



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 08:40 PM UTC

PDB ID : 2MUT / pdb_00002mut
BMRB ID : 25232
Title : Solution structure of the F231L mutant ERCC1-XPF dimerization region
Authors : Faridounnia, M.; Wienk, H.; Kovacic, L.; Folkers, G.E.; Jaspers, N.G.J.;
Kaptein, R.; Hoeijmakers, J.H.J.; Boelens, R.
Deposited on : 2014-09-17

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

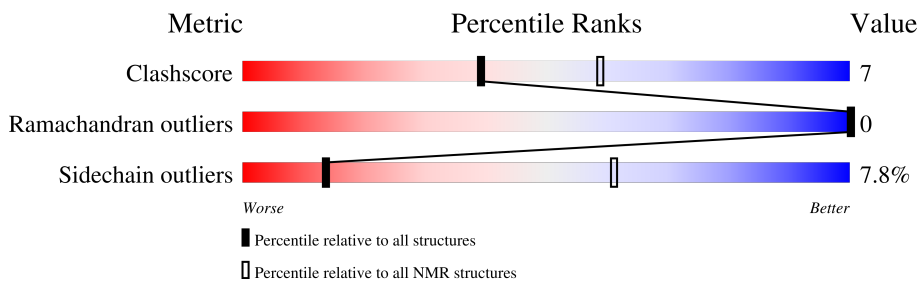
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	96	
2	B	84	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 14 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:230-A:295, B:833-B:894 (128)	0.37	14

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 1 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2846 atoms, of which 1431 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA excision repair protein ERCC-1.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	96	1553	481	784	145	139	4	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	ARG	-	expression tag	UNP P07992
A	213	ILE	-	expression tag	UNP P07992
A	214	ARG	-	expression tag	UNP P07992
A	215	ARG	-	expression tag	UNP P07992
A	216	ARG	-	expression tag	UNP P07992
A	217	TYR	-	expression tag	UNP P07992
A	218	ASN	-	expression tag	UNP P07992
A	219	MET	-	expression tag	UNP P07992
A	231	LEU	PHE	engineered mutation	UNP P07992
A	298	GLY	-	expression tag	UNP P07992
A	299	GLY	-	expression tag	UNP P07992
A	300	LEU	-	expression tag	UNP P07992
A	301	GLU	-	expression tag	UNP P07992
A	302	HIS	-	expression tag	UNP P07992
A	303	HIS	-	expression tag	UNP P07992
A	304	HIS	-	expression tag	UNP P07992
A	305	HIS	-	expression tag	UNP P07992
A	306	HIS	-	expression tag	UNP P07992
A	307	HIS	-	expression tag	UNP P07992

- Molecule 2 is a protein called DNA repair endonuclease XPF.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
2	B	84	1293	405	647	111	126	4	0

There is a discrepancy between the modelled and reference sequences:

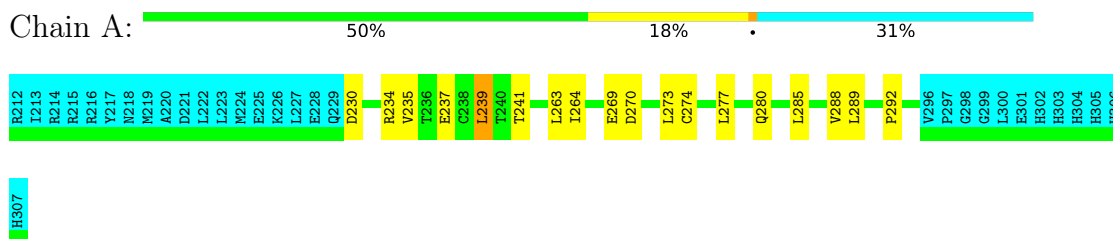
Chain	Residue	Modelled	Actual	Comment	Reference
B	822	MET	-	initiating methionine	UNP Q92889

4 Residue-property plots [i](#)

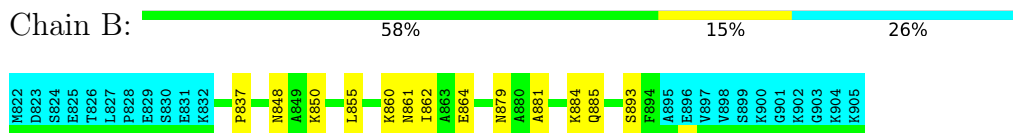
4.1 Average score per residue in the NMR ensemble

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: DNA excision repair protein ERCC-1



- Molecule 2: DNA repair endonuclease XPF

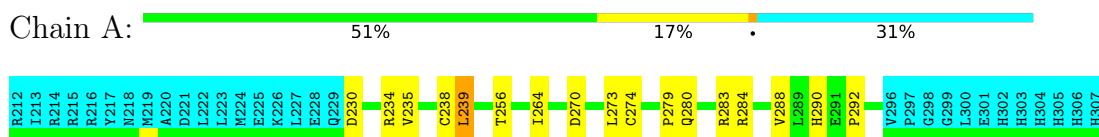


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

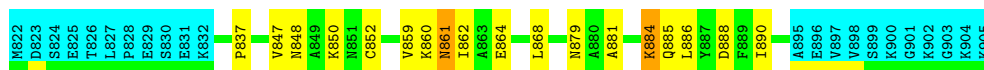
4.2.1 Score per residue for model 1

- Molecule 1: DNA excision repair protein ERCC-1



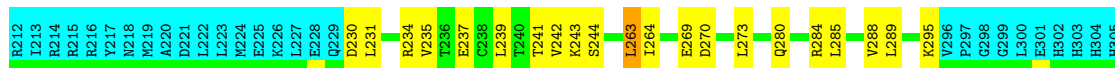
- Molecule 2: DNA repair endonuclease XPF





4.2.2 Score per residue for model 2

- Molecule 1: DNA excision repair protein ERCC-1



- Molecule 2: DNA repair endonuclease XPF



4.2.3 Score per residue for model 3

- Molecule 1: DNA excision repair protein ERCC-1



- Molecule 2: DNA repair endonuclease XPF



4.2.4 Score per residue for model 4

- Molecule 1: DNA excision repair protein ERCC-1



H301
H302
H303
H304
H305
H306
H307

- Molecule 2: DNA repair endonuclease XPF

Chain B:  57% 17% 26%

M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832 K833 V834 M837 Q838 D839 V847 M848 C852 I862 N879 A880 A881 K884 Q885 F889 T892 A895 E896 V897 S898 S899 K900 G901 K902 G903 K904 K905

4.2.5 Score per residue for model 5

- Molecule 1: DNA excision repair protein ERCC-1

Chain A:  52% 17% 31%

R212 L213 R214 R215 R216 R217 V218 W219 N220 D221 E222 L223 L224 W225 E226 K227 L228 E229 Q230 L231 V235 T236 E237 C238 L239 T240 T241 L254 T255 T256 L263 L264 D270 L273 C274 L285 V288 L289 P292 V296 G297 G298 L300 E301 H302 H303 H304 H305 H306 H307

- Molecule 2: DNA repair endonuclease XPF

Chain B:  54% 20% 26%

M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832 K833 V837 M836 D839 F840 L841 L842 K843 M844 L855 V859 K860 M861 I862 N879 A880 A881 K884 Q885 D888 F889 T892 S893 F894 A895 P896 V897 S899 K900 G901 K902 G903 K904 K905

4.2.6 Score per residue for model 6

- Molecule 1: DNA excision repair protein ERCC-1

Chain A:  49% 19% 31%

R212 L213 R214 R215 R216 R217 V218 W219 N220 D221 L222 L223 L224 W225 E226 K227 L228 E229 Q230 V232 V235 T236 E237 C238 L239 T240 T241 L256 E261 Q262 L263 L264 D270 L273 C274 Q280 R284 L285 V288 L289 P292 F295 L294 V296 G297 G298 L300 E301 H302

H303
H304
H305
H306
H307

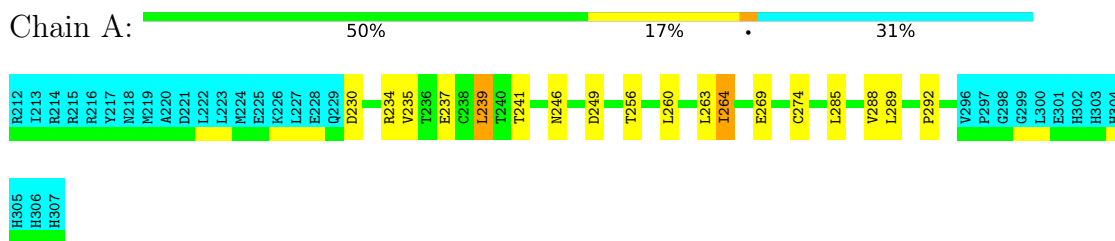
- Molecule 2: DNA repair endonuclease XPF

Chain B:  62% 10% 26%

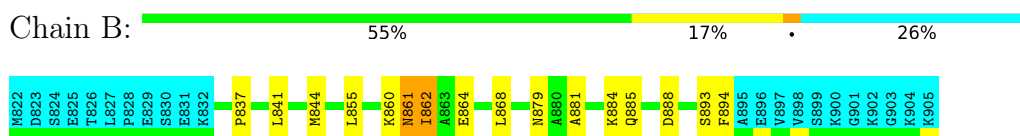
M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832 K833 P837 L855 K860 N861 I862 A865 E864 N879 A880 A881 Q885 S893 F894 A895 E896 V897 V898 S899 K900 G901 K902 G903 K904 K905

4.2.7 Score per residue for model 7

- Molecule 1: DNA excision repair protein ERCC-1

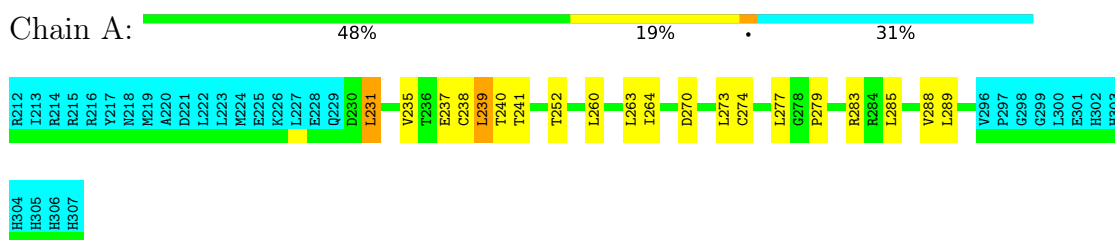


- Molecule 2: DNA repair endonuclease XPF

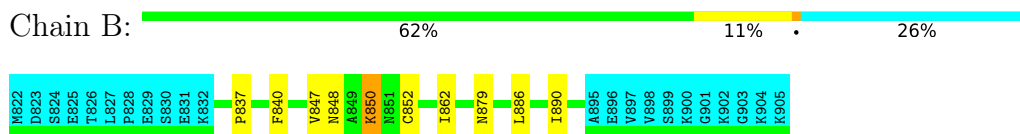


4.2.8 Score per residue for model 8

- Molecule 1: DNA excision repair protein ERCC-1

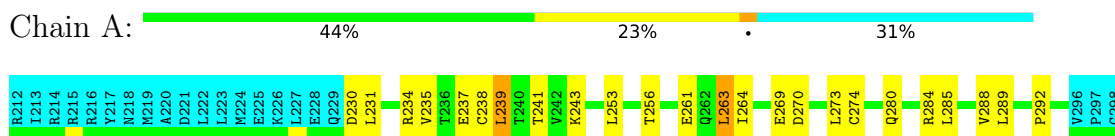


- Molecule 2: DNA repair endonuclease XPF



4.2.9 Score per residue for model 9

- Molecule 1: DNA excision repair protein ERCC-1



G299
L300
E301
H302
H303
H304
H305
H306
H307

- Molecule 2: DNA repair endonuclease XPF

Chain B:  55% 19% 26%

M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832
P837 Q838 Q839 F840 L841 L842 C852 L855 K860 K861 N862 L865 N879 A880 A881 Q885 F889 T892 S893 F894 E895 E896 V897 V898 S899 K900 G901 K902 G903 K904 K905

4.2.10 Score per residue for model 10

- Molecule 1: DNA excision repair protein ERCC-1

Chain A:  50% 15% 31%

R212 I213 R214 R215 R216 R217 Y217 N218 M219 A220 A221 L222 L223 M224 E225 K226 L227 E228 Q229 D230 L231 V235 T236 E237 C238 L239 T240 T241 L260 L263 L264 D270 L273 C274 L277 Q280 R284 L285 V288 L289 P292 V296 P297 Q298 Q299 L300 E301 H302 H303 H304

H305
H306
H307

- Molecule 2: DNA repair endonuclease XPF

Chain B:  56% 17% 26%

M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832
P837 Q838 Q839 F840 L841 L842 C852 K860 N861 I862 A863 E864 N879 K884 Q885 L886 T887 F888 I890 S893 F894 A895 E896 V897 V898 S899 K900 G901 K902 G903 K904 K905

4.2.11 Score per residue for model 11

- Molecule 1: DNA excision repair protein ERCC-1

Chain A:  47% 21% 31%

R212 I213 R214 R215 R216 R217 Y217 N218 M219 A220 A221 L222 L223 M224 E225 K226 L227 E228 Q229 D230 R234 V235 T236 E237 C238 L239 T240 T241 N246 K247 T248 T252 L253 T256 L263 I264 E269 C274 L277 Q280 R284 P292 F293 L294 K295 V296 P297 Q298 G299 L300

E301
H302
H303
H304
H305
H306
H307

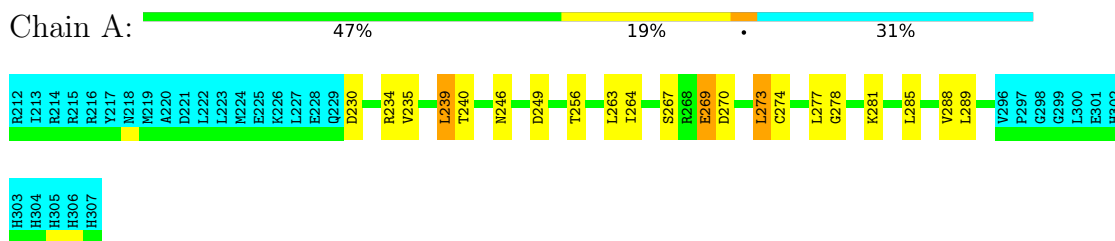
- Molecule 2: DNA repair endonuclease XPF

Chain B:  50% 21% 26%

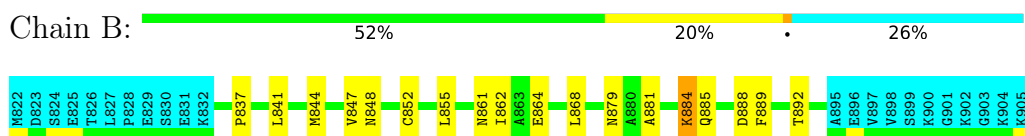
M822 D823 S824 E825 T826 L827 P828 E829 S830 E831 K832
D839 F840 L841 L842 K843 M844 V847 K850 N851 C852 L855 M856 M857 K860 N861 I862 N879 A880 A881 K884 Q885 L886 I890 S893 F894 E895 E896 V897 V898 S899 K900 G901 K902 G903 K904 K905

4.2.12 Score per residue for model 12

- Molecule 1: DNA excision repair protein ERCC-1

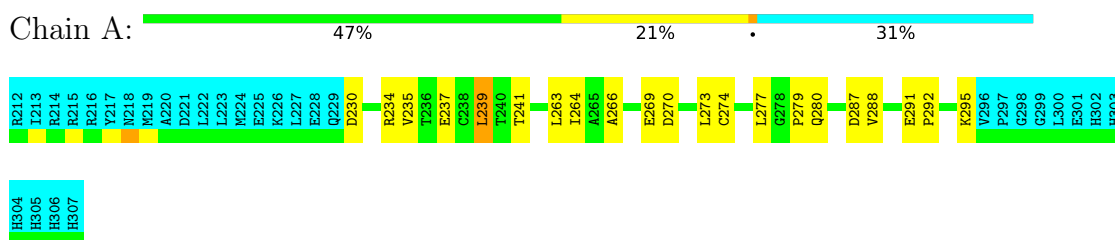


- Molecule 2: DNA repair endonuclease XPF

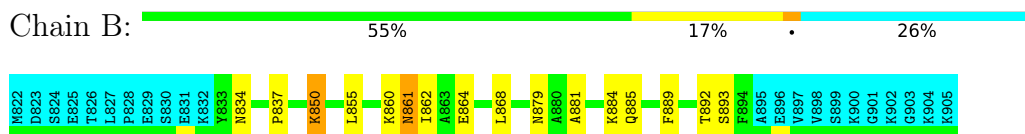


4.2.13 Score per residue for model 13

- Molecule 1: DNA excision repair protein ERCC-1

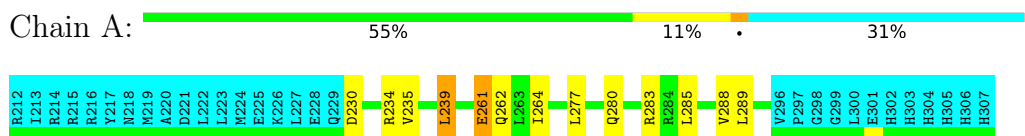


- Molecule 2: DNA repair endonuclease XPF

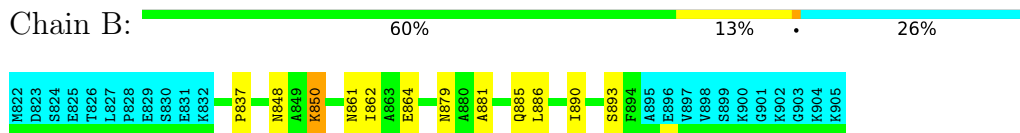


4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: DNA excision repair protein ERCC-1

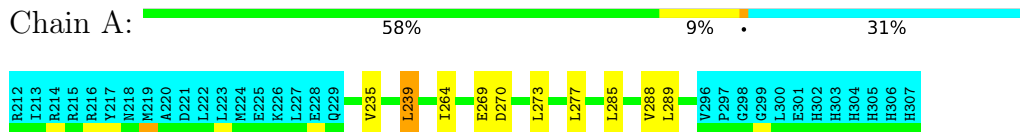


- Molecule 2: DNA repair endonuclease XPF

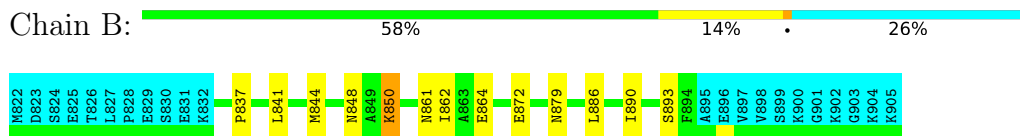


4.2.15 Score per residue for model 15

- Molecule 1: DNA excision repair protein ERCC-1

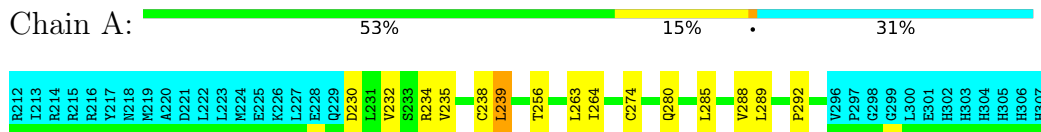


- Molecule 2: DNA repair endonuclease XPF

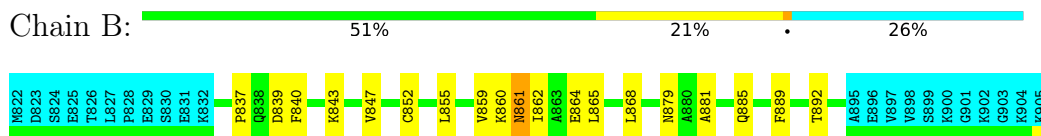


4.2.16 Score per residue for model 16

- Molecule 1: DNA excision repair protein ERCC-1

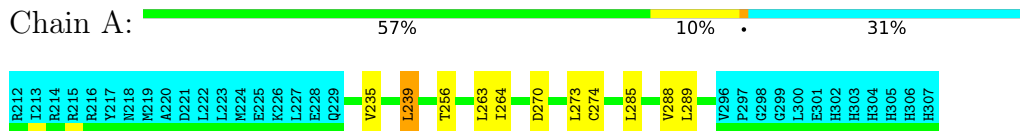


- Molecule 2: DNA repair endonuclease XPF

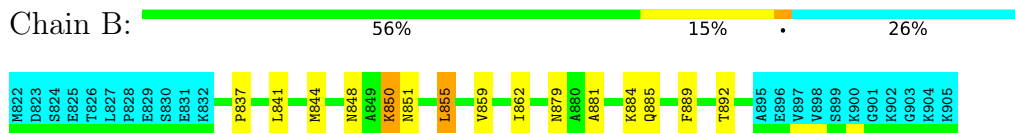


4.2.17 Score per residue for model 17

- Molecule 1: DNA excision repair protein ERCC-1

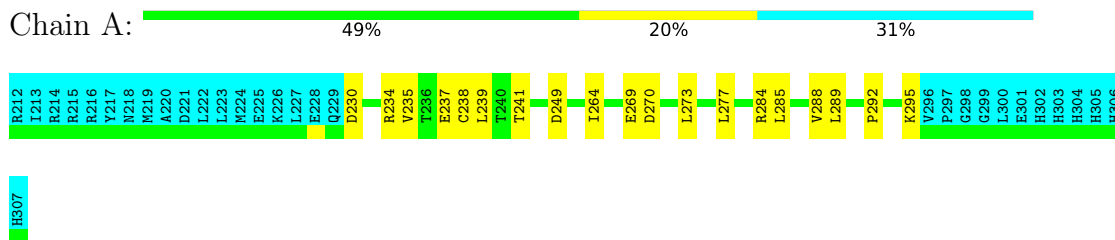


- Molecule 2: DNA repair endonuclease XPF

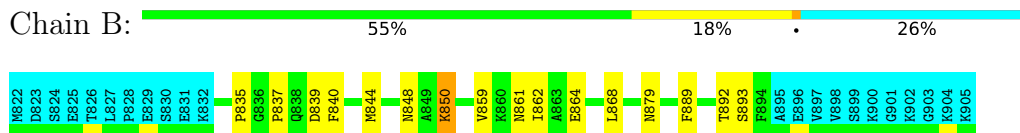


4.2.18 Score per residue for model 18

- Molecule 1: DNA excision repair protein ERCC-1

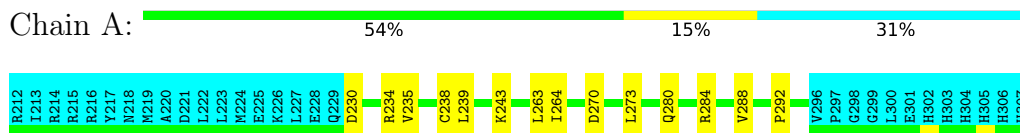


- Molecule 2: DNA repair endonuclease XPF

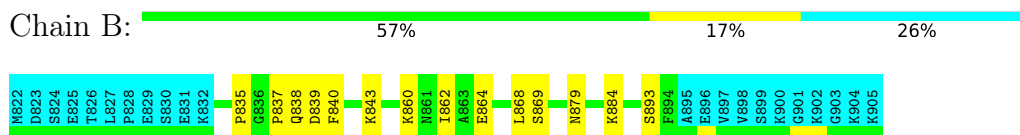


4.2.19 Score per residue for model 19

- Molecule 1: DNA excision repair protein ERCC-1



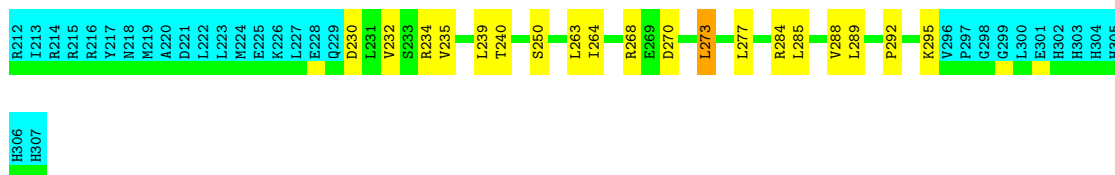
- Molecule 2: DNA repair endonuclease XPF



4.2.20 Score per residue for model 20

- Molecule 1: DNA excision repair protein ERCC-1

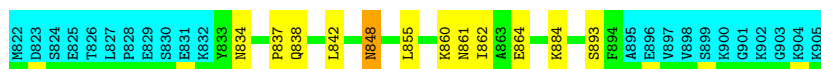




H306
H307

- Molecule 2: DNA repair endonuclease XPF

Chain B: 60% 13% 26%



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CYANA	structure solution	
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	2040
Number of shifts mapped to atoms	2040
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

6 Model quality i

6.1 Standard geometry i

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	1.01±0.02	0±0/516 (0.0± 0.0%)	1.03±0.03	0±0/700 (0.0± 0.0%)
2	B	1.00±0.04	0±0/492 (0.0± 0.1%)	1.12±0.02	0±0/667 (0.0± 0.0%)
All	All	1.00	4/20160 (0.0%)	1.08	2/27340 (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	0.1±0.3
All	All	0	2

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	B	872	GLU	N-CA	-5.89	1.39	1.46	15	1
2	B	855	LEU	C-O	-5.60	1.17	1.24	6	2
2	B	869	SER	N-CA	-5.27	1.39	1.45	19	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(°)	Ideal(°)	Models	
								Worst	Total
2	B	848	ASN	CA-CB-CG	6.77	119.37	112.60	20	1
1	A	249	ASP	CA-CB-CG	5.73	118.33	112.60	18	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	283	ARG	Sidechain	1
1	A	284	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	509	530	530	9±2
2	B	481	476	476	7±2
All	All	19800	20120	20120	287

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:235:VAL:O	1:A:239:LEU:HG	0.62	1.94	1	20
2:B:838:GLN:O	2:B:842:LEU:HG	0.62	1.95	2	3
1:A:249:ASP:HA	1:A:277:LEU:HD21	0.62	1.72	3	1
1:A:256:THR:HG21	1:A:274:CYS:SG	0.57	2.39	1	9
1:A:261:GLU:HG3	2:B:890:ILE:O	0.57	1.99	14	1
1:A:270:ASP:O	1:A:273:LEU:HG	0.56	2.00	10	1
1:A:274:CYS:SG	1:A:277:LEU:HB3	0.56	2.40	13	3
2:B:847:VAL:HG12	2:B:852:CYS:SG	0.55	2.41	4	8
2:B:850:LYS:H	2:B:850:LYS:HD2	0.55	1.62	17	8
2:B:861:ASN:ND2	2:B:864:GLU:HG2	0.55	2.16	7	6
1:A:242:VAL:HG22	1:A:288:VAL:HG21	0.55	1.79	2	1
1:A:261:GLU:OE1	1:A:262:GLN:HG2	0.55	2.02	14	1
1:A:280:GLN:O	1:A:284:ARG:HG2	0.54	2.02	2	8
1:A:295:LYS:HA	2:B:834:ASN:ND2	0.52	2.19	13	5
1:A:230:ASP:O	1:A:234:ARG:HG2	0.52	2.04	3	13
1:A:288:VAL:O	2:B:837:PRO:HB3	0.52	2.05	15	19
1:A:253:LEU:HA	1:A:256:THR:HG22	0.52	1.82	11	2
1:A:292:PRO:HA	2:B:860:LYS:O	0.51	2.06	11	11
1:A:239:LEU:HD22	1:A:263:LEU:HD22	0.51	1.83	17	9
1:A:270:ASP:O	1:A:273:LEU:HB3	0.51	2.06	20	14
1:A:290:HIS:HA	2:B:861:ASN:OD1	0.51	2.05	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:285:LEU:O	1:A:289:LEU:HG	0.50	2.07	8	16
2:B:841:LEU:HA	2:B:844:MET:SD	0.50	2.46	12	6
2:B:884:LYS:HE2	2:B:888:ASP:HB2	0.50	1.84	12	3
1:A:261:GLU:OE2	1:A:262:GLN:HG2	0.49	2.06	4	1
1:A:237:GLU:O	1:A:241:THR:HG23	0.49	2.08	6	11
1:A:238:CYS:HB3	2:B:840:PHE:CE1	0.49	2.42	16	6
2:B:839:ASP:O	2:B:843:LYS:HG2	0.49	2.07	16	4
2:B:881:ALA:O	2:B:885:GLN:HG2	0.49	2.08	7	12
2:B:861:ASN:OD1	2:B:864:GLU:HG2	0.48	2.09	10	6
1:A:235:VAL:HG11	1:A:254:LEU:HD21	0.48	1.86	5	1
2:B:850:LYS:HD3	2:B:850:LYS:H	0.48	1.68	3	1
1:A:231:LEU:O	1:A:235:VAL:HG23	0.47	2.09	10	3
1:A:279:PRO:O	1:A:283:ARG:HG2	0.46	2.10	8	2
1:A:235:VAL:HA	1:A:238:CYS:SG	0.46	2.50	1	1
1:A:231:LEU:O	1:A:235:VAL:HG12	0.46	2.11	5	1
2:B:886:LEU:O	2:B:890:ILE:HG13	0.46	2.11	11	8
2:B:864:GLU:O	2:B:868:LEU:HG	0.45	2.11	13	8
1:A:235:VAL:CG1	1:A:254:LEU:HD21	0.45	2.41	5	1
1:A:253:LEU:HA	1:A:256:THR:CG2	0.45	2.41	11	1
2:B:851:ASN:O	2:B:855:LEU:HB2	0.45	2.12	17	1
1:A:248:THR:O	1:A:251:GLN:HG2	0.44	2.13	4	1
2:B:881:ALA:C	2:B:885:GLN:HE21	0.44	2.19	12	1
2:B:855:LEU:O	2:B:859:VAL:HB	0.44	2.12	5	3
1:A:269:GLU:H	1:A:269:GLU:CD	0.44	2.21	11	1
2:B:884:LYS:CE	2:B:888:ASP:HB2	0.44	2.43	1	1
1:A:252:THR:HG22	1:A:274:CYS:SG	0.44	2.53	4	2
2:B:881:ALA:O	2:B:884:LYS:HB3	0.43	2.13	12	1
1:A:244:SER:OG	1:A:284:ARG:HG3	0.43	2.12	2	1
1:A:260:LEU:O	1:A:264:ILE:HG22	0.43	2.14	7	2
1:A:267:SER:HB2	1:A:269:GLU:OE2	0.43	2.13	12	1
2:B:842:LEU:HD22	2:B:852:CYS:SG	0.43	2.53	9	1
2:B:884:LYS:HE3	2:B:888:ASP:HB2	0.43	1.91	10	1
1:A:246:ASN:OD1	1:A:248:THR:HG22	0.43	2.13	11	1
2:B:850:LYS:H	2:B:850:LYS:CD	0.42	2.26	1	1
2:B:889:PHE:HA	2:B:892:THR:HG22	0.42	1.90	13	9
2:B:835:PRO:HA	2:B:838:GLN:OE1	0.42	2.14	19	1
1:A:266:ALA:HB1	1:A:270:ASP:HB2	0.42	1.90	13	1
1:A:240:THR:HB	1:A:250:SER:OG	0.42	2.15	20	1
1:A:237:GLU:HA	1:A:240:THR:HG22	0.42	1.92	4	1
1:A:246:ASN:O	1:A:249:ASP:HB3	0.42	2.15	7	1
1:A:273:LEU:HD13	1:A:273:LEU:C	0.41	2.40	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:859:VAL:HG13	2:B:864:GLU:HB2	0.41	1.92	1	2
2:B:862:ILE:H	2:B:862:ILE:HD13	0.41	1.76	7	3
1:A:279:PRO:HG2	1:A:280:GLN:OE1	0.41	2.16	13	1
2:B:840:PHE:O	2:B:844:MET:HG2	0.41	2.16	18	1
1:A:284:ARG:HA	1:A:284:ARG:NE	0.41	2.30	20	1
1:A:278:GLY:HA3	1:A:281:LYS:HD3	0.41	1.92	12	1
1:A:287:ASP:O	1:A:291:GLU:HG2	0.41	2.16	13	1
2:B:861:ASN:ND2	2:B:864:GLU:HG3	0.41	2.31	2	1
2:B:835:PRO:O	2:B:839:ASP:HB2	0.40	2.15	18	1
2:B:851:ASN:HB3	2:B:877:LEU:HD22	0.40	1.94	3	1
1:A:253:LEU:HD23	1:A:263:LEU:HD11	0.40	1.94	9	1
1:A:252:THR:O	1:A:256:THR:HG22	0.40	2.17	11	1
1:A:246:ASN:HB2	1:A:249:ASP:OD2	0.40	2.17	12	1
1:A:292:PRO:HG2	1:A:295:LYS:O	0.40	2.17	18	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	66/96 (69%)	63±1 (95±2%)	3±1 (5±2%)	0±0 (0±0%)	100	100
2	B	62/84 (74%)	61±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	100	100
All	All	2560/3600 (71%)	2478 (97%)	82 (3%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	59/86 (69%)	55±1 (93±2%)	4±1 (7±2%)	16	65
2	B	52/71 (73%)	47±1 (91±2%)	5±1 (9±2%)	11	58
All	All	2220/3140 (71%)	2047 (92%)	173 (8%)	14	61

All 26 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	264	ILE	20
2	B	862	ILE	20
2	B	879	ASN	19
1	A	239	LEU	13
2	B	848	ASN	11
1	A	277	LEU	10
2	B	861	ASN	9
1	A	263	LEU	9
1	A	269	GLU	9
2	B	855	LEU	9
2	B	884	LYS	8
2	B	850	LYS	8
1	A	273	LEU	4
1	A	261	GLU	4
1	A	243	LYS	3
1	A	280	GLN	3
1	A	268	ARG	2
2	B	839	ASP	2
1	A	240	THR	2
2	B	865	LEU	2
2	B	838	GLN	1
2	B	860	LYS	1
1	A	231	LEU	1
1	A	260	LEU	1
2	B	857	HIS	1
2	B	859	VAL	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](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 82% 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	2040
Number of shifts mapped to atoms	2040
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	174	-0.62 ± 0.08	Should be checked
$^{13}\text{C}_\beta$	163	0.18 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	148	-0.22 ± 0.08	None needed (< 0.5 ppm)
^{15}N	161	0.23 ± 0.18	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1551 atoms were assigned a chemical shift out of a possible 1739. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	607/634 (96%)	254/256 (99%)	234/256 (91%)	119/122 (98%)
Sidechain	872/999 (87%)	605/653 (93%)	257/310 (83%)	10/36 (28%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	72/106 (68%)	41/54 (76%)	31/48 (65%)	0/4 (0%)
Overall	1551/1739 (89%)	900/963 (93%)	522/614 (85%)	129/162 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 2040 atoms were assigned a chemical shift out of a possible 2474. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	828/894 (93%)	345/362 (95%)	322/360 (89%)	161/172 (94%)
Sidechain	1140/1423 (80%)	787/925 (85%)	342/442 (77%)	11/56 (20%)
Aromatic	72/157 (46%)	41/82 (50%)	31/65 (48%)	0/10 (0%)
Overall	2040/2474 (82%)	1173/1369 (86%)	695/867 (80%)	172/238 (72%)

7.1.4 Statistically unusual chemical shifts [i](#)

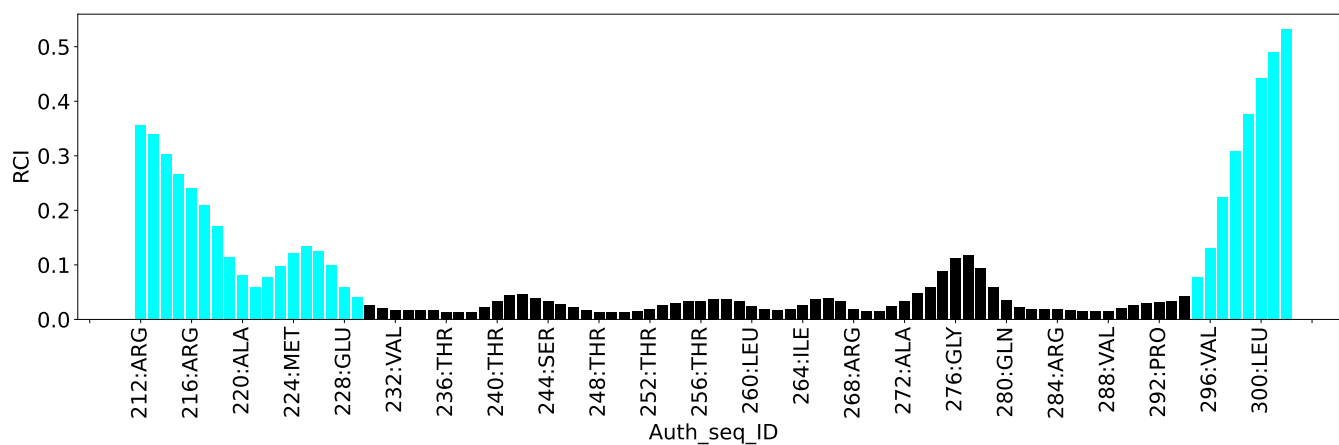
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	213	ILE	CG2	27.27	10.93 – 24.12	7.4
1	B	845	PRO	HD2	1.67	1.93 – 5.38	-5.7
1	B	884	LYS	CG	30.79	19.35 – 30.45	5.3

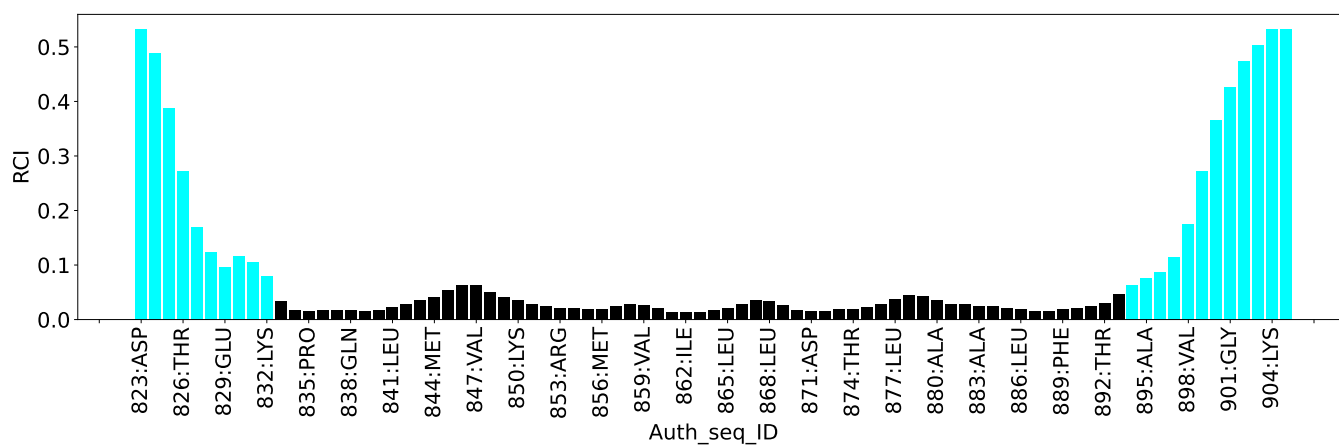
7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3435
Intra-residue ($ i-j =0$)	711
Sequential ($ i-j =1$)	899
Medium range ($ i-j >1$ and $ i-j <5$)	874
Long range ($ i-j \geq 5$)	496
Inter-chain	329
Hydrogen bond restraints	126
Disulfide bond restraints	0
Total dihedral-angle restraints	267
Number of unmapped restraints	0
Number of restraints per residue	20.6
Number of long range restraints per residue ¹	2.8

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	16.8	0.2
0.2-0.5 (Medium)	0.6	0.35
>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.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	8.2	7.61
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis

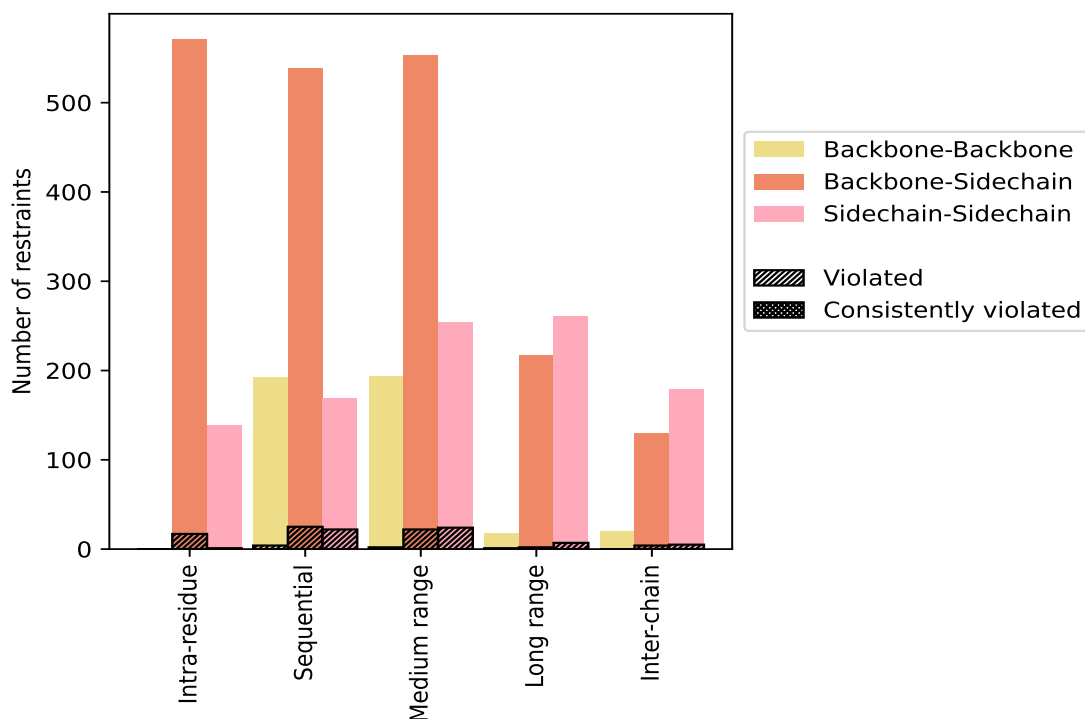
9.1 Summary of distance violations

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	711	20.7	18	2.5	0.5	0	0.0	0.0
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	571	16.6	17	3.0	0.5	0	0.0	0.0
Sidechain-Sidechain	139	4.0	1	0.7	0.0	0	0.0	0.0
Sequential ($i-j =1$)	899	26.2	51	5.7	1.5	0	0.0	0.0
Backbone-Backbone	192	5.6	4	2.1	0.1	0	0.0	0.0
Backbone-Sidechain	538	15.7	25	4.6	0.7	0	0.0	0.0
Sidechain-Sidechain	169	4.9	22	13.0	0.6	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	874	25.4	47	5.4	1.4	0	0.0	0.0
Backbone-Backbone	193	5.6	2	1.0	0.1	0	0.0	0.0
Backbone-Sidechain	427	12.4	21	4.9	0.6	0	0.0	0.0
Sidechain-Sidechain	254	7.4	24	9.4	0.7	0	0.0	0.0
Long range ($i-j \geq 5$)	496	14.4	10	2.0	0.3	0	0.0	0.0
Backbone-Backbone	18	0.5	1	5.6	0.0	0	0.0	0.0
Backbone-Sidechain	217	6.3	2	0.9	0.1	0	0.0	0.0
Sidechain-Sidechain	261	7.6	7	2.7	0.2	0	0.0	0.0
Inter-chain	329	9.6	9	2.7	0.3	0	0.0	0.0
Backbone-Backbone	20	0.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	130	3.8	4	3.1	0.1	0	0.0	0.0
Sidechain-Sidechain	179	5.2	5	2.8	0.1	0	0.0	0.0
Hydrogen bond	126	3.7	1	0.8	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3435	100.0	136	4.0	4.0	0	0.0	0.0
Backbone-Backbone	424	12.3	7	1.7	0.2	0	0.0	0.0
Backbone-Sidechain	2009	58.5	70	3.5	2.0	0	0.0	0.0
Sidechain-Sidechain	1002	29.2	59	5.9	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 disulfid bonds are counted in their appropriate category on the x-axis

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	3	9	5	1	0	18	0.14	0.21	0.03	0.14
2	3	4	5	2	0	14	0.13	0.17	0.02	0.13
3	1	7	5	3	3	19	0.13	0.2	0.03	0.13
4	5	9	4	1	1	20	0.12	0.17	0.02	0.12
5	2	10	6	4	0	22	0.13	0.22	0.03	0.12
6	3	3	8	2	0	16	0.13	0.21	0.03	0.12
7	1	7	7	3	2	20	0.13	0.18	0.02	0.12
8	5	10	4	2	2	23	0.13	0.19	0.02	0.12
9	3	5	4	2	1	15	0.12	0.16	0.02	0.12
10	5	10	3	1	0	19	0.13	0.18	0.02	0.13

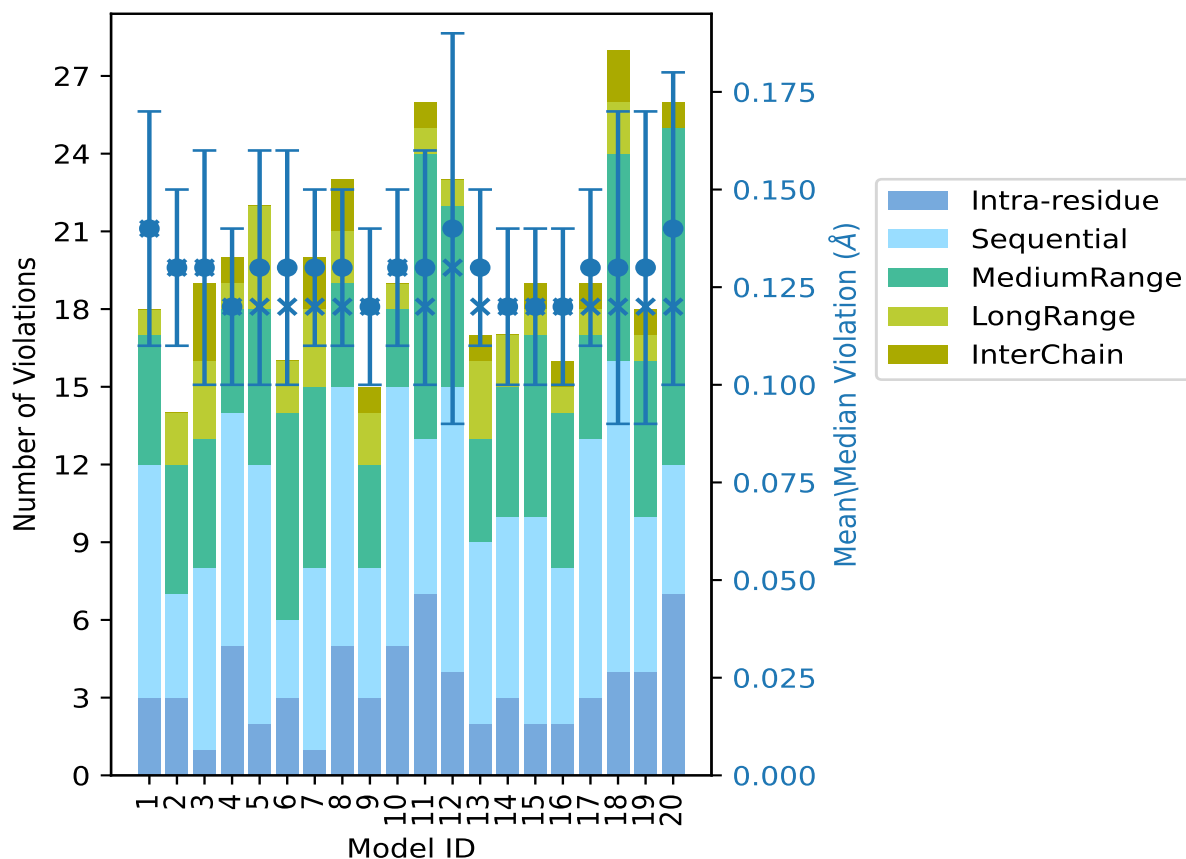
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
11	7	6	11	1	1	26	0.13	0.25	0.03	0.12
12	4	11	7	1	0	23	0.14	0.35	0.05	0.13
13	2	7	4	3	1	17	0.13	0.2	0.02	0.12
14	3	7	5	2	0	17	0.12	0.17	0.02	0.12
15	2	8	7	1	1	19	0.12	0.16	0.02	0.12
16	2	6	6	1	1	16	0.12	0.15	0.02	0.12
17	3	10	4	1	1	19	0.13	0.21	0.02	0.12
18	4	12	8	2	2	28	0.13	0.28	0.04	0.12
19	4	6	6	1	1	18	0.13	0.25	0.04	0.12
20	7	5	13	0	1	26	0.14	0.26	0.04	0.12

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

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



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

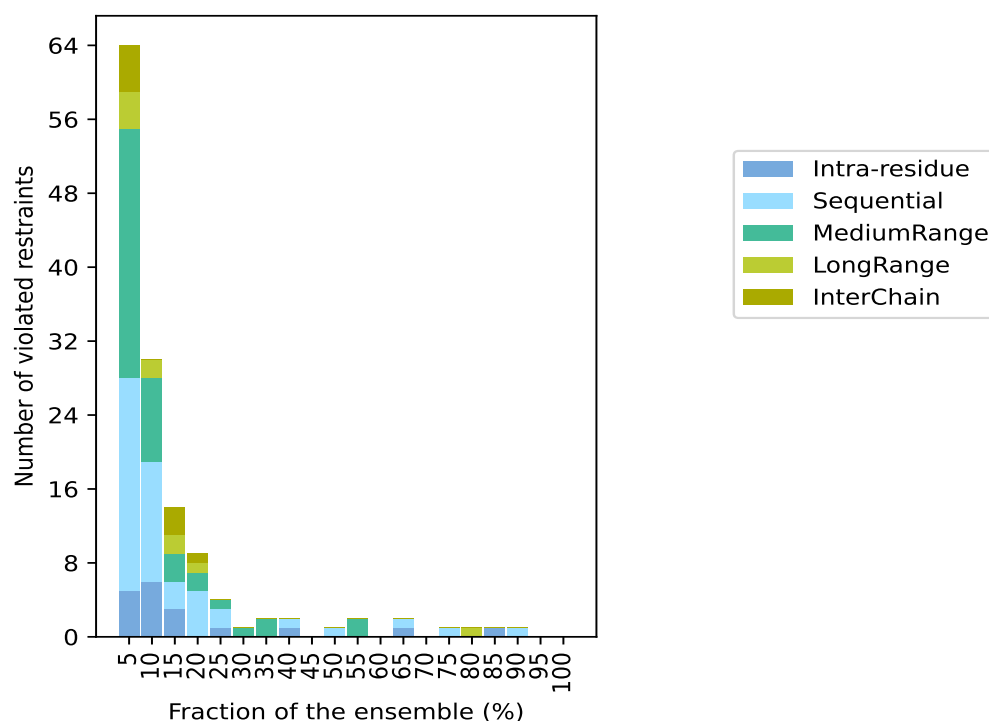
9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3174(IR:693, SQ:848, MR:827, LR:486, IC:320) 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	23	27	4	5	64	1	5.0
6	13	9	2	0	30	2	10.0
3	3	3	2	3	14	3	15.0
0	5	2	1	1	9	4	20.0
1	2	1	0	0	4	5	25.0
0	0	1	0	0	1	6	30.0
0	0	2	0	0	2	7	35.0
1	1	0	0	0	2	8	40.0
0	0	0	0	0	0	9	45.0
0	1	0	0	0	1	10	50.0
0	0	2	0	0	2	11	55.0
0	0	0	0	0	0	12	60.0
1	1	0	0	0	2	13	65.0
0	0	0	0	0	0	14	70.0
0	1	0	0	0	1	15	75.0
0	0	0	1	0	1	16	80.0
1	0	0	0	0	1	17	85.0
0	1	0	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

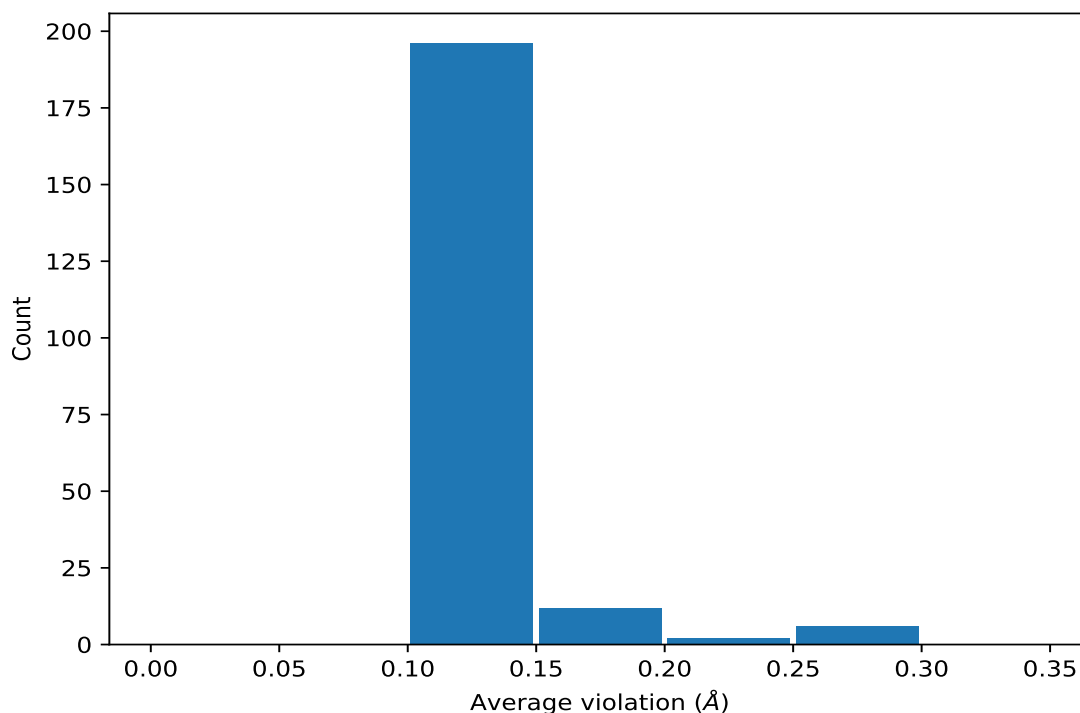
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	18	0.15	0.02	0.15
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	18	0.15	0.02	0.15
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	18	0.15	0.02	0.15
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	18	0.15	0.02	0.15
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	18	0.15	0.02	0.15
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	18	0.15	0.02	0.15
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	17	0.13	0.01	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	17	0.13	0.01	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	17	0.13	0.01	0.13
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	16	0.12	0.01	0.12
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	15	0.13	0.02	0.13
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	15	0.13	0.02	0.13
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	15	0.13	0.02	0.13
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	15	0.13	0.02	0.13
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	15	0.13	0.02	0.13
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	15	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	13	0.13	0.02	0.13
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	13	0.13	0.02	0.12
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	13	0.12	0.01	0.12
(1,3256)	2:884:B:LYS:HE2	2:888:B:ASP:H	11	0.13	0.01	0.14
(1,3256)	2:884:B:LYS:HE3	2:888:B:ASP:H	11	0.13	0.01	0.14
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB2	11	0.12	0.01	0.12
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB3	11	0.12	0.01	0.12
(1,3146)	2:868:B:LEU:HD11	2:869:B:SER:HA	10	0.14	0.02	0.15
(1,3146)	2:868:B:LEU:HD12	2:869:B:SER:HA	10	0.14	0.02	0.15
(1,3146)	2:868:B:LEU:HD13	2:869:B:SER:HA	10	0.14	0.02	0.15
(1,3146)	2:868:B:LEU:HD21	2:869:B:SER:HA	10	0.14	0.02	0.15
(1,3146)	2:868:B:LEU:HD22	2:869:B:SER:HA	10	0.14	0.02	0.15
(1,3146)	2:868:B:LEU:HD23	2:869:B:SER:HA	10	0.14	0.02	0.15
(1,460)	1:248:A:THR:H	1:249:A:ASP:HB3	8	0.15	0.01	0.15
(1,1005)	2:886:B:LEU:H	2:886:B:LEU:HG	8	0.14	0.02	0.13
(1,2739)	1:277:A:LEU:HD11	1:279:A:PRO:HA	7	0.13	0.01	0.12
(1,2739)	1:277:A:LEU:HD12	1:279:A:PRO:HA	7	0.13	0.01	0.12
(1,2739)	1:277:A:LEU:HD13	1:279:A:PRO:HA	7	0.13	0.01	0.12
(1,2739)	1:277:A:LEU:HD21	1:279:A:PRO:HA	7	0.13	0.01	0.12
(1,2739)	1:277:A:LEU:HD22	1:279:A:PRO:HA	7	0.13	0.01	0.12
(1,2739)	1:277:A:LEU:HD23	1:279:A:PRO:HA	7	0.13	0.01	0.12
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE2	7	0.12	0.02	0.11
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE3	7	0.12	0.02	0.11
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE2	7	0.12	0.02	0.11
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE3	7	0.12	0.02	0.11
(1,1163)	1:251:A:GLN:HA	1:254:A:LEU:HG	6	0.14	0.02	0.14
(1,2751)	1:280:A:GLN:HG2	1:281:A:LYS:HA	5	0.17	0.03	0.18
(1,2751)	1:280:A:GLN:HG3	1:281:A:LYS:HA	5	0.17	0.03	0.18
(1,1723)	1:294:A:LEU:HB2	1:296:A:VAL:HA	5	0.12	0.01	0.11
(1,2506)	1:246:A:ASN:HB2	1:247:A:LYS:HA	5	0.12	0.01	0.11
(1,2506)	1:246:A:ASN:HB3	1:247:A:LYS:HA	5	0.12	0.01	0.11
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD11	5	0.11	0.01	0.1
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD12	5	0.11	0.01	0.1
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD13	5	0.11	0.01	0.1
(1,451)	1:246:A:ASN:HD21	1:248:A:THR:H	4	0.14	0.02	0.15
(1,2233)	1:295:A:LYS:HE2	1:296:A:VAL:HA	4	0.14	0.01	0.14
(1,2233)	1:295:A:LYS:HE3	1:296:A:VAL:HA	4	0.14	0.01	0.14
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG21	4	0.13	0.01	0.13
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG22	4	0.13	0.01	0.13
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG23	4	0.13	0.01	0.13
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG21	4	0.13	0.01	0.13
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG22	4	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG23	4	0.13	0.01	0.13
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG21	4	0.13	0.01	0.13
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG22	4	0.13	0.01	0.13
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG23	4	0.13	0.01	0.13
(1,222)	1:235:A:VAL:HB	1:236:A:THR:H	4	0.12	0.01	0.12
(1,707)	1:231:A:LEU:HD11	2:894:B:PHE:H	4	0.12	0.01	0.12
(1,707)	1:231:A:LEU:HD12	2:894:B:PHE:H	4	0.12	0.01	0.12
(1,707)	1:231:A:LEU:HD13	2:894:B:PHE:H	4	0.12	0.01	0.12
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG21	4	0.12	0.01	0.12
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG22	4	0.12	0.01	0.12
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG23	4	0.12	0.01	0.12
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG21	4	0.12	0.01	0.12
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG22	4	0.12	0.01	0.12
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG23	4	0.12	0.01	0.12
(1,444)	2:895:B:ALA:HB1	2:897:B:VAL:H	4	0.11	0.02	0.11
(1,444)	2:895:B:ALA:HB2	2:897:B:VAL:H	4	0.11	0.02	0.11
(1,444)	2:895:B:ALA:HB3	2:897:B:VAL:H	4	0.11	0.02	0.11
(1,2188)	1:239:A:LEU:HB3	1:263:A:LEU:HG	4	0.11	0.0	0.11
(1,1104)	2:838:B:GLN:HG2	2:839:B:ASP:HA	4	0.11	0.01	0.11
(1,763)	1:268:A:ARG:HA	1:282:A:ALA:H	3	0.14	0.04	0.12
(1,2903)	1:301:A:GLU:HG2	1:302:A:HIS:H	3	0.14	0.04	0.11
(1,2903)	1:301:A:GLU:HG3	1:302:A:HIS:H	3	0.14	0.04	0.11
(1,1730)	2:902:B:LYS:HE2	2:903:B:GLY:HA2	3	0.13	0.03	0.11
(1,1730)	2:902:B:LYS:HE2	2:903:B:GLY:HA3	3	0.13	0.03	0.11
(1,1730)	2:902:B:LYS:HE3	2:903:B:GLY:HA2	3	0.13	0.03	0.11
(1,1730)	2:902:B:LYS:HE3	2:903:B:GLY:HA3	3	0.13	0.03	0.11
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD11	3	0.13	0.0	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD12	3	0.13	0.0	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD13	3	0.13	0.0	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD21	3	0.13	0.0	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD22	3	0.13	0.0	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD23	3	0.13	0.0	0.13
(1,2601)	1:260:A:LEU:HD11	2:889:B:PHE:HD1	3	0.13	0.0	0.13
(1,2601)	1:260:A:LEU:HD11	2:889:B:PHE:HD2	3	0.13	0.0	0.13
(1,2601)	1:260:A:LEU:HD12	2:889:B:PHE:HD1	3	0.13	0.0	0.13
(1,2601)	1:260:A:LEU:HD12	2:889:B:PHE:HD2	3	0.13	0.0	0.13
(1,2601)	1:260:A:LEU:HD13	2:889:B:PHE:HD1	3	0.13	0.0	0.13
(1,2601)	1:260:A:LEU:HD13	2:889:B:PHE:HD2	3	0.13	0.0	0.13
(1,2601)	1:260:A:LEU:HD21	2:889:B:PHE:HD1	3	0.13	0.0	0.13
(1,2601)	1:260:A:LEU:HD21	2:889:B:PHE:HD2	3	0.13	0.0	0.13
(1,2601)	1:260:A:LEU:HD22	2:889:B:PHE:HD1	3	0.13	0.0	0.13
(1,2601)	1:260:A:LEU:HD22	2:889:B:PHE:HD2	3	0.13	0.0	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2601)	1:260:A:LEU:HD23	2:889:B:PHE:HD1	3	0.13	0.0	0.13
(1,2601)	1:260:A:LEU:HD23	2:889:B:PHE:HD2	3	0.13	0.0	0.13
(1,704)	2:894:B:PHE:H	2:896:B:GLU:HB2	3	0.12	0.01	0.12
(1,704)	2:894:B:PHE:H	2:896:B:GLU:HB3	3	0.12	0.01	0.12
(1,1018)	1:291:A:GLU:HG2	1:292:A:PRO:HD2	3	0.12	0.01	0.13
(1,1018)	1:291:A:GLU:HG3	1:292:A:PRO:HD2	3	0.12	0.01	0.13
(1,1236)	2:850:B:LYS:H	2:850:B:LYS:HD2	3	0.12	0.01	0.13
(1,1236)	2:850:B:LYS:H	2:850:B:LYS:HD3	3	0.12	0.01	0.13
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD11	3	0.12	0.0	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD12	3	0.12	0.0	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD13	3	0.12	0.0	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD21	3	0.12	0.0	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD22	3	0.12	0.0	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD23	3	0.12	0.0	0.12
(1,901)	1:294:A:LEU:HB3	2:833:B:TYR:HE1	3	0.11	0.0	0.11
(1,901)	1:294:A:LEU:HB3	2:833:B:TYR:HE2	3	0.11	0.0	0.11
(1,1028)	2:862:B:ILE:HA	2:865:B:LEU:HD11	3	0.11	0.01	0.1
(1,1028)	2:862:B:ILE:HA	2:865:B:LEU:HD12	3	0.11	0.01	0.1
(1,1028)	2:862:B:ILE:HA	2:865:B:LEU:HD13	3	0.11	0.01	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD11	3	0.11	0.01	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD12	3	0.11	0.01	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD13	3	0.11	0.01	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD21	3	0.11	0.01	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD22	3	0.11	0.01	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD23	3	0.11	0.01	0.1
(1,2862)	1:295:A:LYS:H	1:295:A:LYS:HB2	3	0.11	0.0	0.11
(1,2862)	1:295:A:LYS:H	1:295:A:LYS:HB3	3	0.11	0.0	0.11
(1,721)	1:240:A:THR:H	2:840:B:PHE:HE1	3	0.1	0.0	0.1
(1,721)	1:240:A:THR:H	2:840:B:PHE:HE2	3	0.1	0.0	0.1
(1,1084)	2:844:B:MET:HB2	2:844:B:MET:HE1	2	0.26	0.01	0.26
(1,1084)	2:844:B:MET:HB2	2:844:B:MET:HE2	2	0.26	0.01	0.26
(1,1084)	2:844:B:MET:HB2	2:844:B:MET:HE3	2	0.26	0.01	0.26
(1,1084)	2:844:B:MET:HB3	2:844:B:MET:HE1	2	0.26	0.01	0.26
(1,1084)	2:844:B:MET:HB3	2:844:B:MET:HE2	2	0.26	0.01	0.26
(1,1084)	2:844:B:MET:HB3	2:844:B:MET:HE3	2	0.26	0.01	0.26
(1,2094)	2:896:B:GLU:HG2	2:897:B:VAL:HA	2	0.21	0.0	0.21
(1,2094)	2:896:B:GLU:HG3	2:897:B:VAL:HA	2	0.21	0.0	0.21
(1,2678)	1:268:A:ARG:HD2	1:286:A:PHE:HB2	2	0.16	0.04	0.16
(1,2678)	1:268:A:ARG:HD3	1:286:A:PHE:HB2	2	0.16	0.04	0.16
(1,589)	2:904:B:LYS:HA	2:905:B:LYS:H	2	0.15	0.0	0.15
(1,379)	1:284:A:ARG:H	1:284:A:ARG:HD3	2	0.14	0.03	0.14
(1,815)	1:297:A:PRO:HA	1:299:A:GLY:H	2	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1454)	2:896:B:GLU:HG2	2:897:B:VAL:HG11	2	0.14	0.0	0.14
(1,1454)	2:896:B:GLU:HG2	2:897:B:VAL:HG12	2	0.14	0.0	0.14
(1,1454)	2:896:B:GLU:HG2	2:897:B:VAL:HG13	2	0.14	0.0	0.14
(1,1454)	2:896:B:GLU:HG3	2:897:B:VAL:HG11	2	0.14	0.0	0.14
(1,1454)	2:896:B:GLU:HG3	2:897:B:VAL:HG12	2	0.14	0.0	0.14
(1,1454)	2:896:B:GLU:HG3	2:897:B:VAL:HG13	2	0.14	0.0	0.14
(1,2617)	1:261:A:GLU:HG2	1:262:A:GLN:HE21	2	0.14	0.02	0.14
(1,2617)	1:261:A:GLU:HG2	1:262:A:GLN:HE22	2	0.14	0.02	0.14
(1,2617)	1:261:A:GLU:HG3	1:262:A:GLN:HE21	2	0.14	0.02	0.14
(1,2617)	1:261:A:GLU:HG3	1:262:A:GLN:HE22	2	0.14	0.02	0.14
(1,1919)	2:831:B:GLU:HG2	2:832:B:LYS:HB2	2	0.13	0.02	0.13
(1,1919)	2:831:B:GLU:HG2	2:832:B:LYS:HB3	2	0.13	0.02	0.13
(1,1235)	2:849:B:ALA:H	2:850:B:LYS:HD2	2	0.12	0.01	0.12
(1,1235)	2:849:B:ALA:H	2:850:B:LYS:HD3	2	0.12	0.01	0.12
(1,1474)	2:848:B:ASN:HD21	2:851:B:ASN:HB2	2	0.12	0.01	0.12
(1,2026)	1:256:A:THR:HA	1:257:A:PHE:HE1	2	0.12	0.02	0.12
(1,2026)	1:256:A:THR:HA	1:257:A:PHE:HE2	2	0.12	0.02	0.12
(1,112)	2:897:B:VAL:HB	2:898:B:VAL:H	2	0.12	0.01	0.12
(1,541)	1:287:A:ASP:HB3	1:289:A:LEU:H	2	0.12	0.01	0.12
(1,1377)	1:258:A:GLY:HA3	1:259:A:SER:HB2	2	0.12	0.0	0.12
(1,1377)	1:258:A:GLY:HA3	1:259:A:SER:HB3	2	0.12	0.0	0.12
(1,1880)	2:870:B:GLN:HA	2:873:B:LEU:HB2	2	0.12	0.0	0.12
(1,2375)	1:232:A:VAL:HG21	1:233:A:SER:HB2	2	0.12	0.0	0.12
(1,2375)	1:232:A:VAL:HG21	1:233:A:SER:HB3	2	0.12	0.0	0.12
(1,2375)	1:232:A:VAL:HG22	1:233:A:SER:HB2	2	0.12	0.0	0.12
(1,2375)	1:232:A:VAL:HG22	1:233:A:SER:HB3	2	0.12	0.0	0.12
(1,2375)	1:232:A:VAL:HG23	1:233:A:SER:HB2	2	0.12	0.0	0.12
(1,2375)	1:232:A:VAL:HG23	1:233:A:SER:HB3	2	0.12	0.0	0.12
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD11	2	0.12	0.0	0.12
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD12	2	0.12	0.0	0.12
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD13	2	0.12	0.0	0.12
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD21	2	0.12	0.0	0.12
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD22	2	0.12	0.0	0.12
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD23	2	0.12	0.0	0.12
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD11	2	0.12	0.0	0.12
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD12	2	0.12	0.0	0.12
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD13	2	0.12	0.0	0.12
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD21	2	0.12	0.0	0.12
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD22	2	0.12	0.0	0.12
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD23	2	0.12	0.0	0.12
(1,3035)	2:848:B:ASN:HD21	2:850:B:LYS:HB2	2	0.12	0.0	0.12
(1,3035)	2:848:B:ASN:HD21	2:850:B:LYS:HB3	2	0.12	0.0	0.12

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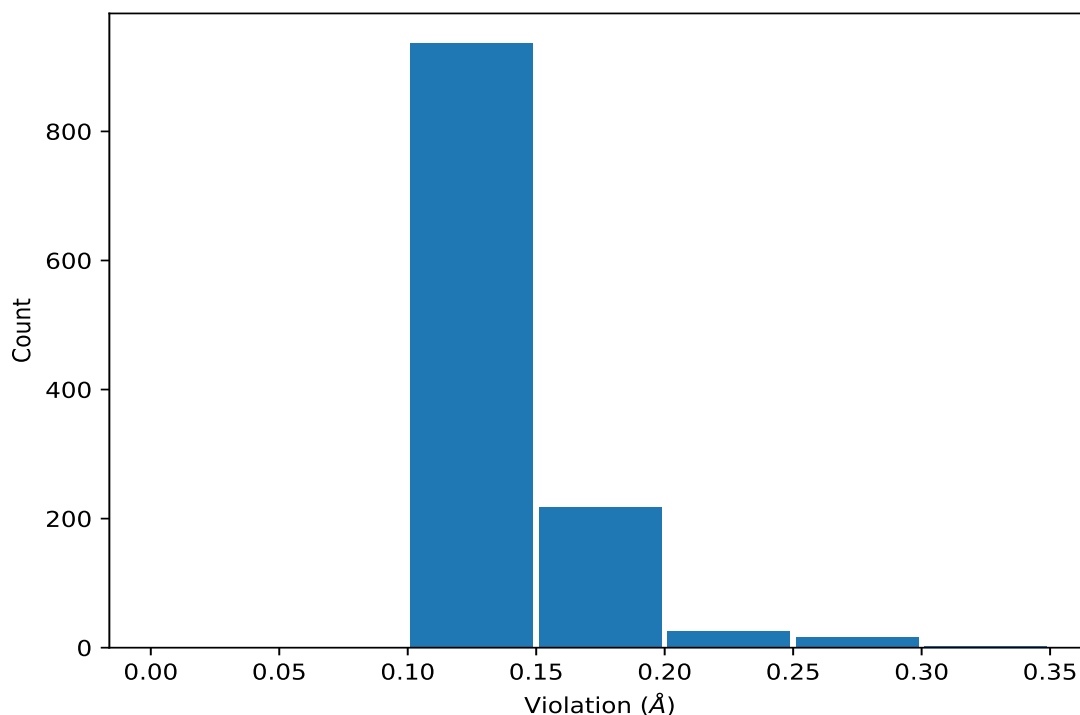
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3035)	2:848:B:ASN:HD22	2:850:B:LYS:HB2	2	0.12	0.0	0.12
(1,3035)	2:848:B:ASN:HD22	2:850:B:LYS:HB3	2	0.12	0.0	0.12
(1,2105)	1:231:A:LEU:HB3	1:232:A:VAL:HB	2	0.11	0.0	0.11
(1,3069)	2:855:B:LEU:HD11	2:866:B:ALA:H	2	0.11	0.0	0.11
(1,3069)	2:855:B:LEU:HD12	2:866:B:ALA:H	2	0.11	0.0	0.11
(1,3069)	2:855:B:LEU:HD13	2:866:B:ALA:H	2	0.11	0.0	0.11
(1,3069)	2:855:B:LEU:HD21	2:866:B:ALA:H	2	0.11	0.0	0.11
(1,3069)	2:855:B:LEU:HD22	2:866:B:ALA:H	2	0.11	0.0	0.11
(1,3069)	2:855:B:LEU:HD23	2:866:B:ALA:H	2	0.11	0.0	0.11
(1,3164)	2:870:B:GLN:HA	2:870:B:GLN:HE21	2	0.11	0.01	0.11
(1,3164)	2:870:B:GLN:HA	2:870:B:GLN:HE22	2	0.11	0.01	0.11
(1,1289)	2:859:B:VAL:HG21	2:861:B:ASN:H	2	0.11	0.0	0.11
(1,1289)	2:859:B:VAL:HG22	2:861:B:ASN:H	2	0.11	0.0	0.11
(1,1289)	2:859:B:VAL:HG23	2:861:B:ASN:H	2	0.11	0.0	0.11
(1,1851)	2:886:B:LEU:HG	2:890:B:ILE:HD11	2	0.11	0.0	0.11
(1,1851)	2:886:B:LEU:HG	2:890:B:ILE:HD12	2	0.11	0.0	0.11
(1,1851)	2:886:B:LEU:HG	2:890:B:ILE:HD13	2	0.11	0.0	0.11
(1,2080)	1:215:A:ARG:HA	1:215:A:ARG:HD2	2	0.11	0.0	0.11
(1,2080)	1:215:A:ARG:HA	1:215:A:ARG:HD3	2	0.11	0.0	0.11
(1,2819)	1:290:A:HIS:H	1:291:A:GLU:HB2	2	0.11	0.0	0.11
(1,2819)	1:290:A:HIS:H	1:291:A:GLU:HB3	2	0.11	0.0	0.11
(1,1118)	2:855:B:LEU:HA	2:855:B:LEU:HD11	2	0.1	0.0	0.1
(1,1118)	2:855:B:LEU:HA	2:855:B:LEU:HD12	2	0.1	0.0	0.1
(1,1118)	2:855:B:LEU:HA	2:855:B:LEU:HD13	2	0.1	0.0	0.1
(1,1376)	2:848:B:ASN:HB2	2:850:B:LYS:HE2	2	0.1	0.0	0.1
(1,1376)	2:848:B:ASN:HB2	2:850:B:LYS:HE3	2	0.1	0.0	0.1
(1,2946)	2:834:B:ASN:HB2	2:835:B:PRO:HG2	2	0.1	0.0	0.1
(1,2946)	2:834:B:ASN:HB2	2:835:B:PRO:HG3	2	0.1	0.0	0.1
(1,2946)	2:834:B:ASN:HB3	2:835:B:PRO:HG2	2	0.1	0.0	0.1
(1,2946)	2:834:B:ASN:HB3	2:835:B:PRO:HG3	2	0.1	0.0	0.1
(1,3102)	2:861:B:ASN:H	2:861:B:ASN:HD21	2	0.1	0.0	0.1
(1,3102)	2:861:B:ASN:H	2:861:B:ASN:HD22	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3247)	2:884:B:LYS:HA	2:885:B:GLN:HE21	12	0.35
(1,3247)	2:884:B:LYS:HA	2:885:B:GLN:HE22	12	0.35
(1,2016)	2:825:B:GLU:HA	2:826:B:THR:H	18	0.28
(1,1084)	2:844:B:MET:HB2	2:844:B:MET:HE1	20	0.26
(1,1084)	2:844:B:MET:HB2	2:844:B:MET:HE2	20	0.26
(1,1084)	2:844:B:MET:HB2	2:844:B:MET:HE3	20	0.26
(1,1084)	2:844:B:MET:HB3	2:844:B:MET:HE1	20	0.26
(1,1084)	2:844:B:MET:HB3	2:844:B:MET:HE2	20	0.26
(1,1084)	2:844:B:MET:HB3	2:844:B:MET:HE3	20	0.26
(1,1084)	2:844:B:MET:HB2	2:844:B:MET:HE1	19	0.25
(1,1084)	2:844:B:MET:HB2	2:844:B:MET:HE2	19	0.25
(1,1084)	2:844:B:MET:HB2	2:844:B:MET:HE3	19	0.25
(1,1084)	2:844:B:MET:HB3	2:844:B:MET:HE1	19	0.25
(1,1084)	2:844:B:MET:HB3	2:844:B:MET:HE2	19	0.25
(1,1084)	2:844:B:MET:HB3	2:844:B:MET:HE3	19	0.25
(1,594)	2:898:B:VAL:H	2:898:B:VAL:HG11	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	2:898:B:VAL:H	2:898:B:VAL:HG12	11	0.25
(1,594)	2:898:B:VAL:H	2:898:B:VAL:HG13	11	0.25
(1,1906)	1:273:A:LEU:HG	1:274:A:CYS:HA	20	0.24
(1,2751)	1:280:A:GLN:HG2	1:281:A:LYS:HA	5	0.22
(1,2751)	1:280:A:GLN:HG3	1:281:A:LYS:HA	5	0.22
(1,2678)	1:268:A:ARG:HD2	1:286:A:PHE:HB2	6	0.21
(1,2678)	1:268:A:ARG:HD3	1:286:A:PHE:HB2	6	0.21
(1,2094)	2:896:B:GLU:HG2	2:897:B:VAL:HA	1	0.21
(1,2094)	2:896:B:GLU:HG3	2:897:B:VAL:HA	1	0.21
(1,2094)	2:896:B:GLU:HG2	2:897:B:VAL:HA	17	0.21
(1,2094)	2:896:B:GLU:HG3	2:897:B:VAL:HA	17	0.21
(1,1888)	2:882:B:ASN:HA	2:885:B:GLN:HG2	12	0.21
(1,1633)	2:881:B:ALA:HB1	2:885:B:GLN:HG2	12	0.21
(1,1633)	2:881:B:ALA:HB2	2:885:B:GLN:HG2	12	0.21
(1,1633)	2:881:B:ALA:HB3	2:885:B:GLN:HG2	12	0.21
(1,2927)	2:829:B:GLU:HG2	2:832:B:LYS:HD2	18	0.2
(1,2927)	2:829:B:GLU:HG2	2:832:B:LYS:HD3	18	0.2
(1,2927)	2:829:B:GLU:HG3	2:832:B:LYS:HD2	18	0.2
(1,2927)	2:829:B:GLU:HG3	2:832:B:LYS:HD3	18	0.2
(1,2903)	1:301:A:GLU:HG2	1:302:A:HIS:H	11	0.2
(1,2903)	1:301:A:GLU:HG3	1:302:A:HIS:H	11	0.2
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	13	0.2
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	13	0.2
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	13	0.2
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	13	0.2
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	13	0.2
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	13	0.2
(1,763)	1:268:A:ARG:HA	1:282:A:ALA:H	3	0.2
(1,2751)	1:280:A:GLN:HG2	1:281:A:LYS:HA	19	0.19
(1,2751)	1:280:A:GLN:HG3	1:281:A:LYS:HA	19	0.19
(1,2368)	1:231:A:LEU:HD11	2:897:B:VAL:H	8	0.19
(1,2368)	1:231:A:LEU:HD12	2:897:B:VAL:H	8	0.19
(1,2368)	1:231:A:LEU:HD13	2:897:B:VAL:H	8	0.19
(1,2368)	1:231:A:LEU:HD21	2:897:B:VAL:H	8	0.19
(1,2368)	1:231:A:LEU:HD22	2:897:B:VAL:H	8	0.19
(1,2368)	1:231:A:LEU:HD23	2:897:B:VAL:H	8	0.19
(1,2143)	1:284:A:ARG:HB2	1:288:A:VAL:HG11	11	0.19
(1,2143)	1:284:A:ARG:HB2	1:288:A:VAL:HG12	11	0.19
(1,2143)	1:284:A:ARG:HB2	1:288:A:VAL:HG13	11	0.19
(1,2143)	1:284:A:ARG:HB3	1:288:A:VAL:HG11	11	0.19
(1,2143)	1:284:A:ARG:HB3	1:288:A:VAL:HG12	11	0.19
(1,2143)	1:284:A:ARG:HB3	1:288:A:VAL:HG13	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	1	0.18
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	1	0.18
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	1	0.18
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	1	0.18
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	1	0.18
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	1	0.18
(1,2751)	1:280:A:GLN:HG2	1:281:A:LYS:HA	8	0.18
(1,2751)	1:280:A:GLN:HG3	1:281:A:LYS:HA	8	0.18
(1,2343)	1:228:A:GLU:HB2	1:231:A:LEU:HB2	5	0.18
(1,2343)	1:228:A:GLU:HB3	1:231:A:LEU:HB2	5	0.18
(1,2236)	2:826:B:THR:HA	2:827:B:LEU:HA	10	0.18
(1,1730)	2:902:B:LYS:HE2	2:903:B:GLY:HA2	7	0.18
(1,1730)	2:902:B:LYS:HE2	2:903:B:GLY:HA3	7	0.18
(1,1730)	2:902:B:LYS:HE3	2:903:B:GLY:HA2	7	0.18
(1,1730)	2:902:B:LYS:HE3	2:903:B:GLY:HA3	7	0.18
(1,1163)	1:251:A:GLN:HA	1:254:A:LEU:HG	12	0.18
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	14	0.17
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	14	0.17
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	14	0.17
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	14	0.17
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	14	0.17
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	14	0.17
(1,3034)	2:848:B:ASN:HB2	2:850:B:LYS:HG2	3	0.17
(1,3034)	2:848:B:ASN:HB2	2:850:B:LYS:HG3	3	0.17
(1,2906)	2:823:B:ASP:HB2	2:825:B:GLU:HA	4	0.17
(1,2906)	2:823:B:ASP:HB3	2:825:B:GLU:HA	4	0.17
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	2	0.17
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	2	0.17
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	2	0.17
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	2	0.17
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	2	0.17
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	2	0.17
(1,460)	1:248:A:THR:H	1:249:A:ASP:HB3	3	0.17
(1,379)	1:284:A:ARG:H	1:284:A:ARG:HD3	20	0.17
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	1	0.16
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	14	0.16
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	20	0.16
(1,3255)	2:884:B:LYS:HG3	2:885:B:GLN:HE21	12	0.16
(1,3255)	2:884:B:LYS:HG3	2:885:B:GLN:HE22	12	0.16
(1,3146)	2:868:B:LEU:HD11	2:869:B:SER:HA	1	0.16
(1,3146)	2:868:B:LEU:HD12	2:869:B:SER:HA	1	0.16
(1,3146)	2:868:B:LEU:HD13	2:869:B:SER:HA	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3146)	2:868:B:LEU:HD21	2:869:B:SER:HA	1	0.16
(1,3146)	2:868:B:LEU:HD22	2:869:B:SER:HA	1	0.16
(1,3146)	2:868:B:LEU:HD23	2:869:B:SER:HA	1	0.16
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	7	0.16
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	7	0.16
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	7	0.16
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	7	0.16
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	7	0.16
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	7	0.16
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	13	0.16
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	13	0.16
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	13	0.16
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	13	0.16
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	13	0.16
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	13	0.16
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	18	0.16
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	18	0.16
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	18	0.16
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	18	0.16
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	18	0.16
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	18	0.16
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	20	0.16
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	20	0.16
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	20	0.16
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	20	0.16
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	20	0.16
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	20	0.16
(1,2881)	1:296:A:VAL:HG11	2:829:B:GLU:HG2	3	0.16
(1,2881)	1:296:A:VAL:HG11	2:829:B:GLU:HG3	3	0.16
(1,2881)	1:296:A:VAL:HG12	2:829:B:GLU:HG2	3	0.16
(1,2881)	1:296:A:VAL:HG12	2:829:B:GLU:HG3	3	0.16
(1,2881)	1:296:A:VAL:HG13	2:829:B:GLU:HG2	3	0.16
(1,2881)	1:296:A:VAL:HG13	2:829:B:GLU:HG3	3	0.16
(1,2881)	1:296:A:VAL:HG21	2:829:B:GLU:HG2	3	0.16
(1,2881)	1:296:A:VAL:HG21	2:829:B:GLU:HG3	3	0.16
(1,2881)	1:296:A:VAL:HG22	2:829:B:GLU:HG2	3	0.16
(1,2881)	1:296:A:VAL:HG22	2:829:B:GLU:HG3	3	0.16
(1,2881)	1:296:A:VAL:HG23	2:829:B:GLU:HG2	3	0.16
(1,2881)	1:296:A:VAL:HG23	2:829:B:GLU:HG3	3	0.16
(1,2617)	1:261:A:GLU:HG2	1:262:A:GLN:HE21	4	0.16
(1,2617)	1:261:A:GLU:HG2	1:262:A:GLN:HE22	4	0.16
(1,2617)	1:261:A:GLU:HG3	1:262:A:GLN:HE21	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2617)	1:261:A:GLU:HG3	1:262:A:GLN:HE22	4	0.16
(1,2511)	1:246:A:ASN:HB2	1:249:A:ASP:HB2	11	0.16
(1,2511)	1:246:A:ASN:HB3	1:249:A:ASP:HB2	11	0.16
(1,2417)	1:238:A:CYS:HB2	1:239:A:LEU:HA	1	0.16
(1,2417)	1:238:A:CYS:HB3	1:239:A:LEU:HA	1	0.16
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	6	0.16
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE2	18	0.16
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE3	18	0.16
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE2	18	0.16
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE3	18	0.16
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	2	0.16
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	9	0.16
(1,1005)	2:886:B:LEU:H	2:886:B:LEU:HG	9	0.16
(1,1005)	2:886:B:LEU:H	2:886:B:LEU:HG	15	0.16
(1,460)	1:248:A:THR:H	1:249:A:ASP:HB3	20	0.16
(1,3256)	2:884:B:LYS:HE2	2:888:B:ASP:H	9	0.15
(1,3256)	2:884:B:LYS:HE3	2:888:B:ASP:H	9	0.15
(1,3146)	2:868:B:LEU:HD11	2:869:B:SER:HA	7	0.15
(1,3146)	2:868:B:LEU:HD12	2:869:B:SER:HA	7	0.15
(1,3146)	2:868:B:LEU:HD13	2:869:B:SER:HA	7	0.15
(1,3146)	2:868:B:LEU:HD21	2:869:B:SER:HA	7	0.15
(1,3146)	2:868:B:LEU:HD22	2:869:B:SER:HA	7	0.15
(1,3146)	2:868:B:LEU:HD23	2:869:B:SER:HA	7	0.15
(1,3146)	2:868:B:LEU:HD11	2:869:B:SER:HA	13	0.15
(1,3146)	2:868:B:LEU:HD12	2:869:B:SER:HA	13	0.15
(1,3146)	2:868:B:LEU:HD13	2:869:B:SER:HA	13	0.15
(1,3146)	2:868:B:LEU:HD21	2:869:B:SER:HA	13	0.15
(1,3146)	2:868:B:LEU:HD22	2:869:B:SER:HA	13	0.15
(1,3146)	2:868:B:LEU:HD23	2:869:B:SER:HA	13	0.15
(1,3146)	2:868:B:LEU:HD11	2:869:B:SER:HA	16	0.15
(1,3146)	2:868:B:LEU:HD12	2:869:B:SER:HA	16	0.15
(1,3146)	2:868:B:LEU:HD13	2:869:B:SER:HA	16	0.15
(1,3146)	2:868:B:LEU:HD21	2:869:B:SER:HA	16	0.15
(1,3146)	2:868:B:LEU:HD22	2:869:B:SER:HA	16	0.15
(1,3146)	2:868:B:LEU:HD23	2:869:B:SER:HA	16	0.15
(1,3146)	2:868:B:LEU:HD11	2:869:B:SER:HA	18	0.15
(1,3146)	2:868:B:LEU:HD12	2:869:B:SER:HA	18	0.15
(1,3146)	2:868:B:LEU:HD13	2:869:B:SER:HA	18	0.15
(1,3146)	2:868:B:LEU:HD21	2:869:B:SER:HA	18	0.15
(1,3146)	2:868:B:LEU:HD22	2:869:B:SER:HA	18	0.15
(1,3146)	2:868:B:LEU:HD23	2:869:B:SER:HA	18	0.15
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	2	0.15
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	2	0.15
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	2	0.15
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	2	0.15
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	2	0.15
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	3	0.15
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	3	0.15
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	3	0.15
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	3	0.15
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	3	0.15
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	3	0.15
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	5	0.15
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	5	0.15
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	5	0.15
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	5	0.15
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	5	0.15
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	5	0.15
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	19	0.15
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	19	0.15
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	19	0.15
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	19	0.15
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	19	0.15
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	19	0.15
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	4	0.15
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	4	0.15
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	4	0.15
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	4	0.15
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	4	0.15
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	4	0.15
(1,2233)	1:295:A:LYS:HE2	1:296:A:VAL:HA	10	0.15
(1,2233)	1:295:A:LYS:HE3	1:296:A:VAL:HA	10	0.15
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB2	15	0.15
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB3	15	0.15
(1,2026)	1:256:A:THR:HA	1:257:A:PHE:HE1	11	0.15
(1,2026)	1:256:A:THR:HA	1:257:A:PHE:HE2	11	0.15
(1,1919)	2:831:B:GLU:HG2	2:832:B:LYS:HB2	5	0.15
(1,1919)	2:831:B:GLU:HG2	2:832:B:LYS:HB3	5	0.15
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	8	0.15
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	8	0.15
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	8	0.15
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	12	0.15
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	12	0.15
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	14	0.15
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	14	0.15
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	14	0.15
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE2	20	0.15
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE3	20	0.15
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE2	20	0.15
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE3	20	0.15
(1,1294)	2:829:B:GLU:HB2	2:830:B:SER:HB2	17	0.15
(1,1294)	2:829:B:GLU:HB2	2:830:B:SER:HB3	17	0.15
(1,1294)	2:829:B:GLU:HB3	2:830:B:SER:HB2	17	0.15
(1,1294)	2:829:B:GLU:HB3	2:830:B:SER:HB3	17	0.15
(1,1270)	1:243:A:LYS:HG2	1:244:A:SER:HB2	12	0.15
(1,1270)	1:243:A:LYS:HG2	1:244:A:SER:HB3	12	0.15
(1,1270)	1:243:A:LYS:HG3	1:244:A:SER:HB2	12	0.15
(1,1270)	1:243:A:LYS:HG3	1:244:A:SER:HB3	12	0.15
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG21	13	0.15
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG22	13	0.15
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG23	13	0.15
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG21	13	0.15
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG22	13	0.15
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG23	13	0.15
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG21	13	0.15
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG22	13	0.15
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG23	13	0.15
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	20	0.15
(1,1005)	2:886:B:LEU:H	2:886:B:LEU:HG	20	0.15
(1,815)	1:297:A:PRO:HA	1:299:A:GLY:H	16	0.15
(1,589)	2:904:B:LYS:HA	2:905:B:LYS:H	1	0.15
(1,460)	1:248:A:THR:H	1:249:A:ASP:HB3	1	0.15
(1,460)	1:248:A:THR:H	1:249:A:ASP:HB3	8	0.15
(1,460)	1:248:A:THR:H	1:249:A:ASP:HB3	9	0.15
(1,451)	1:246:A:ASN:HD21	1:248:A:THR:H	8	0.15
(1,451)	1:246:A:ASN:HD21	1:248:A:THR:H	15	0.15
(1,451)	1:246:A:ASN:HD21	1:248:A:THR:H	20	0.15
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	11	0.14
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	17	0.14
(1,3256)	2:884:B:LYS:HE2	2:888:B:ASP:H	2	0.14
(1,3256)	2:884:B:LYS:HE3	2:888:B:ASP:H	2	0.14
(1,3256)	2:884:B:LYS:HE2	2:888:B:ASP:H	3	0.14
(1,3256)	2:884:B:LYS:HE3	2:888:B:ASP:H	3	0.14
(1,3256)	2:884:B:LYS:HE2	2:888:B:ASP:H	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3256)	2:884:B:LYS:HE3	2:888:B:ASP:H	6	0.14
(1,3256)	2:884:B:LYS:HE2	2:888:B:ASP:H	8	0.14
(1,3256)	2:884:B:LYS:HE3	2:888:B:ASP:H	8	0.14
(1,3256)	2:884:B:LYS:HE2	2:888:B:ASP:H	10	0.14
(1,3256)	2:884:B:LYS:HE3	2:888:B:ASP:H	10	0.14
(1,3146)	2:868:B:LEU:HD11	2:869:B:SER:HA	12	0.14
(1,3146)	2:868:B:LEU:HD12	2:869:B:SER:HA	12	0.14
(1,3146)	2:868:B:LEU:HD13	2:869:B:SER:HA	12	0.14
(1,3146)	2:868:B:LEU:HD21	2:869:B:SER:HA	12	0.14
(1,3146)	2:868:B:LEU:HD22	2:869:B:SER:HA	12	0.14
(1,3146)	2:868:B:LEU:HD23	2:869:B:SER:HA	12	0.14
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	6	0.14
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	6	0.14
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	6	0.14
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	6	0.14
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	6	0.14
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	6	0.14
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	12	0.14
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	12	0.14
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	12	0.14
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	12	0.14
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	12	0.14
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	12	0.14
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	15	0.14
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	15	0.14
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	15	0.14
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	15	0.14
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	15	0.14
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	15	0.14
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	17	0.14
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	17	0.14
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	17	0.14
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	17	0.14
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	17	0.14
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	17	0.14
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD11	20	0.14
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD12	20	0.14
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD13	20	0.14
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD21	20	0.14
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD22	20	0.14
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD23	20	0.14
(1,2751)	1:280:A:GLN:HG2	1:281:A:LYS:HA	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2751)	1:280:A:GLN:HG3	1:281:A:LYS:HA	13	0.14
(1,2751)	1:280:A:GLN:HG2	1:281:A:LYS:HA	15	0.14
(1,2751)	1:280:A:GLN:HG3	1:281:A:LYS:HA	15	0.14
(1,2739)	1:277:A:LEU:HD11	1:279:A:PRO:HA	13	0.14
(1,2739)	1:277:A:LEU:HD12	1:279:A:PRO:HA	13	0.14
(1,2739)	1:277:A:LEU:HD13	1:279:A:PRO:HA	13	0.14
(1,2739)	1:277:A:LEU:HD21	1:279:A:PRO:HA	13	0.14
(1,2739)	1:277:A:LEU:HD22	1:279:A:PRO:HA	13	0.14
(1,2739)	1:277:A:LEU:HD23	1:279:A:PRO:HA	13	0.14
(1,2739)	1:277:A:LEU:HD11	1:279:A:PRO:HA	19	0.14
(1,2739)	1:277:A:LEU:HD12	1:279:A:PRO:HA	19	0.14
(1,2739)	1:277:A:LEU:HD13	1:279:A:PRO:HA	19	0.14
(1,2739)	1:277:A:LEU:HD21	1:279:A:PRO:HA	19	0.14
(1,2739)	1:277:A:LEU:HD22	1:279:A:PRO:HA	19	0.14
(1,2739)	1:277:A:LEU:HD23	1:279:A:PRO:HA	19	0.14
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	14	0.14
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	14	0.14
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	14	0.14
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	14	0.14
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	14	0.14
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	14	0.14
(1,2514)	1:247:A:LYS:HB2	1:248:A:THR:HG21	10	0.14
(1,2514)	1:247:A:LYS:HB2	1:248:A:THR:HG22	10	0.14
(1,2514)	1:247:A:LYS:HB2	1:248:A:THR:HG23	10	0.14
(1,2514)	1:247:A:LYS:HB3	1:248:A:THR:HG21	10	0.14
(1,2514)	1:247:A:LYS:HB3	1:248:A:THR:HG22	10	0.14
(1,2514)	1:247:A:LYS:HB3	1:248:A:THR:HG23	10	0.14
(1,2384)	1:235:A:VAL:H	1:238:A:CYS:HB2	1	0.14
(1,2384)	1:235:A:VAL:H	1:238:A:CYS:HB3	1	0.14
(1,2233)	1:295:A:LYS:HE2	1:296:A:VAL:HA	11	0.14
(1,2233)	1:295:A:LYS:HE3	1:296:A:VAL:HA	11	0.14
(1,2009)	2:884:B:LYS:HG3	2:885:B:GLN:HB2	5	0.14
(1,1723)	1:294:A:LEU:HB2	1:296:A:VAL:HA	4	0.14
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	13	0.14
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	7	0.14
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	7	0.14
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	7	0.14
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	11	0.14
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	11	0.14
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	11	0.14
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	17	0.14
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	17	0.14
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	19	0.14
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	19	0.14
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	19	0.14
(1,1454)	2:896:B:GLU:HG2	2:897:B:VAL:HG11	1	0.14
(1,1454)	2:896:B:GLU:HG2	2:897:B:VAL:HG12	1	0.14
(1,1454)	2:896:B:GLU:HG2	2:897:B:VAL:HG13	1	0.14
(1,1454)	2:896:B:GLU:HG3	2:897:B:VAL:HG11	1	0.14
(1,1454)	2:896:B:GLU:HG3	2:897:B:VAL:HG12	1	0.14
(1,1454)	2:896:B:GLU:HG3	2:897:B:VAL:HG13	1	0.14
(1,1454)	2:896:B:GLU:HG2	2:897:B:VAL:HG11	17	0.14
(1,1454)	2:896:B:GLU:HG2	2:897:B:VAL:HG12	17	0.14
(1,1454)	2:896:B:GLU:HG2	2:897:B:VAL:HG13	17	0.14
(1,1454)	2:896:B:GLU:HG3	2:897:B:VAL:HG11	17	0.14
(1,1454)	2:896:B:GLU:HG3	2:897:B:VAL:HG12	17	0.14
(1,1454)	2:896:B:GLU:HG3	2:897:B:VAL:HG13	17	0.14
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG21	10	0.14
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG22	10	0.14
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG23	10	0.14
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG21	10	0.14
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG22	10	0.14
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG23	10	0.14
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG21	10	0.14
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG22	10	0.14
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG23	10	0.14
(1,1163)	1:251:A:GLN:HA	1:254:A:LEU:HG	3	0.14
(1,1163)	1:251:A:GLN:HA	1:254:A:LEU:HG	7	0.14
(1,707)	1:231:A:LEU:HD11	2:894:B:PHE:H	18	0.14
(1,707)	1:231:A:LEU:HD12	2:894:B:PHE:H	18	0.14
(1,707)	1:231:A:LEU:HD13	2:894:B:PHE:H	18	0.14
(1,704)	2:894:B:PHE:H	2:896:B:GLU:HB2	8	0.14
(1,704)	2:894:B:PHE:H	2:896:B:GLU:HB3	8	0.14
(1,589)	2:904:B:LYS:HA	2:905:B:LYS:H	5	0.14
(1,460)	1:248:A:THR:H	1:249:A:ASP:HB3	15	0.14
(1,444)	2:895:B:ALA:HB1	2:897:B:VAL:H	6	0.14
(1,444)	2:895:B:ALA:HB2	2:897:B:VAL:H	6	0.14
(1,444)	2:895:B:ALA:HB3	2:897:B:VAL:H	6	0.14
(1,223)	2:898:B:VAL:HB	2:899:B:SER:H	17	0.14
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	6	0.13
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	7	0.13
(1,3256)	2:884:B:LYS:HE2	2:888:B:ASP:H	16	0.13
(1,3256)	2:884:B:LYS:HE3	2:888:B:ASP:H	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3146)	2:868:B:LEU:HD11	2:869:B:SER:HA	3	0.13
(1,3146)	2:868:B:LEU:HD12	2:869:B:SER:HA	3	0.13
(1,3146)	2:868:B:LEU:HD13	2:869:B:SER:HA	3	0.13
(1,3146)	2:868:B:LEU:HD21	2:869:B:SER:HA	3	0.13
(1,3146)	2:868:B:LEU:HD22	2:869:B:SER:HA	3	0.13
(1,3146)	2:868:B:LEU:HD23	2:869:B:SER:HA	3	0.13
(1,3146)	2:868:B:LEU:HD11	2:869:B:SER:HA	8	0.13
(1,3146)	2:868:B:LEU:HD12	2:869:B:SER:HA	8	0.13
(1,3146)	2:868:B:LEU:HD13	2:869:B:SER:HA	8	0.13
(1,3146)	2:868:B:LEU:HD21	2:869:B:SER:HA	8	0.13
(1,3146)	2:868:B:LEU:HD22	2:869:B:SER:HA	8	0.13
(1,3146)	2:868:B:LEU:HD23	2:869:B:SER:HA	8	0.13
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	11	0.13
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	11	0.13
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	11	0.13
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	11	0.13
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	11	0.13
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	11	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD11	2	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD12	2	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD13	2	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD21	2	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD22	2	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD23	2	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD11	9	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD12	9	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD13	9	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD21	9	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD22	9	0.13
(1,2953)	2:838:B:GLN:HA	2:842:B:LEU:HD23	9	0.13
(1,2940)	2:831:B:GLU:HG2	2:832:B:LYS:HE2	10	0.13
(1,2940)	2:831:B:GLU:HG2	2:832:B:LYS:HE3	10	0.13
(1,2940)	2:831:B:GLU:HG3	2:832:B:LYS:HE2	10	0.13
(1,2940)	2:831:B:GLU:HG3	2:832:B:LYS:HE3	10	0.13
(1,2917)	2:826:B:THR:HG21	2:827:B:LEU:HD11	10	0.13
(1,2917)	2:826:B:THR:HG21	2:827:B:LEU:HD12	10	0.13
(1,2917)	2:826:B:THR:HG21	2:827:B:LEU:HD13	10	0.13
(1,2917)	2:826:B:THR:HG21	2:827:B:LEU:HD21	10	0.13
(1,2917)	2:826:B:THR:HG21	2:827:B:LEU:HD22	10	0.13
(1,2917)	2:826:B:THR:HG21	2:827:B:LEU:HD23	10	0.13
(1,2917)	2:826:B:THR:HG22	2:827:B:LEU:HD11	10	0.13
(1,2917)	2:826:B:THR:HG22	2:827:B:LEU:HD12	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2917)	2:826:B:THR:HG22	2:827:B:LEU:HD13	10	0.13
(1,2917)	2:826:B:THR:HG22	2:827:B:LEU:HD21	10	0.13
(1,2917)	2:826:B:THR:HG22	2:827:B:LEU:HD22	10	0.13
(1,2917)	2:826:B:THR:HG22	2:827:B:LEU:HD23	10	0.13
(1,2917)	2:826:B:THR:HG23	2:827:B:LEU:HD11	10	0.13
(1,2917)	2:826:B:THR:HG23	2:827:B:LEU:HD12	10	0.13
(1,2917)	2:826:B:THR:HG23	2:827:B:LEU:HD13	10	0.13
(1,2917)	2:826:B:THR:HG23	2:827:B:LEU:HD21	10	0.13
(1,2917)	2:826:B:THR:HG23	2:827:B:LEU:HD22	10	0.13
(1,2917)	2:826:B:THR:HG23	2:827:B:LEU:HD23	10	0.13
(1,2911)	2:825:B:GLU:HB2	2:826:B:THR:HG21	4	0.13
(1,2911)	2:825:B:GLU:HB2	2:826:B:THR:HG22	4	0.13
(1,2911)	2:825:B:GLU:HB2	2:826:B:THR:HG23	4	0.13
(1,2911)	2:825:B:GLU:HB3	2:826:B:THR:HG21	4	0.13
(1,2911)	2:825:B:GLU:HB3	2:826:B:THR:HG22	4	0.13
(1,2911)	2:825:B:GLU:HB3	2:826:B:THR:HG23	4	0.13
(1,2785)	1:287:A:ASP:HB3	1:291:A:GLU:HB2	2	0.13
(1,2785)	1:287:A:ASP:HB3	1:291:A:GLU:HB3	2	0.13
(1,2739)	1:277:A:LEU:HD11	1:279:A:PRO:HA	7	0.13
(1,2739)	1:277:A:LEU:HD12	1:279:A:PRO:HA	7	0.13
(1,2739)	1:277:A:LEU:HD13	1:279:A:PRO:HA	7	0.13
(1,2739)	1:277:A:LEU:HD21	1:279:A:PRO:HA	7	0.13
(1,2739)	1:277:A:LEU:HD22	1:279:A:PRO:HA	7	0.13
(1,2739)	1:277:A:LEU:HD23	1:279:A:PRO:HA	7	0.13
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	1	0.13
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	1	0.13
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	1	0.13
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	1	0.13
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	1	0.13
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	1	0.13
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	5	0.13
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	5	0.13
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	5	0.13
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	5	0.13
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	5	0.13
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	5	0.13
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	7	0.13
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	7	0.13
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	7	0.13
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	7	0.13
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	7	0.13
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	8	0.13
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	8	0.13
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	8	0.13
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	8	0.13
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	8	0.13
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	8	0.13
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	16	0.13
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	16	0.13
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	16	0.13
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	16	0.13
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	16	0.13
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	16	0.13
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	18	0.13
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	18	0.13
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	18	0.13
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	18	0.13
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	18	0.13
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	18	0.13
(1,2601)	1:260:A:LEU:HD11	2:889:B:PHE:HD1	3	0.13
(1,2601)	1:260:A:LEU:HD11	2:889:B:PHE:HD2	3	0.13
(1,2601)	1:260:A:LEU:HD12	2:889:B:PHE:HD1	3	0.13
(1,2601)	1:260:A:LEU:HD12	2:889:B:PHE:HD2	3	0.13
(1,2601)	1:260:A:LEU:HD13	2:889:B:PHE:HD1	3	0.13
(1,2601)	1:260:A:LEU:HD13	2:889:B:PHE:HD2	3	0.13
(1,2601)	1:260:A:LEU:HD21	2:889:B:PHE:HD1	3	0.13
(1,2601)	1:260:A:LEU:HD21	2:889:B:PHE:HD2	3	0.13
(1,2601)	1:260:A:LEU:HD22	2:889:B:PHE:HD1	3	0.13
(1,2601)	1:260:A:LEU:HD22	2:889:B:PHE:HD2	3	0.13
(1,2601)	1:260:A:LEU:HD23	2:889:B:PHE:HD1	3	0.13
(1,2601)	1:260:A:LEU:HD23	2:889:B:PHE:HD2	3	0.13
(1,2601)	1:260:A:LEU:HD11	2:889:B:PHE:HD1	4	0.13
(1,2601)	1:260:A:LEU:HD11	2:889:B:PHE:HD2	4	0.13
(1,2601)	1:260:A:LEU:HD12	2:889:B:PHE:HD1	4	0.13
(1,2601)	1:260:A:LEU:HD12	2:889:B:PHE:HD2	4	0.13
(1,2601)	1:260:A:LEU:HD13	2:889:B:PHE:HD1	4	0.13
(1,2601)	1:260:A:LEU:HD13	2:889:B:PHE:HD2	4	0.13
(1,2601)	1:260:A:LEU:HD21	2:889:B:PHE:HD1	4	0.13
(1,2601)	1:260:A:LEU:HD21	2:889:B:PHE:HD2	4	0.13
(1,2601)	1:260:A:LEU:HD22	2:889:B:PHE:HD1	4	0.13
(1,2601)	1:260:A:LEU:HD22	2:889:B:PHE:HD2	4	0.13
(1,2601)	1:260:A:LEU:HD23	2:889:B:PHE:HD1	4	0.13
(1,2601)	1:260:A:LEU:HD23	2:889:B:PHE:HD2	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG21	17	0.13
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG22	17	0.13
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG23	17	0.13
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG21	17	0.13
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG22	17	0.13
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG23	17	0.13
(1,2506)	1:246:A:ASN:HB2	1:247:A:LYS:HA	15	0.13
(1,2506)	1:246:A:ASN:HB3	1:247:A:LYS:HA	15	0.13
(1,2233)	1:295:A:LYS:HE2	1:296:A:VAL:HA	8	0.13
(1,2233)	1:295:A:LYS:HE3	1:296:A:VAL:HA	8	0.13
(1,2233)	1:295:A:LYS:HE2	1:296:A:VAL:HA	18	0.13
(1,2233)	1:295:A:LYS:HE3	1:296:A:VAL:HA	18	0.13
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB2	1	0.13
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB3	1	0.13
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB2	2	0.13
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB3	2	0.13
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	5	0.13
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	6	0.13
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	12	0.13
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	16	0.13
(1,1723)	1:294:A:LEU:HB2	1:296:A:VAL:HA	20	0.13
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	11	0.13
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	16	0.13
(1,1474)	2:848:B:ASN:HD21	2:851:B:ASN:HB2	19	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	3	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	3	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	3	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	4	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	4	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	4	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	5	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	5	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	5	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	10	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	10	0.13
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	10	0.13
(1,1319)	1:235:A:VAL:HB	1:254:A:LEU:HG	5	0.13
(1,1236)	2:850:B:LYS:H	2:850:B:LYS:HD2	4	0.13
(1,1236)	2:850:B:LYS:H	2:850:B:LYS:HD3	4	0.13
(1,1236)	2:850:B:LYS:H	2:850:B:LYS:HD2	10	0.13
(1,1236)	2:850:B:LYS:H	2:850:B:LYS:HD3	10	0.13
(1,1235)	2:849:B:ALA:H	2:850:B:LYS:HD2	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	2:849:B:ALA:H	2:850:B:LYS:HD3	12	0.13
(1,1163)	1:251:A:GLN:HA	1:254:A:LEU:HG	13	0.13
(1,1163)	1:251:A:GLN:HA	1:254:A:LEU:HG	20	0.13
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	4	0.13
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	7	0.13
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	17	0.13
(1,1018)	1:291:A:GLU:HG2	1:292:A:PRO:HD2	10	0.13
(1,1018)	1:291:A:GLU:HG3	1:292:A:PRO:HD2	10	0.13
(1,1018)	1:291:A:GLU:HG2	1:292:A:PRO:HD2	12	0.13
(1,1018)	1:291:A:GLU:HG3	1:292:A:PRO:HD2	12	0.13
(1,1005)	2:886:B:LEU:H	2:886:B:LEU:HG	1	0.13
(1,1005)	2:886:B:LEU:H	2:886:B:LEU:HG	2	0.13
(1,1005)	2:886:B:LEU:H	2:886:B:LEU:HG	4	0.13
(1,910)	2:823:B:ASP:HA	2:825:B:GLU:H	12	0.13
(1,815)	1:297:A:PRO:HA	1:299:A:GLY:H	11	0.13
(1,541)	1:287:A:ASP:HB3	1:289:A:LEU:H	6	0.13
(1,460)	1:248:A:THR:H	1:249:A:ASP:HB3	12	0.13
(1,222)	1:235:A:VAL:HB	1:236:A:THR:H	5	0.13
(1,222)	1:235:A:VAL:HB	1:236:A:THR:H	12	0.13
(1,112)	2:897:B:VAL:HB	2:898:B:VAL:H	8	0.13
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	16	0.12
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	18	0.12
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	19	0.12
(1,3256)	2:884:B:LYS:HE2	2:888:B:ASP:H	14	0.12
(1,3256)	2:884:B:LYS:HE3	2:888:B:ASP:H	14	0.12
(1,3256)	2:884:B:LYS:HE2	2:888:B:ASP:H	15	0.12
(1,3256)	2:884:B:LYS:HE3	2:888:B:ASP:H	15	0.12
(1,3256)	2:884:B:LYS:HE2	2:888:B:ASP:H	18	0.12
(1,3256)	2:884:B:LYS:HE3	2:888:B:ASP:H	18	0.12
(1,3164)	2:870:B:GLN:HA	2:870:B:GLN:HE21	11	0.12
(1,3164)	2:870:B:GLN:HA	2:870:B:GLN:HE22	11	0.12
(1,3146)	2:868:B:LEU:HD11	2:869:B:SER:HA	19	0.12
(1,3146)	2:868:B:LEU:HD12	2:869:B:SER:HA	19	0.12
(1,3146)	2:868:B:LEU:HD13	2:869:B:SER:HA	19	0.12
(1,3146)	2:868:B:LEU:HD21	2:869:B:SER:HA	19	0.12
(1,3146)	2:868:B:LEU:HD22	2:869:B:SER:HA	19	0.12
(1,3146)	2:868:B:LEU:HD23	2:869:B:SER:HA	19	0.12
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	4	0.12
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	4	0.12
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	4	0.12
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	4	0.12
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	4	0.12
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	8	0.12
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	8	0.12
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	8	0.12
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	8	0.12
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	8	0.12
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	8	0.12
(1,3130)	2:865:B:LEU:HD11	2:866:B:ALA:HA	10	0.12
(1,3130)	2:865:B:LEU:HD12	2:866:B:ALA:HA	10	0.12
(1,3130)	2:865:B:LEU:HD13	2:866:B:ALA:HA	10	0.12
(1,3130)	2:865:B:LEU:HD21	2:866:B:ALA:HA	10	0.12
(1,3130)	2:865:B:LEU:HD22	2:866:B:ALA:HA	10	0.12
(1,3130)	2:865:B:LEU:HD23	2:866:B:ALA:HA	10	0.12
(1,3035)	2:848:B:ASN:HD21	2:850:B:LYS:HB2	20	0.12
(1,3035)	2:848:B:ASN:HD21	2:850:B:LYS:HB3	20	0.12
(1,3035)	2:848:B:ASN:HD22	2:850:B:LYS:HB2	20	0.12
(1,3035)	2:848:B:ASN:HD22	2:850:B:LYS:HB3	20	0.12
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD11	1	0.12
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD12	1	0.12
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD13	1	0.12
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD21	1	0.12
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD22	1	0.12
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD23	1	0.12
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD11	1	0.12
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD12	1	0.12
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD13	1	0.12
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD21	1	0.12
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD22	1	0.12
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD23	1	0.12
(1,2739)	1:277:A:LEU:HD11	1:279:A:PRO:HA	2	0.12
(1,2739)	1:277:A:LEU:HD12	1:279:A:PRO:HA	2	0.12
(1,2739)	1:277:A:LEU:HD13	1:279:A:PRO:HA	2	0.12
(1,2739)	1:277:A:LEU:HD21	1:279:A:PRO:HA	2	0.12
(1,2739)	1:277:A:LEU:HD22	1:279:A:PRO:HA	2	0.12
(1,2739)	1:277:A:LEU:HD23	1:279:A:PRO:HA	2	0.12
(1,2739)	1:277:A:LEU:HD11	1:279:A:PRO:HA	14	0.12
(1,2739)	1:277:A:LEU:HD12	1:279:A:PRO:HA	14	0.12
(1,2739)	1:277:A:LEU:HD13	1:279:A:PRO:HA	14	0.12
(1,2739)	1:277:A:LEU:HD21	1:279:A:PRO:HA	14	0.12
(1,2739)	1:277:A:LEU:HD22	1:279:A:PRO:HA	14	0.12
(1,2739)	1:277:A:LEU:HD23	1:279:A:PRO:HA	14	0.12
(1,2739)	1:277:A:LEU:HD11	1:279:A:PRO:HA	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2739)	1:277:A:LEU:HD12	1:279:A:PRO:HA	18	0.12
(1,2739)	1:277:A:LEU:HD13	1:279:A:PRO:HA	18	0.12
(1,2739)	1:277:A:LEU:HD21	1:279:A:PRO:HA	18	0.12
(1,2739)	1:277:A:LEU:HD22	1:279:A:PRO:HA	18	0.12
(1,2739)	1:277:A:LEU:HD23	1:279:A:PRO:HA	18	0.12
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	15	0.12
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	15	0.12
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	15	0.12
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	15	0.12
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	15	0.12
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	15	0.12
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	17	0.12
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	17	0.12
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	17	0.12
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	17	0.12
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	17	0.12
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	17	0.12
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	19	0.12
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	19	0.12
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	19	0.12
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	19	0.12
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	19	0.12
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	19	0.12
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD11	20	0.12
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD12	20	0.12
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD13	20	0.12
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD21	20	0.12
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD22	20	0.12
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD23	20	0.12
(1,2678)	1:268:A:ARG:HD2	1:286:A:PHE:HB2	13	0.12
(1,2678)	1:268:A:ARG:HD3	1:286:A:PHE:HB2	13	0.12
(1,2617)	1:261:A:GLU:HG2	1:262:A:GLN:HE21	14	0.12
(1,2617)	1:261:A:GLU:HG2	1:262:A:GLN:HE22	14	0.12
(1,2617)	1:261:A:GLU:HG3	1:262:A:GLN:HE21	14	0.12
(1,2617)	1:261:A:GLU:HG3	1:262:A:GLN:HE22	14	0.12
(1,2601)	1:260:A:LEU:HD11	2:889:B:PHE:HD1	8	0.12
(1,2601)	1:260:A:LEU:HD11	2:889:B:PHE:HD2	8	0.12
(1,2601)	1:260:A:LEU:HD12	2:889:B:PHE:HD1	8	0.12
(1,2601)	1:260:A:LEU:HD12	2:889:B:PHE:HD2	8	0.12
(1,2601)	1:260:A:LEU:HD13	2:889:B:PHE:HD1	8	0.12
(1,2601)	1:260:A:LEU:HD13	2:889:B:PHE:HD2	8	0.12
(1,2601)	1:260:A:LEU:HD21	2:889:B:PHE:HD1	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2601)	1:260:A:LEU:HD21	2:889:B:PHE:HD2	8	0.12
(1,2601)	1:260:A:LEU:HD22	2:889:B:PHE:HD1	8	0.12
(1,2601)	1:260:A:LEU:HD22	2:889:B:PHE:HD2	8	0.12
(1,2601)	1:260:A:LEU:HD23	2:889:B:PHE:HD1	8	0.12
(1,2601)	1:260:A:LEU:HD23	2:889:B:PHE:HD2	8	0.12
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG21	18	0.12
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG22	18	0.12
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG23	18	0.12
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG21	18	0.12
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG22	18	0.12
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG23	18	0.12
(1,2509)	1:246:A:ASN:HB2	1:248:A:THR:HG21	10	0.12
(1,2509)	1:246:A:ASN:HB2	1:248:A:THR:HG22	10	0.12
(1,2509)	1:246:A:ASN:HB2	1:248:A:THR:HG23	10	0.12
(1,2509)	1:246:A:ASN:HB3	1:248:A:THR:HG21	10	0.12
(1,2509)	1:246:A:ASN:HB3	1:248:A:THR:HG22	10	0.12
(1,2509)	1:246:A:ASN:HB3	1:248:A:THR:HG23	10	0.12
(1,2506)	1:246:A:ASN:HB2	1:247:A:LYS:HA	3	0.12
(1,2506)	1:246:A:ASN:HB3	1:247:A:LYS:HA	3	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD11	7	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD12	7	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD13	7	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD21	7	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD22	7	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD23	7	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD11	13	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD12	13	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD13	13	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD21	13	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD22	13	0.12
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD23	13	0.12
(1,2375)	1:232:A:VAL:HG21	1:233:A:SER:HB2	9	0.12
(1,2375)	1:232:A:VAL:HG21	1:233:A:SER:HB3	9	0.12
(1,2375)	1:232:A:VAL:HG22	1:233:A:SER:HB2	9	0.12
(1,2375)	1:232:A:VAL:HG22	1:233:A:SER:HB3	9	0.12
(1,2375)	1:232:A:VAL:HG23	1:233:A:SER:HB2	9	0.12
(1,2375)	1:232:A:VAL:HG23	1:233:A:SER:HB3	9	0.12
(1,2317)	1:218:A:ASN:HB2	1:220:A:ALA:H	12	0.12
(1,2317)	1:218:A:ASN:HB3	1:220:A:ALA:H	12	0.12
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB2	7	0.12
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB3	7	0.12
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB3	11	0.12
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB2	17	0.12
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB3	17	0.12
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB2	18	0.12
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB3	18	0.12
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB2	20	0.12
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB3	20	0.12
(1,1961)	2:869:B:SER:H	2:870:B:GLN:HA	5	0.12
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	9	0.12
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	14	0.12
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	17	0.12
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	19	0.12
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	20	0.12
(1,1880)	2:870:B:GLN:HA	2:873:B:LEU:HB2	3	0.12
(1,1741)	2:829:B:GLU:HB2	2:832:B:LYS:HD2	19	0.12
(1,1741)	2:829:B:GLU:HB2	2:832:B:LYS:HD3	19	0.12
(1,1741)	2:829:B:GLU:HB3	2:832:B:LYS:HD2	19	0.12
(1,1741)	2:829:B:GLU:HB3	2:832:B:LYS:HD3	19	0.12
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	1	0.12
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	2	0.12
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	10	0.12
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	14	0.12
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	17	0.12
(1,1474)	2:848:B:ASN:HD21	2:851:B:ASN:HB2	13	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	1	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	1	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	1	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	6	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	6	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	6	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	15	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	15	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	15	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	16	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	16	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	16	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	18	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	18	0.12
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	18	0.12
(1,1377)	1:258:A:GLY:HA3	1:259:A:SER:HB2	14	0.12
(1,1377)	1:258:A:GLY:HA3	1:259:A:SER:HB3	14	0.12
(1,1377)	1:258:A:GLY:HA3	1:259:A:SER:HB2	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:258:A:GLY:HA3	1:259:A:SER:HB3	18	0.12
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD11	9	0.12
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD12	9	0.12
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD13	9	0.12
(1,1235)	2:849:B:ALA:H	2:850:B:LYS:HD2	4	0.12
(1,1235)	2:849:B:ALA:H	2:850:B:LYS:HD3	4	0.12
(1,1223)	2:826:B:THR:HG21	2:827:B:LEU:HG	10	0.12
(1,1223)	2:826:B:THR:HG22	2:827:B:LEU:HG	10	0.12
(1,1223)	2:826:B:THR:HG23	2:827:B:LEU:HG	10	0.12
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG21	8	0.12
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG22	8	0.12
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG23	8	0.12
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG21	8	0.12
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG22	8	0.12
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG23	8	0.12
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG21	8	0.12
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG22	8	0.12
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG23	8	0.12
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG21	19	0.12
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG22	19	0.12
(1,1222)	1:240:A:THR:HG21	1:241:A:THR:HG23	19	0.12
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG21	19	0.12
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG22	19	0.12
(1,1222)	1:240:A:THR:HG22	1:241:A:THR:HG23	19	0.12
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG21	19	0.12
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG22	19	0.12
(1,1222)	1:240:A:THR:HG23	1:241:A:THR:HG23	19	0.12
(1,1163)	1:251:A:GLN:HA	1:254:A:LEU:HG	14	0.12
(1,1104)	2:838:B:GLN:HG2	2:839:B:ASP:HA	20	0.12
(1,1028)	2:862:B:ILE:HA	2:865:B:LEU:HD11	6	0.12
(1,1028)	2:862:B:ILE:HA	2:865:B:LEU:HD12	6	0.12
(1,1028)	2:862:B:ILE:HA	2:865:B:LEU:HD13	6	0.12
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	1	0.12
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	13	0.12
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	14	0.12
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	18	0.12
(1,1005)	2:886:B:LEU:H	2:886:B:LEU:HG	8	0.12
(1,1005)	2:886:B:LEU:H	2:886:B:LEU:HG	11	0.12
(1,883)	2:832:B:LYS:HG2	2:833:B:TYR:HD1	18	0.12
(1,883)	2:832:B:LYS:HG2	2:833:B:TYR:HD2	18	0.12
(1,763)	1:268:A:ARG:HA	1:282:A:ALA:H	8	0.12
(1,707)	1:231:A:LEU:HD11	2:894:B:PHE:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,707)	1:231:A:LEU:HD12	2:894:B:PHE:H	7	0.12
(1,707)	1:231:A:LEU:HD13	2:894:B:PHE:H	7	0.12
(1,704)	2:894:B:PHE:H	2:896:B:GLU:HB2	3	0.12
(1,704)	2:894:B:PHE:H	2:896:B:GLU:HB3	3	0.12
(1,532)	2:848:B:ASN:HD22	2:851:B:ASN:HB2	11	0.12
(1,460)	1:248:A:THR:H	1:249:A:ASP:HB3	5	0.12
(1,222)	1:235:A:VAL:HB	1:236:A:THR:H	7	0.12
(1,222)	1:235:A:VAL:HB	1:236:A:THR:H	13	0.12
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	9	0.11
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	13	0.11
(3,37)	1:241:A:THR:H	1:237:A:GLU:O	15	0.11
(1,3285)	2:893:B:SER:HB2	2:896:B:GLU:HG2	8	0.11
(1,3285)	2:893:B:SER:HB2	2:896:B:GLU:HG3	8	0.11
(1,3285)	2:893:B:SER:HB3	2:896:B:GLU:HG2	8	0.11
(1,3285)	2:893:B:SER:HB3	2:896:B:GLU:HG3	8	0.11
(1,3256)	2:884:B:LYS:HE2	2:888:B:ASP:H	7	0.11
(1,3256)	2:884:B:LYS:HE3	2:888:B:ASP:H	7	0.11
(1,3186)	2:871:B:ASP:H	2:872:B:GLU:HG2	15	0.11
(1,3186)	2:871:B:ASP:H	2:872:B:GLU:HG3	15	0.11
(1,3173)	2:870:B:GLN:HG2	2:872:B:GLU:H	7	0.11
(1,3173)	2:870:B:GLN:HG3	2:872:B:GLU:H	7	0.11
(1,3146)	2:868:B:LEU:HD11	2:869:B:SER:HA	4	0.11
(1,3146)	2:868:B:LEU:HD12	2:869:B:SER:HA	4	0.11
(1,3146)	2:868:B:LEU:HD13	2:869:B:SER:HA	4	0.11
(1,3146)	2:868:B:LEU:HD21	2:869:B:SER:HA	4	0.11
(1,3146)	2:868:B:LEU:HD22	2:869:B:SER:HA	4	0.11
(1,3146)	2:868:B:LEU:HD23	2:869:B:SER:HA	4	0.11
(1,3100)	2:860:B:LYS:HD2	2:864:B:GLU:HG2	6	0.11
(1,3100)	2:860:B:LYS:HD2	2:864:B:GLU:HG3	6	0.11
(1,3100)	2:860:B:LYS:HD3	2:864:B:GLU:HG2	6	0.11
(1,3100)	2:860:B:LYS:HD3	2:864:B:GLU:HG3	6	0.11
(1,3069)	2:855:B:LEU:HD11	2:866:B:ALA:H	5	0.11
(1,3069)	2:855:B:LEU:HD12	2:866:B:ALA:H	5	0.11
(1,3069)	2:855:B:LEU:HD13	2:866:B:ALA:H	5	0.11
(1,3069)	2:855:B:LEU:HD21	2:866:B:ALA:H	5	0.11
(1,3069)	2:855:B:LEU:HD22	2:866:B:ALA:H	5	0.11
(1,3069)	2:855:B:LEU:HD23	2:866:B:ALA:H	5	0.11
(1,3069)	2:855:B:LEU:HD11	2:866:B:ALA:H	9	0.11
(1,3069)	2:855:B:LEU:HD12	2:866:B:ALA:H	9	0.11
(1,3069)	2:855:B:LEU:HD13	2:866:B:ALA:H	9	0.11
(1,3069)	2:855:B:LEU:HD21	2:866:B:ALA:H	9	0.11
(1,3069)	2:855:B:LEU:HD22	2:866:B:ALA:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3069)	2:855:B:LEU:HD23	2:866:B:ALA:H	9	0.11
(1,3035)	2:848:B:ASN:HD21	2:850:B:LYS:HB2	4	0.11
(1,3035)	2:848:B:ASN:HD21	2:850:B:LYS:HB3	4	0.11
(1,3035)	2:848:B:ASN:HD22	2:850:B:LYS:HB2	4	0.11
(1,3035)	2:848:B:ASN:HD22	2:850:B:LYS:HB3	4	0.11
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD11	15	0.11
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD12	15	0.11
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD13	15	0.11
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD21	15	0.11
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD22	15	0.11
(1,2958)	2:838:B:GLN:HE21	2:842:B:LEU:HD23	15	0.11
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD11	15	0.11
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD12	15	0.11
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD13	15	0.11
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD21	15	0.11
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD22	15	0.11
(1,2958)	2:838:B:GLN:HE22	2:842:B:LEU:HD23	15	0.11
(1,2907)	2:823:B:ASP:HB2	2:825:B:GLU:HB2	4	0.11
(1,2907)	2:823:B:ASP:HB2	2:825:B:GLU:HB3	4	0.11
(1,2907)	2:823:B:ASP:HB3	2:825:B:GLU:HB2	4	0.11
(1,2907)	2:823:B:ASP:HB3	2:825:B:GLU:HB3	4	0.11
(1,2903)	1:301:A:GLU:HG2	1:302:A:HIS:H	17	0.11
(1,2903)	1:301:A:GLU:HG3	1:302:A:HIS:H	17	0.11
(1,2862)	1:295:A:LYS:H	1:295:A:LYS:HB2	8	0.11
(1,2862)	1:295:A:LYS:H	1:295:A:LYS:HB3	8	0.11
(1,2862)	1:295:A:LYS:H	1:295:A:LYS:HB2	10	0.11
(1,2862)	1:295:A:LYS:H	1:295:A:LYS:HB3	10	0.11
(1,2819)	1:290:A:HIS:H	1:291:A:GLU:HB2	3	0.11
(1,2819)	1:290:A:HIS:H	1:291:A:GLU:HB3	3	0.11
(1,2748)	1:280:A:GLN:HB2	1:284:A:ARG:HG2	20	0.11
(1,2748)	1:280:A:GLN:HB2	1:284:A:ARG:HG3	20	0.11
(1,2748)	1:280:A:GLN:HB3	1:284:A:ARG:HG2	20	0.11
(1,2748)	1:280:A:GLN:HB3	1:284:A:ARG:HG3	20	0.11
(1,2739)	1:277:A:LEU:HD11	1:279:A:PRO:HA	16	0.11
(1,2739)	1:277:A:LEU:HD12	1:279:A:PRO:HA	16	0.11
(1,2739)	1:277:A:LEU:HD13	1:279:A:PRO:HA	16	0.11
(1,2739)	1:277:A:LEU:HD21	1:279:A:PRO:HA	16	0.11
(1,2739)	1:277:A:LEU:HD22	1:279:A:PRO:HA	16	0.11
(1,2739)	1:277:A:LEU:HD23	1:279:A:PRO:HA	16	0.11
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	6	0.11
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	6	0.11
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	6	0.11
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	6	0.11
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	6	0.11
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG21	11	0.11
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG22	11	0.11
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG23	11	0.11
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG21	11	0.11
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG22	11	0.11
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG23	11	0.11
(1,2523)	1:251:A:GLN:H	1:251:A:GLN:HG2	10	0.11
(1,2523)	1:251:A:GLN:H	1:251:A:GLN:HG3	10	0.11
(1,2506)	1:246:A:ASN:HB2	1:247:A:LYS:HA	8	0.11
(1,2506)	1:246:A:ASN:HB3	1:247:A:LYS:HA	8	0.11
(1,2506)	1:246:A:ASN:HB2	1:247:A:LYS:HA	14	0.11
(1,2506)	1:246:A:ASN:HB3	1:247:A:LYS:HA	14	0.11
(1,2506)	1:246:A:ASN:HB2	1:247:A:LYS:HA	18	0.11
(1,2506)	1:246:A:ASN:HB3	1:247:A:LYS:HA	18	0.11
(1,2414)	1:238:A:CYS:H	1:239:A:LEU:HD11	19	0.11
(1,2414)	1:238:A:CYS:H	1:239:A:LEU:HD12	19	0.11
(1,2414)	1:238:A:CYS:H	1:239:A:LEU:HD13	19	0.11
(1,2414)	1:238:A:CYS:H	1:239:A:LEU:HD21	19	0.11
(1,2414)	1:238:A:CYS:H	1:239:A:LEU:HD22	19	0.11
(1,2414)	1:238:A:CYS:H	1:239:A:LEU:HD23	19	0.11
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD11	12	0.11
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD12	12	0.11
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD13	12	0.11
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD21	12	0.11
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD22	12	0.11
(1,2388)	1:235:A:VAL:HB	1:254:A:LEU:HD23	12	0.11
(1,2375)	1:232:A:VAL:HG21	1:233:A:SER:HB2	16	0.11
(1,2375)	1:232:A:VAL:HG21	1:233:A:SER:HB3	16	0.11
(1,2375)	1:232:A:VAL:HG22	1:233:A:SER:HB2	16	0.11
(1,2375)	1:232:A:VAL:HG22	1:233:A:SER:HB3	16	0.11
(1,2375)	1:232:A:VAL:HG23	1:233:A:SER:HB2	16	0.11
(1,2375)	1:232:A:VAL:HG23	1:233:A:SER:HB3	16	0.11
(1,2248)	2:836:B:GLY:HA3	2:837:B:PRO:HB3	11	0.11
(1,2188)	1:239:A:LEU:HB3	1:263:A:LEU:HG	3	0.11
(1,2188)	1:239:A:LEU:HB3	1:263:A:LEU:HG	7	0.11
(1,2188)	1:239:A:LEU:HB3	1:263:A:LEU:HG	14	0.11
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB2	6	0.11
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB3	6	0.11
(1,2105)	1:231:A:LEU:HB3	1:232:A:VAL:HB	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2105)	1:231:A:LEU:HB3	1:232:A:VAL:HB	12	0.11
(1,2080)	1:215:A:ARG:HA	1:215:A:ARG:HD2	18	0.11
(1,2080)	1:215:A:ARG:HA	1:215:A:ARG:HD3	18	0.11
(1,1919)	2:831:B:GLU:HG2	2:832:B:LYS:HB2	3	0.11
(1,1919)	2:831:B:GLU:HG2	2:832:B:LYS:HB3	3	0.11
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	11	0.11
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	13	0.11
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	18	0.11
(1,1880)	2:870:B:GLN:HA	2:873:B:LEU:HB2	1	0.11
(1,1851)	2:886:B:LEU:HG	2:890:B:ILE:HD11	5	0.11
(1,1851)	2:886:B:LEU:HG	2:890:B:ILE:HD12	5	0.11
(1,1851)	2:886:B:LEU:HG	2:890:B:ILE:HD13	5	0.11
(1,1740)	2:829:B:GLU:HA	2:832:B:LYS:HD2	9	0.11
(1,1740)	2:829:B:GLU:HA	2:832:B:LYS:HD3	9	0.11
(1,1730)	2:902:B:LYS:HE2	2:903:B:GLY:HA2	4	0.11
(1,1730)	2:902:B:LYS:HE2	2:903:B:GLY:HA3	4	0.11
(1,1730)	2:902:B:LYS:HE3	2:903:B:GLY:HA2	4	0.11
(1,1730)	2:902:B:LYS:HE3	2:903:B:GLY:HA3	4	0.11
(1,1730)	2:902:B:LYS:HE2	2:903:B:GLY:HA2	16	0.11
(1,1730)	2:902:B:LYS:HE2	2:903:B:GLY:HA3	16	0.11
(1,1730)	2:902:B:LYS:HE3	2:903:B:GLY:HA2	16	0.11
(1,1730)	2:902:B:LYS:HE3	2:903:B:GLY:HA3	16	0.11
(1,1723)	1:294:A:LEU:HB2	1:296:A:VAL:HA	5	0.11
(1,1723)	1:294:A:LEU:HB2	1:296:A:VAL:HA	11	0.11
(1,1722)	1:253:A:LEU:HG	1:257:A:PHE:HE1	11	0.11
(1,1722)	1:253:A:LEU:HG	1:257:A:PHE:HE2	11	0.11
(1,1719)	1:292:A:PRO:HD2	1:296:A:VAL:H	15	0.11
(1,1587)	1:241:A:THR:HA	2:843:B:LYS:HE2	7	0.11
(1,1587)	1:241:A:THR:HA	2:843:B:LYS:HE3	7	0.11
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	3	0.11
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	4	0.11
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	7	0.11
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	9	0.11
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	18	0.11
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	19	0.11
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE2	11	0.11
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE3	11	0.11
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE2	11	0.11
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE3	11	0.11
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE2	15	0.11
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE3	15	0.11
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE2	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE3	15	0.11
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE2	16	0.11
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE3	16	0.11
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE2	16	0.11
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE3	16	0.11
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE2	17	0.11
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE3	17	0.11
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE2	17	0.11
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE3	17	0.11
(1,1356)	1:235:A:VAL:HB	1:254:A:LEU:HD11	5	0.11
(1,1356)	1:235:A:VAL:HB	1:254:A:LEU:HD12	5	0.11
(1,1356)	1:235:A:VAL:HB	1:254:A:LEU:HD13	5	0.11
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD11	10	0.11
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD12	10	0.11
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD13	10	0.11
(1,1304)	2:855:B:LEU:HB3	2:856:B:MET:HG2	15	0.11
(1,1289)	2:859:B:VAL:HG21	2:861:B:ASN:H	10	0.11
(1,1289)	2:859:B:VAL:HG22	2:861:B:ASN:H	10	0.11
(1,1289)	2:859:B:VAL:HG23	2:861:B:ASN:H	10	0.11
(1,1236)	2:850:B:LYS:H	2:850:B:LYS:HD2	12	0.11
(1,1236)	2:850:B:LYS:H	2:850:B:LYS:HD3	12	0.11
(1,1148)	1:236:A:THR:HG21	1:254:A:LEU:HD21	5	0.11
(1,1148)	1:236:A:THR:HG21	1:254:A:LEU:HD22	5	0.11
(1,1148)	1:236:A:THR:HG21	1:254:A:LEU:HD23	5	0.11
(1,1148)	1:236:A:THR:HG22	1:254:A:LEU:HD21	5	0.11
(1,1148)	1:236:A:THR:HG22	1:254:A:LEU:HD22	5	0.11
(1,1148)	1:236:A:THR:HG22	1:254:A:LEU:HD23	5	0.11
(1,1148)	1:236:A:THR:HG23	1:254:A:LEU:HD21	5	0.11
(1,1148)	1:236:A:THR:HG23	1:254:A:LEU:HD22	5	0.11
(1,1148)	1:236:A:THR:HG23	1:254:A:LEU:HD23	5	0.11
(1,1104)	2:838:B:GLN:HG2	2:839:B:ASP:HA	18	0.11
(1,1077)	2:842:B:LEU:HA	2:842:B:LEU:HD11	2	0.11
(1,1077)	2:842:B:LEU:HA	2:842:B:LEU:HD12	2	0.11
(1,1077)	2:842:B:LEU:HA	2:842:B:LEU:HD13	2	0.11
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	5	0.11
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	8	0.11
(1,1022)	2:842:B:LEU:HB3	2:843:B:LYS:HG2	16	0.11
(1,1018)	1:291:A:GLU:HG2	1:292:A:PRO:HD2	18	0.11
(1,1018)	1:291:A:GLU:HG3	1:292:A:PRO:HD2	18	0.11
(1,1002)	2:879:B:ASN:HB2	2:882:B:ASN:HB3	20	0.11
(1,974)	1:234:A:ARG:HG2	2:889:B:PHE:HD1	11	0.11
(1,974)	1:234:A:ARG:HG2	2:889:B:PHE:HD2	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:234:A:ARG:HG3	2:889:B:PHE:HD1	11	0.11
(1,974)	1:234:A:ARG:HG3	2:889:B:PHE:HD2	11	0.11
(1,901)	1:294:A:LEU:HB3	2:833:B:TYR:HE1	13	0.11
(1,901)	1:294:A:LEU:HB3	2:833:B:TYR:HE2	13	0.11
(1,901)	1:294:A:LEU:HB3	2:833:B:TYR:HE1	17	0.11
(1,901)	1:294:A:LEU:HB3	2:833:B:TYR:HE2	17	0.11
(1,901)	1:294:A:LEU:HB3	2:833:B:TYR:HE1	18	0.11
(1,901)	1:294:A:LEU:HB3	2:833:B:TYR:HE2	18	0.11
(1,763)	1:268:A:ARG:HA	1:282:A:ALA:H	18	0.11
(1,721)	1:240:A:THR:H	2:840:B:PHE:HE1	20	0.11
(1,721)	1:240:A:THR:H	2:840:B:PHE:HE2	20	0.11
(1,707)	1:231:A:LEU:HD11	2:894:B:PHE:H	3	0.11
(1,707)	1:231:A:LEU:HD12	2:894:B:PHE:H	3	0.11
(1,707)	1:231:A:LEU:HD13	2:894:B:PHE:H	3	0.11
(1,707)	1:231:A:LEU:HD11	2:894:B:PHE:H	15	0.11
(1,707)	1:231:A:LEU:HD12	2:894:B:PHE:H	15	0.11
(1,707)	1:231:A:LEU:HD13	2:894:B:PHE:H	15	0.11
(1,704)	2:894:B:PHE:H	2:896:B:GLU:HB2	18	0.11
(1,704)	2:894:B:PHE:H	2:896:B:GLU:HB3	18	0.11
(1,541)	1:287:A:ASP:HB3	1:289:A:LEU:H	11	0.11
(1,451)	1:246:A:ASN:HD21	1:248:A:THR:H	12	0.11
(1,444)	2:895:B:ALA:HB1	2:897:B:VAL:H	20	0.11
(1,444)	2:895:B:ALA:HB2	2:897:B:VAL:H	20	0.11
(1,444)	2:895:B:ALA:HB3	2:897:B:VAL:H	20	0.11
(1,379)	1:284:A:ARG:H	1:284:A:ARG:HD3	11	0.11
(1,112)	2:897:B:VAL:HB	2:898:B:VAL:H	6	0.11
(1,3164)	2:870:B:GLN:HA	2:870:B:GLN:HE21	6	0.1
(1,3164)	2:870:B:GLN:HA	2:870:B:GLN:HE22	6	0.1
(1,3102)	2:861:B:ASN:H	2:861:B:ASN:HD21	8	0.1
(1,3102)	2:861:B:ASN:H	2:861:B:ASN:HD22	8	0.1
(1,3102)	2:861:B:ASN:H	2:861:B:ASN:HD21	20	0.1
(1,3102)	2:861:B:ASN:H	2:861:B:ASN:HD22	20	0.1
(1,3024)	2:847:B:VAL:HG11	2:848:B:ASN:H	12	0.1
(1,3024)	2:847:B:VAL:HG12	2:848:B:ASN:H	12	0.1
(1,3024)	2:847:B:VAL:HG13	2:848:B:ASN:H	12	0.1
(1,3024)	2:847:B:VAL:HG21	2:848:B:ASN:H	12	0.1
(1,3024)	2:847:B:VAL:HG22	2:848:B:ASN:H	12	0.1
(1,3024)	2:847:B:VAL:HG23	2:848:B:ASN:H	12	0.1
(1,2946)	2:834:B:ASN:HB2	2:835:B:PRO:HG2	9	0.1
(1,2946)	2:834:B:ASN:HB2	2:835:B:PRO:HG3	9	0.1
(1,2946)	2:834:B:ASN:HB3	2:835:B:PRO:HG2	9	0.1
(1,2946)	2:834:B:ASN:HB3	2:835:B:PRO:HG3	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2946)	2:834:B:ASN:HB2	2:835:B:PRO:HG2	16	0.1
(1,2946)	2:834:B:ASN:HB2	2:835:B:PRO:HG3	16	0.1
(1,2946)	2:834:B:ASN:HB3	2:835:B:PRO:HG2	16	0.1
(1,2946)	2:834:B:ASN:HB3	2:835:B:PRO:HG3	16	0.1
(1,2903)	1:301:A:GLU:HG2	1:302:A:HIS:H	7	0.1
(1,2903)	1:301:A:GLU:HG3	1:302:A:HIS:H	7	0.1
(1,2862)	1:295:A:LYS:H	1:295:A:LYS:HB2	18	0.1
(1,2862)	1:295:A:LYS:H	1:295:A:LYS:HB3	18	0.1
(1,2830)	1:293:A:PHE:HB2	2:842:B:LEU:HD11	16	0.1
(1,2830)	1:293:A:PHE:HB2	2:842:B:LEU:HD12	16	0.1
(1,2830)	1:293:A:PHE:HB2	2:842:B:LEU:HD13	16	0.1
(1,2830)	1:293:A:PHE:HB2	2:842:B:LEU:HD21	16	0.1
(1,2830)	1:293:A:PHE:HB2	2:842:B:LEU:HD22	16	0.1
(1,2830)	1:293:A:PHE:HB2	2:842:B:LEU:HD23	16	0.1
(1,2819)	1:290:A:HIS:H	1:291:A:GLU:HB2	10	0.1
(1,2819)	1:290:A:HIS:H	1:291:A:GLU:HB3	10	0.1
(1,2752)	1:280:A:GLN:HG2	1:283:A:ARG:HG2	20	0.1
(1,2752)	1:280:A:GLN:HG2	1:283:A:ARG:HG3	20	0.1
(1,2752)	1:280:A:GLN:HG3	1:283:A:ARG:HG2	20	0.1
(1,2752)	1:280:A:GLN:HG3	1:283:A:ARG:HG3	20	0.1
(1,2718)	1:273:A:LEU:HD11	1:274:A:CYS:H	9	0.1
(1,2718)	1:273:A:LEU:HD12	1:274:A:CYS:H	9	0.1
(1,2718)	1:273:A:LEU:HD13	1:274:A:CYS:H	9	0.1
(1,2718)	1:273:A:LEU:HD21	1:274:A:CYS:H	9	0.1
(1,2718)	1:273:A:LEU:HD22	1:274:A:CYS:H	9	0.1
(1,2718)	1:273:A:LEU:HD23	1:274:A:CYS:H	9	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD11	17	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD12	17	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD13	17	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD21	17	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD22	17	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD23	17	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD11	19	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD12	19	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD13	19	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD21	19	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD22	19	0.1
(1,2714)	1:273:A:LEU:H	1:273:A:LEU:HD23	19	0.1
(1,2658)	1:267:A:SER:HA	1:269:A:GLU:HG2	7	0.1
(1,2658)	1:267:A:SER:HA	1:269:A:GLU:HG3	7	0.1
(1,2608)	1:261:A:GLU:H	1:261:A:GLU:HG2	2	0.1
(1,2608)	1:261:A:GLU:H	1:261:A:GLU:HG3	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG21	15	0.1
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG22	15	0.1
(1,2530)	1:251:A:GLN:HG2	1:252:A:THR:HG23	15	0.1
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG21	15	0.1
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG22	15	0.1
(1,2530)	1:251:A:GLN:HG3	1:252:A:THR:HG23	15	0.1
(1,2263)	2:844:B:MET:HE1	2:862:B:ILE:HD11	2	0.1
(1,2263)	2:844:B:MET:HE1	2:862:B:ILE:HD12	2	0.1
(1,2263)	2:844:B:MET:HE1	2:862:B:ILE:HD13	2	0.1
(1,2263)	2:844:B:MET:HE2	2:862:B:ILE:HD11	2	0.1
(1,2263)	2:844:B:MET:HE2	2:862:B:ILE:HD12	2	0.1
(1,2263)	2:844:B:MET:HE2	2:862:B:ILE:HD13	2	0.1
(1,2263)	2:844:B:MET:HE3	2:862:B:ILE:HD11	2	0.1
(1,2263)	2:844:B:MET:HE3	2:862:B:ILE:HD12	2	0.1
(1,2263)	2:844:B:MET:HE3	2:862:B:ILE:HD13	2	0.1
(1,2251)	2:841:B:LEU:HG	2:842:B:LEU:HG	14	0.1
(1,2188)	1:239:A:LEU:HB3	1:263:A:LEU:HG	15	0.1
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB2	5	0.1
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB3	5	0.1
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB2	19	0.1
(1,2138)	2:837:B:PRO:HA	2:839:B:ASP:HB3	19	0.1
(1,2080)	1:215:A:ARG:HA	1:215:A:ARG:HD2	12	0.1
(1,2080)	1:215:A:ARG:HA	1:215:A:ARG:HD3	12	0.1
(1,2026)	1:256:A:THR:HA	1:257:A:PHE:HE1	17	0.1
(1,2026)	1:256:A:THR:HA	1:257:A:PHE:HE2	17	0.1
(1,1907)	2:891:B:HIS:HA	2:891:B:HIS:HE1	4	0.1
(1,1851)	2:886:B:LEU:HG	2:890:B:ILE:HD11	12	0.1
(1,1851)	2:886:B:LEU:HG	2:890:B:ILE:HD12	12	0.1
(1,1851)	2:886:B:LEU:HG	2:890:B:ILE:HD13	12	0.1
(1,1723)	1:294:A:LEU:HB2	1:296:A:VAL:HA	14	0.1
(1,1703)	1:286:A:PHE:HA	1:286:A:PHE:HE1	20	0.1
(1,1703)	1:286:A:PHE:HA	1:286:A:PHE:HE2	20	0.1
(1,1476)	2:841:B:LEU:HB2	2:862:B:ILE:HA	8	0.1
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD21	13	0.1
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD22	13	0.1
(1,1461)	2:842:B:LEU:HA	2:842:B:LEU:HD23	13	0.1
(1,1376)	2:848:B:ASN:HB2	2:850:B:LYS:HE2	17	0.1
(1,1376)	2:848:B:ASN:HB2	2:850:B:LYS:HE3	17	0.1
(1,1376)	2:848:B:ASN:HB2	2:850:B:LYS:HE2	19	0.1
(1,1376)	2:848:B:ASN:HB2	2:850:B:LYS:HE3	19	0.1
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE2	6	0.1
(1,1369)	2:839:B:ASP:HB2	2:843:B:LYS:HE3	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE2	6	0.1
(1,1369)	2:839:B:ASP:HB3	2:843:B:LYS:HE3	6	0.1
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD11	4	0.1
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD12	4	0.1
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD13	4	0.1
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD11	8	0.1
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD12	8	0.1
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD13	8	0.1
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD11	11	0.1
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD12	11	0.1
(1,1353)	1:254:A:LEU:HA	1:254:A:LEU:HD13	11	0.1
(1,1289)	2:859:B:VAL:HG21	2:861:B:ASN:H	20	0.1
(1,1289)	2:859:B:VAL:HG22	2:861:B:ASN:H	20	0.1
(1,1289)	2:859:B:VAL:HG23	2:861:B:ASN:H	20	0.1
(1,1118)	2:855:B:LEU:HA	2:855:B:LEU:HD11	1	0.1
(1,1118)	2:855:B:LEU:HA	2:855:B:LEU:HD12	1	0.1
(1,1118)	2:855:B:LEU:HA	2:855:B:LEU:HD13	1	0.1
(1,1118)	2:855:B:LEU:HA	2:855:B:LEU:HD11	14	0.1
(1,1118)	2:855:B:LEU:HA	2:855:B:LEU:HD12	14	0.1
(1,1118)	2:855:B:LEU:HA	2:855:B:LEU:HD13	14	0.1
(1,1104)	2:838:B:GLN:HG2	2:839:B:ASP:HA	2	0.1
(1,1104)	2:838:B:GLN:HG2	2:839:B:ASP:HA	3	0.1
(1,1028)	2:862:B:ILE:HA	2:865:B:LEU:HD11	5	0.1
(1,1028)	2:862:B:ILE:HA	2:865:B:LEU:HD12	5	0.1
(1,1028)	2:862:B:ILE:HA	2:865:B:LEU:HD13	5	0.1
(1,1028)	2:862:B:ILE:HA	2:865:B:LEU:HD11	18	0.1
(1,1028)	2:862:B:ILE:HA	2:865:B:LEU:HD12	18	0.1
(1,1028)	2:862:B:ILE:HA	2:865:B:LEU:HD13	18	0.1
(1,939)	1:253:A:LEU:HD11	1:256:A:THR:HG21	11	0.1
(1,939)	1:253:A:LEU:HD11	1:256:A:THR:HG22	11	0.1
(1,939)	1:253:A:LEU:HD11	1:256:A:THR:HG23	11	0.1
(1,939)	1:253:A:LEU:HD12	1:256:A:THR:HG21	11	0.1
(1,939)	1:253:A:LEU:HD12	1:256:A:THR:HG22	11	0.1
(1,939)	1:253:A:LEU:HD12	1:256:A:THR:HG23	11	0.1
(1,939)	1:253:A:LEU:HD13	1:256:A:THR:HG21	11	0.1
(1,939)	1:253:A:LEU:HD13	1:256:A:THR:HG22	11	0.1
(1,939)	1:253:A:LEU:HD13	1:256:A:THR:HG23	11	0.1
(1,721)	1:240:A:THR:H	2:840:B:PHE:HE1	9	0.1
(1,721)	1:240:A:THR:H	2:840:B:PHE:HE2	9	0.1
(1,721)	1:240:A:THR:H	2:840:B:PHE:HE1	19	0.1
(1,721)	1:240:A:THR:H	2:840:B:PHE:HE2	19	0.1
(1,444)	2:895:B:ALA:HB1	2:897:B:VAL:H	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,444)	2:895:B:ALA:HB2	2:897:B:VAL:H	5	0.1
(1,444)	2:895:B:ALA:HB3	2:897:B:VAL:H	5	0.1
(1,444)	2:895:B:ALA:HB1	2:897:B:VAL:H	16	0.1
(1,444)	2:895:B:ALA:HB2	2:897:B:VAL:H	16	0.1
(1,444)	2:895:B:ALA:HB3	2:897:B:VAL:H	16	0.1

10 Dihedral-angle violation analysis [i](#)

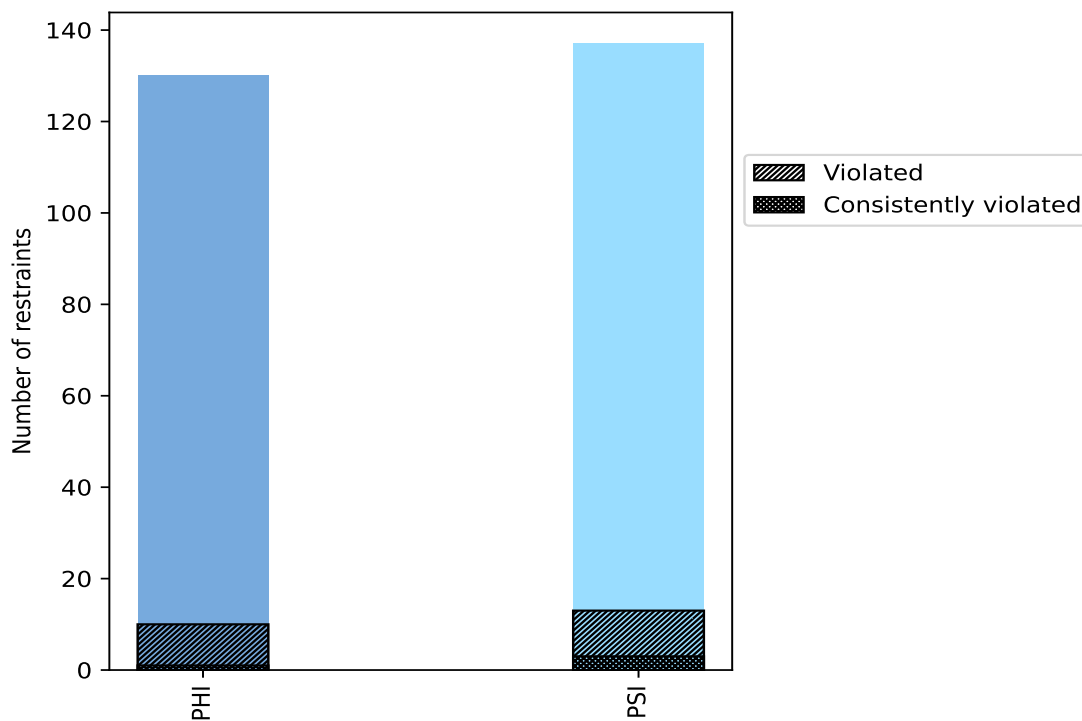
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	130	48.7	10	7.7	3.7	1	0.8	0.4
PSI	137	51.3	13	9.5	4.9	3	2.2	1.1
Total	267	100.0	23	8.6	8.6	4	1.5	1.5

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



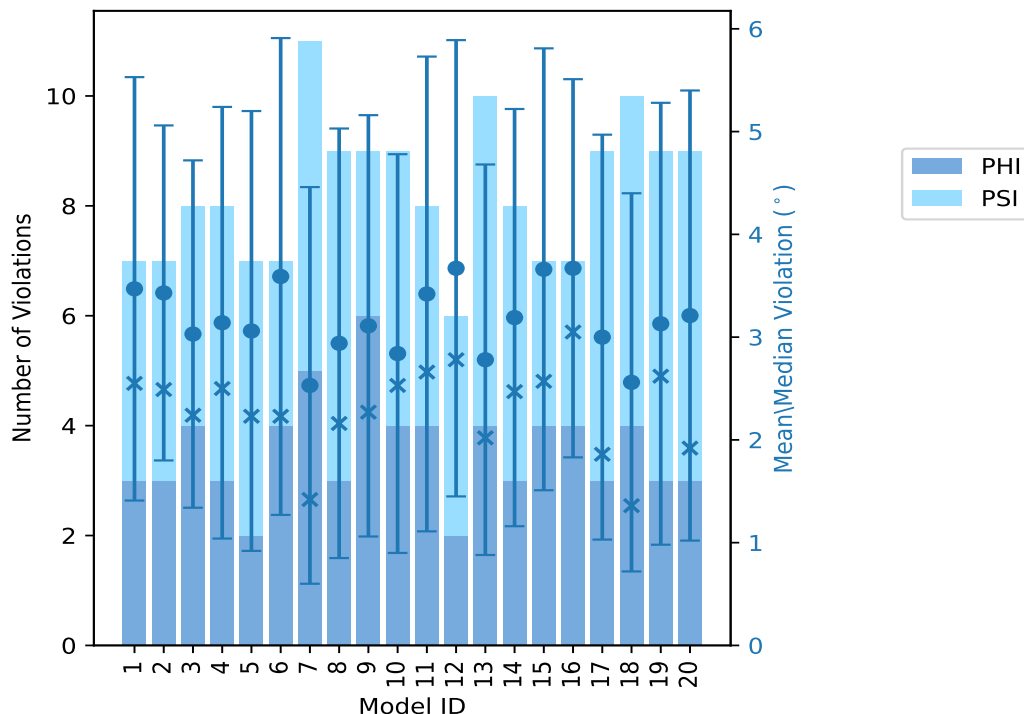
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	3	4	7	3.47	6.57	2.06	2.55
2	3	4	7	3.43	5.94	1.63	2.49
3	4	4	8	3.03	6.01	1.69	2.24
4	3	5	8	3.14	6.84	2.1	2.5
5	2	5	7	3.06	6.58	2.14	2.23
6	4	3	7	3.59	7.61	2.32	2.23
7	5	6	11	2.53	6.45	1.93	1.42
8	3	6	9	2.94	6.85	2.09	2.16
9	6	3	9	3.11	6.88	2.05	2.27
10	4	5	9	2.84	6.96	1.94	2.53
11	4	4	8	3.42	7.56	2.31	2.66
12	2	4	6	3.67	6.91	2.22	2.78
13	4	6	10	2.78	7.16	1.9	2.02
14	3	5	8	3.19	6.38	2.03	2.47
15	4	3	7	3.66	7.44	2.15	2.57
16	4	3	7	3.67	6.86	1.84	3.05
17	3	6	9	3.0	6.76	1.97	1.86
18	4	6	10	2.56	6.32	1.84	1.36
19	3	6	9	3.13	7.52	2.15	2.62
20	3	6	9	3.21	7.51	2.19	1.92

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
4	5	9	1	5.0
0	0	0	2	10.0
0	2	2	3	15.0
0	0	0	4	20.0
3	1	4	5	25.0
0	0	0	6	30.0
0	1	1	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	1	1	11	55.0

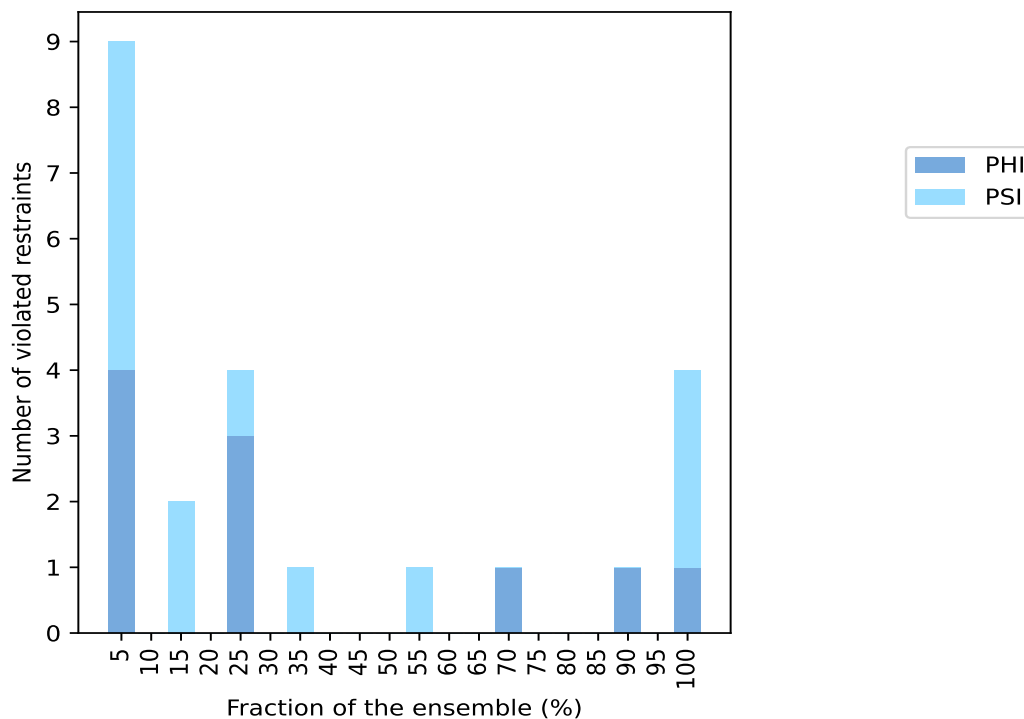
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
1	0	1	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
1	0	1	18	90.0
0	0	0	19	95.0
1	3	4	20	100.0

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)

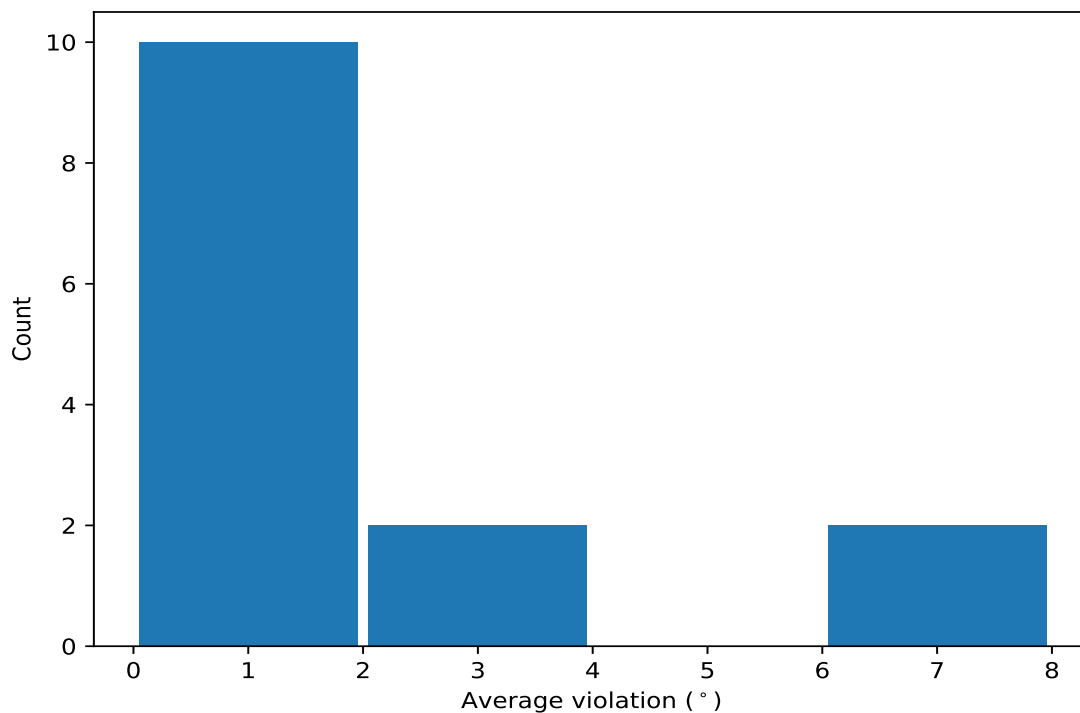


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

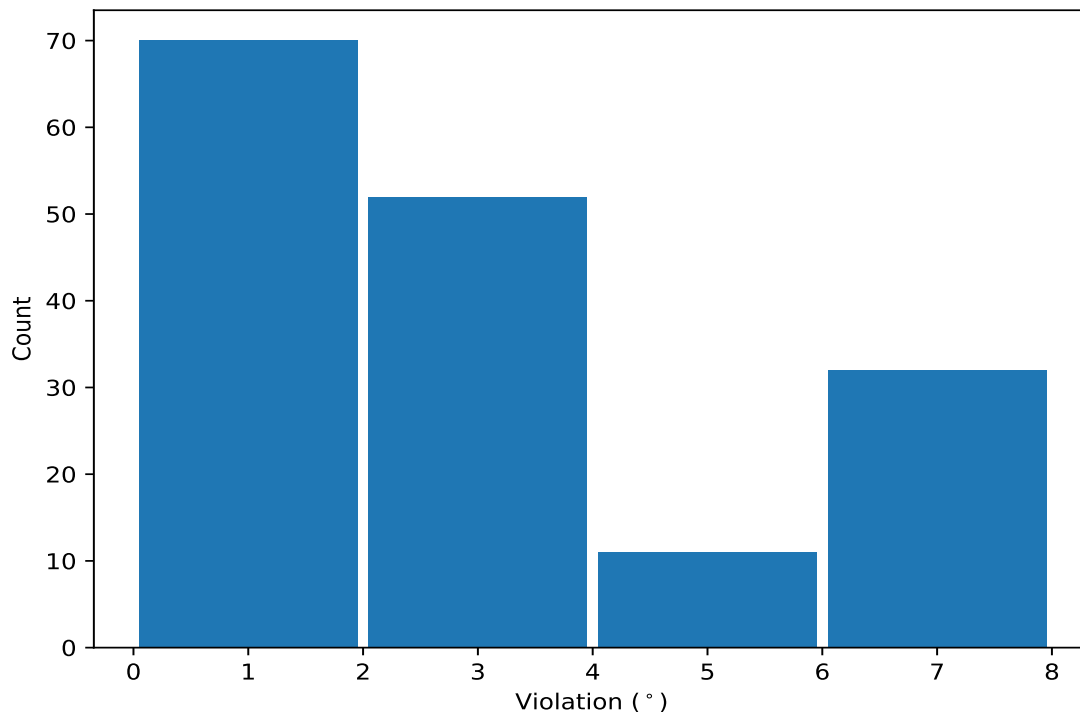
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	20	6.77	0.5	6.84
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	20	6.15	0.58	6.2
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	20	3.48	0.53	3.44
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	20	2.66	0.44	2.62
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	18	1.83	0.37	1.84
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	14	1.76	0.52	1.62
(1,130)	1:287:A:ASP:N	1:287:A:ASP:CA	1:287:A:ASP:C	1:288:A:VAL:N	11	1.46	0.31	1.35
(1,201)	2:860:B:LYS:N	2:860:B:LYS:CA	2:860:B:LYS:C	2:861:B:ASN:N	7	1.37	0.37	1.19
(1,73)	1:256:A:THR:C	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	5	1.58	0.28	1.54
(1,266)	2:896:B:GLU:C	2:897:B:VAL:N	2:897:B:VAL:CA	2:897:B:VAL:C	5	1.49	0.19	1.43
(1,153)	2:832:B:LYS:C	2:833:B:TYR:N	2:833:B:TYR:CA	2:833:B:TYR:C	5	1.44	0.26	1.48
(1,156)	2:834:B:ASN:N	2:834:B:ASN:CA	2:834:B:ASN:C	2:835:B:PRO:N	5	1.3	0.3	1.2
(1,146)	2:828:B:PRO:N	2:828:B:PRO:CA	2:828:B:PRO:C	2:829:B:GLU:N	3	1.85	1.02	1.2
(1,84)	1:262:A:GLN:N	1:262:A:GLN:CA	1:262:A:GLN:C	1:263:A:LEU:N	3	1.05	0.02	1.04

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	6	7.61
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	11	7.56
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	19	7.52
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	20	7.51
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	15	7.44
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	13	7.16
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	10	6.96
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	20	6.92
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	12	6.91
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	9	6.88
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	16	6.86
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	8	6.85
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	4	6.84
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	11	6.81

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	17	6.76
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	5	6.58
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	1	6.57
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	6	6.51
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	12	6.48
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	15	6.46
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	7	6.45
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	14	6.38
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	1	6.33
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	18	6.32
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	8	6.31
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	4	6.26
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	14	6.25
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	7	6.13
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	9	6.11
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	19	6.11
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	5	6.07
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	3	6.01
(1,111)	1:277:A:LEU:N	1:277:A:LEU:CA	1:277:A:LEU:C	1:278:A:GLY:N	2	5.94
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	16	5.8
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	17	5.69
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	3	5.58
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	2	5.56
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	18	5.53
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	10	5.46
(1,112)	1:277:A:LEU:C	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	13	4.95
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	9	4.45
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	14	4.19
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	2	4.05
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	1	3.96
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	16	3.96
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	13	3.9
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	8	3.75
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	17	3.7
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	6	3.67
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	17	3.63
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	11	3.5
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	19	3.37
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	4	3.31
(1,146)	2:828:B:PRO:N	2:828:B:PRO:CA	2:828:B:PRO:C	2:829:B:GLU:N	19	3.29
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	3	3.27
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	18	3.26
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	7	3.24
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	7	3.23
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	12	3.2
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	15	3.13
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	11	3.12
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	16	3.05
(1,106)	1:273:A:LEU:N	1:273:A:LEU:CA	1:273:A:LEU:C	1:274:A:CYS:N	20	2.96
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	18	2.91
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	10	2.89

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	13	2.83
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	5	2.8
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	20	2.78
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	4	2.7
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	10	2.68
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	19	2.62
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	3	2.61
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	14	2.6
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	15	2.57
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	1	2.55
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	10	2.53
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	9	2.51
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	2	2.49
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	15	2.42
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	12	2.37
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	2	2.36
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	14	2.34
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	4	2.29
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	9	2.27
(1,74)	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	1:258:A:GLY:N	5	2.23
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	1	2.23
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	6	2.23
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	11	2.21
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	8	2.19
(1,201)	2:860:B:LYS:N	2:860:B:LYS:CA	2:860:B:LYS:C	2:861:B:ASN:N	8	2.16
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	13	2.14
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	6	2.13
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	16	2.12
(1,73)	1:256:A:THR:C	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	16	2.08
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	15	2.05
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	9	1.98
(1,130)	1:287:A:ASP:N	1:287:A:ASP:CA	1:287:A:ASP:C	1:288:A:VAL:N	2	1.96
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	20	1.92
(1,130)	1:287:A:ASP:N	1:287:A:ASP:CA	1:287:A:ASP:C	1:288:A:VAL:N	13	1.89
(1,156)	2:834:B:ASN:N	2:834:B:ASN:CA	2:834:B:ASN:C	2:835:B:PRO:N	3	1.88
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	17	1.86
(1,153)	2:832:B:LYS:C	2:833:B:TYR:N	2:833:B:TYR:CA	2:833:B:TYR:C	20	1.85
(1,266)	2:896:B:GLU:C	2:897:B:VAL:N	2:897:B:VAL:CA	2:897:B:VAL:C	6	1.83
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	16	1.81
(1,130)	1:287:A:ASP:N	1:287:A:ASP:CA	1:287:A:ASP:C	1:288:A:VAL:N	20	1.8
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	3	1.79
(1,130)	1:287:A:ASP:N	1:287:A:ASP:CA	1:287:A:ASP:C	1:288:A:VAL:N	12	1.73
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	17	1.7
(1,85)	1:262:A:GLN:C	1:263:A:LEU:N	1:263:A:LEU:CA	1:263:A:LEU:C	2	1.62
(1,73)	1:256:A:THR:C	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	7	1.61
(1,109)	1:275:A:PRO:N	1:275:A:PRO:CA	1:275:A:PRO:C	1:276:A:GLY:N	20	1.59
(1,201)	2:860:B:LYS:N	2:860:B:LYS:CA	2:860:B:LYS:C	2:861:B:ASN:N	20	1.58
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	19	1.58
(1,153)	2:832:B:LYS:C	2:833:B:TYR:N	2:833:B:TYR:CA	2:833:B:TYR:C	3	1.56
(1,266)	2:896:B:GLU:C	2:897:B:VAL:N	2:897:B:VAL:CA	2:897:B:VAL:C	3	1.54
(1,73)	1:256:A:THR:C	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	15	1.54

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	11	1.53
(1,153)	2:832:B:LYS:C	2:833:B:TYR:N	2:833:B:TYR:CA	2:833:B:TYR:C	19	1.48
(1,1)	1:218:A:ASN:C	1:219:A:MET:N	1:219:A:MET:CA	1:219:A:MET:C	9	1.44
(1,266)	2:896:B:GLU:C	2:897:B:VAL:N	2:897:B:VAL:CA	2:897:B:VAL:C	14	1.43
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	1	1.43
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	10	1.43
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	7	1.42
(1,201)	2:860:B:LYS:N	2:860:B:LYS:CA	2:860:B:LYS:C	2:861:B:ASN:N	17	1.41
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	4	1.41
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	18	1.41
(1,266)	2:896:B:GLU:C	2:897:B:VAL:N	2:897:B:VAL:CA	2:897:B:VAL:C	7	1.37
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	8	1.37
(1,130)	1:287:A:ASP:N	1:287:A:ASP:CA	1:287:A:ASP:C	1:288:A:VAL:N	4	1.35
(1,130)	1:287:A:ASP:N	1:287:A:ASP:CA	1:287:A:ASP:C	1:288:A:VAL:N	8	1.35
(1,73)	1:256:A:THR:C	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	13	1.35
(1,62)	1:251:A:GLN:N	1:251:A:GLN:CA	1:251:A:GLN:C	1:252:A:THR:N	14	1.35
(1,148)	2:829:B:GLU:N	2:829:B:GLU:CA	2:829:B:GLU:C	2:830:B:SER:N	10	1.34
(1,130)	1:287:A:ASP:N	1:287:A:ASP:CA	1:287:A:ASP:C	1:288:A:VAL:N	5	1.34
(1,45)	1:240:A:THR:C	1:241:A:THR:N	1:241:A:THR:CA	1:241:A:THR:C	12	1.33
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	18	1.32
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	8	1.31
(1,73)	1:256:A:THR:C	1:257:A:PHE:N	1:257:A:PHE:CA	1:257:A:PHE:C	11	1.31
(1,130)	1:287:A:ASP:N	1:287:A:ASP:CA	1:287:A:ASP:C	1:288:A:VAL:N	11	1.29
(1,56)	1:248:A:THR:N	1:248:A:THR:CA	1:248:A:THR:C	1:249:A:ASP:N	18	1.29
(1,266)	2:896:B:GLU:C	2:897:B:VAL:N	2:897:B:VAL:CA	2:897:B:VAL:C	18	1.28
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	13	1.25
(1,153)	2:832:B:LYS:C	2:833:B:TYR:N	2:833:B:TYR:CA	2:833:B:TYR:C	5	1.23
(1,105)	1:272:A:ALA:C	1:273:A:LEU:N	1:273:A:LEU:CA	1:273:A:LEU:C	9	1.22
(1,156)	2:834:B:ASN:N	2:834:B:ASN:CA	2:834:B:ASN:C	2:835:B:PRO:N	18	1.21
(1,147)	2:828:B:PRO:C	2:829:B:GLU:N	2:829:B:GLU:CA	2:829:B:GLU:C	10	1.21
(1,130)	1:287:A:ASP:N	1:287:A:ASP:CA	1:287:A:ASP:C	1:288:A:VAL:N	17	1.21
(1,32)	1:234:A:ARG:N	1:234:A:ARG:CA	1:234:A:ARG:C	1:235:A:VAL:N	13	1.21
(1,156)	2:834:B:ASN:N	2:834:B:ASN:CA	2:834:B:ASN:C	2:835:B:PRO:N	7	1.2
(1,146)	2:828:B:PRO:N	2:828:B:PRO:CA	2:828:B:PRO:C	2:829:B:GLU:N	1	1.2
(1,201)	2:860:B:LYS:N	2:860:B:LYS:CA	2:860:B:LYS:C	2:861:B:ASN:N	19	1.19
(1,201)	2:860:B:LYS:N	2:860:B:LYS:CA	2:860:B:LYS:C	2:861:B:ASN:N	5	1.17
(1,156)	2:834:B:ASN:N	2:834:B:ASN:CA	2:834:B:ASN:C	2:835:B:PRO:N	8	1.16
(1,130)	1:287:A:ASP:N	1:287:A:ASP:CA	1:287:A:ASP:C	1:288:A:VAL:N	7	1.16
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	6	1.15
(1,153)	2:832:B:LYS:C	2:833:B:TYR:N	2:833:B:TYR:CA	2:833:B:TYR:C	9	1.09
(1,84)	1:262:A:GLN:N	1:262:A:GLN:CA	1:262:A:GLN:C	1:263:A:LEU:N	13	1.08
(1,201)	2:860:B:LYS:N	2:860:B:LYS:CA	2:860:B:LYS:C	2:861:B:ASN:N	18	1.06
(1,146)	2:828:B:PRO:N	2:828:B:PRO:CA	2:828:B:PRO:C	2:829:B:GLU:N	10	1.06
(1,156)	2:834:B:ASN:N	2:834:B:ASN:CA	2:834:B:ASN:C	2:835:B:PRO:N	17	1.04
(1,84)	1:262:A:GLN:N	1:262:A:GLN:CA	1:262:A:GLN:C	1:263:A:LEU:N	19	1.04
(1,77)	1:258:A:GLY:C	1:259:A:SER:N	1:259:A:SER:CA	1:259:A:SER:C	7	1.04
(1,84)	1:262:A:GLN:N	1:262:A:GLN:CA	1:262:A:GLN:C	1:263:A:LEU:N	7	1.03
(1,130)	1:287:A:ASP:N	1:287:A:ASP:CA	1:287:A:ASP:C	1:288:A:VAL:N	14	1.01
(1,201)	2:860:B:LYS:N	2:860:B:LYS:CA	2:860:B:LYS:C	2:861:B:ASN:N	4	1.0