Full wwPDB NMR Structure Validation Report (i)

Aug 5, 2026 – 08:05 PM EDT

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 (i) symbol.

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

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

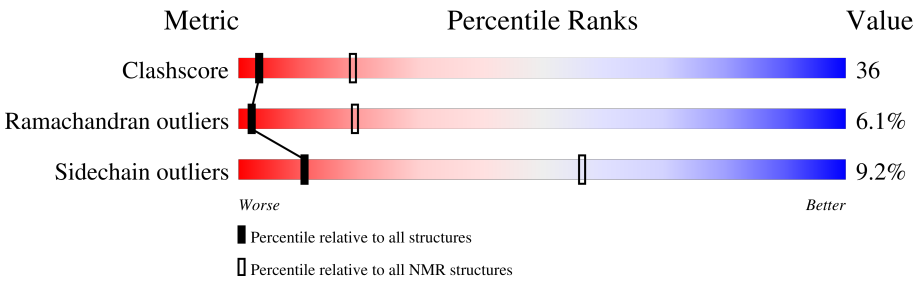
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 22%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	108	48% 43% 7% •

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

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

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 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.

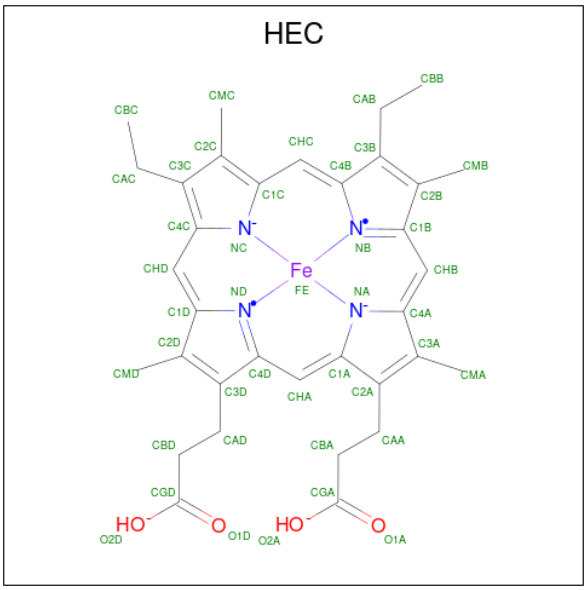
- Molecule 1 is a protein called Cytochrome c iso-1.

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

There are 3 discrepancies between the modelled and reference sequences:

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

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



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

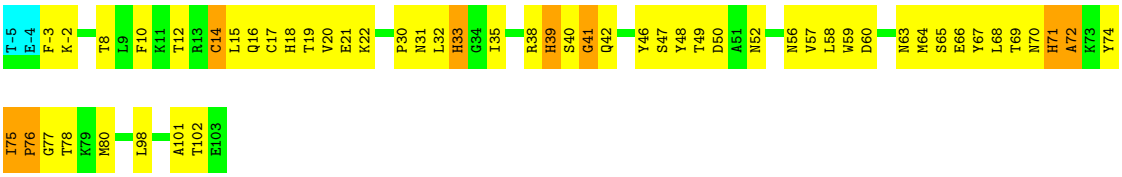
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Cytochrome c iso-1

Chain A:



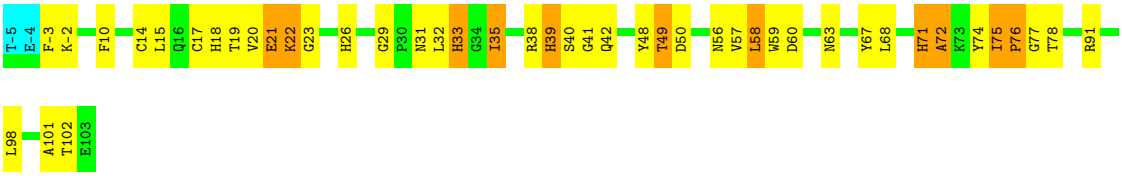
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

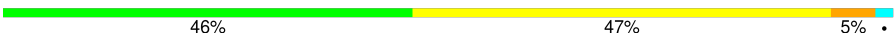
• Molecule 1: Cytochrome c iso-1

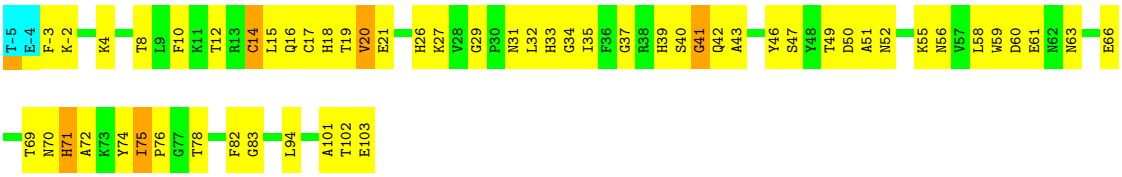
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Cytochrome c iso-1

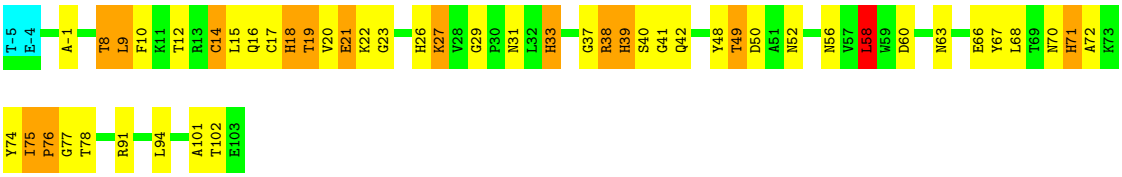
Chain A: 



4.2.3 Score per residue for model 3

- Molecule 1: Cytochrome c iso-1

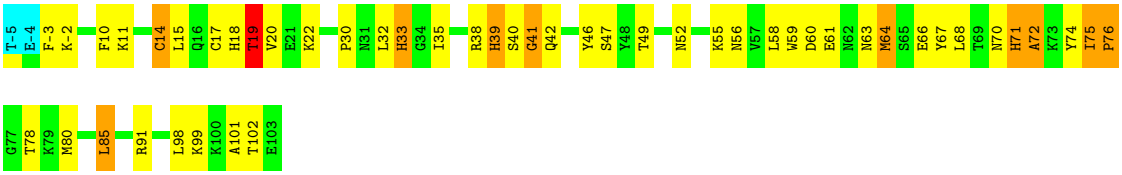
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Cytochrome c iso-1

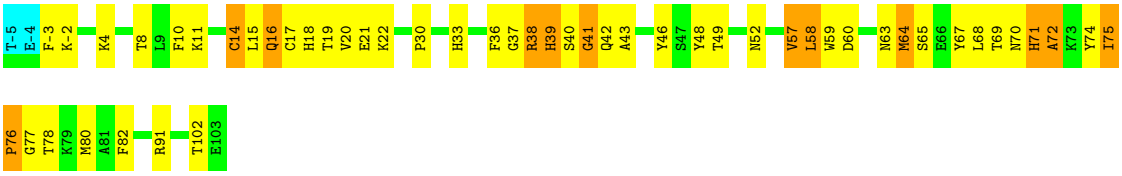
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Cytochrome c iso-1

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Cytochrome c iso-1

Chain A: 51% 37% 9%

T-5 E-4 F-3 K-2 A-1 K4 T8 L9 F10 K11 T12 R13 C14 L15 Q16 C17 H18 T19 V20 L32 H33 G34 I35 F36 G37 R38 H39 S40 G41 Q42 Y46 S47 Y48 T49 N52 L58 W59 D60 E61 N62 N63 M64 S65 E66 Y67 L68 T69 N70 H71 A72 K73 Y74 I75 P76

G77 T78 K79 M80 A81 F82 L94 L98 A101 T102 E103

4.2.7 Score per residue for model 7

- Molecule 1: Cytochrome c iso-1

Chain A: 51% 38% 9%

T-5 E-4 F-3 K-2 A3 K4 A7 T8 L9 F10 K11 T12 R13 C14 L15 Q16 C17 H18 T19 V20 K27 V28 G29 P30 N31 L32 H33 G34 I35 R38 H39 S40 G41 Q42 Y46 S47 Y48 T49 N52 V57 L58 W59 D60 N63 M64 S65 E66 Y67 L68 T69 N70 H71

A72 K73 Y74 I75 P76 G77 T78 F82 G83 K99 K100 A101 T102 E103

4.2.8 Score per residue for model 8

- Molecule 1: Cytochrome c iso-1

Chain A: 51% 40% 7%

T-5 E-4 F-3 K-2 F10 K11 T12 R13 C14 L15 Q16 C17 H18 T19 V20 E21 K22 G23 P30 N31 L32 H33 G34 I35 R38 H39 S40 G41 Q42 Y46 S47 Y48 T49 D50 A51 N56 V57 L58 W59 D60 N63 M64 S65 E66 Y67 L68 T69 N70 H71 A72 I75 P76 G77

T78 L85 K86 K87 E88 K89 D90 R91 A101 T102 E103

4.2.9 Score per residue for model 9

- Molecule 1: Cytochrome c iso-1

Chain A: 51% 36% 11%

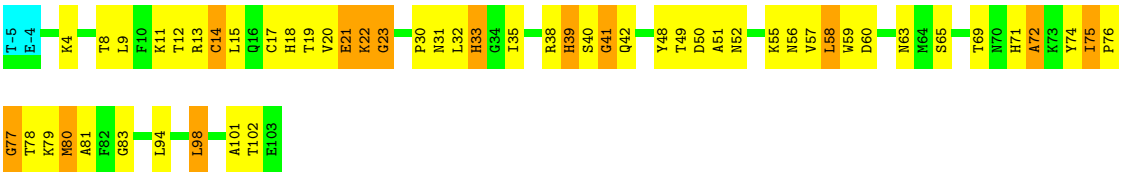
T-5 E-4 F-3 K-2 K4 T8 L9 F10 K11 C14 L15 Q16 C17 H18 T19 V20 E21 K22 P30 N31 L32 H33 G34 I35 R38 H39 S40 G41 Q42 Y46 S47 Y48 T49 N52 K55 N56 V57 L58 W59 D60 N63 M64 Y67 L68 H71 A72 K73 Y74 I75

P76 G77 T78 K79 M80 R91 L94 L98 A101 T102 E103

4.2.10 Score per residue for model 10

- Molecule 1: Cytochrome c iso-1

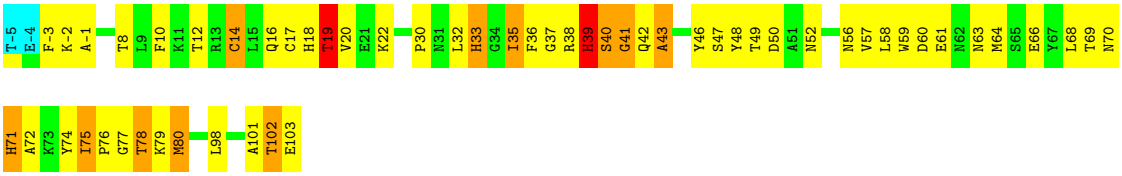
Chain A: 48% 38% 12%



4.2.11 Score per residue for model 11

- Molecule 1: Cytochrome c iso-1

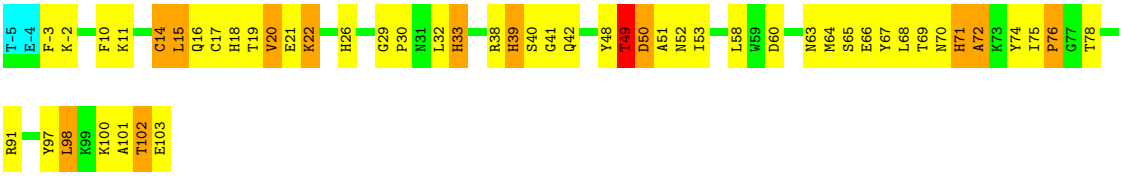
Chain A: 46% 40% 10%



4.2.12 Score per residue for model 12

- Molecule 1: Cytochrome c iso-1

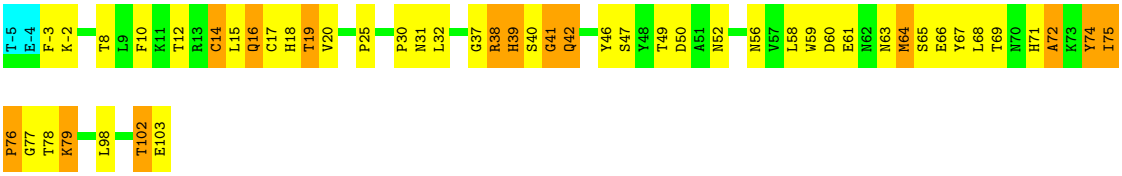
Chain A: 50% 36% 11%



4.2.13 Score per residue for model 13

- Molecule 1: Cytochrome c iso-1

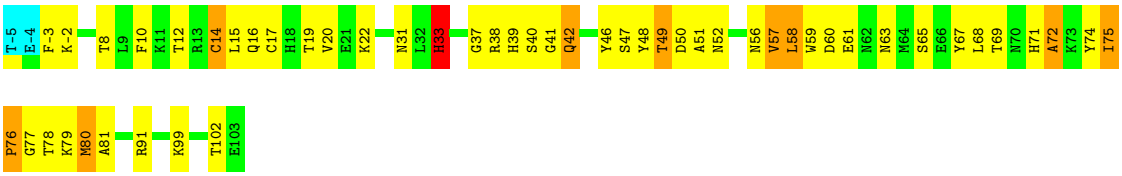
Chain A: 52% 33% 13%



4.2.14 Score per residue for model 14

- Molecule 1: Cytochrome c iso-1

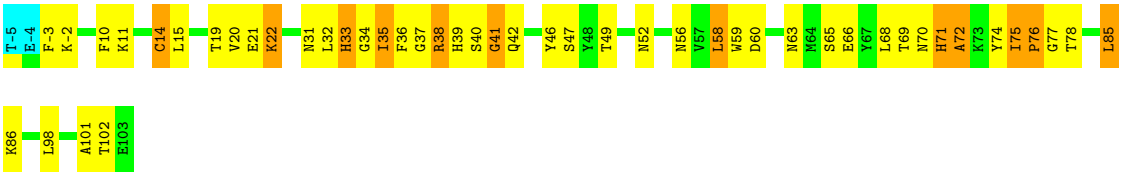
Chain A: 51% 38% 8%



4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Cytochrome c iso-1

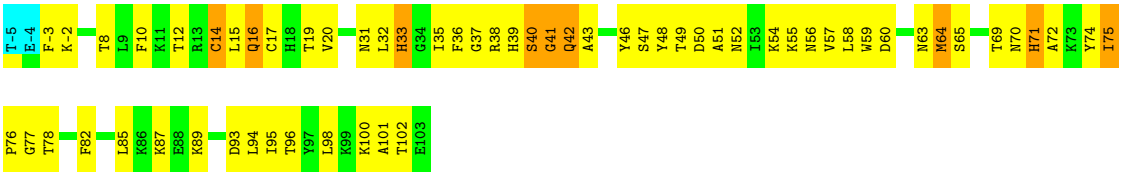
Chain A: 54% 33% 11%



4.2.16 Score per residue for model 16

- Molecule 1: Cytochrome c iso-1

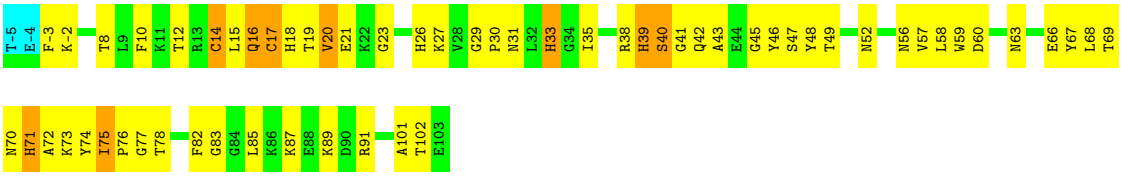
Chain A: 42% 48% 8%



4.2.17 Score per residue for model 17

- Molecule 1: Cytochrome c iso-1

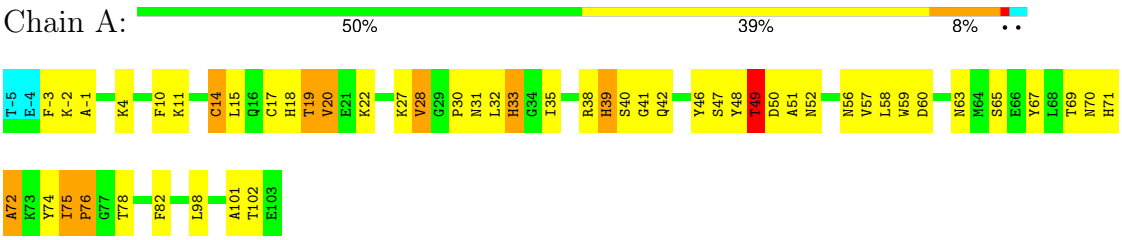
Chain A: 43% 47% 8%



4.2.18 Score per residue for model 18

- Molecule 1: Cytochrome c iso-1

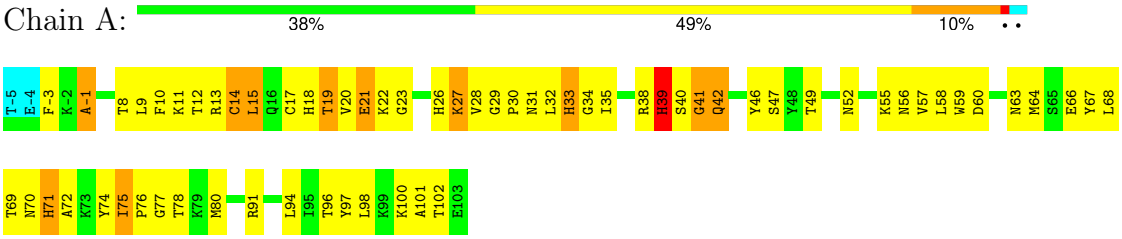
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Cytochrome c iso-1

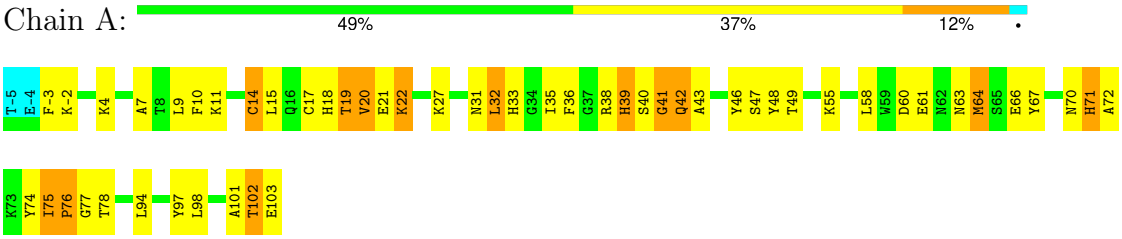
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Cytochrome c iso-1

Chain A:



5 Refinement protocol and experimental data overview (i)

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

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

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

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

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	616
Number of shifts mapped to atoms	616
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	22%

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(^{o})	Ideal(^{o})	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 (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	86/88 (98%)	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	50,50,50	0.81±0.01	2±0 (4±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	HEC	A	104	1	68,82,82	0.84±0.01	0±0 (0±0%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	104	HEC	O2A-CGA	2.58	1.22	1.30	13	20
2	A	104	HEC	O2D-CGD	2.56	1.22	1.30	5	20

There are no bond-angle outliers.

All unique chiral outliers are listed below.

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

There are no torsion outliers.

There are no ring outliers.

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

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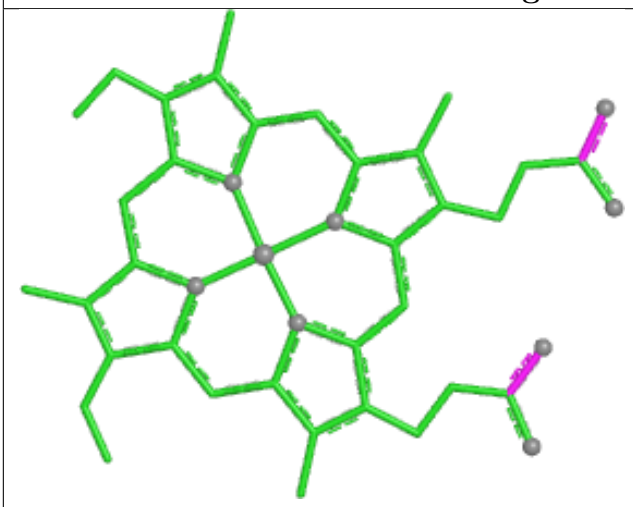
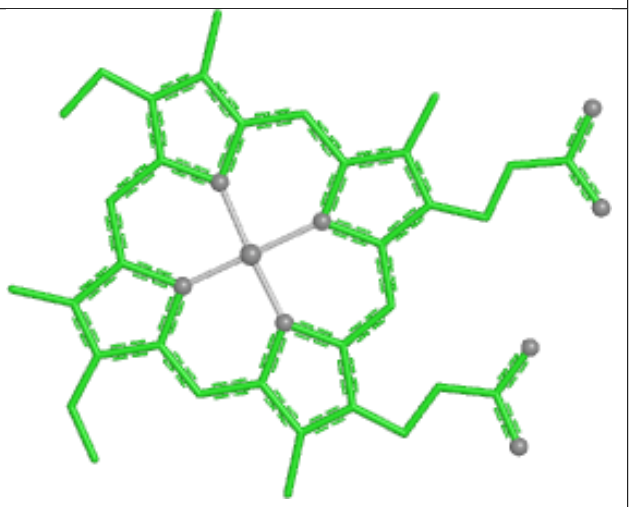
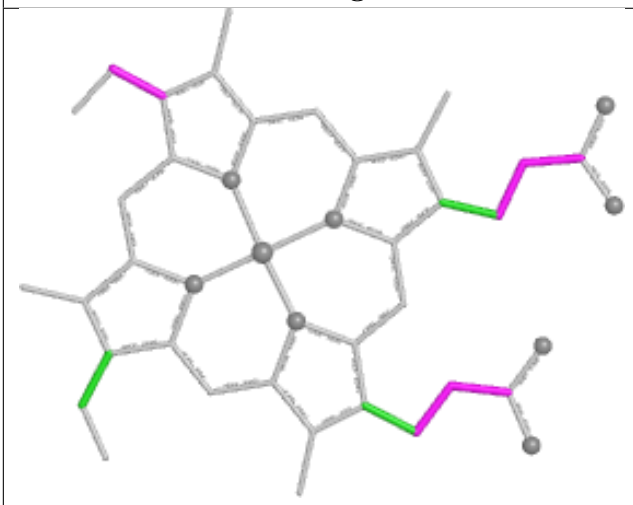


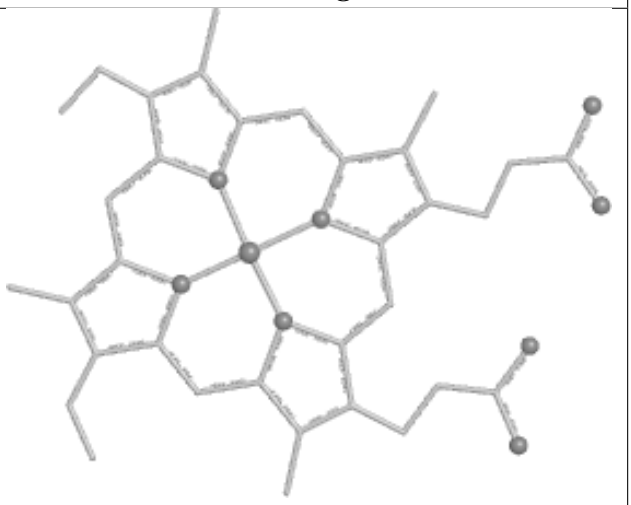
Bond lengths



Bond angles



Torsions



Rings

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 22% for the well-defined parts and 21% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	616
Number of shifts mapped to atoms	616
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

- Can not parse the chemical shift value. All 304 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	-3	PHE	HB2	2.720	0.000	.
1	A	-3	PHE	HB3	3.008	0.000	.
1	A	-3	PHE	HD1	7.148	0.014	.
1	A	-3	PHE	HE1	7.416	0.002	.
1	A	-2	LYS	HB2	1.227	0.001	.
1	A	-2	LYS	HB3	1.499	0.012	.
1	A	-2	LYS	HE3	2.661	0.001	.
1	A	-2	LYS	HG2	1.023	0.001	.
1	A	-2	LYS	HG3	1.092	0.001	.
1	A	1	GLY	HA2	3.701	0.005	.
1	A	1	GLY	HA3	4.284	0.002	.
1	A	2	SER	HB2	3.892	0.000	.
1	A	4	LYS	HB2	1.861	0.002	.
1	A	4	LYS	HB3	1.922	0.001	.
1	A	4	LYS	HG2	1.333	0.002	.
1	A	4	LYS	HG3	1.414	0.001	.
1	A	5	LYS	HB2	1.861	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	LYS	HD2	1.506	0.001	.
1	A	5	LYS	HD3	1.593	0.000	.
1	A	5	LYS	HE2	2.872	0.000	.
1	A	5	LYS	HG2	1.355	0.000	.
1	A	6	GLY	HA2	4.337	0.010	.
1	A	6	GLY	HA3	3.600	0.016	.
1	A	9	LEU	HB2	1.509	0.000	.
1	A	9	LEU	HB3	2.274	0.001	.
1	A	9	LEU	HD11	1.013	0.010	.
1	A	9	LEU	HD12	1.013	0.010	.
1	A	9	LEU	HD13	1.013	0.010	.
1	A	9	LEU	HD21	1.231	0.021	.
1	A	9	LEU	HD22	1.231	0.021	.
1	A	9	LEU	HD23	1.231	0.021	.
1	A	10	PHE	HB2	2.939	0.004	.
1	A	10	PHE	HB3	3.028	0.017	.
1	A	10	PHE	HD2	7.208	0.001	.
1	A	10	PHE	HE1	6.618	0.001	.
1	A	10	PHE	HE2	6.236	0.001	.
1	A	11	LYS	HB2	1.678	0.002	.
1	A	11	LYS	HB3	2.063	0.002	.
1	A	11	LYS	HG2	1.331	0.001	.
1	A	11	LYS	HG3	1.412	0.003	.
1	A	13	ARG	HB2	2.500	0.002	.
1	A	13	ARG	HB3	2.706	0.001	.
1	A	13	ARG	HD2	3.347	0.000	.
1	A	13	ARG	HD3	3.503	0.000	.
1	A	13	ARG	HG2	1.942	0.001	.
1	A	13	ARG	HG3	2.158	0.000	.
1	A	14	CYS	HB2	1.110	0.004	.
1	A	14	CYS	HB3	1.803	0.002	.
1	A	15	LEU	HB2	1.358	0.000	.
1	A	15	LEU	HB3	1.872	0.001	.
1	A	15	LEU	HD11	0.962	0.007	.
1	A	15	LEU	HD12	0.962	0.007	.
1	A	15	LEU	HD13	0.962	0.007	.
1	A	15	LEU	HD21	1.119	0.021	.
1	A	15	LEU	HD22	1.119	0.021	.
1	A	15	LEU	HD23	1.119	0.021	.
1	A	16	GLN	HB2	2.009	0.001	.
1	A	16	GLN	HB3	2.248	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	16	GLN	HE21	7.061	0.000	.
1	A	16	GLN	HE22	7.647	0.000	.
1	A	16	GLN	HG2	2.498	0.005	.
1	A	16	GLN	HG3	2.788	0.003	.
1	A	17	CYS	HB2	1.099	0.003	.
1	A	17	CYS	HB3	1.517	0.003	.
1	A	18	HIS	HB2	0.765	0.002	.
1	A	18	HIS	HB3	1.032	0.007	.
1	A	20	VAL	HG11	0.233	0.011	.
1	A	20	VAL	HG12	0.233	0.011	.
1	A	20	VAL	HG13	0.233	0.011	.
1	A	20	VAL	HG21	0.461	0.021	.
1	A	20	VAL	HG22	0.461	0.021	.
1	A	20	VAL	HG23	0.461	0.021	.
1	A	21	GLU	HB2	1.884	0.001	.
1	A	22	LYS	HB2	0.422	0.011	.
1	A	22	LYS	HB3	1.250	0.017	.
1	A	22	LYS	HD2	1.403	0.012	.
1	A	22	LYS	HE2	2.803	0.018	.
1	A	22	LYS	HG2	0.743	0.012	.
1	A	22	LYS	HG3	0.932	0.014	.
1	A	23	GLY	HA2	3.508	0.001	.
1	A	23	GLY	HA3	3.893	0.003	.
1	A	24	GLY	HA2	3.182	0.001	.
1	A	25	PRO	HB2	2.173	0.000	.
1	A	26	HIS	HB2	2.878	0.000	.
1	A	26	HIS	HB3	3.052	0.003	.
1	A	27	LYS	HB2	0.950	0.009	.
1	A	27	LYS	HB3	1.096	0.004	.
1	A	27	LYS	HD2	1.883	0.000	.
1	A	27	LYS	HE2	3.410	0.003	.
1	A	27	LYS	HG2	1.588	0.000	.
1	A	28	VAL	HG11	1.281	0.001	.
1	A	28	VAL	HG12	1.281	0.001	.
1	A	28	VAL	HG13	1.281	0.001	.
1	A	28	VAL	HG21	1.750	0.017	.
1	A	28	VAL	HG22	1.750	0.017	.
1	A	28	VAL	HG23	1.750	0.017	.
1	A	29	GLY	HA2	-0.032	0.030	.
1	A	29	GLY	HA3	3.563	0.017	.
1	A	30	PRO	HB2	0.368	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	PRO	HB3	1.251	0.002	.
1	A	30	PRO	HD2	1.336	0.000	.
1	A	30	PRO	HD3	1.834	0.000	.
1	A	30	PRO	HG2	0.792	0.001	.
1	A	31	ASN	HB2	1.938	0.001	.
1	A	31	ASN	HB3	2.107	0.001	.
1	A	31	ASN	HD21	7.901	0.002	.
1	A	32	LEU	HB2	1.225	0.002	.
1	A	32	LEU	HD11	-0.891	0.010	.
1	A	32	LEU	HD12	-0.891	0.010	.
1	A	32	LEU	HD13	-0.891	0.010	.
1	A	32	LEU	HD21	-0.691	0.011	.
1	A	32	LEU	HD22	-0.691	0.011	.
1	A	32	LEU	HD23	-0.691	0.011	.
1	A	33	HIS	HB3	2.991	0.002	.
1	A	34	GLY	HA2	4.208	0.002	.
1	A	35	ILE	HG12	0.942	0.004	.
1	A	35	ILE	HG13	1.276	0.005	.
1	A	36	PHE	HB2	2.979	0.001	.
1	A	36	PHE	HB3	3.059	0.002	.
1	A	36	PHE	HD2	7.211	0.003	.
1	A	36	PHE	HE2	6.771	0.002	.
1	A	37	GLY	HA2	4.229	0.014	.
1	A	38	ARG	HB2	1.957	0.009	.
1	A	38	ARG	HB3	2.008	0.007	.
1	A	38	ARG	HD2	2.937	0.021	.
1	A	38	ARG	HD3	3.133	0.030	.
1	A	38	ARG	HG2	1.835	0.013	.
1	A	38	ARG	HG3	2.168	0.020	.
1	A	39	HIS	HB2	2.719	0.002	.
1	A	39	HIS	HB3	2.873	0.001	.
1	A	40	SER	HB2	3.602	0.000	.
1	A	40	SER	HB3	3.766	0.000	.
1	A	41	GLY	HA2	3.491	0.012	.
1	A	41	GLY	HA3	1.353	0.000	.
1	A	42	GLN	HB2	1.853	0.002	.
1	A	42	GLN	HE21	6.762	0.003	.
1	A	42	GLN	HG2	2.206	0.001	.
1	A	42	GLN	HG3	2.384	0.003	.
1	A	44	GLU	HB2	2.072	0.000	.
1	A	44	GLU	HB3	2.398	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	44	GLU	HG2	2.310	0.000	.
1	A	45	GLY	HA2	3.501	0.003	.
1	A	46	TYR	HB2	0.881	0.007	.
1	A	46	TYR	HB3	2.163	0.001	.
1	A	46	TYR	HD1	6.231	0.002	.
1	A	46	TYR	HE1	6.891	0.009	.
1	A	47	SER	HB2	3.401	0.003	.
1	A	47	SER	HB3	3.564	0.000	.
1	A	48	TYR	HB2	2.926	0.011	.
1	A	48	TYR	HB3	3.726	0.001	.
1	A	48	TYR	HD1	7.478	0.000	.
1	A	48	TYR	HD2	8.028	0.000	.
1	A	48	TYR	HE1	7.244	0.041	.
1	A	48	TYR	HE2	7.060	0.026	.
1	A	50	ASP	HB2	2.673	0.002	.
1	A	52	ASN	HB2	2.932	0.000	.
1	A	52	ASN	HB3	3.128	0.000	.
1	A	53	ILE	HG12	1.073	0.011	.
1	A	54	LYS	HB2	1.723	0.001	.
1	A	54	LYS	HB3	1.860	0.000	.
1	A	54	LYS	HD2	1.587	0.003	.
1	A	54	LYS	HG2	1.442	0.005	.
1	A	54	LYS	HG3	1.516	0.006	.
1	A	55	LYS	HB2	1.799	0.002	.
1	A	55	LYS	HB3	1.907	0.006	.
1	A	56	ASN	HB2	3.015	0.000	.
1	A	56	ASN	HD21	6.297	0.013	.
1	A	56	ASN	HD22	7.789	0.003	.
1	A	57	VAL	HG11	-0.262	0.007	.
1	A	57	VAL	HG12	-0.262	0.007	.
1	A	57	VAL	HG13	-0.262	0.007	.
1	A	57	VAL	HG21	0.425	0.007	.
1	A	57	VAL	HG22	0.425	0.007	.
1	A	57	VAL	HG23	0.425	0.007	.
1	A	58	LEU	HB2	1.627	0.008	.
1	A	58	LEU	HB3	0.827	0.012	.
1	A	58	LEU	HD11	0.248	0.004	.
1	A	58	LEU	HD12	0.248	0.004	.
1	A	58	LEU	HD13	0.248	0.004	.
1	A	58	LEU	HD21	0.650	0.017	.
1	A	58	LEU	HD22	0.650	0.017	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	58	LEU	HD23	0.650	0.017	.
1	A	59	TRP	HB2	2.597	0.005	.
1	A	59	TRP	HB3	3.167	0.007	.
1	A	60	ASP	HB2	2.819	0.000	.
1	A	60	ASP	HB3	3.069	0.001	.
1	A	61	GLU	HB2	1.085	0.009	.
1	A	61	GLU	HB3	1.516	0.003	.
1	A	61	GLU	HG2	2.722	0.005	.
1	A	61	GLU	HG3	2.886	0.003	.
1	A	62	ASN	HB2	2.875	0.001	.
1	A	62	ASN	HB3	2.950	0.000	.
1	A	63	ASN	HB2	2.871	0.000	.
1	A	63	ASN	HB3	3.071	0.002	.
1	A	63	ASN	HD21	7.583	0.024	.
1	A	63	ASN	HD22	7.015	0.020	.
1	A	64	MET	HB2	2.242	0.002	.
1	A	64	MET	HB3	2.740	0.003	.
1	A	66	GLU	HB2	2.082	0.024	.
1	A	66	GLU	HB3	2.306	0.002	.
1	A	67	TYR	HB2	3.036	0.003	.
1	A	67	TYR	HB3	3.146	0.009	.
1	A	67	TYR	HD1	7.161	0.005	.
1	A	67	TYR	HD2	7.222	0.007	.
1	A	67	TYR	HE1	7.389	0.001	.
1	A	67	TYR	HE2	7.651	0.003	.
1	A	68	LEU	HB2	1.243	0.002	.
1	A	68	LEU	HB3	1.804	0.004	.
1	A	68	LEU	HD11	1.118	0.003	.
1	A	68	LEU	HD12	1.118	0.003	.
1	A	68	LEU	HD13	1.118	0.003	.
1	A	68	LEU	HD21	0.251	0.003	.
1	A	68	LEU	HD22	0.251	0.003	.
1	A	68	LEU	HD23	0.251	0.003	.
1	A	70	ASN	HB2	2.646	0.000	.
1	A	70	ASN	HB3	2.705	0.000	.
1	A	71	HIS	HB2	3.046	0.018	.
1	A	71	HIS	HB3	2.829	0.014	.
1	A	73	LYS	HB2	1.677	0.005	.
1	A	73	LYS	HB3	1.746	0.000	.
1	A	74	TYR	HB2	3.158	0.005	.
1	A	74	TYR	HD2	7.223	0.005	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	74	TYR	HE2	6.672	0.026	.
1	A	76	PRO	HB2	2.226	0.000	.
1	A	76	PRO	HB3	1.955	0.000	.
1	A	76	PRO	HD2	3.001	0.000	.
1	A	76	PRO	HG2	0.621	0.000	.
1	A	77	GLY	HA2	3.627	0.008	.
1	A	77	GLY	HA3	4.280	0.000	.
1	A	80	MET	HB2	-2.402	0.003	.
1	A	80	MET	HB3	-0.477	0.004	.
1	A	80	MET	HG2	-3.760	0.001	.
1	A	80	MET	HG3	-2.531	0.002	.
1	A	82	PHE	HB2	0.630	0.013	.
1	A	82	PHE	HB3	2.153	0.000	.
1	A	82	PHE	HD1	6.780	0.006	.
1	A	82	PHE	HE1	7.353	0.003	.
1	A	84	GLY	HA2	3.841	0.002	.
1	A	84	GLY	HA3	4.321	0.005	.
1	A	85	LEU	HB2	1.511	0.002	.
1	A	85	LEU	HB3	1.652	0.002	.
1	A	85	LEU	HD11	1.095	0.001	.
1	A	85	LEU	HD12	1.095	0.001	.
1	A	85	LEU	HD13	1.095	0.001	.
1	A	85	LEU	HD21	1.083	0.025	.
1	A	85	LEU	HD22	1.083	0.025	.
1	A	85	LEU	HD23	1.083	0.025	.
1	A	86	LYS	HB2	1.799	0.001	.
1	A	86	LYS	HG2	1.191	0.003	.
1	A	87	LYS	HB2	1.827	0.002	.
1	A	87	LYS	HB3	1.885	0.000	.
1	A	87	LYS	HD2	1.573	0.000	.
1	A	87	LYS	HD3	1.421	0.000	.
1	A	87	LYS	HG2	1.573	0.000	.
1	A	87	LYS	HG3	1.421	0.000	.
1	A	88	GLU	HB2	2.004	0.016	.
1	A	88	GLU	HB3	2.236	0.018	.
1	A	88	GLU	HG2	2.490	0.017	.
1	A	88	GLU	HG3	2.769	0.019	.
1	A	89	LYS	HB2	1.720	0.004	.
1	A	89	LYS	HB3	1.858	0.001	.
1	A	89	LYS	HG2	1.492	0.000	.
1	A	89	LYS	HG3	1.567	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	90	ASP	HB2	2.633	0.020	.
1	A	90	ASP	HB3	2.957	0.017	.
1	A	91	ARG	HB2	2.222	0.003	.
1	A	91	ARG	HB3	2.012	0.003	.
1	A	91	ARG	HG2	1.229	0.002	.
1	A	91	ARG	HG3	1.741	0.002	.
1	A	92	ASN	HB2	2.805	0.001	.
1	A	92	ASN	HB3	3.005	0.002	.
1	A	92	ASN	HD21	7.082	0.000	.
1	A	92	ASN	HD22	7.216	0.000	.
1	A	93	ASP	HB2	3.053	0.018	.
1	A	93	ASP	HB3	2.799	0.010	.
1	A	94	LEU	HB2	2.209	0.000	.
1	A	94	LEU	HB3	2.058	0.000	.
1	A	94	LEU	HD11	1.219	0.000	.
1	A	94	LEU	HD12	1.219	0.000	.
1	A	94	LEU	HD13	1.219	0.000	.
1	A	94	LEU	HD21	1.501	0.006	.
1	A	94	LEU	HD22	1.501	0.006	.
1	A	94	LEU	HD23	1.501	0.006	.
1	A	95	ILE	HG12	2.054	0.015	.
1	A	97	TYR	HB2	3.692	0.008	.
1	A	97	TYR	HB3	3.851	0.003	.
1	A	97	TYR	HD2	7.001	0.003	.
1	A	97	TYR	HE2	6.242	0.013	.
1	A	98	LEU	HB2	1.916	0.002	.
1	A	98	LEU	HB3	2.008	0.010	.
1	A	98	LEU	HD11	0.827	0.008	.
1	A	98	LEU	HD12	0.827	0.008	.
1	A	98	LEU	HD13	0.827	0.008	.
1	A	98	LEU	HD21	0.865	0.006	.
1	A	98	LEU	HD22	0.865	0.006	.
1	A	98	LEU	HD23	0.865	0.006	.
1	A	99	LYS	HB2	1.361	0.001	.
1	A	99	LYS	HB3	1.566	0.005	.
1	A	99	LYS	HE2	2.609	0.002	.
1	A	100	LYS	HB2	1.418	0.015	.
1	A	100	LYS	HB3	1.810	0.018	.
1	A	100	LYS	HE2	2.914	0.021	.
1	A	103	GLU	HB2	1.972	0.016	.
1	A	103	GLU	HB3	2.285	0.014	.

7.1.2 Chemical shift referencing (i)

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

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 22%, i.e. 311 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	193/536 (36%)	193/221 (87%)	0/212 (0%)	0/103 (0%)
Sidechain	98/752 (13%)	98/484 (20%)	0/235 (0%)	0/33 (0%)
Aromatic	20/136 (15%)	20/66 (30%)	0/60 (0%)	0/10 (0%)
Overall	311/1424 (22%)	311/771 (40%)	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 21%, i.e. 311 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	193/546 (35%)	193/225 (86%)	0/216 (0%)	0/105 (0%)
Sidechain	98/765 (13%)	98/492 (20%)	0/240 (0%)	0/33 (0%)
Aromatic	20/136 (15%)	20/66 (30%)	0/60 (0%)	0/10 (0%)
Overall	311/1447 (21%)	311/783 (40%)	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.

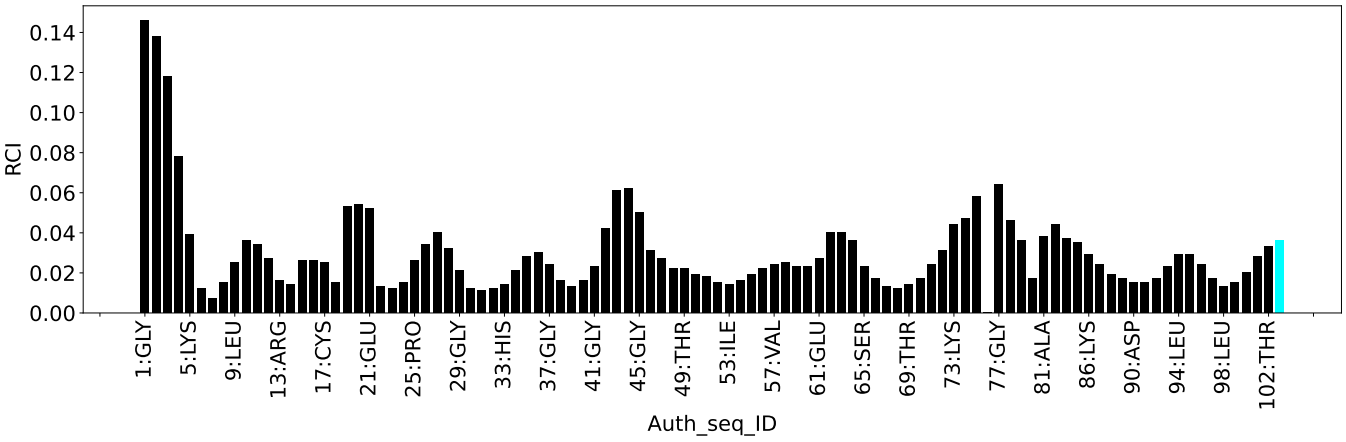
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	18	HIS	HD2	-0.06	4.65 – 9.35	-15.0
1	A	80	MET	HE1	-3.75	-0.03 – 3.80	-14.7
1	A	80	MET	HE2	-3.75	-0.03 – 3.80	-14.7
1	A	80	MET	HE3	-3.75	-0.03 – 3.80	-14.7

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from

the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	1367
Intra-residue (|i-j|=0)	442
Sequential (|i-j|=1)	306
Medium range (|i-j|>1 and |i-j|<5)	272
Long range (|i-j|≥5)	284
Inter-chain	63
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	12.5
Number of long range restraints per residue[1]	2.6

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

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	10.4	0.2
0.2-0.5 (Medium)	3.4	0.5
>0.5 (Large)	0.9	0.94

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

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

9 Distance violation analysis (i)

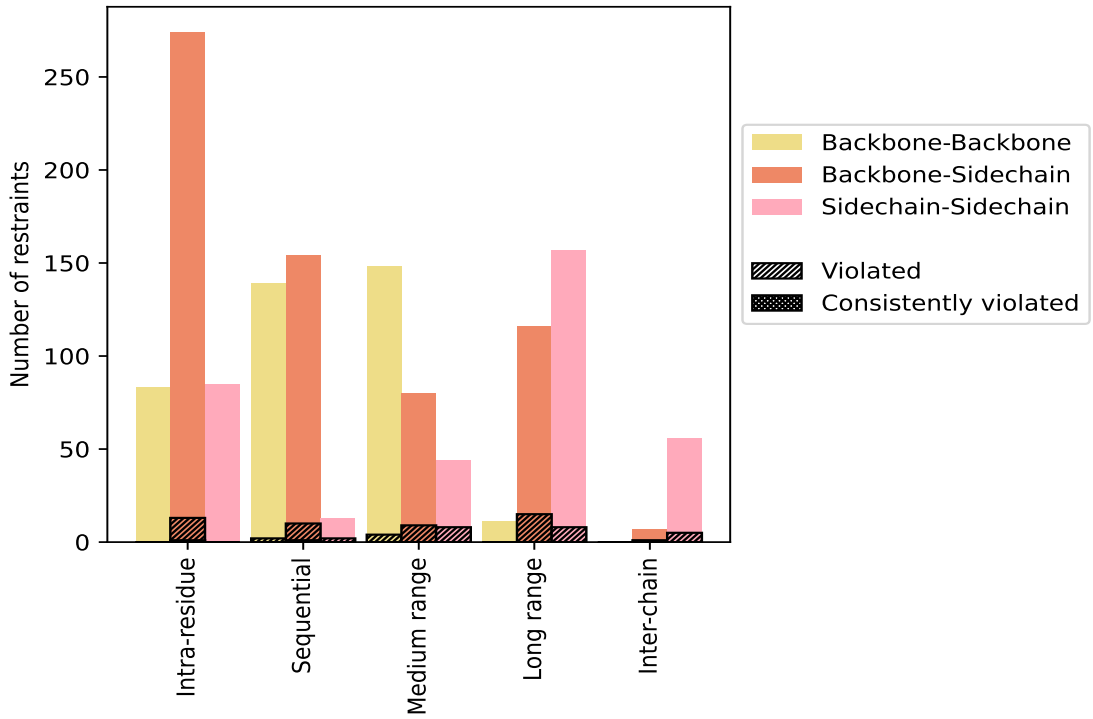
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	442	32.3	13	2.9	1.0	1	0.2	0.1
Backbone-Backbone	83	6.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	274	20.0	13	4.7	1.0	1	0.4	0.1
Sidechain-Sidechain	85	6.2	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	306	22.4	14	4.6	1.0	1	0.3	0.1
Backbone-Backbone	139	10.2	2	1.4	0.1	0	0.0	0.0
Backbone-Sidechain	154	11.3	10	6.5	0.7	1	0.6	0.1
Sidechain-Sidechain	13	1.0	2	15.4	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	272	19.9	21	7.7	1.5	0	0.0	0.0
Backbone-Backbone	148	10.8	4	2.7	0.3	0	0.0	0.0
Backbone-Sidechain	80	5.9	9	11.2	0.7	0	0.0	0.0
Sidechain-Sidechain	44	3.2	8	18.2	0.6	0	0.0	0.0
Long range (|i-j|≥5)	284	20.8	23	8.1	1.7	0	0.0	0.0
Backbone-Backbone	11	0.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	116	8.5	15	12.9	1.1	0	0.0	0.0
Sidechain-Sidechain	157	11.5	8	5.1	0.6	0	0.0	0.0
Inter-chain	63	4.6	6	9.5	0.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	7	0.5	1	14.3	0.1	0	0.0	0.0
Sidechain-Sidechain	56	4.1	5	8.9	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	1367	100.0	77	5.6	5.6	2	0.1	0.1
Backbone-Backbone	381	27.9	6	1.6	0.4	0	0.0	0.0
Backbone-Sidechain	631	46.2	48	7.6	3.5	2	0.3	0.1
Sidechain-Sidechain	355	26.0	23	6.5	1.7	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	4	4	5	6	2	21	0.19	0.91	0.17	0.13
2	5	2	1	4	1	13	0.22	0.83	0.2	0.12
3	6	2	2	7	3	20	0.19	0.66	0.13	0.14
4	3	5	2	3	1	14	0.21	0.85	0.19	0.14
5	2	3	1	6	5	17	0.23	0.83	0.22	0.14
6	2	3	4	4	1	14	0.19	0.7	0.15	0.14
7	5	4	6	7	1	23	0.17	0.66	0.12	0.12
8	4	6	4	5	2	21	0.16	0.59	0.1	0.12
9	3	3	5	6	1	18	0.21	0.78	0.16	0.16
10	3	3	2	7	1	16	0.2	0.86	0.18	0.14

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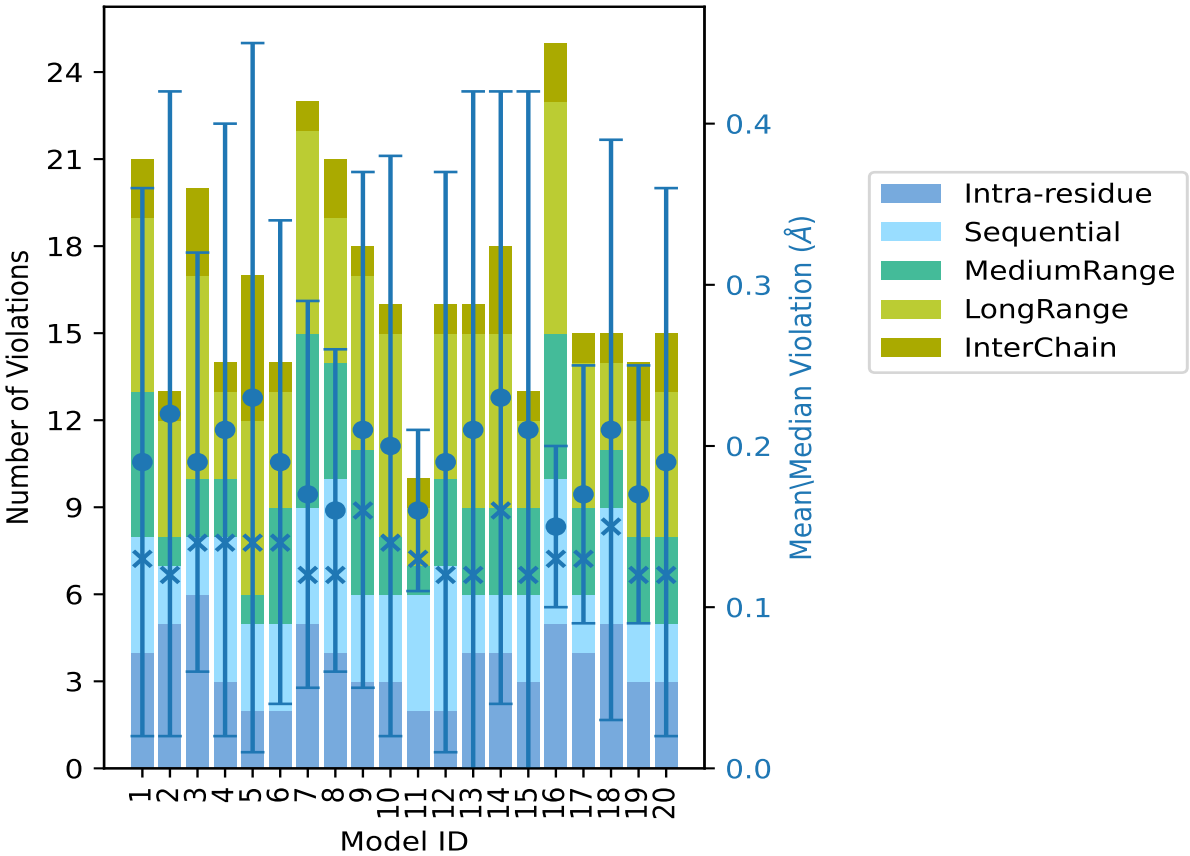
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	2	4	1	2	1	10	0.16	0.26	0.05	0.13
12	2	5	3	5	1	16	0.19	0.84	0.18	0.12
13	4	2	3	6	1	16	0.21	0.94	0.21	0.12
14	4	2	3	6	3	18	0.23	0.79	0.19	0.16
15	3	3	3	3	1	13	0.21	0.88	0.21	0.12
16	5	5	5	8	2	25	0.15	0.3	0.05	0.13
17	4	2	3	5	1	15	0.17	0.41	0.08	0.13
18	5	4	2	3	1	15	0.21	0.84	0.18	0.15
19	3	2	3	4	2	14	0.17	0.42	0.08	0.12
20	3	2	3	5	2	15	0.19	0.79	0.17	0.12

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

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



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

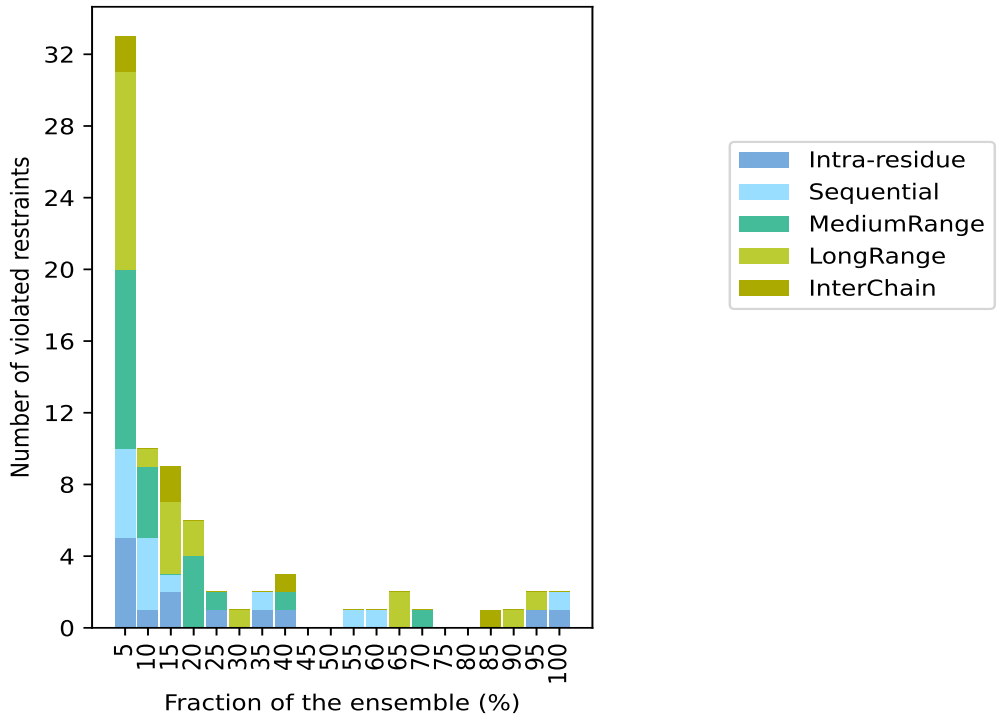
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1290(IR:429, SQ:292, MR:251, LR:261, IC:57) 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]	%
5	5	10	11	2	33	1	5.0
1	4	4	1	0	10	2	10.0
2	1	0	4	2	9	3	15.0
0	0	4	2	0	6	4	20.0
1	0	1	0	0	2	5	25.0
0	0	0	1	0	1	6	30.0
1	1	0	0	0	2	7	35.0
1	0	1	0	1	3	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	1	0	0	0	1	11	55.0
0	1	0	0	0	1	12	60.0
0	0	0	2	0	2	13	65.0
0	0	1	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	1	1	17	85.0
0	0	0	1	0	1	18	90.0
1	0	0	1	0	2	19	95.0
1	1	0	0	0	2	20	100.0

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

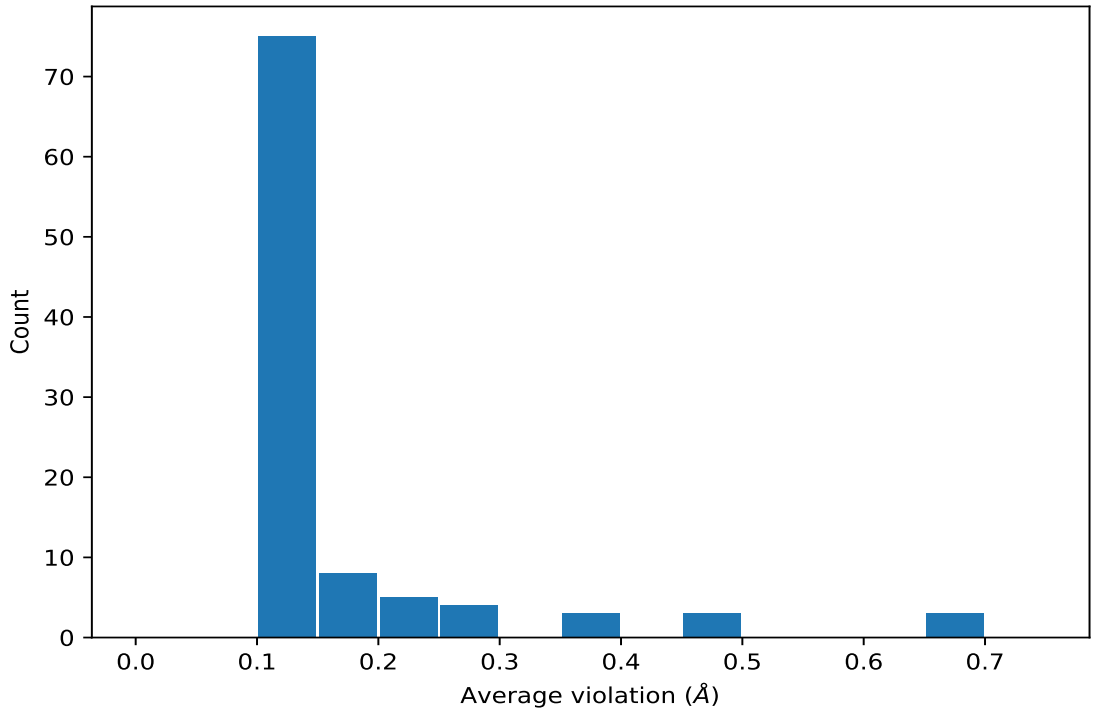
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	20	0.25	0.01	0.25
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	20	0.25	0.01	0.25
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	20	0.25	0.01	0.25
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	20	0.22	0.01	0.22
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	20	0.22	0.01	0.22
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	19	0.66	0.27	0.78
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	19	0.66	0.27	0.78
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	19	0.66	0.27	0.78
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	19	0.12	0.0	0.12
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	18	0.15	0.04	0.13
(1,1354)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	17	0.38	0.18	0.36
(1,1354)	2:104:A:HEC:HMA1	1:59:A:TRP:HE3	17	0.38	0.18	0.36
(1,1354)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	17	0.38	0.18	0.36
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	14	0.14	0.02	0.15
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	14	0.14	0.02	0.15
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	13	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	13	0.14	0.03	0.12
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	13	0.14	0.03	0.12
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	13	0.14	0.03	0.12
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	13	0.14	0.03	0.12
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	13	0.14	0.03	0.12
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	13	0.14	0.03	0.12
(1,971)	1:74:A:TYR:HD1	1:75:A:ILE:H	12	0.14	0.04	0.13
(1,971)	1:74:A:TYR:HD2	1:75:A:ILE:H	12	0.14	0.04	0.13
(1,120)	1:8:A:THR:HB	1:9:A:LEU:H	11	0.11	0.01	0.11
(1,619)	1:49:A:THR:HG21	1:49:A:THR:H	8	0.13	0.03	0.13
(1,619)	1:49:A:THR:HG22	1:49:A:THR:H	8	0.13	0.03	0.13
(1,619)	1:49:A:THR:HG23	1:49:A:THR:H	8	0.13	0.03	0.13
(1,376)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	8	0.12	0.02	0.12
(1,376)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	8	0.12	0.02	0.12
(1,627)	1:49:A:THR:HG21	1:52:A:ASN:H	8	0.12	0.03	0.12
(1,627)	1:49:A:THR:HG22	1:52:A:ASN:H	8	0.12	0.03	0.12
(1,627)	1:49:A:THR:HG23	1:52:A:ASN:H	8	0.12	0.03	0.12
(1,539)	1:40:A:SER:HB2	1:40:A:SER:H	7	0.13	0.03	0.12
(1,644)	1:51:A:ALA:HA	1:52:A:ASN:H	7	0.1	0.0	0.1
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	6	0.11	0.01	0.11
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	6	0.11	0.01	0.11
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	6	0.11	0.01	0.11
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	6	0.11	0.01	0.11
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	6	0.11	0.01	0.11
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	6	0.11	0.01	0.11
(1,965)	1:74:A:TYR:HA	1:74:A:TYR:HD1	5	0.17	0.01	0.17
(1,965)	1:74:A:TYR:HA	1:74:A:TYR:HD2	5	0.17	0.01	0.17
(1,861)	1:64:A:MET:HB2	1:60:A:ASP:H	5	0.14	0.03	0.14
(1,861)	1:64:A:MET:HB3	1:60:A:ASP:H	5	0.14	0.03	0.14
(1,580)	1:43:A:ALA:HB1	1:46:A:TYR:HD2	4	0.15	0.04	0.12
(1,580)	1:43:A:ALA:HB2	1:46:A:TYR:HD2	4	0.15	0.04	0.12
(1,580)	1:43:A:ALA:HB3	1:46:A:TYR:HD2	4	0.15	0.04	0.12
(1,568)	1:42:A:GLN:HE21	1:39:A:HIS:H	4	0.14	0.03	0.12
(1,568)	1:42:A:GLN:HE22	1:39:A:HIS:H	4	0.14	0.03	0.12
(1,268)	1:19:A:THR:HA	1:17:A:CYS:H	4	0.12	0.02	0.12
(1,535)	1:39:A:HIS:HA	1:59:A:TRP:HD1	4	0.12	0.02	0.12
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD11	4	0.12	0.01	0.12
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD12	4	0.12	0.01	0.12
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD13	4	0.12	0.01	0.12
(1,205)	1:14:A:CYS:HA	1:18:A:HIS:HB2	4	0.12	0.03	0.1
(1,205)	1:14:A:CYS:HA	1:18:A:HIS:HB3	4	0.12	0.03	0.1
(1,1031)	1:80:A:MET:HE1	2:104:A:HEC:HBA2	3	0.49	0.24	0.46

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1031)	1:80:A:MET:HE3	2:104:A:HEC:HBA2	3	0.49	0.24	0.46
(1,1031)	1:80:A:MET:HE2	2:104:A:HEC:HBB1	3	0.49	0.24	0.46
(1,560)	1:42:A:GLN:HB2	1:42:A:GLN:H	3	0.27	0.01	0.27
(1,489)	1:35:A:ILE:HG21	2:104:A:HEC:HAA1	3	0.23	0.02	0.22
(1,489)	1:35:A:ILE:HG22	2:104:A:HEC:HAA1	3	0.23	0.02	0.22
(1,489)	1:35:A:ILE:HG23	2:104:A:HEC:HAA1	3	0.23	0.02	0.22
(1,1313)	1:101:A:ALA:HB1	1:20:A:VAL:H	3	0.15	0.03	0.16
(1,1313)	1:101:A:ALA:HB2	1:20:A:VAL:H	3	0.15	0.03	0.16
(1,1313)	1:101:A:ALA:HB3	1:20:A:VAL:H	3	0.15	0.03	0.16
(1,653)	1:51:A:ALA:HB1	1:78:A:THR:H	3	0.14	0.03	0.13
(1,653)	1:51:A:ALA:HB2	1:78:A:THR:H	3	0.14	0.03	0.13
(1,653)	1:51:A:ALA:HB3	1:78:A:THR:H	3	0.14	0.03	0.13
(1,460)	1:33:A:HIS:HD2	1:34:A:GLY:H	3	0.13	0.03	0.12
(1,932)	1:71:A:HIS:HB3	1:71:A:HIS:H	3	0.12	0.01	0.11
(1,482)	1:35:A:ILE:HD11	1:59:A:TRP:HH2	3	0.12	0.01	0.11
(1,482)	1:35:A:ILE:HD12	1:59:A:TRP:HH2	3	0.12	0.01	0.11
(1,482)	1:35:A:ILE:HD13	1:59:A:TRP:HH2	3	0.12	0.01	0.11
(1,370)	1:28:A:VAL:HA	1:46:A:TYR:HD1	3	0.1	0.0	0.1
(1,370)	1:28:A:VAL:HA	1:46:A:TYR:HD2	3	0.1	0.0	0.1
(1,418)	1:32:A:LEU:HA	1:34:A:GLY:H	2	0.19	0.04	0.19
(1,315)	1:22:A:LYS:HD2	1:23:A:GLY:H	2	0.18	0.02	0.18
(1,315)	1:22:A:LYS:HD3	1:23:A:GLY:H	2	0.18	0.02	0.18
(1,108)	1:8:A:THR:HG21	1:8:A:THR:HA	2	0.17	0.01	0.17
(1,108)	1:8:A:THR:HG22	1:8:A:THR:HA	2	0.17	0.01	0.17
(1,108)	1:8:A:THR:HG23	1:8:A:THR:HA	2	0.17	0.01	0.17
(1,267)	1:19:A:THR:HG21	1:21:A:GLU:H	2	0.15	0.02	0.15
(1,267)	1:19:A:THR:HG22	1:21:A:GLU:H	2	0.15	0.02	0.15
(1,267)	1:19:A:THR:HG23	1:21:A:GLU:H	2	0.15	0.02	0.15
(1,945)	1:71:A:HIS:HB2	1:74:A:TYR:HE1	2	0.13	0.0	0.13
(1,945)	1:71:A:HIS:HB2	1:74:A:TYR:HE2	2	0.13	0.0	0.13
(1,945)	1:71:A:HIS:HB3	1:74:A:TYR:HE1	2	0.13	0.0	0.13
(1,945)	1:71:A:HIS:HB3	1:74:A:TYR:HE2	2	0.13	0.0	0.13
(1,293)	1:21:A:GLU:H	1:20:A:VAL:H	2	0.12	0.02	0.12
(1,954)	1:72:A:ALA:HA	1:78:A:THR:HG21	2	0.12	0.0	0.12
(1,954)	1:72:A:ALA:HA	1:78:A:THR:HG22	2	0.12	0.0	0.12
(1,954)	1:72:A:ALA:HA	1:78:A:THR:HG23	2	0.12	0.0	0.12
(1,235)	1:16:A:GLN:HG3	1:18:A:HIS:H	2	0.11	0.01	0.11
(1,121)	1:8:A:THR:HG21	1:9:A:LEU:H	2	0.11	0.0	0.11
(1,121)	1:8:A:THR:HG22	1:9:A:LEU:H	2	0.11	0.0	0.11
(1,121)	1:8:A:THR:HG23	1:9:A:LEU:H	2	0.11	0.0	0.11
(1,483)	1:35:A:ILE:HD11	1:36:A:PHE:HZ	2	0.11	0.0	0.11
(1,483)	1:35:A:ILE:HD12	1:36:A:PHE:HZ	2	0.11	0.0	0.11

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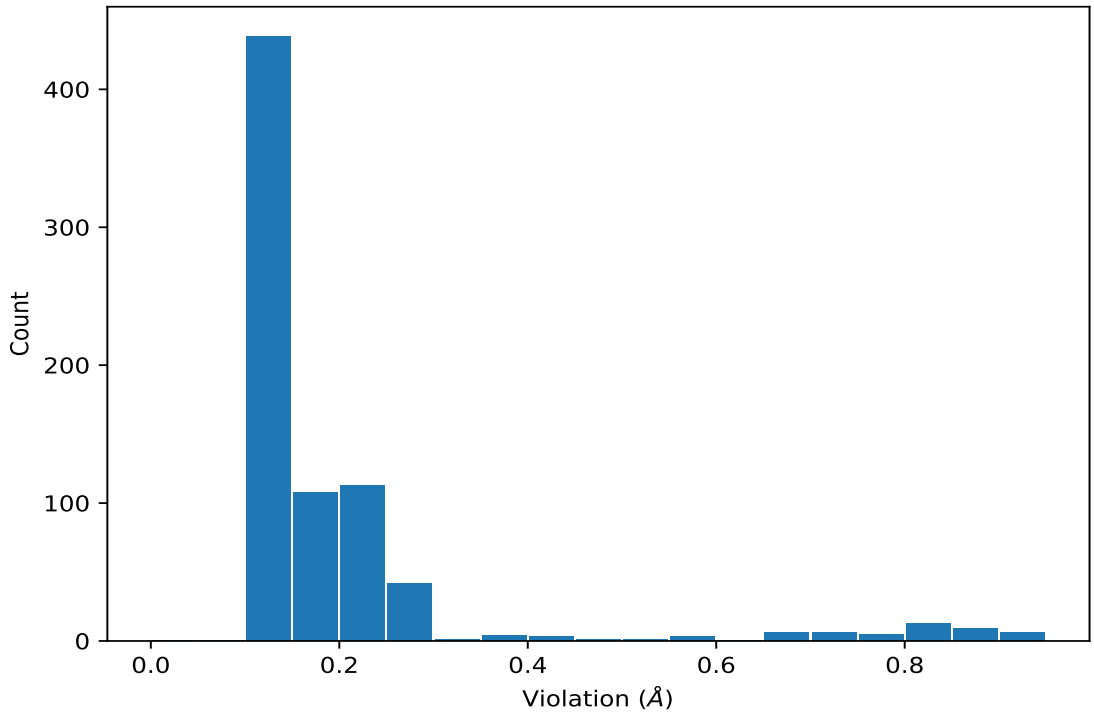
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,483)	1:35:A:ILE:HD13	1:36:A:PHE:HZ	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	13	0.94
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	13	0.94
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	13	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	1	0.91
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	1	0.91
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	1	0.91
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	15	0.88
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	15	0.88
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	15	0.88
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	10	0.86
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	10	0.86
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	10	0.86
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	4	0.85
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	4	0.85
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	4	0.85
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	12	0.84
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	12	0.84
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	12	0.84
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	18	0.84
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	18	0.84
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	18	0.84
(1,1354)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	5	0.83
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	2	0.83
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	2	0.83
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	2	0.83
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	5	0.82
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	5	0.82
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	5	0.82
(1,1354)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	14	0.79
(1,1031)	1:80:A:MET:HE2	2:104:A:HEC:HBB1	20	0.79
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	9	0.78
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	9	0.78
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	9	0.78
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	14	0.72
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	14	0.72
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	14	0.72
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	6	0.7
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	6	0.7
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	6	0.7
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	3	0.66
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	3	0.66
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	3	0.66
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	7	0.66
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	7	0.66
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	7	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	8	0.59
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	8	0.59
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	8	0.59
(1,1354)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	13	0.5
(1,1031)	1:80:A:MET:HE3	2:104:A:HEC:HBA2	9	0.46
(1,1354)	2:104:A:HEC:HMA1	1:59:A:TRP:HE3	2	0.42
(1,1354)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	19	0.42
(1,1354)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	17	0.41
(1,1354)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	3	0.39
(1,1354)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	18	0.37
(1,1354)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	15	0.36
(1,1354)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	1	0.35
(1,1354)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	16	0.3
(1,1354)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	12	0.29
(1,1354)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	10	0.28
(1,560)	1:42:A:GLN:HB2	1:42:A:GLN:H	17	0.28
(1,560)	1:42:A:GLN:HB2	1:42:A:GLN:H	9	0.27
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	11	0.26
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	11	0.26
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	11	0.26
(1,560)	1:42:A:GLN:HB2	1:42:A:GLN:H	7	0.26
(1,489)	1:35:A:ILE:HG21	2:104:A:HEC:HAA1	14	0.26
(1,489)	1:35:A:ILE:HG22	2:104:A:HEC:HAA1	14	0.26
(1,489)	1:35:A:ILE:HG23	2:104:A:HEC:HAA1	14	0.26
(1,1354)	2:104:A:HEC:HMA2	1:59:A:TRP:HE3	4	0.25
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	2	0.25
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	2	0.25
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	2	0.25
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	4	0.25
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	4	0.25
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	4	0.25
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	6	0.25
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	6	0.25
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	6	0.25
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	7	0.25
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	7	0.25
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	7	0.25
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	9	0.25
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	9	0.25
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	9	0.25
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	13	0.25
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	13	0.25
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	14	0.25
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	14	0.25
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	14	0.25
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	16	0.25
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	16	0.25
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	16	0.25
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	18	0.25
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	18	0.25
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	18	0.25
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	19	0.25
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	19	0.25
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	19	0.25
(1,1274)	1:98:A:LEU:HD11	1:32:A:LEU:H	13	0.24
(1,1274)	1:98:A:LEU:HD12	1:32:A:LEU:H	13	0.24
(1,1274)	1:98:A:LEU:HD13	1:32:A:LEU:H	13	0.24
(1,1274)	1:98:A:LEU:HD21	1:32:A:LEU:H	13	0.24
(1,1274)	1:98:A:LEU:HD22	1:32:A:LEU:H	13	0.24
(1,1274)	1:98:A:LEU:HD23	1:32:A:LEU:H	13	0.24
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	1	0.24
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	1	0.24
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	1	0.24
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	3	0.24
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	3	0.24
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	3	0.24
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	5	0.24
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	5	0.24
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	5	0.24
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	8	0.24
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	8	0.24
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	8	0.24
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	10	0.24
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	10	0.24
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	10	0.24
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	12	0.24
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	12	0.24
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	12	0.24
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	17	0.24
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	17	0.24
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	17	0.24
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	20	0.24
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	20	0.24
(1,971)	1:74:A:TYR:HD1	1:75:A:ILE:H	11	0.24
(1,971)	1:74:A:TYR:HD2	1:75:A:ILE:H	11	0.24
(1,1186)	1:95:A:ILE:HG21	1:95:A:ILE:H	15	0.23
(1,1186)	1:95:A:ILE:HG22	1:95:A:ILE:H	15	0.23
(1,1186)	1:95:A:ILE:HG23	1:95:A:ILE:H	15	0.23
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	9	0.23
(1,418)	1:32:A:LEU:HA	1:34:A:GLY:H	7	0.23
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	1	0.23
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	1	0.23
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	4	0.23
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	4	0.23
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	6	0.23
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	6	0.23
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	7	0.23
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	7	0.23
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	10	0.23
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	10	0.23
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	12	0.23
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	12	0.23
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	18	0.23
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	18	0.23
(1,971)	1:74:A:TYR:HD1	1:75:A:ILE:H	16	0.22
(1,971)	1:74:A:TYR:HD2	1:75:A:ILE:H	16	0.22
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	4	0.22
(1,580)	1:43:A:ALA:HB1	1:46:A:TYR:HD2	20	0.22
(1,580)	1:43:A:ALA:HB2	1:46:A:TYR:HD2	20	0.22
(1,580)	1:43:A:ALA:HB3	1:46:A:TYR:HD2	20	0.22
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	19	0.22
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	19	0.22
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	19	0.22
(1,489)	1:35:A:ILE:HG21	2:104:A:HEC:HAA1	3	0.22
(1,489)	1:35:A:ILE:HG22	2:104:A:HEC:HAA1	3	0.22
(1,489)	1:35:A:ILE:HG23	2:104:A:HEC:HAA1	3	0.22
(1,489)	1:35:A:ILE:HG21	2:104:A:HEC:HAA1	5	0.22
(1,489)	1:35:A:ILE:HG22	2:104:A:HEC:HAA1	5	0.22
(1,489)	1:35:A:ILE:HG23	2:104:A:HEC:HAA1	5	0.22
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	2	0.22
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	2	0.22
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	8	0.22
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	8	0.22
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	9	0.22
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	14	0.22
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	14	0.22
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	15	0.22
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	15	0.22
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	16	0.22
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	16	0.22
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	17	0.22
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	17	0.22
(1,1031)	1:80:A:MET:HE1	2:104:A:HEC:HBA2	8	0.21
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	1	0.21
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	3	0.21
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	3	0.21
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	5	0.21
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	5	0.21
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	11	0.21
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	11	0.21
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	13	0.21
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	13	0.21
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	20	0.21
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	20	0.21
(1,1354)	2:104:A:HEC:HMA1	1:59:A:TRP:HE3	6	0.2
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	14	0.2
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	14	0.2
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	14	0.2
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	14	0.2
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	14	0.2
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	14	0.2
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	16	0.2
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	16	0.2
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	16	0.2
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	16	0.2
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	16	0.2
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	16	0.2
(1,766)	1:58:A:LEU:HG	1:37:A:GLY:H	6	0.2
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	17	0.2
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	17	0.2
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	17	0.2
(1,315)	1:22:A:LYS:HD2	1:23:A:GLY:H	12	0.2
(1,315)	1:22:A:LYS:HD3	1:23:A:GLY:H	12	0.2
(1,61)	1:4:A:LYS:HG2	1:5:A:LYS:H	19	0.2
(1,61)	1:4:A:LYS:HG3	1:5:A:LYS:H	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,627)	1:49:A:THR:HG21	1:52:A:ASN:H	3	0.19
(1,627)	1:49:A:THR:HG22	1:52:A:ASN:H	3	0.19
(1,627)	1:49:A:THR:HG23	1:52:A:ASN:H	3	0.19
(1,568)	1:42:A:GLN:HE21	1:39:A:HIS:H	9	0.19
(1,568)	1:42:A:GLN:HE22	1:39:A:HIS:H	9	0.19
(1,539)	1:40:A:SER:HB2	1:40:A:SER:H	18	0.19
(1,1354)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	11	0.18
(1,1313)	1:101:A:ALA:HB1	1:20:A:VAL:H	14	0.18
(1,1313)	1:101:A:ALA:HB2	1:20:A:VAL:H	14	0.18
(1,1313)	1:101:A:ALA:HB3	1:20:A:VAL:H	14	0.18
(1,971)	1:74:A:TYR:HD1	1:75:A:ILE:H	20	0.18
(1,971)	1:74:A:TYR:HD2	1:75:A:ILE:H	20	0.18
(1,965)	1:74:A:TYR:HA	1:74:A:TYR:HD1	2	0.18
(1,965)	1:74:A:TYR:HA	1:74:A:TYR:HD2	2	0.18
(1,965)	1:74:A:TYR:HA	1:74:A:TYR:HD1	8	0.18
(1,965)	1:74:A:TYR:HA	1:74:A:TYR:HD2	8	0.18
(1,653)	1:51:A:ALA:HB1	1:78:A:THR:H	10	0.18
(1,653)	1:51:A:ALA:HB2	1:78:A:THR:H	10	0.18
(1,653)	1:51:A:ALA:HB3	1:78:A:THR:H	10	0.18
(1,539)	1:40:A:SER:HB2	1:40:A:SER:H	1	0.18
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	5	0.18
(1,205)	1:14:A:CYS:HA	1:18:A:HIS:HB2	10	0.18
(1,205)	1:14:A:CYS:HA	1:18:A:HIS:HB3	10	0.18
(1,108)	1:8:A:THR:HG21	1:8:A:THR:HA	3	0.18
(1,108)	1:8:A:THR:HG22	1:8:A:THR:HA	3	0.18
(1,108)	1:8:A:THR:HG23	1:8:A:THR:HA	3	0.18
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	4	0.17
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	4	0.17
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	4	0.17
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	4	0.17
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	4	0.17
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	4	0.17
(1,1062)	1:85:A:LEU:HB3	1:85:A:LEU:H	16	0.17
(1,965)	1:74:A:TYR:HA	1:74:A:TYR:HD1	19	0.17
(1,965)	1:74:A:TYR:HA	1:74:A:TYR:HD2	19	0.17
(1,861)	1:64:A:MET:HB2	1:60:A:ASP:H	9	0.17
(1,861)	1:64:A:MET:HB3	1:60:A:ASP:H	9	0.17
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	12	0.17
(1,619)	1:49:A:THR:HG21	1:49:A:THR:H	3	0.17
(1,619)	1:49:A:THR:HG22	1:49:A:THR:H	3	0.17
(1,619)	1:49:A:THR:HG23	1:49:A:THR:H	3	0.17
(1,460)	1:33:A:HIS:HD2	1:34:A:GLY:H	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	9	0.17
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	14	0.17
(1,315)	1:22:A:LYS:HD2	1:23:A:GLY:H	8	0.17
(1,315)	1:22:A:LYS:HD3	1:23:A:GLY:H	8	0.17
(1,267)	1:19:A:THR:HG21	1:21:A:GLU:H	8	0.17
(1,267)	1:19:A:THR:HG22	1:21:A:GLU:H	8	0.17
(1,267)	1:19:A:THR:HG23	1:21:A:GLU:H	8	0.17
(1,1313)	1:101:A:ALA:HB1	1:20:A:VAL:H	16	0.16
(1,1313)	1:101:A:ALA:HB2	1:20:A:VAL:H	16	0.16
(1,1313)	1:101:A:ALA:HB3	1:20:A:VAL:H	16	0.16
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	9	0.16
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	9	0.16
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	9	0.16
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	9	0.16
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	9	0.16
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	9	0.16
(1,965)	1:74:A:TYR:HA	1:74:A:TYR:HD1	17	0.16
(1,965)	1:74:A:TYR:HA	1:74:A:TYR:HD2	17	0.16
(1,861)	1:64:A:MET:HB2	1:60:A:ASP:H	20	0.16
(1,861)	1:64:A:MET:HB3	1:60:A:ASP:H	20	0.16
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	14	0.16
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	6	0.16
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	6	0.16
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	10	0.16
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	10	0.16
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	14	0.16
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	14	0.16
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	7	0.16
(1,376)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	16	0.16
(1,376)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	16	0.16
(1,108)	1:8:A:THR:HG21	1:8:A:THR:HA	7	0.16
(1,108)	1:8:A:THR:HG22	1:8:A:THR:HA	7	0.16
(1,108)	1:8:A:THR:HG23	1:8:A:THR:HA	7	0.16
(1,965)	1:74:A:TYR:HA	1:74:A:TYR:HD1	3	0.15
(1,965)	1:74:A:TYR:HA	1:74:A:TYR:HD2	3	0.15
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	2	0.15
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	8	0.15
(1,627)	1:49:A:THR:HG21	1:52:A:ASN:H	16	0.15
(1,627)	1:49:A:THR:HG22	1:52:A:ASN:H	16	0.15
(1,627)	1:49:A:THR:HG23	1:52:A:ASN:H	16	0.15
(1,619)	1:49:A:THR:HG21	1:49:A:THR:H	1	0.15
(1,619)	1:49:A:THR:HG22	1:49:A:THR:H	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	1:49:A:THR:HG23	1:49:A:THR:H	1	0.15
(1,619)	1:49:A:THR:HG21	1:49:A:THR:H	14	0.15
(1,619)	1:49:A:THR:HG22	1:49:A:THR:H	14	0.15
(1,619)	1:49:A:THR:HG23	1:49:A:THR:H	14	0.15
(1,619)	1:49:A:THR:HG21	1:49:A:THR:H	18	0.15
(1,619)	1:49:A:THR:HG22	1:49:A:THR:H	18	0.15
(1,619)	1:49:A:THR:HG23	1:49:A:THR:H	18	0.15
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	16	0.15
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	16	0.15
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	16	0.15
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	1	0.15
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	1	0.15
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	4	0.15
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	4	0.15
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	12	0.15
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	12	0.15
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	15	0.15
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	15	0.15
(1,535)	1:39:A:HIS:HA	1:59:A:TRP:HD1	5	0.15
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	3	0.15
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	19	0.15
(1,418)	1:32:A:LEU:HA	1:34:A:GLY:H	18	0.15
(1,268)	1:19:A:THR:HA	1:17:A:CYS:H	7	0.15
(1,203)	1:14:A:CYS:HA	1:15:A:LEU:HG	1	0.15
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	10	0.14
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	10	0.14
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	10	0.14
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	10	0.14
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	10	0.14
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	10	0.14
(1,1087)	1:87:A:LYS:HB2	1:90:A:ASP:HB2	6	0.14
(1,1087)	1:87:A:LYS:HB2	1:90:A:ASP:HB3	6	0.14
(1,1087)	1:87:A:LYS:HB3	1:90:A:ASP:HB2	6	0.14
(1,1087)	1:87:A:LYS:HB3	1:90:A:ASP:HB3	6	0.14
(1,971)	1:74:A:TYR:HD1	1:75:A:ILE:H	10	0.14
(1,971)	1:74:A:TYR:HD2	1:75:A:ILE:H	10	0.14
(1,932)	1:71:A:HIS:HB3	1:71:A:HIS:H	16	0.14
(1,861)	1:64:A:MET:HB2	1:60:A:ASP:H	14	0.14
(1,861)	1:64:A:MET:HB3	1:60:A:ASP:H	14	0.14
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	18	0.14
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD11	5	0.14
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD12	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD13	5	0.14
(1,568)	1:42:A:GLN:HE21	1:39:A:HIS:H	17	0.14
(1,568)	1:42:A:GLN:HE22	1:39:A:HIS:H	17	0.14
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	8	0.14
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	8	0.14
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	13	0.14
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	13	0.14
(1,412)	1:32:A:LEU:HD11	1:32:A:LEU:H	7	0.14
(1,412)	1:32:A:LEU:HD12	1:32:A:LEU:H	7	0.14
(1,412)	1:32:A:LEU:HD13	1:32:A:LEU:H	7	0.14
(1,412)	1:32:A:LEU:HD21	1:32:A:LEU:H	7	0.14
(1,412)	1:32:A:LEU:HD22	1:32:A:LEU:H	7	0.14
(1,412)	1:32:A:LEU:HD23	1:32:A:LEU:H	7	0.14
(1,376)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	5	0.14
(1,376)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	5	0.14
(1,376)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	7	0.14
(1,376)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	7	0.14
(1,268)	1:19:A:THR:HA	1:17:A:CYS:H	16	0.14
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	5	0.13
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	5	0.13
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	5	0.13
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	5	0.13
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	5	0.13
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	5	0.13
(1,971)	1:74:A:TYR:HD1	1:75:A:ILE:H	1	0.13
(1,971)	1:74:A:TYR:HD2	1:75:A:ILE:H	1	0.13
(1,971)	1:74:A:TYR:HD1	1:75:A:ILE:H	9	0.13
(1,971)	1:74:A:TYR:HD2	1:75:A:ILE:H	9	0.13
(1,971)	1:74:A:TYR:HD1	1:75:A:ILE:H	18	0.13
(1,971)	1:74:A:TYR:HD2	1:75:A:ILE:H	18	0.13
(1,971)	1:74:A:TYR:HD1	1:75:A:ILE:H	19	0.13
(1,971)	1:74:A:TYR:HD2	1:75:A:ILE:H	19	0.13
(1,945)	1:71:A:HIS:HB2	1:74:A:TYR:HE1	9	0.13
(1,945)	1:71:A:HIS:HB2	1:74:A:TYR:HE2	9	0.13
(1,945)	1:71:A:HIS:HB3	1:74:A:TYR:HE1	9	0.13
(1,945)	1:71:A:HIS:HB3	1:74:A:TYR:HE2	9	0.13
(1,945)	1:71:A:HIS:HB2	1:74:A:TYR:HE1	16	0.13
(1,945)	1:71:A:HIS:HB2	1:74:A:TYR:HE2	16	0.13
(1,945)	1:71:A:HIS:HB3	1:74:A:TYR:HE1	16	0.13
(1,945)	1:71:A:HIS:HB3	1:74:A:TYR:HE2	16	0.13
(1,840)	1:63:A:ASN:HD22	1:60:A:ASP:H	3	0.13
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	7	0.13
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	17	0.13
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	1	0.13
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	1	0.13
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	1	0.13
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	1	0.13
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	1	0.13
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	1	0.13
(1,653)	1:51:A:ALA:HB1	1:78:A:THR:H	14	0.13
(1,653)	1:51:A:ALA:HB2	1:78:A:THR:H	14	0.13
(1,653)	1:51:A:ALA:HB3	1:78:A:THR:H	14	0.13
(1,580)	1:43:A:ALA:HB1	1:46:A:TYR:HD2	11	0.13
(1,580)	1:43:A:ALA:HB2	1:46:A:TYR:HD2	11	0.13
(1,580)	1:43:A:ALA:HB3	1:46:A:TYR:HD2	11	0.13
(1,579)	1:43:A:ALA:HB1	1:48:A:TYR:HD2	20	0.13
(1,579)	1:43:A:ALA:HB2	1:48:A:TYR:HD2	20	0.13
(1,579)	1:43:A:ALA:HB3	1:48:A:TYR:HD2	20	0.13
(1,535)	1:39:A:HIS:HA	1:59:A:TRP:HD1	6	0.13
(1,482)	1:35:A:ILE:HD11	1:59:A:TRP:HH2	9	0.13
(1,482)	1:35:A:ILE:HD12	1:59:A:TRP:HH2	9	0.13
(1,482)	1:35:A:ILE:HD13	1:59:A:TRP:HH2	9	0.13
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	11	0.13
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	12	0.13
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	15	0.13
(1,345)	1:27:A:LYS:H	1:27:A:LYS:HE2	3	0.13
(1,345)	1:27:A:LYS:H	1:27:A:LYS:HE3	3	0.13
(1,293)	1:21:A:GLU:H	1:20:A:VAL:H	4	0.13
(1,267)	1:19:A:THR:HG21	1:21:A:GLU:H	1	0.13
(1,267)	1:19:A:THR:HG22	1:21:A:GLU:H	1	0.13
(1,267)	1:19:A:THR:HG23	1:21:A:GLU:H	1	0.13
(1,120)	1:8:A:THR:HB	1:9:A:LEU:H	4	0.13
(1,120)	1:8:A:THR:HB	1:9:A:LEU:H	11	0.13
(1,1324)	1:102:A:THR:HG21	1:36:A:PHE:H	2	0.12
(1,1324)	1:102:A:THR:HG22	1:36:A:PHE:H	2	0.12
(1,1324)	1:102:A:THR:HG23	1:36:A:PHE:H	2	0.12
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	1	0.12
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	1	0.12
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	1	0.12
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	1	0.12
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	1	0.12
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	1	0.12
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	8	0.12
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	8	0.12
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	8	0.12
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	8	0.12
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	8	0.12
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	11	0.12
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	11	0.12
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	11	0.12
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	11	0.12
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	11	0.12
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	11	0.12
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	19	0.12
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	19	0.12
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	19	0.12
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	19	0.12
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	19	0.12
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	19	0.12
(1,1192)	1:95:A:ILE:H	1:-3:A:PHE:HZ	3	0.12
(1,1101)	1:88:A:GLU:HA	1:92:A:ASN:H	6	0.12
(1,971)	1:74:A:TYR:HD1	1:75:A:ILE:H	4	0.12
(1,971)	1:74:A:TYR:HD2	1:75:A:ILE:H	4	0.12
(1,954)	1:72:A:ALA:HA	1:78:A:THR:HG21	12	0.12
(1,954)	1:72:A:ALA:HA	1:78:A:THR:HG22	12	0.12
(1,954)	1:72:A:ALA:HA	1:78:A:THR:HG23	12	0.12
(1,937)	1:71:A:HIS:H	1:73:A:LYS:H	13	0.12
(1,861)	1:64:A:MET:HB2	1:60:A:ASP:H	4	0.12
(1,861)	1:64:A:MET:HB3	1:60:A:ASP:H	4	0.12
(1,761)	1:58:A:LEU:HB3	1:39:A:HIS:HA	2	0.12
(1,752)	1:58:A:LEU:HD11	1:58:A:LEU:H	16	0.12
(1,752)	1:58:A:LEU:HD12	1:58:A:LEU:H	16	0.12
(1,752)	1:58:A:LEU:HD13	1:58:A:LEU:H	16	0.12
(1,752)	1:58:A:LEU:HD21	1:58:A:LEU:H	16	0.12
(1,752)	1:58:A:LEU:HD22	1:58:A:LEU:H	16	0.12
(1,752)	1:58:A:LEU:HD23	1:58:A:LEU:H	16	0.12
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	10	0.12
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	15	0.12
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	16	0.12
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	16	0.12
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	16	0.12
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	16	0.12
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	16	0.12
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	16	0.12
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD11	7	0.12
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD12	7	0.12
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD13	7	0.12
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD11	10	0.12
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD12	10	0.12
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD13	10	0.12
(1,653)	1:51:A:ALA:HB1	1:78:A:THR:H	17	0.12
(1,653)	1:51:A:ALA:HB2	1:78:A:THR:H	17	0.12
(1,653)	1:51:A:ALA:HB3	1:78:A:THR:H	17	0.12
(1,627)	1:49:A:THR:HG21	1:52:A:ASN:H	2	0.12
(1,627)	1:49:A:THR:HG22	1:52:A:ASN:H	2	0.12
(1,627)	1:49:A:THR:HG23	1:52:A:ASN:H	2	0.12
(1,627)	1:49:A:THR:HG21	1:52:A:ASN:H	6	0.12
(1,627)	1:49:A:THR:HG22	1:52:A:ASN:H	6	0.12
(1,627)	1:49:A:THR:HG23	1:52:A:ASN:H	6	0.12
(1,627)	1:49:A:THR:HG21	1:52:A:ASN:H	7	0.12
(1,627)	1:49:A:THR:HG22	1:52:A:ASN:H	7	0.12
(1,627)	1:49:A:THR:HG23	1:52:A:ASN:H	7	0.12
(1,580)	1:43:A:ALA:HB1	1:46:A:TYR:HD2	16	0.12
(1,580)	1:43:A:ALA:HB2	1:46:A:TYR:HD2	16	0.12
(1,580)	1:43:A:ALA:HB3	1:46:A:TYR:HD2	16	0.12
(1,580)	1:43:A:ALA:HB1	1:46:A:TYR:HD2	19	0.12
(1,580)	1:43:A:ALA:HB2	1:46:A:TYR:HD2	19	0.12
(1,580)	1:43:A:ALA:HB3	1:46:A:TYR:HD2	19	0.12
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	19	0.12
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	19	0.12
(1,539)	1:40:A:SER:HB2	1:40:A:SER:H	13	0.12
(1,539)	1:40:A:SER:HB2	1:40:A:SER:H	20	0.12
(1,522)	1:38:A:ARG:HG2	1:42:A:GLN:HG2	1	0.12
(1,522)	1:38:A:ARG:HG2	1:42:A:GLN:HG3	1	0.12
(1,522)	1:38:A:ARG:HG3	1:42:A:GLN:HG2	1	0.12
(1,522)	1:38:A:ARG:HG3	1:42:A:GLN:HG3	1	0.12
(1,460)	1:33:A:HIS:HD2	1:34:A:GLY:H	7	0.12
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	8	0.12
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	10	0.12
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	20	0.12
(1,427)	1:32:A:LEU:HD11	1:18:A:HIS:HD2	7	0.12
(1,427)	1:32:A:LEU:HD12	1:18:A:HIS:HD2	7	0.12
(1,427)	1:32:A:LEU:HD13	1:18:A:HIS:HD2	7	0.12
(1,376)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	3	0.12
(1,376)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	8	0.12
(1,376)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	8	0.12
(1,287)	1:20:A:VAL:HG11	1:18:A:HIS:HD1	7	0.12
(1,287)	1:20:A:VAL:HG12	1:18:A:HIS:HD1	7	0.12
(1,287)	1:20:A:VAL:HG13	1:18:A:HIS:HD1	7	0.12
(1,287)	1:20:A:VAL:HG21	1:18:A:HIS:HD1	7	0.12
(1,287)	1:20:A:VAL:HG22	1:18:A:HIS:HD1	7	0.12
(1,287)	1:20:A:VAL:HG23	1:18:A:HIS:HD1	7	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	1	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	2	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	3	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	6	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	7	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	8	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	9	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	10	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	11	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	13	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	14	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	15	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	16	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	17	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	18	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	19	0.12
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	20	0.12
(1,235)	1:16:A:GLN:HG3	1:18:A:HIS:H	5	0.12
(1,215)	1:15:A:LEU:HD11	1:15:A:LEU:H	12	0.12
(1,215)	1:15:A:LEU:HD12	1:15:A:LEU:H	12	0.12
(1,215)	1:15:A:LEU:HD13	1:15:A:LEU:H	12	0.12
(1,215)	1:15:A:LEU:HD21	1:15:A:LEU:H	12	0.12
(1,215)	1:15:A:LEU:HD22	1:15:A:LEU:H	12	0.12
(1,215)	1:15:A:LEU:HD23	1:15:A:LEU:H	12	0.12
(1,120)	1:8:A:THR:HB	1:9:A:LEU:H	1	0.12
(1,7)	1:-3:A:PHE:HD1	1:96:A:THR:H	16	0.12
(1,7)	1:-3:A:PHE:HD2	1:96:A:THR:H	16	0.12
(1,1354)	2:104:A:HEC:HMA3	1:59:A:TRP:HE3	20	0.11
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	3	0.11
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	3	0.11
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	3	0.11
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	3	0.11
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	3	0.11
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	18	0.11
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	18	0.11
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	18	0.11
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	18	0.11
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	18	0.11
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	18	0.11
(1,1027)	1:80:A:MET:HE1	1:82:A:PHE:HE1	20	0.11
(1,1027)	1:80:A:MET:HE1	1:82:A:PHE:HE2	20	0.11
(1,1027)	1:80:A:MET:HE2	1:82:A:PHE:HE1	20	0.11
(1,1027)	1:80:A:MET:HE2	1:82:A:PHE:HE2	20	0.11
(1,1027)	1:80:A:MET:HE3	1:82:A:PHE:HE1	20	0.11
(1,1027)	1:80:A:MET:HE3	1:82:A:PHE:HE2	20	0.11
(1,993)	1:76:A:PRO:HG2	2:104:A:HEC:HHA	5	0.11
(1,993)	1:76:A:PRO:HG3	2:104:A:HEC:HHA	5	0.11
(1,971)	1:74:A:TYR:HD1	1:75:A:ILE:H	5	0.11
(1,971)	1:74:A:TYR:HD2	1:75:A:ILE:H	5	0.11
(1,971)	1:74:A:TYR:HD1	1:75:A:ILE:H	7	0.11
(1,971)	1:74:A:TYR:HD2	1:75:A:ILE:H	7	0.11
(1,954)	1:72:A:ALA:HA	1:78:A:THR:HG21	17	0.11
(1,954)	1:72:A:ALA:HA	1:78:A:THR:HG22	17	0.11
(1,954)	1:72:A:ALA:HA	1:78:A:THR:HG23	17	0.11
(1,932)	1:71:A:HIS:HB3	1:71:A:HIS:H	13	0.11
(1,932)	1:71:A:HIS:HB3	1:71:A:HIS:H	18	0.11
(1,907)	1:68:A:LEU:HG	1:69:A:THR:H	13	0.11
(1,788)	1:59:A:TRP:HZ3	2:104:A:HEC:HAA1	5	0.11
(1,779)	1:58:A:LEU:HD11	1:56:A:ASN:HD21	1	0.11
(1,779)	1:58:A:LEU:HD11	1:56:A:ASN:HD22	1	0.11
(1,779)	1:58:A:LEU:HD12	1:56:A:ASN:HD21	1	0.11
(1,779)	1:58:A:LEU:HD12	1:56:A:ASN:HD22	1	0.11
(1,779)	1:58:A:LEU:HD13	1:56:A:ASN:HD21	1	0.11
(1,779)	1:58:A:LEU:HD13	1:56:A:ASN:HD22	1	0.11
(1,779)	1:58:A:LEU:HD21	1:56:A:ASN:HD21	1	0.11
(1,779)	1:58:A:LEU:HD21	1:56:A:ASN:HD22	1	0.11
(1,779)	1:58:A:LEU:HD22	1:56:A:ASN:HD21	1	0.11
(1,779)	1:58:A:LEU:HD22	1:56:A:ASN:HD22	1	0.11
(1,779)	1:58:A:LEU:HD23	1:56:A:ASN:HD21	1	0.11
(1,779)	1:58:A:LEU:HD23	1:56:A:ASN:HD22	1	0.11
(1,775)	1:58:A:LEU:HD11	1:56:A:ASN:HD21	1	0.11
(1,775)	1:58:A:LEU:HD11	1:56:A:ASN:HD22	1	0.11
(1,775)	1:58:A:LEU:HD12	1:56:A:ASN:HD21	1	0.11
(1,775)	1:58:A:LEU:HD12	1:56:A:ASN:HD22	1	0.11
(1,775)	1:58:A:LEU:HD13	1:56:A:ASN:HD21	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,775)	1:58:A:LEU:HD13	1:56:A:ASN:HD22	1	0.11
(1,775)	1:58:A:LEU:HD21	1:56:A:ASN:HD21	1	0.11
(1,775)	1:58:A:LEU:HD21	1:56:A:ASN:HD22	1	0.11
(1,775)	1:58:A:LEU:HD22	1:56:A:ASN:HD21	1	0.11
(1,775)	1:58:A:LEU:HD22	1:56:A:ASN:HD22	1	0.11
(1,775)	1:58:A:LEU:HD23	1:56:A:ASN:HD21	1	0.11
(1,775)	1:58:A:LEU:HD23	1:56:A:ASN:HD22	1	0.11
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	3	0.11
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	13	0.11
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	19	0.11
(1,670)	1:52:A:ASN:HA	1:59:A:TRP:HE1	20	0.11
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	6	0.11
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	6	0.11
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	6	0.11
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	6	0.11
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	6	0.11
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	6	0.11
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	9	0.11
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	9	0.11
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	9	0.11
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	9	0.11
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	9	0.11
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	9	0.11
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	10	0.11
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	10	0.11
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	10	0.11
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	10	0.11
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	10	0.11
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	10	0.11
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD11	13	0.11
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD12	13	0.11
(1,668)	1:52:A:ASN:HA	1:75:A:ILE:HD13	13	0.11
(1,644)	1:51:A:ALA:HA	1:52:A:ASN:H	9	0.11
(1,619)	1:49:A:THR:HG21	1:49:A:THR:H	2	0.11
(1,619)	1:49:A:THR:HG22	1:49:A:THR:H	2	0.11
(1,619)	1:49:A:THR:HG23	1:49:A:THR:H	2	0.11
(1,568)	1:42:A:GLN:HE21	1:39:A:HIS:H	7	0.11
(1,568)	1:42:A:GLN:HE22	1:39:A:HIS:H	7	0.11
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	7	0.11
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	7	0.11
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	9	0.11
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	17	0.11
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	17	0.11
(1,539)	1:40:A:SER:HB2	1:40:A:SER:H	2	0.11
(1,539)	1:40:A:SER:HB2	1:40:A:SER:H	8	0.11
(1,535)	1:39:A:HIS:HA	1:59:A:TRP:HD1	3	0.11
(1,529)	1:39:A:HIS:H	1:38:A:ARG:HB3	16	0.11
(1,529)	1:39:A:HIS:H	1:38:A:ARG:HB2	16	0.11
(1,485)	1:35:A:ILE:HG12	1:36:A:PHE:HE1	14	0.11
(1,485)	1:35:A:ILE:HG12	1:36:A:PHE:HE2	14	0.11
(1,485)	1:35:A:ILE:HG13	1:36:A:PHE:HE1	14	0.11
(1,485)	1:35:A:ILE:HG13	1:36:A:PHE:HE2	14	0.11
(1,483)	1:35:A:ILE:HD11	1:36:A:PHE:HZ	16	0.11
(1,483)	1:35:A:ILE:HD12	1:36:A:PHE:HZ	16	0.11
(1,483)	1:35:A:ILE:HD13	1:36:A:PHE:HZ	16	0.11
(1,482)	1:35:A:ILE:HD11	1:59:A:TRP:HH2	7	0.11
(1,482)	1:35:A:ILE:HD12	1:59:A:TRP:HH2	7	0.11
(1,482)	1:35:A:ILE:HD13	1:59:A:TRP:HH2	7	0.11
(1,482)	1:35:A:ILE:HD11	1:59:A:TRP:HH2	16	0.11
(1,482)	1:35:A:ILE:HD12	1:59:A:TRP:HH2	16	0.11
(1,482)	1:35:A:ILE:HD13	1:59:A:TRP:HH2	16	0.11
(1,460)	1:33:A:HIS:HD2	1:34:A:GLY:H	12	0.11
(1,376)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	1	0.11
(1,376)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	1	0.11
(1,376)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	19	0.11
(1,376)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	19	0.11
(1,370)	1:28:A:VAL:HA	1:46:A:TYR:HD1	16	0.11
(1,370)	1:28:A:VAL:HA	1:46:A:TYR:HD2	16	0.11
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	4	0.11
(1,274)	1:20:A:VAL:HB	1:20:A:VAL:HA	5	0.11
(1,268)	1:19:A:THR:HA	1:17:A:CYS:H	15	0.11
(1,121)	1:8:A:THR:HG21	1:9:A:LEU:H	12	0.11
(1,121)	1:8:A:THR:HG22	1:9:A:LEU:H	12	0.11
(1,121)	1:8:A:THR:HG23	1:9:A:LEU:H	12	0.11
(1,120)	1:8:A:THR:HB	1:9:A:LEU:H	6	0.11
(1,120)	1:8:A:THR:HB	1:9:A:LEU:H	8	0.11
(1,120)	1:8:A:THR:HB	1:9:A:LEU:H	10	0.11
(1,120)	1:8:A:THR:HB	1:9:A:LEU:H	15	0.11
(1,120)	1:8:A:THR:HB	1:9:A:LEU:H	16	0.11
(1,120)	1:8:A:THR:HB	1:9:A:LEU:H	17	0.11
(1,120)	1:8:A:THR:HB	1:9:A:LEU:H	18	0.11
(1,1313)	1:101:A:ALA:HB1	1:20:A:VAL:H	3	0.1
(1,1313)	1:101:A:ALA:HB2	1:20:A:VAL:H	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:101:A:ALA:HB3	1:20:A:VAL:H	3	0.1
(1,1275)	1:98:A:LEU:HD11	1:33:A:HIS:HE1	12	0.1
(1,1275)	1:98:A:LEU:HD12	1:33:A:HIS:HE1	12	0.1
(1,1275)	1:98:A:LEU:HD13	1:33:A:HIS:HE1	12	0.1
(1,1275)	1:98:A:LEU:HD21	1:33:A:HIS:HE1	12	0.1
(1,1275)	1:98:A:LEU:HD22	1:33:A:HIS:HE1	12	0.1
(1,1275)	1:98:A:LEU:HD23	1:33:A:HIS:HE1	12	0.1
(1,992)	1:76:A:PRO:HG2	1:59:A:TRP:HE1	17	0.1
(1,992)	1:76:A:PRO:HG3	1:59:A:TRP:HE1	17	0.1
(1,971)	1:74:A:TYR:HD1	1:75:A:ILE:H	6	0.1
(1,971)	1:74:A:TYR:HD2	1:75:A:ILE:H	6	0.1
(1,938)	1:71:A:HIS:H	1:74:A:TYR:HD1	13	0.1
(1,938)	1:71:A:HIS:H	1:74:A:TYR:HD2	13	0.1
(1,861)	1:64:A:MET:HB2	1:60:A:ASP:H	18	0.1
(1,861)	1:64:A:MET:HB3	1:60:A:ASP:H	18	0.1
(1,791)	1:59:A:TRP:HZ2	1:64:A:MET:HE1	7	0.1
(1,791)	1:59:A:TRP:HZ2	1:64:A:MET:HE2	7	0.1
(1,791)	1:59:A:TRP:HZ2	1:64:A:MET:HE3	7	0.1
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG21	13	0.1
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG22	13	0.1
(1,669)	1:52:A:ASN:HB2	1:75:A:ILE:HG23	13	0.1
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG21	13	0.1
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG22	13	0.1
(1,669)	1:52:A:ASN:HB3	1:75:A:ILE:HG23	13	0.1
(1,644)	1:51:A:ALA:HA	1:52:A:ASN:H	2	0.1
(1,644)	1:51:A:ALA:HA	1:52:A:ASN:H	4	0.1
(1,644)	1:51:A:ALA:HA	1:52:A:ASN:H	5	0.1
(1,644)	1:51:A:ALA:HA	1:52:A:ASN:H	7	0.1
(1,644)	1:51:A:ALA:HA	1:52:A:ASN:H	8	0.1
(1,644)	1:51:A:ALA:HA	1:52:A:ASN:H	15	0.1
(1,627)	1:49:A:THR:HG21	1:52:A:ASN:H	8	0.1
(1,627)	1:49:A:THR:HG22	1:52:A:ASN:H	8	0.1
(1,627)	1:49:A:THR:HG23	1:52:A:ASN:H	8	0.1
(1,627)	1:49:A:THR:HG21	1:52:A:ASN:H	15	0.1
(1,627)	1:49:A:THR:HG22	1:52:A:ASN:H	15	0.1
(1,627)	1:49:A:THR:HG23	1:52:A:ASN:H	15	0.1
(1,627)	1:49:A:THR:HG21	1:52:A:ASN:H	19	0.1
(1,627)	1:49:A:THR:HG22	1:52:A:ASN:H	19	0.1
(1,627)	1:49:A:THR:HG23	1:52:A:ASN:H	19	0.1
(1,619)	1:49:A:THR:HG21	1:49:A:THR:H	4	0.1
(1,619)	1:49:A:THR:HG22	1:49:A:THR:H	4	0.1
(1,619)	1:49:A:THR:HG23	1:49:A:THR:H	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	1:49:A:THR:HG21	1:49:A:THR:H	10	0.1
(1,619)	1:49:A:THR:HG22	1:49:A:THR:H	10	0.1
(1,619)	1:49:A:THR:HG23	1:49:A:THR:H	10	0.1
(1,619)	1:49:A:THR:HG21	1:49:A:THR:H	15	0.1
(1,619)	1:49:A:THR:HG22	1:49:A:THR:H	15	0.1
(1,619)	1:49:A:THR:HG23	1:49:A:THR:H	15	0.1
(1,568)	1:42:A:GLN:HE21	1:39:A:HIS:H	12	0.1
(1,568)	1:42:A:GLN:HE22	1:39:A:HIS:H	12	0.1
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE1	16	0.1
(1,566)	1:42:A:GLN:H	1:46:A:TYR:HE2	16	0.1
(1,539)	1:40:A:SER:HB2	1:40:A:SER:H	14	0.1
(1,535)	1:39:A:HIS:HA	1:59:A:TRP:HD1	20	0.1
(1,483)	1:35:A:ILE:HD11	1:36:A:PHE:HZ	8	0.1
(1,483)	1:35:A:ILE:HD12	1:36:A:PHE:HZ	8	0.1
(1,483)	1:35:A:ILE:HD13	1:36:A:PHE:HZ	8	0.1
(1,448)	1:32:A:LEU:HG	1:101:A:ALA:H	1	0.1
(1,376)	1:29:A:GLY:HA2	2:104:A:HEC:HAC	14	0.1
(1,376)	1:29:A:GLY:HA3	2:104:A:HEC:HAC	14	0.1
(1,375)	1:29:A:GLY:HA2	1:46:A:TYR:HB2	13	0.1
(1,375)	1:29:A:GLY:HA2	1:46:A:TYR:HB3	13	0.1
(1,375)	1:29:A:GLY:HA3	1:46:A:TYR:HB2	13	0.1
(1,375)	1:29:A:GLY:HA3	1:46:A:TYR:HB3	13	0.1
(1,370)	1:28:A:VAL:HA	1:46:A:TYR:HD1	8	0.1
(1,370)	1:28:A:VAL:HA	1:46:A:TYR:HD2	8	0.1
(1,370)	1:28:A:VAL:HA	1:46:A:TYR:HD1	20	0.1
(1,370)	1:28:A:VAL:HA	1:46:A:TYR:HD2	20	0.1
(1,317)	1:22:A:LYS:HE2	1:23:A:GLY:H	3	0.1
(1,317)	1:22:A:LYS:HE3	1:23:A:GLY:H	3	0.1
(1,293)	1:21:A:GLU:H	1:20:A:VAL:H	11	0.1
(1,268)	1:19:A:THR:HA	1:17:A:CYS:H	14	0.1
(1,235)	1:16:A:GLN:HG3	1:18:A:HIS:H	17	0.1
(1,205)	1:14:A:CYS:HA	1:18:A:HIS:HB2	8	0.1
(1,205)	1:14:A:CYS:HA	1:18:A:HIS:HB3	8	0.1
(1,205)	1:14:A:CYS:HA	1:18:A:HIS:HB2	9	0.1
(1,205)	1:14:A:CYS:HA	1:18:A:HIS:HB3	9	0.1
(1,205)	1:14:A:CYS:HA	1:18:A:HIS:HB2	12	0.1
(1,205)	1:14:A:CYS:HA	1:18:A:HIS:HB3	12	0.1
(1,158)	1:10:A:PHE:HZ	1:18:A:HIS:HD1	1	0.1
(1,121)	1:8:A:THR:HG21	1:9:A:LEU:H	8	0.1
(1,121)	1:8:A:THR:HG22	1:9:A:LEU:H	8	0.1
(1,121)	1:8:A:THR:HG23	1:9:A:LEU:H	8	0.1
(1,120)	1:8:A:THR:HB	1:9:A:LEU:H	12	0.1

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found