:H	2	0.12
(1,1744)	1:102:A:THR:HG22	1:36:A:PHE:H	2	0.12
(1,1744)	1:102:A:THR:HG23	1:36:A:PHE:H	2	0.12
(1,1724)	1:100:A:LYS:HE2	1:101:A:ALA:H	16	0.12
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	1	0.12
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	1	0.12
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	1	0.12
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	1	0.12
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	1	0.12
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	1	0.12
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	8	0.12
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	8	0.12
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	8	0.12
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	8	0.12
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	8	0.12
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	8	0.12
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	11	0.12
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	11	0.12
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	11	0.12
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	11	0.12
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	11	0.12
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	11	0.12
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	19	0.12
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	19	0.12
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	19	0.12
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	19	0.12
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	19	0.12
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	19	0.12
(1,1648)	1:98:A:LEU:HB3	1:98:A:LEU:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1648)	1:98:A:LEU:HB3	1:98:A:LEU:H	17	0.12
(1,1587)	1:95:A:ILE:H	1:3:A:PHE:HZ	3	0.12
(1,1470)	1:88:A:GLU:HA	1:92:A:ASN:H	6	0.12
(1,1308)	1:74:A:TYR:HD1	1:75:A:ILE:H	4	0.12
(1,1308)	1:74:A:TYR:HD2	1:75:A:ILE:H	4	0.12
(1,1289)	1:72:A:ALA:HA	1:78:A:THR:HG21	12	0.12
(1,1289)	1:72:A:ALA:HA	1:78:A:THR:HG22	12	0.12
(1,1289)	1:72:A:ALA:HA	1:78:A:THR:HG23	12	0.12
(1,1272)	1:71:A:HIS:H	1:73:A:LYS:H	13	0.12
(1,1234)	1:68:A:LEU:HD11	2:104:A:HEC:HMA1	20	0.12
(1,1234)	1:68:A:LEU:HD11	2:104:A:HEC:HMA2	20	0.12
(1,1234)	1:68:A:LEU:HD11	2:104:A:HEC:HMA3	20	0.12
(1,1234)	1:68:A:LEU:HD12	2:104:A:HEC:HMA1	20	0.12
(1,1234)	1:68:A:LEU:HD12	2:104:A:HEC:HMA2	20	0.12
(1,1234)	1:68:A:LEU:HD12	2:104:A:HEC:HMA3	20	0.12
(1,1234)	1:68:A:LEU:HD13	2:104:A:HEC:HMA1	20	0.12
(1,1234)	1:68:A:LEU:HD13	2:104:A:HEC:HMA2	20	0.12
(1,1234)	1:68:A:LEU:HD13	2:104:A:HEC:HMA3	20	0.12
(1,1166)	1:64:A:MET:HB2	1:60:A:ASP:H	4	0.12
(1,1166)	1:64:A:MET:HB3	1:60:A:ASP:H	4	0.12
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	3	0.12
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	5	0.12
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	10	0.12
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	13	0.12
(1,1033)	1:58:A:LEU:HB3	1:39:A:HIS:HA	2	0.12
(1,1017)	1:58:A:LEU:HD11	1:58:A:LEU:H	16	0.12
(1,1017)	1:58:A:LEU:HD12	1:58:A:LEU:H	16	0.12
(1,1017)	1:58:A:LEU:HD13	1:58:A:LEU:H	16	0.12
(1,1017)	1:58:A:LEU:HD21	1:58:A:LEU:H	16	0.12
(1,1017)	1:58:A:LEU:HD22	1:58:A:LEU:H	16	0.12
(1,1017)	1:58:A:LEU:HD23	1:58:A:LEU:H	16	0.12
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	10	0.12
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	15	0.12
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	16	0.12
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	16	0.12
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	16	0.12
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	16	0.12
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	16	0.12
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	16	0.12
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	16	0.12
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD11	7	0.12
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD12	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD13	7	0.12
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD11	10	0.12
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD12	10	0.12
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD13	10	0.12
(1,882)	1:51:A:ALA:HB1	1:78:A:THR:H	17	0.12
(1,882)	1:51:A:ALA:HB2	1:78:A:THR:H	17	0.12
(1,882)	1:51:A:ALA:HB3	1:78:A:THR:H	17	0.12
(1,881)	1:51:A:ALA:HB1	1:77:A:GLY:HA2	17	0.12
(1,881)	1:51:A:ALA:HB2	1:77:A:GLY:HA2	17	0.12
(1,881)	1:51:A:ALA:HB3	1:77:A:GLY:HA2	17	0.12
(1,854)	1:49:A:THR:HG21	1:52:A:ASN:H	2	0.12
(1,854)	1:49:A:THR:HG22	1:52:A:ASN:H	2	0.12
(1,854)	1:49:A:THR:HG23	1:52:A:ASN:H	2	0.12
(1,854)	1:49:A:THR:HG21	1:52:A:ASN:H	6	0.12
(1,854)	1:49:A:THR:HG22	1:52:A:ASN:H	6	0.12
(1,854)	1:49:A:THR:HG23	1:52:A:ASN:H	6	0.12
(1,854)	1:49:A:THR:HG21	1:52:A:ASN:H	7	0.12
(1,854)	1:49:A:THR:HG22	1:52:A:ASN:H	7	0.12
(1,854)	1:49:A:THR:HG23	1:52:A:ASN:H	7	0.12
(1,792)	1:43:A:ALA:HB1	1:46:A:TYR:HD2	16	0.12
(1,792)	1:43:A:ALA:HB2	1:46:A:TYR:HD2	16	0.12
(1,792)	1:43:A:ALA:HB3	1:46:A:TYR:HD2	16	0.12
(1,792)	1:43:A:ALA:HB1	1:46:A:TYR:HD2	19	0.12
(1,792)	1:43:A:ALA:HB2	1:46:A:TYR:HD2	19	0.12
(1,792)	1:43:A:ALA:HB3	1:46:A:TYR:HD2	19	0.12
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	19	0.12
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	19	0.12
(1,762)	1:41:A:GLY:HA2	1:42:A:GLN:HE21	17	0.12
(1,762)	1:41:A:GLY:HA2	1:42:A:GLN:HE22	17	0.12
(1,738)	1:40:A:SER:HB2	1:40:A:SER:H	13	0.12
(1,738)	1:40:A:SER:HB2	1:40:A:SER:H	20	0.12
(1,715)	1:38:A:ARG:HG2	1:42:A:GLN:HG2	1	0.12
(1,715)	1:38:A:ARG:HG2	1:42:A:GLN:HG3	1	0.12
(1,715)	1:38:A:ARG:HG3	1:42:A:GLN:HG2	1	0.12
(1,715)	1:38:A:ARG:HG3	1:42:A:GLN:HG3	1	0.12
(1,634)	1:33:A:HIS:HD2	1:34:A:GLY:H	7	0.12
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	8	0.12
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	10	0.12
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	20	0.12
(1,611)	1:32:A:LEU:HD21	2:104:A:HEC:HMA1	7	0.12
(1,611)	1:32:A:LEU:HD21	2:104:A:HEC:HMA2	7	0.12
(1,611)	1:32:A:LEU:HD21	2:104:A:HEC:HMA3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,611)	1:32:A:LEU:HD22	2:104:A:HEC:HMA1	7	0.12
(1,611)	1:32:A:LEU:HD22	2:104:A:HEC:HMA2	7	0.12
(1,611)	1:32:A:LEU:HD22	2:104:A:HEC:HMA3	7	0.12
(1,611)	1:32:A:LEU:HD23	2:104:A:HEC:HMA1	7	0.12
(1,611)	1:32:A:LEU:HD23	2:104:A:HEC:HMA2	7	0.12
(1,611)	1:32:A:LEU:HD23	2:104:A:HEC:HMA3	7	0.12
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	14	0.12
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	14	0.12
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	14	0.12
(1,583)	1:32:A:LEU:HD11	1:18:A:HIS:HD2	7	0.12
(1,583)	1:32:A:LEU:HD12	1:18:A:HIS:HD2	7	0.12
(1,583)	1:32:A:LEU:HD13	1:18:A:HIS:HD2	7	0.12
(1,579)	1:32:A:LEU:HD11	1:18:A:HIS:HB2	5	0.12
(1,579)	1:32:A:LEU:HD12	1:18:A:HIS:HB2	5	0.12
(1,579)	1:32:A:LEU:HD13	1:18:A:HIS:HB2	5	0.12
(1,512)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	3	0.12
(1,512)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	3	0.12
(1,512)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	8	0.12
(1,512)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	8	0.12
(1,396)	1:20:A:VAL:HG21	1:24:A:GLY:H	13	0.12
(1,396)	1:20:A:VAL:HG22	1:24:A:GLY:H	13	0.12
(1,396)	1:20:A:VAL:HG23	1:24:A:GLY:H	13	0.12
(1,394)	1:20:A:VAL:HG11	1:18:A:HIS:HD1	7	0.12
(1,394)	1:20:A:VAL:HG12	1:18:A:HIS:HD1	7	0.12
(1,394)	1:20:A:VAL:HG13	1:18:A:HIS:HD1	7	0.12
(1,394)	1:20:A:VAL:HG21	1:18:A:HIS:HD1	7	0.12
(1,394)	1:20:A:VAL:HG22	1:18:A:HIS:HD1	7	0.12
(1,394)	1:20:A:VAL:HG23	1:18:A:HIS:HD1	7	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	1	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	2	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	3	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	6	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	7	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	8	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	9	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	10	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	11	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	13	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	14	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	15	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	16	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	18	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	19	0.12
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	20	0.12
(1,361)	1:18:A:HIS:HD2	1:32:A:LEU:HD11	7	0.12
(1,361)	1:18:A:HIS:HD2	1:32:A:LEU:HD12	7	0.12
(1,361)	1:18:A:HIS:HD2	1:32:A:LEU:HD13	7	0.12
(1,323)	1:16:A:GLN:HG3	1:18:A:HIS:H	5	0.12
(1,294)	1:15:A:LEU:HD11	1:15:A:LEU:H	12	0.12
(1,294)	1:15:A:LEU:HD12	1:15:A:LEU:H	12	0.12
(1,294)	1:15:A:LEU:HD13	1:15:A:LEU:H	12	0.12
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD21	16	0.12
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD22	16	0.12
(1,268)	1:13:A:ARG:HA	1:15:A:LEU:HD23	16	0.12
(1,202)	1:10:A:PHE:HA	1:13:A:ARG:HB3	2	0.12
(1,184)	1:9:A:LEU:HB2	1:10:A:PHE:H	9	0.12
(1,184)	1:9:A:LEU:HB2	1:10:A:PHE:H	13	0.12
(1,184)	1:9:A:LEU:HB2	1:10:A:PHE:H	14	0.12
(1,184)	1:9:A:LEU:HB2	1:10:A:PHE:H	20	0.12
(1,160)	1:8:A:THR:HB	1:9:A:LEU:H	1	0.12
(1,11)	1:-3:A:PHE:HD1	1:96:A:THR:H	16	0.12
(1,11)	1:-3:A:PHE:HD2	1:96:A:THR:H	16	0.12
(1,1779)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	20	0.11
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	3	0.11
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	3	0.11
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	3	0.11
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	3	0.11
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	3	0.11
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	3	0.11
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	18	0.11
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	18	0.11
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	18	0.11
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	18	0.11
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	18	0.11
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	18	0.11
(1,1648)	1:98:A:LEU:HB3	1:98:A:LEU:H	1	0.11
(1,1648)	1:98:A:LEU:HB3	1:98:A:LEU:H	3	0.11
(1,1648)	1:98:A:LEU:HB3	1:98:A:LEU:H	4	0.11
(1,1648)	1:98:A:LEU:HB3	1:98:A:LEU:H	6	0.11
(1,1648)	1:98:A:LEU:HB3	1:98:A:LEU:H	9	0.11
(1,1648)	1:98:A:LEU:HB3	1:98:A:LEU:H	11	0.11
(1,1648)	1:98:A:LEU:HB3	1:98:A:LEU:H	13	0.11
(1,1648)	1:98:A:LEU:HB3	1:98:A:LEU:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1648)	1:98:A:LEU:HB3	1:98:A:LEU:H	19	0.11
(1,1568)	1:94:A:LEU:HB3	1:95:A:ILE:H	15	0.11
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	10	0.11
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	3	0.11
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	6	0.11
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	11	0.11
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	14	0.11
(1,1490)	1:90:A:ASP:HB3	1:90:A:ASP:H	16	0.11
(1,1474)	1:89:A:LYS:HB3	1:89:A:LYS:H	8	0.11
(1,1474)	1:89:A:LYS:HB3	1:89:A:LYS:H	11	0.11
(1,1406)	1:82:A:PHE:HE1	1:85:A:LEU:HD21	11	0.11
(1,1406)	1:82:A:PHE:HE1	1:85:A:LEU:HD22	11	0.11
(1,1406)	1:82:A:PHE:HE1	1:85:A:LEU:HD23	11	0.11
(1,1406)	1:82:A:PHE:HE2	1:85:A:LEU:HD21	11	0.11
(1,1406)	1:82:A:PHE:HE2	1:85:A:LEU:HD22	11	0.11
(1,1406)	1:82:A:PHE:HE2	1:85:A:LEU:HD23	11	0.11
(1,1405)	1:82:A:PHE:HE1	1:85:A:LEU:HD11	4	0.11
(1,1405)	1:82:A:PHE:HE1	1:85:A:LEU:HD12	4	0.11
(1,1405)	1:82:A:PHE:HE1	1:85:A:LEU:HD13	4	0.11
(1,1405)	1:82:A:PHE:HE2	1:85:A:LEU:HD11	4	0.11
(1,1405)	1:82:A:PHE:HE2	1:85:A:LEU:HD12	4	0.11
(1,1405)	1:82:A:PHE:HE2	1:85:A:LEU:HD13	4	0.11
(1,1397)	1:82:A:PHE:HD1	1:84:A:GLY:HA3	2	0.11
(1,1397)	1:82:A:PHE:HD2	1:84:A:GLY:HA3	2	0.11
(1,1397)	1:82:A:PHE:HD1	1:84:A:GLY:HA3	17	0.11
(1,1397)	1:82:A:PHE:HD2	1:84:A:GLY:HA3	17	0.11
(1,1371)	1:80:A:MET:HE1	1:82:A:PHE:HE1	20	0.11
(1,1371)	1:80:A:MET:HE1	1:82:A:PHE:HE2	20	0.11
(1,1371)	1:80:A:MET:HE2	1:82:A:PHE:HE1	20	0.11
(1,1371)	1:80:A:MET:HE2	1:82:A:PHE:HE2	20	0.11
(1,1371)	1:80:A:MET:HE3	1:82:A:PHE:HE1	20	0.11
(1,1371)	1:80:A:MET:HE3	1:82:A:PHE:HE2	20	0.11
(1,1331)	1:76:A:PRO:HG2	2:104:A:HEC:HHA	5	0.11
(1,1331)	1:76:A:PRO:HG3	2:104:A:HEC:HHA	5	0.11
(1,1308)	1:74:A:TYR:HD1	1:75:A:ILE:H	5	0.11
(1,1308)	1:74:A:TYR:HD2	1:75:A:ILE:H	5	0.11
(1,1308)	1:74:A:TYR:HD1	1:75:A:ILE:H	7	0.11
(1,1308)	1:74:A:TYR:HD2	1:75:A:ILE:H	7	0.11
(1,1289)	1:72:A:ALA:HA	1:78:A:THR:HG21	17	0.11
(1,1289)	1:72:A:ALA:HA	1:78:A:THR:HG22	17	0.11
(1,1289)	1:72:A:ALA:HA	1:78:A:THR:HG23	17	0.11
(1,1265)	1:71:A:HIS:HB3	1:71:A:HIS:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1265)	1:71:A:HIS:HB3	1:71:A:HIS:H	18	0.11
(1,1234)	1:68:A:LEU:HD11	2:104:A:HEC:HMA1	16	0.11
(1,1234)	1:68:A:LEU:HD11	2:104:A:HEC:HMA2	16	0.11
(1,1234)	1:68:A:LEU:HD11	2:104:A:HEC:HMA3	16	0.11
(1,1234)	1:68:A:LEU:HD12	2:104:A:HEC:HMA1	16	0.11
(1,1234)	1:68:A:LEU:HD12	2:104:A:HEC:HMA2	16	0.11
(1,1234)	1:68:A:LEU:HD12	2:104:A:HEC:HMA3	16	0.11
(1,1234)	1:68:A:LEU:HD13	2:104:A:HEC:HMA1	16	0.11
(1,1234)	1:68:A:LEU:HD13	2:104:A:HEC:HMA2	16	0.11
(1,1234)	1:68:A:LEU:HD13	2:104:A:HEC:HMA3	16	0.11
(1,1234)	1:68:A:LEU:HD11	2:104:A:HEC:HMA1	19	0.11
(1,1234)	1:68:A:LEU:HD11	2:104:A:HEC:HMA2	19	0.11
(1,1234)	1:68:A:LEU:HD11	2:104:A:HEC:HMA3	19	0.11
(1,1234)	1:68:A:LEU:HD12	2:104:A:HEC:HMA1	19	0.11
(1,1234)	1:68:A:LEU:HD12	2:104:A:HEC:HMA2	19	0.11
(1,1234)	1:68:A:LEU:HD12	2:104:A:HEC:HMA3	19	0.11
(1,1234)	1:68:A:LEU:HD13	2:104:A:HEC:HMA1	19	0.11
(1,1234)	1:68:A:LEU:HD13	2:104:A:HEC:HMA2	19	0.11
(1,1234)	1:68:A:LEU:HD13	2:104:A:HEC:HMA3	19	0.11
(1,1230)	1:68:A:LEU:HB3	1:69:A:THR:H	6	0.11
(1,1229)	1:68:A:LEU:HG	1:69:A:THR:H	13	0.11
(1,1063)	1:59:A:TRP:HB3	1:59:A:TRP:HD1	8	0.11
(1,1059)	1:58:A:LEU:HD11	1:56:A:ASN:HD21	1	0.11
(1,1059)	1:58:A:LEU:HD11	1:56:A:ASN:HD22	1	0.11
(1,1059)	1:58:A:LEU:HD12	1:56:A:ASN:HD21	1	0.11
(1,1059)	1:58:A:LEU:HD12	1:56:A:ASN:HD22	1	0.11
(1,1059)	1:58:A:LEU:HD13	1:56:A:ASN:HD21	1	0.11
(1,1059)	1:58:A:LEU:HD13	1:56:A:ASN:HD22	1	0.11
(1,1059)	1:58:A:LEU:HD21	1:56:A:ASN:HD21	1	0.11
(1,1059)	1:58:A:LEU:HD21	1:56:A:ASN:HD22	1	0.11
(1,1059)	1:58:A:LEU:HD22	1:56:A:ASN:HD21	1	0.11
(1,1059)	1:58:A:LEU:HD22	1:56:A:ASN:HD22	1	0.11
(1,1059)	1:58:A:LEU:HD23	1:56:A:ASN:HD21	1	0.11
(1,1059)	1:58:A:LEU:HD23	1:56:A:ASN:HD22	1	0.11
(1,1051)	1:58:A:LEU:HD11	1:56:A:ASN:HD21	1	0.11
(1,1051)	1:58:A:LEU:HD11	1:56:A:ASN:HD22	1	0.11
(1,1051)	1:58:A:LEU:HD12	1:56:A:ASN:HD21	1	0.11
(1,1051)	1:58:A:LEU:HD12	1:56:A:ASN:HD22	1	0.11
(1,1051)	1:58:A:LEU:HD13	1:56:A:ASN:HD21	1	0.11
(1,1051)	1:58:A:LEU:HD13	1:56:A:ASN:HD22	1	0.11
(1,1051)	1:58:A:LEU:HD21	1:56:A:ASN:HD21	1	0.11
(1,1051)	1:58:A:LEU:HD21	1:56:A:ASN:HD22	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1051)	1:58:A:LEU:HD22	1:56:A:ASN:HD21	1	0.11
(1,1051)	1:58:A:LEU:HD22	1:56:A:ASN:HD22	1	0.11
(1,1051)	1:58:A:LEU:HD23	1:56:A:ASN:HD21	1	0.11
(1,1051)	1:58:A:LEU:HD23	1:56:A:ASN:HD22	1	0.11
(1,972)	1:56:A:ASN:HD21	1:39:A:HIS:HD2	11	0.11
(1,972)	1:56:A:ASN:HD21	1:39:A:HIS:HD2	17	0.11
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	1	0.11
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	4	0.11
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	7	0.11
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	11	0.11
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	17	0.11
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	18	0.11
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	19	0.11
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	3	0.11
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	13	0.11
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	19	0.11
(1,907)	1:52:A:ASN:HA	1:59:A:TRP:HE1	20	0.11
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	6	0.11
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	6	0.11
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	6	0.11
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	6	0.11
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	6	0.11
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	6	0.11
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	9	0.11
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	9	0.11
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	9	0.11
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	9	0.11
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	9	0.11
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	9	0.11
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	10	0.11
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	10	0.11
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	10	0.11
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	10	0.11
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	10	0.11
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	10	0.11
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD11	13	0.11
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD12	13	0.11
(1,905)	1:52:A:ASN:HA	1:75:A:ILE:HD13	13	0.11
(1,871)	1:51:A:ALA:HA	1:52:A:ASN:H	9	0.11
(1,846)	1:49:A:THR:HG21	1:49:A:THR:H	2	0.11
(1,846)	1:49:A:THR:HG22	1:49:A:THR:H	2	0.11
(1,846)	1:49:A:THR:HG23	1:49:A:THR:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,779)	1:42:A:GLN:HE21	1:39:A:HIS:H	7	0.11
(1,779)	1:42:A:GLN:HE22	1:39:A:HIS:H	7	0.11
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	7	0.11
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	7	0.11
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	9	0.11
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	9	0.11
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	17	0.11
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	17	0.11
(1,738)	1:40:A:SER:HB2	1:40:A:SER:H	2	0.11
(1,738)	1:40:A:SER:HB2	1:40:A:SER:H	8	0.11
(1,733)	1:39:A:HIS:HA	1:59:A:TRP:HD1	3	0.11
(1,660)	1:35:A:ILE:HG12	1:36:A:PHE:HE1	14	0.11
(1,660)	1:35:A:ILE:HG12	1:36:A:PHE:HE2	14	0.11
(1,660)	1:35:A:ILE:HG13	1:36:A:PHE:HE1	14	0.11
(1,660)	1:35:A:ILE:HG13	1:36:A:PHE:HE2	14	0.11
(1,658)	1:35:A:ILE:HD11	1:36:A:PHE:HZ	16	0.11
(1,658)	1:35:A:ILE:HD12	1:36:A:PHE:HZ	16	0.11
(1,658)	1:35:A:ILE:HD13	1:36:A:PHE:HZ	16	0.11
(1,657)	1:35:A:ILE:HD11	1:59:A:TRP:HH2	7	0.11
(1,657)	1:35:A:ILE:HD12	1:59:A:TRP:HH2	7	0.11
(1,657)	1:35:A:ILE:HD13	1:59:A:TRP:HH2	7	0.11
(1,657)	1:35:A:ILE:HD11	1:59:A:TRP:HH2	16	0.11
(1,657)	1:35:A:ILE:HD12	1:59:A:TRP:HH2	16	0.11
(1,657)	1:35:A:ILE:HD13	1:59:A:TRP:HH2	16	0.11
(1,634)	1:33:A:HIS:HD2	1:34:A:GLY:H	12	0.11
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	9	0.11
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	9	0.11
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	9	0.11
(1,607)	1:32:A:LEU:HD21	2:104:A:HEC:HHA	15	0.11
(1,607)	1:32:A:LEU:HD22	2:104:A:HEC:HHA	15	0.11
(1,607)	1:32:A:LEU:HD23	2:104:A:HEC:HHA	15	0.11
(1,579)	1:32:A:LEU:HD11	1:18:A:HIS:HB2	4	0.11
(1,579)	1:32:A:LEU:HD12	1:18:A:HIS:HB2	4	0.11
(1,579)	1:32:A:LEU:HD13	1:18:A:HIS:HB2	4	0.11
(1,579)	1:32:A:LEU:HD11	1:18:A:HIS:HB2	9	0.11
(1,579)	1:32:A:LEU:HD12	1:18:A:HIS:HB2	9	0.11
(1,579)	1:32:A:LEU:HD13	1:18:A:HIS:HB2	9	0.11
(1,579)	1:32:A:LEU:HD11	1:18:A:HIS:HB2	12	0.11
(1,579)	1:32:A:LEU:HD12	1:18:A:HIS:HB2	12	0.11
(1,579)	1:32:A:LEU:HD13	1:18:A:HIS:HB2	12	0.11
(1,579)	1:32:A:LEU:HD11	1:18:A:HIS:HB2	19	0.11
(1,579)	1:32:A:LEU:HD12	1:18:A:HIS:HB2	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:32:A:LEU:HD13	1:18:A:HIS:HB2	19	0.11
(1,512)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	1	0.11
(1,512)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	1	0.11
(1,512)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	19	0.11
(1,512)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	19	0.11
(1,504)	1:28:A:VAL:HA	1:46:A:TYR:HD1	16	0.11
(1,504)	1:28:A:VAL:HA	1:46:A:TYR:HD2	16	0.11
(1,500)	1:28:A:VAL:HG21	2:104:A:HEC:HHD	3	0.11
(1,500)	1:28:A:VAL:HG22	2:104:A:HEC:HHD	3	0.11
(1,500)	1:28:A:VAL:HG23	2:104:A:HEC:HHD	3	0.11
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	4	0.11
(1,377)	1:20:A:VAL:HB	1:20:A:VAL:HA	5	0.11
(1,368)	1:19:A:THR:HA	1:17:A:CYS:H	15	0.11
(1,217)	1:11:A:LYS:HB3	1:11:A:LYS:H	10	0.11
(1,202)	1:10:A:PHE:HA	1:13:A:ARG:HB3	11	0.11
(1,202)	1:10:A:PHE:HA	1:13:A:ARG:HB3	18	0.11
(1,184)	1:9:A:LEU:HB2	1:10:A:PHE:H	19	0.11
(1,161)	1:8:A:THR:HG21	1:9:A:LEU:H	12	0.11
(1,161)	1:8:A:THR:HG22	1:9:A:LEU:H	12	0.11
(1,161)	1:8:A:THR:HG23	1:9:A:LEU:H	12	0.11
(1,160)	1:8:A:THR:HB	1:9:A:LEU:H	6	0.11
(1,160)	1:8:A:THR:HB	1:9:A:LEU:H	8	0.11
(1,160)	1:8:A:THR:HB	1:9:A:LEU:H	10	0.11
(1,160)	1:8:A:THR:HB	1:9:A:LEU:H	15	0.11
(1,160)	1:8:A:THR:HB	1:9:A:LEU:H	16	0.11
(1,160)	1:8:A:THR:HB	1:9:A:LEU:H	17	0.11
(1,160)	1:8:A:THR:HB	1:9:A:LEU:H	18	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	1	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	2	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	3	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	4	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	5	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	6	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	7	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	8	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	10	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	11	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	12	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	13	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	14	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	15	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	17	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	18	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	19	0.11
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	20	0.11
(1,1733)	1:101:A:ALA:HB1	1:20:A:VAL:H	3	0.1
(1,1733)	1:101:A:ALA:HB2	1:20:A:VAL:H	3	0.1
(1,1733)	1:101:A:ALA:HB3	1:20:A:VAL:H	3	0.1
(1,1688)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	12	0.1
(1,1688)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	12	0.1
(1,1688)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	12	0.1
(1,1688)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	12	0.1
(1,1688)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	12	0.1
(1,1688)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	12	0.1
(1,1568)	1:94:A:LEU:HB3	1:95:A:ILE:H	12	0.1
(1,1554)	1:94:A:LEU:HB3	1:94:A:LEU:H	10	0.1
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	2	0.1
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	3	0.1
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	5	0.1
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	7	0.1
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	8	0.1
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	9	0.1
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	11	0.1
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	12	0.1
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	14	0.1
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	15	0.1
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	16	0.1
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	17	0.1
(1,1539)	1:93:A:ASP:HB3	1:93:A:ASP:H	19	0.1
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	2	0.1
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	4	0.1
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	5	0.1
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	7	0.1
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	8	0.1
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	10	0.1
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	12	0.1
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	15	0.1
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	18	0.1
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	19	0.1
(1,1525)	1:92:A:ASN:HB3	1:92:A:ASN:H	20	0.1
(1,1490)	1:90:A:ASP:HB3	1:90:A:ASP:H	3	0.1
(1,1490)	1:90:A:ASP:HB3	1:90:A:ASP:H	5	0.1
(1,1490)	1:90:A:ASP:HB3	1:90:A:ASP:H	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1490)	1:90:A:ASP:HB3	1:90:A:ASP:H	18	0.1
(1,1490)	1:90:A:ASP:HB3	1:90:A:ASP:H	19	0.1
(1,1490)	1:90:A:ASP:HB3	1:90:A:ASP:H	20	0.1
(1,1474)	1:89:A:LYS:HB3	1:89:A:LYS:H	1	0.1
(1,1474)	1:89:A:LYS:HB3	1:89:A:LYS:H	3	0.1
(1,1474)	1:89:A:LYS:HB3	1:89:A:LYS:H	7	0.1
(1,1474)	1:89:A:LYS:HB3	1:89:A:LYS:H	9	0.1
(1,1474)	1:89:A:LYS:HB3	1:89:A:LYS:H	10	0.1
(1,1474)	1:89:A:LYS:HB3	1:89:A:LYS:H	12	0.1
(1,1474)	1:89:A:LYS:HB3	1:89:A:LYS:H	19	0.1
(1,1406)	1:82:A:PHE:HE1	1:85:A:LEU:HD21	8	0.1
(1,1406)	1:82:A:PHE:HE1	1:85:A:LEU:HD22	8	0.1
(1,1406)	1:82:A:PHE:HE1	1:85:A:LEU:HD23	8	0.1
(1,1406)	1:82:A:PHE:HE2	1:85:A:LEU:HD21	8	0.1
(1,1406)	1:82:A:PHE:HE2	1:85:A:LEU:HD22	8	0.1
(1,1406)	1:82:A:PHE:HE2	1:85:A:LEU:HD23	8	0.1
(1,1330)	1:76:A:PRO:HG2	1:59:A:TRP:HE1	17	0.1
(1,1330)	1:76:A:PRO:HG3	1:59:A:TRP:HE1	17	0.1
(1,1308)	1:74:A:TYR:HD1	1:75:A:ILE:H	6	0.1
(1,1308)	1:74:A:TYR:HD2	1:75:A:ILE:H	6	0.1
(1,1273)	1:71:A:HIS:H	1:74:A:TYR:HD1	13	0.1
(1,1273)	1:71:A:HIS:H	1:74:A:TYR:HD2	13	0.1
(1,1207)	1:71:A:HIS:HB3	1:67:A:TYR:HE1	16	0.1
(1,1207)	1:71:A:HIS:HB3	1:67:A:TYR:HE2	16	0.1
(1,1205)	1:71:A:HIS:HB2	1:67:A:TYR:HD1	6	0.1
(1,1205)	1:71:A:HIS:HB2	1:67:A:TYR:HD2	6	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	1	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	2	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	3	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	4	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	5	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	7	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	8	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	9	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	10	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	13	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	14	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	15	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	16	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	18	0.1
(1,1174)	1:66:A:GLU:HB3	1:66:A:GLU:H	19	0.1
(1,1166)	1:64:A:MET:HB2	1:60:A:ASP:H	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1166)	1:64:A:MET:HB3	1:60:A:ASP:H	18	0.1
(1,1075)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	7	0.1
(1,1075)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	7	0.1
(1,1075)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	7	0.1
(1,1052)	1:58:A:LEU:HD11	1:59:A:TRP:H	3	0.1
(1,1052)	1:58:A:LEU:HD12	1:59:A:TRP:H	3	0.1
(1,1052)	1:58:A:LEU:HD13	1:59:A:TRP:H	3	0.1
(1,988)	1:57:A:VAL:HG21	1:39:A:HIS:HA	14	0.1
(1,988)	1:57:A:VAL:HG22	1:39:A:HIS:HA	14	0.1
(1,988)	1:57:A:VAL:HG23	1:39:A:HIS:HA	14	0.1
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	2	0.1
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	3	0.1
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	5	0.1
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	6	0.1
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	8	0.1
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	9	0.1
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	10	0.1
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	12	0.1
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	13	0.1
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	14	0.1
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	15	0.1
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	16	0.1
(1,932)	1:54:A:LYS:HB3	1:54:A:LYS:H	20	0.1
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	13	0.1
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	13	0.1
(1,906)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	13	0.1
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	13	0.1
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	13	0.1
(1,906)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	13	0.1
(1,871)	1:51:A:ALA:HA	1:52:A:ASN:H	2	0.1
(1,871)	1:51:A:ALA:HA	1:52:A:ASN:H	4	0.1
(1,871)	1:51:A:ALA:HA	1:52:A:ASN:H	5	0.1
(1,871)	1:51:A:ALA:HA	1:52:A:ASN:H	7	0.1
(1,871)	1:51:A:ALA:HA	1:52:A:ASN:H	8	0.1
(1,871)	1:51:A:ALA:HA	1:52:A:ASN:H	15	0.1
(1,854)	1:49:A:THR:HG21	1:52:A:ASN:H	8	0.1
(1,854)	1:49:A:THR:HG22	1:52:A:ASN:H	8	0.1
(1,854)	1:49:A:THR:HG23	1:52:A:ASN:H	8	0.1
(1,854)	1:49:A:THR:HG21	1:52:A:ASN:H	15	0.1
(1,854)	1:49:A:THR:HG22	1:52:A:ASN:H	15	0.1
(1,854)	1:49:A:THR:HG23	1:52:A:ASN:H	15	0.1
(1,854)	1:49:A:THR:HG21	1:52:A:ASN:H	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,854)	1:49:A:THR:HG22	1:52:A:ASN:H	19	0.1
(1,854)	1:49:A:THR:HG23	1:52:A:ASN:H	19	0.1
(1,846)	1:49:A:THR:HG21	1:49:A:THR:H	4	0.1
(1,846)	1:49:A:THR:HG22	1:49:A:THR:H	4	0.1
(1,846)	1:49:A:THR:HG23	1:49:A:THR:H	4	0.1
(1,846)	1:49:A:THR:HG21	1:49:A:THR:H	10	0.1
(1,846)	1:49:A:THR:HG22	1:49:A:THR:H	10	0.1
(1,846)	1:49:A:THR:HG23	1:49:A:THR:H	10	0.1
(1,846)	1:49:A:THR:HG21	1:49:A:THR:H	15	0.1
(1,846)	1:49:A:THR:HG22	1:49:A:THR:H	15	0.1
(1,846)	1:49:A:THR:HG23	1:49:A:THR:H	15	0.1
(1,779)	1:42:A:GLN:HE21	1:39:A:HIS:H	12	0.1
(1,779)	1:42:A:GLN:HE22	1:39:A:HIS:H	12	0.1
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE1	16	0.1
(1,777)	1:42:A:GLN:H	1:46:A:TYR:HE2	16	0.1
(1,738)	1:40:A:SER:HB2	1:40:A:SER:H	14	0.1
(1,733)	1:39:A:HIS:HA	1:59:A:TRP:HD1	20	0.1
(1,716)	1:38:A:ARG:HD3	1:39:A:HIS:HD2	5	0.1
(1,658)	1:35:A:ILE:HD11	1:36:A:PHE:HZ	8	0.1
(1,658)	1:35:A:ILE:HD12	1:36:A:PHE:HZ	8	0.1
(1,658)	1:35:A:ILE:HD13	1:36:A:PHE:HZ	8	0.1
(1,619)	1:32:A:LEU:HG	1:101:A:ALA:H	1	0.1
(1,512)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	14	0.1
(1,512)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	14	0.1
(1,511)	1:29:A:GLY:HA2	1:46:A:TYR:HB2	13	0.1
(1,511)	1:29:A:GLY:HA2	1:46:A:TYR:HB3	13	0.1
(1,511)	1:29:A:GLY:HA3	1:46:A:TYR:HB2	13	0.1
(1,511)	1:29:A:GLY:HA3	1:46:A:TYR:HB3	13	0.1
(1,504)	1:28:A:VAL:HA	1:46:A:TYR:HD1	8	0.1
(1,504)	1:28:A:VAL:HA	1:46:A:TYR:HD2	8	0.1
(1,504)	1:28:A:VAL:HA	1:46:A:TYR:HD1	20	0.1
(1,504)	1:28:A:VAL:HA	1:46:A:TYR:HD2	20	0.1
(1,433)	1:22:A:LYS:HE2	1:23:A:GLY:H	3	0.1
(1,433)	1:22:A:LYS:HE3	1:23:A:GLY:H	3	0.1
(1,401)	1:21:A:GLU:H	1:20:A:VAL:H	11	0.1
(1,396)	1:20:A:VAL:HG21	1:24:A:GLY:H	14	0.1
(1,396)	1:20:A:VAL:HG22	1:24:A:GLY:H	14	0.1
(1,396)	1:20:A:VAL:HG23	1:24:A:GLY:H	14	0.1
(1,388)	1:20:A:VAL:HG21	1:10:A:PHE:HD1	12	0.1
(1,388)	1:20:A:VAL:HG21	1:10:A:PHE:HD2	12	0.1
(1,388)	1:20:A:VAL:HG22	1:10:A:PHE:HD1	12	0.1
(1,388)	1:20:A:VAL:HG22	1:10:A:PHE:HD2	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:20:A:VAL:HG23	1:10:A:PHE:HD1	12	0.1
(1,388)	1:20:A:VAL:HG23	1:10:A:PHE:HD2	12	0.1
(1,368)	1:19:A:THR:HA	1:17:A:CYS:H	14	0.1
(1,323)	1:16:A:GLN:HG3	1:18:A:HIS:H	17	0.1
(1,279)	1:14:A:CYS:HA	1:18:A:HIS:HB2	8	0.1
(1,279)	1:14:A:CYS:HA	1:18:A:HIS:HB3	8	0.1
(1,279)	1:14:A:CYS:HA	1:18:A:HIS:HB2	9	0.1
(1,279)	1:14:A:CYS:HA	1:18:A:HIS:HB3	9	0.1
(1,279)	1:14:A:CYS:HA	1:18:A:HIS:HB2	12	0.1
(1,279)	1:14:A:CYS:HA	1:18:A:HIS:HB3	12	0.1
(1,215)	1:10:A:PHE:HZ	1:18:A:HIS:HD1	1	0.1
(1,202)	1:10:A:PHE:HA	1:13:A:ARG:HB3	4	0.1
(1,202)	1:10:A:PHE:HA	1:13:A:ARG:HB3	16	0.1
(1,202)	1:10:A:PHE:HA	1:13:A:ARG:HB3	19	0.1
(1,161)	1:8:A:THR:HG21	1:9:A:LEU:H	8	0.1
(1,161)	1:8:A:THR:HG22	1:9:A:LEU:H	8	0.1
(1,161)	1:8:A:THR:HG23	1:9:A:LEU:H	8	0.1
(1,160)	1:8:A:THR:HB	1:9:A:LEU:H	12	0.1
(1,92)	1:5:A:LYS:HB3	1:5:A:LYS:H	9	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found