Full wwPDB NMR Structure Validation Report (i)

May 7, 2025 – 04:33 pm BST

PDB ID	:	9FTD / pdb_00009ftd
BMRB ID	:	34924
Title	:	Solution structure of BmSA1, the major surface antigen from Babesia microti
Authors	:	Barthe, P.; Roumestand, C.; Mouhand, A.; Delbecq, S.
Deposited on	:	2024-06-24

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:

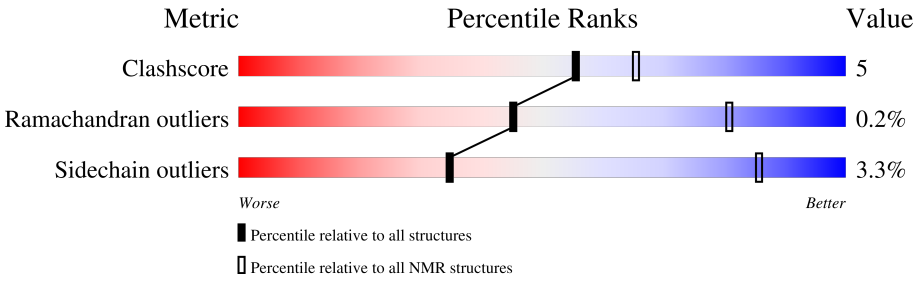
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 81%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	254	86% 8% 6%

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:62-A:136, A:146-A:308 (238)	0.96	20

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

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

The models can be grouped into 5 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3979 atoms, of which 2005 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	254	3979	1214	2005	336	419	5	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	GLY	-	expression tag	UNP A0A0K3AT66
A	56	HIS	-	expression tag	UNP A0A0K3AT66
A	57	MET	-	expression tag	UNP A0A0K3AT66

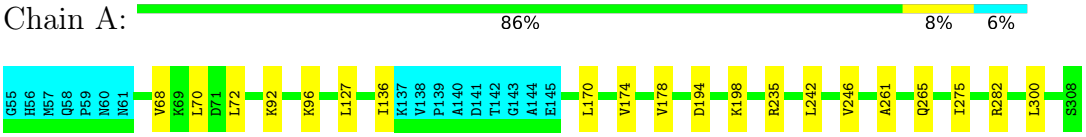
4 Residue-property plots

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: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

Chain A:



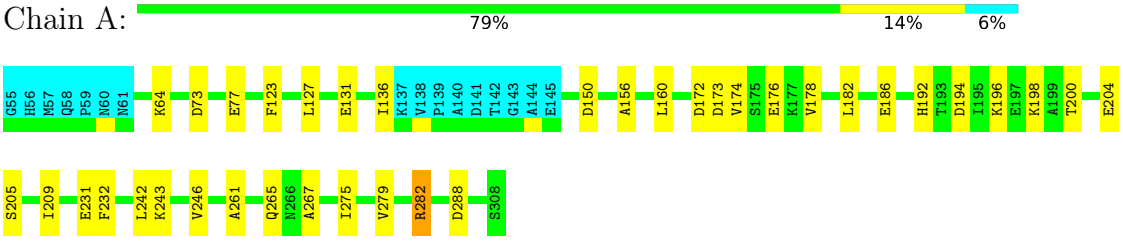
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

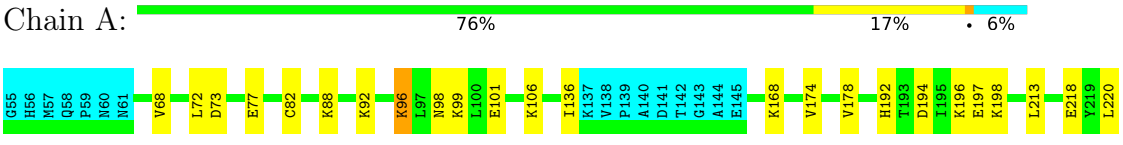
Chain A:

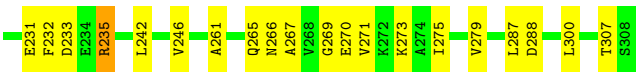


4.2.2 Score per residue for model 2

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

Chain A:

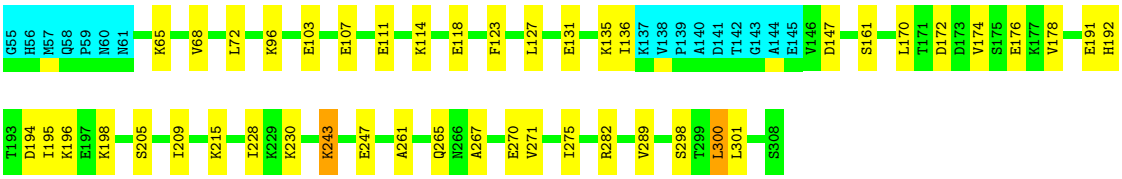




4.2.3 Score per residue for model 3

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

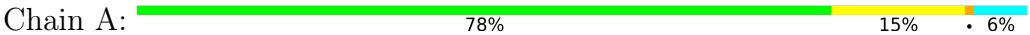
Chain A:

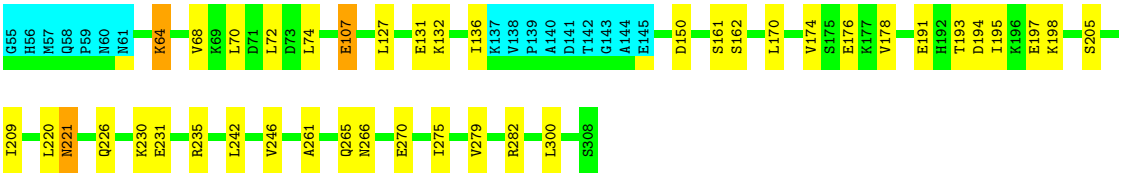


4.2.4 Score per residue for model 4

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

Chain A:

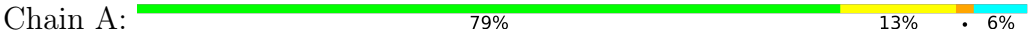


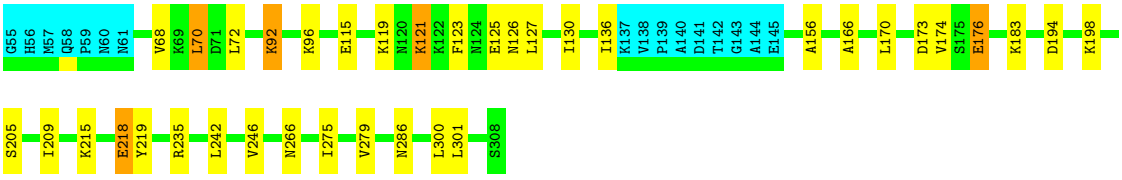


4.2.5 Score per residue for model 5

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

Chain A:

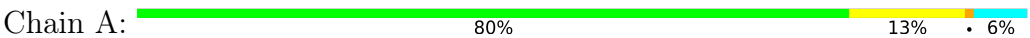


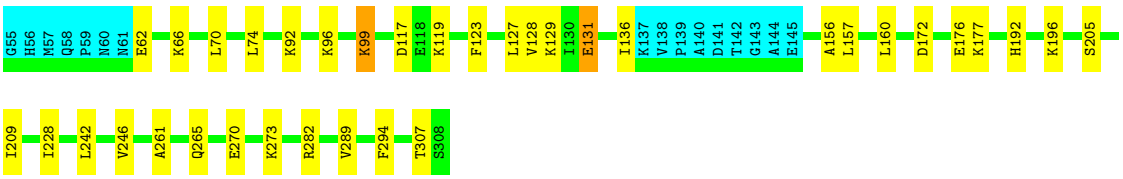


4.2.6 Score per residue for model 6

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

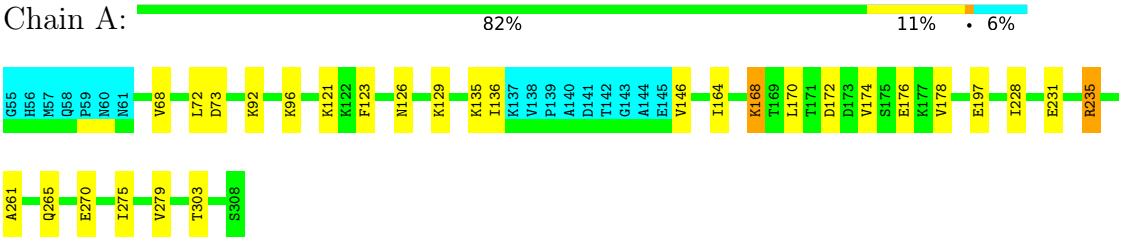
Chain A:





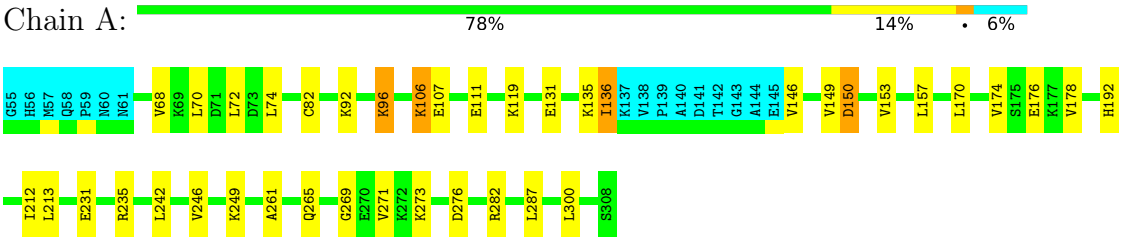
4.2.7 Score per residue for model 7

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue



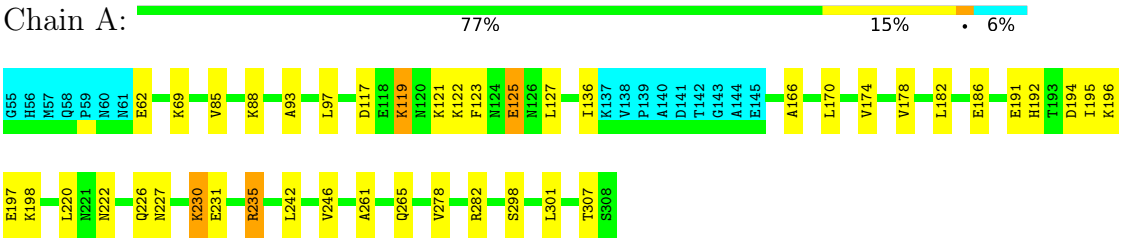
4.2.8 Score per residue for model 8

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue



4.2.9 Score per residue for model 9

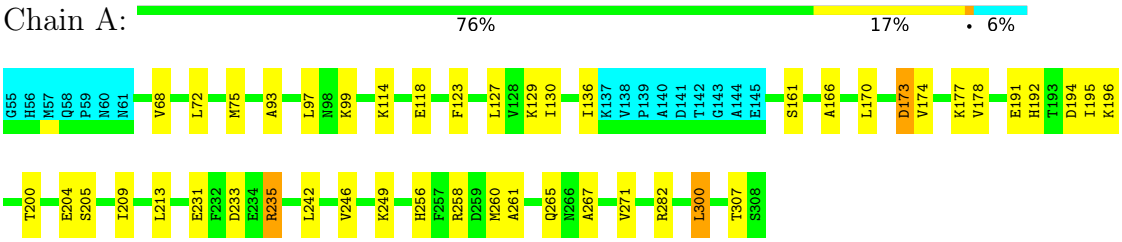
• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue



4.2.10 Score per residue for model 10

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

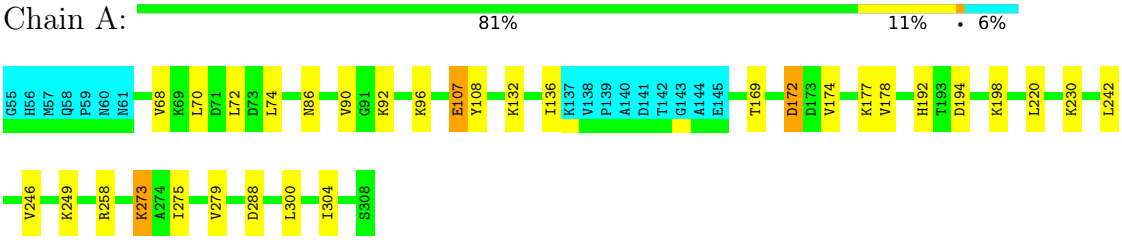
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

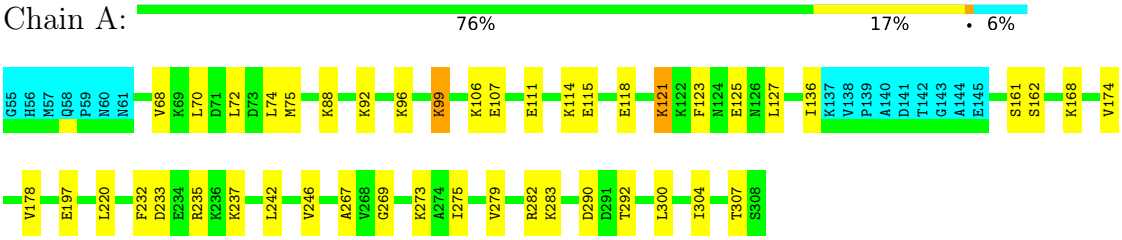
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

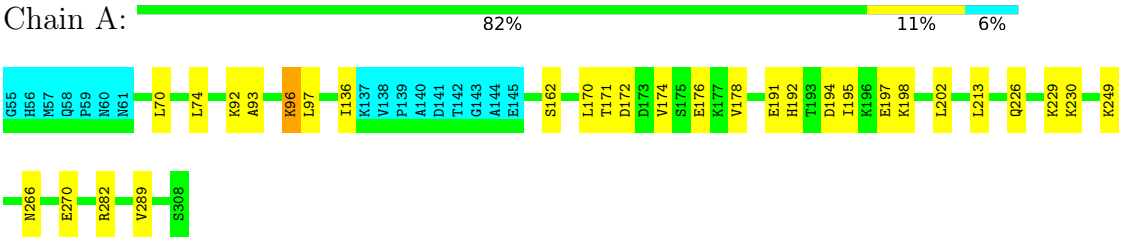
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

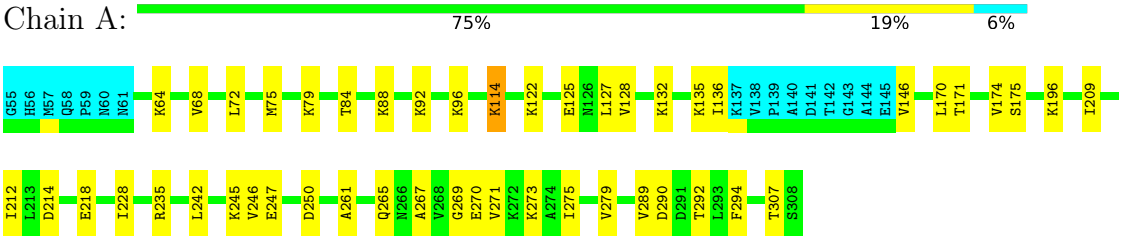
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

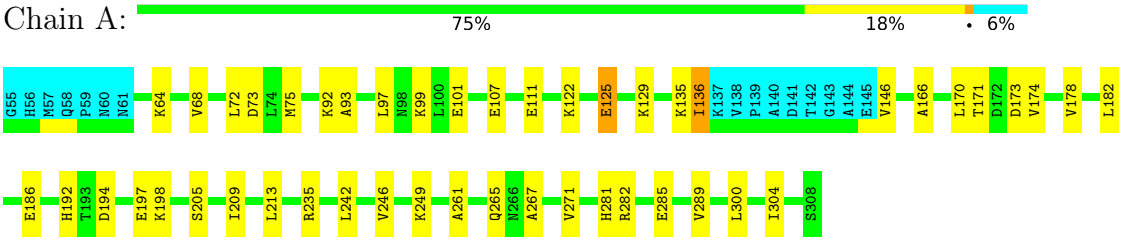
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

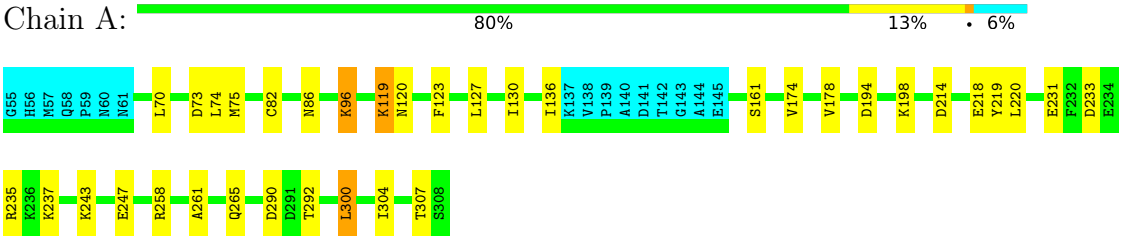
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

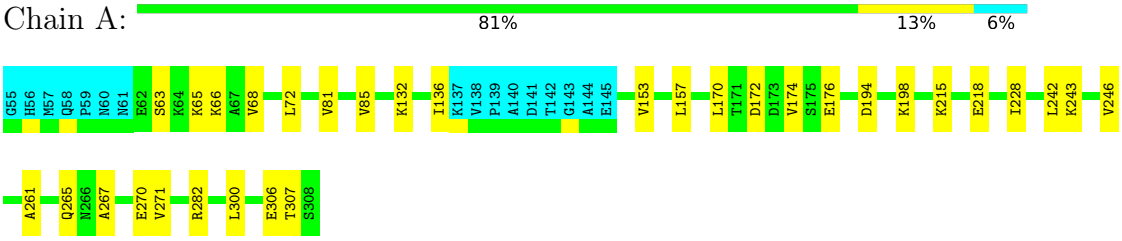
Chain A:



4.2.17 Score per residue for model 17

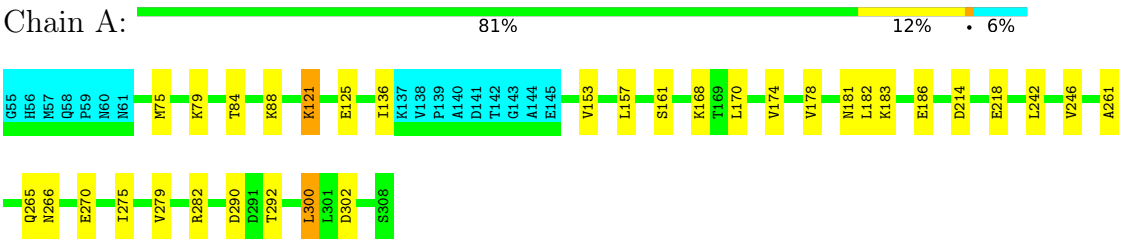
• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue

Chain A:



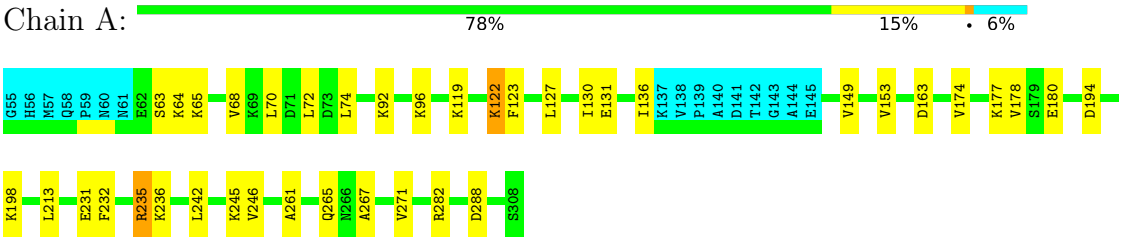
4.2.18 Score per residue for model 18

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue



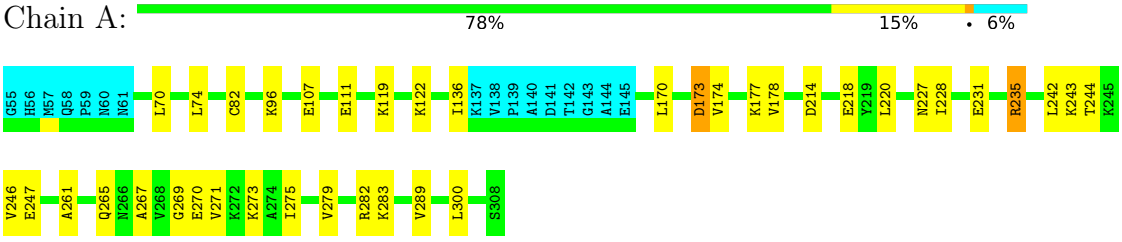
4.2.19 Score per residue for model 19

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue



4.2.20 Score per residue for model 20 (medoid)

• Molecule 1: BmGPI12, BMN1 family, BMN1-9, BmSA1 orthologue



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CYANA	structure calculation	
CNS	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	2734
Number of shifts mapped to atoms	2734
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality

6.1 Standard geometry

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	0.95±0.02	1±1/1869 (0.0± 0.0%)	1.01±0.02	0±0/2506 (0.0± 0.0%)
All	All	0.95	13/37380 (0.0%)	1.01	2/50120 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.7±0.6
All	All	0	14

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
1	A	101	GLU	C-N	-8.14	1.21	1.33	15	1
1	A	307	THR	N-CA	-6.62	1.38	1.46	17	4
1	A	162	SER	N-CA	-6.27	1.38	1.46	4	3
1	A	64	LYS	N-CA	-5.83	1.39	1.46	14	1
1	A	282	ARG	NE-CZ	5.31	1.38	1.33	1	1
1	A	306	GLU	C-N	-5.31	1.26	1.33	17	1
1	A	101	GLU	N-CA	-5.31	1.39	1.46	15	1
1	A	231	GLU	N-CA	-5.14	1.40	1.46	1	1

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	221	ASN	CA-CB-CG	5.64	118.24	112.60	4	1
1	A	172	ASP	CA-CB-CG	5.05	117.65	112.60	11	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	282	ARG	Sidechain	9
1	A	235	ARG	Sidechain	4
1	A	258	ARG	Sidechain	1

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	1859	1898	1898	18±3
All	All	37180	37960	37960	358

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:282:ARG:HD3	1:A:289:VAL:HG21	0.66	1.68	20	1
1:A:194:ASP:O	1:A:198:LYS:HG2	0.65	1.92	11	12
1:A:214:ASP:O	1:A:218:GLU:HG2	0.62	1.94	14	3
1:A:92:LYS:O	1:A:96:LYS:HG2	0.60	1.97	6	6
1:A:107:GLU:O	1:A:111:GLU:HG2	0.60	1.96	15	5
1:A:156:ALA:O	1:A:160:LEU:HG	0.59	1.97	6	2
1:A:68:VAL:O	1:A:72:LEU:HG	0.59	1.97	19	13
1:A:231:GLU:O	1:A:235:ARG:HD3	0.58	1.98	2	3
1:A:261:ALA:O	1:A:265:GLN:HG2	0.57	1.99	14	16
1:A:88:LYS:O	1:A:92:LYS:HG2	0.56	2.00	12	1
1:A:166:ALA:O	1:A:170:LEU:HG	0.54	2.02	15	3
1:A:106:LYS:HD2	1:A:107:GLU:N	0.54	2.17	12	1
1:A:96:LYS:HB3	1:A:178:VAL:HG21	0.54	1.79	13	2
1:A:62:GLU:O	1:A:66:LYS:HG2	0.54	2.03	6	1
1:A:231:GLU:O	1:A:235:ARG:HG2	0.53	2.04	16	4
1:A:99:LYS:HA	1:A:99:LYS:NZ	0.53	2.18	6	2
1:A:123:PHE:O	1:A:127:LEU:HG	0.53	2.03	10	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:THR:O	1:A:88:LYS:HG2	0.53	2.04	14	2
1:A:192:HIS:CE1	1:A:249:LYS:HB3	0.52	2.40	8	5
1:A:194:ASP:O	1:A:197:GLU:HG2	0.52	2.05	15	1
1:A:114:LYS:O	1:A:118:GLU:HG2	0.52	2.05	12	3
1:A:205:SER:O	1:A:209:ILE:HG12	0.51	2.05	1	5
1:A:196:LYS:NZ	1:A:247:GLU:HA	0.51	2.19	3	2
1:A:75:MET:SD	1:A:130:ILE:HB	0.51	2.46	16	1
1:A:70:LEU:O	1:A:74:LEU:HG	0.51	2.04	4	7
1:A:242:LEU:O	1:A:246:VAL:HG23	0.51	2.05	14	16
1:A:174:VAL:O	1:A:178:VAL:HG23	0.51	2.06	18	16
1:A:149:VAL:HB	1:A:153:VAL:HG21	0.51	1.83	19	1
1:A:269:GLY:O	1:A:273:LYS:HD3	0.50	2.06	14	1
1:A:82:CYS:SG	1:A:300:LEU:HD21	0.50	2.46	20	3
1:A:107:GLU:CD	1:A:107:GLU:H	0.50	2.14	11	1
1:A:231:GLU:O	1:A:235:ARG:HD2	0.50	2.06	7	2
1:A:79:LYS:NZ	1:A:127:LEU:HA	0.50	2.21	14	1
1:A:178:VAL:O	1:A:182:LEU:HG	0.50	2.07	18	1
1:A:92:LYS:O	1:A:96:LYS:HD2	0.49	2.07	8	2
1:A:99:LYS:HA	1:A:99:LYS:HE2	0.49	1.83	10	2
1:A:119:LYS:HD3	1:A:163:ASP:HA	0.49	1.84	19	1
1:A:275:ILE:O	1:A:279:VAL:HG23	0.49	2.06	2	10
1:A:161:SER:HA	1:A:300:LEU:HD23	0.49	1.84	10	4
1:A:215:LYS:O	1:A:218:GLU:HG3	0.49	2.08	5	1
1:A:92:LYS:HG3	1:A:197:GLU:OE1	0.49	2.07	13	1
1:A:70:LEU:HD11	1:A:219:TYR:CG	0.49	2.43	16	1
1:A:115:GLU:O	1:A:119:LYS:HG3	0.49	2.08	5	1
1:A:173:ASP:O	1:A:177:LYS:HD3	0.49	2.07	20	2
1:A:267:ALA:O	1:A:271:VAL:HG23	0.49	2.08	14	7
1:A:153:VAL:O	1:A:157:LEU:HG	0.49	2.07	18	3
1:A:290:ASP:OD1	1:A:292:THR:HB	0.48	2.09	12	2
1:A:282:ARG:HB2	1:A:289:VAL:CG2	0.48	2.39	15	1
1:A:73:ASP:O	1:A:77:GLU:HG2	0.48	2.07	2	2
1:A:226:GLN:O	1:A:230:LYS:HG2	0.48	2.08	4	2
1:A:269:GLY:O	1:A:273:LYS:HG2	0.48	2.09	8	1
1:A:117:ASP:O	1:A:121:LYS:HG2	0.48	2.08	9	1
1:A:196:LYS:HE2	1:A:246:VAL:O	0.48	2.09	2	1
1:A:192:HIS:NE2	1:A:196:LYS:HE2	0.48	2.22	3	2
1:A:290:ASP:OD2	1:A:292:THR:HB	0.48	2.09	18	2
1:A:279:VAL:O	1:A:283:LYS:HG2	0.48	2.09	20	1
1:A:228:ILE:HG23	1:A:270:GLU:HB3	0.48	1.84	20	6
1:A:243:LYS:O	1:A:247:GLU:HG2	0.48	2.09	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:LYS:HD2	1:A:171:THR:CG2	0.48	2.38	15	2
1:A:170:LEU:O	1:A:174:VAL:HG23	0.47	2.09	4	11
1:A:169:THR:HA	1:A:172:ASP:OD2	0.47	2.09	11	1
1:A:128:VAL:O	1:A:132:LYS:HB2	0.47	2.08	14	1
1:A:213:LEU:HD12	1:A:271:VAL:HG22	0.47	1.86	10	5
1:A:93:ALA:O	1:A:97:LEU:HG	0.47	2.08	10	4
1:A:70:LEU:HG	1:A:219:TYR:CD2	0.47	2.44	5	1
1:A:269:GLY:O	1:A:273:LYS:HG3	0.47	2.10	12	3
1:A:119:LYS:HD3	1:A:120:ASN:N	0.47	2.25	16	1
1:A:122:LYS:O	1:A:125:GLU:HG3	0.47	2.09	9	3
1:A:119:LYS:HA	1:A:119:LYS:NZ	0.46	2.25	9	1
1:A:205:SER:O	1:A:209:ILE:HG13	0.46	2.10	5	2
1:A:243:LYS:O	1:A:247:GLU:HG3	0.46	2.10	16	2
1:A:161:SER:HA	1:A:300:LEU:CD2	0.46	2.41	3	4
1:A:121:LYS:O	1:A:125:GLU:HG2	0.46	2.09	5	3
1:A:127:LEU:O	1:A:131:GLU:HG2	0.46	2.10	3	3
1:A:75:MET:SD	1:A:79:LYS:HD3	0.46	2.51	18	1
1:A:243:LYS:HG3	1:A:244:THR:N	0.45	2.26	20	1
1:A:135:LYS:HA	1:A:146:VAL:O	0.45	2.11	8	4
1:A:209:ILE:HA	1:A:212:ILE:HD12	0.45	1.87	14	1
1:A:289:VAL:HG13	1:A:294:PHE:CE2	0.45	2.47	6	2
1:A:266:ASN:O	1:A:270:GLU:HG2	0.45	2.12	4	4
1:A:168:LYS:HE3	1:A:303:THR:O	0.45	2.11	7	1
1:A:177:LYS:O	1:A:180:GLU:HG2	0.45	2.11	19	1
1:A:172:ASP:O	1:A:176:GLU:HG2	0.45	2.10	17	3
1:A:183:LYS:HE2	1:A:186:GLU:OE1	0.45	2.12	18	1
1:A:172:ASP:O	1:A:176:GLU:HG3	0.45	2.11	6	3
1:A:191:GLU:O	1:A:195:ILE:HG12	0.45	2.12	3	5
1:A:81:VAL:O	1:A:85:VAL:HG23	0.44	2.11	17	1
1:A:192:HIS:NE2	1:A:196:LYS:HE3	0.44	2.28	1	3
1:A:200:THR:O	1:A:204:GLU:HG2	0.44	2.13	1	2
1:A:86:ASN:OD1	1:A:119:LYS:HE3	0.44	2.12	16	1
1:A:123:PHE:CZ	1:A:127:LEU:HD21	0.44	2.47	3	1
1:A:82:CYS:SG	1:A:300:LEU:HD11	0.44	2.53	16	1
1:A:130:ILE:HA	1:A:153:VAL:HG22	0.44	1.90	19	1
1:A:227:ASN:O	1:A:230:LYS:HG3	0.44	2.11	9	1
1:A:171:THR:O	1:A:174:VAL:HB	0.44	2.12	13	1
1:A:270:GLU:O	1:A:273:LYS:HB3	0.44	2.13	6	1
1:A:114:LYS:HE3	1:A:114:LYS:HA	0.44	1.90	14	1
1:A:182:LEU:HB3	1:A:186:GLU:HB2	0.44	1.88	15	2
1:A:119:LYS:HE2	1:A:119:LYS:HA	0.44	1.89	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:222:ASN:O	1:A:226:GLN:HG2	0.44	2.13	9	1
1:A:96:LYS:HA	1:A:96:LYS:HE2	0.44	1.90	12	1
1:A:281:HIS:O	1:A:285:GLU:HG2	0.44	2.13	15	1
1:A:198:LYS:O	1:A:202:LEU:HG	0.43	2.12	13	1
1:A:126:ASN:O	1:A:129:LYS:HG2	0.43	2.14	7	1
1:A:233:ASP:O	1:A:237:LYS:HB2	0.43	2.13	16	2
1:A:273:LYS:HA	1:A:273:LYS:NZ	0.43	2.29	11	1
1:A:122:LYS:HE3	1:A:122:LYS:HA	0.43	1.90	19	1
1:A:271:VAL:O	1:A:275:ILE:HG12	0.43	2.13	20	2
1:A:192:HIS:CE1	1:A:196:LYS:HD2	0.43	2.48	10	1
1:A:300:LEU:O	1:A:304:ILE:HG12	0.43	2.14	11	4
1:A:298:SER:O	1:A:301:LEU:HB3	0.43	2.14	3	2
1:A:123:PHE:CE1	1:A:164:ILE:HD11	0.43	2.49	7	1
1:A:173:ASP:O	1:A:176:GLU:HG3	0.42	2.13	5	1
1:A:215:LYS:O	1:A:218:GLU:HG2	0.42	2.12	17	1
1:A:182:LEU:HD12	1:A:186:GLU:CB	0.42	2.44	1	1
1:A:128:VAL:O	1:A:131:GLU:HG3	0.42	2.14	6	1
1:A:126:ASN:HA	1:A:129:LYS:HG2	0.42	1.91	7	1
1:A:278:VAL:O	1:A:282:ARG:HG3	0.42	2.15	9	1
1:A:256:HIS:O	1:A:260:MET:HG3	0.42	2.15	10	1
1:A:282:ARG:HB2	1:A:289:VAL:HG21	0.42	1.91	3	3
1:A:75:MET:CE	1:A:130:ILE:HB	0.42	2.44	10	1
1:A:258:ARG:HD3	1:A:258:ARG:C	0.42	2.40	10	1
1:A:64:LYS:O	1:A:68:VAL:HG23	0.42	2.15	15	1
1:A:232:PHE:CD2	1:A:267:ALA:HB1	0.42	2.50	1	3
1:A:213:LEU:HD21	1:A:229:LYS:HA	0.42	1.90	13	1
1:A:63:SER:HA	1:A:66:LYS:CD	0.42	2.45	17	1
1:A:214:ASP:O	1:A:218:GLU:HG3	0.42	2.15	16	1
1:A:166:ALA:O	1:A:170:LEU:HD23	0.41	2.15	5	1
1:A:70:LEU:O	1:A:74:LEU:HD13	0.41	2.14	8	1
1:A:135:LYS:HE2	1:A:147:ASP:OD2	0.41	2.15	3	1
1:A:245:LYS:HA	1:A:245:LYS:HE2	0.41	1.91	19	1
1:A:86:ASN:O	1:A:90:VAL:HG23	0.41	2.16	11	1
1:A:108:TYR:CZ	1:A:177:LYS:HG3	0.41	2.51	11	1
1:A:230:LYS:HD2	1:A:230:LYS:C	0.41	2.40	11	1
1:A:130:ILE:HG22	1:A:156:ALA:HB1	0.41	1.93	5	1
1:A:74:LEU:HG	1:A:212:ILE:HG23	0.41	1.92	8	1
1:A:232:PHE:O	1:A:236:LYS:HG2	0.41	2.16	19	1
1:A:149:VAL:O	1:A:150:ASP:HB3	0.40	2.16	8	1
1:A:75:MET:HA	1:A:75:MET:HE3	0.40	1.93	12	1
1:A:70:LEU:O	1:A:74:LEU:HD23	0.40	2.16	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:193:THR:O	1:A:197:GLU:HG2	0.40	2.17	4	1
1:A:106:LYS:HD3	1:A:107:GLU:N	0.40	2.30	8	1
1:A:85:VAL:O	1:A:88:LYS:HG3	0.40	2.17	9	1
1:A:92:LYS:HE2	1:A:175:SER:OG	0.40	2.17	14	1
1:A:92:LYS:HD3	1:A:92:LYS:C	0.40	2.40	15	1
1:A:107:GLU:H	1:A:107:GLU:CD	0.40	2.25	4	1
1:A:126:ASN:O	1:A:130:ILE:HG23	0.40	2.17	5	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	237/254 (93%)	232±1 (98±0%)	4±1 (2±0%)	0±1 (0±0%)	45	81
All	All	4740/5080 (93%)	4648 (98%)	84 (2%)	8 (0%)	45	81

All 3 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	288	ASP	4
1	A	150	ASP	3
1	A	101	GLU	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	213/225 (95%)	206±2 (97±1%)	7±2 (3±1%)	35	86
All	All	4260/4500 (95%)	4119 (97%)	141 (3%)	35	86

All 58 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	136	ILE	20
1	A	220	LEU	7
1	A	96	LYS	6
1	A	300	LEU	6
1	A	235	ARG	6
1	A	173	ASP	4
1	A	168	LYS	4
1	A	197	GLU	4
1	A	307	THR	4
1	A	121	LYS	4
1	A	119	LYS	4
1	A	131	GLU	3
1	A	243	LYS	3
1	A	65	LYS	3
1	A	132	LYS	3
1	A	176	GLU	3
1	A	99	LYS	3
1	A	129	LYS	3
1	A	73	ASP	3
1	A	106	LYS	2
1	A	218	GLU	2
1	A	233	ASP	2
1	A	287	LEU	2
1	A	230	LYS	2
1	A	107	GLU	2
1	A	125	GLU	2
1	A	75	MET	2
1	A	122	LYS	2
1	A	88	LYS	1
1	A	98	ASN	1
1	A	103	GLU	1
1	A	170	LEU	1
1	A	215	LYS	1
1	A	64	LYS	1
1	A	221	ASN	1
1	A	70	LEU	1
1	A	92	LYS	1
1	A	183	LYS	1
1	A	266	ASN	1
1	A	286	ASN	1
1	A	301	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	117	ASP	1
1	A	157	LEU	1
1	A	177	LYS	1
1	A	276	ASP	1
1	A	62	GLU	1
1	A	69	LYS	1
1	A	194	ASP	1
1	A	258	ARG	1
1	A	273	LYS	1
1	A	115	GLU	1
1	A	283	LYS	1
1	A	114	LYS	1
1	A	245	LYS	1
1	A	250	ASP	1
1	A	181	ASN	1
1	A	302	ASP	1
1	A	227	ASN	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

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

Total number of shifts	2734
Number of shifts mapped to atoms	2734
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	252	-0.79 ± 0.11	Should be checked
$^{13}C_{\beta}$	244	0.26 ± 0.06	None needed (< 0.5 ppm)
$^{13}C'$	252	-0.57 ± 0.09	Should be applied
^{15}N	247	-0.27 ± 0.12	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 2587 atoms were assigned a chemical shift out of a possible 3195. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1195/1197 (100%)	482/483 (100%)	476/476 (100%)	237/238 (100%)
Sidechain	1352/1903 (71%)	1099/1219 (90%)	231/616 (38%)	22/68 (32%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	40/95 (42%)	40/48 (83%)	0/43 (0%)	0/4 (0%)
Overall	2587/3195 (81%)	1621/1750 (93%)	707/1135 (62%)	259/310 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 2733 atoms were assigned a chemical shift out of a possible 3383. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1259/1275 (99%)	508/515 (99%)	504/508 (99%)	247/252 (98%)
Sidechain	1432/2006 (71%)	1163/1285 (91%)	244/649 (38%)	25/72 (35%)
Aromatic	42/102 (41%)	42/52 (81%)	0/45 (0%)	0/5 (0%)
Overall	2733/3383 (81%)	1713/1852 (92%)	748/1202 (62%)	272/329 (83%)

7.1.4 Statistically unusual chemical shifts (i)

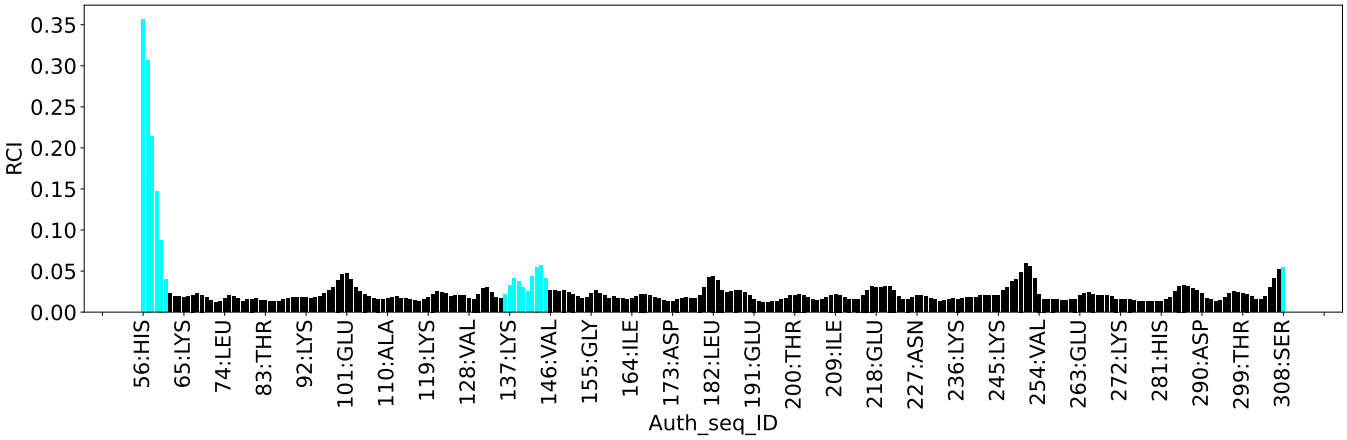
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	126	ASN	HD21	10.21	4.94 – 9.72	6.0

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
56:HIS
65:LYS
74:LEU
83:THR
92:LYS
101:GLU
110:ALA
119:LYS
128:VAL
137:LYS
146:VAL
155:GLY
164:ILE
173:ASP
182:LEU
191:GLU
200:THR
209:ILE
218:GLU
227:ASN
236:LYS
245:LYS
254:VAL
263:GLU
272:LYS
281:HIS
290:ASP
299:THR
308:SER
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3847
Intra-residue (|i-j|=0)	898
Sequential (|i-j|=1)	1214
Medium range (|i-j|>1 and |i-j|<5)	932
Long range (|i-j|≥5)	521
Inter-chain	0
Hydrogen bond restraints	282
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	15.1
Number of long range restraints per residue[1]	2.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	15.7	0.2
0.2-0.5 (Medium)	1.1	0.29
>0.5 (Large)	None	None

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)

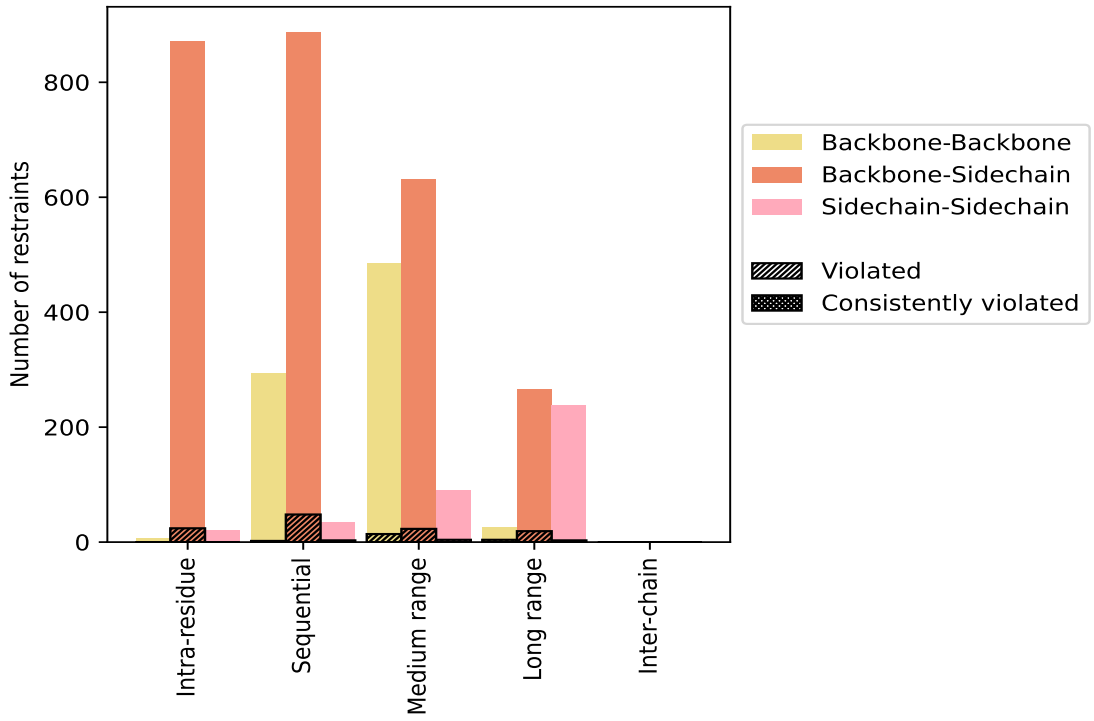
9.1 Summary of distance violations (i)

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)	898	23.3	24	2.7	0.6	0	0.0	0.0
Backbone-Backbone	6	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	871	22.6	24	2.8	0.6	0	0.0	0.0
Sidechain-Sidechain	21	0.5	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	1214	31.6	53	4.4	1.4	0	0.0	0.0
Backbone-Backbone	293	7.6	2	0.7	0.1	0	0.0	0.0
Backbone-Sidechain	887	23.1	48	5.4	1.2	0	0.0	0.0
Sidechain-Sidechain	34	0.9	3	8.8	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	932	24.2	32	3.4	0.8	0	0.0	0.0
Backbone-Backbone	485	12.6	14	2.9	0.4	0	0.0	0.0
Backbone-Sidechain	357	9.3	14	3.9	0.4	0	0.0	0.0
Sidechain-Sidechain	90	2.3	4	4.4	0.1	0	0.0	0.0
Long range (|i-j|≥5)	521	13.5	26	5.0	0.7	0	0.0	0.0
Backbone-Backbone	26	0.7	4	15.4	0.1	0	0.0	0.0
Backbone-Sidechain	257	6.7	19	7.4	0.5	0	0.0	0.0
Sidechain-Sidechain	238	6.2	3	1.3	0.1	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	282	7.3	9	3.2	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3847	100.0	144	3.7	3.7	0	0.0	0.0
Backbone-Backbone	810	21.1	20	2.5	0.5	0	0.0	0.0
Backbone-Sidechain	2654	69.0	114	4.3	3.0	0	0.0	0.0
Sidechain-Sidechain	383	10.0	10	2.6	0.3	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



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	4	4	9	3	0	20	0.15	0.27	0.05	0.13
2	3	5	9	4	0	21	0.13	0.2	0.02	0.12
3	4	7	6	5	0	22	0.13	0.17	0.02	0.13
4	4	8	5	1	0	18	0.13	0.28	0.04	0.12
5	5	5	7	4	0	21	0.13	0.18	0.03	0.12
6	5	12	9	2	0	28	0.15	0.25	0.04	0.14
7	4	8	6	1	0	19	0.15	0.27	0.05	0.15
8	3	8	7	2	0	20	0.13	0.23	0.03	0.11
9	4	6	6	2	0	18	0.12	0.22	0.03	0.11
10	2	6	3	3	0	14	0.13	0.17	0.02	0.12

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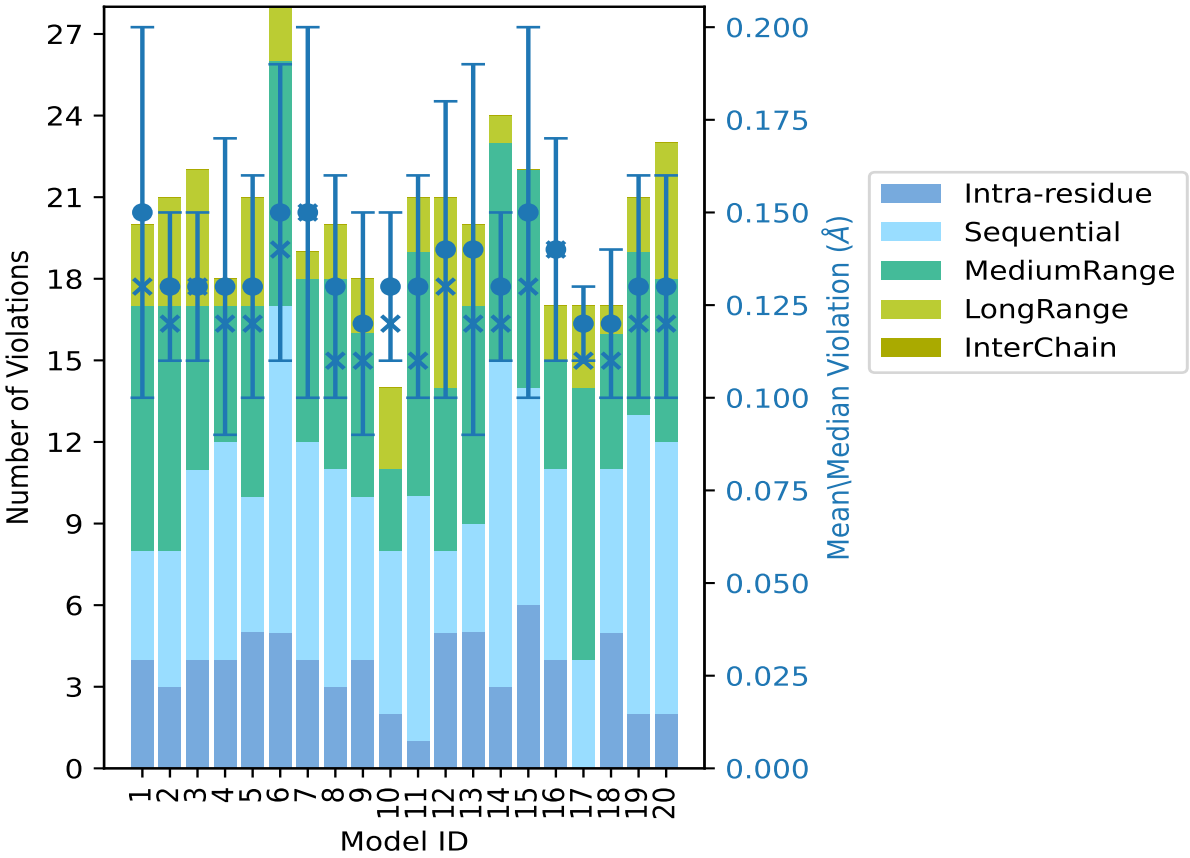
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	1	9	9	2	0	21	0.13	0.22	0.03	0.11
12	5	3	6	7	0	21	0.14	0.28	0.04	0.13
13	5	4	8	3	0	20	0.14	0.27	0.05	0.12
14	3	12	8	1	0	24	0.13	0.19	0.02	0.12
15	6	8	8	0	0	22	0.15	0.29	0.05	0.13
16	4	7	4	2	0	17	0.14	0.19	0.03	0.14
17	0	4	10	3	0	17	0.12	0.13	0.01	0.11
18	5	6	5	1	0	17	0.12	0.17	0.02	0.11
19	2	11	6	2	0	21	0.13	0.21	0.03	0.12
20	2	10	6	5	0	23	0.13	0.2	0.03	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



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

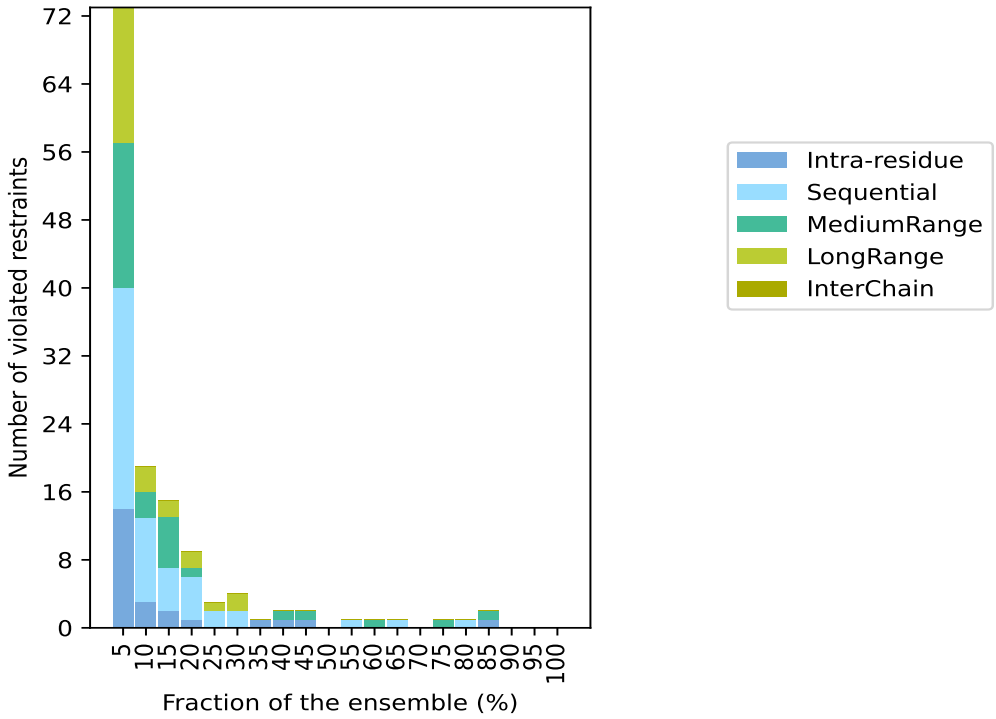
9.3 Distance violation statistics for the ensemble (i)

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, 3430(IR:874, SQ:1161, MR:900, LR:495, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
14	26	17	16	0	73	1	5.0
3	10	3	3	0	19	2	10.0
2	5	6	2	0	15	3	15.0
1	5	1	2	0	9	4	20.0
0	2	0	1	0	3	5	25.0
0	2	0	2	0	4	6	30.0
1	0	0	0	0	1	7	35.0
1	0	1	0	0	2	8	40.0
1	0	1	0	0	2	9	45.0
0	0	0	0	0	0	10	50.0
0	1	0	0	0	1	11	55.0
0	0	1	0	0	1	12	60.0
0	1	0	0	0	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	1	0	0	1	15	75.0
0	1	0	0	0	1	16	80.0
1	0	1	0	0	2	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	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

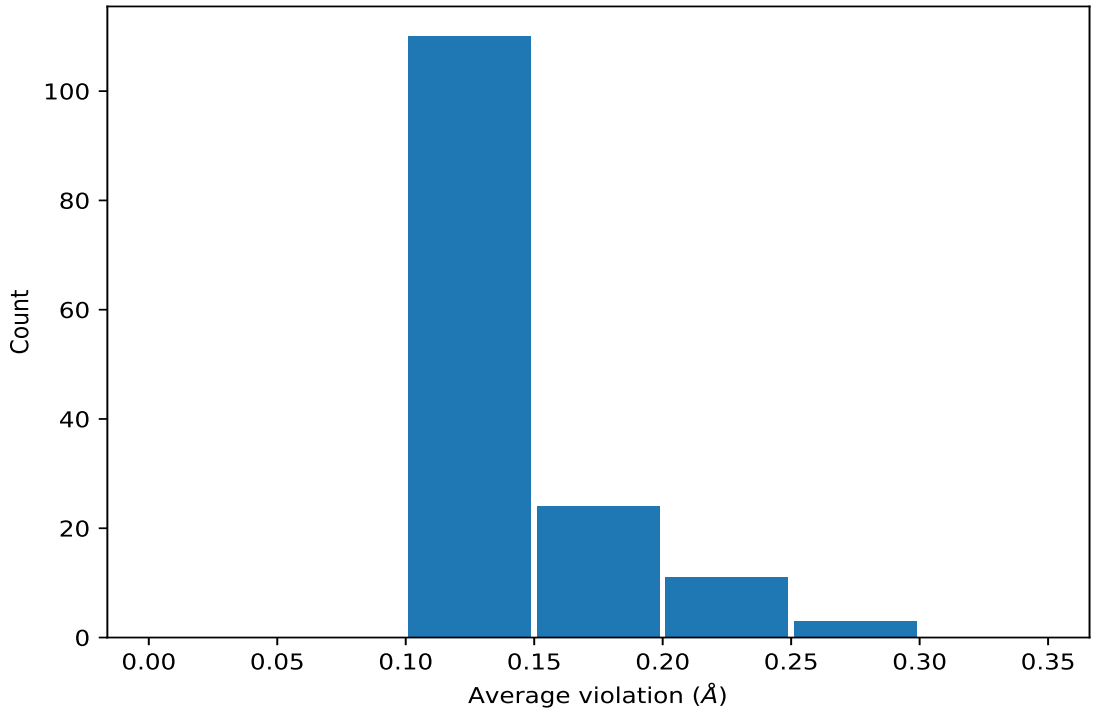
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	17	0.16	0.01	0.16
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	17	0.14	0.03	0.14
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	16	0.11	0.01	0.11
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	15	0.14	0.01	0.13
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	13	0.12	0.01	0.12
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	13	0.12	0.01	0.12
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	13	0.12	0.01	0.11
(1,3490)	1:300:A:LEU:HD21	1:303:A:THR:H	12	0.2	0.02	0.2
(1,3490)	1:300:A:LEU:HD22	1:303:A:THR:H	12	0.2	0.02	0.2
(1,3490)	1:300:A:LEU:HD23	1:303:A:THR:H	12	0.2	0.02	0.2
(1,2134)	1:212:A:ILE:HD11	1:213:A:LEU:H	11	0.12	0.02	0.12
(1,2134)	1:212:A:ILE:HD12	1:213:A:LEU:H	11	0.12	0.02	0.12
(1,2134)	1:212:A:ILE:HD13	1:213:A:LEU:H	11	0.12	0.02	0.12
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG2	9	0.15	0.01	0.15
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG3	9	0.15	0.01	0.15
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD1	9	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD2	9	0.12	0.01	0.12
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD1	9	0.12	0.01	0.12
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD2	9	0.12	0.01	0.12
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD1	9	0.12	0.01	0.12
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD2	9	0.12	0.01	0.12
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD21	8	0.13	0.02	0.13
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD22	8	0.13	0.02	0.13
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD21	8	0.13	0.02	0.13
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD22	8	0.13	0.02	0.13
(1,3009)	1:265:A:GLN:H	1:265:A:GLN:HG3	8	0.12	0.01	0.12
(1,3422)	1:295:A:SER:H	1:295:A:SER:HB3	7	0.16	0.01	0.16
(2,143)	1:179:A:SER:H	1:176:A:GLU:O	7	0.11	0.01	0.11
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD11	6	0.14	0.02	0.14
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD12	6	0.14	0.02	0.14
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD13	6	0.14	0.02	0.14
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD21	6	0.14	0.02	0.14
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD22	6	0.14	0.02	0.14
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD23	6	0.14	0.02	0.14
(1,1138)	1:133:A:ARG:HA	1:150:A:ASP:HA	6	0.13	0.02	0.13
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD11	6	0.12	0.01	0.12
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD12	6	0.12	0.01	0.12
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD13	6	0.12	0.01	0.12
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD11	6	0.11	0.01	0.11
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD12	6	0.11	0.01	0.11
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD13	6	0.11	0.01	0.11
(1,549)	1:96:A:LYS:HE2	1:97:A:LEU:H	5	0.21	0.02	0.21
(1,549)	1:96:A:LYS:HE3	1:97:A:LEU:H	5	0.21	0.02	0.21
(1,884)	1:116:A:ILE:HG21	1:121:A:LYS:H	5	0.12	0.01	0.12
(1,884)	1:116:A:ILE:HG22	1:121:A:LYS:H	5	0.12	0.01	0.12
(1,884)	1:116:A:ILE:HG23	1:121:A:LYS:H	5	0.12	0.01	0.12
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD11	5	0.11	0.01	0.11
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD12	5	0.11	0.01	0.11
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD13	5	0.11	0.01	0.11
(1,2804)	1:250:A:ASP:H	1:250:A:ASP:HB3	4	0.17	0.01	0.17
(1,1237)	1:137:A:LYS:HE2	1:138:A:VAL:H	4	0.15	0.03	0.15
(1,1237)	1:137:A:LYS:HE3	1:138:A:VAL:H	4	0.15	0.03	0.15
(1,425)	1:88:A:LYS:HB2	1:89:A:LEU:H	4	0.15	0.02	0.15
(1,425)	1:88:A:LYS:HB3	1:89:A:LEU:H	4	0.15	0.02	0.15
(1,45)	1:63:A:SER:H	1:64:A:LYS:HG2	4	0.14	0.01	0.14
(1,45)	1:63:A:SER:H	1:64:A:LYS:HG3	4	0.14	0.01	0.14
(1,3235)	1:282:A:ARG:H	1:289:A:VAL:HB	4	0.12	0.01	0.12
(2,185)	1:219:A:TYR:H	1:216:A:LEU:O	4	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1259)	1:138:A:VAL:H	1:143:A:GLY:HA2	4	0.12	0.01	0.12
(1,1259)	1:138:A:VAL:H	1:143:A:GLY:HA3	4	0.12	0.01	0.12
(1,2230)	1:218:A:GLU:HG2	1:219:A:TYR:H	4	0.11	0.0	0.11
(1,1442)	1:158:A:SER:HA	1:161:A:SER:H	4	0.11	0.0	0.11
(1,1474)	1:160:A:LEU:HD21	1:161:A:SER:H	4	0.11	0.0	0.11
(1,1474)	1:160:A:LEU:HD22	1:161:A:SER:H	4	0.11	0.0	0.11
(1,1474)	1:160:A:LEU:HD23	1:161:A:SER:H	4	0.11	0.0	0.11
(1,1493)	1:162:A:SER:H	1:162:A:SER:HB3	3	0.28	0.0	0.28
(1,1741)	1:183:A:LYS:HE2	1:184:A:ASP:H	3	0.16	0.02	0.15
(1,1741)	1:183:A:LYS:HE3	1:184:A:ASP:H	3	0.16	0.02	0.15
(1,55)	1:64:A:LYS:H	1:64:A:LYS:HG2	3	0.15	0.01	0.16
(1,55)	1:64:A:LYS:H	1:64:A:LYS:HG3	3	0.15	0.01	0.16
(1,3292)	1:287:A:LEU:HG	1:288:A:ASP:H	3	0.14	0.0	0.14
(1,1053)	1:127:A:LEU:HD11	1:128:A:VAL:H	3	0.13	0.04	0.11
(1,1053)	1:127:A:LEU:HD12	1:128:A:VAL:H	3	0.13	0.04	0.11
(1,1053)	1:127:A:LEU:HD13	1:128:A:VAL:H	3	0.13	0.04	0.11
(1,1053)	1:127:A:LEU:HD21	1:128:A:VAL:H	3	0.13	0.04	0.11
(1,1053)	1:127:A:LEU:HD22	1:128:A:VAL:H	3	0.13	0.04	0.11
(1,1053)	1:127:A:LEU:HD23	1:128:A:VAL:H	3	0.13	0.04	0.11
(1,1078)	1:129:A:LYS:HA	1:132:A:LYS:H	3	0.13	0.01	0.13
(1,3108)	1:275:A:ILE:HD11	1:276:A:ASP:H	3	0.13	0.02	0.13
(1,3108)	1:275:A:ILE:HD12	1:276:A:ASP:H	3	0.13	0.02	0.13
(1,3108)	1:275:A:ILE:HD13	1:276:A:ASP:H	3	0.13	0.02	0.13
(1,1743)	1:183:A:LYS:HG2	1:186:A:GLU:H	3	0.12	0.03	0.1
(1,1743)	1:183:A:LYS:HG3	1:186:A:GLU:H	3	0.12	0.03	0.1
(1,2306)	1:220:A:LEU:HD21	1:278:A:VAL:HA	3	0.12	0.02	0.11
(1,2306)	1:220:A:LEU:HD22	1:278:A:VAL:HA	3	0.12	0.02	0.11
(1,2306)	1:220:A:LEU:HD23	1:278:A:VAL:HA	3	0.12	0.02	0.11
(1,2421)	1:227:A:ASN:H	1:230:A:LYS:HB2	3	0.12	0.01	0.11
(1,2421)	1:227:A:ASN:H	1:230:A:LYS:HB3	3	0.12	0.01	0.11
(1,365)	1:85:A:VAL:HA	1:88:A:LYS:HB2	3	0.11	0.01	0.11
(1,365)	1:85:A:VAL:HA	1:88:A:LYS:HB3	3	0.11	0.01	0.11
(1,1555)	1:168:A:LYS:HG2	1:169:A:THR:H	3	0.11	0.0	0.11
(1,1555)	1:168:A:LYS:HG3	1:169:A:THR:H	3	0.11	0.0	0.11
(1,1261)	1:138:A:VAL:H	1:144:A:ALA:H	3	0.1	0.0	0.1
(1,3551)	1:306:A:GLU:HG3	1:308:A:SER:H	3	0.1	0.0	0.1
(1,1895)	1:195:A:ILE:HA	1:199:A:ALA:HB1	3	0.1	0.0	0.1
(1,1895)	1:195:A:ILE:HA	1:199:A:ALA:HB2	3	0.1	0.0	0.1
(1,1895)	1:195:A:ILE:HA	1:199:A:ALA:HB3	3	0.1	0.0	0.1
(1,2480)	1:231:A:GLU:H	1:231:A:GLU:HG2	2	0.28	0.01	0.28
(1,2480)	1:231:A:GLU:H	1:231:A:GLU:HG3	2	0.28	0.01	0.28
(1,1472)	1:160:A:LEU:HD11	1:162:A:SER:H	2	0.2	0.01	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1472)	1:160:A:LEU:HD12	1:162:A:SER:H	2	0.2	0.01	0.2
(1,1472)	1:160:A:LEU:HD13	1:162:A:SER:H	2	0.2	0.01	0.2
(1,1472)	1:160:A:LEU:HD21	1:162:A:SER:H	2	0.2	0.01	0.2
(1,1472)	1:160:A:LEU:HD22	1:162:A:SER:H	2	0.2	0.01	0.2
(1,1472)	1:160:A:LEU:HD23	1:162:A:SER:H	2	0.2	0.01	0.2
(1,1108)	1:131:A:GLU:HG2	1:132:A:LYS:H	2	0.17	0.0	0.17
(1,1108)	1:131:A:GLU:HG3	1:132:A:LYS:H	2	0.17	0.0	0.17
(1,1471)	1:160:A:LEU:HD11	1:161:A:SER:H	2	0.17	0.04	0.17
(1,1471)	1:160:A:LEU:HD12	1:161:A:SER:H	2	0.17	0.04	0.17
(1,1471)	1:160:A:LEU:HD13	1:161:A:SER:H	2	0.17	0.04	0.17
(1,1471)	1:160:A:LEU:HD21	1:161:A:SER:H	2	0.17	0.04	0.17
(1,1471)	1:160:A:LEU:HD22	1:161:A:SER:H	2	0.17	0.04	0.17
(1,1471)	1:160:A:LEU:HD23	1:161:A:SER:H	2	0.17	0.04	0.17
(1,2399)	1:227:A:ASN:HA	1:227:A:ASN:HD21	2	0.17	0.02	0.17
(1,2399)	1:227:A:ASN:HA	1:227:A:ASN:HD22	2	0.17	0.02	0.17
(1,2229)	1:218:A:GLU:HG3	1:219:A:TYR:H	2	0.16	0.02	0.16
(1,979)	1:122:A:LYS:HG2	1:125:A:GLU:HG2	2	0.14	0.02	0.14
(1,979)	1:122:A:LYS:HG2	1:125:A:GLU:HG3	2	0.14	0.02	0.14
(1,979)	1:122:A:LYS:HG3	1:125:A:GLU:HG2	2	0.14	0.02	0.14
(1,979)	1:122:A:LYS:HG3	1:125:A:GLU:HG3	2	0.14	0.02	0.14
(1,3501)	1:301:A:LEU:HD11	1:302:A:ASP:H	2	0.14	0.01	0.14
(1,3501)	1:301:A:LEU:HD12	1:302:A:ASP:H	2	0.14	0.01	0.14
(1,3501)	1:301:A:LEU:HD13	1:302:A:ASP:H	2	0.14	0.01	0.14
(1,3501)	1:301:A:LEU:HD21	1:302:A:ASP:H	2	0.14	0.01	0.14
(1,3501)	1:301:A:LEU:HD22	1:302:A:ASP:H	2	0.14	0.01	0.14
(1,3501)	1:301:A:LEU:HD23	1:302:A:ASP:H	2	0.14	0.01	0.14
(1,2464)	1:230:A:LYS:HG3	1:231:A:GLU:H	2	0.12	0.01	0.12
(1,2630)	1:239:A:LEU:H	1:263:A:GLU:HG2	2	0.12	0.01	0.12
(1,2630)	1:239:A:LEU:H	1:263:A:GLU:HG3	2	0.12	0.01	0.12
(1,2994)	1:265:A:GLN:HA	1:268:A:VAL:H	2	0.12	0.01	0.12
(1,3286)	1:286:A:ASN:H	1:287:A:LEU:HD21	2	0.12	0.01	0.12
(1,3286)	1:286:A:ASN:H	1:287:A:LEU:HD22	2	0.12	0.01	0.12
(1,3286)	1:286:A:ASN:H	1:287:A:LEU:HD23	2	0.12	0.01	0.12
(1,363)	1:84:A:THR:H	1:164:A:ILE:HD11	2	0.12	0.02	0.12
(1,363)	1:84:A:THR:H	1:164:A:ILE:HD12	2	0.12	0.02	0.12
(1,363)	1:84:A:THR:H	1:164:A:ILE:HD13	2	0.12	0.02	0.12
(1,618)	1:100:A:LEU:HB2	1:105:A:HIS:HA	2	0.12	0.0	0.12
(1,618)	1:100:A:LEU:HB3	1:105:A:HIS:HA	2	0.12	0.0	0.12
(1,672)	1:101:A:GLU:HB3	1:102:A:GLY:H	2	0.12	0.0	0.12
(1,1241)	1:137:A:LYS:H	1:137:A:LYS:HE2	2	0.11	0.0	0.11
(1,1241)	1:137:A:LYS:H	1:137:A:LYS:HE3	2	0.11	0.0	0.11
(1,3539)	1:305:A:ILE:HG21	1:306:A:GLU:H	2	0.11	0.0	0.11

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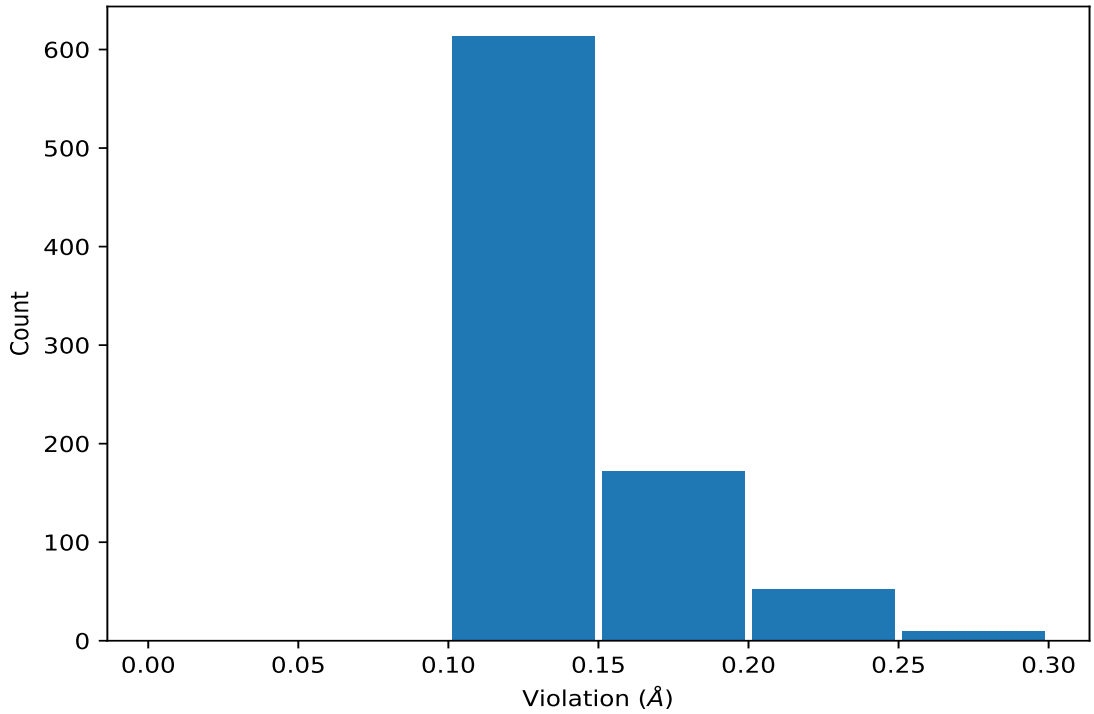
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3539)	1:305:A:ILE:HG22	1:306:A:GLU:H	2	0.11	0.0	0.11
(1,3539)	1:305:A:ILE:HG23	1:306:A:GLU:H	2	0.11	0.0	0.11
(1,2465)	1:230:A:LYS:HG2	1:231:A:GLU:H	2	0.11	0.0	0.11
(2,281)	1:306:A:GLU:H	1:302:A:ASP:O	2	0.11	0.0	0.11
(1,1606)	1:172:A:ASP:HB2	1:173:A:ASP:H	2	0.1	0.0	0.1
(1,1606)	1:172:A:ASP:HB3	1:173:A:ASP:H	2	0.1	0.0	0.1

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

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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

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)
(1,2480)	1:231:A:GLU:H	1:231:A:GLU:HG2	15	0.29
(1,2480)	1:231:A:GLU:H	1:231:A:GLU:HG3	15	0.29
(1,1493)	1:162:A:SER:H	1:162:A:SER:HB3	4	0.28
(1,1493)	1:162:A:SER:H	1:162:A:SER:HB3	12	0.28
(1,2480)	1:231:A:GLU:H	1:231:A:GLU:HG2	1	0.27
(1,2480)	1:231:A:GLU:H	1:231:A:GLU:HG3	1	0.27
(1,1493)	1:162:A:SER:H	1:162:A:SER:HB3	13	0.27
(1,1076)	1:128:A:VAL:H	1:129:A:LYS:HB2	7	0.27
(1,549)	1:96:A:LYS:HE2	1:97:A:LEU:H	6	0.25
(1,549)	1:96:A:LYS:HE3	1:97:A:LEU:H	6	0.25
(1,2662)	1:242:A:LEU:HG	1:260:A:MET:H	6	0.24
(1,289)	1:79:A:LYS:H	1:79:A:LYS:HE2	15	0.24
(1,289)	1:79:A:LYS:H	1:79:A:LYS:HE3	15	0.24
(1,3490)	1:300:A:LEU:HD21	1:303:A:THR:H	8	0.23
(1,3490)	1:300:A:LEU:HD22	1:303:A:THR:H	8	0.23
(1,3490)	1:300:A:LEU:HD23	1:303:A:THR:H	8	0.23
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	1	0.23
(1,677)	1:101:A:GLU:H	1:102:A:GLY:H	15	0.23
(1,3490)	1:300:A:LEU:HD21	1:303:A:THR:H	9	0.22
(1,3490)	1:300:A:LEU:HD22	1:303:A:THR:H	9	0.22
(1,3490)	1:300:A:LEU:HD23	1:303:A:THR:H	9	0.22
(1,2805)	1:250:A:ASP:H	1:250:A:ASP:HB2	13	0.22
(1,549)	1:96:A:LYS:HE2	1:97:A:LEU:H	11	0.22
(1,549)	1:96:A:LYS:HE3	1:97:A:LEU:H	11	0.22
(1,3490)	1:300:A:LEU:HD21	1:303:A:THR:H	6	0.21
(1,3490)	1:300:A:LEU:HD22	1:303:A:THR:H	6	0.21
(1,3490)	1:300:A:LEU:HD23	1:303:A:THR:H	6	0.21
(1,3490)	1:300:A:LEU:HD21	1:303:A:THR:H	7	0.21
(1,3490)	1:300:A:LEU:HD22	1:303:A:THR:H	7	0.21
(1,3490)	1:300:A:LEU:HD23	1:303:A:THR:H	7	0.21
(1,3490)	1:300:A:LEU:HD21	1:303:A:THR:H	19	0.21
(1,3490)	1:300:A:LEU:HD22	1:303:A:THR:H	19	0.21
(1,3490)	1:300:A:LEU:HD23	1:303:A:THR:H	19	0.21
(1,1561)	1:168:A:LYS:H	1:168:A:LYS:HE2	13	0.21
(1,1561)	1:168:A:LYS:H	1:168:A:LYS:HE3	13	0.21
(1,1472)	1:160:A:LEU:HD11	1:162:A:SER:H	1	0.21
(1,1472)	1:160:A:LEU:HD12	1:162:A:SER:H	1	0.21
(1,1472)	1:160:A:LEU:HD13	1:162:A:SER:H	1	0.21
(1,1472)	1:160:A:LEU:HD21	1:162:A:SER:H	1	0.21
(1,1472)	1:160:A:LEU:HD22	1:162:A:SER:H	1	0.21
(1,1472)	1:160:A:LEU:HD23	1:162:A:SER:H	1	0.21
(1,1471)	1:160:A:LEU:HD11	1:161:A:SER:H	6	0.21
(1,1471)	1:160:A:LEU:HD12	1:161:A:SER:H	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1471)	1:160:A:LEU:HD13	1:161:A:SER:H	6	0.21
(1,1471)	1:160:A:LEU:HD21	1:161:A:SER:H	6	0.21
(1,1471)	1:160:A:LEU:HD22	1:161:A:SER:H	6	0.21
(1,1471)	1:160:A:LEU:HD23	1:161:A:SER:H	6	0.21
(1,549)	1:96:A:LYS:HE2	1:97:A:LEU:H	19	0.21
(1,549)	1:96:A:LYS:HE3	1:97:A:LEU:H	19	0.21
(1,3490)	1:300:A:LEU:HD21	1:303:A:THR:H	2	0.2
(1,3490)	1:300:A:LEU:HD22	1:303:A:THR:H	2	0.2
(1,3490)	1:300:A:LEU:HD23	1:303:A:THR:H	2	0.2
(1,3490)	1:300:A:LEU:HD21	1:303:A:THR:H	15	0.2
(1,3490)	1:300:A:LEU:HD22	1:303:A:THR:H	15	0.2
(1,3490)	1:300:A:LEU:HD23	1:303:A:THR:H	15	0.2
(1,1726)	1:182:A:LEU:HD11	1:187:A:ALA:H	1	0.2
(1,1726)	1:182:A:LEU:HD12	1:187:A:ALA:H	1	0.2
(1,1726)	1:182:A:LEU:HD13	1:187:A:ALA:H	1	0.2
(1,1726)	1:182:A:LEU:HD21	1:187:A:ALA:H	1	0.2
(1,1726)	1:182:A:LEU:HD22	1:187:A:ALA:H	1	0.2
(1,1726)	1:182:A:LEU:HD23	1:187:A:ALA:H	1	0.2
(1,180)	1:72:A:LEU:HG	1:73:A:ASP:H	20	0.2
(1,3542)	1:305:A:ILE:H	1:305:A:ILE:HG12	6	0.19
(1,3542)	1:305:A:ILE:H	1:305:A:ILE:HG13	6	0.19
(1,3490)	1:300:A:LEU:HD21	1:303:A:THR:H	11	0.19
(1,3490)	1:300:A:LEU:HD22	1:303:A:THR:H	11	0.19
(1,3490)	1:300:A:LEU:HD23	1:303:A:THR:H	11	0.19
(1,3490)	1:300:A:LEU:HD21	1:303:A:THR:H	13	0.19
(1,3490)	1:300:A:LEU:HD22	1:303:A:THR:H	13	0.19
(1,3490)	1:300:A:LEU:HD23	1:303:A:THR:H	13	0.19
(1,3490)	1:300:A:LEU:HD21	1:303:A:THR:H	14	0.19
(1,3490)	1:300:A:LEU:HD22	1:303:A:THR:H	14	0.19
(1,3490)	1:300:A:LEU:HD23	1:303:A:THR:H	14	0.19
(1,2399)	1:227:A:ASN:HA	1:227:A:ASN:HD21	16	0.19
(1,2399)	1:227:A:ASN:HA	1:227:A:ASN:HD22	16	0.19
(1,1741)	1:183:A:LYS:HE2	1:184:A:ASP:H	8	0.19
(1,1741)	1:183:A:LYS:HE3	1:184:A:ASP:H	8	0.19
(1,1472)	1:160:A:LEU:HD11	1:162:A:SER:H	6	0.19
(1,1472)	1:160:A:LEU:HD12	1:162:A:SER:H	6	0.19
(1,1472)	1:160:A:LEU:HD13	1:162:A:SER:H	6	0.19
(1,1472)	1:160:A:LEU:HD21	1:162:A:SER:H	6	0.19
(1,1472)	1:160:A:LEU:HD22	1:162:A:SER:H	6	0.19
(1,1472)	1:160:A:LEU:HD23	1:162:A:SER:H	6	0.19
(1,1237)	1:137:A:LYS:HE2	1:138:A:VAL:H	16	0.19
(1,1237)	1:137:A:LYS:HE3	1:138:A:VAL:H	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1053)	1:127:A:LEU:HD11	1:128:A:VAL:H	7	0.19
(1,1053)	1:127:A:LEU:HD12	1:128:A:VAL:H	7	0.19
(1,1053)	1:127:A:LEU:HD13	1:128:A:VAL:H	7	0.19
(1,1053)	1:127:A:LEU:HD21	1:128:A:VAL:H	7	0.19
(1,1053)	1:127:A:LEU:HD22	1:128:A:VAL:H	7	0.19
(1,1053)	1:127:A:LEU:HD23	1:128:A:VAL:H	7	0.19
(1,549)	1:96:A:LYS:HE2	1:97:A:LEU:H	7	0.19
(1,549)	1:96:A:LYS:HE3	1:97:A:LEU:H	7	0.19
(1,3490)	1:300:A:LEU:HD21	1:303:A:THR:H	1	0.18
(1,3490)	1:300:A:LEU:HD22	1:303:A:THR:H	1	0.18
(1,3490)	1:300:A:LEU:HD23	1:303:A:THR:H	1	0.18
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	15	0.18
(1,2804)	1:250:A:ASP:H	1:250:A:ASP:HB3	1	0.18
(1,2804)	1:250:A:ASP:H	1:250:A:ASP:HB3	5	0.18
(1,2229)	1:218:A:GLU:HG3	1:219:A:TYR:H	20	0.18
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	7	0.18
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	16	0.18
(1,549)	1:96:A:LYS:HE2	1:97:A:LEU:H	5	0.18
(1,549)	1:96:A:LYS:HE3	1:97:A:LEU:H	5	0.18
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD11	6	0.18
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD12	6	0.18
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD13	6	0.18
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD21	6	0.18
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD22	6	0.18
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD23	6	0.18
(1,3490)	1:300:A:LEU:HD21	1:303:A:THR:H	20	0.17
(1,3490)	1:300:A:LEU:HD22	1:303:A:THR:H	20	0.17
(1,3490)	1:300:A:LEU:HD23	1:303:A:THR:H	20	0.17
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	2	0.17
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	5	0.17
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	9	0.17
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	10	0.17
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	16	0.17
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	18	0.17
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	19	0.17
(1,3422)	1:295:A:SER:H	1:295:A:SER:HB3	10	0.17
(1,3422)	1:295:A:SER:H	1:295:A:SER:HB3	16	0.17
(1,3227)	1:282:A:ARG:HE	1:289:A:VAL:HB	20	0.17
(1,1743)	1:183:A:LYS:HG2	1:186:A:GLU:H	18	0.17
(1,1743)	1:183:A:LYS:HG3	1:186:A:GLU:H	18	0.17
(1,1138)	1:133:A:ARG:HA	1:150:A:ASP:HA	12	0.17
(1,1108)	1:131:A:GLU:HG2	1:132:A:LYS:H	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1108)	1:131:A:GLU:HG3	1:132:A:LYS:H	7	0.17
(1,1108)	1:131:A:GLU:HG2	1:132:A:LYS:H	14	0.17
(1,1108)	1:131:A:GLU:HG3	1:132:A:LYS:H	14	0.17
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	7	0.17
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	13	0.17
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD21	15	0.17
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD22	15	0.17
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD21	15	0.17
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD22	15	0.17
(1,457)	1:90:A:VAL:HA	1:94:A:LYS:HE2	6	0.17
(1,457)	1:90:A:VAL:HA	1:94:A:LYS:HE3	6	0.17
(1,425)	1:88:A:LYS:HB2	1:89:A:LEU:H	11	0.17
(1,425)	1:88:A:LYS:HB3	1:89:A:LEU:H	11	0.17
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG2	6	0.17
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG3	6	0.17
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG2	13	0.17
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG3	13	0.17
(1,2)	1:57:A:MET:HA	1:59:A:PRO:HD2	3	0.17
(1,2)	1:57:A:MET:HA	1:59:A:PRO:HD3	3	0.17
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	6	0.16
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	11	0.16
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	12	0.16
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	13	0.16
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	20	0.16
(1,3422)	1:295:A:SER:H	1:295:A:SER:HB3	8	0.16
(1,3422)	1:295:A:SER:H	1:295:A:SER:HB3	9	0.16
(1,3422)	1:295:A:SER:H	1:295:A:SER:HB3	12	0.16
(1,2804)	1:250:A:ASP:H	1:250:A:ASP:HB3	19	0.16
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	10	0.16
(1,1237)	1:137:A:LYS:HE2	1:138:A:VAL:H	19	0.16
(1,1237)	1:137:A:LYS:HE3	1:138:A:VAL:H	19	0.16
(1,979)	1:122:A:LYS:HG2	1:125:A:GLU:HG2	5	0.16
(1,979)	1:122:A:LYS:HG2	1:125:A:GLU:HG3	5	0.16
(1,979)	1:122:A:LYS:HG3	1:125:A:GLU:HG2	5	0.16
(1,979)	1:122:A:LYS:HG3	1:125:A:GLU:HG3	5	0.16
(1,679)	1:102:A:GLY:H	1:103:A:GLU:HA	14	0.16
(1,425)	1:88:A:LYS:HB2	1:89:A:LEU:H	2	0.16
(1,425)	1:88:A:LYS:HB3	1:89:A:LEU:H	2	0.16
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD11	12	0.16
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD12	12	0.16
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD13	12	0.16
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD21	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD22	12	0.16
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD23	12	0.16
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG2	4	0.16
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG3	4	0.16
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG2	8	0.16
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG3	8	0.16
(1,55)	1:64:A:LYS:H	1:64:A:LYS:HG2	12	0.16
(1,55)	1:64:A:LYS:H	1:64:A:LYS:HG3	12	0.16
(1,55)	1:64:A:LYS:H	1:64:A:LYS:HG2	14	0.16
(1,55)	1:64:A:LYS:H	1:64:A:LYS:HG3	14	0.16
(1,45)	1:63:A:SER:H	1:64:A:LYS:HG2	14	0.16
(1,45)	1:63:A:SER:H	1:64:A:LYS:HG3	14	0.16
(1,3501)	1:301:A:LEU:HD11	1:302:A:ASP:H	8	0.15
(1,3501)	1:301:A:LEU:HD12	1:302:A:ASP:H	8	0.15
(1,3501)	1:301:A:LEU:HD13	1:302:A:ASP:H	8	0.15
(1,3501)	1:301:A:LEU:HD21	1:302:A:ASP:H	8	0.15
(1,3501)	1:301:A:LEU:HD22	1:302:A:ASP:H	8	0.15
(1,3501)	1:301:A:LEU:HD23	1:302:A:ASP:H	8	0.15
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	1	0.15
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	3	0.15
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	4	0.15
(1,3454)	1:297:A:LEU:H	1:297:A:LEU:HG	7	0.15
(1,3422)	1:295:A:SER:H	1:295:A:SER:HB3	5	0.15
(1,3422)	1:295:A:SER:H	1:295:A:SER:HB3	7	0.15
(1,3108)	1:275:A:ILE:HD11	1:276:A:ASP:H	3	0.15
(1,3108)	1:275:A:ILE:HD12	1:276:A:ASP:H	3	0.15
(1,3108)	1:275:A:ILE:HD13	1:276:A:ASP:H	3	0.15
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	4	0.15
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	4	0.15
(1,2804)	1:250:A:ASP:H	1:250:A:ASP:HB3	14	0.15
(1,2399)	1:227:A:ASN:HA	1:227:A:ASN:HD21	3	0.15
(1,2399)	1:227:A:ASN:HA	1:227:A:ASN:HD22	3	0.15
(1,2306)	1:220:A:LEU:HD21	1:278:A:VAL:HA	12	0.15
(1,2306)	1:220:A:LEU:HD22	1:278:A:VAL:HA	12	0.15
(1,2306)	1:220:A:LEU:HD23	1:278:A:VAL:HA	12	0.15
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	5	0.15
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	12	0.15
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	13	0.15
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	15	0.15
(1,2134)	1:212:A:ILE:HD11	1:213:A:LEU:H	10	0.15
(1,2134)	1:212:A:ILE:HD12	1:213:A:LEU:H	10	0.15
(1,2134)	1:212:A:ILE:HD13	1:213:A:LEU:H	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1741)	1:183:A:LYS:HE2	1:184:A:ASP:H	2	0.15
(1,1741)	1:183:A:LYS:HE3	1:184:A:ASP:H	2	0.15
(1,1138)	1:133:A:ARG:HA	1:150:A:ASP:HA	19	0.15
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD21	1	0.15
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD22	1	0.15
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD21	1	0.15
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD22	1	0.15
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD21	12	0.15
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD22	12	0.15
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD21	12	0.15
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD22	12	0.15
(1,716)	1:106:A:LYS:HG3	1:107:A:GLU:H	15	0.15
(1,706)	1:105:A:HIS:H	1:106:A:LYS:HB2	3	0.15
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG2	5	0.15
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG3	5	0.15
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG2	7	0.15
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG3	7	0.15
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG2	15	0.15
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG3	15	0.15
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG2	16	0.15
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG3	16	0.15
(1,49)	1:64:A:LYS:HB2	1:65:A:LYS:H	4	0.15
(1,49)	1:64:A:LYS:HB3	1:65:A:LYS:H	4	0.15
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	16	0.14
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	18	0.14
(2,185)	1:219:A:TYR:H	1:216:A:LEU:O	4	0.14
(2,185)	1:219:A:TYR:H	1:216:A:LEU:O	14	0.14
(1,3292)	1:287:A:LEU:HG	1:288:A:ASP:H	3	0.14
(1,3292)	1:287:A:LEU:HG	1:288:A:ASP:H	16	0.14
(1,3235)	1:282:A:ARG:H	1:289:A:VAL:HB	3	0.14
(1,3009)	1:265:A:GLN:H	1:265:A:GLN:HG3	6	0.14
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	6	0.14
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	6	0.14
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD1	19	0.14
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD2	19	0.14
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD1	19	0.14
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD2	19	0.14
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD1	19	0.14
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD2	19	0.14
(1,2229)	1:218:A:GLU:HG3	1:219:A:TYR:H	14	0.14
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	2	0.14
(1,2134)	1:212:A:ILE:HD11	1:213:A:LEU:H	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2134)	1:212:A:ILE:HD12	1:213:A:LEU:H	11	0.14
(1,2134)	1:212:A:ILE:HD13	1:213:A:LEU:H	11	0.14
(1,1741)	1:183:A:LYS:HE2	1:184:A:ASP:H	10	0.14
(1,1741)	1:183:A:LYS:HE3	1:184:A:ASP:H	10	0.14
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD11	16	0.14
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD12	16	0.14
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD13	16	0.14
(1,1259)	1:138:A:VAL:H	1:143:A:GLY:HA2	12	0.14
(1,1259)	1:138:A:VAL:H	1:143:A:GLY:HA3	12	0.14
(1,1120)	1:132:A:LYS:HG3	1:133:A:ARG:H	9	0.14
(1,1078)	1:129:A:LYS:HA	1:132:A:LYS:H	14	0.14
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	1	0.14
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	2	0.14
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	10	0.14
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	11	0.14
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD21	2	0.14
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD22	2	0.14
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD21	2	0.14
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD22	2	0.14
(1,839)	1:114:A:LYS:HE2	1:115:A:GLU:H	8	0.14
(1,839)	1:114:A:LYS:HE3	1:115:A:GLU:H	8	0.14
(1,673)	1:101:A:GLU:HB2	1:102:A:GLY:H	15	0.14
(1,521)	1:94:A:LYS:HG2	1:95:A:SER:H	6	0.14
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD11	4	0.14
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD12	4	0.14
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD13	4	0.14
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD21	4	0.14
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD22	4	0.14
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD23	4	0.14
(1,55)	1:64:A:LYS:H	1:64:A:LYS:HG2	6	0.14
(1,55)	1:64:A:LYS:H	1:64:A:LYS:HG3	6	0.14
(1,45)	1:63:A:SER:H	1:64:A:LYS:HG2	6	0.14
(1,45)	1:63:A:SER:H	1:64:A:LYS:HG3	6	0.14
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	2	0.13
(1,3501)	1:301:A:LEU:HD11	1:302:A:ASP:H	15	0.13
(1,3501)	1:301:A:LEU:HD12	1:302:A:ASP:H	15	0.13
(1,3501)	1:301:A:LEU:HD13	1:302:A:ASP:H	15	0.13
(1,3501)	1:301:A:LEU:HD21	1:302:A:ASP:H	15	0.13
(1,3501)	1:301:A:LEU:HD22	1:302:A:ASP:H	15	0.13
(1,3501)	1:301:A:LEU:HD23	1:302:A:ASP:H	15	0.13
(1,3292)	1:287:A:LEU:HG	1:288:A:ASP:H	14	0.13
(1,3286)	1:286:A:ASN:H	1:287:A:LEU:HD21	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3286)	1:286:A:ASN:H	1:287:A:LEU:HD22	20	0.13
(1,3286)	1:286:A:ASN:H	1:287:A:LEU:HD23	20	0.13
(1,3108)	1:275:A:ILE:HD11	1:276:A:ASP:H	20	0.13
(1,3108)	1:275:A:ILE:HD12	1:276:A:ASP:H	20	0.13
(1,3108)	1:275:A:ILE:HD13	1:276:A:ASP:H	20	0.13
(1,3009)	1:265:A:GLN:H	1:265:A:GLN:HG3	3	0.13
(1,2994)	1:265:A:GLN:HA	1:268:A:VAL:H	2	0.13
(1,2630)	1:239:A:LEU:H	1:263:A:GLU:HG2	8	0.13
(1,2630)	1:239:A:LEU:H	1:263:A:GLU:HG3	8	0.13
(1,2464)	1:230:A:LYS:HG3	1:231:A:GLU:H	6	0.13
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD1	11	0.13
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD2	11	0.13
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD1	11	0.13
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD2	11	0.13
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD1	11	0.13
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD2	11	0.13
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD1	17	0.13
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD2	17	0.13
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD1	17	0.13
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD2	17	0.13
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD1	17	0.13
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD2	17	0.13
(1,2421)	1:227:A:ASN:H	1:230:A:LYS:HB2	12	0.13
(1,2421)	1:227:A:ASN:H	1:230:A:LYS:HB3	12	0.13
(1,2276)	1:220:A:LEU:HD11	1:222:A:ASN:HA	12	0.13
(1,2276)	1:220:A:LEU:HD12	1:222:A:ASN:HA	12	0.13
(1,2276)	1:220:A:LEU:HD13	1:222:A:ASN:HA	12	0.13
(1,2276)	1:220:A:LEU:HD21	1:222:A:ASN:HA	12	0.13
(1,2276)	1:220:A:LEU:HD22	1:222:A:ASN:HA	12	0.13
(1,2276)	1:220:A:LEU:HD23	1:222:A:ASN:HA	12	0.13
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	4	0.13
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	17	0.13
(1,2134)	1:212:A:ILE:HD11	1:213:A:LEU:H	5	0.13
(1,2134)	1:212:A:ILE:HD12	1:213:A:LEU:H	5	0.13
(1,2134)	1:212:A:ILE:HD13	1:213:A:LEU:H	5	0.13
(1,2134)	1:212:A:ILE:HD11	1:213:A:LEU:H	17	0.13
(1,2134)	1:212:A:ILE:HD12	1:213:A:LEU:H	17	0.13
(1,2134)	1:212:A:ILE:HD13	1:213:A:LEU:H	17	0.13
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD11	14	0.13
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD12	14	0.13
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD13	14	0.13
(1,1820)	1:191:A:GLU:HB2	1:195:A:ILE:HG12	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1820)	1:191:A:GLU:HB2	1:195:A:ILE:HG13	17	0.13
(1,1820)	1:191:A:GLU:HB3	1:195:A:ILE:HG12	17	0.13
(1,1820)	1:191:A:GLU:HB3	1:195:A:ILE:HG13	17	0.13
(1,1746)	1:183:A:LYS:H	1:183:A:LYS:HD2	3	0.13
(1,1746)	1:183:A:LYS:H	1:183:A:LYS:HD3	3	0.13
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD11	3	0.13
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD12	3	0.13
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD13	3	0.13
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD11	18	0.13
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD12	18	0.13
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD13	18	0.13
(1,1471)	1:160:A:LEU:HD11	1:161:A:SER:H	1	0.13
(1,1471)	1:160:A:LEU:HD12	1:161:A:SER:H	1	0.13
(1,1471)	1:160:A:LEU:HD13	1:161:A:SER:H	1	0.13
(1,1471)	1:160:A:LEU:HD21	1:161:A:SER:H	1	0.13
(1,1471)	1:160:A:LEU:HD22	1:161:A:SER:H	1	0.13
(1,1471)	1:160:A:LEU:HD23	1:161:A:SER:H	1	0.13
(1,1305)	1:145:A:GLU:HG3	1:146:A:VAL:H	4	0.13
(1,1237)	1:137:A:LYS:HE2	1:138:A:VAL:H	3	0.13
(1,1237)	1:137:A:LYS:HE3	1:138:A:VAL:H	3	0.13
(1,1158)	1:133:A:ARG:H	1:149:A:VAL:HA	1	0.13
(1,1138)	1:133:A:ARG:HA	1:150:A:ASP:HA	3	0.13
(1,1138)	1:133:A:ARG:HA	1:150:A:ASP:HA	14	0.13
(1,1078)	1:129:A:LYS:HA	1:132:A:LYS:H	17	0.13
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	3	0.13
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	5	0.13
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	6	0.13
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	9	0.13
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	15	0.13
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	19	0.13
(1,884)	1:116:A:ILE:HG21	1:121:A:LYS:H	3	0.13
(1,884)	1:116:A:ILE:HG22	1:121:A:LYS:H	3	0.13
(1,884)	1:116:A:ILE:HG23	1:121:A:LYS:H	3	0.13
(1,482)	1:90:A:VAL:H	1:171:A:THR:HG21	12	0.13
(1,482)	1:90:A:VAL:H	1:171:A:THR:HG22	12	0.13
(1,482)	1:90:A:VAL:H	1:171:A:THR:HG23	12	0.13
(1,425)	1:88:A:LYS:HB2	1:89:A:LEU:H	9	0.13
(1,425)	1:88:A:LYS:HB3	1:89:A:LEU:H	9	0.13
(1,425)	1:88:A:LYS:HB2	1:89:A:LEU:H	17	0.13
(1,425)	1:88:A:LYS:HB3	1:89:A:LEU:H	17	0.13
(1,363)	1:84:A:THR:H	1:164:A:ILE:HD11	2	0.13
(1,363)	1:84:A:THR:H	1:164:A:ILE:HD12	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:84:A:THR:H	1:164:A:ILE:HD13	2	0.13
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD11	19	0.13
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD12	19	0.13
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD13	19	0.13
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD21	19	0.13
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD22	19	0.13
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD23	19	0.13
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD11	20	0.13
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD12	20	0.13
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD13	20	0.13
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD21	20	0.13
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD22	20	0.13
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD23	20	0.13
(1,189)	1:72:A:LEU:H	1:149:A:VAL:HG11	10	0.13
(1,189)	1:72:A:LEU:H	1:149:A:VAL:HG12	10	0.13
(1,189)	1:72:A:LEU:H	1:149:A:VAL:HG13	10	0.13
(1,189)	1:72:A:LEU:H	1:149:A:VAL:HG21	10	0.13
(1,189)	1:72:A:LEU:H	1:149:A:VAL:HG22	10	0.13
(1,189)	1:72:A:LEU:H	1:149:A:VAL:HG23	10	0.13
(1,138)	1:70:A:LEU:HD11	1:278:A:VAL:HB	5	0.13
(1,138)	1:70:A:LEU:HD12	1:278:A:VAL:HB	5	0.13
(1,138)	1:70:A:LEU:HD13	1:278:A:VAL:HB	5	0.13
(1,138)	1:70:A:LEU:HD21	1:278:A:VAL:HB	5	0.13
(1,138)	1:70:A:LEU:HD22	1:278:A:VAL:HB	5	0.13
(1,138)	1:70:A:LEU:HD23	1:278:A:VAL:HB	5	0.13
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG2	1	0.13
(1,120)	1:69:A:LYS:H	1:69:A:LYS:HG3	1	0.13
(1,45)	1:63:A:SER:H	1:64:A:LYS:HG2	12	0.13
(1,45)	1:63:A:SER:H	1:64:A:LYS:HG3	12	0.13
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	3	0.12
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	15	0.12
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	20	0.12
(2,143)	1:179:A:SER:H	1:176:A:GLU:O	3	0.12
(2,143)	1:179:A:SER:H	1:176:A:GLU:O	17	0.12
(2,49)	1:95:A:SER:H	1:91:A:GLY:O	5	0.12
(1,3235)	1:282:A:ARG:H	1:289:A:VAL:HB	2	0.12
(1,3235)	1:282:A:ARG:H	1:289:A:VAL:HB	13	0.12
(1,3009)	1:265:A:GLN:H	1:265:A:GLN:HG3	14	0.12
(1,3009)	1:265:A:GLN:H	1:265:A:GLN:HG3	15	0.12
(1,3009)	1:265:A:GLN:H	1:265:A:GLN:HG3	20	0.12
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	1	0.12
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	3	0.12
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	3	0.12
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	11	0.12
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	11	0.12
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	15	0.12
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	15	0.12
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	19	0.12
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	19	0.12
(1,2464)	1:230:A:LYS:HG3	1:231:A:GLU:H	15	0.12
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD1	4	0.12
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD2	4	0.12
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD1	4	0.12
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD2	4	0.12
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD1	4	0.12
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD2	4	0.12
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD1	12	0.12
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD2	12	0.12
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD1	12	0.12
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD2	12	0.12
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD1	12	0.12
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD2	12	0.12
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD1	14	0.12
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD2	14	0.12
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD1	14	0.12
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD2	14	0.12
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD1	14	0.12
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD2	14	0.12
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD1	20	0.12
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD2	20	0.12
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD1	20	0.12
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD2	20	0.12
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD1	20	0.12
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD2	20	0.12
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	6	0.12
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	9	0.12
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	11	0.12
(1,2134)	1:212:A:ILE:HD11	1:213:A:LEU:H	7	0.12
(1,2134)	1:212:A:ILE:HD12	1:213:A:LEU:H	7	0.12
(1,2134)	1:212:A:ILE:HD13	1:213:A:LEU:H	7	0.12
(1,2134)	1:212:A:ILE:HD11	1:213:A:LEU:H	8	0.12
(1,2134)	1:212:A:ILE:HD12	1:213:A:LEU:H	8	0.12
(1,2134)	1:212:A:ILE:HD13	1:213:A:LEU:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2134)	1:212:A:ILE:HD11	1:213:A:LEU:H	13	0.12
(1,2134)	1:212:A:ILE:HD12	1:213:A:LEU:H	13	0.12
(1,2134)	1:212:A:ILE:HD13	1:213:A:LEU:H	13	0.12
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD11	2	0.12
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD12	2	0.12
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD13	2	0.12
(1,1740)	1:183:A:LYS:HD2	1:184:A:ASP:H	18	0.12
(1,1740)	1:183:A:LYS:HD3	1:184:A:ASP:H	18	0.12
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD11	17	0.12
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD12	17	0.12
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD13	17	0.12
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	5	0.12
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	6	0.12
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	14	0.12
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	16	0.12
(1,1259)	1:138:A:VAL:H	1:143:A:GLY:HA2	19	0.12
(1,1259)	1:138:A:VAL:H	1:143:A:GLY:HA3	19	0.12
(1,1237)	1:137:A:LYS:HE2	1:138:A:VAL:H	14	0.12
(1,1237)	1:137:A:LYS:HE3	1:138:A:VAL:H	14	0.12
(1,1078)	1:129:A:LYS:HA	1:132:A:LYS:H	1	0.12
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	12	0.12
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	16	0.12
(1,1057)	1:127:A:LEU:HG	1:129:A:LYS:H	20	0.12
(1,979)	1:122:A:LYS:HG2	1:125:A:GLU:HG2	4	0.12
(1,979)	1:122:A:LYS:HG2	1:125:A:GLU:HG3	4	0.12
(1,979)	1:122:A:LYS:HG3	1:125:A:GLU:HG2	4	0.12
(1,979)	1:122:A:LYS:HG3	1:125:A:GLU:HG3	4	0.12
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD21	6	0.12
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD22	6	0.12
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD21	6	0.12
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD22	6	0.12
(1,884)	1:116:A:ILE:HG21	1:121:A:LYS:H	1	0.12
(1,884)	1:116:A:ILE:HG22	1:121:A:LYS:H	1	0.12
(1,884)	1:116:A:ILE:HG23	1:121:A:LYS:H	1	0.12
(1,884)	1:116:A:ILE:HG21	1:121:A:LYS:H	10	0.12
(1,884)	1:116:A:ILE:HG22	1:121:A:LYS:H	10	0.12
(1,884)	1:116:A:ILE:HG23	1:121:A:LYS:H	10	0.12
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD11	1	0.12
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD12	1	0.12
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD13	1	0.12
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD11	20	0.12
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD12	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD13	20	0.12
(1,838)	1:114:A:LYS:HD2	1:115:A:GLU:H	14	0.12
(1,838)	1:114:A:LYS:HD3	1:115:A:GLU:H	14	0.12
(1,672)	1:101:A:GLU:HB3	1:102:A:GLY:H	20	0.12
(1,667)	1:100:A:LEU:H	1:100:A:LEU:HD21	15	0.12
(1,667)	1:100:A:LEU:H	1:100:A:LEU:HD22	15	0.12
(1,667)	1:100:A:LEU:H	1:100:A:LEU:HD23	15	0.12
(1,618)	1:100:A:LEU:HB2	1:105:A:HIS:HA	9	0.12
(1,618)	1:100:A:LEU:HB3	1:105:A:HIS:HA	9	0.12
(1,432)	1:88:A:LYS:H	1:88:A:LYS:HE2	2	0.12
(1,432)	1:88:A:LYS:H	1:88:A:LYS:HE3	2	0.12
(1,365)	1:85:A:VAL:HA	1:88:A:LYS:HB2	11	0.12
(1,365)	1:85:A:VAL:HA	1:88:A:LYS:HB3	11	0.12
(1,232)	1:76:A:LYS:HA	1:79:A:LYS:H	6	0.12
(1,45)	1:63:A:SER:H	1:64:A:LYS:HG2	19	0.12
(1,45)	1:63:A:SER:H	1:64:A:LYS:HG3	19	0.12
(2,281)	1:306:A:GLU:H	1:302:A:ASP:O	13	0.11
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	5	0.11
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	6	0.11
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	8	0.11
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	14	0.11
(2,167)	1:207:A:ASN:H	1:203:A:GLN:O	20	0.11
(2,143)	1:179:A:SER:H	1:176:A:GLU:O	8	0.11
(2,143)	1:179:A:SER:H	1:176:A:GLU:O	14	0.11
(2,143)	1:179:A:SER:H	1:176:A:GLU:O	16	0.11
(2,143)	1:179:A:SER:H	1:176:A:GLU:O	18	0.11
(2,107)	1:158:A:SER:H	1:154:A:ALA:O	5	0.11
(2,93)	1:131:A:GLU:H	1:127:A:LEU:O	17	0.11
(2,91)	1:130:A:ILE:H	1:126:A:ASN:O	7	0.11
(1,3551)	1:306:A:GLU:HG3	1:308:A:SER:H	11	0.11
(1,3539)	1:305:A:ILE:HG21	1:306:A:GLU:H	9	0.11
(1,3539)	1:305:A:ILE:HG22	1:306:A:GLU:H	9	0.11
(1,3539)	1:305:A:ILE:HG23	1:306:A:GLU:H	9	0.11
(1,3539)	1:305:A:ILE:HG21	1:306:A:GLU:H	13	0.11
(1,3539)	1:305:A:ILE:HG22	1:306:A:GLU:H	13	0.11
(1,3539)	1:305:A:ILE:HG23	1:306:A:GLU:H	13	0.11
(1,3286)	1:286:A:ASN:H	1:287:A:LEU:HD21	11	0.11
(1,3286)	1:286:A:ASN:H	1:287:A:LEU:HD22	11	0.11
(1,3286)	1:286:A:ASN:H	1:287:A:LEU:HD23	11	0.11
(1,3175)	1:279:A:VAL:HG11	1:292:A:THR:H	13	0.11
(1,3175)	1:279:A:VAL:HG12	1:292:A:THR:H	13	0.11
(1,3175)	1:279:A:VAL:HG13	1:292:A:THR:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3175)	1:279:A:VAL:HG21	1:292:A:THR:H	13	0.11
(1,3175)	1:279:A:VAL:HG22	1:292:A:THR:H	13	0.11
(1,3175)	1:279:A:VAL:HG23	1:292:A:THR:H	13	0.11
(1,3118)	1:275:A:ILE:H	1:275:A:ILE:HD11	18	0.11
(1,3118)	1:275:A:ILE:H	1:275:A:ILE:HD12	18	0.11
(1,3118)	1:275:A:ILE:H	1:275:A:ILE:HD13	18	0.11
(1,3108)	1:275:A:ILE:HD11	1:276:A:ASP:H	9	0.11
(1,3108)	1:275:A:ILE:HD12	1:276:A:ASP:H	9	0.11
(1,3108)	1:275:A:ILE:HD13	1:276:A:ASP:H	9	0.11
(1,2994)	1:265:A:GLN:HA	1:268:A:VAL:H	13	0.11
(1,2846)	1:253:A:TYR:HE1	1:254:A:VAL:HB	14	0.11
(1,2846)	1:253:A:TYR:HE2	1:254:A:VAL:HB	14	0.11
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	5	0.11
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	5	0.11
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	8	0.11
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	8	0.11
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	16	0.11
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	16	0.11
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	17	0.11
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	17	0.11
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	18	0.11
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	18	0.11
(1,2670)	1:242:A:LEU:H	1:260:A:MET:HB2	8	0.11
(1,2670)	1:242:A:LEU:H	1:260:A:MET:HB3	8	0.11
(1,2630)	1:239:A:LEU:H	1:263:A:GLU:HG2	13	0.11
(1,2630)	1:239:A:LEU:H	1:263:A:GLU:HG3	13	0.11
(1,2503)	1:232:A:PHE:HD1	1:268:A:VAL:H	20	0.11
(1,2503)	1:232:A:PHE:HD2	1:268:A:VAL:H	20	0.11
(1,2465)	1:230:A:LYS:HG2	1:231:A:GLU:H	2	0.11
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD1	2	0.11
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD2	2	0.11
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD1	2	0.11
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD2	2	0.11
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD1	2	0.11
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD2	2	0.11
(1,2421)	1:227:A:ASN:H	1:230:A:LYS:HB2	3	0.11
(1,2421)	1:227:A:ASN:H	1:230:A:LYS:HB3	3	0.11
(1,2421)	1:227:A:ASN:H	1:230:A:LYS:HB2	9	0.11
(1,2421)	1:227:A:ASN:H	1:230:A:LYS:HB3	9	0.11
(1,2321)	1:220:A:LEU:H	1:221:A:ASN:HD21	6	0.11
(1,2321)	1:220:A:LEU:H	1:221:A:ASN:HD22	6	0.11
(1,2306)	1:220:A:LEU:HD21	1:278:A:VAL:HA	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2306)	1:220:A:LEU:HD22	1:278:A:VAL:HA	16	0.11
(1,2306)	1:220:A:LEU:HD23	1:278:A:VAL:HA	16	0.11
(1,2306)	1:220:A:LEU:HD21	1:278:A:VAL:HA	20	0.11
(1,2306)	1:220:A:LEU:HD22	1:278:A:VAL:HA	20	0.11
(1,2306)	1:220:A:LEU:HD23	1:278:A:VAL:HA	20	0.11
(1,2230)	1:218:A:GLU:HG2	1:219:A:TYR:H	3	0.11
(1,2230)	1:218:A:GLU:HG2	1:219:A:TYR:H	6	0.11
(1,2230)	1:218:A:GLU:HG2	1:219:A:TYR:H	10	0.11
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	8	0.11
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	18	0.11
(1,2227)	1:218:A:GLU:HA	1:221:A:ASN:H	20	0.11
(1,2134)	1:212:A:ILE:HD11	1:213:A:LEU:H	16	0.11
(1,2134)	1:212:A:ILE:HD12	1:213:A:LEU:H	16	0.11
(1,2134)	1:212:A:ILE:HD13	1:213:A:LEU:H	16	0.11
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD11	4	0.11
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD12	4	0.11
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD13	4	0.11
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD11	20	0.11
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD12	20	0.11
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD13	20	0.11
(1,2057)	1:205:A:SER:H	1:205:A:SER:HG	7	0.11
(1,1997)	1:202:A:LEU:HD11	1:206:A:CYS:H	14	0.11
(1,1997)	1:202:A:LEU:HD12	1:206:A:CYS:H	14	0.11
(1,1997)	1:202:A:LEU:HD13	1:206:A:CYS:H	14	0.11
(1,1997)	1:202:A:LEU:HD21	1:206:A:CYS:H	14	0.11
(1,1997)	1:202:A:LEU:HD22	1:206:A:CYS:H	14	0.11
(1,1997)	1:202:A:LEU:HD23	1:206:A:CYS:H	14	0.11
(1,1920)	1:196:A:LYS:HA	1:199:A:ALA:H	3	0.11
(1,1895)	1:195:A:ILE:HA	1:199:A:ALA:HB1	19	0.11
(1,1895)	1:195:A:ILE:HA	1:199:A:ALA:HB2	19	0.11
(1,1895)	1:195:A:ILE:HA	1:199:A:ALA:HB3	19	0.11
(1,1555)	1:168:A:LYS:HG2	1:169:A:THR:H	6	0.11
(1,1555)	1:168:A:LYS:HG3	1:169:A:THR:H	6	0.11
(1,1555)	1:168:A:LYS:HG2	1:169:A:THR:H	11	0.11
(1,1555)	1:168:A:LYS:HG3	1:169:A:THR:H	11	0.11
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD11	5	0.11
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD12	5	0.11
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD13	5	0.11
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD11	12	0.11
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD12	12	0.11
(1,1488)	1:161:A:SER:H	1:300:A:LEU:HD13	12	0.11
(1,1474)	1:160:A:LEU:HD21	1:161:A:SER:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1474)	1:160:A:LEU:HD22	1:161:A:SER:H	2	0.11
(1,1474)	1:160:A:LEU:HD23	1:161:A:SER:H	2	0.11
(1,1474)	1:160:A:LEU:HD21	1:161:A:SER:H	19	0.11
(1,1474)	1:160:A:LEU:HD22	1:161:A:SER:H	19	0.11
(1,1474)	1:160:A:LEU:HD23	1:161:A:SER:H	19	0.11
(1,1442)	1:158:A:SER:HA	1:161:A:SER:H	9	0.11
(1,1442)	1:158:A:SER:HA	1:161:A:SER:H	10	0.11
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	3	0.11
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	4	0.11
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	8	0.11
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	10	0.11
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	11	0.11
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	13	0.11
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	18	0.11
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	19	0.11
(1,1261)	1:138:A:VAL:H	1:144:A:ALA:H	2	0.11
(1,1259)	1:138:A:VAL:H	1:143:A:GLY:HA2	11	0.11
(1,1259)	1:138:A:VAL:H	1:143:A:GLY:HA3	11	0.11
(1,1241)	1:137:A:LYS:H	1:137:A:LYS:HE2	2	0.11
(1,1241)	1:137:A:LYS:H	1:137:A:LYS:HE3	2	0.11
(1,1241)	1:137:A:LYS:H	1:137:A:LYS:HE2	9	0.11
(1,1241)	1:137:A:LYS:H	1:137:A:LYS:HE3	9	0.11
(1,1138)	1:133:A:ARG:HA	1:150:A:ASP:HA	17	0.11
(1,1138)	1:133:A:ARG:HA	1:150:A:ASP:HA	20	0.11
(1,1121)	1:132:A:LYS:HG2	1:133:A:ARG:H	8	0.11
(1,1096)	1:130:A:ILE:HG21	1:131:A:GLU:H	20	0.11
(1,1096)	1:130:A:ILE:HG22	1:131:A:GLU:H	20	0.11
(1,1096)	1:130:A:ILE:HG23	1:131:A:GLU:H	20	0.11
(1,1053)	1:127:A:LEU:HD11	1:128:A:VAL:H	11	0.11
(1,1053)	1:127:A:LEU:HD12	1:128:A:VAL:H	11	0.11
(1,1053)	1:127:A:LEU:HD13	1:128:A:VAL:H	11	0.11
(1,1053)	1:127:A:LEU:HD21	1:128:A:VAL:H	11	0.11
(1,1053)	1:127:A:LEU:HD22	1:128:A:VAL:H	11	0.11
(1,1053)	1:127:A:LEU:HD23	1:128:A:VAL:H	11	0.11
(1,1050)	1:127:A:LEU:HA	1:130:A:ILE:H	14	0.11
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD21	4	0.11
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD22	4	0.11
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD21	4	0.11
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD22	4	0.11
(1,884)	1:116:A:ILE:HG21	1:121:A:LYS:H	6	0.11
(1,884)	1:116:A:ILE:HG22	1:121:A:LYS:H	6	0.11
(1,884)	1:116:A:ILE:HG23	1:121:A:LYS:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,884)	1:116:A:ILE:HG21	1:121:A:LYS:H	12	0.11
(1,884)	1:116:A:ILE:HG22	1:121:A:LYS:H	12	0.11
(1,884)	1:116:A:ILE:HG23	1:121:A:LYS:H	12	0.11
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD11	8	0.11
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD12	8	0.11
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD13	8	0.11
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD11	11	0.11
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD12	11	0.11
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD13	11	0.11
(1,685)	1:103:A:GLU:H	1:103:A:GLU:HG2	8	0.11
(1,685)	1:103:A:GLU:H	1:103:A:GLU:HG3	8	0.11
(1,672)	1:101:A:GLU:HB3	1:102:A:GLY:H	19	0.11
(1,618)	1:100:A:LEU:HB2	1:105:A:HIS:HA	5	0.11
(1,618)	1:100:A:LEU:HB3	1:105:A:HIS:HA	5	0.11
(1,538)	1:95:A:SER:HA	1:98:A:ASN:H	15	0.11
(1,426)	1:88:A:LYS:HB3	1:89:A:LEU:H	5	0.11
(1,365)	1:85:A:VAL:HA	1:88:A:LYS:HB2	17	0.11
(1,365)	1:85:A:VAL:HA	1:88:A:LYS:HB3	17	0.11
(1,218)	1:75:A:MET:HA	1:78:A:THR:H	5	0.11
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD11	16	0.11
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD12	16	0.11
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD13	16	0.11
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD21	16	0.11
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD22	16	0.11
(1,201)	1:73:A:ASP:H	1:74:A:LEU:HD23	16	0.11
(1,72)	1:66:A:LYS:HA	1:69:A:LYS:H	17	0.11
(2,281)	1:306:A:GLU:H	1:302:A:ASP:O	8	0.1
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	11	0.1
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	13	0.1
(2,259)	1:285:A:GLU:H	1:282:A:ARG:O	19	0.1
(2,185)	1:219:A:TYR:H	1:216:A:LEU:O	9	0.1
(2,185)	1:219:A:TYR:H	1:216:A:LEU:O	18	0.1
(2,143)	1:179:A:SER:H	1:176:A:GLU:O	11	0.1
(1,3551)	1:306:A:GLU:HG3	1:308:A:SER:H	1	0.1
(1,3551)	1:306:A:GLU:HG3	1:308:A:SER:H	19	0.1
(1,3318)	1:289:A:VAL:HG21	1:294:A:PHE:HZ	20	0.1
(1,3318)	1:289:A:VAL:HG22	1:294:A:PHE:HZ	20	0.1
(1,3318)	1:289:A:VAL:HG23	1:294:A:PHE:HZ	20	0.1
(1,3290)	1:287:A:LEU:HB2	1:289:A:VAL:H	1	0.1
(1,3290)	1:287:A:LEU:HB3	1:289:A:VAL:H	1	0.1
(1,3281)	1:286:A:ASN:H	1:286:A:ASN:HD21	4	0.1
(1,3281)	1:286:A:ASN:H	1:286:A:ASN:HD22	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3235)	1:282:A:ARG:H	1:289:A:VAL:HB	11	0.1
(1,3009)	1:265:A:GLN:H	1:265:A:GLN:HG3	9	0.1
(1,3009)	1:265:A:GLN:H	1:265:A:GLN:HG3	12	0.1
(1,3009)	1:265:A:GLN:H	1:265:A:GLN:HG3	18	0.1
(1,2845)	1:253:A:TYR:HE1	1:254:A:VAL:HA	9	0.1
(1,2845)	1:253:A:TYR:HE2	1:254:A:VAL:HA	9	0.1
(1,2786)	1:249:A:LYS:HG2	1:250:A:ASP:HB2	19	0.1
(1,2786)	1:249:A:LYS:HG2	1:250:A:ASP:HB3	19	0.1
(1,2786)	1:249:A:LYS:HG3	1:250:A:ASP:HB2	19	0.1
(1,2786)	1:249:A:LYS:HG3	1:250:A:ASP:HB3	19	0.1
(1,2737)	1:246:A:VAL:HG11	1:258:A:ARG:H	3	0.1
(1,2737)	1:246:A:VAL:HG12	1:258:A:ARG:H	3	0.1
(1,2737)	1:246:A:VAL:HG13	1:258:A:ARG:H	3	0.1
(1,2621)	1:239:A:LEU:HG	1:241:A:SER:H	17	0.1
(1,2465)	1:230:A:LYS:HG2	1:231:A:GLU:H	16	0.1
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD1	6	0.1
(1,2433)	1:228:A:ILE:HG21	1:232:A:PHE:HD2	6	0.1
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD1	6	0.1
(1,2433)	1:228:A:ILE:HG22	1:232:A:PHE:HD2	6	0.1
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD1	6	0.1
(1,2433)	1:228:A:ILE:HG23	1:232:A:PHE:HD2	6	0.1
(1,2405)	1:227:A:ASN:HB2	1:228:A:ILE:HD11	10	0.1
(1,2405)	1:227:A:ASN:HB2	1:228:A:ILE:HD12	10	0.1
(1,2405)	1:227:A:ASN:HB2	1:228:A:ILE:HD13	10	0.1
(1,2405)	1:227:A:ASN:HB3	1:228:A:ILE:HD11	10	0.1
(1,2405)	1:227:A:ASN:HB3	1:228:A:ILE:HD12	10	0.1
(1,2405)	1:227:A:ASN:HB3	1:228:A:ILE:HD13	10	0.1
(1,2230)	1:218:A:GLU:HG2	1:219:A:TYR:H	4	0.1
(1,2169)	1:213:A:LEU:HD11	1:271:A:VAL:H	2	0.1
(1,2169)	1:213:A:LEU:HD12	1:271:A:VAL:H	2	0.1
(1,2169)	1:213:A:LEU:HD13	1:271:A:VAL:H	2	0.1
(1,2169)	1:213:A:LEU:HD21	1:271:A:VAL:H	2	0.1
(1,2169)	1:213:A:LEU:HD22	1:271:A:VAL:H	2	0.1
(1,2169)	1:213:A:LEU:HD23	1:271:A:VAL:H	2	0.1
(1,2158)	1:213:A:LEU:HD11	1:232:A:PHE:HA	9	0.1
(1,2158)	1:213:A:LEU:HD12	1:232:A:PHE:HA	9	0.1
(1,2158)	1:213:A:LEU:HD13	1:232:A:PHE:HA	9	0.1
(1,2158)	1:213:A:LEU:HD21	1:232:A:PHE:HA	9	0.1
(1,2158)	1:213:A:LEU:HD22	1:232:A:PHE:HA	9	0.1
(1,2158)	1:213:A:LEU:HD23	1:232:A:PHE:HA	9	0.1
(1,2134)	1:212:A:ILE:HD11	1:213:A:LEU:H	1	0.1
(1,2134)	1:212:A:ILE:HD12	1:213:A:LEU:H	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2134)	1:212:A:ILE:HD13	1:213:A:LEU:H	1	0.1
(1,2134)	1:212:A:ILE:HD11	1:213:A:LEU:H	18	0.1
(1,2134)	1:212:A:ILE:HD12	1:213:A:LEU:H	18	0.1
(1,2134)	1:212:A:ILE:HD13	1:213:A:LEU:H	18	0.1
(1,2134)	1:212:A:ILE:HD11	1:213:A:LEU:H	20	0.1
(1,2134)	1:212:A:ILE:HD12	1:213:A:LEU:H	20	0.1
(1,2134)	1:212:A:ILE:HD13	1:213:A:LEU:H	20	0.1
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD11	6	0.1
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD12	6	0.1
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD13	6	0.1
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD11	18	0.1
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD12	18	0.1
(1,2127)	1:211:A:THR:H	1:212:A:ILE:HD13	18	0.1
(1,1895)	1:195:A:ILE:HA	1:199:A:ALA:HB1	11	0.1
(1,1895)	1:195:A:ILE:HA	1:199:A:ALA:HB2	11	0.1
(1,1895)	1:195:A:ILE:HA	1:199:A:ALA:HB3	11	0.1
(1,1895)	1:195:A:ILE:HA	1:199:A:ALA:HB1	15	0.1
(1,1895)	1:195:A:ILE:HA	1:199:A:ALA:HB2	15	0.1
(1,1895)	1:195:A:ILE:HA	1:199:A:ALA:HB3	15	0.1
(1,1743)	1:183:A:LYS:HG2	1:186:A:GLU:H	1	0.1
(1,1743)	1:183:A:LYS:HG3	1:186:A:GLU:H	1	0.1
(1,1743)	1:183:A:LYS:HG2	1:186:A:GLU:H	2	0.1
(1,1743)	1:183:A:LYS:HG3	1:186:A:GLU:H	2	0.1
(1,1606)	1:172:A:ASP:HB2	1:173:A:ASP:H	13	0.1
(1,1606)	1:172:A:ASP:HB3	1:173:A:ASP:H	13	0.1
(1,1606)	1:172:A:ASP:HB2	1:173:A:ASP:H	14	0.1
(1,1606)	1:172:A:ASP:HB3	1:173:A:ASP:H	14	0.1
(1,1555)	1:168:A:LYS:HG2	1:169:A:THR:H	19	0.1
(1,1555)	1:168:A:LYS:HG3	1:169:A:THR:H	19	0.1
(1,1549)	1:168:A:LYS:HA	1:171:A:THR:H	13	0.1
(1,1487)	1:161:A:SER:H	1:300:A:LEU:HD11	12	0.1
(1,1487)	1:161:A:SER:H	1:300:A:LEU:HD12	12	0.1
(1,1487)	1:161:A:SER:H	1:300:A:LEU:HD13	12	0.1
(1,1487)	1:161:A:SER:H	1:300:A:LEU:HD21	12	0.1
(1,1487)	1:161:A:SER:H	1:300:A:LEU:HD22	12	0.1
(1,1487)	1:161:A:SER:H	1:300:A:LEU:HD23	12	0.1
(1,1474)	1:160:A:LEU:HD21	1:161:A:SER:H	7	0.1
(1,1474)	1:160:A:LEU:HD22	1:161:A:SER:H	7	0.1
(1,1474)	1:160:A:LEU:HD23	1:161:A:SER:H	7	0.1
(1,1474)	1:160:A:LEU:HD21	1:161:A:SER:H	10	0.1
(1,1474)	1:160:A:LEU:HD22	1:161:A:SER:H	10	0.1
(1,1474)	1:160:A:LEU:HD23	1:161:A:SER:H	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1442)	1:158:A:SER:HA	1:161:A:SER:H	7	0.1
(1,1442)	1:158:A:SER:HA	1:161:A:SER:H	13	0.1
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	7	0.1
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	9	0.1
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	15	0.1
(1,1275)	1:139:A:PRO:HG3	1:140:A:ALA:H	17	0.1
(1,1261)	1:138:A:VAL:H	1:144:A:ALA:H	5	0.1
(1,1261)	1:138:A:VAL:H	1:144:A:ALA:H	17	0.1
(1,1259)	1:138:A:VAL:H	1:143:A:GLY:HA2	10	0.1
(1,1259)	1:138:A:VAL:H	1:143:A:GLY:HA3	10	0.1
(1,1163)	1:134:A:LYS:HD2	1:135:A:LYS:H	7	0.1
(1,1163)	1:134:A:LYS:HD3	1:135:A:LYS:H	7	0.1
(1,1150)	1:133:A:ARG:HD2	1:147:A:ASP:H	4	0.1
(1,1150)	1:133:A:ARG:HD3	1:147:A:ASP:H	4	0.1
(1,1081)	1:129:A:LYS:HG3	1:130:A:ILE:H	18	0.1
(1,1053)	1:127:A:LEU:HD11	1:128:A:VAL:H	12	0.1
(1,1053)	1:127:A:LEU:HD12	1:128:A:VAL:H	12	0.1
(1,1053)	1:127:A:LEU:HD13	1:128:A:VAL:H	12	0.1
(1,1053)	1:127:A:LEU:HD21	1:128:A:VAL:H	12	0.1
(1,1053)	1:127:A:LEU:HD22	1:128:A:VAL:H	12	0.1
(1,1053)	1:127:A:LEU:HD23	1:128:A:VAL:H	12	0.1
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD21	8	0.1
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD22	8	0.1
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD21	8	0.1
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD22	8	0.1
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD21	17	0.1
(1,945)	1:120:A:ASN:HD21	1:124:A:ASN:HD22	17	0.1
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD21	17	0.1
(1,945)	1:120:A:ASN:HD22	1:124:A:ASN:HD22	17	0.1
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD11	14	0.1
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD12	14	0.1
(1,865)	1:115:A:GLU:H	1:116:A:ILE:HD13	14	0.1
(1,841)	1:114:A:LYS:HG3	1:115:A:GLU:H	4	0.1
(1,804)	1:111:A:GLU:H	1:111:A:GLU:HG3	18	0.1
(1,721)	1:106:A:LYS:H	1:106:A:LYS:HD2	5	0.1
(1,721)	1:106:A:LYS:H	1:106:A:LYS:HD3	5	0.1
(1,711)	1:106:A:LYS:HA	1:110:A:ALA:H	15	0.1
(1,705)	1:105:A:HIS:H	1:106:A:LYS:HB3	15	0.1
(1,551)	1:96:A:LYS:H	1:96:A:LYS:HG2	18	0.1
(1,551)	1:96:A:LYS:H	1:96:A:LYS:HG3	18	0.1
(1,365)	1:85:A:VAL:HA	1:88:A:LYS:HB2	2	0.1
(1,365)	1:85:A:VAL:HA	1:88:A:LYS:HB3	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:84:A:THR:H	1:164:A:ILE:HD11	7	0.1
(1,363)	1:84:A:THR:H	1:164:A:ILE:HD12	7	0.1
(1,363)	1:84:A:THR:H	1:164:A:ILE:HD13	7	0.1
(1,204)	1:74:A:LEU:HA	1:77:A:GLU:H	8	0.1
(1,194)	1:73:A:ASP:HA	1:76:A:LYS:H	7	0.1
(1,62)	1:65:A:LYS:HB3	1:66:A:LYS:H	19	0.1

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found