



Full wwPDB NMR Structure Validation Report ⓘ

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BMRB ID : 34899
Title : NMR solution structure of the CysD2 domain of MUC2
Authors : Recktenwald, C.; Karlsson, B.G.; Garcia-Bonnete, M.-J.; Katona, G.; Jensen, M.; Lymer, R.; Baeckstroem, M.; Johansson, M.E.V.; Hansson, G.C.; Trillo-Muyo, S.
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<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

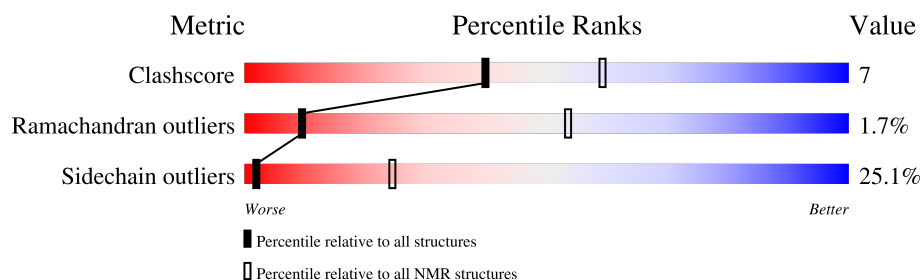
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

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	142	

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 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:1785-A:1793, A:1804-A:1852, A:1864-A:1876 (71)	0.94	2

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 4, 5, 6, 7, 8, 9, 10
2	1, 3

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1440 atoms, of which 701 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mucin-2.

Mol	Chain	Residues	Atoms						Trace
1	A	100	Total	C	H	N	O	S	0
			1439	464	701	122	140	12	

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1751	ASP	-	expression tag	UNP Q02817
A	1752	ALA	-	expression tag	UNP Q02817
A	1753	ALA	-	expression tag	UNP Q02817
A	1754	GLN	-	expression tag	UNP Q02817
A	1755	PRO	-	expression tag	UNP Q02817
A	1756	ALA	-	expression tag	UNP Q02817
A	1757	ARG	-	expression tag	UNP Q02817
A	1758	ARG	-	expression tag	UNP Q02817
A	1759	ALA	-	expression tag	UNP Q02817
A	1760	VAL	-	expression tag	UNP Q02817
A	1761	ARG	-	expression tag	UNP Q02817
A	1762	SER	-	expression tag	UNP Q02817
A	1763	SER	-	expression tag	UNP Q02817
A	1764	SER	-	expression tag	UNP Q02817
A	1765	GLU	-	expression tag	UNP Q02817
A	1766	LEU	-	expression tag	UNP Q02817
A	1767	THR	-	expression tag	UNP Q02817
A	1768	SER	-	expression tag	UNP Q02817
A	1769	GLU	-	expression tag	UNP Q02817
A	1770	GLN	-	expression tag	UNP Q02817
A	1771	LYS	-	expression tag	UNP Q02817
A	1772	LEU	-	expression tag	UNP Q02817
A	1773	ILE	-	expression tag	UNP Q02817
A	1774	SER	-	expression tag	UNP Q02817
A	1775	GLU	-	expression tag	UNP Q02817
A	1776	GLU	-	expression tag	UNP Q02817
A	1777	ASP	-	expression tag	UNP Q02817
A	1778	LEU	-	expression tag	UNP Q02817
A	1779	SER	-	expression tag	UNP Q02817
A	1780	SER	-	expression tag	UNP Q02817

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

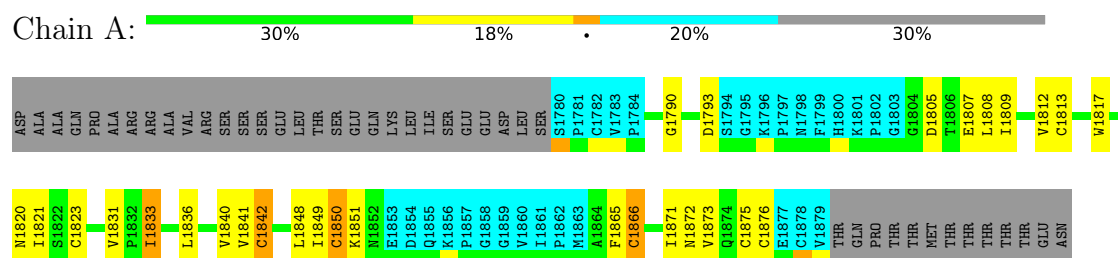
Mol	Chain	Residues	Atoms	
2	A	1	Total	Ca
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Mucin-2

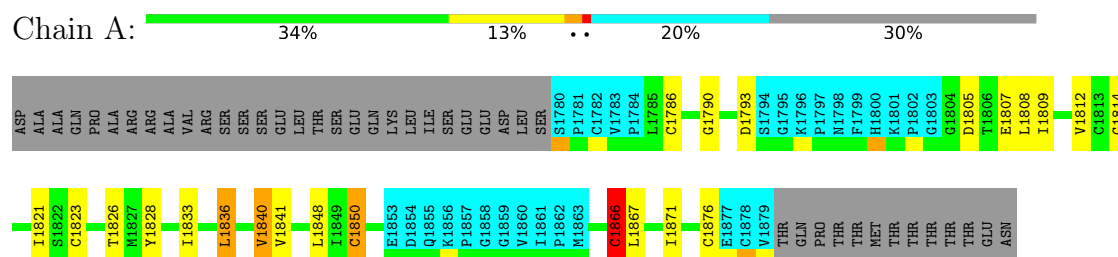


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

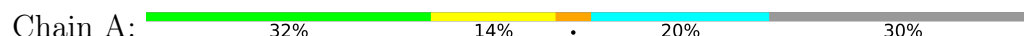
4.2.1 Score per residue for model 1

- Molecule 1: Mucin-2



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Mucin-2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *ENERGY MINIMIZATION*.

Of the 200 calculated structures, 10 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
YASARA	refinement	2.5
CYANA	structure calculation	3.0

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	812
Number of shifts mapped to atoms	812
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	1.59±0.21	8±4/540 (1.5± 0.8%)	1.50±0.15	8±4/741 (1.0± 0.5%)
All	All	1.61	80/5400 (1.5%)	1.50	75/7410 (1.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	1842	CYS	CA-CB	10.28	1.66	1.53	7	3
1	A	1841	VAL	CA-CB	-10.26	1.40	1.53	9	1
1	A	1820	ASN	C-O	-9.97	1.12	1.24	6	5
1	A	1872	ASN	CA-C	-9.61	1.41	1.52	8	6
1	A	1851	LYS	C-O	-9.14	1.13	1.23	7	1
1	A	1844	VAL	CA-CB	-8.79	1.42	1.54	6	1
1	A	1849	ILE	CA-CB	8.09	1.62	1.53	8	2
1	A	1808	LEU	CA-CB	-7.86	1.43	1.53	3	1
1	A	1850	CYS	CA-CB	-7.79	1.42	1.53	7	3
1	A	1873	VAL	CA-C	-7.10	1.44	1.52	3	2
1	A	1821	ILE	CA-CB	6.87	1.67	1.55	8	3
1	A	1817	TRP	CG-CD2	6.86	1.56	1.43	6	6
1	A	1823	CYS	CA-C	6.79	1.60	1.52	7	1
1	A	1871	ILE	N-CA	-6.78	1.38	1.46	9	6
1	A	1872	ASN	N-CA	6.62	1.54	1.46	8	1
1	A	1840	VAL	N-CA	-6.42	1.39	1.46	1	2
1	A	1842	CYS	C-O	-6.39	1.16	1.23	6	1
1	A	1840	VAL	C-O	-6.38	1.16	1.23	7	1
1	A	1840	VAL	C-N	-6.20	1.24	1.33	10	2
1	A	1820	ASN	N-CA	6.20	1.53	1.45	8	2
1	A	1836	LEU	CG-CD1	-6.17	1.32	1.52	6	1
1	A	1842	CYS	CA-C	6.03	1.60	1.53	7	1
1	A	1844	VAL	N-CA	6.00	1.53	1.46	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	1809	ILE	CA-CB	5.99	1.63	1.54	7	1
1	A	1874	GLN	C-O	5.88	1.30	1.23	7	1
1	A	1833	ILE	CB-CG1	5.79	1.65	1.53	2	2
1	A	1873	VAL	CA-CB	-5.73	1.45	1.55	5	2
1	A	1836	LEU	CB-CG	5.65	1.64	1.53	9	1
1	A	1871	ILE	CA-C	-5.65	1.45	1.52	8	2
1	A	1820	ASN	CA-C	-5.64	1.45	1.52	4	1
1	A	1870	GLU	CA-C	-5.62	1.45	1.52	7	1
1	A	1848	LEU	CB-CG	-5.56	1.42	1.53	9	1
1	A	1841	VAL	C-O	5.56	1.30	1.24	9	1
1	A	1833	ILE	N-CA	-5.52	1.40	1.46	7	1
1	A	1869	TYR	CA-CB	5.51	1.62	1.53	7	2
1	A	1822	SER	CA-CB	-5.49	1.45	1.53	3	3
1	A	1825	ALA	CA-CB	5.47	1.61	1.53	9	1
1	A	1791	TRP	CE2-CZ2	5.40	1.51	1.39	3	1
1	A	1839	THR	CA-C	-5.40	1.46	1.53	5	1
1	A	1833	ILE	C-O	5.29	1.30	1.24	9	1
1	A	1848	LEU	CA-CB	-5.19	1.45	1.53	3	1
1	A	1821	ILE	N-CA	-5.18	1.40	1.46	8	1
1	A	1791	TRP	CD2-CE2	5.15	1.50	1.41	8	1
1	A	1851	LYS	N-CA	-5.08	1.40	1.46	3	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
1	A	1804	GLY	N-CA-C	11.63	127.39	113.79	6	1
1	A	1790	GLY	N-CA-C	-11.16	99.79	112.29	6	10
1	A	1831	VAL	N-CA-C	8.88	117.57	107.89	9	6
1	A	1804	GLY	CA-C-O	-8.80	111.90	119.56	7	2
1	A	1812	VAL	N-CA-C	8.61	119.21	111.81	9	3
1	A	1792	LEU	N-CA-C	8.53	121.47	107.23	8	2
1	A	1816	GLY	N-CA-C	-7.92	105.11	113.58	10	1
1	A	1840	VAL	CA-CB-CG2	7.66	123.42	110.40	6	1
1	A	1872	ASN	N-CA-C	-7.46	96.74	108.90	8	7
1	A	1870	GLU	N-CA-CB	-6.95	100.58	111.56	7	3
1	A	1874	GLN	N-CA-C	-6.90	98.44	109.76	10	1
1	A	1840	VAL	N-CA-CB	6.78	123.83	112.44	6	3
1	A	1842	CYS	N-CA-C	-6.68	94.46	107.62	9	1
1	A	1868	ASN	N-CA-C	6.63	118.86	110.24	9	1
1	A	1793	ASP	N-CA-C	6.35	117.80	107.32	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	1847	GLY	CA-C-O	-6.35	116.48	122.13	7	2
1	A	1814	GLY	CA-C-N	-6.24	112.05	119.84	10	2
1	A	1814	GLY	C-N-CA	-6.24	112.05	119.84	10	2
1	A	1840	VAL	CB-CA-C	-6.14	101.21	110.55	6	2
1	A	1817	TRP	N-CA-C	6.00	119.33	109.85	10	1
1	A	1813	CYS	N-CA-C	5.91	120.79	112.93	8	2
1	A	1817	TRP	CD2-CE2-CZ2	-5.89	116.51	122.40	8	2
1	A	1810	GLY	N-CA-C	5.88	119.75	112.64	7	1
1	A	1833	ILE	O-C-N	-5.85	116.20	121.87	8	1
1	A	1840	VAL	N-CA-C	-5.77	99.98	108.99	10	2
1	A	1807	GLU	CA-C-N	5.71	130.26	122.84	3	1
1	A	1807	GLU	C-N-CA	5.71	130.26	122.84	3	1
1	A	1843	ASP	N-CA-C	5.67	118.48	109.24	6	2
1	A	1790	GLY	CA-C-O	5.59	127.59	122.39	3	1
1	A	1867	LEU	N-CA-C	-5.58	102.63	110.50	8	2
1	A	1791	TRP	N-CA-C	-5.56	101.41	109.59	3	1
1	A	1809	ILE	CB-CA-C	-5.50	105.00	111.94	7	1
1	A	1846	VAL	N-CA-C	5.43	118.87	113.71	3	1
1	A	1815	PRO	N-CA-C	5.42	119.09	110.21	4	1
1	A	1813	CYS	N-CA-CB	-5.36	101.89	110.19	5	1
1	A	1840	VAL	O-C-N	5.28	128.90	123.04	7	1
1	A	1820	ASN	N-CA-C	5.27	118.41	109.76	10	1
1	A	1869	TYR	CA-CB-CG	-5.06	104.78	113.90	9	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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	528	497	505	7±2
2	A	1	0	0	1±1
All	All	5290	4970	5050	73

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:1850:CYS:CB	1:A:1866:CYS:HG	0.69	1.98	6	4
1:A:1833:ILE:HD12	1:A:1840:VAL:HG11	0.69	1.64	5	1
1:A:1840:VAL:HG12	1:A:1850:CYS:SG	0.67	2.29	9	1
1:A:1850:CYS:HG	1:A:1866:CYS:CB	0.65	2.05	7	4
1:A:1793:ASP:OD1	2:A:1901:CA:CA	0.63	1.76	9	3
1:A:1823:CYS:SG	1:A:1842:CYS:CB	0.63	2.87	10	5
1:A:1807:GLU:OE1	2:A:1901:CA:CA	0.62	1.77	2	6
1:A:1823:CYS:SG	1:A:1842:CYS:HB2	0.59	2.37	10	3
1:A:1833:ILE:HD12	1:A:1840:VAL:HG21	0.59	1.74	9	2
1:A:1823:CYS:HG	1:A:1842:CYS:CB	0.59	2.07	7	2
1:A:1848:LEU:C	1:A:1849:ILE:HD13	0.57	2.24	8	1
1:A:1850:CYS:HB3	1:A:1869:TYR:CZ	0.56	2.35	9	1
1:A:1823:CYS:HB2	1:A:1833:ILE:HD11	0.56	1.77	9	1
1:A:1869:TYR:C	1:A:1869:TYR:CD1	0.55	2.85	3	1
1:A:1821:ILE:HG21	1:A:1844:VAL:HA	0.53	1.80	7	1
1:A:1813:CYS:HG	1:A:1875:CYS:CB	0.52	2.15	3	2
1:A:1848:LEU:HD12	1:A:1849:ILE:N	0.52	2.20	8	6
1:A:1850:CYS:C	1:A:1866:CYS:SG	0.51	2.94	9	1
1:A:1823:CYS:CB	1:A:1842:CYS:HB2	0.48	2.37	10	2
1:A:1813:CYS:CB	1:A:1875:CYS:HG	0.48	2.17	10	1
1:A:1848:LEU:HD23	1:A:1869:TYR:CE1	0.48	2.43	3	1
1:A:1842:CYS:HB3	1:A:1848:LEU:HD13	0.47	1.85	8	1
1:A:1842:CYS:HA	1:A:1848:LEU:HA	0.47	1.86	8	1
1:A:1850:CYS:CB	1:A:1866:CYS:SG	0.47	3.01	10	1
1:A:1786:CYS:HG	1:A:1876:CYS:CB	0.47	2.20	2	1
1:A:1809:ILE:HD12	1:A:1810:GLY:N	0.45	2.26	6	3
1:A:1805:ASP:HB3	1:A:1869:TYR:CE1	0.45	2.47	9	1
1:A:1828:TYR:CD1	1:A:1836:LEU:HD13	0.44	2.46	6	1
1:A:1840:VAL:HG12	1:A:1841:VAL:N	0.44	2.27	4	5
1:A:1865:PHE:O	1:A:1866:CYS:C	0.43	2.61	10	2
1:A:1836:LEU:HD13	1:A:1836:LEU:H	0.42	1.75	1	1
1:A:1850:CYS:SG	1:A:1866:CYS:CB	0.41	3.08	6	1
1:A:1809:ILE:HG13	1:A:1873:VAL:HG11	0.41	1.93	3	1
1:A:1828:TYR:CD2	1:A:1836:LEU:HG	0.41	2.51	1	1
1:A:1836:LEU:CD1	1:A:1836:LEU:H	0.41	2.28	3	1
1:A:1805:ASP:HB2	1:A:1850:CYS:SG	0.41	2.55	6	1
1:A:1786:CYS:CB	1:A:1876:CYS:SG	0.40	3.09	4	1
1:A:1833:ILE:CD1	1:A:1840:VAL:HG11	0.40	2.43	5	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	71/142 (50%)	64±1 (90±1%)	6±1 (8±2%)	1±1 (2±1%)	9	53
All	All	710/1420 (50%)	640 (90%)	58 (8%)	12 (2%)	9	53

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	1866	CYS	6
1	A	1814	GLY	3
1	A	1865	PHE	3

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	59/122 (48%)	44±2 (75±3%)	15±2 (25±3%)	2	24
All	All	590/1220 (48%)	442 (75%)	148 (25%)	2	24

All 41 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	1833	ILE	10
1	A	1808	LEU	9
1	A	1812	VAL	9
1	A	1836	LEU	9
1	A	1876	CYS	8
1	A	1823	CYS	6
1	A	1820	ASN	5

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Mol	Chain	Res	Type	Models (Total)
1	A	1842	CYS	5
1	A	1805	ASP	4
1	A	1821	ILE	4
1	A	1826	THR	4
1	A	1848	LEU	4
1	A	1793	ASP	4
1	A	1807	GLU	4
1	A	1851	LYS	4
1	A	1872	ASN	4
1	A	1875	CYS	4
1	A	1813	CYS	4
1	A	1786	CYS	3
1	A	1809	ILE	3
1	A	1850	CYS	3
1	A	1846	VAL	3
1	A	1873	VAL	3
1	A	1792	LEU	3
1	A	1865	PHE	3
1	A	1866	CYS	2
1	A	1867	LEU	2
1	A	1852	ASN	2
1	A	1806	THR	2
1	A	1822	SER	2
1	A	1840	VAL	2
1	A	1838	GLN	2
1	A	1831	VAL	2
1	A	1835	GLN	2
1	A	1824	ARG	2
1	A	1870	GLU	1
1	A	1827	MET	1
1	A	1844	VAL	1
1	A	1830	ASP	1
1	A	1849	ILE	1
1	A	1839	THR	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 65% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *nef_chemical_shift_list_ShiftList_1*

7.1.1 Bookkeeping

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

Total number of shifts	812
Number of shifts mapped to atoms	812
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	83	0.06 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	72	-0.42 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	2	—	None (insufficient data)
^{15}N	71	-0.94 ± 0.57	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 77%, i.e. 684 atoms were assigned a chemical shift out of a possible 889. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	268/357 (75%)	138/147 (94%)	70/142 (49%)	60/68 (88%)
Sidechain	374/468 (80%)	257/308 (83%)	117/148 (79%)	0/12 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	42/64 (66%)	30/31 (97%)	9/30 (30%)	3/3 (100%)
Overall	684/889 (77%)	425/486 (87%)	196/320 (61%)	63/83 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 65%, i.e. 811 atoms were assigned a chemical shift out of a possible 1242. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	317/494 (64%)	161/203 (79%)	85/200 (42%)	71/91 (78%)
Sidechain	452/667 (68%)	309/437 (71%)	143/213 (67%)	0/17 (0%)
Aromatic	42/81 (52%)	30/40 (75%)	9/37 (24%)	3/4 (75%)
Overall	811/1242 (65%)	500/680 (74%)	237/450 (53%)	74/112 (66%)

7.1.4 Statistically unusual chemical shifts [i](#)

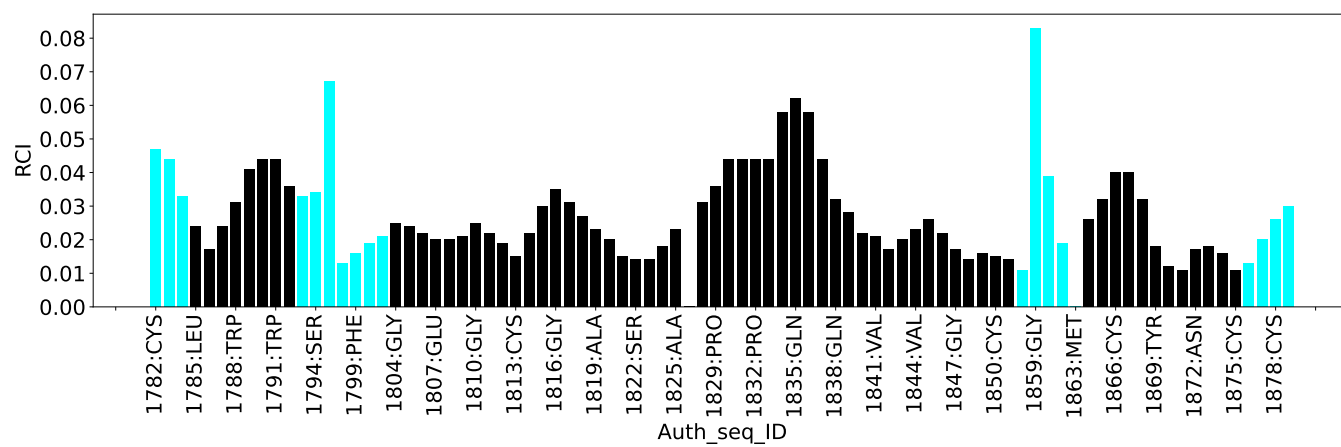
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	1789	THR	HG1	6.14	0.08 – 2.19	23.7
1	A	1874	GLN	HB2	-1.31	0.80 – 3.29	-13.5
1	A	1872	ASN	HB2	-0.03	1.27 – 4.34	-9.2
1	A	1874	GLN	HG2	0.48	1.01 – 3.62	-7.0
1	A	1794	SER	H	11.14	5.45 – 11.10	5.1

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	732
Intra-residue ($ i-j =0$)	340
Sequential ($ i-j =1$)	203
Medium range ($ i-j >1$ and $ i-j <5$)	39
Long range ($ i-j \geq 5$)	150
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	151
Number of unmapped restraints	0
Number of restraints per residue	6.2
Number of long range restraints per residue ¹	1.0

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)	49.9	0.2
0.2-0.5 (Medium)	103.2	0.5
>0.5 (Large)	90.0	10.47

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)	1.7	7.1
10.0-20.0 (Medium)	1.9	19.46
>20.0 (Large)	2.2	130.56

9 Distance violation analysis ⓘ

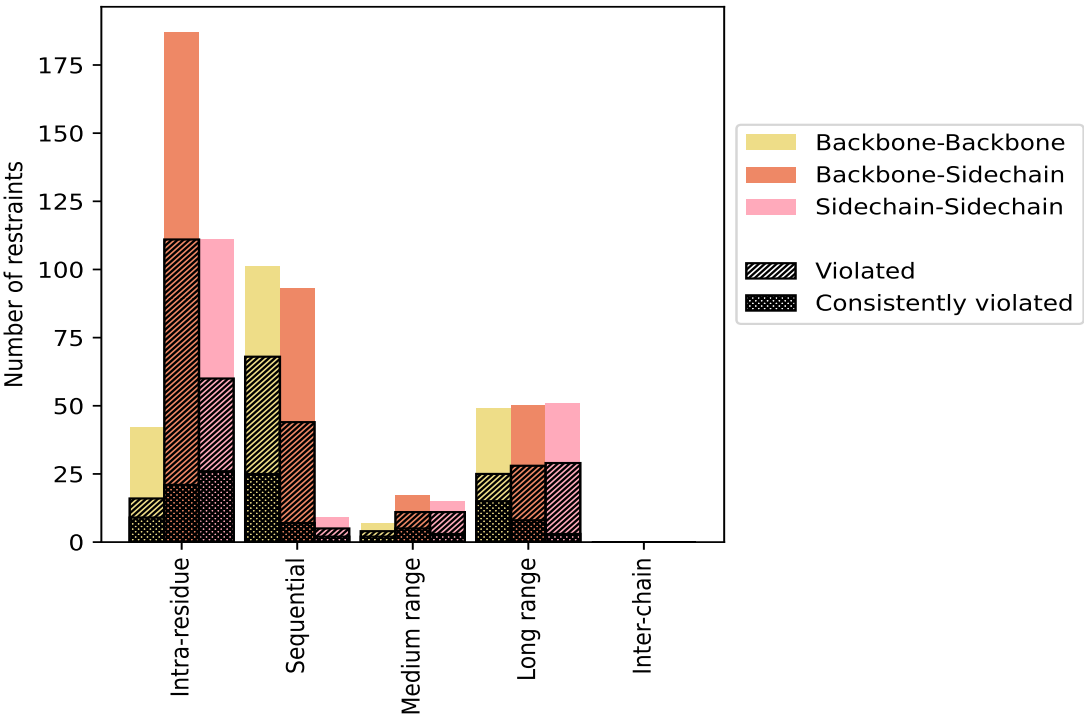
9.1 Summary of distance violations ⓘ

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)	340	46.4	187	55.0	25.5	56	16.5	7.7
Backbone-Backbone	42	5.7	16	38.1	2.2	9	21.4	1.2
Backbone-Sidechain	187	25.5	111	59.4	15.2	21	11.2	2.9
Sidechain-Sidechain	111	15.2	60	54.1	8.2	26	23.4	3.6
Sequential (i-j =1)	203	27.7	117	57.6	16.0	34	16.7	4.6
Backbone-Backbone	101	13.8	68	67.3	9.3	25	24.8	3.4
Backbone-Sidechain	93	12.7	44	47.3	6.0	7	7.5	1.0
Sidechain-Sidechain	9	1.2	5	55.6	0.7	2	22.2	0.3
Medium range (i-j >1 & i-j <5)	39	5.3	26	66.7	3.6	10	25.6	1.4
Backbone-Backbone	7	1.0	4	57.1	0.5	2	28.6	0.3
Backbone-Sidechain	17	2.3	11	64.7	1.5	5	29.4	0.7
Sidechain-Sidechain	15	2.0	11	73.3	1.5	3	20.0	0.4
Long range (i-j ≥5)	150	20.5	82	54.7	11.2	26	17.3	3.6
Backbone-Backbone	49	6.7	25	51.0	3.4	15	30.6	2.0
Backbone-Sidechain	50	6.8	28	56.0	3.8	8	16.0	1.1
Sidechain-Sidechain	51	7.0	29	56.9	4.0	3	5.9	0.4
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	732	100.0	412	56.3	56.3	126	17.2	17.2
Backbone-Backbone	199	27.2	113	56.8	15.4	51	25.6	7.0
Backbone-Sidechain	347	47.4	194	55.9	26.5	41	11.8	5.6
Sidechain-Sidechain	186	25.4	105	56.5	14.3	34	18.3	4.6

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

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



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

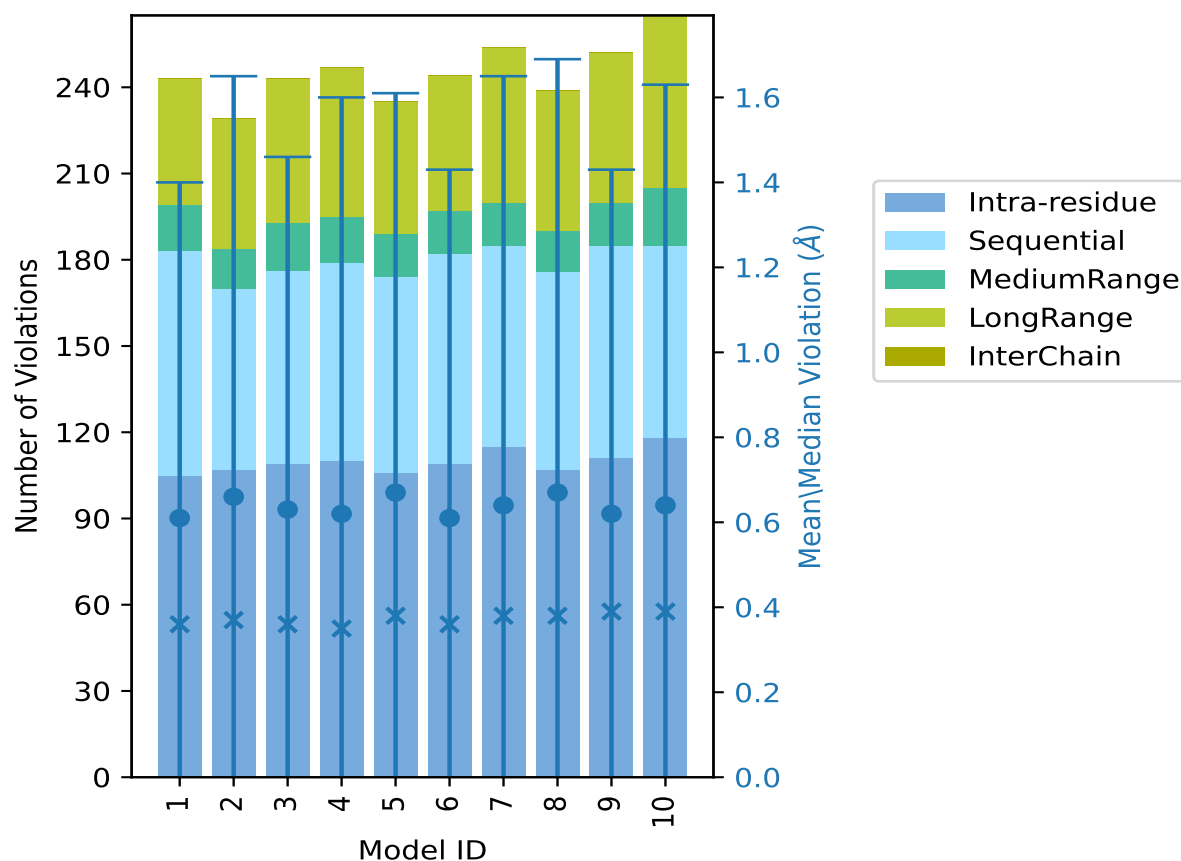
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	105	78	16	44	0	243	0.61	5.89	0.79	0.36
2	107	63	14	45	0	229	0.66	8.99	0.99	0.37
3	109	67	17	50	0	243	0.63	7.33	0.83	0.36
4	110	69	16	52	0	247	0.62	8.63	0.98	0.35
5	106	68	15	46	0	235	0.67	7.17	0.94	0.38
6	109	73	15	47	0	244	0.61	6.35	0.82	0.36
7	115	70	15	54	0	254	0.64	10.47	1.01	0.38
8	107	69	14	49	0	239	0.67	8.88	1.02	0.38
9	111	74	15	52	0	252	0.62	6.43	0.81	0.39
10	118	67	20	60	0	265	0.64	10.44	0.99	0.39

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 [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 320(IR:153, SQ:86, MR:13, LR:68, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
28	11	5	7	0	51	1	10.0
22	13	1	9	0	45	2	20.0
16	11	2	8	0	37	3	30.0

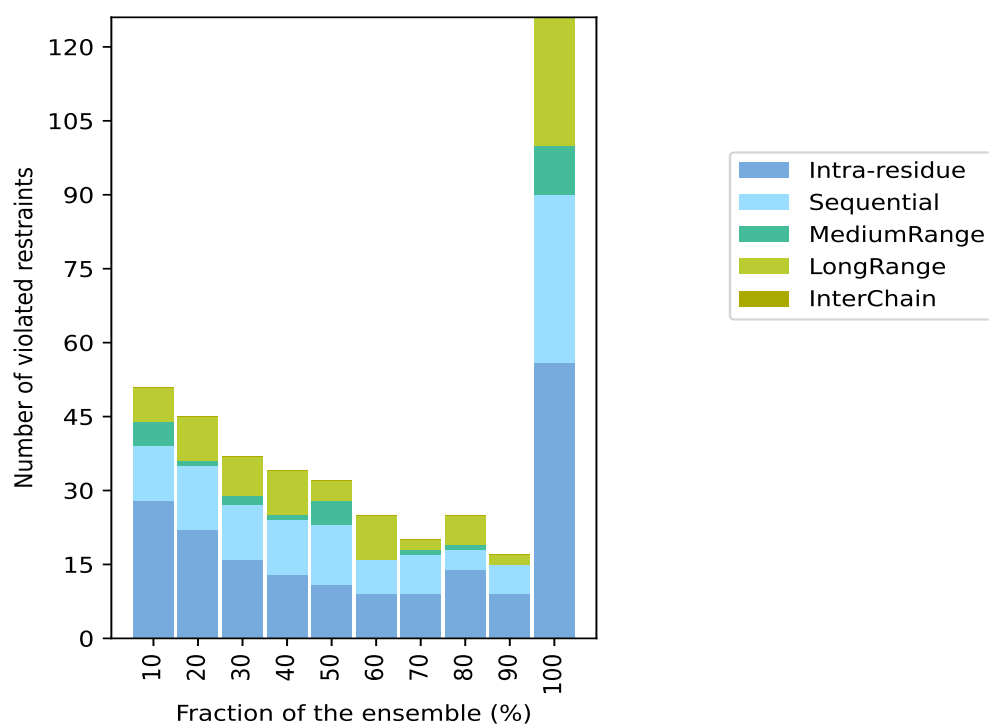
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
13	11	1	9	0	34	4	40.0
11	12	5	4	0	32	5	50.0
9	7	0	9	0	25	6	60.0
9	8	1	2	0	20	7	70.0
14	4	1	6	0	25	8	80.0
9	6	0	2	0	17	9	90.0
56	34	10	26	0	126	10	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](#)

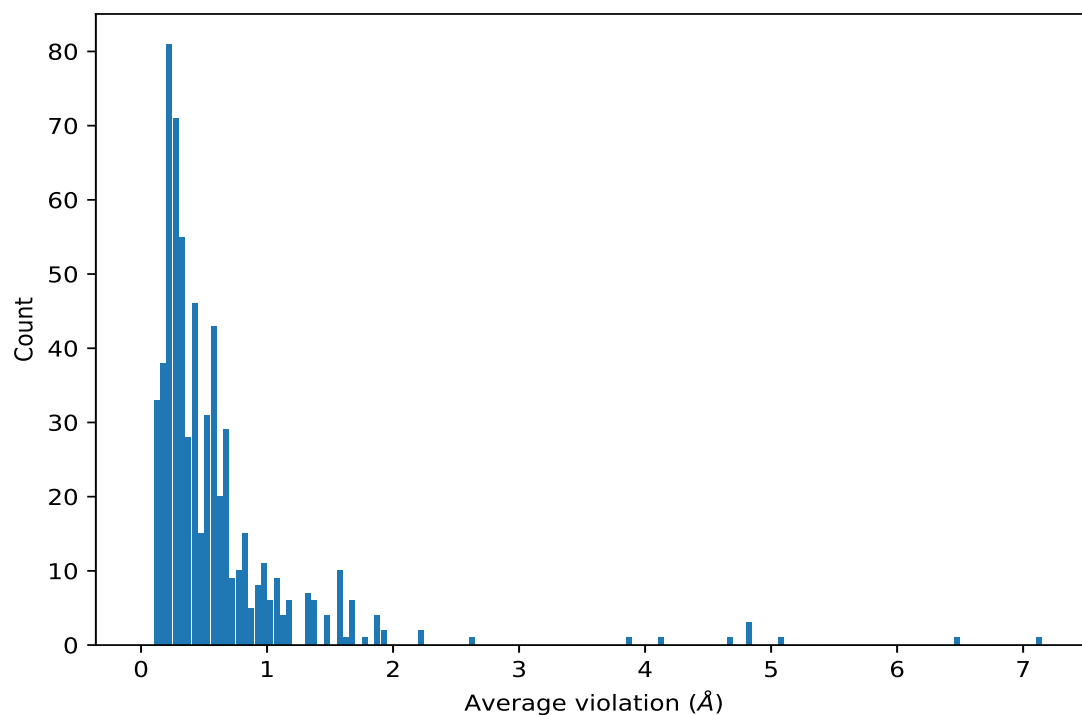


9.4 Most violated distance restraints in the ensemble [i](#)

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)
(1,293)	1:1795:A:GLY:H	1:1799:A:PHE:HA	10	7.14	2.61	7.9
(1,335)	1:1805:A:ASP:H	1:1870:A:GLU:HA	10	6.45	0.41	6.39
(1,267)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	10	5.08	0.27	5.0
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG21	10	4.81	0.9	4.72
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG22	10	4.81	0.9	4.72
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG23	10	4.81	0.9	4.72
(1,266)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	10	4.68	0.27	4.6
(1,218)	1:1818:A:ALA:H	1:1874:A:GLN:H	10	4.12	0.41	4.26
(1,228)	1:1818:A:ALA:H	1:1874:A:GLN:H	10	3.89	0.42	4.03
(1,422)	1:1787:A:ASN:HA	1:1820:A:ASN:H	10	2.61	0.36	2.52
(1,689)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD3	10	2.24	0.06	2.23
(1,689)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD3	10	2.24	0.06	2.23
(1,685)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD2	10	1.93	0.2	1.88
(1,685)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD2	10	1.93	0.2	1.88
(1,427)	1:1818:A:ALA:HB1	1:1820:A:ASN:H	10	1.9	0.31	1.84

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,427)	1:1818:A:ALA:HB2	1:1820:A:ASN:H	10	1.9	0.31	1.84
(1,427)	1:1818:A:ALA:HB3	1:1820:A:ASN:H	10	1.9	0.31	1.84
(1,699)	1:1821:A:ILE:HA	1:1872:A:ASN:HB2	10	1.85	0.18	1.94
(1,367)	1:1810:A:GLY:H	1:1811:A:ASP:HA	10	1.75	0.12	1.78
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG21	10	1.69	0.77	1.68
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG22	10	1.69	0.77	1.68
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG23	10	1.69	0.77	1.68
(1,409)	1:1815:A:PRO:HD2	1:1816:A:GLY:H	10	1.64	0.2	1.7
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD11	10	1.59	0.52	1.83
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD12	10	1.59	0.52	1.83
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD13	10	1.59	0.52	1.83
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD11	10	1.59	0.52	1.83
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD12	10	1.59	0.52	1.83
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD13	10	1.59	0.52	1.83
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD11	10	1.59	0.52	1.83
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD12	10	1.59	0.52	1.83
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD13	10	1.59	0.52	1.83
(1,325)	1:1792:A:LEU:HA	1:1794:A:SER:H	10	1.56	0.36	1.54
(1,724)	1:1788:A:TRP:HB3	1:1788:A:TRP:HH2	10	1.46	0.03	1.45
(1,412)	1:1816:A:GLY:H	1:1817:A:TRP:H	10	1.3	0.27	1.3
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG11	10	1.19	0.57	1.16
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG12	10	1.19	0.57	1.16
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG13	10	1.19	0.57	1.16
(1,406)	1:1815:A:PRO:HA	1:1816:A:GLY:H	10	1.15	0.07	1.13
(1,441)	1:1825:A:ALA:HB1	1:1828:A:TYR:HB2	10	1.14	0.06	1.13
(1,441)	1:1825:A:ALA:HB2	1:1828:A:TYR:HB2	10	1.14	0.06	1.13
(1,441)	1:1825:A:ALA:HB3	1:1828:A:TYR:HB2	10	1.14	0.06	1.13
(1,548)	1:1820:A:ASN:H	1:1874:A:GLN:HB3	10	1.05	0.14	1.03
(1,613)	1:1791:A:TRP:HA	1:1791:A:TRP:HE3	10	0.97	0.12	0.94
(1,185)	1:1819:A:ALA:H	1:1820:A:ASN:H	10	0.96	0.07	0.98
(1,295)	1:1788:A:TRP:H	1:1788:A:TRP:HB2	10	0.95	0.07	0.96
(1,290)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	10	0.93	0.11	0.91
(1,354)	1:1812:A:VAL:H	1:1813:A:CYS:HA	10	0.89	0.15	0.85
(1,421)	1:1819:A:ALA:H	1:1820:A:ASN:H	10	0.89	0.07	0.91
(1,594)	1:1799:A:PHE:H	1:1799:A:PHE:HA	10	0.85	0.06	0.82
(1,24)	1:1865:A:PHE:HA	1:1865:A:PHE:HB3	10	0.83	0.12	0.87
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG21	10	0.82	0.2	0.84
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG22	10	0.82	0.2	0.84
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG23	10	0.82	0.2	0.84
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	10	0.8	0.25	0.76
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	10	0.8	0.25	0.76
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	10	0.8	0.25	0.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,494)	1:1842:A:CYS:HA	1:1843:A:ASP:HB3	10	0.76	0.13	0.72
(1,407)	1:1815:A:PRO:HD3	1:1816:A:GLY:H	10	0.75	0.11	0.79
(1,615)	1:1812:A:VAL:H	1:1813:A:CYS:HA	10	0.75	0.15	0.7
(1,386)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	10	0.73	0.07	0.75
(1,263)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	10	0.73	0.08	0.72
(1,595)	1:1869:A:TYR:HA	1:1869:A:TYR:HB3	10	0.7	0.08	0.68
(1,424)	1:1820:A:ASN:H	1:1820:A:ASN:HB2	10	0.69	0.1	0.68
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG21	10	0.68	0.18	0.68
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG22	10	0.68	0.18	0.68
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG23	10	0.68	0.18	0.68
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG21	10	0.68	0.18	0.68
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG22	10	0.68	0.18	0.68
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG23	10	0.68	0.18	0.68
(1,505)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	10	0.68	0.08	0.67
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	10	0.66	0.25	0.62
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	10	0.66	0.25	0.62
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	10	0.66	0.25	0.62
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	10	0.65	0.14	0.67
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	10	0.65	0.14	0.67
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	10	0.64	0.14	0.66
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	10	0.64	0.14	0.66
(1,436)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	10	0.64	0.03	0.64
(1,86)	1:1812:A:VAL:HG11	1:1813:A:CYS:H	10	0.62	0.31	0.57
(1,86)	1:1812:A:VAL:HG12	1:1813:A:CYS:H	10	0.62	0.31	0.57
(1,86)	1:1812:A:VAL:HG13	1:1813:A:CYS:H	10	0.62	0.31	0.57
(1,402)	1:1871:A:ILE:H	1:1871:A:ILE:HA	10	0.61	0.06	0.6
(1,728)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	10	0.59	0.1	0.61
(1,610)	1:1806:A:THR:HA	1:1807:A:GLU:H	10	0.57	0.05	0.56
(1,611)	1:1850:A:CYS:HA	1:1851:A:LYS:H	10	0.57	0.09	0.55
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG11	10	0.56	0.17	0.56
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG12	10	0.56	0.17	0.56
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG13	10	0.56	0.17	0.56
(1,383)	1:1808:A:LEU:H	1:1808:A:LEU:HB2	10	0.55	0.07	0.58
(1,356)	1:1809:A:ILE:H	1:1810:A:GLY:H	10	0.55	0.1	0.56
(1,276)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	10	0.55	0.16	0.5
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE1	10	0.53	0.02	0.52
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE2	10	0.53	0.02	0.52
(1,726)	1:1874:A:GLN:H	1:1874:A:GLN:HB3	10	0.52	0.24	0.46
(1,672)	1:1874:A:GLN:HG2	1:1874:A:GLN:HG3	10	0.51	0.04	0.52
(1,357)	1:1809:A:ILE:H	1:1847:A:GLY:HA3	10	0.51	0.21	0.48
(1,547)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	10	0.5	0.1	0.53
(1,189)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	10	0.5	0.11	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,309)	1:1788:A:TRP:HB3	1:1790:A:GLY:H	10	0.5	0.05	0.5
(1,151)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	10	0.5	0.07	0.52
(1,80)	1:1847:A:GLY:HA2	1:1848:A:LEU:H	10	0.47	0.09	0.46
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	10	0.45	0.14	0.52
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	10	0.45	0.14	0.52
(1,214)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	10	0.44	0.25	0.28
(1,214)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	10	0.44	0.25	0.28
(1,214)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	10	0.44	0.25	0.28
(1,113)	1:1822:A:SER:H	1:1822:A:SER:HB2	10	0.44	0.15	0.48
(1,328)	1:1791:A:TRP:HZ2	1:1822:A:SER:HB3	10	0.43	0.2	0.46
(1,662)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	10	0.43	0.28	0.23
(1,662)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	10	0.43	0.28	0.23
(1,662)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	10	0.43	0.28	0.23
(1,618)	1:1851:A:LYS:HA	1:1852:A:ASN:H	10	0.43	0.07	0.42
(1,366)	1:1809:A:ILE:H	1:1810:A:GLY:H	10	0.42	0.1	0.43
(1,241)	1:1791:A:TRP:HH2	1:1822:A:SER:HB3	10	0.42	0.11	0.41
(1,200)	1:1821:A:ILE:H	1:1822:A:SER:H	10	0.41	0.09	0.42
(1,6)	1:1822:A:SER:H	1:1872:A:ASN:H	10	0.41	0.15	0.42
(1,4)	1:1794:A:SER:H	1:1795:A:GLY:H	10	0.4	0.07	0.4
(1,275)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	10	0.4	0.03	0.4
(1,645)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	10	0.4	0.02	0.4
(1,526)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	10	0.4	0.02	0.4
(1,612)	1:1824:A:ARG:HA	1:1825:A:ALA:H	10	0.39	0.11	0.38
(1,534)	1:1850:A:CYS:HA	1:1850:A:CYS:HB2	10	0.39	0.14	0.38
(1,246)	1:1869:A:TYR:H	1:1869:A:TYR:HA	10	0.38	0.02	0.38
(1,514)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	10	0.38	0.06	0.36
(1,283)	1:1871:A:ILE:H	1:1871:A:ILE:HG13	10	0.38	0.12	0.34
(1,365)	1:1810:A:GLY:H	1:1810:A:GLY:HA3	10	0.37	0.03	0.38
(1,279)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	10	0.37	0.05	0.34
(1,46)	1:1788:A:TRP:HA	1:1789:A:THR:H	10	0.36	0.04	0.36
(1,516)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	10	0.36	0.03	0.36
(1,300)	1:1788:A:TRP:HA	1:1789:A:THR:H	10	0.35	0.04	0.36
(1,569)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	10	0.35	0.12	0.38
(1,492)	1:1842:A:CYS:HA	1:1847:A:GLY:HA2	10	0.35	0.12	0.3
(1,464)	1:1832:A:PRO:HB2	1:1835:A:GLN:H	10	0.35	0.04	0.34
(1,517)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	10	0.34	0.03	0.35
(1,506)	1:1842:A:CYS:HA	1:1849:A:ILE:H	10	0.34	0.15	0.33
(1,264)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	10	0.34	0.05	0.32
(1,206)	1:1842:A:CYS:HA	1:1849:A:ILE:H	10	0.34	0.15	0.33
(1,520)	1:1820:A:ASN:HB2	1:1820:A:ASN:HB3	10	0.34	0.03	0.33
(1,280)	1:1786:A:CYS:HA	1:1787:A:ASN:H	10	0.33	0.04	0.34
(1,223)	1:1829:A:PRO:HG2	1:1830:A:ASP:H	10	0.33	0.12	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,513)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	10	0.32	0.01	0.32
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG11	10	0.32	0.06	0.33
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG12	10	0.32	0.06	0.33
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG13	10	0.32	0.06	0.33
(1,467)	1:1834:A:GLY:HA3	1:1835:A:GLN:H	10	0.32	0.05	0.32
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG21	10	0.31	0.07	0.29
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG22	10	0.31	0.07	0.29
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG23	10	0.31	0.07	0.29
(1,511)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	10	0.3	0.06	0.28
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG21	10	0.3	0.14	0.26
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG22	10	0.3	0.14	0.26
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG23	10	0.3	0.14	0.26
(1,292)	1:1787:A:ASN:HA	1:1788:A:TRP:H	10	0.3	0.06	0.28
(1,478)	1:1839:A:THR:H	1:1839:A:THR:HA	10	0.29	0.02	0.3
(1,272)	1:1786:A:CYS:HA	1:1787:A:ASN:H	10	0.28	0.03	0.29
(1,281)	1:1871:A:ILE:H	1:1871:A:ILE:HA	10	0.28	0.06	0.28
(1,702)	1:1851:A:LYS:HA	1:1852:A:ASN:H	10	0.28	0.07	0.27
(1,512)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	10	0.27	0.01	0.27
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG11	10	0.27	0.05	0.27
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG12	10	0.27	0.05	0.27
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG13	10	0.27	0.05	0.27
(1,162)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	10	0.26	0.04	0.26
(1,147)	1:1791:A:TRP:HZ2	1:1791:A:TRP:HZ3	10	0.25	0.04	0.26
(1,479)	1:1838:A:GLN:HA	1:1839:A:THR:H	10	0.25	0.06	0.24
(1,518)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	10	0.25	0.04	0.26
(1,257)	1:1829:A:PRO:HD2	1:1829:A:PRO:HD3	10	0.23	0.03	0.22
(1,343)	1:1870:A:GLU:H	1:1870:A:GLU:HA	10	0.22	0.05	0.22
(1,439)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	10	0.22	0.03	0.22
(1,705)	1:1792:A:LEU:H	1:1792:A:LEU:HA	10	0.22	0.03	0.22
(1,390)	1:1823:A:CYS:HA	1:1823:A:CYS:HB3	10	0.21	0.09	0.16
(1,521)	1:1865:A:PHE:HB2	1:1865:A:PHE:HB3	10	0.21	0.0	0.21
(1,260)	1:1829:A:PRO:HD2	1:1829:A:PRO:HG2	10	0.2	0.06	0.2
(1,437)	1:1878:A:CYS:HB2	1:1878:A:CYS:HB3	10	0.18	0.0	0.18
(1,1)	1:1793:A:ASP:HA	1:1794:A:SER:H	10	0.17	0.05	0.17
(1,438)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	10	0.17	0.03	0.16
(1,337)	1:1806:A:THR:H	1:1806:A:THR:HA	10	0.15	0.03	0.15
(1,362)	1:1808:A:LEU:HD21	1:1809:A:ILE:H	9	1.4	0.11	1.4
(1,362)	1:1808:A:LEU:HD22	1:1809:A:ILE:H	9	1.4	0.11	1.4
(1,362)	1:1808:A:LEU:HD23	1:1809:A:ILE:H	9	1.4	0.11	1.4
(1,87)	1:1808:A:LEU:H	1:1808:A:LEU:HG	9	0.76	0.25	0.79
(1,27)	1:1865:A:PHE:H	1:1865:A:PHE:HB3	9	0.55	0.21	0.49
(1,529)	1:1865:A:PHE:HB2	1:1866:A:CYS:H	9	0.5	0.13	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,529)	1:1866:A:CYS:H	1:1866:A:CYS:HB2	9	0.5	0.13	0.56
(1,49)	1:1789:A:THR:H	1:1874:A:GLN:HA	9	0.3	0.07	0.29
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	9	0.28	0.12	0.37
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	9	0.28	0.12	0.37
(1,119)	1:1821:A:ILE:H	1:1822:A:SER:H	9	0.24	0.06	0.25
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG21	9	0.23	0.08	0.19
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG22	9	0.23	0.08	0.19
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG23	9	0.23	0.08	0.19
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	9	0.22	0.04	0.23
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	9	0.22	0.04	0.23
(1,204)	1:1848:A:LEU:HA	1:1849:A:ILE:H	9	0.22	0.08	0.25
(1,614)	1:1821:A:ILE:HA	1:1873:A:VAL:HA	9	0.21	0.05	0.22
(1,282)	1:1787:A:ASN:H	1:1787:A:ASN:HB2	9	0.21	0.09	0.16
(1,3)	1:1794:A:SER:H	1:1795:A:GLY:H	9	0.21	0.06	0.2
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	9	0.2	0.04	0.21
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	9	0.2	0.04	0.21
(1,245)	1:1868:A:ASN:HA	1:1869:A:TYR:H	9	0.19	0.04	0.2
(1,400)	1:1848:A:LEU:H	1:1848:A:LEU:HA	9	0.16	0.03	0.18
(1,47)	1:1789:A:THR:H	1:1789:A:THR:HA	9	0.12	0.02	0.12
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD1	8	0.68	0.42	0.68
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD1	8	0.68	0.42	0.68
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD1	8	0.68	0.42	0.68
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD2	8	0.68	0.42	0.68
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD2	8	0.68	0.42	0.68
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD2	8	0.68	0.42	0.68
(1,573)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	8	0.64	0.28	0.68
(1,115)	1:1822:A:SER:H	1:1872:A:ASN:HB2	8	0.57	0.15	0.6
(1,247)	1:1869:A:TYR:H	1:1869:A:TYR:HB2	8	0.56	0.12	0.61
(1,600)	1:1869:A:TYR:HB3	1:1870:A:GLU:H	8	0.52	0.17	0.48
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	8	0.45	0.19	0.38
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	8	0.45	0.19	0.38
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	8	0.45	0.19	0.38
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	8	0.45	0.19	0.38
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	8	0.45	0.19	0.38
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	8	0.45	0.19	0.38
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD21	8	0.43	0.18	0.52
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD22	8	0.43	0.18	0.52
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD23	8	0.43	0.18	0.52
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	8	0.41	0.24	0.25
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	8	0.41	0.24	0.25
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	8	0.41	0.24	0.25
(1,374)	1:1808:A:LEU:HD21	1:1810:A:GLY:H	8	0.4	0.23	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,374)	1:1808:A:LEU:HD22	1:1810:A:GLY:H	8	0.4	0.23	0.35
(1,374)	1:1808:A:LEU:HD23	1:1810:A:GLY:H	8	0.4	0.23	0.35
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB2	8	0.37	0.03	0.36
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB3	8	0.37	0.03	0.36
(1,43)	1:1791:A:TRP:HE3	1:1872:A:ASN:HB3	8	0.35	0.05	0.36
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	8	0.32	0.19	0.24
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	8	0.32	0.19	0.24
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	8	0.32	0.19	0.24
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	8	0.32	0.19	0.24
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	8	0.32	0.19	0.24
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	8	0.32	0.19	0.24
(1,183)	1:1817:A:TRP:HD1	1:1818:A:ALA:H	8	0.32	0.08	0.3
(1,268)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	8	0.28	0.15	0.23
(1,472)	1:1836:A:LEU:H	1:1836:A:LEU:HG	8	0.28	0.14	0.28
(1,5)	1:1822:A:SER:H	1:1872:A:ASN:H	8	0.27	0.11	0.25
(1,461)	1:1835:A:GLN:H	1:1835:A:GLN:HB2	8	0.27	0.05	0.25
(1,537)	1:1875:A:CYS:HA	1:1875:A:CYS:HB3	8	0.24	0.06	0.25
(1,639)	1:1789:A:THR:HB	1:1789:A:THR:HG1	8	0.23	0.07	0.21
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG21	8	0.22	0.13	0.16
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG22	8	0.22	0.13	0.16
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG23	8	0.22	0.13	0.16
(1,124)	1:1821:A:ILE:HA	1:1822:A:SER:H	8	0.19	0.06	0.16
(1,160)	1:1817:A:TRP:HE3	1:1817:A:TRP:HH2	8	0.17	0.05	0.18
(1,515)	1:1850:A:CYS:HB2	1:1850:A:CYS:HB3	8	0.15	0.03	0.15
(1,163)	1:1788:A:TRP:HB3	1:1788:A:TRP:HE3	8	0.15	0.03	0.15
(1,259)	1:1829:A:PRO:HD3	1:1829:A:PRO:HG3	8	0.14	0.02	0.15
(1,589)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	7	0.84	0.03	0.83
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD11	7	0.75	0.11	0.82
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD12	7	0.75	0.11	0.82
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD13	7	0.75	0.11	0.82
(1,219)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	7	0.75	0.03	0.74
(1,333)	1:1805:A:ASP:H	1:1850:A:CYS:HB2	7	0.67	0.21	0.62
(1,321)	1:1792:A:LEU:HB2	1:1793:A:ASP:H	7	0.67	0.16	0.67
(1,431)	1:1824:A:ARG:H	1:1824:A:ARG:HB2	7	0.65	0.16	0.71
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG21	7	0.64	0.31	0.51
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG22	7	0.64	0.31	0.51
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG23	7	0.64	0.31	0.51
(1,587)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	7	0.63	0.06	0.65
(1,229)	1:1799:A:PHE:H	1:1800:A:HIS:H	7	0.45	0.15	0.42
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG21	7	0.4	0.15	0.41
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG22	7	0.4	0.15	0.41
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG23	7	0.4	0.15	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,16)	1:1817:A:TRP:HB2	1:1817:A:TRP:HE3	7	0.36	0.04	0.35
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD11	7	0.36	0.1	0.4
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD12	7	0.36	0.1	0.4
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD13	7	0.36	0.1	0.4
(1,145)	1:1799:A:PHE:H	1:1800:A:HIS:H	7	0.35	0.15	0.32
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD11	7	0.33	0.13	0.28
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD12	7	0.33	0.13	0.28
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD13	7	0.33	0.13	0.28
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD11	7	0.33	0.13	0.28
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD12	7	0.33	0.13	0.28
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD13	7	0.33	0.13	0.28
(1,527)	1:1817:A:TRP:HB3	1:1817:A:TRP:HE3	7	0.33	0.05	0.35
(1,191)	1:1871:A:ILE:HA	1:1872:A:ASN:H	7	0.27	0.1	0.22
(1,8)	1:1871:A:ILE:HA	1:1872:A:ASN:H	7	0.24	0.1	0.19
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD1	7	0.21	0.08	0.23
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD1	7	0.21	0.08	0.23
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD1	7	0.21	0.08	0.23
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD2	7	0.21	0.08	0.23
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD2	7	0.21	0.08	0.23
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD2	7	0.21	0.08	0.23
(1,490)	1:1842:A:CYS:HA	1:1842:A:CYS:HB2	7	0.18	0.07	0.16
(1,110)	1:1821:A:ILE:HA	1:1822:A:SER:H	7	0.15	0.05	0.12
(1,663)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	6	1.38	0.05	1.39
(1,663)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	6	1.38	0.05	1.39
(1,663)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	6	1.38	0.05	1.39
(1,215)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	6	1.31	0.05	1.32
(1,215)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	6	1.31	0.05	1.32
(1,215)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	6	1.31	0.05	1.32
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG11	6	1.3	0.32	1.26
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG12	6	1.3	0.32	1.26
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG13	6	1.3	0.32	1.26
(1,646)	1:1840:A:VAL:HG21	1:1850:A:CYS:HB3	6	1.17	0.56	1.3
(1,646)	1:1840:A:VAL:HG22	1:1850:A:CYS:HB3	6	1.17	0.56	1.3
(1,646)	1:1840:A:VAL:HG23	1:1850:A:CYS:HB3	6	1.17	0.56	1.3
(1,373)	1:1809:A:ILE:HD11	1:1810:A:GLY:H	6	1.07	0.42	1.29
(1,373)	1:1809:A:ILE:HD12	1:1810:A:GLY:H	6	1.07	0.42	1.29
(1,373)	1:1809:A:ILE:HD13	1:1810:A:GLY:H	6	1.07	0.42	1.29
(1,657)	1:1848:A:LEU:HD21	1:1849:A:ILE:HA	6	1.01	0.14	1.0
(1,657)	1:1848:A:LEU:HD22	1:1849:A:ILE:HA	6	1.01	0.14	1.0
(1,657)	1:1848:A:LEU:HD23	1:1849:A:ILE:HA	6	1.01	0.14	1.0
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD11	6	0.57	0.05	0.56
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD12	6	0.57	0.05	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD13	6	0.57	0.05	0.56
(1,76)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	6	0.48	0.17	0.51
(1,608)	1:1848:A:LEU:HD21	1:1869:A:TYR:HB2	6	0.4	0.07	0.43
(1,608)	1:1848:A:LEU:HD22	1:1869:A:TYR:HB2	6	0.4	0.07	0.43
(1,608)	1:1848:A:LEU:HD23	1:1869:A:TYR:HB2	6	0.4	0.07	0.43
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD21	6	0.37	0.21	0.34
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD22	6	0.37	0.21	0.34
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD23	6	0.37	0.21	0.34
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD21	6	0.37	0.21	0.34
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD22	6	0.37	0.21	0.34
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD23	6	0.37	0.21	0.34
(1,7)	1:1791:A:TRP:HZ3	1:1872:A:ASN:H	6	0.32	0.13	0.37
(1,345)	1:1870:A:GLU:H	1:1870:A:GLU:HB3	6	0.31	0.04	0.3
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD21	6	0.31	0.06	0.29
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD22	6	0.31	0.06	0.29
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD23	6	0.31	0.06	0.29
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD21	6	0.31	0.06	0.29
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD22	6	0.31	0.06	0.29
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD23	6	0.31	0.06	0.29
(1,352)	1:1812:A:VAL:H	1:1813:A:CYS:H	6	0.3	0.09	0.31
(1,99)	1:1791:A:TRP:HZ3	1:1824:A:ARG:H	6	0.26	0.07	0.26
(1,81)	1:1805:A:ASP:H	1:1850:A:CYS:H	6	0.25	0.12	0.2
(1,284)	1:1871:A:ILE:H	1:1871:A:ILE:HG12	6	0.24	0.08	0.25
(1,190)	1:1848:A:LEU:HA	1:1849:A:ILE:H	6	0.22	0.05	0.24
(1,413)	1:1830:A:ASP:H	1:1830:A:ASP:HB3	6	0.22	0.11	0.2
(1,79)	1:1850:A:CYS:H	1:1850:A:CYS:HB2	6	0.21	0.07	0.22
(1,181)	1:1830:A:ASP:H	1:1831:A:VAL:H	6	0.19	0.04	0.2
(1,552)	1:1833:A:ILE:H	1:1833:A:ILE:HA	6	0.19	0.04	0.2
(1,161)	1:1817:A:TRP:HE3	1:1817:A:TRP:HZ2	6	0.17	0.04	0.18
(1,277)	1:1786:A:CYS:HA	1:1786:A:CYS:HB2	6	0.16	0.04	0.16
(1,707)	1:1791:A:TRP:HB2	1:1791:A:TRP:HD1	6	0.15	0.03	0.16
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG11	5	1.05	0.46	1.38
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG12	5	1.05	0.46	1.38
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG13	5	1.05	0.46	1.38
(1,62)	1:1840:A:VAL:HG11	1:1841:A:VAL:H	5	1.0	0.04	0.98
(1,62)	1:1840:A:VAL:HG12	1:1841:A:VAL:H	5	1.0	0.04	0.98
(1,62)	1:1840:A:VAL:HG13	1:1841:A:VAL:H	5	1.0	0.04	0.98
(1,71)	1:1840:A:VAL:HG11	1:1841:A:VAL:H	5	0.98	0.04	0.96
(1,71)	1:1840:A:VAL:HG12	1:1841:A:VAL:H	5	0.98	0.04	0.96
(1,71)	1:1840:A:VAL:HG13	1:1841:A:VAL:H	5	0.98	0.04	0.96
(1,75)	1:1840:A:VAL:HG11	1:1842:A:CYS:H	5	0.96	0.15	1.01
(1,75)	1:1840:A:VAL:HG12	1:1842:A:CYS:H	5	0.96	0.15	1.01

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,75)	1:1840:A:VAL:HG13	1:1842:A:CYS:H	5	0.96	0.15	1.01
(1,528)	1:1866:A:CYS:H	1:1866:A:CYS:HB3	5	0.76	0.22	0.61
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD11	5	0.74	0.3	0.73
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD12	5	0.74	0.3	0.73
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD13	5	0.74	0.3	0.73
(1,54)	1:1840:A:VAL:HG11	1:1842:A:CYS:HB2	5	0.66	0.17	0.59
(1,54)	1:1840:A:VAL:HG12	1:1842:A:CYS:HB2	5	0.66	0.17	0.59
(1,54)	1:1840:A:VAL:HG13	1:1842:A:CYS:HB2	5	0.66	0.17	0.59
(1,561)	1:1827:A:MET:HE1	1:1828:A:TYR:HE1	5	0.57	0.19	0.64
(1,561)	1:1827:A:MET:HE2	1:1828:A:TYR:HE1	5	0.57	0.19	0.64
(1,561)	1:1827:A:MET:HE3	1:1828:A:TYR:HE1	5	0.57	0.19	0.64
(1,561)	1:1827:A:MET:HE1	1:1828:A:TYR:HE2	5	0.57	0.19	0.64
(1,561)	1:1827:A:MET:HE2	1:1828:A:TYR:HE2	5	0.57	0.19	0.64
(1,561)	1:1827:A:MET:HE3	1:1828:A:TYR:HE2	5	0.57	0.19	0.64
(1,227)	1:1873:A:VAL:HG21	1:1874:A:GLN:H	5	0.57	0.15	0.6
(1,227)	1:1873:A:VAL:HG22	1:1874:A:GLN:H	5	0.57	0.15	0.6
(1,227)	1:1873:A:VAL:HG23	1:1874:A:GLN:H	5	0.57	0.15	0.6
(1,564)	1:1840:A:VAL:HG11	1:1842:A:CYS:HB2	5	0.55	0.17	0.48
(1,564)	1:1840:A:VAL:HG12	1:1842:A:CYS:HB2	5	0.55	0.17	0.48
(1,564)	1:1840:A:VAL:HG13	1:1842:A:CYS:HB2	5	0.55	0.17	0.48
(1,686)	1:1827:A:MET:HE1	1:1828:A:TYR:HE1	5	0.53	0.19	0.6
(1,686)	1:1827:A:MET:HE2	1:1828:A:TYR:HE1	5	0.53	0.19	0.6
(1,686)	1:1827:A:MET:HE3	1:1828:A:TYR:HE1	5	0.53	0.19	0.6
(1,686)	1:1827:A:MET:HE1	1:1828:A:TYR:HE2	5	0.53	0.19	0.6
(1,686)	1:1827:A:MET:HE2	1:1828:A:TYR:HE2	5	0.53	0.19	0.6
(1,686)	1:1827:A:MET:HE3	1:1828:A:TYR:HE2	5	0.53	0.19	0.6
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG11	5	0.52	0.12	0.48
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG12	5	0.52	0.12	0.48
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG13	5	0.52	0.12	0.48
(1,45)	1:1789:A:THR:H	1:1789:A:THR:HG1	5	0.5	0.37	0.25
(1,647)	1:1840:A:VAL:HG21	1:1850:A:CYS:HB2	5	0.4	0.17	0.37
(1,647)	1:1840:A:VAL:HG22	1:1850:A:CYS:HB2	5	0.4	0.17	0.37
(1,647)	1:1840:A:VAL:HG23	1:1850:A:CYS:HB2	5	0.4	0.17	0.37
(1,252)	1:1877:A:GLU:H	1:1877:A:GLU:HG2	5	0.39	0.11	0.4
(1,192)	1:1789:A:THR:HG1	1:1873:A:VAL:H	5	0.37	0.24	0.22
(1,353)	1:1812:A:VAL:H	1:1813:A:CYS:H	5	0.27	0.06	0.27
(1,193)	1:1791:A:TRP:HZ3	1:1824:A:ARG:H	5	0.25	0.04	0.25
(1,667)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	5	0.23	0.05	0.2
(1,388)	1:1791:A:TRP:HZ3	1:1823:A:CYS:HA	5	0.23	0.07	0.23
(1,139)	1:1817:A:TRP:HA	1:1817:A:TRP:HD1	5	0.22	0.03	0.21
(1,410)	1:1815:A:PRO:HG2	1:1816:A:GLY:H	5	0.21	0.06	0.18
(1,107)	1:1820:A:ASN:HB2	1:1821:A:ILE:H	5	0.19	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,122)	1:1805:A:ASP:HA	1:1806:A:THR:H	5	0.19	0.05	0.19
(1,20)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	5	0.17	0.03	0.16
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB1	5	0.16	0.04	0.17
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB2	5	0.16	0.04	0.17
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB3	5	0.16	0.04	0.17
(1,477)	1:1839:A:THR:HA	1:1840:A:VAL:H	5	0.16	0.03	0.16
(1,544)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	5	0.15	0.02	0.15
(1,638)	1:1793:A:ASP:HA	1:1794:A:SER:H	5	0.14	0.04	0.13
(1,584)	1:1791:A:TRP:HB3	1:1791:A:TRP:HE3	5	0.13	0.02	0.12
(1,453)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	5	0.12	0.02	0.11
(1,417)	1:1818:A:ALA:HA	1:1819:A:ALA:H	5	0.11	0.02	0.11
(1,656)	1:1848:A:LEU:HD11	1:1849:A:ILE:HA	4	0.98	0.04	1.0
(1,656)	1:1848:A:LEU:HD12	1:1849:A:ILE:HA	4	0.98	0.04	1.0
(1,656)	1:1848:A:LEU:HD13	1:1849:A:ILE:HA	4	0.98	0.04	1.0
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD11	4	0.91	0.26	1.01
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD12	4	0.91	0.26	1.01
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD13	4	0.91	0.26	1.01
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD21	4	0.89	0.05	0.88
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD22	4	0.89	0.05	0.88
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD23	4	0.89	0.05	0.88
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	4	0.74	0.21	0.8
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	4	0.74	0.21	0.8
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	4	0.74	0.21	0.8
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD21	4	0.61	0.11	0.56
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD22	4	0.61	0.11	0.56
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD23	4	0.61	0.11	0.56
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD11	4	0.61	0.09	0.6
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD12	4	0.61	0.09	0.6
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD13	4	0.61	0.09	0.6
(1,83)	1:1848:A:LEU:H	1:1848:A:LEU:HB2	4	0.6	0.08	0.62
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD21	4	0.6	0.11	0.55
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD22	4	0.6	0.11	0.55
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD23	4	0.6	0.11	0.55
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB1	4	0.56	0.15	0.64
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB2	4	0.56	0.15	0.64
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB3	4	0.56	0.15	0.64
(1,731)	1:1840:A:VAL:HG11	1:1848:A:LEU:HG	4	0.51	0.13	0.54
(1,731)	1:1840:A:VAL:HG12	1:1848:A:LEU:HG	4	0.51	0.13	0.54
(1,731)	1:1840:A:VAL:HG13	1:1848:A:LEU:HG	4	0.51	0.13	0.54
(1,29)	1:1789:A:THR:HG1	1:1873:A:VAL:H	4	0.4	0.23	0.34
(1,426)	1:1819:A:ALA:HB1	1:1820:A:ASN:H	4	0.39	0.15	0.47
(1,426)	1:1819:A:ALA:HB2	1:1820:A:ASN:H	4	0.39	0.15	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,426)	1:1819:A:ALA:HB3	1:1820:A:ASN:H	4	0.39	0.15	0.47
(1,432)	1:1824:A:ARG:HB3	1:1825:A:ALA:H	4	0.36	0.15	0.29
(1,106)	1:1820:A:ASN:HB3	1:1821:A:ILE:H	4	0.34	0.1	0.36
(1,26)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD1	4	0.3	0.03	0.31
(1,26)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD2	4	0.3	0.03	0.31
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG11	4	0.29	0.1	0.27
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG12	4	0.29	0.1	0.27
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG13	4	0.29	0.1	0.27
(1,210)	1:1840:A:VAL:HB	1:1841:A:VAL:H	4	0.29	0.11	0.26
(1,66)	1:1840:A:VAL:HG21	1:1850:A:CYS:HA	4	0.28	0.17	0.18
(1,66)	1:1840:A:VAL:HG22	1:1850:A:CYS:HA	4	0.28	0.17	0.18
(1,66)	1:1840:A:VAL:HG23	1:1850:A:CYS:HA	4	0.28	0.17	0.18
(1,522)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD1	4	0.27	0.03	0.28
(1,522)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD2	4	0.27	0.03	0.28
(1,592)	1:1799:A:PHE:H	1:1799:A:PHE:HB2	4	0.24	0.12	0.22
(1,253)	1:1877:A:GLU:H	1:1877:A:GLU:HB2	4	0.24	0.08	0.21
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG21	4	0.22	0.04	0.22
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG22	4	0.22	0.04	0.22
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG23	4	0.22	0.04	0.22
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG21	4	0.22	0.04	0.22
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG22	4	0.22	0.04	0.22
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG23	4	0.22	0.04	0.22
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG21	4	0.22	0.04	0.22
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG22	4	0.22	0.04	0.22
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG23	4	0.22	0.04	0.22
(1,712)	1:1791:A:TRP:HZ3	1:1872:A:ASN:H	4	0.22	0.05	0.2
(1,254)	1:1877:A:GLU:H	1:1877:A:GLU:HB3	4	0.21	0.06	0.22
(1,186)	1:1845:A:SER:H	1:1846:A:VAL:H	4	0.21	0.05	0.22
(1,525)	1:1865:A:PHE:HA	1:1865:A:PHE:HB2	4	0.2	0.05	0.22
(1,224)	1:1873:A:VAL:HA	1:1874:A:GLN:H	4	0.17	0.04	0.18
(1,619)	1:1851:A:LYS:H	1:1851:A:LYS:HA	4	0.16	0.04	0.16
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD11	4	0.16	0.03	0.18
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD12	4	0.16	0.03	0.18
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD13	4	0.16	0.03	0.18
(1,34)	1:1791:A:TRP:HA	1:1792:A:LEU:H	4	0.16	0.06	0.15
(1,621)	1:1869:A:TYR:HA	1:1870:A:GLU:H	4	0.16	0.03	0.16
(1,187)	1:1846:A:VAL:H	1:1847:A:GLY:H	4	0.14	0.03	0.13
(1,617)	1:1847:A:GLY:HA3	1:1848:A:LEU:H	4	0.12	0.01	0.12
(1,142)	1:1788:A:TRP:HB2	1:1788:A:TRP:HD1	4	0.12	0.01	0.11
(1,549)	1:1833:A:ILE:H	1:1833:A:ILE:HG13	3	1.08	0.22	1.03
(1,433)	1:1824:A:ARG:HB2	1:1825:A:ALA:H	3	1.05	0.29	1.23
(1,665)	1:1842:A:CYS:HB3	1:1848:A:LEU:HD21	3	0.9	0.17	0.87

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,665)	1:1842:A:CYS:HB3	1:1848:A:LEU:HD22	3	0.9	0.17	0.87
(1,665)	1:1842:A:CYS:HB3	1:1848:A:LEU:HD23	3	0.9	0.17	0.87
(1,18)	1:1817:A:TRP:HA	1:1817:A:TRP:HE3	3	0.73	0.17	0.65
(1,563)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD21	3	0.56	0.1	0.61
(1,563)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD22	3	0.56	0.1	0.61
(1,563)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD23	3	0.56	0.1	0.61
(1,376)	1:1812:A:VAL:H	1:1812:A:VAL:HG11	3	0.54	0.02	0.54
(1,376)	1:1812:A:VAL:H	1:1812:A:VAL:HG12	3	0.54	0.02	0.54
(1,376)	1:1812:A:VAL:H	1:1812:A:VAL:HG13	3	0.54	0.02	0.54
(1,118)	1:1822:A:SER:H	1:1873:A:VAL:HG11	3	0.53	0.29	0.42
(1,118)	1:1822:A:SER:H	1:1873:A:VAL:HG12	3	0.53	0.29	0.42
(1,118)	1:1822:A:SER:H	1:1873:A:VAL:HG13	3	0.53	0.29	0.42
(1,531)	1:1817:A:TRP:HB3	1:1817:A:TRP:HD1	3	0.49	0.05	0.46
(1,664)	1:1848:A:LEU:HD21	1:1869:A:TYR:HB3	3	0.48	0.48	0.18
(1,664)	1:1848:A:LEU:HD22	1:1869:A:TYR:HB3	3	0.48	0.48	0.18
(1,664)	1:1848:A:LEU:HD23	1:1869:A:TYR:HB3	3	0.48	0.48	0.18
(1,380)	1:1813:A:CYS:H	1:1813:A:CYS:HB3	3	0.44	0.11	0.49
(1,572)	1:1842:A:CYS:HA	1:1842:A:CYS:HB3	3	0.43	0.04	0.4
(1,174)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD21	3	0.4	0.08	0.37
(1,174)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD22	3	0.4	0.08	0.37
(1,174)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD23	3	0.4	0.08	0.37
(1,174)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD21	3	0.4	0.08	0.37
(1,174)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD22	3	0.4	0.08	0.37
(1,174)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD23	3	0.4	0.08	0.37
(1,329)	1:1800:A:HIS:H	1:1800:A:HIS:HB2	3	0.4	0.12	0.45
(1,17)	1:1817:A:TRP:HB3	1:1817:A:TRP:HE3	3	0.33	0.0	0.33
(1,85)	1:1812:A:VAL:HG21	1:1813:A:CYS:H	3	0.31	0.08	0.33
(1,85)	1:1812:A:VAL:HG22	1:1813:A:CYS:H	3	0.31	0.08	0.33
(1,85)	1:1812:A:VAL:HG23	1:1813:A:CYS:H	3	0.31	0.08	0.33
(1,629)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD11	3	0.31	0.14	0.29
(1,629)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD12	3	0.31	0.14	0.29
(1,629)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD13	3	0.31	0.14	0.29
(1,629)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD11	3	0.31	0.14	0.29
(1,629)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD12	3	0.31	0.14	0.29
(1,629)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD13	3	0.31	0.14	0.29
(1,10)	1:1872:A:ASN:H	1:1872:A:ASN:HB2	3	0.3	0.16	0.3
(1,668)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD21	3	0.3	0.03	0.31
(1,668)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD22	3	0.3	0.03	0.31
(1,668)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD23	3	0.3	0.03	0.31
(1,117)	1:1821:A:ILE:HG12	1:1822:A:SER:H	3	0.27	0.2	0.13
(1,653)	1:1833:A:ILE:HG21	1:1836:A:LEU:HD11	3	0.26	0.07	0.28
(1,653)	1:1833:A:ILE:HG21	1:1836:A:LEU:HD12	3	0.26	0.07	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,653)	1:1833:A:ILE:HG21	1:1836:A:LEU:HD13	3	0.26	0.07	0.28
(1,653)	1:1833:A:ILE:HG22	1:1836:A:LEU:HD11	3	0.26	0.07	0.28
(1,653)	1:1833:A:ILE:HG22	1:1836:A:LEU:HD12	3	0.26	0.07	0.28
(1,653)	1:1833:A:ILE:HG22	1:1836:A:LEU:HD13	3	0.26	0.07	0.28
(1,653)	1:1833:A:ILE:HG23	1:1836:A:LEU:HD11	3	0.26	0.07	0.28
(1,653)	1:1833:A:ILE:HG23	1:1836:A:LEU:HD12	3	0.26	0.07	0.28
(1,653)	1:1833:A:ILE:HG23	1:1836:A:LEU:HD13	3	0.26	0.07	0.28
(1,491)	1:1842:A:CYS:HA	1:1842:A:CYS:HB3	3	0.26	0.04	0.23
(1,255)	1:1782:A:CYS:HA	1:1782:A:CYS:HB2	3	0.25	0.07	0.27
(1,652)	1:1848:A:LEU:HB3	1:1848:A:LEU:HD11	3	0.23	0.03	0.21
(1,652)	1:1848:A:LEU:HB3	1:1848:A:LEU:HD12	3	0.23	0.03	0.21
(1,652)	1:1848:A:LEU:HB3	1:1848:A:LEU:HD13	3	0.23	0.03	0.21
(1,387)	1:1791:A:TRP:HE3	1:1871:A:ILE:HA	3	0.22	0.08	0.28
(1,138)	1:1817:A:TRP:HD1	1:1819:A:ALA:HA	3	0.2	0.07	0.18
(1,273)	1:1823:A:CYS:HA	1:1823:A:CYS:HB2	3	0.2	0.02	0.2
(1,156)	1:1791:A:TRP:HB2	1:1791:A:TRP:HE3	3	0.18	0.09	0.13
(1,250)	1:1876:A:CYS:HA	1:1877:A:GLU:H	3	0.18	0.03	0.16
(1,78)	1:1841:A:VAL:HA	1:1842:A:CYS:H	3	0.17	0.09	0.11
(1,196)	1:1789:A:THR:H	1:1790:A:GLY:H	3	0.17	0.04	0.19
(1,338)	1:1805:A:ASP:HA	1:1806:A:THR:H	3	0.16	0.02	0.16
(1,271)	1:1876:A:CYS:HA	1:1877:A:GLU:H	3	0.15	0.03	0.13
(1,96)	1:1809:A:ILE:H	1:1809:A:ILE:HG12	3	0.15	0.03	0.15
(1,567)	1:1793:A:ASP:H	1:1793:A:ASP:HB3	3	0.14	0.03	0.13
(1,316)	1:1790:A:GLY:HA2	1:1791:A:TRP:H	3	0.13	0.01	0.12
(1,447)	1:1828:A:TYR:HA	1:1829:A:PRO:HD2	3	0.13	0.03	0.11
(1,182)	1:1830:A:ASP:H	1:1831:A:VAL:H	3	0.1	0.0	0.1
(1,635)	1:1836:A:LEU:H	1:1836:A:LEU:HD11	2	1.66	0.02	1.66
(1,635)	1:1836:A:LEU:H	1:1836:A:LEU:HD12	2	1.66	0.02	1.66
(1,635)	1:1836:A:LEU:H	1:1836:A:LEU:HD13	2	1.66	0.02	1.66
(1,469)	1:1836:A:LEU:H	1:1836:A:LEU:HD11	2	1.48	0.03	1.48
(1,469)	1:1836:A:LEU:H	1:1836:A:LEU:HD12	2	1.48	0.03	1.48
(1,469)	1:1836:A:LEU:H	1:1836:A:LEU:HD13	2	1.48	0.03	1.48
(1,630)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD11	2	0.8	0.16	0.8
(1,630)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD12	2	0.8	0.16	0.8
(1,630)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD13	2	0.8	0.16	0.8
(1,630)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD11	2	0.8	0.16	0.8
(1,630)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD12	2	0.8	0.16	0.8
(1,630)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD13	2	0.8	0.16	0.8
(1,599)	1:1869:A:TYR:HB2	1:1870:A:GLU:H	2	0.76	0.05	0.76
(1,697)	1:1789:A:THR:HG1	1:1789:A:THR:HG21	2	0.68	0.01	0.68
(1,697)	1:1789:A:THR:HG1	1:1789:A:THR:HG22	2	0.68	0.01	0.68
(1,697)	1:1789:A:THR:HG1	1:1789:A:THR:HG23	2	0.68	0.01	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,623)	1:1865:A:PHE:HD1	1:1866:A:CYS:H	2	0.62	0.04	0.62
(1,623)	1:1865:A:PHE:HD2	1:1866:A:CYS:H	2	0.62	0.04	0.62
(1,604)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD11	2	0.57	0.16	0.57
(1,604)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD12	2	0.57	0.16	0.57
(1,604)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD13	2	0.57	0.16	0.57
(1,604)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD11	2	0.57	0.16	0.57
(1,604)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD12	2	0.57	0.16	0.57
(1,604)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD13	2	0.57	0.16	0.57
(1,701)	1:1870:A:GLU:HA	1:1870:A:GLU:HB2	2	0.42	0.01	0.42
(1,414)	1:1830:A:ASP:H	1:1830:A:ASP:HB2	2	0.36	0.03	0.36
(1,700)	1:1821:A:ILE:HA	1:1821:A:ILE:HG12	2	0.32	0.02	0.32
(1,721)	1:1791:A:TRP:HE3	1:1872:A:ASN:HB2	2	0.3	0.01	0.3
(1,369)	1:1808:A:LEU:HB3	1:1810:A:GLY:H	2	0.3	0.09	0.3
(1,651)	1:1836:A:LEU:HB3	1:1836:A:LEU:HD11	2	0.29	0.11	0.29
(1,651)	1:1836:A:LEU:HB3	1:1836:A:LEU:HD12	2	0.29	0.11	0.29
(1,651)	1:1836:A:LEU:HB3	1:1836:A:LEU:HD13	2	0.29	0.11	0.29
(1,596)	1:1869:A:TYR:HA	1:1869:A:TYR:HB2	2	0.29	0.12	0.29
(1,74)	1:1840:A:VAL:H	1:1840:A:VAL:HG21	2	0.28	0.04	0.28
(1,74)	1:1840:A:VAL:H	1:1840:A:VAL:HG22	2	0.28	0.04	0.28
(1,74)	1:1840:A:VAL:H	1:1840:A:VAL:HG23	2	0.28	0.04	0.28
(1,538)	1:1879:A:VAL:H	1:1879:A:VAL:HG21	2	0.27	0.12	0.27
(1,538)	1:1879:A:VAL:H	1:1879:A:VAL:HG22	2	0.27	0.12	0.27
(1,538)	1:1879:A:VAL:H	1:1879:A:VAL:HG23	2	0.27	0.12	0.27
(1,230)	1:1799:A:PHE:HA	1:1800:A:HIS:H	2	0.25	0.04	0.25
(1,334)	1:1805:A:ASP:H	1:1805:A:ASP:HB2	2	0.25	0.13	0.25
(1,232)	1:1799:A:PHE:H	1:1799:A:PHE:HB2	2	0.24	0.04	0.24
(1,571)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD21	2	0.24	0.02	0.24
(1,571)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD22	2	0.24	0.02	0.24
(1,571)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD23	2	0.24	0.02	0.24
(1,607)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD21	2	0.24	0.02	0.24
(1,607)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD22	2	0.24	0.02	0.24
(1,607)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD23	2	0.24	0.02	0.24
(1,428)	1:1820:A:ASN:H	1:1874:A:GLN:HB2	2	0.23	0.07	0.23
(1,173)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD11	2	0.22	0.1	0.22
(1,173)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD12	2	0.22	0.1	0.22
(1,173)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD13	2	0.22	0.1	0.22
(1,173)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD11	2	0.22	0.1	0.22
(1,173)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD12	2	0.22	0.1	0.22
(1,173)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD13	2	0.22	0.1	0.22
(1,355)	1:1813:A:CYS:H	1:1814:A:GLY:H	2	0.22	0.01	0.22
(1,9)	1:1871:A:ILE:HB	1:1872:A:ASN:H	2	0.2	0.01	0.2
(1,484)	1:1838:A:GLN:HB3	1:1839:A:THR:H	2	0.2	0.06	0.2

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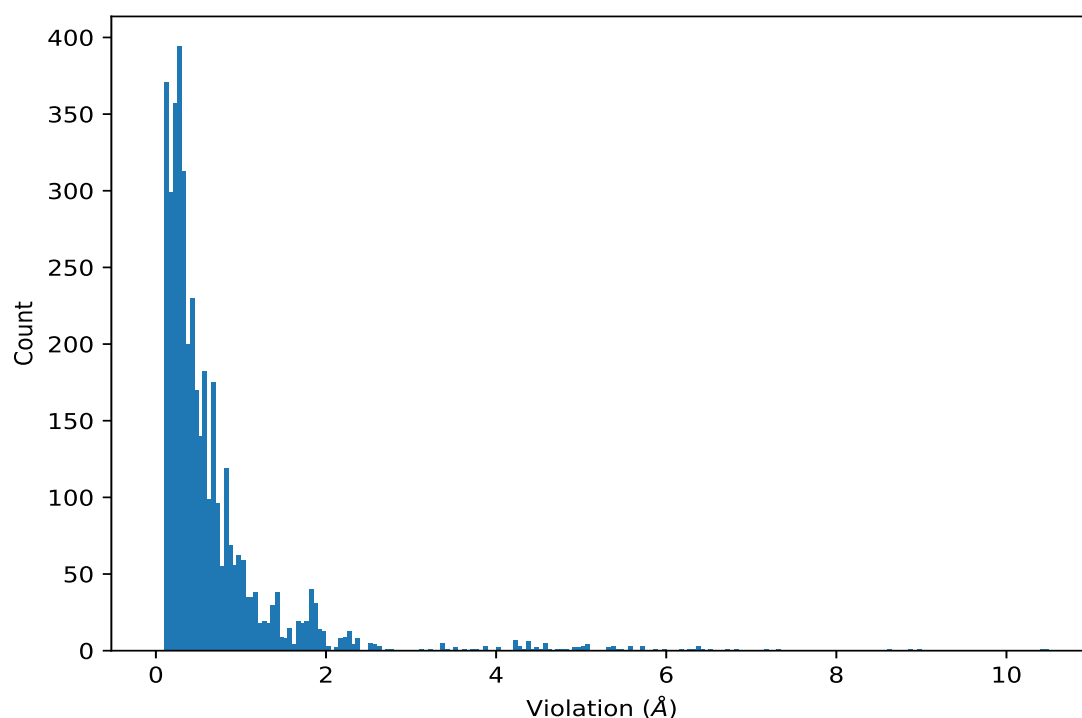
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,503)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	2	0.2	0.02	0.2
(1,570)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD11	2	0.2	0.06	0.2
(1,570)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD12	2	0.2	0.06	0.2
(1,570)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD13	2	0.2	0.06	0.2
(1,199)	1:1813:A:CYS:H	1:1814:A:GLY:H	2	0.18	0.01	0.18
(1,358)	1:1808:A:LEU:HA	1:1809:A:ILE:H	2	0.18	0.02	0.18
(1,197)	1:1789:A:THR:H	1:1873:A:VAL:H	2	0.18	0.06	0.18
(1,562)	1:1842:A:CYS:HA	1:1842:A:CYS:HB2	2	0.17	0.02	0.17
(1,104)	1:1820:A:ASN:HA	1:1821:A:ILE:H	2	0.16	0.02	0.16
(1,577)	1:1878:A:CYS:HA	1:1878:A:CYS:HB2	2	0.16	0.02	0.16
(1,207)	1:1840:A:VAL:HA	1:1841:A:VAL:H	2	0.16	0.02	0.16
(1,416)	1:1829:A:PRO:HD2	1:1830:A:ASP:H	2	0.15	0.01	0.15
(1,650)	1:1848:A:LEU:HD11	1:1848:A:LEU:HG	2	0.15	0.01	0.15
(1,650)	1:1848:A:LEU:HD12	1:1848:A:LEU:HG	2	0.15	0.01	0.15
(1,650)	1:1848:A:LEU:HD13	1:1848:A:LEU:HG	2	0.15	0.01	0.15
(1,101)	1:1823:A:CYS:HA	1:1824:A:ARG:H	2	0.15	0.0	0.15
(1,398)	1:1823:A:CYS:HA	1:1824:A:ARG:H	2	0.15	0.0	0.15
(1,541)	1:1823:A:CYS:HA	1:1823:A:CYS:HB2	2	0.14	0.02	0.14
(1,723)	1:1788:A:TRP:HE3	1:1788:A:TRP:HH2	2	0.14	0.0	0.14
(1,305)	1:1790:A:GLY:H	1:1790:A:GLY:HA2	2	0.14	0.02	0.14
(1,233)	1:1799:A:PHE:H	1:1799:A:PHE:HA	2	0.12	0.01	0.12
(1,425)	1:1820:A:ASN:H	1:1820:A:ASN:HB3	2	0.12	0.02	0.12
(1,727)	1:1874:A:GLN:HB3	1:1874:A:GLN:HG2	2	0.12	0.0	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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



9.5.2 Table : All distance violations [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)
(1,293)	1:1795:A:GLY:H	1:1799:A:PHE:HA	7	10.47
(1,293)	1:1795:A:GLY:H	1:1799:A:PHE:HA	10	10.44
(1,293)	1:1795:A:GLY:H	1:1799:A:PHE:HA	2	8.99
(1,293)	1:1795:A:GLY:H	1:1799:A:PHE:HA	8	8.88
(1,293)	1:1795:A:GLY:H	1:1799:A:PHE:HA	4	8.63
(1,335)	1:1805:A:ASP:H	1:1870:A:GLU:HA	3	7.33
(1,293)	1:1795:A:GLY:H	1:1799:A:PHE:HA	5	7.17
(1,335)	1:1805:A:ASP:H	1:1870:A:GLU:HA	8	6.84
(1,335)	1:1805:A:ASP:H	1:1870:A:GLU:HA	4	6.74
(1,335)	1:1805:A:ASP:H	1:1870:A:GLU:HA	5	6.51
(1,335)	1:1805:A:ASP:H	1:1870:A:GLU:HA	9	6.43
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG21	10	6.36
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG22	10	6.36
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG23	10	6.36
(1,335)	1:1805:A:ASP:H	1:1870:A:GLU:HA	6	6.35
(1,335)	1:1805:A:ASP:H	1:1870:A:GLU:HA	7	6.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,335)	1:1805:A:ASP:H	1:1870:A:GLU:HA	10	6.18
(1,335)	1:1805:A:ASP:H	1:1870:A:GLU:HA	2	5.96
(1,335)	1:1805:A:ASP:H	1:1870:A:GLU:HA	1	5.89
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG21	4	5.72
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG22	4	5.72
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG23	4	5.72
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG21	8	5.56
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG22	8	5.56
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG23	8	5.56
(1,267)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	2	5.49
(1,267)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	8	5.42
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG21	7	5.39
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG22	7	5.39
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG23	7	5.39
(1,267)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	4	5.33
(1,267)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	5	5.31
(1,266)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	2	5.09
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG21	9	5.06
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG22	9	5.06
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG23	9	5.06
(1,267)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	1	5.03
(1,266)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	8	5.02
(1,293)	1:1795:A:GLY:H	1:1799:A:PHE:HA	6	5.0
(1,267)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	9	4.96
(1,267)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	7	4.95
(1,266)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	4	4.93
(1,266)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	5	4.91
(1,267)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	6	4.84
(1,267)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	10	4.76
(1,267)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	3	4.73
(1,266)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	1	4.63
(1,293)	1:1795:A:GLY:H	1:1799:A:PHE:HA	3	4.6
(1,218)	1:1818:A:ALA:H	1:1874:A:GLN:H	5	4.59
(1,218)	1:1818:A:ALA:H	1:1874:A:GLN:H	8	4.58
(1,266)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	9	4.57
(1,266)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	7	4.55
(1,293)	1:1795:A:GLY:H	1:1799:A:PHE:HA	1	4.53
(1,218)	1:1818:A:ALA:H	1:1874:A:GLN:H	6	4.49
(1,218)	1:1818:A:ALA:H	1:1874:A:GLN:H	7	4.45
(1,266)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	6	4.44
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG21	2	4.39
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG22	2	4.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG23	2	4.39
(1,266)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	10	4.36
(1,228)	1:1818:A:ALA:H	1:1874:A:GLN:H	5	4.36
(1,228)	1:1818:A:ALA:H	1:1874:A:GLN:H	8	4.36
(1,266)	1:1823:A:CYS:HA	1:1847:A:GLY:HA3	3	4.33
(1,228)	1:1818:A:ALA:H	1:1874:A:GLN:H	6	4.27
(1,218)	1:1818:A:ALA:H	1:1874:A:GLN:H	2	4.26
(1,218)	1:1818:A:ALA:H	1:1874:A:GLN:H	9	4.25
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG21	5	4.24
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG22	5	4.24
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG23	5	4.24
(1,228)	1:1818:A:ALA:H	1:1874:A:GLN:H	7	4.23
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG21	1	4.21
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG22	1	4.21
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG23	1	4.21
(1,228)	1:1818:A:ALA:H	1:1874:A:GLN:H	2	4.03
(1,228)	1:1818:A:ALA:H	1:1874:A:GLN:H	9	4.02
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG21	6	3.86
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG22	6	3.86
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG23	6	3.86
(1,218)	1:1818:A:ALA:H	1:1874:A:GLN:H	10	3.75
(1,218)	1:1818:A:ALA:H	1:1874:A:GLN:H	4	3.73
(1,218)	1:1818:A:ALA:H	1:1874:A:GLN:H	3	3.63
(1,228)	1:1818:A:ALA:H	1:1874:A:GLN:H	10	3.52
(1,228)	1:1818:A:ALA:H	1:1874:A:GLN:H	4	3.5
(1,218)	1:1818:A:ALA:H	1:1874:A:GLN:H	1	3.43
(1,228)	1:1818:A:ALA:H	1:1874:A:GLN:H	3	3.4
(1,422)	1:1787:A:ASN:HA	1:1820:A:ASN:H	4	3.37
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG21	3	3.36
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG22	3	3.36
(1,222)	1:1818:A:ALA:H	1:1844:A:VAL:HG23	3	3.36
(1,228)	1:1818:A:ALA:H	1:1874:A:GLN:H	1	3.21
(1,422)	1:1787:A:ASN:HA	1:1820:A:ASN:H	10	3.13
(1,422)	1:1787:A:ASN:HA	1:1820:A:ASN:H	3	2.77
(1,293)	1:1795:A:GLY:H	1:1799:A:PHE:HA	9	2.7
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG21	5	2.6
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG22	5	2.6
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG23	5	2.6
(1,422)	1:1787:A:ASN:HA	1:1820:A:ASN:H	5	2.59
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG21	8	2.56
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG22	8	2.56
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG23	8	2.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,422)	1:1787:A:ASN:HA	1:1820:A:ASN:H	8	2.55
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG21	4	2.54
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG22	4	2.54
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG23	4	2.54
(1,422)	1:1787:A:ASN:HA	1:1820:A:ASN:H	7	2.5
(1,422)	1:1787:A:ASN:HA	1:1820:A:ASN:H	9	2.4
(1,427)	1:1818:A:ALA:HB1	1:1820:A:ASN:H	1	2.38
(1,427)	1:1818:A:ALA:HB2	1:1820:A:ASN:H	1	2.38
(1,427)	1:1818:A:ALA:HB3	1:1820:A:ASN:H	1	2.38
(1,427)	1:1818:A:ALA:HB1	1:1820:A:ASN:H	3	2.35
(1,427)	1:1818:A:ALA:HB2	1:1820:A:ASN:H	3	2.35
(1,427)	1:1818:A:ALA:HB3	1:1820:A:ASN:H	3	2.35
(1,422)	1:1787:A:ASN:HA	1:1820:A:ASN:H	2	2.35
(1,689)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD3	1	2.34
(1,689)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD3	1	2.34
(1,689)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD3	3	2.33
(1,689)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD3	3	2.33
(1,685)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD2	3	2.3
(1,685)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD2	3	2.3
(1,685)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD2	5	2.29
(1,685)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD2	5	2.29
(1,689)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD3	8	2.28
(1,689)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD3	8	2.28
(1,427)	1:1818:A:ALA:HB1	1:1820:A:ASN:H	10	2.27
(1,427)	1:1818:A:ALA:HB2	1:1820:A:ASN:H	10	2.27
(1,427)	1:1818:A:ALA:HB3	1:1820:A:ASN:H	10	2.27
(1,422)	1:1787:A:ASN:HA	1:1820:A:ASN:H	1	2.26
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG21	3	2.26
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG22	3	2.26
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG23	3	2.26
(1,689)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD3	2	2.24
(1,689)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD3	2	2.24
(1,689)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD3	9	2.24
(1,689)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD3	9	2.24
(1,689)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD3	5	2.22
(1,689)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD3	5	2.22
(1,325)	1:1792:A:LEU:HA	1:1794:A:SER:H	9	2.22
(1,689)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD3	4	2.2
(1,689)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD3	4	2.2
(1,689)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD3	6	2.18
(1,689)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD3	6	2.18
(1,689)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD3	10	2.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,689)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD3	10	2.18
(1,422)	1:1787:A:ASN:HA	1:1820:A:ASN:H	6	2.18
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG21	7	2.18
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG22	7	2.18
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG23	7	2.18
(1,689)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD3	7	2.14
(1,689)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD3	7	2.14
(1,699)	1:1821:A:ILE:HA	1:1872:A:ASN:HB2	6	2.03
(1,699)	1:1821:A:ILE:HA	1:1872:A:ASN:HB2	7	2.01
(1,699)	1:1821:A:ILE:HA	1:1872:A:ASN:HB2	1	2.0
(1,685)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD2	1	1.99
(1,685)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD2	1	1.99
(1,699)	1:1821:A:ILE:HA	1:1872:A:ASN:HB2	4	1.98
(1,699)	1:1821:A:ILE:HA	1:1872:A:ASN:HB2	8	1.96
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD11	10	1.96
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD12	10	1.96
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD13	10	1.96
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD11	10	1.96
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD12	10	1.96
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD13	10	1.96
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD11	10	1.96
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD12	10	1.96
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD13	10	1.96
(1,367)	1:1810:A:GLY:H	1:1811:A:ASP:HA	7	1.95
(1,325)	1:1792:A:LEU:HA	1:1794:A:SER:H	5	1.93
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD11	2	1.92
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD12	2	1.92
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD13	2	1.92
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD11	2	1.92
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD12	2	1.92
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD13	2	1.92
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD11	2	1.92
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD12	2	1.92
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD13	2	1.92
(1,699)	1:1821:A:ILE:HA	1:1872:A:ASN:HB2	2	1.91
(1,685)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD2	7	1.91
(1,685)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD2	7	1.91
(1,685)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD2	8	1.89
(1,685)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD2	8	1.89
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG11	3	1.88
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG12	3	1.88
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG13	3	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:1818:A:ALA:HB1	1:1820:A:ASN:H	6	1.88
(1,427)	1:1818:A:ALA:HB2	1:1820:A:ASN:H	6	1.88
(1,427)	1:1818:A:ALA:HB3	1:1820:A:ASN:H	6	1.88
(1,685)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD2	4	1.86
(1,685)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD2	4	1.86
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD11	4	1.86
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD12	4	1.86
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD13	4	1.86
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD11	4	1.86
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD12	4	1.86
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD13	4	1.86
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD11	4	1.86
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD12	4	1.86
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD13	4	1.86
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG11	9	1.85
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG12	9	1.85
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG13	9	1.85
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD11	5	1.85
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD12	5	1.85
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD13	5	1.85
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD11	5	1.85
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD12	5	1.85
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD13	5	1.85
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD11	5	1.85
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD12	5	1.85
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD13	5	1.85
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG11	3	1.84
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG12	3	1.84
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG13	3	1.84
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD11	9	1.84
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD12	9	1.84
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD13	9	1.84
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD11	9	1.84
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD12	9	1.84
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD13	9	1.84
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD11	9	1.84
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD12	9	1.84
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD13	9	1.84
(1,427)	1:1818:A:ALA:HB1	1:1820:A:ASN:H	9	1.84
(1,427)	1:1818:A:ALA:HB2	1:1820:A:ASN:H	9	1.84
(1,427)	1:1818:A:ALA:HB3	1:1820:A:ASN:H	9	1.84
(1,685)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD2	2	1.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD2	2	1.83
(1,427)	1:1818:A:ALA:HB1	1:1820:A:ASN:H	7	1.83
(1,427)	1:1818:A:ALA:HB2	1:1820:A:ASN:H	7	1.83
(1,427)	1:1818:A:ALA:HB3	1:1820:A:ASN:H	7	1.83
(1,409)	1:1815:A:PRO:HD2	1:1816:A:GLY:H	9	1.83
(1,367)	1:1810:A:GLY:H	1:1811:A:ASP:HA	1	1.83
(1,699)	1:1821:A:ILE:HA	1:1872:A:ASN:HB2	9	1.82
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD11	8	1.82
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD12	8	1.82
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD13	8	1.82
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD11	8	1.82
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD12	8	1.82
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD13	8	1.82
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD11	8	1.82
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD12	8	1.82
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD13	8	1.82
(1,367)	1:1810:A:GLY:H	1:1811:A:ASP:HA	2	1.82
(1,409)	1:1815:A:PRO:HD2	1:1816:A:GLY:H	2	1.81
(1,325)	1:1792:A:LEU:HA	1:1794:A:SER:H	10	1.81
(1,685)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD2	9	1.8
(1,685)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD2	9	1.8
(1,409)	1:1815:A:PRO:HD2	1:1816:A:GLY:H	5	1.8
(1,409)	1:1815:A:PRO:HD2	1:1816:A:GLY:H	7	1.8
(1,367)	1:1810:A:GLY:H	1:1811:A:ASP:HA	5	1.8
(1,409)	1:1815:A:PRO:HD2	1:1816:A:GLY:H	8	1.79
(1,367)	1:1810:A:GLY:H	1:1811:A:ASP:HA	9	1.79
(1,699)	1:1821:A:ILE:HA	1:1872:A:ASN:HB2	10	1.77
(1,367)	1:1810:A:GLY:H	1:1811:A:ASP:HA	3	1.76
(1,685)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD2	6	1.75
(1,685)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD2	6	1.75
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG11	10	1.75
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG12	10	1.75
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG13	10	1.75
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD11	7	1.75
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD12	7	1.75
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD13	7	1.75
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD11	7	1.75
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD12	7	1.75
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD13	7	1.75
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD11	7	1.75
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD12	7	1.75
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD13	7	1.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:1810:A:GLY:H	1:1811:A:ASP:HA	8	1.75
(1,325)	1:1792:A:LEU:HA	1:1794:A:SER:H	2	1.74
(1,646)	1:1840:A:VAL:HG21	1:1850:A:CYS:HB3	9	1.73
(1,646)	1:1840:A:VAL:HG22	1:1850:A:CYS:HB3	9	1.73
(1,646)	1:1840:A:VAL:HG23	1:1850:A:CYS:HB3	9	1.73
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD11	6	1.71
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD12	6	1.71
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD13	6	1.71
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD11	6	1.71
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD12	6	1.71
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD13	6	1.71
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD11	6	1.71
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD12	6	1.71
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD13	6	1.71
(1,427)	1:1818:A:ALA:HB1	1:1820:A:ASN:H	8	1.71
(1,427)	1:1818:A:ALA:HB2	1:1820:A:ASN:H	8	1.71
(1,427)	1:1818:A:ALA:HB3	1:1820:A:ASN:H	8	1.71
(1,412)	1:1816:A:GLY:H	1:1817:A:TRP:H	1	1.71
(1,412)	1:1816:A:GLY:H	1:1817:A:TRP:H	3	1.71
(1,367)	1:1810:A:GLY:H	1:1811:A:ASP:HA	4	1.7
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG11	7	1.69
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG12	7	1.69
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG13	7	1.69
(1,646)	1:1840:A:VAL:HG21	1:1850:A:CYS:HB3	7	1.69
(1,646)	1:1840:A:VAL:HG22	1:1850:A:CYS:HB3	7	1.69
(1,646)	1:1840:A:VAL:HG23	1:1850:A:CYS:HB3	7	1.69
(1,427)	1:1818:A:ALA:HB1	1:1820:A:ASN:H	5	1.69
(1,427)	1:1818:A:ALA:HB2	1:1820:A:ASN:H	5	1.69
(1,427)	1:1818:A:ALA:HB3	1:1820:A:ASN:H	5	1.69
(1,685)	1:1828:A:TYR:HE1	1:1829:A:PRO:HD2	10	1.68
(1,685)	1:1828:A:TYR:HE2	1:1829:A:PRO:HD2	10	1.68
(1,635)	1:1836:A:LEU:H	1:1836:A:LEU:HD11	1	1.68
(1,635)	1:1836:A:LEU:H	1:1836:A:LEU:HD12	1	1.68
(1,635)	1:1836:A:LEU:H	1:1836:A:LEU:HD13	1	1.68
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG11	6	1.66
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG12	6	1.66
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG13	6	1.66
(1,325)	1:1792:A:LEU:HA	1:1794:A:SER:H	7	1.66
(1,635)	1:1836:A:LEU:H	1:1836:A:LEU:HD11	3	1.64
(1,635)	1:1836:A:LEU:H	1:1836:A:LEU:HD12	3	1.64
(1,635)	1:1836:A:LEU:H	1:1836:A:LEU:HD13	3	1.64
(1,409)	1:1815:A:PRO:HD2	1:1816:A:GLY:H	1	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:1810:A:GLY:H	1:1811:A:ASP:HA	6	1.58
(1,362)	1:1808:A:LEU:HD21	1:1809:A:ILE:H	5	1.56
(1,362)	1:1808:A:LEU:HD22	1:1809:A:ILE:H	5	1.56
(1,362)	1:1808:A:LEU:HD23	1:1809:A:ILE:H	5	1.56
(1,362)	1:1808:A:LEU:HD21	1:1809:A:ILE:H	10	1.56
(1,362)	1:1808:A:LEU:HD22	1:1809:A:ILE:H	10	1.56
(1,362)	1:1808:A:LEU:HD23	1:1809:A:ILE:H	10	1.56
(1,699)	1:1821:A:ILE:HA	1:1872:A:ASN:HB2	5	1.55
(1,646)	1:1840:A:VAL:HG21	1:1850:A:CYS:HB3	10	1.55
(1,646)	1:1840:A:VAL:HG22	1:1850:A:CYS:HB3	10	1.55
(1,646)	1:1840:A:VAL:HG23	1:1850:A:CYS:HB3	10	1.55
(1,427)	1:1818:A:ALA:HB1	1:1820:A:ASN:H	2	1.55
(1,427)	1:1818:A:ALA:HB2	1:1820:A:ASN:H	2	1.55
(1,427)	1:1818:A:ALA:HB3	1:1820:A:ASN:H	2	1.55
(1,409)	1:1815:A:PRO:HD2	1:1816:A:GLY:H	3	1.55
(1,724)	1:1788:A:TRP:HB3	1:1788:A:TRP:HH2	6	1.53
(1,409)	1:1815:A:PRO:HD2	1:1816:A:GLY:H	4	1.52
(1,367)	1:1810:A:GLY:H	1:1811:A:ASP:HA	10	1.52
(1,724)	1:1788:A:TRP:HB3	1:1788:A:TRP:HH2	7	1.51
(1,469)	1:1836:A:LEU:H	1:1836:A:LEU:HD11	1	1.51
(1,469)	1:1836:A:LEU:H	1:1836:A:LEU:HD12	1	1.51
(1,469)	1:1836:A:LEU:H	1:1836:A:LEU:HD13	1	1.51
(1,409)	1:1815:A:PRO:HD2	1:1816:A:GLY:H	6	1.51
(1,699)	1:1821:A:ILE:HA	1:1872:A:ASN:HB2	3	1.49
(1,724)	1:1788:A:TRP:HB3	1:1788:A:TRP:HH2	9	1.48
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG11	8	1.48
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG12	8	1.48
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG13	8	1.48
(1,724)	1:1788:A:TRP:HB3	1:1788:A:TRP:HH2	5	1.46
(1,469)	1:1836:A:LEU:H	1:1836:A:LEU:HD11	3	1.46
(1,469)	1:1836:A:LEU:H	1:1836:A:LEU:HD12	3	1.46
(1,469)	1:1836:A:LEU:H	1:1836:A:LEU:HD13	3	1.46
(1,724)	1:1788:A:TRP:HB3	1:1788:A:TRP:HH2	2	1.45
(1,724)	1:1788:A:TRP:HB3	1:1788:A:TRP:HH2	4	1.45
(1,427)	1:1818:A:ALA:HB1	1:1820:A:ASN:H	4	1.45
(1,427)	1:1818:A:ALA:HB2	1:1820:A:ASN:H	4	1.45
(1,427)	1:1818:A:ALA:HB3	1:1820:A:ASN:H	4	1.45
(1,724)	1:1788:A:TRP:HB3	1:1788:A:TRP:HH2	8	1.44
(1,362)	1:1808:A:LEU:HD21	1:1809:A:ILE:H	2	1.44
(1,362)	1:1808:A:LEU:HD22	1:1809:A:ILE:H	2	1.44
(1,362)	1:1808:A:LEU:HD23	1:1809:A:ILE:H	2	1.44
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG11	5	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG12	5	1.44
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG13	5	1.44
(1,724)	1:1788:A:TRP:HB3	1:1788:A:TRP:HH2	1	1.43
(1,724)	1:1788:A:TRP:HB3	1:1788:A:TRP:HH2	10	1.43
(1,663)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	3	1.43
(1,663)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	3	1.43
(1,663)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	3	1.43
(1,663)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	4	1.43
(1,663)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	4	1.43
(1,663)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	4	1.43
(1,373)	1:1809:A:ILE:HD11	1:1810:A:GLY:H	10	1.43
(1,373)	1:1809:A:ILE:HD12	1:1810:A:GLY:H	10	1.43
(1,373)	1:1809:A:ILE:HD13	1:1810:A:GLY:H	10	1.43
(1,362)	1:1808:A:LEU:HD21	1:1809:A:ILE:H	6	1.43
(1,362)	1:1808:A:LEU:HD22	1:1809:A:ILE:H	6	1.43
(1,362)	1:1808:A:LEU:HD23	1:1809:A:ILE:H	6	1.43
(1,325)	1:1792:A:LEU:HA	1:1794:A:SER:H	1	1.43
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG11	2	1.43
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG12	2	1.43
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG13	2	1.43
(1,724)	1:1788:A:TRP:HB3	1:1788:A:TRP:HH2	3	1.42
(1,663)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	2	1.42
(1,663)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	2	1.42
(1,663)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	2	1.42
(1,373)	1:1809:A:ILE:HD11	1:1810:A:GLY:H	9	1.42
(1,373)	1:1809:A:ILE:HD12	1:1810:A:GLY:H	9	1.42
(1,373)	1:1809:A:ILE:HD13	1:1810:A:GLY:H	9	1.42
(1,412)	1:1816:A:GLY:H	1:1817:A:TRP:H	8	1.41
(1,362)	1:1808:A:LEU:HD21	1:1809:A:ILE:H	9	1.4
(1,362)	1:1808:A:LEU:HD22	1:1809:A:ILE:H	9	1.4
(1,362)	1:1808:A:LEU:HD23	1:1809:A:ILE:H	9	1.4
(1,325)	1:1792:A:LEU:HA	1:1794:A:SER:H	8	1.38
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG11	8	1.38
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG12	8	1.38
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG13	8	1.38
(1,549)	1:1833:A:ILE:H	1:1833:A:ILE:HG13	6	1.37
(1,412)	1:1816:A:GLY:H	1:1817:A:TRP:H	7	1.37
(1,663)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	6	1.36
(1,663)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	6	1.36
(1,663)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	6	1.36
(1,362)	1:1808:A:LEU:HD21	1:1809:A:ILE:H	1	1.36
(1,362)	1:1808:A:LEU:HD22	1:1809:A:ILE:H	1	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,362)	1:1808:A:LEU:HD23	1:1809:A:ILE:H	1	1.36
(1,215)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	3	1.36
(1,215)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	3	1.36
(1,215)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	3	1.36
(1,373)	1:1809:A:ILE:HD11	1:1810:A:GLY:H	5	1.35
(1,373)	1:1809:A:ILE:HD12	1:1810:A:GLY:H	5	1.35
(1,373)	1:1809:A:ILE:HD13	1:1810:A:GLY:H	5	1.35
(1,362)	1:1808:A:LEU:HD21	1:1809:A:ILE:H	8	1.35
(1,362)	1:1808:A:LEU:HD22	1:1809:A:ILE:H	8	1.35
(1,362)	1:1808:A:LEU:HD23	1:1809:A:ILE:H	8	1.35
(1,215)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	2	1.35
(1,215)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	2	1.35
(1,215)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	2	1.35
(1,215)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	4	1.35
(1,215)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	4	1.35
(1,215)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	4	1.35
(1,663)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	5	1.34
(1,663)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	5	1.34
(1,663)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	5	1.34
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG21	10	1.34
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG22	10	1.34
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG23	10	1.34
(1,362)	1:1808:A:LEU:HD21	1:1809:A:ILE:H	4	1.34
(1,362)	1:1808:A:LEU:HD22	1:1809:A:ILE:H	4	1.34
(1,362)	1:1808:A:LEU:HD23	1:1809:A:ILE:H	4	1.34
(1,548)	1:1820:A:ASN:H	1:1874:A:GLN:HB3	10	1.33
(1,412)	1:1816:A:GLY:H	1:1817:A:TRP:H	5	1.33
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	3	1.31
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	3	1.31
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	3	1.31
(1,663)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	8	1.3
(1,663)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	8	1.3
(1,663)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	8	1.3
(1,406)	1:1815:A:PRO:HA	1:1816:A:GLY:H	1	1.3
(1,657)	1:1848:A:LEU:HD21	1:1849:A:ILE:HA	3	1.29
(1,657)	1:1848:A:LEU:HD22	1:1849:A:ILE:HA	3	1.29
(1,657)	1:1848:A:LEU:HD23	1:1849:A:ILE:HA	3	1.29
(1,613)	1:1791:A:TRP:HA	1:1791:A:TRP:HE3	3	1.28
(1,433)	1:1824:A:ARG:HB2	1:1825:A:ALA:H	8	1.28
(1,215)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	6	1.28
(1,215)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	6	1.28
(1,215)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	6	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	5	1.27
(1,215)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	5	1.27
(1,215)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	5	1.27
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG11	4	1.26
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG12	4	1.26
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG13	4	1.26
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG11	5	1.26
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG12	5	1.26
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG13	5	1.26
(1,412)	1:1816:A:GLY:H	1:1817:A:TRP:H	2	1.26
(1,325)	1:1792:A:LEU:HA	1:1794:A:SER:H	3	1.26
(1,441)	1:1825:A:ALA:HB1	1:1828:A:TYR:HB2	2	1.24
(1,441)	1:1825:A:ALA:HB2	1:1828:A:TYR:HB2	2	1.24
(1,441)	1:1825:A:ALA:HB3	1:1828:A:TYR:HB2	2	1.24
(1,433)	1:1824:A:ARG:HB2	1:1825:A:ALA:H	7	1.23
(1,406)	1:1815:A:PRO:HA	1:1816:A:GLY:H	3	1.23
(1,373)	1:1809:A:ILE:HD11	1:1810:A:GLY:H	6	1.23
(1,373)	1:1809:A:ILE:HD12	1:1810:A:GLY:H	6	1.23
(1,373)	1:1809:A:ILE:HD13	1:1810:A:GLY:H	6	1.23
(1,215)	1:1848:A:LEU:HD11	1:1849:A:ILE:H	8	1.23
(1,215)	1:1848:A:LEU:HD12	1:1849:A:ILE:H	8	1.23
(1,215)	1:1848:A:LEU:HD13	1:1849:A:ILE:H	8	1.23
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD11	8	1.22
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD12	8	1.22
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD13	8	1.22
(1,441)	1:1825:A:ALA:HB1	1:1828:A:TYR:HB2	9	1.21
(1,441)	1:1825:A:ALA:HB2	1:1828:A:TYR:HB2	9	1.21
(1,441)	1:1825:A:ALA:HB3	1:1828:A:TYR:HB2	9	1.21
(1,406)	1:1815:A:PRO:HA	1:1816:A:GLY:H	6	1.21
(1,412)	1:1816:A:GLY:H	1:1817:A:TRP:H	9	1.2
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD1	8	1.19
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD1	8	1.19
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD1	8	1.19
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD2	8	1.19
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD2	8	1.19
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD2	8	1.19
(1,548)	1:1820:A:ASN:H	1:1874:A:GLN:HB3	6	1.19
(1,412)	1:1816:A:GLY:H	1:1817:A:TRP:H	10	1.19
(1,409)	1:1815:A:PRO:HD2	1:1816:A:GLY:H	10	1.19
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG21	9	1.19
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG22	9	1.19
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG23	9	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD1	10	1.18
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD1	10	1.18
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD1	10	1.18
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD2	10	1.18
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD2	10	1.18
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD2	10	1.18
(1,406)	1:1815:A:PRO:HA	1:1816:A:GLY:H	4	1.18
(1,441)	1:1825:A:ALA:HB1	1:1828:A:TYR:HB2	7	1.17
(1,441)	1:1825:A:ALA:HB2	1:1828:A:TYR:HB2	7	1.17
(1,441)	1:1825:A:ALA:HB3	1:1828:A:TYR:HB2	7	1.17
(1,664)	1:1848:A:LEU:HD21	1:1869:A:TYR:HB3	9	1.16
(1,664)	1:1848:A:LEU:HD22	1:1869:A:TYR:HB3	9	1.16
(1,664)	1:1848:A:LEU:HD23	1:1869:A:TYR:HB3	9	1.16
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	3	1.16
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	3	1.16
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	3	1.16
(1,441)	1:1825:A:ALA:HB1	1:1828:A:TYR:HB2	6	1.16
(1,441)	1:1825:A:ALA:HB2	1:1828:A:TYR:HB2	6	1.16
(1,441)	1:1825:A:ALA:HB3	1:1828:A:TYR:HB2	6	1.16
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG21	1	1.16
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG22	1	1.16
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG23	1	1.16
(1,362)	1:1808:A:LEU:HD21	1:1809:A:ILE:H	7	1.16
(1,362)	1:1808:A:LEU:HD22	1:1809:A:ILE:H	7	1.16
(1,362)	1:1808:A:LEU:HD23	1:1809:A:ILE:H	7	1.16
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD11	3	1.15
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD12	3	1.15
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD13	3	1.15
(1,548)	1:1820:A:ASN:H	1:1874:A:GLN:HB3	1	1.15
(1,290)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	1	1.15
(1,441)	1:1825:A:ALA:HB1	1:1828:A:TYR:HB2	10	1.14
(1,441)	1:1825:A:ALA:HB2	1:1828:A:TYR:HB2	10	1.14
(1,441)	1:1825:A:ALA:HB3	1:1828:A:TYR:HB2	10	1.14
(1,406)	1:1815:A:PRO:HA	1:1816:A:GLY:H	5	1.14
(1,441)	1:1825:A:ALA:HB1	1:1828:A:TYR:HB2	5	1.13
(1,441)	1:1825:A:ALA:HB2	1:1828:A:TYR:HB2	5	1.13
(1,441)	1:1825:A:ALA:HB3	1:1828:A:TYR:HB2	5	1.13
(1,665)	1:1842:A:CYS:HB3	1:1848:A:LEU:HD21	1	1.12
(1,665)	1:1842:A:CYS:HB3	1:1848:A:LEU:HD22	1	1.12
(1,665)	1:1842:A:CYS:HB3	1:1848:A:LEU:HD23	1	1.12
(1,441)	1:1825:A:ALA:HB1	1:1828:A:TYR:HB2	8	1.12
(1,441)	1:1825:A:ALA:HB2	1:1828:A:TYR:HB2	8	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,441)	1:1825:A:ALA:HB3	1:1828:A:TYR:HB2	8	1.12
(1,406)	1:1815:A:PRO:HA	1:1816:A:GLY:H	8	1.12
(1,441)	1:1825:A:ALA:HB1	1:1828:A:TYR:HB2	4	1.11
(1,441)	1:1825:A:ALA:HB2	1:1828:A:TYR:HB2	4	1.11
(1,441)	1:1825:A:ALA:HB3	1:1828:A:TYR:HB2	4	1.11
(1,406)	1:1815:A:PRO:HA	1:1816:A:GLY:H	7	1.11
(1,354)	1:1812:A:VAL:H	1:1813:A:CYS:HA	2	1.11
(1,290)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	3	1.11
(1,75)	1:1840:A:VAL:HG11	1:1842:A:CYS:H	1	1.11
(1,75)	1:1840:A:VAL:HG12	1:1842:A:CYS:H	1	1.11
(1,75)	1:1840:A:VAL:HG13	1:1842:A:CYS:H	1	1.11
(1,75)	1:1840:A:VAL:HG11	1:1842:A:CYS:H	5	1.11
(1,75)	1:1840:A:VAL:HG12	1:1842:A:CYS:H	5	1.11
(1,75)	1:1840:A:VAL:HG13	1:1842:A:CYS:H	5	1.11
(1,406)	1:1815:A:PRO:HA	1:1816:A:GLY:H	9	1.1
(1,406)	1:1815:A:PRO:HA	1:1816:A:GLY:H	10	1.1
(1,354)	1:1812:A:VAL:H	1:1813:A:CYS:HA	8	1.1
(1,87)	1:1808:A:LEU:H	1:1808:A:LEU:HG	1	1.1
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG21	2	1.09
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG22	2	1.09
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG23	2	1.09
(1,325)	1:1792:A:LEU:HA	1:1794:A:SER:H	6	1.09
(1,86)	1:1812:A:VAL:HG11	1:1813:A:CYS:H	6	1.09
(1,86)	1:1812:A:VAL:HG12	1:1813:A:CYS:H	6	1.09
(1,86)	1:1812:A:VAL:HG13	1:1813:A:CYS:H	6	1.09
(1,548)	1:1820:A:ASN:H	1:1874:A:GLN:HB3	3	1.08
(1,528)	1:1866:A:CYS:H	1:1866:A:CYS:HB3	2	1.08
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG11	10	1.08
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG12	10	1.08
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG13	10	1.08
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG21	10	1.08
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG22	10	1.08
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG23	10	1.08
(1,325)	1:1792:A:LEU:HA	1:1794:A:SER:H	4	1.08
(1,62)	1:1840:A:VAL:HG11	1:1841:A:VAL:H	5	1.08
(1,62)	1:1840:A:VAL:HG12	1:1841:A:VAL:H	5	1.08
(1,62)	1:1840:A:VAL:HG13	1:1841:A:VAL:H	5	1.08
(1,354)	1:1812:A:VAL:H	1:1813:A:CYS:HA	5	1.07
(1,45)	1:1789:A:THR:H	1:1789:A:THR:HG1	9	1.07
(1,333)	1:1805:A:ASP:H	1:1850:A:CYS:HB2	9	1.06
(1,185)	1:1819:A:ALA:H	1:1820:A:ASN:H	6	1.06
(1,71)	1:1840:A:VAL:HG11	1:1841:A:VAL:H	5	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:1840:A:VAL:HG12	1:1841:A:VAL:H	5	1.06
(1,71)	1:1840:A:VAL:HG13	1:1841:A:VAL:H	5	1.06
(1,441)	1:1825:A:ALA:HB1	1:1828:A:TYR:HB2	3	1.05
(1,441)	1:1825:A:ALA:HB2	1:1828:A:TYR:HB2	3	1.05
(1,441)	1:1825:A:ALA:HB3	1:1828:A:TYR:HB2	3	1.05
(1,406)	1:1815:A:PRO:HA	1:1816:A:GLY:H	2	1.05
(1,295)	1:1788:A:TRP:H	1:1788:A:TRP:HB2	10	1.05
(1,185)	1:1819:A:ALA:H	1:1820:A:ASN:H	8	1.05
(1,86)	1:1812:A:VAL:HG11	1:1813:A:CYS:H	10	1.05
(1,86)	1:1812:A:VAL:HG12	1:1813:A:CYS:H	10	1.05
(1,86)	1:1812:A:VAL:HG13	1:1813:A:CYS:H	10	1.05
(1,657)	1:1848:A:LEU:HD21	1:1849:A:ILE:HA	4	1.04
(1,657)	1:1848:A:LEU:HD22	1:1849:A:ILE:HA	4	1.04
(1,657)	1:1848:A:LEU:HD23	1:1849:A:ILE:HA	4	1.04
(1,657)	1:1848:A:LEU:HD21	1:1849:A:ILE:HA	8	1.04
(1,657)	1:1848:A:LEU:HD22	1:1849:A:ILE:HA	8	1.04
(1,657)	1:1848:A:LEU:HD23	1:1849:A:ILE:HA	8	1.04
(1,646)	1:1840:A:VAL:HG21	1:1850:A:CYS:HB3	3	1.04
(1,646)	1:1840:A:VAL:HG22	1:1850:A:CYS:HB3	3	1.04
(1,646)	1:1840:A:VAL:HG23	1:1850:A:CYS:HB3	3	1.04
(1,613)	1:1791:A:TRP:HA	1:1791:A:TRP:HE3	5	1.04
(1,441)	1:1825:A:ALA:HB1	1:1828:A:TYR:HB2	1	1.04
(1,441)	1:1825:A:ALA:HB2	1:1828:A:TYR:HB2	1	1.04
(1,441)	1:1825:A:ALA:HB3	1:1828:A:TYR:HB2	1	1.04
(1,549)	1:1833:A:ILE:H	1:1833:A:ILE:HG13	9	1.03
(1,548)	1:1820:A:ASN:H	1:1874:A:GLN:HB3	2	1.03
(1,548)	1:1820:A:ASN:H	1:1874:A:GLN:HB3	9	1.03
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	5	1.02
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	5	1.02
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	5	1.02
(1,295)	1:1788:A:TRP:H	1:1788:A:TRP:HB2	3	1.02
(1,656)	1:1848:A:LEU:HD11	1:1849:A:ILE:HA	7	1.01
(1,656)	1:1848:A:LEU:HD12	1:1849:A:ILE:HA	7	1.01
(1,656)	1:1848:A:LEU:HD13	1:1849:A:ILE:HA	7	1.01
(1,573)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	3	1.01
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD11	2	1.01
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD12	2	1.01
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD13	2	1.01
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD11	4	1.01
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD12	4	1.01
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD13	4	1.01
(1,548)	1:1820:A:ASN:H	1:1874:A:GLN:HB3	8	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:1840:A:VAL:HG11	1:1842:A:CYS:H	8	1.01
(1,75)	1:1840:A:VAL:HG12	1:1842:A:CYS:H	8	1.01
(1,75)	1:1840:A:VAL:HG13	1:1842:A:CYS:H	8	1.01
(1,24)	1:1865:A:PHE:HA	1:1865:A:PHE:HB3	6	1.01
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD1	9	1.0
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD1	9	1.0
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD1	9	1.0
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD2	9	1.0
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD2	9	1.0
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD2	9	1.0
(1,656)	1:1848:A:LEU:HD11	1:1849:A:ILE:HA	9	1.0
(1,656)	1:1848:A:LEU:HD12	1:1849:A:ILE:HA	9	1.0
(1,656)	1:1848:A:LEU:HD13	1:1849:A:ILE:HA	9	1.0
(1,656)	1:1848:A:LEU:HD11	1:1849:A:ILE:HA	10	1.0
(1,656)	1:1848:A:LEU:HD12	1:1849:A:ILE:HA	10	1.0
(1,656)	1:1848:A:LEU:HD13	1:1849:A:ILE:HA	10	1.0
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	1	1.0
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	1	1.0
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	1	1.0
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG21	2	1.0
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG22	2	1.0
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG23	2	1.0
(1,295)	1:1788:A:TRP:H	1:1788:A:TRP:HB2	4	1.0
(1,185)	1:1819:A:ALA:H	1:1820:A:ASN:H	7	1.0
(1,185)	1:1819:A:ALA:H	1:1820:A:ASN:H	9	1.0
(1,62)	1:1840:A:VAL:HG11	1:1841:A:VAL:H	4	1.0
(1,62)	1:1840:A:VAL:HG12	1:1841:A:VAL:H	4	1.0
(1,62)	1:1840:A:VAL:HG13	1:1841:A:VAL:H	4	1.0
(1,726)	1:1874:A:GLN:H	1:1874:A:GLN:HB3	1	0.99
(1,528)	1:1866:A:CYS:H	1:1866:A:CYS:HB3	5	0.99
(1,421)	1:1819:A:ALA:H	1:1820:A:ASN:H	6	0.99
(1,295)	1:1788:A:TRP:H	1:1788:A:TRP:HB2	2	0.99
(1,87)	1:1808:A:LEU:H	1:1808:A:LEU:HG	6	0.99
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD1	7	0.98
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD1	7	0.98
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD1	7	0.98
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD2	7	0.98
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD2	7	0.98
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD2	7	0.98
(1,613)	1:1791:A:TRP:HA	1:1791:A:TRP:HE3	4	0.98
(1,421)	1:1819:A:ALA:H	1:1820:A:ASN:H	8	0.98
(1,295)	1:1788:A:TRP:H	1:1788:A:TRP:HB2	1	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:1819:A:ALA:H	1:1820:A:ASN:H	2	0.98
(1,185)	1:1819:A:ALA:H	1:1820:A:ASN:H	5	0.98
(1,71)	1:1840:A:VAL:HG11	1:1841:A:VAL:H	4	0.98
(1,71)	1:1840:A:VAL:HG12	1:1841:A:VAL:H	4	0.98
(1,71)	1:1840:A:VAL:HG13	1:1841:A:VAL:H	4	0.98
(1,62)	1:1840:A:VAL:HG11	1:1841:A:VAL:H	8	0.98
(1,62)	1:1840:A:VAL:HG12	1:1841:A:VAL:H	8	0.98
(1,62)	1:1840:A:VAL:HG13	1:1841:A:VAL:H	8	0.98
(1,615)	1:1812:A:VAL:H	1:1813:A:CYS:HA	2	0.97
(1,613)	1:1791:A:TRP:HA	1:1791:A:TRP:HE3	6	0.97
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD21	9	0.97
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD22	9	0.97
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD23	9	0.97
(1,86)	1:1812:A:VAL:HG11	1:1813:A:CYS:H	4	0.97
(1,86)	1:1812:A:VAL:HG12	1:1813:A:CYS:H	4	0.97
(1,86)	1:1812:A:VAL:HG13	1:1813:A:CYS:H	4	0.97
(1,62)	1:1840:A:VAL:HG11	1:1841:A:VAL:H	1	0.97
(1,62)	1:1840:A:VAL:HG12	1:1841:A:VAL:H	1	0.97
(1,62)	1:1840:A:VAL:HG13	1:1841:A:VAL:H	1	0.97
(1,62)	1:1840:A:VAL:HG11	1:1841:A:VAL:H	2	0.97
(1,62)	1:1840:A:VAL:HG12	1:1841:A:VAL:H	2	0.97
(1,62)	1:1840:A:VAL:HG13	1:1841:A:VAL:H	2	0.97
(1,657)	1:1848:A:LEU:HD21	1:1849:A:ILE:HA	2	0.96
(1,657)	1:1848:A:LEU:HD22	1:1849:A:ILE:HA	2	0.96
(1,657)	1:1848:A:LEU:HD23	1:1849:A:ILE:HA	2	0.96
(1,630)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD11	6	0.96
(1,630)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD12	6	0.96
(1,630)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD13	6	0.96
(1,630)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD11	6	0.96
(1,630)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD12	6	0.96
(1,630)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD13	6	0.96
(1,615)	1:1812:A:VAL:H	1:1813:A:CYS:HA	8	0.96
(1,600)	1:1869:A:TYR:HB3	1:1870:A:GLU:H	10	0.96
(1,548)	1:1820:A:ASN:H	1:1874:A:GLN:HB3	5	0.96
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	1	0.96
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	1	0.96
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	1	0.96
(1,412)	1:1816:A:GLY:H	1:1817:A:TRP:H	6	0.96
(1,71)	1:1840:A:VAL:HG11	1:1841:A:VAL:H	1	0.96
(1,71)	1:1840:A:VAL:HG12	1:1841:A:VAL:H	1	0.96
(1,71)	1:1840:A:VAL:HG13	1:1841:A:VAL:H	1	0.96
(1,71)	1:1840:A:VAL:HG11	1:1841:A:VAL:H	8	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:1840:A:VAL:HG12	1:1841:A:VAL:H	8	0.96
(1,71)	1:1840:A:VAL:HG13	1:1841:A:VAL:H	8	0.96
(1,54)	1:1840:A:VAL:HG11	1:1842:A:CYS:HB2	6	0.96
(1,54)	1:1840:A:VAL:HG12	1:1842:A:CYS:HB2	6	0.96
(1,54)	1:1840:A:VAL:HG13	1:1842:A:CYS:HB2	6	0.96
(1,18)	1:1817:A:TRP:HA	1:1817:A:TRP:HE3	10	0.96
(1,613)	1:1791:A:TRP:HA	1:1791:A:TRP:HE3	9	0.95
(1,594)	1:1799:A:PHE:H	1:1799:A:PHE:HA	7	0.95
(1,494)	1:1842:A:CYS:HA	1:1843:A:ASP:HB3	6	0.95
(1,295)	1:1788:A:TRP:H	1:1788:A:TRP:HB2	5	0.95
(1,290)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	9	0.95
(1,71)	1:1840:A:VAL:HG11	1:1841:A:VAL:H	2	0.95
(1,71)	1:1840:A:VAL:HG12	1:1841:A:VAL:H	2	0.95
(1,71)	1:1840:A:VAL:HG13	1:1841:A:VAL:H	2	0.95
(1,613)	1:1791:A:TRP:HA	1:1791:A:TRP:HE3	8	0.94
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	10	0.94
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	10	0.94
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	10	0.94
(1,421)	1:1819:A:ALA:H	1:1820:A:ASN:H	9	0.94
(1,354)	1:1812:A:VAL:H	1:1813:A:CYS:HA	3	0.94
(1,290)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	2	0.94
(1,657)	1:1848:A:LEU:HD21	1:1849:A:ILE:HA	6	0.93
(1,657)	1:1848:A:LEU:HD22	1:1849:A:ILE:HA	6	0.93
(1,657)	1:1848:A:LEU:HD23	1:1849:A:ILE:HA	6	0.93
(1,594)	1:1799:A:PHE:H	1:1799:A:PHE:HA	2	0.93
(1,421)	1:1819:A:ALA:H	1:1820:A:ASN:H	7	0.93
(1,185)	1:1819:A:ALA:H	1:1820:A:ASN:H	1	0.93
(1,615)	1:1812:A:VAL:H	1:1813:A:CYS:HA	5	0.92
(1,613)	1:1791:A:TRP:HA	1:1791:A:TRP:HE3	7	0.92
(1,594)	1:1799:A:PHE:H	1:1799:A:PHE:HA	10	0.92
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG21	4	0.92
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG22	4	0.92
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG23	4	0.92
(1,295)	1:1788:A:TRP:H	1:1788:A:TRP:HB2	9	0.92
(1,263)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	8	0.92
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG21	5	0.92
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG22	5	0.92
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG23	5	0.92
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG21	5	0.92
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG22	5	0.92
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG23	5	0.92
(1,118)	1:1822:A:SER:H	1:1873:A:VAL:HG11	10	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:1822:A:SER:H	1:1873:A:VAL:HG12	10	0.92
(1,118)	1:1822:A:SER:H	1:1873:A:VAL:HG13	10	0.92
(1,24)	1:1865:A:PHE:HA	1:1865:A:PHE:HB3	5	0.92
(1,656)	1:1848:A:LEU:HD11	1:1849:A:ILE:HA	1	0.91
(1,656)	1:1848:A:LEU:HD12	1:1849:A:ILE:HA	1	0.91
(1,656)	1:1848:A:LEU:HD13	1:1849:A:ILE:HA	1	0.91
(1,613)	1:1791:A:TRP:HA	1:1791:A:TRP:HE3	1	0.91
(1,613)	1:1791:A:TRP:HA	1:1791:A:TRP:HE3	10	0.91
(1,494)	1:1842:A:CYS:HA	1:1843:A:ASP:HB3	10	0.91
(1,421)	1:1819:A:ALA:H	1:1820:A:ASN:H	2	0.91
(1,421)	1:1819:A:ALA:H	1:1820:A:ASN:H	5	0.91
(1,290)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	7	0.91
(1,290)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	10	0.91
(1,548)	1:1820:A:ASN:H	1:1874:A:GLN:HB3	4	0.9
(1,494)	1:1842:A:CYS:HA	1:1843:A:ASP:HB3	7	0.9
(1,424)	1:1820:A:ASN:H	1:1820:A:ASN:HB2	10	0.9
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG21	6	0.9
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG22	6	0.9
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG23	6	0.9
(1,24)	1:1865:A:PHE:HA	1:1865:A:PHE:HB3	2	0.9
(1,595)	1:1869:A:TYR:HA	1:1869:A:TYR:HB3	9	0.89
(1,494)	1:1842:A:CYS:HA	1:1843:A:ASP:HB3	9	0.89
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD21	1	0.89
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD22	1	0.89
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD23	1	0.89
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG21	1	0.89
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG22	1	0.89
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG23	1	0.89
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG21	1	0.89
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG22	1	0.89
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG23	1	0.89
(1,185)	1:1819:A:ALA:H	1:1820:A:ASN:H	4	0.89
(1,677)	1:1874:A:GLN:HG2	1:1875:A:CYS:H	10	0.88
(1,573)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	4	0.88
(1,407)	1:1815:A:PRO:HD3	1:1816:A:GLY:H	4	0.88
(1,321)	1:1792:A:LEU:HB2	1:1793:A:ASP:H	1	0.88
(1,290)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	6	0.88
(1,276)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	8	0.88
(1,24)	1:1865:A:PHE:HA	1:1865:A:PHE:HB3	4	0.88
(1,24)	1:1865:A:PHE:HA	1:1865:A:PHE:HB3	9	0.88
(1,665)	1:1842:A:CYS:HB3	1:1848:A:LEU:HD21	7	0.87
(1,665)	1:1842:A:CYS:HB3	1:1848:A:LEU:HD22	7	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,665)	1:1842:A:CYS:HB3	1:1848:A:LEU:HD23	7	0.87
(1,589)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	7	0.87
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	5	0.87
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	5	0.87
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	5	0.87
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG21	9	0.87
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG22	9	0.87
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG23	9	0.87
(1,354)	1:1812:A:VAL:H	1:1813:A:CYS:HA	10	0.87
(1,295)	1:1788:A:TRP:H	1:1788:A:TRP:HB2	6	0.87
(1,290)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	4	0.87
(1,662)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	9	0.86
(1,662)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	9	0.86
(1,662)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	9	0.86
(1,589)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	8	0.86
(1,589)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	9	0.86
(1,573)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	2	0.86
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	1	0.86
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	1	0.86
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	1	0.86
(1,505)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	8	0.86
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD21	7	0.86
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD22	7	0.86
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD23	7	0.86
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG11	7	0.86
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG12	7	0.86
(1,429)	1:1820:A:ASN:H	1:1873:A:VAL:HG13	7	0.86
(1,421)	1:1819:A:ALA:H	1:1820:A:ASN:H	1	0.86
(1,321)	1:1792:A:LEU:HB2	1:1793:A:ASP:H	9	0.86
(1,295)	1:1788:A:TRP:H	1:1788:A:TRP:HB2	7	0.86
(1,295)	1:1788:A:TRP:H	1:1788:A:TRP:HB2	8	0.86
(1,290)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	5	0.86
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG21	4	0.86
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG22	4	0.86
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG23	4	0.86
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG21	4	0.86
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG22	4	0.86
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG23	4	0.86
(1,185)	1:1819:A:ALA:H	1:1820:A:ASN:H	3	0.86
(1,185)	1:1819:A:ALA:H	1:1820:A:ASN:H	10	0.86
(1,87)	1:1808:A:LEU:H	1:1808:A:LEU:HG	4	0.86
(1,75)	1:1840:A:VAL:HG11	1:1842:A:CYS:H	2	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:1840:A:VAL:HG12	1:1842:A:CYS:H	2	0.86
(1,75)	1:1840:A:VAL:HG13	1:1842:A:CYS:H	2	0.86
(1,27)	1:1865:A:PHE:H	1:1865:A:PHE:HB3	8	0.86
(1,24)	1:1865:A:PHE:HA	1:1865:A:PHE:HB3	1	0.86
(1,24)	1:1865:A:PHE:HA	1:1865:A:PHE:HB3	3	0.86
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	6	0.85
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	6	0.85
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	6	0.85
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	6	0.85
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	6	0.85
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	6	0.85
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD21	10	0.85
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD22	10	0.85
(1,444)	1:1824:A:ARG:H	1:1848:A:LEU:HD23	10	0.85
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG21	8	0.85
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG22	8	0.85
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG23	8	0.85
(1,431)	1:1824:A:ARG:H	1:1824:A:ARG:HB2	5	0.85
(1,328)	1:1791:A:TRP:HZ2	1:1822:A:SER:HB3	7	0.85
(1,87)	1:1808:A:LEU:H	1:1808:A:LEU:HG	2	0.85
(1,594)	1:1799:A:PHE:H	1:1799:A:PHE:HA	1	0.84
(1,564)	1:1840:A:VAL:HG11	1:1842:A:CYS:HB2	6	0.84
(1,564)	1:1840:A:VAL:HG12	1:1842:A:CYS:HB2	6	0.84
(1,564)	1:1840:A:VAL:HG13	1:1842:A:CYS:HB2	6	0.84
(1,549)	1:1833:A:ILE:H	1:1833:A:ILE:HG13	3	0.84
(1,548)	1:1820:A:ASN:H	1:1874:A:GLN:HB3	7	0.84
(1,407)	1:1815:A:PRO:HD3	1:1816:A:GLY:H	10	0.84
(1,374)	1:1808:A:LEU:HD21	1:1810:A:GLY:H	8	0.84
(1,374)	1:1808:A:LEU:HD22	1:1810:A:GLY:H	8	0.84
(1,374)	1:1808:A:LEU:HD23	1:1810:A:GLY:H	8	0.84
(1,333)	1:1805:A:ASP:H	1:1850:A:CYS:HB2	3	0.84
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	5	0.84
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	5	0.84
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD11	5	0.83
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD12	5	0.83
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD13	5	0.83
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD11	9	0.83
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD12	9	0.83
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD13	9	0.83
(1,646)	1:1840:A:VAL:HG21	1:1850:A:CYS:HB3	6	0.83
(1,646)	1:1840:A:VAL:HG22	1:1850:A:CYS:HB3	6	0.83
(1,646)	1:1840:A:VAL:HG23	1:1850:A:CYS:HB3	6	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:1799:A:PHE:H	1:1799:A:PHE:HA	3	0.83
(1,589)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	4	0.83
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	3	0.83
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	3	0.83
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	5	0.83
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	5	0.83
(1,354)	1:1812:A:VAL:H	1:1813:A:CYS:HA	9	0.83
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG21	6	0.83
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG22	6	0.83
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG23	6	0.83
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG21	6	0.83
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG22	6	0.83
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG23	6	0.83
(1,214)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	9	0.83
(1,214)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	9	0.83
(1,214)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	9	0.83
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	3	0.83
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	3	0.83
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD11	6	0.83
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD12	6	0.83
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD13	6	0.83
(1,27)	1:1865:A:PHE:H	1:1865:A:PHE:HB3	7	0.83
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	1	0.82
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	1	0.82
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	1	0.82
(1,657)	1:1848:A:LEU:HD21	1:1849:A:ILE:HA	5	0.82
(1,657)	1:1848:A:LEU:HD22	1:1849:A:ILE:HA	5	0.82
(1,657)	1:1848:A:LEU:HD23	1:1849:A:ILE:HA	5	0.82
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD11	2	0.82
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD12	2	0.82
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD13	2	0.82
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD11	8	0.82
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD12	8	0.82
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD13	8	0.82
(1,613)	1:1791:A:TRP:HA	1:1791:A:TRP:HE3	2	0.82
(1,594)	1:1799:A:PHE:H	1:1799:A:PHE:HA	6	0.82
(1,589)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	6	0.82
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG21	3	0.82
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG22	3	0.82
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG23	3	0.82
(1,421)	1:1819:A:ALA:H	1:1820:A:ASN:H	4	0.82
(1,412)	1:1816:A:GLY:H	1:1817:A:TRP:H	4	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:1815:A:PRO:HD3	1:1816:A:GLY:H	6	0.82
(1,386)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	6	0.82
(1,386)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	9	0.82
(1,263)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	6	0.82
(1,599)	1:1869:A:TYR:HB2	1:1870:A:GLU:H	3	0.81
(1,589)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	5	0.81
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	9	0.81
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	9	0.81
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	9	0.81
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	7	0.81
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	7	0.81
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	7	0.81
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG21	5	0.81
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG22	5	0.81
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG23	5	0.81
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG21	7	0.81
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG22	7	0.81
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG23	7	0.81
(1,407)	1:1815:A:PRO:HD3	1:1816:A:GLY:H	8	0.81
(1,354)	1:1812:A:VAL:H	1:1813:A:CYS:HA	1	0.81
(1,354)	1:1812:A:VAL:H	1:1813:A:CYS:HA	6	0.81
(1,45)	1:1789:A:THR:H	1:1789:A:THR:HG1	7	0.81
(1,27)	1:1865:A:PHE:H	1:1865:A:PHE:HB3	10	0.81
(1,662)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	1	0.8
(1,662)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	1	0.8
(1,662)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	1	0.8
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD21	10	0.8
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD22	10	0.8
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD23	10	0.8
(1,594)	1:1799:A:PHE:H	1:1799:A:PHE:HA	4	0.8
(1,594)	1:1799:A:PHE:H	1:1799:A:PHE:HA	5	0.8
(1,594)	1:1799:A:PHE:H	1:1799:A:PHE:HA	8	0.8
(1,589)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	2	0.8
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	10	0.8
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	10	0.8
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	10	0.8
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	10	0.8
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	10	0.8
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	10	0.8
(1,276)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	4	0.8
(1,726)	1:1874:A:GLN:H	1:1874:A:GLN:HB3	3	0.79
(1,615)	1:1812:A:VAL:H	1:1813:A:CYS:HA	3	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:1799:A:PHE:H	1:1799:A:PHE:HA	9	0.79
(1,421)	1:1819:A:ALA:H	1:1820:A:ASN:H	3	0.79
(1,421)	1:1819:A:ALA:H	1:1820:A:ASN:H	10	0.79
(1,407)	1:1815:A:PRO:HD3	1:1816:A:GLY:H	2	0.79
(1,407)	1:1815:A:PRO:HD3	1:1816:A:GLY:H	9	0.79
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD21	10	0.79
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD22	10	0.79
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD23	10	0.79
(1,357)	1:1809:A:ILE:H	1:1847:A:GLY:HA3	3	0.79
(1,87)	1:1808:A:LEU:H	1:1808:A:LEU:HG	5	0.79
(1,726)	1:1874:A:GLN:H	1:1874:A:GLN:HB3	10	0.78
(1,595)	1:1869:A:TYR:HA	1:1869:A:TYR:HB3	2	0.78
(1,219)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	7	0.78
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG11	2	0.78
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG12	2	0.78
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG13	2	0.78
(1,505)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	6	0.77
(1,424)	1:1820:A:ASN:H	1:1820:A:ASN:HB2	4	0.77
(1,386)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	1	0.77
(1,386)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	5	0.77
(1,354)	1:1812:A:VAL:H	1:1813:A:CYS:HA	7	0.77
(1,219)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	8	0.77
(1,219)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	9	0.77
(1,214)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	1	0.77
(1,214)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	1	0.77
(1,214)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	1	0.77
(1,192)	1:1789:A:THR:HG1	1:1873:A:VAL:H	9	0.77
(1,115)	1:1822:A:SER:H	1:1872:A:ASN:HB2	8	0.77
(1,573)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	9	0.76
(1,407)	1:1815:A:PRO:HD3	1:1816:A:GLY:H	7	0.76
(1,386)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	3	0.76
(1,357)	1:1809:A:ILE:H	1:1847:A:GLY:HA3	1	0.76
(1,333)	1:1805:A:ASP:H	1:1850:A:CYS:HB2	8	0.76
(1,290)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	8	0.76
(1,561)	1:1827:A:MET:HE1	1:1828:A:TYR:HE1	7	0.75
(1,561)	1:1827:A:MET:HE2	1:1828:A:TYR:HE1	7	0.75
(1,561)	1:1827:A:MET:HE3	1:1828:A:TYR:HE1	7	0.75
(1,561)	1:1827:A:MET:HE1	1:1828:A:TYR:HE2	7	0.75
(1,561)	1:1827:A:MET:HE2	1:1828:A:TYR:HE2	7	0.75
(1,561)	1:1827:A:MET:HE3	1:1828:A:TYR:HE2	7	0.75
(1,431)	1:1824:A:ARG:H	1:1824:A:ARG:HB2	2	0.75
(1,431)	1:1824:A:ARG:H	1:1824:A:ARG:HB2	3	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:1820:A:ASN:H	1:1820:A:ASN:HB2	8	0.75
(1,407)	1:1815:A:PRO:HD3	1:1816:A:GLY:H	5	0.75
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD11	1	0.75
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD12	1	0.75
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD13	1	0.75
(1,263)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	1	0.75
(1,263)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	2	0.75
(1,263)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	5	0.75
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG11	5	0.75
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG12	5	0.75
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG13	5	0.75
(1,662)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	10	0.74
(1,662)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	10	0.74
(1,662)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	10	0.74
(1,604)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD11	6	0.74
(1,604)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD12	6	0.74
(1,604)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD13	6	0.74
(1,604)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD11	6	0.74
(1,604)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD12	6	0.74
(1,604)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD13	6	0.74
(1,386)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	10	0.74
(1,219)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	4	0.74
(1,115)	1:1822:A:SER:H	1:1872:A:ASN:HB2	7	0.74
(1,29)	1:1789:A:THR:HG1	1:1873:A:VAL:H	9	0.74
(1,595)	1:1869:A:TYR:HA	1:1869:A:TYR:HB3	4	0.73
(1,561)	1:1827:A:MET:HE1	1:1828:A:TYR:HE1	10	0.73
(1,561)	1:1827:A:MET:HE2	1:1828:A:TYR:HE1	10	0.73
(1,561)	1:1827:A:MET:HE3	1:1828:A:TYR:HE1	10	0.73
(1,561)	1:1827:A:MET:HE1	1:1828:A:TYR:HE2	10	0.73
(1,561)	1:1827:A:MET:HE2	1:1828:A:TYR:HE2	10	0.73
(1,561)	1:1827:A:MET:HE3	1:1828:A:TYR:HE2	10	0.73
(1,219)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	6	0.73
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG11	8	0.73
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG12	8	0.73
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG13	8	0.73
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD11	3	0.73
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD12	3	0.73
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD13	3	0.73
(1,728)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	5	0.72
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD11	4	0.72
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD12	4	0.72
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD13	4	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD11	3	0.72
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD12	3	0.72
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD13	3	0.72
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD11	3	0.72
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD12	3	0.72
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD13	3	0.72
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD11	3	0.72
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD12	3	0.72
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD13	3	0.72
(1,615)	1:1812:A:VAL:H	1:1813:A:CYS:HA	10	0.72
(1,587)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	5	0.72
(1,494)	1:1842:A:CYS:HA	1:1843:A:ASP:HB3	3	0.72
(1,494)	1:1842:A:CYS:HA	1:1843:A:ASP:HB3	5	0.72
(1,227)	1:1873:A:VAL:HG21	1:1874:A:GLN:H	9	0.72
(1,227)	1:1873:A:VAL:HG22	1:1874:A:GLN:H	9	0.72
(1,227)	1:1873:A:VAL:HG23	1:1874:A:GLN:H	9	0.72
(1,219)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	5	0.72
(1,189)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	1	0.72
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	6	0.72
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	6	0.72
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	6	0.72
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	6	0.72
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	6	0.72
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	6	0.72
(1,75)	1:1840:A:VAL:HG11	1:1842:A:CYS:H	4	0.72
(1,75)	1:1840:A:VAL:HG12	1:1842:A:CYS:H	4	0.72
(1,75)	1:1840:A:VAL:HG13	1:1842:A:CYS:H	4	0.72
(1,686)	1:1827:A:MET:HE1	1:1828:A:TYR:HE1	7	0.71
(1,686)	1:1827:A:MET:HE2	1:1828:A:TYR:HE1	7	0.71
(1,686)	1:1827:A:MET:HE3	1:1828:A:TYR:HE1	7	0.71
(1,686)	1:1827:A:MET:HE1	1:1828:A:TYR:HE2	7	0.71
(1,686)	1:1827:A:MET:HE2	1:1828:A:TYR:HE2	7	0.71
(1,686)	1:1827:A:MET:HE3	1:1828:A:TYR:HE2	7	0.71
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	10	0.71
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	10	0.71
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	10	0.71
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	10	0.71
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	10	0.71
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	10	0.71
(1,611)	1:1850:A:CYS:HA	1:1851:A:LYS:H	6	0.71
(1,599)	1:1869:A:TYR:HB2	1:1870:A:GLU:H	9	0.71
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	1	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	1	0.71
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	6	0.71
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	6	0.71
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	6	0.71
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG21	2	0.71
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG22	2	0.71
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG23	2	0.71
(1,431)	1:1824:A:ARG:H	1:1824:A:ARG:HB2	1	0.71
(1,424)	1:1820:A:ASN:H	1:1820:A:ASN:HB2	1	0.71
(1,424)	1:1820:A:ASN:H	1:1820:A:ASN:HB2	3	0.71
(1,386)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	8	0.71
(1,219)	1:1817:A:TRP:HB2	1:1818:A:ALA:H	2	0.71
(1,214)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	10	0.71
(1,214)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	10	0.71
(1,214)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	10	0.71
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	1	0.71
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	1	0.71
(1,87)	1:1808:A:LEU:H	1:1808:A:LEU:HG	9	0.71
(1,87)	1:1808:A:LEU:H	1:1808:A:LEU:HG	10	0.71
(1,76)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	3	0.71
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG11	7	0.71
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG12	7	0.71
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG13	7	0.71
(1,728)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	3	0.7
(1,665)	1:1842:A:CYS:HB3	1:1848:A:LEU:HD21	10	0.7
(1,665)	1:1842:A:CYS:HB3	1:1848:A:LEU:HD22	10	0.7
(1,665)	1:1842:A:CYS:HB3	1:1848:A:LEU:HD23	10	0.7
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD11	7	0.7
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD12	7	0.7
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD13	7	0.7
(1,647)	1:1840:A:VAL:HG21	1:1850:A:CYS:HB2	4	0.7
(1,647)	1:1840:A:VAL:HG22	1:1850:A:CYS:HB2	4	0.7
(1,647)	1:1840:A:VAL:HG23	1:1850:A:CYS:HB2	4	0.7
(1,505)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	1	0.7
(1,374)	1:1808:A:LEU:HD21	1:1810:A:GLY:H	7	0.7
(1,374)	1:1808:A:LEU:HD22	1:1810:A:GLY:H	7	0.7
(1,374)	1:1808:A:LEU:HD23	1:1810:A:GLY:H	7	0.7
(1,357)	1:1809:A:ILE:H	1:1847:A:GLY:HA3	2	0.7
(1,321)	1:1792:A:LEU:HB2	1:1793:A:ASP:H	5	0.7
(1,263)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	4	0.7
(1,263)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	9	0.7
(1,247)	1:1869:A:TYR:H	1:1869:A:TYR:HB2	8	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:1808:A:LEU:H	1:1808:A:LEU:HG	8	0.7
(1,54)	1:1840:A:VAL:HG11	1:1842:A:CYS:HB2	10	0.7
(1,54)	1:1840:A:VAL:HG12	1:1842:A:CYS:HB2	10	0.7
(1,54)	1:1840:A:VAL:HG13	1:1842:A:CYS:HB2	10	0.7
(1,686)	1:1827:A:MET:HE1	1:1828:A:TYR:HE1	10	0.69
(1,686)	1:1827:A:MET:HE2	1:1828:A:TYR:HE1	10	0.69
(1,686)	1:1827:A:MET:HE3	1:1828:A:TYR:HE1	10	0.69
(1,686)	1:1827:A:MET:HE1	1:1828:A:TYR:HE2	10	0.69
(1,686)	1:1827:A:MET:HE2	1:1828:A:TYR:HE2	10	0.69
(1,686)	1:1827:A:MET:HE3	1:1828:A:TYR:HE2	10	0.69
(1,610)	1:1806:A:THR:HA	1:1807:A:GLU:H	1	0.69
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	2	0.69
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	2	0.69
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	2	0.69
(1,529)	1:1865:A:PHE:HB2	1:1866:A:CYS:H	4	0.69
(1,529)	1:1866:A:CYS:H	1:1866:A:CYS:HB2	4	0.69
(1,505)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	2	0.69
(1,505)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	5	0.69
(1,436)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	10	0.69
(1,402)	1:1871:A:ILE:H	1:1871:A:ILE:HA	1	0.69
(1,402)	1:1871:A:ILE:H	1:1871:A:ILE:HA	10	0.69
(1,386)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	2	0.69
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG21	3	0.69
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG22	3	0.69
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG23	3	0.69
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG21	3	0.69
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG22	3	0.69
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG23	3	0.69
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	8	0.69
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	8	0.69
(1,83)	1:1848:A:LEU:H	1:1848:A:LEU:HB2	7	0.69
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG11	4	0.69
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG12	4	0.69
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG13	4	0.69
(1,728)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	1	0.68
(1,697)	1:1789:A:THR:HG1	1:1789:A:THR:HG21	7	0.68
(1,697)	1:1789:A:THR:HG1	1:1789:A:THR:HG22	7	0.68
(1,697)	1:1789:A:THR:HG1	1:1789:A:THR:HG23	7	0.68
(1,662)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	7	0.68
(1,662)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	7	0.68
(1,662)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	7	0.68
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD21	9	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD22	9	0.68
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD23	9	0.68
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD21	9	0.68
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD22	9	0.68
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD23	9	0.68
(1,615)	1:1812:A:VAL:H	1:1813:A:CYS:HA	9	0.68
(1,595)	1:1869:A:TYR:HA	1:1869:A:TYR:HB3	3	0.68
(1,595)	1:1869:A:TYR:HA	1:1869:A:TYR:HB3	8	0.68
(1,595)	1:1869:A:TYR:HA	1:1869:A:TYR:HB3	10	0.68
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	8	0.68
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	8	0.68
(1,506)	1:1842:A:CYS:HA	1:1849:A:ILE:H	8	0.68
(1,357)	1:1809:A:ILE:H	1:1847:A:GLY:HA3	6	0.68
(1,263)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	7	0.68
(1,206)	1:1842:A:CYS:HA	1:1849:A:ILE:H	8	0.68
(1,189)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	3	0.68
(1,697)	1:1789:A:THR:HG1	1:1789:A:THR:HG21	9	0.67
(1,697)	1:1789:A:THR:HG1	1:1789:A:THR:HG22	9	0.67
(1,697)	1:1789:A:THR:HG1	1:1789:A:THR:HG23	9	0.67
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG11	5	0.67
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG12	5	0.67
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG13	5	0.67
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD11	6	0.67
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD12	6	0.67
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD13	6	0.67
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	7	0.67
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	7	0.67
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	7	0.67
(1,615)	1:1812:A:VAL:H	1:1813:A:CYS:HA	1	0.67
(1,611)	1:1850:A:CYS:HA	1:1851:A:LYS:H	9	0.67
(1,595)	1:1869:A:TYR:HA	1:1869:A:TYR:HB3	5	0.67
(1,595)	1:1869:A:TYR:HA	1:1869:A:TYR:HB3	6	0.67
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	7	0.67
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	7	0.67
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	9	0.67
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	9	0.67
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	9	0.67
(1,529)	1:1865:A:PHE:HB2	1:1866:A:CYS:H	3	0.67
(1,529)	1:1866:A:CYS:H	1:1866:A:CYS:HB2	3	0.67
(1,436)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	4	0.67
(1,321)	1:1792:A:LEU:HB2	1:1793:A:ASP:H	3	0.67
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG21	10	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG22	10	0.67
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG23	10	0.67
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG21	10	0.67
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG22	10	0.67
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG23	10	0.67
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	4	0.67
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	4	0.67
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	7	0.67
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	7	0.67
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB1	3	0.67
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB2	3	0.67
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB3	3	0.67
(1,113)	1:1822:A:SER:H	1:1822:A:SER:HB2	3	0.67
(1,24)	1:1865:A:PHE:HA	1:1865:A:PHE:HB3	10	0.67
(1,731)	1:1840:A:VAL:HG11	1:1848:A:LEU:HG	9	0.66
(1,731)	1:1840:A:VAL:HG12	1:1848:A:LEU:HG	9	0.66
(1,731)	1:1840:A:VAL:HG13	1:1848:A:LEU:HG	9	0.66
(1,728)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	2	0.66
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	10	0.66
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	10	0.66
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	10	0.66
(1,623)	1:1865:A:PHE:HD1	1:1866:A:CYS:H	10	0.66
(1,623)	1:1865:A:PHE:HD2	1:1866:A:CYS:H	10	0.66
(1,615)	1:1812:A:VAL:H	1:1813:A:CYS:HA	6	0.66
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	4	0.66
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	4	0.66
(1,494)	1:1842:A:CYS:HA	1:1843:A:ASP:HB3	8	0.66
(1,402)	1:1871:A:ILE:H	1:1871:A:ILE:HA	2	0.66
(1,356)	1:1809:A:ILE:H	1:1810:A:GLY:H	3	0.66
(1,356)	1:1809:A:ILE:H	1:1810:A:GLY:H	5	0.66
(1,356)	1:1809:A:ILE:H	1:1810:A:GLY:H	6	0.66
(1,229)	1:1799:A:PHE:H	1:1800:A:HIS:H	4	0.66
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	9	0.66
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	9	0.66
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB1	1	0.66
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB2	1	0.66
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB3	1	0.66
(1,86)	1:1812:A:VAL:HG11	1:1813:A:CYS:H	8	0.66
(1,86)	1:1812:A:VAL:HG12	1:1813:A:CYS:H	8	0.66
(1,86)	1:1812:A:VAL:HG13	1:1813:A:CYS:H	8	0.66
(1,24)	1:1865:A:PHE:HA	1:1865:A:PHE:HB3	7	0.66
(1,24)	1:1865:A:PHE:HA	1:1865:A:PHE:HB3	8	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	4	0.65
(1,670)	1:1823:A:CYS:HB3	1:1848:A:LEU:HD21	3	0.65
(1,670)	1:1823:A:CYS:HB3	1:1848:A:LEU:HD22	3	0.65
(1,670)	1:1823:A:CYS:HB3	1:1848:A:LEU:HD23	3	0.65
(1,611)	1:1850:A:CYS:HA	1:1851:A:LYS:H	8	0.65
(1,595)	1:1869:A:TYR:HA	1:1869:A:TYR:HB3	1	0.65
(1,587)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	2	0.65
(1,587)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	8	0.65
(1,587)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	9	0.65
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	9	0.65
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	9	0.65
(1,563)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD21	10	0.65
(1,563)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD22	10	0.65
(1,563)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD23	10	0.65
(1,505)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	9	0.65
(1,436)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	3	0.65
(1,436)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	5	0.65
(1,436)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	8	0.65
(1,431)	1:1824:A:ARG:H	1:1824:A:ARG:HB2	10	0.65
(1,424)	1:1820:A:ASN:H	1:1820:A:ASN:HB2	5	0.65
(1,402)	1:1871:A:ILE:H	1:1871:A:ILE:HA	9	0.65
(1,356)	1:1809:A:ILE:H	1:1810:A:GLY:H	1	0.65
(1,247)	1:1869:A:TYR:H	1:1869:A:TYR:HB2	5	0.65
(1,214)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	7	0.65
(1,214)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	7	0.65
(1,214)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	7	0.65
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG11	1	0.65
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG12	1	0.65
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG13	1	0.65
(1,18)	1:1817:A:TRP:HA	1:1817:A:TRP:HE3	3	0.65
(1,561)	1:1827:A:MET:HE1	1:1828:A:TYR:HE1	9	0.64
(1,561)	1:1827:A:MET:HE2	1:1828:A:TYR:HE1	9	0.64
(1,561)	1:1827:A:MET:HE3	1:1828:A:TYR:HE1	9	0.64
(1,561)	1:1827:A:MET:HE1	1:1828:A:TYR:HE2	9	0.64
(1,561)	1:1827:A:MET:HE2	1:1828:A:TYR:HE2	9	0.64
(1,561)	1:1827:A:MET:HE3	1:1828:A:TYR:HE2	9	0.64
(1,547)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	5	0.64
(1,534)	1:1850:A:CYS:HA	1:1850:A:CYS:HB2	7	0.64
(1,505)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	4	0.64
(1,494)	1:1842:A:CYS:HA	1:1843:A:ASP:HB3	2	0.64
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG21	9	0.64
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG22	9	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG23	9	0.64
(1,433)	1:1824:A:ARG:HB2	1:1825:A:ALA:H	9	0.64
(1,386)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	4	0.64
(1,263)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	10	0.64
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG21	2	0.64
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG22	2	0.64
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG23	2	0.64
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG21	2	0.64
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG22	2	0.64
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG23	2	0.64
(1,227)	1:1873:A:VAL:HG21	1:1874:A:GLN:H	2	0.64
(1,227)	1:1873:A:VAL:HG22	1:1874:A:GLN:H	2	0.64
(1,227)	1:1873:A:VAL:HG23	1:1874:A:GLN:H	2	0.64
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG11	8	0.63
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG12	8	0.63
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG13	8	0.63
(1,630)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD11	10	0.63
(1,630)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD12	10	0.63
(1,630)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD13	10	0.63
(1,630)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD11	10	0.63
(1,630)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD12	10	0.63
(1,630)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD13	10	0.63
(1,615)	1:1812:A:VAL:H	1:1813:A:CYS:HA	7	0.63
(1,587)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	7	0.63
(1,505)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	7	0.63
(1,494)	1:1842:A:CYS:HA	1:1843:A:ASP:HB3	4	0.63
(1,436)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	6	0.63
(1,436)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	7	0.63
(1,383)	1:1808:A:LEU:H	1:1808:A:LEU:HB2	4	0.63
(1,383)	1:1808:A:LEU:H	1:1808:A:LEU:HB2	9	0.63
(1,373)	1:1809:A:ILE:HD11	1:1810:A:GLY:H	2	0.63
(1,373)	1:1809:A:ILE:HD12	1:1810:A:GLY:H	2	0.63
(1,373)	1:1809:A:ILE:HD13	1:1810:A:GLY:H	2	0.63
(1,339)	1:1806:A:THR:H	1:1806:A:THR:HG21	7	0.63
(1,339)	1:1806:A:THR:H	1:1806:A:THR:HG22	7	0.63
(1,339)	1:1806:A:THR:H	1:1806:A:THR:HG23	7	0.63
(1,321)	1:1792:A:LEU:HB2	1:1793:A:ASP:H	4	0.63
(1,247)	1:1869:A:TYR:H	1:1869:A:TYR:HB2	10	0.63
(1,229)	1:1799:A:PHE:H	1:1800:A:HIS:H	8	0.63
(1,115)	1:1822:A:SER:H	1:1872:A:ASN:HB2	4	0.63
(1,83)	1:1848:A:LEU:H	1:1848:A:LEU:HB2	10	0.63
(1,611)	1:1850:A:CYS:HA	1:1851:A:LYS:H	2	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG21	2	0.62
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG22	2	0.62
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG23	2	0.62
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD21	7	0.62
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD22	7	0.62
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD23	7	0.62
(1,432)	1:1824:A:ARG:HB3	1:1825:A:ALA:H	1	0.62
(1,424)	1:1820:A:ASN:H	1:1820:A:ASN:HB2	2	0.62
(1,424)	1:1820:A:ASN:H	1:1820:A:ASN:HB2	7	0.62
(1,383)	1:1808:A:LEU:H	1:1808:A:LEU:HB2	5	0.62
(1,357)	1:1809:A:ILE:H	1:1847:A:GLY:HA3	5	0.62
(1,354)	1:1812:A:VAL:H	1:1813:A:CYS:HA	4	0.62
(1,333)	1:1805:A:ASP:H	1:1850:A:CYS:HB2	10	0.62
(1,283)	1:1871:A:ILE:H	1:1871:A:ILE:HG13	9	0.62
(1,83)	1:1848:A:LEU:H	1:1848:A:LEU:HB2	1	0.62
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG11	2	0.61
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG12	2	0.61
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG13	2	0.61
(1,610)	1:1806:A:THR:HA	1:1807:A:GLU:H	2	0.61
(1,573)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	7	0.61
(1,563)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD21	7	0.61
(1,563)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD22	7	0.61
(1,563)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD23	7	0.61
(1,547)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	3	0.61
(1,528)	1:1866:A:CYS:H	1:1866:A:CYS:HB3	10	0.61
(1,436)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	9	0.61
(1,424)	1:1820:A:ASN:H	1:1820:A:ASN:HB2	6	0.61
(1,402)	1:1871:A:ILE:H	1:1871:A:ILE:HA	6	0.61
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD11	7	0.61
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD12	7	0.61
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD13	7	0.61
(1,386)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	7	0.61
(1,383)	1:1808:A:LEU:H	1:1808:A:LEU:HB2	2	0.61
(1,263)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	3	0.61
(1,247)	1:1869:A:TYR:H	1:1869:A:TYR:HB2	6	0.61
(1,247)	1:1869:A:TYR:H	1:1869:A:TYR:HB2	7	0.61
(1,241)	1:1791:A:TRP:HH2	1:1822:A:SER:HB3	7	0.61
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB1	10	0.61
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB2	10	0.61
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB3	10	0.61
(1,115)	1:1822:A:SER:H	1:1872:A:ASN:HB2	6	0.61
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD11	1	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD12	1	0.61
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD13	1	0.61
(1,6)	1:1822:A:SER:H	1:1872:A:ASN:H	3	0.61
(1,686)	1:1827:A:MET:HE1	1:1828:A:TYR:HE1	9	0.6
(1,686)	1:1827:A:MET:HE2	1:1828:A:TYR:HE1	9	0.6
(1,686)	1:1827:A:MET:HE3	1:1828:A:TYR:HE1	9	0.6
(1,686)	1:1827:A:MET:HE1	1:1828:A:TYR:HE2	9	0.6
(1,686)	1:1827:A:MET:HE2	1:1828:A:TYR:HE2	9	0.6
(1,686)	1:1827:A:MET:HE3	1:1828:A:TYR:HE2	9	0.6
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG11	4	0.6
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG12	4	0.6
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG13	4	0.6
(1,610)	1:1806:A:THR:HA	1:1807:A:GLU:H	4	0.6
(1,610)	1:1806:A:THR:HA	1:1807:A:GLU:H	9	0.6
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	2	0.6
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	2	0.6
(1,547)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	1	0.6
(1,534)	1:1850:A:CYS:HA	1:1850:A:CYS:HB2	10	0.6
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	2	0.6
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	2	0.6
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD21	9	0.6
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD22	9	0.6
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD23	9	0.6
(1,407)	1:1815:A:PRO:HD3	1:1816:A:GLY:H	3	0.6
(1,383)	1:1808:A:LEU:H	1:1808:A:LEU:HB2	8	0.6
(1,328)	1:1791:A:TRP:HZ2	1:1822:A:SER:HB3	4	0.6
(1,227)	1:1873:A:VAL:HG21	1:1874:A:GLN:H	10	0.6
(1,227)	1:1873:A:VAL:HG22	1:1874:A:GLN:H	10	0.6
(1,227)	1:1873:A:VAL:HG23	1:1874:A:GLN:H	10	0.6
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	2	0.6
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	2	0.6
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG11	3	0.6
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG12	3	0.6
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG13	3	0.6
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG11	1	0.59
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG12	1	0.59
(1,678)	1:1807:A:GLU:H	1:1840:A:VAL:HG13	1	0.59
(1,623)	1:1865:A:PHE:HD1	1:1866:A:CYS:H	7	0.59
(1,623)	1:1865:A:PHE:HD2	1:1866:A:CYS:H	7	0.59
(1,612)	1:1824:A:ARG:HA	1:1825:A:ALA:H	2	0.59
(1,595)	1:1869:A:TYR:HA	1:1869:A:TYR:HB3	7	0.59
(1,564)	1:1840:A:VAL:HG11	1:1842:A:CYS:HB2	10	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,564)	1:1840:A:VAL:HG12	1:1842:A:CYS:HB2	10	0.59
(1,564)	1:1840:A:VAL:HG13	1:1842:A:CYS:HB2	10	0.59
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	4	0.59
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	4	0.59
(1,505)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	10	0.59
(1,494)	1:1842:A:CYS:HA	1:1843:A:ASP:HB3	1	0.59
(1,436)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	1	0.59
(1,436)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	2	0.59
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD11	9	0.59
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD12	9	0.59
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD13	9	0.59
(1,356)	1:1809:A:ILE:H	1:1810:A:GLY:H	9	0.59
(1,309)	1:1788:A:TRP:HB3	1:1790:A:GLY:H	3	0.59
(1,227)	1:1873:A:VAL:HG21	1:1874:A:GLN:H	6	0.59
(1,227)	1:1873:A:VAL:HG22	1:1874:A:GLN:H	6	0.59
(1,227)	1:1873:A:VAL:HG23	1:1874:A:GLN:H	6	0.59
(1,151)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	6	0.59
(1,151)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	9	0.59
(1,115)	1:1822:A:SER:H	1:1872:A:ASN:HB2	1	0.59
(1,86)	1:1812:A:VAL:HG11	1:1813:A:CYS:H	5	0.59
(1,86)	1:1812:A:VAL:HG12	1:1813:A:CYS:H	5	0.59
(1,86)	1:1812:A:VAL:HG13	1:1813:A:CYS:H	5	0.59
(1,76)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	4	0.59
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG11	1	0.59
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG12	1	0.59
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG13	1	0.59
(1,54)	1:1840:A:VAL:HG11	1:1842:A:CYS:HB2	7	0.59
(1,54)	1:1840:A:VAL:HG12	1:1842:A:CYS:HB2	7	0.59
(1,54)	1:1840:A:VAL:HG13	1:1842:A:CYS:HB2	7	0.59
(1,54)	1:1840:A:VAL:HG11	1:1842:A:CYS:HB2	9	0.59
(1,54)	1:1840:A:VAL:HG12	1:1842:A:CYS:HB2	9	0.59
(1,54)	1:1840:A:VAL:HG13	1:1842:A:CYS:HB2	9	0.59
(1,6)	1:1822:A:SER:H	1:1872:A:ASN:H	10	0.59
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD21	1	0.58
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD22	1	0.58
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD23	1	0.58
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD11	2	0.58
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD12	2	0.58
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD13	2	0.58
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	8	0.58
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	8	0.58
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	8	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	2	0.58
(1,528)	1:1866:A:CYS:H	1:1866:A:CYS:HB3	7	0.58
(1,402)	1:1871:A:ILE:H	1:1871:A:ILE:HA	4	0.58
(1,321)	1:1792:A:LEU:HB2	1:1793:A:ASP:H	6	0.58
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	10	0.58
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	10	0.58
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	10	0.58
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	10	0.58
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	10	0.58
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	10	0.58
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE1	1	0.58
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE2	1	0.58
(1,113)	1:1822:A:SER:H	1:1822:A:SER:HB2	5	0.58
(1,80)	1:1847:A:GLY:HA2	1:1848:A:LEU:H	8	0.58
(1,66)	1:1840:A:VAL:HG21	1:1850:A:CYS:HA	9	0.58
(1,66)	1:1840:A:VAL:HG22	1:1850:A:CYS:HA	9	0.58
(1,66)	1:1840:A:VAL:HG23	1:1850:A:CYS:HA	9	0.58
(1,6)	1:1822:A:SER:H	1:1872:A:ASN:H	5	0.58
(1,728)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	6	0.57
(1,672)	1:1874:A:GLN:HG2	1:1874:A:GLN:HG3	3	0.57
(1,610)	1:1806:A:THR:HA	1:1807:A:GLU:H	10	0.57
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	6	0.57
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	6	0.57
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	6	0.57
(1,547)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	4	0.57
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	1	0.57
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	1	0.57
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	3	0.57
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	3	0.57
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	5	0.57
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	5	0.57
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD21	4	0.57
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD22	4	0.57
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD23	4	0.57
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD21	1	0.57
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD22	1	0.57
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD23	1	0.57
(1,268)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	8	0.57
(1,252)	1:1877:A:GLU:H	1:1877:A:GLU:HG2	8	0.57
(1,80)	1:1847:A:GLY:HA2	1:1848:A:LEU:H	4	0.57
(1,18)	1:1817:A:TRP:HA	1:1817:A:TRP:HE3	1	0.57
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD11	4	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD12	4	0.56
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD13	4	0.56
(1,611)	1:1850:A:CYS:HA	1:1851:A:LYS:H	5	0.56
(1,587)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	4	0.56
(1,569)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	9	0.56
(1,531)	1:1817:A:TRP:HB3	1:1817:A:TRP:HD1	10	0.56
(1,529)	1:1865:A:PHE:HB2	1:1866:A:CYS:H	2	0.56
(1,529)	1:1866:A:CYS:H	1:1866:A:CYS:HB2	2	0.56
(1,529)	1:1865:A:PHE:HB2	1:1866:A:CYS:H	5	0.56
(1,529)	1:1866:A:CYS:H	1:1866:A:CYS:HB2	5	0.56
(1,529)	1:1865:A:PHE:HB2	1:1866:A:CYS:H	7	0.56
(1,529)	1:1866:A:CYS:H	1:1866:A:CYS:HB2	7	0.56
(1,528)	1:1866:A:CYS:H	1:1866:A:CYS:HB3	3	0.56
(1,492)	1:1842:A:CYS:HA	1:1847:A:GLY:HA2	10	0.56
(1,402)	1:1871:A:ILE:H	1:1871:A:ILE:HA	8	0.56
(1,383)	1:1808:A:LEU:H	1:1808:A:LEU:HB2	6	0.56
(1,376)	1:1812:A:VAL:H	1:1812:A:VAL:HG11	6	0.56
(1,376)	1:1812:A:VAL:H	1:1812:A:VAL:HG12	6	0.56
(1,376)	1:1812:A:VAL:H	1:1812:A:VAL:HG13	6	0.56
(1,333)	1:1805:A:ASP:H	1:1850:A:CYS:HB2	7	0.56
(1,309)	1:1788:A:TRP:HB3	1:1790:A:GLY:H	10	0.56
(1,276)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	6	0.56
(1,145)	1:1799:A:PHE:H	1:1800:A:HIS:H	4	0.56
(1,117)	1:1821:A:ILE:HG12	1:1822:A:SER:H	10	0.56
(1,86)	1:1812:A:VAL:HG11	1:1813:A:CYS:H	2	0.56
(1,86)	1:1812:A:VAL:HG12	1:1813:A:CYS:H	2	0.56
(1,86)	1:1812:A:VAL:HG13	1:1813:A:CYS:H	2	0.56
(1,80)	1:1847:A:GLY:HA2	1:1848:A:LEU:H	2	0.56
(1,76)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	2	0.56
(1,731)	1:1840:A:VAL:HG11	1:1848:A:LEU:HG	7	0.55
(1,731)	1:1840:A:VAL:HG12	1:1848:A:LEU:HG	7	0.55
(1,731)	1:1840:A:VAL:HG13	1:1848:A:LEU:HG	7	0.55
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD11	5	0.55
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD12	5	0.55
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD13	5	0.55
(1,610)	1:1806:A:THR:HA	1:1807:A:GLU:H	5	0.55
(1,610)	1:1806:A:THR:HA	1:1807:A:GLU:H	7	0.55
(1,600)	1:1869:A:TYR:HB3	1:1870:A:GLU:H	1	0.55
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	2	0.55
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	2	0.55
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	2	0.55
(1,505)	1:1842:A:CYS:HA	1:1848:A:LEU:HA	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:1842:A:CYS:HA	1:1847:A:GLY:HA2	4	0.55
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD21	8	0.55
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD22	8	0.55
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD23	8	0.55
(1,431)	1:1824:A:ARG:H	1:1824:A:ARG:HB2	6	0.55
(1,424)	1:1820:A:ASN:H	1:1820:A:ASN:HB2	9	0.55
(1,402)	1:1871:A:ILE:H	1:1871:A:ILE:HA	3	0.55
(1,402)	1:1871:A:ILE:H	1:1871:A:ILE:HA	7	0.55
(1,383)	1:1808:A:LEU:H	1:1808:A:LEU:HB2	3	0.55
(1,380)	1:1813:A:CYS:H	1:1813:A:CYS:HB3	9	0.55
(1,276)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	7	0.55
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG21	3	0.55
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG22	3	0.55
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG23	3	0.55
(1,229)	1:1799:A:PHE:H	1:1800:A:HIS:H	5	0.55
(1,223)	1:1829:A:PRO:HG2	1:1830:A:ASP:H	2	0.55
(1,115)	1:1822:A:SER:H	1:1872:A:ASN:HB2	2	0.55
(1,726)	1:1874:A:GLN:H	1:1874:A:GLN:HB3	6	0.54
(1,672)	1:1874:A:GLN:HG2	1:1874:A:GLN:HG3	5	0.54
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD21	9	0.54
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD22	9	0.54
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD23	9	0.54
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD11	3	0.54
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD12	3	0.54
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD13	3	0.54
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD21	6	0.54
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD22	6	0.54
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD23	6	0.54
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD21	6	0.54
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD22	6	0.54
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD23	6	0.54
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG21	8	0.54
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG22	8	0.54
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG23	8	0.54
(1,443)	1:1821:A:ILE:H	1:1821:A:ILE:HB	10	0.54
(1,376)	1:1812:A:VAL:H	1:1812:A:VAL:HG11	10	0.54
(1,376)	1:1812:A:VAL:H	1:1812:A:VAL:HG12	10	0.54
(1,376)	1:1812:A:VAL:H	1:1812:A:VAL:HG13	10	0.54
(1,366)	1:1809:A:ILE:H	1:1810:A:GLY:H	3	0.54
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE1	3	0.54
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE2	3	0.54
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE1	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE2	8	0.54
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE1	10	0.54
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE2	10	0.54
(1,151)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	1	0.54
(1,672)	1:1874:A:GLN:HG2	1:1874:A:GLN:HG3	1	0.53
(1,672)	1:1874:A:GLN:HG2	1:1874:A:GLN:HG3	8	0.53
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD21	7	0.53
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD22	7	0.53
(1,660)	1:1848:A:LEU:HA	1:1848:A:LEU:HD23	7	0.53
(1,611)	1:1850:A:CYS:HA	1:1851:A:LYS:H	1	0.53
(1,610)	1:1806:A:THR:HA	1:1807:A:GLU:H	6	0.53
(1,587)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	6	0.53
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD21	9	0.53
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD22	9	0.53
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD23	9	0.53
(1,366)	1:1809:A:ILE:H	1:1810:A:GLY:H	1	0.53
(1,366)	1:1809:A:ILE:H	1:1810:A:GLY:H	5	0.53
(1,366)	1:1809:A:ILE:H	1:1810:A:GLY:H	6	0.53
(1,361)	1:1808:A:LEU:HB3	1:1809:A:ILE:H	7	0.53
(1,356)	1:1809:A:ILE:H	1:1810:A:GLY:H	10	0.53
(1,276)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	5	0.53
(1,247)	1:1869:A:TYR:H	1:1869:A:TYR:HB2	1	0.53
(1,241)	1:1791:A:TRP:HH2	1:1822:A:SER:HB3	3	0.53
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE1	6	0.53
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE2	6	0.53
(1,151)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	3	0.53
(1,151)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	5	0.53
(1,145)	1:1799:A:PHE:H	1:1800:A:HIS:H	8	0.53
(1,113)	1:1822:A:SER:H	1:1822:A:SER:HB2	6	0.53
(1,80)	1:1847:A:GLY:HA2	1:1848:A:LEU:H	7	0.53
(1,27)	1:1865:A:PHE:H	1:1865:A:PHE:HB3	1	0.53
(1,731)	1:1840:A:VAL:HG11	1:1848:A:LEU:HG	10	0.52
(1,731)	1:1840:A:VAL:HG12	1:1848:A:LEU:HG	10	0.52
(1,731)	1:1840:A:VAL:HG13	1:1848:A:LEU:HG	10	0.52
(1,672)	1:1874:A:GLN:HG2	1:1874:A:GLN:HG3	7	0.52
(1,618)	1:1851:A:LYS:HA	1:1852:A:ASN:H	5	0.52
(1,611)	1:1850:A:CYS:HA	1:1851:A:LYS:H	7	0.52
(1,610)	1:1806:A:THR:HA	1:1807:A:GLU:H	3	0.52
(1,462)	1:1835:A:GLN:H	1:1835:A:GLN:HB3	5	0.52
(1,402)	1:1871:A:ILE:H	1:1871:A:ILE:HA	5	0.52
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD21	7	0.52
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD22	7	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:1848:A:LEU:HA	1:1848:A:LEU:HD23	7	0.52
(1,376)	1:1812:A:VAL:H	1:1812:A:VAL:HG11	4	0.52
(1,376)	1:1812:A:VAL:H	1:1812:A:VAL:HG12	4	0.52
(1,376)	1:1812:A:VAL:H	1:1812:A:VAL:HG13	4	0.52
(1,309)	1:1788:A:TRP:HB3	1:1790:A:GLY:H	5	0.52
(1,241)	1:1791:A:TRP:HH2	1:1822:A:SER:HB3	2	0.52
(1,200)	1:1821:A:ILE:H	1:1822:A:SER:H	5	0.52
(1,200)	1:1821:A:ILE:H	1:1822:A:SER:H	10	0.52
(1,192)	1:1789:A:THR:HG1	1:1873:A:VAL:H	7	0.52
(1,189)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	9	0.52
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE1	4	0.52
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE2	4	0.52
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE1	9	0.52
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE2	9	0.52
(1,728)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	9	0.51
(1,672)	1:1874:A:GLN:HG2	1:1874:A:GLN:HG3	2	0.51
(1,672)	1:1874:A:GLN:HG2	1:1874:A:GLN:HG3	6	0.51
(1,672)	1:1874:A:GLN:HG2	1:1874:A:GLN:HG3	9	0.51
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD11	10	0.51
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD12	10	0.51
(1,655)	1:1836:A:LEU:HA	1:1836:A:LEU:HD13	10	0.51
(1,610)	1:1806:A:THR:HA	1:1807:A:GLU:H	8	0.51
(1,600)	1:1869:A:TYR:HB3	1:1870:A:GLU:H	2	0.51
(1,573)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	6	0.51
(1,569)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	10	0.51
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG21	8	0.51
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG22	8	0.51
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG23	8	0.51
(1,472)	1:1836:A:LEU:H	1:1836:A:LEU:HG	5	0.51
(1,356)	1:1809:A:ILE:H	1:1810:A:GLY:H	4	0.51
(1,329)	1:1800:A:HIS:H	1:1800:A:HIS:HB2	2	0.51
(1,309)	1:1788:A:TRP:HB3	1:1790:A:GLY:H	4	0.51
(1,283)	1:1871:A:ILE:H	1:1871:A:ILE:HG13	3	0.51
(1,241)	1:1791:A:TRP:HH2	1:1822:A:SER:HB3	10	0.51
(1,223)	1:1829:A:PRO:HG2	1:1830:A:ASP:H	7	0.51
(1,189)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	2	0.51
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD11	7	0.51
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD12	7	0.51
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD13	7	0.51
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD11	7	0.51
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD12	7	0.51
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD13	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD21	9	0.51
(1,174)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD22	9	0.51
(1,174)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD23	9	0.51
(1,174)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD21	9	0.51
(1,174)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD22	9	0.51
(1,174)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD23	9	0.51
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE1	7	0.51
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE2	7	0.51
(1,151)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	10	0.51
(1,4)	1:1794:A:SER:H	1:1795:A:GLY:H	3	0.51
(1,672)	1:1874:A:GLN:HG2	1:1874:A:GLN:HG3	4	0.5
(1,618)	1:1851:A:LYS:HA	1:1852:A:ASN:H	3	0.5
(1,618)	1:1851:A:LYS:HA	1:1852:A:ASN:H	4	0.5
(1,618)	1:1851:A:LYS:HA	1:1852:A:ASN:H	8	0.5
(1,612)	1:1824:A:ARG:HA	1:1825:A:ALA:H	5	0.5
(1,611)	1:1850:A:CYS:HA	1:1851:A:LYS:H	4	0.5
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG21	5	0.5
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG22	5	0.5
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG23	5	0.5
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD11	10	0.5
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD12	10	0.5
(1,395)	1:1848:A:LEU:HA	1:1848:A:LEU:HD13	10	0.5
(1,328)	1:1791:A:TRP:HZ2	1:1822:A:SER:HB3	1	0.5
(1,328)	1:1791:A:TRP:HZ2	1:1822:A:SER:HB3	8	0.5
(1,309)	1:1788:A:TRP:HB3	1:1790:A:GLY:H	6	0.5
(1,309)	1:1788:A:TRP:HB3	1:1790:A:GLY:H	7	0.5
(1,283)	1:1871:A:ILE:H	1:1871:A:ILE:HG13	7	0.5
(1,183)	1:1817:A:TRP:HD1	1:1818:A:ALA:H	8	0.5
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE1	5	0.5
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE2	5	0.5
(1,113)	1:1822:A:SER:H	1:1822:A:SER:HB2	2	0.5
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD11	8	0.49
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD12	8	0.49
(1,659)	1:1842:A:CYS:HA	1:1848:A:LEU:HD13	8	0.49
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD21	8	0.49
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD22	8	0.49
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD23	8	0.49
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD21	8	0.49
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD22	8	0.49
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD23	8	0.49
(1,629)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD11	7	0.49
(1,629)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD12	7	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,629)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD13	7	0.49
(1,629)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD11	7	0.49
(1,629)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD12	7	0.49
(1,629)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD13	7	0.49
(1,612)	1:1824:A:ARG:HA	1:1825:A:ALA:H	4	0.49
(1,572)	1:1842:A:CYS:HA	1:1842:A:CYS:HB3	5	0.49
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	4	0.49
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	4	0.49
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	4	0.49
(1,547)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	6	0.49
(1,514)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	9	0.49
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG21	10	0.49
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG22	10	0.49
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG23	10	0.49
(1,426)	1:1819:A:ALA:HB1	1:1820:A:ASN:H	3	0.49
(1,426)	1:1819:A:ALA:HB2	1:1820:A:ASN:H	3	0.49
(1,426)	1:1819:A:ALA:HB3	1:1820:A:ASN:H	3	0.49
(1,407)	1:1815:A:PRO:HD3	1:1816:A:GLY:H	1	0.49
(1,380)	1:1813:A:CYS:H	1:1813:A:CYS:HB3	7	0.49
(1,268)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	4	0.49
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG21	9	0.49
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG22	9	0.49
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG23	9	0.49
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG21	9	0.49
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG22	9	0.49
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG23	9	0.49
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD11	6	0.49
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD12	6	0.49
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD13	6	0.49
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD11	6	0.49
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD12	6	0.49
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD13	6	0.49
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE1	2	0.49
(1,171)	1:1828:A:TYR:HB3	1:1828:A:TYR:HE2	2	0.49
(1,113)	1:1822:A:SER:H	1:1822:A:SER:HB2	1	0.49
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG21	10	0.49
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG22	10	0.49
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG23	10	0.49
(1,29)	1:1789:A:THR:HG1	1:1873:A:VAL:H	7	0.49
(1,27)	1:1865:A:PHE:H	1:1865:A:PHE:HB3	9	0.49
(1,10)	1:1872:A:ASN:H	1:1872:A:ASN:HB2	5	0.49
(1,728)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:1812:A:VAL:H	1:1813:A:CYS:HA	4	0.48
(1,600)	1:1869:A:TYR:HB3	1:1870:A:GLU:H	4	0.48
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD11	6	0.48
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD12	6	0.48
(1,565)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD13	6	0.48
(1,564)	1:1840:A:VAL:HG11	1:1842:A:CYS:HB2	7	0.48
(1,564)	1:1840:A:VAL:HG12	1:1842:A:CYS:HB2	7	0.48
(1,564)	1:1840:A:VAL:HG13	1:1842:A:CYS:HB2	7	0.48
(1,564)	1:1840:A:VAL:HG11	1:1842:A:CYS:HB2	9	0.48
(1,564)	1:1840:A:VAL:HG12	1:1842:A:CYS:HB2	9	0.48
(1,564)	1:1840:A:VAL:HG13	1:1842:A:CYS:HB2	9	0.48
(1,561)	1:1827:A:MET:HE1	1:1828:A:TYR:HE1	8	0.48
(1,561)	1:1827:A:MET:HE2	1:1828:A:TYR:HE1	8	0.48
(1,561)	1:1827:A:MET:HE3	1:1828:A:TYR:HE1	8	0.48
(1,561)	1:1827:A:MET:HE1	1:1828:A:TYR:HE2	8	0.48
(1,561)	1:1827:A:MET:HE2	1:1828:A:TYR:HE2	8	0.48
(1,561)	1:1827:A:MET:HE3	1:1828:A:TYR:HE2	8	0.48
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	7	0.48
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	7	0.48
(1,560)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	7	0.48
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	6	0.48
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	6	0.48
(1,514)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	7	0.48
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD21	2	0.48
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD22	2	0.48
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD23	2	0.48
(1,426)	1:1819:A:ALA:HB1	1:1820:A:ASN:H	10	0.48
(1,426)	1:1819:A:ALA:HB2	1:1820:A:ASN:H	10	0.48
(1,426)	1:1819:A:ALA:HB3	1:1820:A:ASN:H	10	0.48
(1,383)	1:1808:A:LEU:H	1:1808:A:LEU:HB2	1	0.48
(1,328)	1:1791:A:TRP:HZ2	1:1822:A:SER:HB3	10	0.48
(1,309)	1:1788:A:TRP:HB3	1:1790:A:GLY:H	1	0.48
(1,309)	1:1788:A:TRP:HB3	1:1790:A:GLY:H	9	0.48
(1,276)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	2	0.48
(1,276)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	9	0.48
(1,189)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	7	0.48
(1,189)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	10	0.48
(1,81)	1:1805:A:ASP:H	1:1850:A:CYS:H	6	0.48
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG11	6	0.48
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG12	6	0.48
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG13	6	0.48
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG11	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG12	10	0.48
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG13	10	0.48
(1,7)	1:1791:A:TRP:HZ3	1:1872:A:ASN:H	5	0.48
(1,4)	1:1794:A:SER:H	1:1795:A:GLY:H	1	0.48
(1,4)	1:1794:A:SER:H	1:1795:A:GLY:H	8	0.48
(1,728)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	7	0.47
(1,611)	1:1850:A:CYS:HA	1:1851:A:LYS:H	3	0.47
(1,608)	1:1848:A:LEU:HD21	1:1869:A:TYR:HB2	5	0.47
(1,608)	1:1848:A:LEU:HD22	1:1869:A:TYR:HB2	5	0.47
(1,608)	1:1848:A:LEU:HD23	1:1869:A:TYR:HB2	5	0.47
(1,608)	1:1848:A:LEU:HD21	1:1869:A:TYR:HB2	8	0.47
(1,608)	1:1848:A:LEU:HD22	1:1869:A:TYR:HB2	8	0.47
(1,608)	1:1848:A:LEU:HD23	1:1869:A:TYR:HB2	8	0.47
(1,600)	1:1869:A:TYR:HB3	1:1870:A:GLU:H	7	0.47
(1,151)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	8	0.47
(1,83)	1:1848:A:LEU:H	1:1848:A:LEU:HB2	9	0.47
(1,726)	1:1874:A:GLN:H	1:1874:A:GLN:HB3	2	0.46
(1,726)	1:1874:A:GLN:H	1:1874:A:GLN:HB3	9	0.46
(1,647)	1:1840:A:VAL:HG21	1:1850:A:CYS:HB2	1	0.46
(1,647)	1:1840:A:VAL:HG22	1:1850:A:CYS:HB2	1	0.46
(1,647)	1:1840:A:VAL:HG23	1:1850:A:CYS:HB2	1	0.46
(1,531)	1:1817:A:TRP:HB3	1:1817:A:TRP:HD1	1	0.46
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG21	6	0.46
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG22	6	0.46
(1,440)	1:1828:A:TYR:HB2	1:1831:A:VAL:HG23	6	0.46
(1,426)	1:1819:A:ALA:HB1	1:1820:A:ASN:H	1	0.46
(1,426)	1:1819:A:ALA:HB2	1:1820:A:ASN:H	1	0.46
(1,426)	1:1819:A:ALA:HB3	1:1820:A:ASN:H	1	0.46
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG21	1	0.46
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG22	1	0.46
(1,391)	1:1823:A:CYS:HA	1:1873:A:VAL:HG23	1	0.46
(1,366)	1:1809:A:ILE:H	1:1810:A:GLY:H	9	0.46
(1,309)	1:1788:A:TRP:HB3	1:1790:A:GLY:H	8	0.46
(1,279)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	8	0.46
(1,276)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	1	0.46
(1,275)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	4	0.46
(1,210)	1:1840:A:VAL:HB	1:1841:A:VAL:H	9	0.46
(1,151)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	2	0.46
(1,113)	1:1822:A:SER:H	1:1822:A:SER:HB2	9	0.46
(1,86)	1:1812:A:VAL:HG11	1:1813:A:CYS:H	1	0.46
(1,86)	1:1812:A:VAL:HG12	1:1813:A:CYS:H	1	0.46
(1,86)	1:1812:A:VAL:HG13	1:1813:A:CYS:H	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:1812:A:VAL:HG11	1:1813:A:CYS:H	3	0.46
(1,86)	1:1812:A:VAL:HG12	1:1813:A:CYS:H	3	0.46
(1,86)	1:1812:A:VAL:HG13	1:1813:A:CYS:H	3	0.46
(1,80)	1:1847:A:GLY:HA2	1:1848:A:LEU:H	3	0.46
(1,80)	1:1847:A:GLY:HA2	1:1848:A:LEU:H	5	0.46
(1,80)	1:1847:A:GLY:HA2	1:1848:A:LEU:H	10	0.46
(1,76)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	9	0.46
(1,6)	1:1822:A:SER:H	1:1872:A:ASN:H	2	0.46
(1,608)	1:1848:A:LEU:HD21	1:1869:A:TYR:HB2	4	0.45
(1,608)	1:1848:A:LEU:HD22	1:1869:A:TYR:HB2	4	0.45
(1,608)	1:1848:A:LEU:HD23	1:1869:A:TYR:HB2	4	0.45
(1,531)	1:1817:A:TRP:HB3	1:1817:A:TRP:HD1	3	0.45
(1,529)	1:1865:A:PHE:HB2	1:1866:A:CYS:H	10	0.45
(1,529)	1:1866:A:CYS:H	1:1866:A:CYS:HB2	10	0.45
(1,492)	1:1842:A:CYS:HA	1:1847:A:GLY:HA2	7	0.45
(1,383)	1:1808:A:LEU:H	1:1808:A:LEU:HB2	7	0.45
(1,333)	1:1805:A:ASP:H	1:1850:A:CYS:HB2	6	0.45
(1,329)	1:1800:A:HIS:H	1:1800:A:HIS:HB2	10	0.45
(1,328)	1:1791:A:TRP:HZ2	1:1822:A:SER:HB3	3	0.45
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG21	8	0.45
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG22	8	0.45
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG23	8	0.45
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG21	8	0.45
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG22	8	0.45
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG23	8	0.45
(1,200)	1:1821:A:ILE:H	1:1822:A:SER:H	9	0.45
(1,189)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	6	0.45
(1,145)	1:1799:A:PHE:H	1:1800:A:HIS:H	5	0.45
(1,106)	1:1820:A:ASN:HB3	1:1821:A:ILE:H	5	0.45
(1,54)	1:1840:A:VAL:HG11	1:1842:A:CYS:HB2	3	0.45
(1,54)	1:1840:A:VAL:HG12	1:1842:A:CYS:HB2	3	0.45
(1,54)	1:1840:A:VAL:HG13	1:1842:A:CYS:HB2	3	0.45
(1,27)	1:1865:A:PHE:H	1:1865:A:PHE:HB3	4	0.45
(1,728)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	8	0.44
(1,686)	1:1827:A:MET:HE1	1:1828:A:TYR:HE1	8	0.44
(1,686)	1:1827:A:MET:HE2	1:1828:A:TYR:HE1	8	0.44
(1,686)	1:1827:A:MET:HE3	1:1828:A:TYR:HE1	8	0.44
(1,686)	1:1827:A:MET:HE1	1:1828:A:TYR:HE2	8	0.44
(1,686)	1:1827:A:MET:HE2	1:1828:A:TYR:HE2	8	0.44
(1,686)	1:1827:A:MET:HE3	1:1828:A:TYR:HE2	8	0.44
(1,612)	1:1824:A:ARG:HA	1:1825:A:ALA:H	9	0.44
(1,529)	1:1865:A:PHE:HB2	1:1866:A:CYS:H	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,529)	1:1866:A:CYS:H	1:1866:A:CYS:HB2	8	0.44
(1,506)	1:1842:A:CYS:HA	1:1849:A:ILE:H	5	0.44
(1,356)	1:1809:A:ILE:H	1:1810:A:GLY:H	7	0.44
(1,279)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	4	0.44
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG21	5	0.44
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG22	5	0.44
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG23	5	0.44
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG21	8	0.44
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG22	8	0.44
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG23	8	0.44
(1,241)	1:1791:A:TRP:HH2	1:1822:A:SER:HB3	8	0.44
(1,206)	1:1842:A:CYS:HA	1:1849:A:ILE:H	5	0.44
(1,200)	1:1821:A:ILE:H	1:1822:A:SER:H	2	0.44
(1,200)	1:1821:A:ILE:H	1:1822:A:SER:H	3	0.44
(1,189)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	4	0.44
(1,88)	1:1787:A:ASN:H	1:1875:A:CYS:H	10	0.44
(1,80)	1:1847:A:GLY:HA2	1:1848:A:LEU:H	6	0.44
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG11	9	0.44
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG12	9	0.44
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG13	9	0.44
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG11	3	0.44
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG12	3	0.44
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG13	3	0.44
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG11	9	0.44
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG12	9	0.44
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG13	9	0.44
(1,701)	1:1870:A:GLU:HA	1:1870:A:GLU:HB2	5	0.43
(1,563)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD21	9	0.43
(1,563)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD22	9	0.43
(1,563)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD23	9	0.43
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	8	0.43
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	8	0.43
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	8	0.43
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG21	1	0.43
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG22	1	0.43
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG23	1	0.43
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG21	3	0.43
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG22	3	0.43
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG23	3	0.43
(1,365)	1:1810:A:GLY:H	1:1810:A:GLY:HA3	3	0.43
(1,275)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	5	0.43
(1,264)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,189)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	5	0.43
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	10	0.43
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	10	0.43
(1,115)	1:1822:A:SER:H	1:1872:A:ASN:HB2	9	0.43
(1,49)	1:1789:A:THR:H	1:1874:A:GLN:HA	8	0.43
(1,46)	1:1788:A:TRP:HA	1:1789:A:THR:H	3	0.43
(1,27)	1:1865:A:PHE:H	1:1865:A:PHE:HB3	3	0.43
(1,16)	1:1817:A:TRP:HB2	1:1817:A:TRP:HE3	6	0.43
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD11	3	0.42
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD12	3	0.42
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD13	3	0.42
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD11	6	0.42
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD12	6	0.42
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD13	6	0.42
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD11	1	0.42
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD12	1	0.42
(1,654)	1:1831:A:VAL:HG21	1:1836:A:LEU:HD13	1	0.42
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD11	1	0.42
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD12	1	0.42
(1,654)	1:1831:A:VAL:HG22	1:1836:A:LEU:HD13	1	0.42
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD11	1	0.42
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD12	1	0.42
(1,654)	1:1831:A:VAL:HG23	1:1836:A:LEU:HD13	1	0.42
(1,645)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	4	0.42
(1,645)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	7	0.42
(1,645)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	9	0.42
(1,618)	1:1851:A:LYS:HA	1:1852:A:ASN:H	9	0.42
(1,611)	1:1850:A:CYS:HA	1:1851:A:LYS:H	10	0.42
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	10	0.42
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	10	0.42
(1,547)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	9	0.42
(1,534)	1:1850:A:CYS:HA	1:1850:A:CYS:HB2	6	0.42
(1,526)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	4	0.42
(1,526)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	7	0.42
(1,526)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	9	0.42
(1,516)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	4	0.42
(1,472)	1:1836:A:LEU:H	1:1836:A:LEU:HG	10	0.42
(1,383)	1:1808:A:LEU:H	1:1808:A:LEU:HB2	10	0.42
(1,352)	1:1812:A:VAL:H	1:1813:A:CYS:H	7	0.42
(1,333)	1:1805:A:ASP:H	1:1850:A:CYS:HB2	2	0.42
(1,309)	1:1788:A:TRP:HB3	1:1790:A:GLY:H	2	0.42
(1,300)	1:1788:A:TRP:HA	1:1789:A:THR:H	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:1787:A:ASN:HA	1:1788:A:TRP:H	4	0.42
(1,246)	1:1869:A:TYR:H	1:1869:A:TYR:HA	9	0.42
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD21	9	0.42
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD22	9	0.42
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD23	9	0.42
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD21	9	0.42
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD22	9	0.42
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD23	9	0.42
(1,229)	1:1799:A:PHE:H	1:1800:A:HIS:H	9	0.42
(1,118)	1:1822:A:SER:H	1:1873:A:VAL:HG11	1	0.42
(1,118)	1:1822:A:SER:H	1:1873:A:VAL:HG12	1	0.42
(1,118)	1:1822:A:SER:H	1:1873:A:VAL:HG13	1	0.42
(1,6)	1:1822:A:SER:H	1:1872:A:ASN:H	9	0.42
(1,5)	1:1822:A:SER:H	1:1872:A:ASN:H	3	0.42
(1,701)	1:1870:A:GLU:HA	1:1870:A:GLU:HB2	6	0.41
(1,645)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	1	0.41
(1,645)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	6	0.41
(1,618)	1:1851:A:LYS:HA	1:1852:A:ASN:H	2	0.41
(1,608)	1:1848:A:LEU:HD21	1:1869:A:TYR:HB2	9	0.41
(1,608)	1:1848:A:LEU:HD22	1:1869:A:TYR:HB2	9	0.41
(1,608)	1:1848:A:LEU:HD23	1:1869:A:TYR:HB2	9	0.41
(1,604)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD11	10	0.41
(1,604)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD12	10	0.41
(1,604)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD13	10	0.41
(1,604)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD11	10	0.41
(1,604)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD12	10	0.41
(1,604)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD13	10	0.41
(1,600)	1:1869:A:TYR:HB3	1:1870:A:GLU:H	6	0.41
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG21	5	0.41
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG22	5	0.41
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG23	5	0.41
(1,526)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	1	0.41
(1,511)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	9	0.41
(1,464)	1:1832:A:PRO:HB2	1:1835:A:GLN:H	7	0.41
(1,356)	1:1809:A:ILE:H	1:1810:A:GLY:H	2	0.41
(1,275)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	1	0.41
(1,264)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	4	0.41
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG21	7	0.41
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG22	7	0.41
(1,240)	1:1828:A:TYR:HE1	1:1831:A:VAL:HG23	7	0.41
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG21	7	0.41
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG22	7	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,240)	1:1828:A:TYR:HE2	1:1831:A:VAL:HG23	7	0.41
(1,200)	1:1821:A:ILE:H	1:1822:A:SER:H	6	0.41
(1,183)	1:1817:A:TRP:HD1	1:1818:A:ALA:H	5	0.41
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD11	8	0.41
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD12	8	0.41
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD13	8	0.41
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD11	8	0.41
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD12	8	0.41
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD13	8	0.41
(1,151)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	4	0.41
(1,113)	1:1822:A:SER:H	1:1822:A:SER:HB2	4	0.41
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG21	8	0.41
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG22	8	0.41
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG23	8	0.41
(1,46)	1:1788:A:TRP:HA	1:1789:A:THR:H	5	0.41
(1,43)	1:1791:A:TRP:HE3	1:1872:A:ASN:HB3	2	0.41
(1,16)	1:1817:A:TRP:HB2	1:1817:A:TRP:HE3	4	0.41
(1,7)	1:1791:A:TRP:HZ3	1:1872:A:ASN:H	8	0.41
(1,6)	1:1822:A:SER:H	1:1872:A:ASN:H	1	0.41
(1,4)	1:1794:A:SER:H	1:1795:A:GLY:H	4	0.41
(1,4)	1:1794:A:SER:H	1:1795:A:GLY:H	6	0.41
(1,726)	1:1874:A:GLN:H	1:1874:A:GLN:HB3	7	0.4
(1,672)	1:1874:A:GLN:HG2	1:1874:A:GLN:HG3	10	0.4
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD11	2	0.4
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD12	2	0.4
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD13	2	0.4
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD11	4	0.4
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD12	4	0.4
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD13	4	0.4
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD11	8	0.4
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD12	8	0.4
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD13	8	0.4
(1,651)	1:1836:A:LEU:HB3	1:1836:A:LEU:HD11	6	0.4
(1,651)	1:1836:A:LEU:HB3	1:1836:A:LEU:HD12	6	0.4
(1,651)	1:1836:A:LEU:HB3	1:1836:A:LEU:HD13	6	0.4
(1,645)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	5	0.4
(1,645)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	10	0.4
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB2	4	0.4
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB3	4	0.4
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB2	6	0.4
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB3	6	0.4
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	7	0.4
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	7	0.4
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	7	0.4
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	7	0.4
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	7	0.4
(1,618)	1:1851:A:LYS:HA	1:1852:A:ASN:H	10	0.4
(1,600)	1:1869:A:TYR:HB3	1:1870:A:GLU:H	8	0.4
(1,596)	1:1869:A:TYR:HA	1:1869:A:TYR:HB2	3	0.4
(1,592)	1:1799:A:PHE:H	1:1799:A:PHE:HB2	6	0.4
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	6	0.4
(1,583)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	6	0.4
(1,572)	1:1842:A:CYS:HA	1:1842:A:CYS:HB3	1	0.4
(1,572)	1:1842:A:CYS:HA	1:1842:A:CYS:HB3	8	0.4
(1,547)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	10	0.4
(1,534)	1:1850:A:CYS:HA	1:1850:A:CYS:HB2	9	0.4
(1,526)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	5	0.4
(1,526)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	6	0.4
(1,526)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	10	0.4
(1,517)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	2	0.4
(1,516)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	5	0.4
(1,511)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	7	0.4
(1,506)	1:1842:A:CYS:HA	1:1849:A:ILE:H	6	0.4
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG11	9	0.4
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG12	9	0.4
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG13	9	0.4
(1,467)	1:1834:A:GLY:HA3	1:1835:A:GLN:H	7	0.4
(1,366)	1:1809:A:ILE:H	1:1810:A:GLY:H	10	0.4
(1,300)	1:1788:A:TRP:HA	1:1789:A:THR:H	5	0.4
(1,292)	1:1787:A:ASN:HA	1:1788:A:TRP:H	10	0.4
(1,279)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	2	0.4
(1,279)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	10	0.4
(1,275)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	2	0.4
(1,275)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	3	0.4
(1,252)	1:1877:A:GLU:H	1:1877:A:GLU:HG2	3	0.4
(1,252)	1:1877:A:GLU:H	1:1877:A:GLU:HG2	4	0.4
(1,246)	1:1869:A:TYR:H	1:1869:A:TYR:HA	10	0.4
(1,200)	1:1821:A:ILE:H	1:1822:A:SER:H	4	0.4
(1,200)	1:1821:A:ILE:H	1:1822:A:SER:H	7	0.4
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE1	6	0.4
(1,168)	1:1828:A:TYR:HA	1:1828:A:TYR:HE2	6	0.4
(1,85)	1:1812:A:VAL:HG21	1:1813:A:CYS:H	10	0.4
(1,85)	1:1812:A:VAL:HG22	1:1813:A:CYS:H	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:1812:A:VAL:HG23	1:1813:A:CYS:H	10	0.4
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG21	7	0.4
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG22	7	0.4
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG23	7	0.4
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG21	5	0.4
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG22	5	0.4
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG23	5	0.4
(1,46)	1:1788:A:TRP:HA	1:1789:A:THR:H	1	0.4
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	2	0.4
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	2	0.4
(1,5)	1:1822:A:SER:H	1:1872:A:ASN:H	10	0.4
(1,639)	1:1789:A:THR:HB	1:1789:A:THR:HG1	5	0.39
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB2	10	0.39
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB3	10	0.39
(1,612)	1:1824:A:ARG:HA	1:1825:A:ALA:H	3	0.39
(1,569)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	2	0.39
(1,569)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	5	0.39
(1,569)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	7	0.39
(1,547)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	7	0.39
(1,538)	1:1879:A:VAL:H	1:1879:A:VAL:HG21	3	0.39
(1,538)	1:1879:A:VAL:H	1:1879:A:VAL:HG22	3	0.39
(1,538)	1:1879:A:VAL:H	1:1879:A:VAL:HG23	3	0.39
(1,534)	1:1850:A:CYS:HA	1:1850:A:CYS:HB2	3	0.39
(1,520)	1:1820:A:ASN:HB2	1:1820:A:ASN:HB3	4	0.39
(1,506)	1:1842:A:CYS:HA	1:1849:A:ILE:H	2	0.39
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	9	0.39
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	9	0.39
(1,501)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	9	0.39
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG11	1	0.39
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG12	1	0.39
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG13	1	0.39
(1,472)	1:1836:A:LEU:H	1:1836:A:LEU:HG	6	0.39
(1,414)	1:1830:A:ASP:H	1:1830:A:ASP:HB2	6	0.39
(1,369)	1:1808:A:LEU:HB3	1:1810:A:GLY:H	10	0.39
(1,365)	1:1810:A:GLY:H	1:1810:A:GLY:HA3	8	0.39
(1,356)	1:1809:A:ILE:H	1:1810:A:GLY:H	8	0.39
(1,328)	1:1791:A:TRP:HZ2	1:1822:A:SER:HB3	2	0.39
(1,300)	1:1788:A:TRP:HA	1:1789:A:THR:H	1	0.39
(1,282)	1:1787:A:ASN:H	1:1787:A:ASN:HB2	10	0.39
(1,276)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	10	0.39
(1,275)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	7	0.39
(1,275)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,247)	1:1869:A:TYR:H	1:1869:A:TYR:HB2	4	0.39
(1,246)	1:1869:A:TYR:H	1:1869:A:TYR:HA	3	0.39
(1,246)	1:1869:A:TYR:H	1:1869:A:TYR:HA	8	0.39
(1,206)	1:1842:A:CYS:HA	1:1849:A:ILE:H	6	0.39
(1,191)	1:1871:A:ILE:HA	1:1872:A:ASN:H	4	0.39
(1,191)	1:1871:A:ILE:HA	1:1872:A:ASN:H	8	0.39
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG11	7	0.39
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG12	7	0.39
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG13	7	0.39
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG11	6	0.39
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG12	6	0.39
(1,57)	1:1838:A:GLN:HB3	1:1840:A:VAL:HG13	6	0.39
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG11	4	0.39
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG12	4	0.39
(1,56)	1:1838:A:GLN:HB2	1:1840:A:VAL:HG13	4	0.39
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	4	0.39
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	4	0.39
(1,7)	1:1791:A:TRP:HZ3	1:1872:A:ASN:H	4	0.39
(1,5)	1:1822:A:SER:H	1:1872:A:ASN:H	5	0.39
(1,4)	1:1794:A:SER:H	1:1795:A:GLY:H	7	0.39
(1,702)	1:1851:A:LYS:HA	1:1852:A:ASN:H	5	0.38
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD1	5	0.38
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD1	5	0.38
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD1	5	0.38
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD2	5	0.38
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD2	5	0.38
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD2	5	0.38
(1,645)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	3	0.38
(1,645)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	8	0.38
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	5	0.38
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	5	0.38
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	5	0.38
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	5	0.38
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	5	0.38
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	5	0.38
(1,600)	1:1869:A:TYR:HB3	1:1870:A:GLU:H	5	0.38
(1,534)	1:1850:A:CYS:HA	1:1850:A:CYS:HB2	4	0.38
(1,527)	1:1817:A:TRP:HB3	1:1817:A:TRP:HE3	7	0.38
(1,526)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	3	0.38
(1,526)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	8	0.38
(1,514)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	3	0.38
(1,464)	1:1832:A:PRO:HB2	1:1835:A:GLN:H	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,464)	1:1832:A:PRO:HB2	1:1835:A:GLN:H	5	0.38
(1,464)	1:1832:A:PRO:HB2	1:1835:A:GLN:H	9	0.38
(1,366)	1:1809:A:ILE:H	1:1810:A:GLY:H	4	0.38
(1,365)	1:1810:A:GLY:H	1:1810:A:GLY:HA3	1	0.38
(1,365)	1:1810:A:GLY:H	1:1810:A:GLY:HA3	4	0.38
(1,365)	1:1810:A:GLY:H	1:1810:A:GLY:HA3	7	0.38
(1,345)	1:1870:A:GLU:H	1:1870:A:GLU:HB3	10	0.38
(1,334)	1:1805:A:ASP:H	1:1805:A:ASP:HB2	1	0.38
(1,280)	1:1786:A:CYS:HA	1:1787:A:ASN:H	5	0.38
(1,280)	1:1786:A:CYS:HA	1:1787:A:ASN:H	6	0.38
(1,275)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	8	0.38
(1,275)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	10	0.38
(1,246)	1:1869:A:TYR:H	1:1869:A:TYR:HA	2	0.38
(1,246)	1:1869:A:TYR:H	1:1869:A:TYR:HA	7	0.38
(1,241)	1:1791:A:TRP:HH2	1:1822:A:SER:HB3	1	0.38
(1,223)	1:1829:A:PRO:HG2	1:1830:A:ASP:H	8	0.38
(1,206)	1:1842:A:CYS:HA	1:1849:A:ILE:H	2	0.38
(1,106)	1:1820:A:ASN:HB3	1:1821:A:ILE:H	3	0.38
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG11	10	0.38
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG12	10	0.38
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG13	10	0.38
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG21	2	0.38
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG22	2	0.38
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG23	2	0.38
(1,46)	1:1788:A:TRP:HA	1:1789:A:THR:H	9	0.38
(1,43)	1:1791:A:TRP:HE3	1:1872:A:ASN:HB3	7	0.38
(1,43)	1:1791:A:TRP:HE3	1:1872:A:ASN:HB3	8	0.38
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	1	0.38
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	1	0.38
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	5	0.38
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	5	0.38
(1,4)	1:1794:A:SER:H	1:1795:A:GLY:H	10	0.38
(1,647)	1:1840:A:VAL:HG21	1:1850:A:CYS:HB2	2	0.37
(1,647)	1:1840:A:VAL:HG22	1:1850:A:CYS:HB2	2	0.37
(1,647)	1:1840:A:VAL:HG23	1:1850:A:CYS:HB2	2	0.37
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	4	0.37
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	4	0.37
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	4	0.37
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	4	0.37
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	4	0.37
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	4	0.37
(1,618)	1:1851:A:LYS:HA	1:1852:A:ASN:H	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG21	5	0.37
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG22	5	0.37
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG23	5	0.37
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG21	4	0.37
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG22	4	0.37
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG23	4	0.37
(1,527)	1:1817:A:TRP:HB3	1:1817:A:TRP:HE3	2	0.37
(1,520)	1:1820:A:ASN:HB2	1:1820:A:ASN:HB3	10	0.37
(1,517)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	7	0.37
(1,516)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	1	0.37
(1,461)	1:1835:A:GLN:H	1:1835:A:GLN:HB2	6	0.37
(1,413)	1:1830:A:ASP:H	1:1830:A:ASP:HB3	1	0.37
(1,374)	1:1808:A:LEU:HD21	1:1810:A:GLY:H	1	0.37
(1,374)	1:1808:A:LEU:HD22	1:1810:A:GLY:H	1	0.37
(1,374)	1:1808:A:LEU:HD23	1:1810:A:GLY:H	1	0.37
(1,373)	1:1809:A:ILE:HD11	1:1810:A:GLY:H	4	0.37
(1,373)	1:1809:A:ILE:HD12	1:1810:A:GLY:H	4	0.37
(1,373)	1:1809:A:ILE:HD13	1:1810:A:GLY:H	4	0.37
(1,365)	1:1810:A:GLY:H	1:1810:A:GLY:HA3	6	0.37
(1,365)	1:1810:A:GLY:H	1:1810:A:GLY:HA3	10	0.37
(1,352)	1:1812:A:VAL:H	1:1813:A:CYS:H	4	0.37
(1,321)	1:1792:A:LEU:HB2	1:1793:A:ASP:H	10	0.37
(1,300)	1:1788:A:TRP:HA	1:1789:A:THR:H	9	0.37
(1,281)	1:1871:A:ILE:H	1:1871:A:ILE:HA	1	0.37
(1,264)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	2	0.37
(1,264)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	10	0.37
(1,253)	1:1877:A:GLU:H	1:1877:A:GLU:HB2	5	0.37
(1,246)	1:1869:A:TYR:H	1:1869:A:TYR:HA	1	0.37
(1,246)	1:1869:A:TYR:H	1:1869:A:TYR:HA	4	0.37
(1,174)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD21	6	0.37
(1,174)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD22	6	0.37
(1,174)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD23	6	0.37
(1,174)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD21	6	0.37
(1,174)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD22	6	0.37
(1,174)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD23	6	0.37
(1,151)	1:1791:A:TRP:HZ3	1:1871:A:ILE:HA	7	0.37
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG21	6	0.37
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG22	6	0.37
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG23	6	0.37
(1,49)	1:1789:A:THR:H	1:1874:A:GLN:HA	5	0.37
(1,46)	1:1788:A:TRP:HA	1:1789:A:THR:H	2	0.37
(1,43)	1:1791:A:TRP:HE3	1:1872:A:ASN:HB3	10	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	3	0.37
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	3	0.37
(1,16)	1:1817:A:TRP:HB2	1:1817:A:TRP:HE3	8	0.37
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD11	5	0.36
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD12	5	0.36
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD13	5	0.36
(1,645)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	2	0.36
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB2	3	0.36
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB3	3	0.36
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB2	9	0.36
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB3	9	0.36
(1,612)	1:1824:A:ARG:HA	1:1825:A:ALA:H	8	0.36
(1,573)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	10	0.36
(1,569)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	8	0.36
(1,527)	1:1817:A:TRP:HB3	1:1817:A:TRP:HE3	5	0.36
(1,520)	1:1820:A:ASN:HB2	1:1820:A:ASN:HB3	5	0.36
(1,517)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	1	0.36
(1,517)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	3	0.36
(1,516)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	2	0.36
(1,516)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	3	0.36
(1,516)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	7	0.36
(1,516)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	9	0.36
(1,514)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	2	0.36
(1,514)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	6	0.36
(1,467)	1:1834:A:GLY:HA3	1:1835:A:GLN:H	9	0.36
(1,390)	1:1823:A:CYS:HA	1:1823:A:CYS:HB3	8	0.36
(1,374)	1:1808:A:LEU:HD21	1:1810:A:GLY:H	2	0.36
(1,374)	1:1808:A:LEU:HD22	1:1810:A:GLY:H	2	0.36
(1,374)	1:1808:A:LEU:HD23	1:1810:A:GLY:H	2	0.36
(1,300)	1:1788:A:TRP:HA	1:1789:A:THR:H	2	0.36
(1,281)	1:1871:A:ILE:H	1:1871:A:ILE:HA	10	0.36
(1,275)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	6	0.36
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG21	1	0.36
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG22	1	0.36
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG23	1	0.36
(1,247)	1:1869:A:TYR:H	1:1869:A:TYR:HB2	2	0.36
(1,191)	1:1871:A:ILE:HA	1:1872:A:ASN:H	5	0.36
(1,99)	1:1791:A:TRP:HZ3	1:1824:A:ARG:H	1	0.36
(1,89)	1:1787:A:ASN:H	1:1875:A:CYS:H	10	0.36
(1,46)	1:1788:A:TRP:HA	1:1789:A:THR:H	6	0.36
(1,46)	1:1788:A:TRP:HA	1:1789:A:THR:H	8	0.36
(1,43)	1:1791:A:TRP:HE3	1:1872:A:ASN:HB3	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:1871:A:ILE:HA	1:1872:A:ASN:H	8	0.36
(1,702)	1:1851:A:LYS:HA	1:1852:A:ASN:H	3	0.35
(1,702)	1:1851:A:LYS:HA	1:1852:A:ASN:H	4	0.35
(1,702)	1:1851:A:LYS:HA	1:1852:A:ASN:H	8	0.35
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB2	1	0.35
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB3	1	0.35
(1,612)	1:1824:A:ARG:HA	1:1825:A:ALA:H	1	0.35
(1,547)	1:1874:A:GLN:HB2	1:1874:A:GLN:HB3	8	0.35
(1,527)	1:1817:A:TRP:HB3	1:1817:A:TRP:HE3	4	0.35
(1,526)	1:1866:A:CYS:HB2	1:1866:A:CYS:HB3	2	0.35
(1,520)	1:1820:A:ASN:HB2	1:1820:A:ASN:HB3	8	0.35
(1,517)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	4	0.35
(1,517)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	9	0.35
(1,517)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	10	0.35
(1,516)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	10	0.35
(1,514)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	5	0.35
(1,514)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	8	0.35
(1,513)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	8	0.35
(1,492)	1:1842:A:CYS:HA	1:1847:A:GLY:HA2	2	0.35
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG11	4	0.35
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG12	4	0.35
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG13	4	0.35
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG11	8	0.35
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG12	8	0.35
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG13	8	0.35
(1,479)	1:1838:A:GLN:HA	1:1839:A:THR:H	6	0.35
(1,467)	1:1834:A:GLY:HA3	1:1835:A:GLN:H	10	0.35
(1,365)	1:1810:A:GLY:H	1:1810:A:GLY:HA3	9	0.35
(1,353)	1:1812:A:VAL:H	1:1813:A:CYS:H	7	0.35
(1,300)	1:1788:A:TRP:HA	1:1789:A:THR:H	6	0.35
(1,300)	1:1788:A:TRP:HA	1:1789:A:THR:H	8	0.35
(1,284)	1:1871:A:ILE:H	1:1871:A:ILE:HG12	9	0.35
(1,283)	1:1871:A:ILE:H	1:1871:A:ILE:HG13	1	0.35
(1,283)	1:1871:A:ILE:H	1:1871:A:ILE:HG13	5	0.35
(1,280)	1:1786:A:CYS:HA	1:1787:A:ASN:H	2	0.35
(1,280)	1:1786:A:CYS:HA	1:1787:A:ASN:H	10	0.35
(1,279)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	9	0.35
(1,276)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	3	0.35
(1,246)	1:1869:A:TYR:H	1:1869:A:TYR:HA	5	0.35
(1,246)	1:1869:A:TYR:H	1:1869:A:TYR:HA	6	0.35
(1,241)	1:1791:A:TRP:HH2	1:1822:A:SER:HB3	9	0.35
(1,229)	1:1799:A:PHE:H	1:1800:A:HIS:H	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:1820:A:ASN:HB3	1:1821:A:ILE:H	4	0.35
(1,80)	1:1847:A:GLY:HA2	1:1848:A:LEU:H	1	0.35
(1,49)	1:1789:A:THR:H	1:1874:A:GLN:HA	9	0.35
(1,16)	1:1817:A:TRP:HB2	1:1817:A:TRP:HE3	2	0.35
(1,8)	1:1871:A:ILE:HA	1:1872:A:ASN:H	4	0.35
(1,7)	1:1791:A:TRP:HZ3	1:1872:A:ASN:H	6	0.35
(1,4)	1:1794:A:SER:H	1:1795:A:GLY:H	2	0.35
(1,653)	1:1833:A:ILE:HG21	1:1836:A:LEU:HD11	10	0.34
(1,653)	1:1833:A:ILE:HG21	1:1836:A:LEU:HD12	10	0.34
(1,653)	1:1833:A:ILE:HG21	1:1836:A:LEU:HD13	10	0.34
(1,653)	1:1833:A:ILE:HG22	1:1836:A:LEU:HD11	10	0.34
(1,653)	1:1833:A:ILE:HG22	1:1836:A:LEU:HD12	10	0.34
(1,653)	1:1833:A:ILE:HG22	1:1836:A:LEU:HD13	10	0.34
(1,653)	1:1833:A:ILE:HG23	1:1836:A:LEU:HD11	10	0.34
(1,653)	1:1833:A:ILE:HG23	1:1836:A:LEU:HD12	10	0.34
(1,653)	1:1833:A:ILE:HG23	1:1836:A:LEU:HD13	10	0.34
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB2	8	0.34
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB3	8	0.34
(1,618)	1:1851:A:LYS:HA	1:1852:A:ASN:H	7	0.34
(1,564)	1:1840:A:VAL:HG11	1:1842:A:CYS:HB2	3	0.34
(1,564)	1:1840:A:VAL:HG12	1:1842:A:CYS:HB2	3	0.34
(1,564)	1:1840:A:VAL:HG13	1:1842:A:CYS:HB2	3	0.34
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	4	0.34
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	4	0.34
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	4	0.34
(1,534)	1:1850:A:CYS:HA	1:1850:A:CYS:HB2	8	0.34
(1,527)	1:1817:A:TRP:HB3	1:1817:A:TRP:HE3	9	0.34
(1,516)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	8	0.34
(1,514)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	1	0.34
(1,514)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	4	0.34
(1,464)	1:1832:A:PRO:HB2	1:1835:A:GLN:H	4	0.34
(1,374)	1:1808:A:LEU:HD21	1:1810:A:GLY:H	9	0.34
(1,374)	1:1808:A:LEU:HD22	1:1810:A:GLY:H	9	0.34
(1,374)	1:1808:A:LEU:HD23	1:1810:A:GLY:H	9	0.34
(1,365)	1:1810:A:GLY:H	1:1810:A:GLY:HA3	2	0.34
(1,365)	1:1810:A:GLY:H	1:1810:A:GLY:HA3	5	0.34
(1,357)	1:1809:A:ILE:H	1:1847:A:GLY:HA3	7	0.34
(1,357)	1:1809:A:ILE:H	1:1847:A:GLY:HA3	9	0.34
(1,357)	1:1809:A:ILE:H	1:1847:A:GLY:HA3	10	0.34
(1,281)	1:1871:A:ILE:H	1:1871:A:ILE:HA	2	0.34
(1,280)	1:1786:A:CYS:HA	1:1787:A:ASN:H	9	0.34
(1,279)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:1786:A:CYS:HA	1:1787:A:ASN:H	5	0.34
(1,241)	1:1791:A:TRP:HH2	1:1822:A:SER:HB3	4	0.34
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD21	7	0.34
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD22	7	0.34
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD23	7	0.34
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD21	7	0.34
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD22	7	0.34
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD23	7	0.34
(1,223)	1:1829:A:PRO:HG2	1:1830:A:ASP:H	3	0.34
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG11	10	0.34
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG12	10	0.34
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG13	10	0.34
(1,43)	1:1791:A:TRP:HE3	1:1872:A:ASN:HB3	1	0.34
(1,17)	1:1817:A:TRP:HB3	1:1817:A:TRP:HE3	1	0.34
(1,16)	1:1817:A:TRP:HB2	1:1817:A:TRP:HE3	9	0.34
(1,700)	1:1821:A:ILE:HA	1:1821:A:ILE:HG12	8	0.33
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB2	7	0.33
(1,637)	1:1794:A:SER:H	1:1794:A:SER:HB3	7	0.33
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	9	0.33
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	9	0.33
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	9	0.33
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	9	0.33
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	9	0.33
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	9	0.33
(1,608)	1:1848:A:LEU:HD21	1:1869:A:TYR:HB2	2	0.33
(1,608)	1:1848:A:LEU:HD22	1:1869:A:TYR:HB2	2	0.33
(1,608)	1:1848:A:LEU:HD23	1:1869:A:TYR:HB2	2	0.33
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD11	7	0.33
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD12	7	0.33
(1,558)	1:1833:A:ILE:HA	1:1836:A:LEU:HD13	7	0.33
(1,537)	1:1875:A:CYS:HA	1:1875:A:CYS:HB3	6	0.33
(1,534)	1:1850:A:CYS:HA	1:1850:A:CYS:HB2	1	0.33
(1,520)	1:1820:A:ASN:HB2	1:1820:A:ASN:HB3	1	0.33
(1,520)	1:1820:A:ASN:HB2	1:1820:A:ASN:HB3	3	0.33
(1,520)	1:1820:A:ASN:HB2	1:1820:A:ASN:HB3	9	0.33
(1,513)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	3	0.33
(1,513)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	9	0.33
(1,506)	1:1842:A:CYS:HA	1:1849:A:ILE:H	1	0.33
(1,506)	1:1842:A:CYS:HA	1:1849:A:ILE:H	4	0.33
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG11	2	0.33
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG12	2	0.33
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG13	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG11	7	0.33
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG12	7	0.33
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG13	7	0.33
(1,479)	1:1838:A:GLN:HA	1:1839:A:THR:H	10	0.33
(1,467)	1:1834:A:GLY:HA3	1:1835:A:GLN:H	2	0.33
(1,467)	1:1834:A:GLY:HA3	1:1835:A:GLN:H	3	0.33
(1,464)	1:1832:A:PRO:HB2	1:1835:A:GLN:H	6	0.33
(1,464)	1:1832:A:PRO:HB2	1:1835:A:GLN:H	8	0.33
(1,414)	1:1830:A:ASP:H	1:1830:A:ASP:HB2	8	0.33
(1,413)	1:1830:A:ASP:H	1:1830:A:ASP:HB3	9	0.33
(1,352)	1:1812:A:VAL:H	1:1813:A:CYS:H	9	0.33
(1,345)	1:1870:A:GLU:H	1:1870:A:GLU:HB3	2	0.33
(1,283)	1:1871:A:ILE:H	1:1871:A:ILE:HG13	2	0.33
(1,282)	1:1787:A:ASN:H	1:1787:A:ASN:HB2	3	0.33
(1,281)	1:1871:A:ILE:H	1:1871:A:ILE:HA	9	0.33
(1,280)	1:1786:A:CYS:HA	1:1787:A:ASN:H	7	0.33
(1,280)	1:1786:A:CYS:HA	1:1787:A:ASN:H	8	0.33
(1,279)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	3	0.33
(1,279)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	5	0.33
(1,272)	1:1786:A:CYS:HA	1:1787:A:ASN:H	6	0.33
(1,264)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	9	0.33
(1,255)	1:1782:A:CYS:HA	1:1782:A:CYS:HB2	8	0.33
(1,206)	1:1842:A:CYS:HA	1:1849:A:ILE:H	1	0.33
(1,206)	1:1842:A:CYS:HA	1:1849:A:ILE:H	4	0.33
(1,193)	1:1791:A:TRP:HZ3	1:1824:A:ARG:H	1	0.33
(1,189)	1:1788:A:TRP:H	1:1788:A:TRP:HD1	8	0.33
(1,174)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD21	8	0.33
(1,174)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD22	8	0.33
(1,174)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD23	8	0.33
(1,174)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD21	8	0.33
(1,174)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD22	8	0.33
(1,174)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD23	8	0.33
(1,162)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	6	0.33
(1,119)	1:1821:A:ILE:H	1:1822:A:SER:H	5	0.33
(1,119)	1:1821:A:ILE:H	1:1822:A:SER:H	10	0.33
(1,85)	1:1812:A:VAL:HG21	1:1813:A:CYS:H	6	0.33
(1,85)	1:1812:A:VAL:HG22	1:1813:A:CYS:H	6	0.33
(1,85)	1:1812:A:VAL:HG23	1:1813:A:CYS:H	6	0.33
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG11	4	0.33
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG12	4	0.33
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG13	4	0.33
(1,46)	1:1788:A:TRP:HA	1:1789:A:THR:H	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD1	8	0.33
(1,26)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD2	8	0.33
(1,17)	1:1817:A:TRP:HB3	1:1817:A:TRP:HE3	3	0.33
(1,17)	1:1817:A:TRP:HB3	1:1817:A:TRP:HE3	10	0.33
(1,16)	1:1817:A:TRP:HB2	1:1817:A:TRP:HE3	5	0.33
(1,6)	1:1822:A:SER:H	1:1872:A:ASN:H	7	0.33
(1,4)	1:1794:A:SER:H	1:1795:A:GLY:H	9	0.33
(1,668)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD21	5	0.32
(1,668)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD22	5	0.32
(1,668)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD23	5	0.32
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	8	0.32
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	8	0.32
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	8	0.32
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	8	0.32
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	8	0.32
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	8	0.32
(1,618)	1:1851:A:LYS:HA	1:1852:A:ASN:H	6	0.32
(1,612)	1:1824:A:ARG:HA	1:1825:A:ALA:H	7	0.32
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG21	10	0.32
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG22	10	0.32
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG23	10	0.32
(1,529)	1:1865:A:PHE:HB2	1:1866:A:CYS:H	1	0.32
(1,529)	1:1866:A:CYS:H	1:1866:A:CYS:HB2	1	0.32
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	7	0.32
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	7	0.32
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	10	0.32
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	10	0.32
(1,520)	1:1820:A:ASN:HB2	1:1820:A:ASN:HB3	7	0.32
(1,516)	1:1786:A:CYS:HB2	1:1786:A:CYS:HB3	6	0.32
(1,514)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	10	0.32
(1,513)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	1	0.32
(1,513)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	2	0.32
(1,513)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	6	0.32
(1,513)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	7	0.32
(1,491)	1:1842:A:CYS:HA	1:1842:A:CYS:HB3	5	0.32
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG11	5	0.32
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG12	5	0.32
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG13	5	0.32
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG21	1	0.32
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG22	1	0.32
(1,481)	1:1839:A:THR:H	1:1839:A:THR:HG23	1	0.32
(1,464)	1:1832:A:PRO:HB2	1:1835:A:GLN:H	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:1835:A:GLN:H	1:1835:A:GLN:HB2	8	0.32
(1,431)	1:1824:A:ARG:H	1:1824:A:ARG:HB2	4	0.32
(1,390)	1:1823:A:CYS:HA	1:1823:A:CYS:HB3	5	0.32
(1,300)	1:1788:A:TRP:HA	1:1789:A:THR:H	7	0.32
(1,284)	1:1871:A:ILE:H	1:1871:A:ILE:HG12	10	0.32
(1,283)	1:1871:A:ILE:H	1:1871:A:ILE:HG13	8	0.32
(1,264)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	7	0.32
(1,252)	1:1877:A:GLU:H	1:1877:A:GLU:HG2	10	0.32
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD1	1	0.32
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD1	1	0.32
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD1	1	0.32
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD2	1	0.32
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD2	1	0.32
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD2	1	0.32
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD1	5	0.32
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD1	5	0.32
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD1	5	0.32
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD2	5	0.32
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD2	5	0.32
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD2	5	0.32
(1,204)	1:1848:A:LEU:HA	1:1849:A:ILE:H	9	0.32
(1,173)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD11	7	0.32
(1,173)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD12	7	0.32
(1,173)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD13	7	0.32
(1,173)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD11	7	0.32
(1,173)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD12	7	0.32
(1,173)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD13	7	0.32
(1,145)	1:1799:A:PHE:H	1:1800:A:HIS:H	9	0.32
(1,113)	1:1822:A:SER:H	1:1822:A:SER:HB2	7	0.32
(1,81)	1:1805:A:ASP:H	1:1850:A:CYS:H	4	0.32
(1,74)	1:1840:A:VAL:H	1:1840:A:VAL:HG21	10	0.32
(1,74)	1:1840:A:VAL:H	1:1840:A:VAL:HG22	10	0.32
(1,74)	1:1840:A:VAL:H	1:1840:A:VAL:HG23	10	0.32
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG11	8	0.32
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG12	8	0.32
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG13	8	0.32
(1,43)	1:1791:A:TRP:HE3	1:1872:A:ASN:HB3	4	0.32
(1,27)	1:1865:A:PHE:H	1:1865:A:PHE:HB3	5	0.32
(1,26)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD1	7	0.32
(1,26)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD2	7	0.32
(1,16)	1:1817:A:TRP:HB2	1:1817:A:TRP:HE3	7	0.32
(1,8)	1:1871:A:ILE:HA	1:1872:A:ASN:H	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:1791:A:TRP:HE3	1:1872:A:ASN:HB2	3	0.31
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD1	2	0.31
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD1	2	0.31
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD1	2	0.31
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD2	2	0.31
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD2	2	0.31
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD2	2	0.31
(1,668)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD21	10	0.31
(1,668)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD22	10	0.31
(1,668)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD23	10	0.31
(1,667)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	5	0.31
(1,592)	1:1799:A:PHE:H	1:1799:A:PHE:HB2	2	0.31
(1,537)	1:1875:A:CYS:HA	1:1875:A:CYS:HB3	2	0.31
(1,527)	1:1817:A:TRP:HB3	1:1817:A:TRP:HE3	8	0.31
(1,518)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	2	0.31
(1,513)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	4	0.31
(1,513)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	5	0.31
(1,511)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	3	0.31
(1,479)	1:1838:A:GLN:HA	1:1839:A:THR:H	7	0.31
(1,478)	1:1839:A:THR:H	1:1839:A:THR:HA	1	0.31
(1,478)	1:1839:A:THR:H	1:1839:A:THR:HA	2	0.31
(1,478)	1:1839:A:THR:H	1:1839:A:THR:HA	4	0.31
(1,478)	1:1839:A:THR:H	1:1839:A:THR:HA	7	0.31
(1,472)	1:1836:A:LEU:H	1:1836:A:LEU:HG	2	0.31
(1,461)	1:1835:A:GLN:H	1:1835:A:GLN:HB2	2	0.31
(1,439)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	8	0.31
(1,432)	1:1824:A:ARG:HB3	1:1825:A:ALA:H	3	0.31
(1,390)	1:1823:A:CYS:HA	1:1823:A:CYS:HB3	6	0.31
(1,388)	1:1791:A:TRP:HZ3	1:1823:A:CYS:HA	4	0.31
(1,374)	1:1808:A:LEU:HD21	1:1810:A:GLY:H	5	0.31
(1,374)	1:1808:A:LEU:HD22	1:1810:A:GLY:H	5	0.31
(1,374)	1:1808:A:LEU:HD23	1:1810:A:GLY:H	5	0.31
(1,366)	1:1809:A:ILE:H	1:1810:A:GLY:H	7	0.31
(1,353)	1:1812:A:VAL:H	1:1813:A:CYS:H	4	0.31
(1,345)	1:1870:A:GLU:H	1:1870:A:GLU:HB3	3	0.31
(1,343)	1:1870:A:GLU:H	1:1870:A:GLU:HA	8	0.31
(1,283)	1:1871:A:ILE:H	1:1871:A:ILE:HG13	4	0.31
(1,280)	1:1786:A:CYS:HA	1:1787:A:ASN:H	1	0.31
(1,279)	1:1786:A:CYS:HA	1:1786:A:CYS:HA	6	0.31
(1,264)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	3	0.31
(1,264)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	5	0.31
(1,231)	1:1800:A:HIS:H	1:1800:A:HIS:HB3	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	1:1840:A:VAL:HB	1:1841:A:VAL:H	7	0.31
(1,200)	1:1821:A:ILE:H	1:1822:A:SER:H	1	0.31
(1,183)	1:1817:A:TRP:HD1	1:1818:A:ALA:H	3	0.31
(1,183)	1:1817:A:TRP:HD1	1:1818:A:ALA:H	9	0.31
(1,156)	1:1791:A:TRP:HB2	1:1791:A:TRP:HE3	3	0.31
(1,153)	1:1791:A:TRP:HA	1:1791:A:TRP:HE3	3	0.31
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB1	4	0.31
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB2	4	0.31
(1,140)	1:1817:A:TRP:HD1	1:1819:A:ALA:HB3	4	0.31
(1,124)	1:1821:A:ILE:HA	1:1822:A:SER:H	8	0.31
(1,79)	1:1850:A:CYS:H	1:1850:A:CYS:HB2	10	0.31
(1,76)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	7	0.31
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG11	2	0.31
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG12	2	0.31
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG13	2	0.31
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG11	5	0.31
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG12	5	0.31
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG13	5	0.31
(1,49)	1:1789:A:THR:H	1:1874:A:GLN:HA	2	0.31
(1,46)	1:1788:A:TRP:HA	1:1789:A:THR:H	10	0.31
(1,731)	1:1840:A:VAL:HG11	1:1848:A:LEU:HG	3	0.3
(1,731)	1:1840:A:VAL:HG12	1:1848:A:LEU:HG	3	0.3
(1,731)	1:1840:A:VAL:HG13	1:1848:A:LEU:HG	3	0.3
(1,726)	1:1874:A:GLN:H	1:1874:A:GLN:HB3	8	0.3
(1,721)	1:1791:A:TRP:HE3	1:1872:A:ASN:HB2	5	0.3
(1,700)	1:1821:A:ILE:HA	1:1821:A:ILE:HG12	7	0.3
(1,608)	1:1848:A:LEU:HD21	1:1869:A:TYR:HB2	6	0.3
(1,608)	1:1848:A:LEU:HD22	1:1869:A:TYR:HB2	6	0.3
(1,608)	1:1848:A:LEU:HD23	1:1869:A:TYR:HB2	6	0.3
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG21	9	0.3
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG22	9	0.3
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG23	9	0.3
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	9	0.3
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	9	0.3
(1,522)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD1	8	0.3
(1,522)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD2	8	0.3
(1,517)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	6	0.3
(1,513)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	10	0.3
(1,512)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	8	0.3
(1,492)	1:1842:A:CYS:HA	1:1847:A:GLY:HA2	1	0.3
(1,492)	1:1842:A:CYS:HA	1:1847:A:GLY:HA2	5	0.3
(1,490)	1:1842:A:CYS:HA	1:1842:A:CYS:HB2	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:1839:A:THR:H	1:1839:A:THR:HA	8	0.3
(1,478)	1:1839:A:THR:H	1:1839:A:THR:HA	9	0.3
(1,467)	1:1834:A:GLY:HA3	1:1835:A:GLN:H	4	0.3
(1,464)	1:1832:A:PRO:HB2	1:1835:A:GLN:H	3	0.3
(1,428)	1:1820:A:ASN:H	1:1874:A:GLN:HB2	7	0.3
(1,388)	1:1791:A:TRP:HZ3	1:1823:A:CYS:HA	10	0.3
(1,343)	1:1870:A:GLU:H	1:1870:A:GLU:HA	4	0.3
(1,300)	1:1788:A:TRP:HA	1:1789:A:THR:H	10	0.3
(1,292)	1:1787:A:ASN:HA	1:1788:A:TRP:H	3	0.3
(1,283)	1:1871:A:ILE:H	1:1871:A:ILE:HG13	10	0.3
(1,279)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	1	0.3
(1,272)	1:1786:A:CYS:HA	1:1787:A:ASN:H	2	0.3
(1,272)	1:1786:A:CYS:HA	1:1787:A:ASN:H	10	0.3
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD21	8	0.3
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD22	8	0.3
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD23	8	0.3
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD21	8	0.3
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD22	8	0.3
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD23	8	0.3
(1,183)	1:1817:A:TRP:HD1	1:1818:A:ALA:H	1	0.3
(1,162)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	1	0.3
(1,162)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	8	0.3
(1,113)	1:1822:A:SER:H	1:1822:A:SER:HB2	10	0.3
(1,78)	1:1841:A:VAL:HA	1:1842:A:CYS:H	10	0.3
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG21	10	0.3
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG22	10	0.3
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG23	10	0.3
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD11	4	0.3
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD12	4	0.3
(1,37)	1:1792:A:LEU:H	1:1792:A:LEU:HD13	4	0.3
(1,26)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD1	10	0.3
(1,26)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD2	10	0.3
(1,10)	1:1872:A:ASN:H	1:1872:A:ASN:HB2	3	0.3
(1,4)	1:1794:A:SER:H	1:1795:A:GLY:H	5	0.3
(1,3)	1:1794:A:SER:H	1:1795:A:GLY:H	3	0.3
(1,726)	1:1874:A:GLN:H	1:1874:A:GLN:HB3	5	0.29
(1,712)	1:1791:A:TRP:HZ3	1:1872:A:ASN:H	5	0.29
(1,629)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD11	10	0.29
(1,629)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD12	10	0.29
(1,629)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD13	10	0.29
(1,629)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD11	10	0.29
(1,629)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD12	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,629)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD13	10	0.29
(1,522)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD1	7	0.29
(1,522)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD2	7	0.29
(1,520)	1:1820:A:ASN:HB2	1:1820:A:ASN:HB3	2	0.29
(1,517)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	5	0.29
(1,517)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	8	0.29
(1,506)	1:1842:A:CYS:HA	1:1849:A:ILE:H	10	0.29
(1,492)	1:1842:A:CYS:HA	1:1847:A:GLY:HA2	3	0.29
(1,478)	1:1839:A:THR:H	1:1839:A:THR:HA	5	0.29
(1,467)	1:1834:A:GLY:HA3	1:1835:A:GLN:H	1	0.29
(1,467)	1:1834:A:GLY:HA3	1:1835:A:GLN:H	8	0.29
(1,464)	1:1832:A:PRO:HB2	1:1835:A:GLN:H	10	0.29
(1,380)	1:1813:A:CYS:H	1:1813:A:CYS:HB3	6	0.29
(1,366)	1:1809:A:ILE:H	1:1810:A:GLY:H	2	0.29
(1,281)	1:1871:A:ILE:H	1:1871:A:ILE:HA	6	0.29
(1,280)	1:1786:A:CYS:HA	1:1787:A:ASN:H	3	0.29
(1,272)	1:1786:A:CYS:HA	1:1787:A:ASN:H	9	0.29
(1,260)	1:1829:A:PRO:HD2	1:1829:A:PRO:HG2	6	0.29
(1,232)	1:1799:A:PHE:H	1:1799:A:PHE:HB2	6	0.29
(1,230)	1:1799:A:PHE:HA	1:1800:A:HIS:H	9	0.29
(1,223)	1:1829:A:PRO:HG2	1:1830:A:ASP:H	9	0.29
(1,206)	1:1842:A:CYS:HA	1:1849:A:ILE:H	10	0.29
(1,204)	1:1848:A:LEU:HA	1:1849:A:ILE:H	10	0.29
(1,147)	1:1791:A:TRP:HZ2	1:1791:A:TRP:HZ3	1	0.29
(1,147)	1:1791:A:TRP:HZ2	1:1791:A:TRP:HZ3	2	0.29
(1,147)	1:1791:A:TRP:HZ2	1:1791:A:TRP:HZ3	10	0.29
(1,138)	1:1817:A:TRP:HD1	1:1819:A:ALA:HA	10	0.29
(1,99)	1:1791:A:TRP:HZ3	1:1824:A:ARG:H	10	0.29
(1,80)	1:1847:A:GLY:HA2	1:1848:A:LEU:H	9	0.29
(1,49)	1:1789:A:THR:H	1:1874:A:GLN:HA	6	0.29
(1,46)	1:1788:A:TRP:HA	1:1789:A:THR:H	4	0.29
(1,6)	1:1822:A:SER:H	1:1872:A:ASN:H	6	0.29
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG21	7	0.28
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG22	7	0.28
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG23	7	0.28
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG21	7	0.28
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG22	7	0.28
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG23	7	0.28
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG21	7	0.28
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG22	7	0.28
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG23	7	0.28
(1,653)	1:1833:A:ILE:HG21	1:1836:A:LEU:HD11	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:1833:A:ILE:HG21	1:1836:A:LEU:HD12	9	0.28
(1,653)	1:1833:A:ILE:HG21	1:1836:A:LEU:HD13	9	0.28
(1,653)	1:1833:A:ILE:HG22	1:1836:A:LEU:HD11	9	0.28
(1,653)	1:1833:A:ILE:HG22	1:1836:A:LEU:HD12	9	0.28
(1,653)	1:1833:A:ILE:HG22	1:1836:A:LEU:HD13	9	0.28
(1,653)	1:1833:A:ILE:HG23	1:1836:A:LEU:HD11	9	0.28
(1,653)	1:1833:A:ILE:HG23	1:1836:A:LEU:HD12	9	0.28
(1,653)	1:1833:A:ILE:HG23	1:1836:A:LEU:HD13	9	0.28
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	2	0.28
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	2	0.28
(1,631)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	2	0.28
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	2	0.28
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	2	0.28
(1,631)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	2	0.28
(1,614)	1:1821:A:ILE:HA	1:1873:A:VAL:HA	1	0.28
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG21	10	0.28
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG22	10	0.28
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG23	10	0.28
(1,529)	1:1865:A:PHE:HB2	1:1866:A:CYS:H	9	0.28
(1,529)	1:1866:A:CYS:H	1:1866:A:CYS:HB2	9	0.28
(1,520)	1:1820:A:ASN:HB2	1:1820:A:ASN:HB3	6	0.28
(1,512)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	3	0.28
(1,512)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	9	0.28
(1,511)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	2	0.28
(1,511)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	5	0.28
(1,511)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	6	0.28
(1,413)	1:1830:A:ASP:H	1:1830:A:ASP:HB3	3	0.28
(1,410)	1:1815:A:PRO:HG2	1:1816:A:GLY:H	1	0.28
(1,387)	1:1791:A:TRP:HE3	1:1871:A:ILE:HA	3	0.28
(1,387)	1:1791:A:TRP:HE3	1:1871:A:ILE:HA	5	0.28
(1,352)	1:1812:A:VAL:H	1:1813:A:CYS:H	1	0.28
(1,345)	1:1870:A:GLU:H	1:1870:A:GLU:HB3	1	0.28
(1,345)	1:1870:A:GLU:H	1:1870:A:GLU:HB3	8	0.28
(1,345)	1:1870:A:GLU:H	1:1870:A:GLU:HB3	9	0.28
(1,300)	1:1788:A:TRP:HA	1:1789:A:THR:H	4	0.28
(1,292)	1:1787:A:ASN:HA	1:1788:A:TRP:H	1	0.28
(1,292)	1:1787:A:ASN:HA	1:1788:A:TRP:H	5	0.28
(1,292)	1:1787:A:ASN:HA	1:1788:A:TRP:H	8	0.28
(1,284)	1:1871:A:ILE:H	1:1871:A:ILE:HG12	7	0.28
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG21	6	0.28
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG22	6	0.28
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG23	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:1786:A:CYS:HA	1:1787:A:ASN:H	7	0.28
(1,272)	1:1786:A:CYS:HA	1:1787:A:ASN:H	8	0.28
(1,264)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	6	0.28
(1,254)	1:1877:A:GLU:H	1:1877:A:GLU:HB3	7	0.28
(1,241)	1:1791:A:TRP:HH2	1:1822:A:SER:HB3	5	0.28
(1,229)	1:1799:A:PHE:H	1:1800:A:HIS:H	6	0.28
(1,227)	1:1873:A:VAL:HG21	1:1874:A:GLN:H	1	0.28
(1,227)	1:1873:A:VAL:HG22	1:1874:A:GLN:H	1	0.28
(1,227)	1:1873:A:VAL:HG23	1:1874:A:GLN:H	1	0.28
(1,223)	1:1829:A:PRO:HG2	1:1830:A:ASP:H	1	0.28
(1,214)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	5	0.28
(1,214)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	5	0.28
(1,214)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	5	0.28
(1,204)	1:1848:A:LEU:HA	1:1849:A:ILE:H	3	0.28
(1,204)	1:1848:A:LEU:HA	1:1849:A:ILE:H	7	0.28
(1,190)	1:1848:A:LEU:HA	1:1849:A:ILE:H	9	0.28
(1,183)	1:1817:A:TRP:HD1	1:1818:A:ALA:H	2	0.28
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD11	3	0.28
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD12	3	0.28
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD13	3	0.28
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD11	3	0.28
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD12	3	0.28
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD13	3	0.28
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD11	5	0.28
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD12	5	0.28
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD13	5	0.28
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD11	5	0.28
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD12	5	0.28
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD13	5	0.28
(1,162)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	2	0.28
(1,162)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	5	0.28
(1,147)	1:1791:A:TRP:HZ2	1:1791:A:TRP:HZ3	9	0.28
(1,115)	1:1822:A:SER:H	1:1872:A:ASN:HB2	10	0.28
(1,99)	1:1791:A:TRP:HZ3	1:1824:A:ARG:H	3	0.28
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG11	1	0.28
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG12	1	0.28
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG13	1	0.28
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG21	3	0.28
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG22	3	0.28
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG23	3	0.28
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	6	0.28
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:1793:A:ASP:HA	1:1794:A:SER:H	8	0.28
(1,702)	1:1851:A:LYS:HA	1:1852:A:ASN:H	2	0.27
(1,702)	1:1851:A:LYS:HA	1:1852:A:ASN:H	9	0.27
(1,652)	1:1848:A:LEU:HB3	1:1848:A:LEU:HD11	7	0.27
(1,652)	1:1848:A:LEU:HB3	1:1848:A:LEU:HD12	7	0.27
(1,652)	1:1848:A:LEU:HB3	1:1848:A:LEU:HD13	7	0.27
(1,647)	1:1840:A:VAL:HG21	1:1850:A:CYS:HB2	8	0.27
(1,647)	1:1840:A:VAL:HG22	1:1850:A:CYS:HB2	8	0.27
(1,647)	1:1840:A:VAL:HG23	1:1850:A:CYS:HB2	8	0.27
(1,614)	1:1821:A:ILE:HA	1:1873:A:VAL:HA	9	0.27
(1,612)	1:1824:A:ARG:HA	1:1825:A:ALA:H	10	0.27
(1,537)	1:1875:A:CYS:HA	1:1875:A:CYS:HB3	9	0.27
(1,522)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD1	10	0.27
(1,522)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD2	10	0.27
(1,518)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	3	0.27
(1,518)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	7	0.27
(1,512)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	1	0.27
(1,512)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	2	0.27
(1,512)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	6	0.27
(1,512)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	7	0.27
(1,511)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	1	0.27
(1,511)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	8	0.27
(1,506)	1:1842:A:CYS:HA	1:1849:A:ILE:H	7	0.27
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG11	10	0.27
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG12	10	0.27
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG13	10	0.27
(1,479)	1:1838:A:GLN:HA	1:1839:A:THR:H	9	0.27
(1,478)	1:1839:A:THR:H	1:1839:A:THR:HA	3	0.27
(1,478)	1:1839:A:THR:H	1:1839:A:THR:HA	6	0.27
(1,478)	1:1839:A:THR:H	1:1839:A:THR:HA	10	0.27
(1,467)	1:1834:A:GLY:HA3	1:1835:A:GLN:H	6	0.27
(1,432)	1:1824:A:ARG:HB3	1:1825:A:ALA:H	10	0.27
(1,410)	1:1815:A:PRO:HG2	1:1816:A:GLY:H	10	0.27
(1,390)	1:1823:A:CYS:HA	1:1823:A:CYS:HB3	10	0.27
(1,366)	1:1809:A:ILE:H	1:1810:A:GLY:H	8	0.27
(1,360)	1:1809:A:ILE:H	1:1809:A:ILE:HG12	4	0.27
(1,353)	1:1812:A:VAL:H	1:1813:A:CYS:H	9	0.27
(1,352)	1:1812:A:VAL:H	1:1813:A:CYS:H	6	0.27
(1,292)	1:1787:A:ASN:HA	1:1788:A:TRP:H	2	0.27
(1,292)	1:1787:A:ASN:HA	1:1788:A:TRP:H	6	0.27
(1,264)	1:1786:A:CYS:HA	1:1876:A:CYS:HA	1	0.27
(1,257)	1:1829:A:PRO:HD2	1:1829:A:PRO:HD3	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:1782:A:CYS:HA	1:1782:A:CYS:HB2	9	0.27
(1,245)	1:1868:A:ASN:HA	1:1869:A:TYR:H	9	0.27
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD21	4	0.27
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD22	4	0.27
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD23	4	0.27
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD21	4	0.27
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD22	4	0.27
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD23	4	0.27
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD21	5	0.27
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD22	5	0.27
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD23	5	0.27
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD21	5	0.27
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD22	5	0.27
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD23	5	0.27
(1,223)	1:1829:A:PRO:HG2	1:1830:A:ASP:H	4	0.27
(1,214)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	3	0.27
(1,214)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	3	0.27
(1,214)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	3	0.27
(1,214)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	8	0.27
(1,214)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	8	0.27
(1,214)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	8	0.27
(1,206)	1:1842:A:CYS:HA	1:1849:A:ILE:H	7	0.27
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	7	0.27
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	7	0.27
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	7	0.27
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	7	0.27
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	7	0.27
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	7	0.27
(1,79)	1:1850:A:CYS:H	1:1850:A:CYS:HB2	9	0.27
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG11	3	0.27
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG12	3	0.27
(1,68)	1:1840:A:VAL:HA	1:1840:A:VAL:HG13	3	0.27
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG21	1	0.27
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG22	1	0.27
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG23	1	0.27
(1,49)	1:1789:A:THR:H	1:1874:A:GLN:HA	1	0.27
(1,49)	1:1789:A:THR:H	1:1874:A:GLN:HA	7	0.27
(1,27)	1:1865:A:PHE:H	1:1865:A:PHE:HB3	2	0.27
(1,5)	1:1822:A:SER:H	1:1872:A:ASN:H	2	0.27
(1,3)	1:1794:A:SER:H	1:1795:A:GLY:H	1	0.27
(1,3)	1:1794:A:SER:H	1:1795:A:GLY:H	8	0.27
(1,705)	1:1792:A:LEU:H	1:1792:A:LEU:HA	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,702)	1:1851:A:LYS:HA	1:1852:A:ASN:H	10	0.26
(1,668)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD21	7	0.26
(1,668)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD22	7	0.26
(1,668)	1:1842:A:CYS:HB2	1:1848:A:LEU:HD23	7	0.26
(1,667)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	6	0.26
(1,666)	1:1848:A:LEU:HD21	1:1850:A:CYS:HB2	4	0.26
(1,666)	1:1848:A:LEU:HD22	1:1850:A:CYS:HB2	4	0.26
(1,666)	1:1848:A:LEU:HD23	1:1850:A:CYS:HB2	4	0.26
(1,639)	1:1789:A:THR:HB	1:1789:A:THR:HG1	2	0.26
(1,614)	1:1821:A:ILE:HA	1:1873:A:VAL:HA	6	0.26
(1,607)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD21	2	0.26
(1,607)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD22	2	0.26
(1,607)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD23	2	0.26
(1,571)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD21	2	0.26
(1,571)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD22	2	0.26
(1,571)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD23	2	0.26
(1,570)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD11	9	0.26
(1,570)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD12	9	0.26
(1,570)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD13	9	0.26
(1,552)	1:1833:A:ILE:H	1:1833:A:ILE:HA	10	0.26
(1,518)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	1	0.26
(1,518)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	10	0.26
(1,512)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	4	0.26
(1,512)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	5	0.26
(1,511)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	4	0.26
(1,492)	1:1842:A:CYS:HA	1:1847:A:GLY:HA2	8	0.26
(1,490)	1:1842:A:CYS:HA	1:1842:A:CYS:HB2	10	0.26
(1,484)	1:1838:A:GLN:HB3	1:1839:A:THR:H	7	0.26
(1,479)	1:1838:A:GLN:HA	1:1839:A:THR:H	2	0.26
(1,438)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	8	0.26
(1,357)	1:1809:A:ILE:H	1:1847:A:GLY:HA3	4	0.26
(1,357)	1:1809:A:ILE:H	1:1847:A:GLY:HA3	8	0.26
(1,281)	1:1871:A:ILE:H	1:1871:A:ILE:HA	4	0.26
(1,280)	1:1786:A:CYS:HA	1:1787:A:ASN:H	4	0.26
(1,272)	1:1786:A:CYS:HA	1:1787:A:ASN:H	1	0.26
(1,260)	1:1829:A:PRO:HD2	1:1829:A:PRO:HG2	3	0.26
(1,257)	1:1829:A:PRO:HD2	1:1829:A:PRO:HD3	6	0.26
(1,256)	1:1782:A:CYS:HA	1:1782:A:CYS:HB3	3	0.26
(1,241)	1:1791:A:TRP:HH2	1:1822:A:SER:HB3	6	0.26
(1,223)	1:1829:A:PRO:HG2	1:1830:A:ASP:H	10	0.26
(1,193)	1:1791:A:TRP:HZ3	1:1824:A:ARG:H	10	0.26
(1,186)	1:1845:A:SER:H	1:1846:A:VAL:H	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,183)	1:1817:A:TRP:HD1	1:1818:A:ALA:H	6	0.26
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	1	0.26
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	1	0.26
(1,147)	1:1791:A:TRP:HZ2	1:1791:A:TRP:HZ3	5	0.26
(1,147)	1:1791:A:TRP:HZ2	1:1791:A:TRP:HZ3	6	0.26
(1,139)	1:1817:A:TRP:HA	1:1817:A:TRP:HD1	4	0.26
(1,110)	1:1821:A:ILE:HA	1:1822:A:SER:H	8	0.26
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG11	6	0.26
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG12	6	0.26
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG13	6	0.26
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG11	9	0.26
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG12	9	0.26
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG13	9	0.26
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG21	4	0.26
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG22	4	0.26
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG23	4	0.26
(1,49)	1:1789:A:THR:H	1:1874:A:GLN:HA	3	0.26
(1,705)	1:1792:A:LEU:H	1:1792:A:LEU:HA	1	0.25
(1,705)	1:1792:A:LEU:H	1:1792:A:LEU:HA	8	0.25
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD1	1	0.25
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD1	1	0.25
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD1	1	0.25
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD2	1	0.25
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD2	1	0.25
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD2	1	0.25
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	5	0.25
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	5	0.25
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	5	0.25
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	9	0.25
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	9	0.25
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	9	0.25
(1,569)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	1	0.25
(1,537)	1:1875:A:CYS:HA	1:1875:A:CYS:HB3	7	0.25
(1,537)	1:1875:A:CYS:HA	1:1875:A:CYS:HB3	8	0.25
(1,518)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	4	0.25
(1,518)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	9	0.25
(1,512)	1:1788:A:TRP:HB2	1:1788:A:TRP:HB3	10	0.25
(1,472)	1:1836:A:LEU:H	1:1836:A:LEU:HG	8	0.25
(1,461)	1:1835:A:GLN:H	1:1835:A:GLN:HB2	1	0.25
(1,461)	1:1835:A:GLN:H	1:1835:A:GLN:HB2	4	0.25
(1,439)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	3	0.25
(1,432)	1:1824:A:ARG:HB3	1:1825:A:ALA:H	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:1870:A:GLU:H	1:1870:A:GLU:HA	5	0.25
(1,292)	1:1787:A:ASN:HA	1:1788:A:TRP:H	7	0.25
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG21	4	0.25
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG22	4	0.25
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG23	4	0.25
(1,272)	1:1786:A:CYS:HA	1:1787:A:ASN:H	3	0.25
(1,268)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	6	0.25
(1,257)	1:1829:A:PRO:HD2	1:1829:A:PRO:HD3	7	0.25
(1,257)	1:1829:A:PRO:HD2	1:1829:A:PRO:HD3	10	0.25
(1,253)	1:1877:A:GLU:H	1:1877:A:GLU:HB2	1	0.25
(1,252)	1:1877:A:GLU:H	1:1877:A:GLU:HG2	2	0.25
(1,229)	1:1799:A:PHE:H	1:1800:A:HIS:H	1	0.25
(1,204)	1:1848:A:LEU:HA	1:1849:A:ILE:H	1	0.25
(1,193)	1:1791:A:TRP:HZ3	1:1824:A:ARG:H	3	0.25
(1,190)	1:1848:A:LEU:HA	1:1849:A:ILE:H	10	0.25
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	5	0.25
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	5	0.25
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	5	0.25
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	5	0.25
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	5	0.25
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	5	0.25
(1,162)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	9	0.25
(1,145)	1:1799:A:PHE:H	1:1800:A:HIS:H	3	0.25
(1,139)	1:1817:A:TRP:HA	1:1817:A:TRP:HD1	9	0.25
(1,122)	1:1805:A:ASP:HA	1:1806:A:THR:H	4	0.25
(1,119)	1:1821:A:ILE:H	1:1822:A:SER:H	2	0.25
(1,119)	1:1821:A:ILE:H	1:1822:A:SER:H	3	0.25
(1,119)	1:1821:A:ILE:H	1:1822:A:SER:H	9	0.25
(1,99)	1:1791:A:TRP:HZ3	1:1824:A:ARG:H	7	0.25
(1,86)	1:1812:A:VAL:HG11	1:1813:A:CYS:H	9	0.25
(1,86)	1:1812:A:VAL:HG12	1:1813:A:CYS:H	9	0.25
(1,86)	1:1812:A:VAL:HG13	1:1813:A:CYS:H	9	0.25
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG11	10	0.25
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG12	10	0.25
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG13	10	0.25
(1,45)	1:1789:A:THR:H	1:1789:A:THR:HG1	3	0.25
(1,705)	1:1792:A:LEU:H	1:1792:A:LEU:HA	7	0.24
(1,643)	1:1861:A:ILE:H	1:1861:A:ILE:HB	7	0.24
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	1	0.24
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	1	0.24
(1,561)	1:1827:A:MET:HE1	1:1828:A:TYR:HE1	2	0.24
(1,561)	1:1827:A:MET:HE2	1:1828:A:TYR:HE1	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:1827:A:MET:HE3	1:1828:A:TYR:HE1	2	0.24
(1,561)	1:1827:A:MET:HE1	1:1828:A:TYR:HE2	2	0.24
(1,561)	1:1827:A:MET:HE2	1:1828:A:TYR:HE2	2	0.24
(1,561)	1:1827:A:MET:HE3	1:1828:A:TYR:HE2	2	0.24
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG21	3	0.24
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG22	3	0.24
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG23	3	0.24
(1,525)	1:1865:A:PHE:HA	1:1865:A:PHE:HB2	7	0.24
(1,524)	1:1865:A:PHE:H	1:1865:A:PHE:HB2	6	0.24
(1,511)	1:1823:A:CYS:HB2	1:1823:A:CYS:HB3	10	0.24
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG11	6	0.24
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG12	6	0.24
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG13	6	0.24
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD21	5	0.24
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD22	5	0.24
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD23	5	0.24
(1,329)	1:1800:A:HIS:H	1:1800:A:HIS:HB2	7	0.24
(1,328)	1:1791:A:TRP:HZ2	1:1822:A:SER:HB3	6	0.24
(1,282)	1:1787:A:ASN:H	1:1787:A:ASN:HB2	2	0.24
(1,268)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	7	0.24
(1,260)	1:1829:A:PRO:HD2	1:1829:A:PRO:HG2	10	0.24
(1,254)	1:1877:A:GLU:H	1:1877:A:GLU:HB3	6	0.24
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD21	2	0.24
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD22	2	0.24
(1,238)	1:1828:A:TYR:HD1	1:1836:A:LEU:HD23	2	0.24
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD21	2	0.24
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD22	2	0.24
(1,238)	1:1828:A:TYR:HD2	1:1836:A:LEU:HD23	2	0.24
(1,223)	1:1829:A:PRO:HG2	1:1830:A:ASP:H	6	0.24
(1,214)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	4	0.24
(1,214)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	4	0.24
(1,214)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	4	0.24
(1,190)	1:1848:A:LEU:HA	1:1849:A:ILE:H	3	0.24
(1,190)	1:1848:A:LEU:HA	1:1849:A:ILE:H	7	0.24
(1,181)	1:1830:A:ASP:H	1:1831:A:VAL:H	1	0.24
(1,181)	1:1830:A:ASP:H	1:1831:A:VAL:H	4	0.24
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	4	0.24
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	4	0.24
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	4	0.24
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	4	0.24
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	4	0.24
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	7	0.24
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	7	0.24
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	8	0.24
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	8	0.24
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	9	0.24
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	9	0.24
(1,162)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	3	0.24
(1,162)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	4	0.24
(1,162)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	7	0.24
(1,160)	1:1817:A:TRP:HE3	1:1817:A:TRP:HH2	10	0.24
(1,147)	1:1791:A:TRP:HZ2	1:1791:A:TRP:HZ3	7	0.24
(1,118)	1:1822:A:SER:H	1:1873:A:VAL:HG11	2	0.24
(1,118)	1:1822:A:SER:H	1:1873:A:VAL:HG12	2	0.24
(1,118)	1:1822:A:SER:H	1:1873:A:VAL:HG13	2	0.24
(1,99)	1:1791:A:TRP:HZ3	1:1824:A:ARG:H	2	0.24
(1,74)	1:1840:A:VAL:H	1:1840:A:VAL:HG21	7	0.24
(1,74)	1:1840:A:VAL:H	1:1840:A:VAL:HG22	7	0.24
(1,74)	1:1840:A:VAL:H	1:1840:A:VAL:HG23	7	0.24
(1,43)	1:1791:A:TRP:HE3	1:1872:A:ASN:HB3	6	0.24
(1,34)	1:1791:A:TRP:HA	1:1792:A:LEU:H	9	0.24
(1,26)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD1	6	0.24
(1,26)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD2	6	0.24
(1,705)	1:1792:A:LEU:H	1:1792:A:LEU:HA	2	0.23
(1,682)	1:1860:A:VAL:HA	1:1860:A:VAL:HG11	5	0.23
(1,682)	1:1860:A:VAL:HA	1:1860:A:VAL:HG12	5	0.23
(1,682)	1:1860:A:VAL:HA	1:1860:A:VAL:HG13	5	0.23
(1,662)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	5	0.23
(1,662)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	5	0.23
(1,662)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	5	0.23
(1,662)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	8	0.23
(1,662)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	8	0.23
(1,662)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	8	0.23
(1,639)	1:1789:A:THR:HB	1:1789:A:THR:HG1	1	0.23
(1,619)	1:1851:A:LYS:H	1:1851:A:LYS:HA	6	0.23
(1,614)	1:1821:A:ILE:HA	1:1873:A:VAL:HA	2	0.23
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	8	0.23
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	8	0.23
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	9	0.23
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	9	0.23
(1,571)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD21	4	0.23
(1,571)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD22	4	0.23
(1,571)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD23	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,537)	1:1875:A:CYS:HA	1:1875:A:CYS:HB3	5	0.23
(1,534)	1:1850:A:CYS:HA	1:1850:A:CYS:HB2	5	0.23
(1,525)	1:1865:A:PHE:HA	1:1865:A:PHE:HB2	8	0.23
(1,491)	1:1842:A:CYS:HA	1:1842:A:CYS:HB3	1	0.23
(1,491)	1:1842:A:CYS:HA	1:1842:A:CYS:HB3	8	0.23
(1,467)	1:1834:A:GLY:HA3	1:1835:A:GLN:H	5	0.23
(1,388)	1:1791:A:TRP:HZ3	1:1823:A:CYS:HA	1	0.23
(1,343)	1:1870:A:GLU:H	1:1870:A:GLU:HA	3	0.23
(1,343)	1:1870:A:GLU:H	1:1870:A:GLU:HA	6	0.23
(1,281)	1:1871:A:ILE:H	1:1871:A:ILE:HA	8	0.23
(1,273)	1:1823:A:CYS:HA	1:1823:A:CYS:HB2	9	0.23
(1,260)	1:1829:A:PRO:HD2	1:1829:A:PRO:HG2	7	0.23
(1,250)	1:1876:A:CYS:HA	1:1877:A:GLU:H	7	0.23
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD1	2	0.23
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD1	2	0.23
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD1	2	0.23
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD2	2	0.23
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD2	2	0.23
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD2	2	0.23
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD1	8	0.23
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD1	8	0.23
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD1	8	0.23
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD2	8	0.23
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD2	8	0.23
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD2	8	0.23
(1,197)	1:1789:A:THR:H	1:1873:A:VAL:H	4	0.23
(1,186)	1:1845:A:SER:H	1:1846:A:VAL:H	1	0.23
(1,181)	1:1830:A:ASP:H	1:1831:A:VAL:H	9	0.23
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	3	0.23
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	3	0.23
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	5	0.23
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	5	0.23
(1,160)	1:1817:A:TRP:HE3	1:1817:A:TRP:HH2	4	0.23
(1,147)	1:1791:A:TRP:HZ2	1:1791:A:TRP:HZ3	4	0.23
(1,124)	1:1821:A:ILE:HA	1:1822:A:SER:H	9	0.23
(1,122)	1:1805:A:ASP:HA	1:1806:A:THR:H	10	0.23
(1,79)	1:1850:A:CYS:H	1:1850:A:CYS:HB2	5	0.23
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG21	9	0.23
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG22	9	0.23
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG23	9	0.23
(1,20)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	5	0.23
(1,5)	1:1822:A:SER:H	1:1872:A:ASN:H	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG21	3	0.22
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG22	3	0.22
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG23	3	0.22
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG21	3	0.22
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG22	3	0.22
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG23	3	0.22
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG21	3	0.22
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG22	3	0.22
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG23	3	0.22
(1,712)	1:1791:A:TRP:HZ3	1:1872:A:ASN:H	8	0.22
(1,705)	1:1792:A:LEU:H	1:1792:A:LEU:HA	4	0.22
(1,702)	1:1851:A:LYS:HA	1:1852:A:ASN:H	1	0.22
(1,662)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	3	0.22
(1,662)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	3	0.22
(1,662)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	3	0.22
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	4	0.22
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	4	0.22
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	4	0.22
(1,647)	1:1840:A:VAL:HG21	1:1850:A:CYS:HB2	5	0.22
(1,647)	1:1840:A:VAL:HG22	1:1850:A:CYS:HB2	5	0.22
(1,647)	1:1840:A:VAL:HG23	1:1850:A:CYS:HB2	5	0.22
(1,639)	1:1789:A:THR:HB	1:1789:A:THR:HG1	10	0.22
(1,614)	1:1821:A:ILE:HA	1:1873:A:VAL:HA	3	0.22
(1,612)	1:1824:A:ARG:HA	1:1825:A:ALA:H	6	0.22
(1,607)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD21	4	0.22
(1,607)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD22	4	0.22
(1,607)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD23	4	0.22
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	7	0.22
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	7	0.22
(1,569)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	4	0.22
(1,569)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	6	0.22
(1,527)	1:1817:A:TRP:HB3	1:1817:A:TRP:HE3	6	0.22
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	8	0.22
(1,523)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	8	0.22
(1,503)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	9	0.22
(1,502)	1:1840:A:VAL:HG11	1:1842:A:CYS:HA	3	0.22
(1,502)	1:1840:A:VAL:HG12	1:1842:A:CYS:HA	3	0.22
(1,502)	1:1840:A:VAL:HG13	1:1842:A:CYS:HA	3	0.22
(1,492)	1:1842:A:CYS:HA	1:1847:A:GLY:HA2	6	0.22
(1,479)	1:1838:A:GLN:HA	1:1839:A:THR:H	1	0.22
(1,461)	1:1835:A:GLN:H	1:1835:A:GLN:HB2	7	0.22
(1,461)	1:1835:A:GLN:H	1:1835:A:GLN:HB2	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:1835:A:GLN:H	1:1835:A:GLN:HB2	10	0.22
(1,439)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	1	0.22
(1,439)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	7	0.22
(1,439)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	9	0.22
(1,394)	1:1840:A:VAL:HG11	1:1848:A:LEU:HA	3	0.22
(1,394)	1:1840:A:VAL:HG12	1:1848:A:LEU:HA	3	0.22
(1,394)	1:1840:A:VAL:HG13	1:1848:A:LEU:HA	3	0.22
(1,355)	1:1813:A:CYS:H	1:1814:A:GLY:H	6	0.22
(1,353)	1:1812:A:VAL:H	1:1813:A:CYS:H	1	0.22
(1,284)	1:1871:A:ILE:H	1:1871:A:ILE:HG12	1	0.22
(1,281)	1:1871:A:ILE:H	1:1871:A:ILE:HA	3	0.22
(1,281)	1:1871:A:ILE:H	1:1871:A:ILE:HA	7	0.22
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG21	10	0.22
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG22	10	0.22
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG23	10	0.22
(1,272)	1:1786:A:CYS:HA	1:1787:A:ASN:H	4	0.22
(1,268)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	5	0.22
(1,260)	1:1829:A:PRO:HD2	1:1829:A:PRO:HG2	5	0.22
(1,257)	1:1829:A:PRO:HD2	1:1829:A:PRO:HD3	4	0.22
(1,257)	1:1829:A:PRO:HD2	1:1829:A:PRO:HD3	8	0.22
(1,245)	1:1868:A:ASN:HA	1:1869:A:TYR:H	8	0.22
(1,214)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	2	0.22
(1,214)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	2	0.22
(1,214)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	2	0.22
(1,193)	1:1791:A:TRP:HZ3	1:1824:A:ARG:H	7	0.22
(1,192)	1:1789:A:THR:HG1	1:1873:A:VAL:H	3	0.22
(1,192)	1:1789:A:THR:HG1	1:1873:A:VAL:H	4	0.22
(1,191)	1:1871:A:ILE:HA	1:1872:A:ASN:H	7	0.22
(1,183)	1:1817:A:TRP:HD1	1:1818:A:ALA:H	7	0.22
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	4	0.22
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	4	0.22
(1,161)	1:1817:A:TRP:HE3	1:1817:A:TRP:HZ2	10	0.22
(1,147)	1:1791:A:TRP:HZ2	1:1791:A:TRP:HZ3	8	0.22
(1,124)	1:1821:A:ILE:HA	1:1822:A:SER:H	7	0.22
(1,119)	1:1821:A:ILE:H	1:1822:A:SER:H	6	0.22
(1,107)	1:1820:A:ASN:HB2	1:1821:A:ILE:H	2	0.22
(1,107)	1:1820:A:ASN:HB2	1:1821:A:ILE:H	10	0.22
(1,79)	1:1850:A:CYS:H	1:1850:A:CYS:HB2	7	0.22
(1,76)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	6	0.22
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG11	3	0.22
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG12	3	0.22
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG13	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG21	7	0.22
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG22	7	0.22
(1,50)	1:1789:A:THR:H	1:1789:A:THR:HG23	7	0.22
(1,5)	1:1822:A:SER:H	1:1872:A:ASN:H	1	0.22
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG21	10	0.21
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG22	10	0.21
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG23	10	0.21
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG21	10	0.21
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG22	10	0.21
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG23	10	0.21
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG21	10	0.21
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG22	10	0.21
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG23	10	0.21
(1,726)	1:1874:A:GLN:H	1:1874:A:GLN:HB3	4	0.21
(1,705)	1:1792:A:LEU:H	1:1792:A:LEU:HA	10	0.21
(1,652)	1:1848:A:LEU:HB3	1:1848:A:LEU:HD11	9	0.21
(1,652)	1:1848:A:LEU:HB3	1:1848:A:LEU:HD12	9	0.21
(1,652)	1:1848:A:LEU:HB3	1:1848:A:LEU:HD13	9	0.21
(1,638)	1:1793:A:ASP:HA	1:1794:A:SER:H	8	0.21
(1,616)	1:1878:A:CYS:HA	1:1879:A:VAL:H	3	0.21
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	3	0.21
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	3	0.21
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	5	0.21
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	5	0.21
(1,569)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	3	0.21
(1,525)	1:1865:A:PHE:HA	1:1865:A:PHE:HB2	10	0.21
(1,522)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD1	6	0.21
(1,522)	1:1865:A:PHE:HB2	1:1865:A:PHE:HD2	6	0.21
(1,521)	1:1865:A:PHE:HB2	1:1865:A:PHE:HB3	2	0.21
(1,521)	1:1865:A:PHE:HB2	1:1865:A:PHE:HB3	3	0.21
(1,521)	1:1865:A:PHE:HB2	1:1865:A:PHE:HB3	4	0.21
(1,521)	1:1865:A:PHE:HB2	1:1865:A:PHE:HB3	5	0.21
(1,521)	1:1865:A:PHE:HB2	1:1865:A:PHE:HB3	6	0.21
(1,521)	1:1865:A:PHE:HB2	1:1865:A:PHE:HB3	7	0.21
(1,521)	1:1865:A:PHE:HB2	1:1865:A:PHE:HB3	8	0.21
(1,521)	1:1865:A:PHE:HB2	1:1865:A:PHE:HB3	9	0.21
(1,521)	1:1865:A:PHE:HB2	1:1865:A:PHE:HB3	10	0.21
(1,479)	1:1838:A:GLN:HA	1:1839:A:THR:H	5	0.21
(1,479)	1:1838:A:GLN:HA	1:1839:A:THR:H	8	0.21
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD21	10	0.21
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD22	10	0.21
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD23	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	4	0.21
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB1	6	0.21
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB2	6	0.21
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB3	6	0.21
(1,369)	1:1808:A:LEU:HB3	1:1810:A:GLY:H	4	0.21
(1,355)	1:1813:A:CYS:H	1:1814:A:GLY:H	10	0.21
(1,343)	1:1870:A:GLU:H	1:1870:A:GLU:HA	1	0.21
(1,337)	1:1806:A:THR:H	1:1806:A:THR:HA	7	0.21
(1,328)	1:1791:A:TRP:HZ2	1:1822:A:SER:HB3	9	0.21
(1,282)	1:1787:A:ASN:H	1:1787:A:ASN:HB2	1	0.21
(1,257)	1:1829:A:PRO:HD2	1:1829:A:PRO:HD3	5	0.21
(1,257)	1:1829:A:PRO:HD2	1:1829:A:PRO:HD3	9	0.21
(1,245)	1:1868:A:ASN:HA	1:1869:A:TYR:H	10	0.21
(1,230)	1:1799:A:PHE:HA	1:1800:A:HIS:H	6	0.21
(1,196)	1:1789:A:THR:H	1:1790:A:GLY:H	7	0.21
(1,193)	1:1791:A:TRP:HZ3	1:1824:A:ARG:H	2	0.21
(1,191)	1:1871:A:ILE:HA	1:1872:A:ASN:H	3	0.21
(1,190)	1:1848:A:LEU:HA	1:1849:A:ILE:H	1	0.21
(1,186)	1:1845:A:SER:H	1:1846:A:VAL:H	7	0.21
(1,160)	1:1817:A:TRP:HE3	1:1817:A:TRP:HH2	3	0.21
(1,139)	1:1817:A:TRP:HA	1:1817:A:TRP:HD1	7	0.21
(1,85)	1:1812:A:VAL:HG21	1:1813:A:CYS:H	4	0.21
(1,85)	1:1812:A:VAL:HG22	1:1813:A:CYS:H	4	0.21
(1,85)	1:1812:A:VAL:HG23	1:1813:A:CYS:H	4	0.21
(1,81)	1:1805:A:ASP:H	1:1850:A:CYS:H	7	0.21
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG21	2	0.21
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG22	2	0.21
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG23	2	0.21
(1,1)	1:1793:A:ASP:HA	1:1794:A:SER:H	5	0.21
(1,705)	1:1792:A:LEU:H	1:1792:A:LEU:HA	3	0.2
(1,686)	1:1827:A:MET:HE1	1:1828:A:TYR:HE1	2	0.2
(1,686)	1:1827:A:MET:HE2	1:1828:A:TYR:HE1	2	0.2
(1,686)	1:1827:A:MET:HE3	1:1828:A:TYR:HE1	2	0.2
(1,686)	1:1827:A:MET:HE1	1:1828:A:TYR:HE2	2	0.2
(1,686)	1:1827:A:MET:HE2	1:1828:A:TYR:HE2	2	0.2
(1,686)	1:1827:A:MET:HE3	1:1828:A:TYR:HE2	2	0.2
(1,667)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	8	0.2
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	2	0.2
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	2	0.2
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	2	0.2
(1,652)	1:1848:A:LEU:HB3	1:1848:A:LEU:HD11	10	0.2
(1,652)	1:1848:A:LEU:HB3	1:1848:A:LEU:HD12	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:1848:A:LEU:HB3	1:1848:A:LEU:HD13	10	0.2
(1,639)	1:1789:A:THR:HB	1:1789:A:THR:HG1	8	0.2
(1,627)	1:1789:A:THR:HB	1:1789:A:THR:HG1	5	0.2
(1,621)	1:1869:A:TYR:HA	1:1870:A:GLU:H	4	0.2
(1,614)	1:1821:A:ILE:HA	1:1873:A:VAL:HA	8	0.2
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	4	0.2
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	4	0.2
(1,552)	1:1833:A:ILE:H	1:1833:A:ILE:HA	1	0.2
(1,552)	1:1833:A:ILE:H	1:1833:A:ILE:HA	5	0.2
(1,552)	1:1833:A:ILE:H	1:1833:A:ILE:HA	8	0.2
(1,521)	1:1865:A:PHE:HB2	1:1865:A:PHE:HB3	1	0.2
(1,518)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	6	0.2
(1,515)	1:1850:A:CYS:HB2	1:1850:A:CYS:HB3	3	0.2
(1,477)	1:1839:A:THR:HA	1:1840:A:VAL:H	5	0.2
(1,439)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	2	0.2
(1,439)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	10	0.2
(1,374)	1:1808:A:LEU:HD21	1:1810:A:GLY:H	6	0.2
(1,374)	1:1808:A:LEU:HD22	1:1810:A:GLY:H	6	0.2
(1,374)	1:1808:A:LEU:HD23	1:1810:A:GLY:H	6	0.2
(1,358)	1:1808:A:LEU:HA	1:1809:A:ILE:H	3	0.2
(1,353)	1:1812:A:VAL:H	1:1813:A:CYS:H	6	0.2
(1,292)	1:1787:A:ASN:HA	1:1788:A:TRP:H	9	0.2
(1,284)	1:1871:A:ILE:H	1:1871:A:ILE:HG12	2	0.2
(1,281)	1:1871:A:ILE:H	1:1871:A:ILE:HA	5	0.2
(1,277)	1:1786:A:CYS:HA	1:1786:A:CYS:HB2	1	0.2
(1,273)	1:1823:A:CYS:HA	1:1823:A:CYS:HB2	4	0.2
(1,271)	1:1876:A:CYS:HA	1:1877:A:GLU:H	7	0.2
(1,245)	1:1868:A:ASN:HA	1:1869:A:TYR:H	1	0.2
(1,245)	1:1868:A:ASN:HA	1:1869:A:TYR:H	3	0.2
(1,232)	1:1799:A:PHE:H	1:1799:A:PHE:HB2	2	0.2
(1,224)	1:1873:A:VAL:HA	1:1874:A:GLN:H	3	0.2
(1,224)	1:1873:A:VAL:HA	1:1874:A:GLN:H	7	0.2
(1,214)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	6	0.2
(1,214)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	6	0.2
(1,214)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	6	0.2
(1,210)	1:1840:A:VAL:HB	1:1841:A:VAL:H	10	0.2
(1,200)	1:1821:A:ILE:H	1:1822:A:SER:H	8	0.2
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	9	0.2
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	9	0.2
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	9	0.2
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	9	0.2
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	9	0.2
(1,163)	1:1788:A:TRP:HB3	1:1788:A:TRP:HE3	10	0.2
(1,161)	1:1817:A:TRP:HE3	1:1817:A:TRP:HZ2	3	0.2
(1,139)	1:1817:A:TRP:HA	1:1817:A:TRP:HD1	2	0.2
(1,119)	1:1821:A:ILE:H	1:1822:A:SER:H	4	0.2
(1,119)	1:1821:A:ILE:H	1:1822:A:SER:H	7	0.2
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG11	6	0.2
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG12	6	0.2
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG13	6	0.2
(1,45)	1:1789:A:THR:H	1:1789:A:THR:HG1	4	0.2
(1,29)	1:1789:A:THR:HG1	1:1873:A:VAL:H	3	0.2
(1,9)	1:1871:A:ILE:HB	1:1872:A:ASN:H	10	0.2
(1,6)	1:1822:A:SER:H	1:1872:A:ASN:H	4	0.2
(1,3)	1:1794:A:SER:H	1:1795:A:GLY:H	4	0.2
(1,3)	1:1794:A:SER:H	1:1795:A:GLY:H	6	0.2
(1,712)	1:1791:A:TRP:HZ3	1:1872:A:ASN:H	4	0.19
(1,707)	1:1791:A:TRP:HB2	1:1791:A:TRP:HD1	5	0.19
(1,702)	1:1851:A:LYS:HA	1:1852:A:ASN:H	7	0.19
(1,667)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	2	0.19
(1,667)	1:1874:A:GLN:HA	1:1874:A:GLN:HG2	9	0.19
(1,662)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	4	0.19
(1,662)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	4	0.19
(1,662)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	4	0.19
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD21	8	0.19
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD22	8	0.19
(1,658)	1:1842:A:CYS:HA	1:1848:A:LEU:HD23	8	0.19
(1,614)	1:1821:A:ILE:HA	1:1873:A:VAL:HA	5	0.19
(1,562)	1:1842:A:CYS:HA	1:1842:A:CYS:HB2	3	0.19
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG21	8	0.19
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG22	8	0.19
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG23	8	0.19
(1,518)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	5	0.19
(1,518)	1:1813:A:CYS:HB2	1:1813:A:CYS:HB3	8	0.19
(1,492)	1:1842:A:CYS:HA	1:1847:A:GLY:HA2	9	0.19
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG11	3	0.19
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG12	3	0.19
(1,486)	1:1841:A:VAL:H	1:1841:A:VAL:HG13	3	0.19
(1,479)	1:1838:A:GLN:HA	1:1839:A:THR:H	4	0.19
(1,439)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	5	0.19
(1,439)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	6	0.19
(1,438)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	3	0.19
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB1	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB2	9	0.19
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB3	9	0.19
(1,400)	1:1848:A:LEU:H	1:1848:A:LEU:HA	2	0.19
(1,400)	1:1848:A:LEU:H	1:1848:A:LEU:HA	5	0.19
(1,400)	1:1848:A:LEU:H	1:1848:A:LEU:HA	6	0.19
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD11	3	0.19
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD12	3	0.19
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD13	3	0.19
(1,343)	1:1870:A:GLU:H	1:1870:A:GLU:HA	2	0.19
(1,338)	1:1805:A:ASP:HA	1:1806:A:THR:H	4	0.19
(1,277)	1:1786:A:CYS:HA	1:1786:A:CYS:HB2	3	0.19
(1,277)	1:1786:A:CYS:HA	1:1786:A:CYS:HB2	10	0.19
(1,260)	1:1829:A:PRO:HD2	1:1829:A:PRO:HG2	2	0.19
(1,257)	1:1829:A:PRO:HD2	1:1829:A:PRO:HD3	1	0.19
(1,254)	1:1877:A:GLU:H	1:1877:A:GLU:HB3	1	0.19
(1,210)	1:1840:A:VAL:HB	1:1841:A:VAL:H	6	0.19
(1,199)	1:1813:A:CYS:H	1:1814:A:GLY:H	6	0.19
(1,196)	1:1789:A:THR:H	1:1790:A:GLY:H	4	0.19
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	8	0.19
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	8	0.19
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	8	0.19
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	8	0.19
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	8	0.19
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	8	0.19
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD11	10	0.19
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD12	10	0.19
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD13	10	0.19
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD11	10	0.19
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD12	10	0.19
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD13	10	0.19
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	2	0.19
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	2	0.19
(1,161)	1:1817:A:TRP:HE3	1:1817:A:TRP:HZ2	4	0.19
(1,160)	1:1817:A:TRP:HE3	1:1817:A:TRP:HH2	1	0.19
(1,122)	1:1805:A:ASP:HA	1:1806:A:THR:H	1	0.19
(1,104)	1:1820:A:ASN:HA	1:1821:A:ILE:H	6	0.19
(1,81)	1:1805:A:ASP:H	1:1850:A:CYS:H	10	0.19
(1,66)	1:1840:A:VAL:HG21	1:1850:A:CYS:HA	1	0.19
(1,66)	1:1840:A:VAL:HG22	1:1850:A:CYS:HA	1	0.19
(1,66)	1:1840:A:VAL:HG23	1:1850:A:CYS:HA	1	0.19
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG11	9	0.19
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG12	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:1840:A:VAL:H	1:1840:A:VAL:HG13	9	0.19
(1,49)	1:1789:A:THR:H	1:1874:A:GLN:HA	10	0.19
(1,34)	1:1791:A:TRP:HA	1:1792:A:LEU:H	6	0.19
(1,29)	1:1789:A:THR:HG1	1:1873:A:VAL:H	4	0.19
(1,9)	1:1871:A:ILE:HB	1:1872:A:ASN:H	1	0.19
(1,8)	1:1871:A:ILE:HA	1:1872:A:ASN:H	7	0.19
(1,7)	1:1791:A:TRP:HZ3	1:1872:A:ASN:H	3	0.19
(1,3)	1:1794:A:SER:H	1:1795:A:GLY:H	7	0.19
(1,1)	1:1793:A:ASP:HA	1:1794:A:SER:H	7	0.19
(1,705)	1:1792:A:LEU:H	1:1792:A:LEU:HA	5	0.18
(1,664)	1:1848:A:LEU:HD21	1:1869:A:TYR:HB3	3	0.18
(1,664)	1:1848:A:LEU:HD22	1:1869:A:TYR:HB3	3	0.18
(1,664)	1:1848:A:LEU:HD23	1:1869:A:TYR:HB3	3	0.18
(1,662)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	2	0.18
(1,662)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	2	0.18
(1,662)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	2	0.18
(1,651)	1:1836:A:LEU:HB3	1:1836:A:LEU:HD11	10	0.18
(1,651)	1:1836:A:LEU:HB3	1:1836:A:LEU:HD12	10	0.18
(1,651)	1:1836:A:LEU:HB3	1:1836:A:LEU:HD13	10	0.18
(1,639)	1:1789:A:THR:HB	1:1789:A:THR:HG1	4	0.18
(1,639)	1:1789:A:THR:HB	1:1789:A:THR:HG1	6	0.18
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD21	1	0.18
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD22	1	0.18
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD23	1	0.18
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD21	1	0.18
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD22	1	0.18
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD23	1	0.18
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD21	3	0.18
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD22	3	0.18
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD23	3	0.18
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD21	3	0.18
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD22	3	0.18
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD23	3	0.18
(1,597)	1:1869:A:TYR:HA	1:1869:A:TYR:HB2	3	0.18
(1,577)	1:1878:A:CYS:HA	1:1878:A:CYS:HB2	1	0.18
(1,567)	1:1793:A:ASP:H	1:1793:A:ASP:HB3	4	0.18
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG21	6	0.18
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG22	6	0.18
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG23	6	0.18
(1,544)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	6	0.18
(1,537)	1:1875:A:CYS:HA	1:1875:A:CYS:HB3	4	0.18
(1,515)	1:1850:A:CYS:HB2	1:1850:A:CYS:HB3	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:1839:A:THR:HA	1:1840:A:VAL:H	1	0.18
(1,437)	1:1878:A:CYS:HB2	1:1878:A:CYS:HB3	1	0.18
(1,437)	1:1878:A:CYS:HB2	1:1878:A:CYS:HB3	2	0.18
(1,437)	1:1878:A:CYS:HB2	1:1878:A:CYS:HB3	3	0.18
(1,437)	1:1878:A:CYS:HB2	1:1878:A:CYS:HB3	4	0.18
(1,437)	1:1878:A:CYS:HB2	1:1878:A:CYS:HB3	5	0.18
(1,437)	1:1878:A:CYS:HB2	1:1878:A:CYS:HB3	6	0.18
(1,437)	1:1878:A:CYS:HB2	1:1878:A:CYS:HB3	7	0.18
(1,437)	1:1878:A:CYS:HB2	1:1878:A:CYS:HB3	8	0.18
(1,437)	1:1878:A:CYS:HB2	1:1878:A:CYS:HB3	9	0.18
(1,437)	1:1878:A:CYS:HB2	1:1878:A:CYS:HB3	10	0.18
(1,410)	1:1815:A:PRO:HG2	1:1816:A:GLY:H	3	0.18
(1,410)	1:1815:A:PRO:HG2	1:1816:A:GLY:H	6	0.18
(1,400)	1:1848:A:LEU:H	1:1848:A:LEU:HA	7	0.18
(1,400)	1:1848:A:LEU:H	1:1848:A:LEU:HA	8	0.18
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD11	4	0.18
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD12	4	0.18
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD13	4	0.18
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD11	8	0.18
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD12	8	0.18
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD13	8	0.18
(1,382)	1:1808:A:LEU:H	1:1808:A:LEU:HB3	10	0.18
(1,343)	1:1870:A:GLU:H	1:1870:A:GLU:HA	7	0.18
(1,343)	1:1870:A:GLU:H	1:1870:A:GLU:HA	9	0.18
(1,337)	1:1806:A:THR:H	1:1806:A:THR:HA	6	0.18
(1,337)	1:1806:A:THR:H	1:1806:A:THR:HA	8	0.18
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG21	2	0.18
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG22	2	0.18
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG23	2	0.18
(1,268)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	9	0.18
(1,257)	1:1829:A:PRO:HD2	1:1829:A:PRO:HD3	3	0.18
(1,243)	1:1824:A:ARG:HA	1:1825:A:ALA:H	2	0.18
(1,207)	1:1840:A:VAL:HA	1:1841:A:VAL:H	9	0.18
(1,199)	1:1813:A:CYS:H	1:1814:A:GLY:H	10	0.18
(1,191)	1:1871:A:ILE:HA	1:1872:A:ASN:H	6	0.18
(1,187)	1:1846:A:VAL:H	1:1847:A:GLY:H	8	0.18
(1,161)	1:1817:A:TRP:HE3	1:1817:A:TRP:HZ2	1	0.18
(1,145)	1:1799:A:PHE:H	1:1800:A:HIS:H	6	0.18
(1,139)	1:1817:A:TRP:HA	1:1817:A:TRP:HD1	6	0.18
(1,138)	1:1817:A:TRP:HD1	1:1819:A:ALA:HA	3	0.18
(1,110)	1:1821:A:ILE:HA	1:1822:A:SER:H	7	0.18
(1,110)	1:1821:A:ILE:HA	1:1822:A:SER:H	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:1820:A:ASN:HB2	1:1821:A:ILE:H	6	0.18
(1,107)	1:1820:A:ASN:HB2	1:1821:A:ILE:H	7	0.18
(1,96)	1:1809:A:ILE:H	1:1809:A:ILE:HG12	7	0.18
(1,66)	1:1840:A:VAL:HG21	1:1850:A:CYS:HA	4	0.18
(1,66)	1:1840:A:VAL:HG22	1:1850:A:CYS:HA	4	0.18
(1,66)	1:1840:A:VAL:HG23	1:1850:A:CYS:HA	4	0.18
(1,8)	1:1871:A:ILE:HA	1:1872:A:ASN:H	3	0.18
(1,6)	1:1822:A:SER:H	1:1872:A:ASN:H	8	0.18
(1,1)	1:1793:A:ASP:HA	1:1794:A:SER:H	2	0.18
(1,1)	1:1793:A:ASP:HA	1:1794:A:SER:H	3	0.18
(1,707)	1:1791:A:TRP:HB2	1:1791:A:TRP:HD1	4	0.17
(1,705)	1:1792:A:LEU:H	1:1792:A:LEU:HA	6	0.17
(1,702)	1:1851:A:LYS:HA	1:1852:A:ASN:H	6	0.17
(1,653)	1:1833:A:ILE:HG21	1:1836:A:LEU:HD11	5	0.17
(1,653)	1:1833:A:ILE:HG21	1:1836:A:LEU:HD12	5	0.17
(1,653)	1:1833:A:ILE:HG21	1:1836:A:LEU:HD13	5	0.17
(1,653)	1:1833:A:ILE:HG22	1:1836:A:LEU:HD11	5	0.17
(1,653)	1:1833:A:ILE:HG22	1:1836:A:LEU:HD12	5	0.17
(1,653)	1:1833:A:ILE:HG22	1:1836:A:LEU:HD13	5	0.17
(1,653)	1:1833:A:ILE:HG23	1:1836:A:LEU:HD11	5	0.17
(1,653)	1:1833:A:ILE:HG23	1:1836:A:LEU:HD12	5	0.17
(1,653)	1:1833:A:ILE:HG23	1:1836:A:LEU:HD13	5	0.17
(1,644)	1:1846:A:VAL:H	1:1846:A:VAL:HB	7	0.17
(1,619)	1:1851:A:LYS:H	1:1851:A:LYS:HA	10	0.17
(1,614)	1:1821:A:ILE:HA	1:1873:A:VAL:HA	4	0.17
(1,596)	1:1869:A:TYR:HA	1:1869:A:TYR:HB2	9	0.17
(1,584)	1:1791:A:TRP:HB3	1:1791:A:TRP:HE3	9	0.17
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	2	0.17
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	2	0.17
(1,515)	1:1850:A:CYS:HB2	1:1850:A:CYS:HB3	8	0.17
(1,503)	1:1793:A:ASP:HA	1:1793:A:ASP:HB2	10	0.17
(1,498)	1:1841:A:VAL:HG21	1:1842:A:CYS:HA	3	0.17
(1,498)	1:1841:A:VAL:HG22	1:1842:A:CYS:HA	3	0.17
(1,498)	1:1841:A:VAL:HG23	1:1842:A:CYS:HA	3	0.17
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD21	6	0.17
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD22	6	0.17
(1,470)	1:1836:A:LEU:H	1:1836:A:LEU:HD23	6	0.17
(1,447)	1:1828:A:TYR:HA	1:1829:A:PRO:HD2	9	0.17
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB1	7	0.17
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB2	7	0.17
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB3	7	0.17
(1,400)	1:1848:A:LEU:H	1:1848:A:LEU:HA	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:1823:A:CYS:HA	1:1823:A:CYS:HB3	7	0.17
(1,283)	1:1871:A:ILE:H	1:1871:A:ILE:HG13	6	0.17
(1,273)	1:1823:A:CYS:HA	1:1823:A:CYS:HB2	2	0.17
(1,268)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	2	0.17
(1,260)	1:1829:A:PRO:HD2	1:1829:A:PRO:HG2	1	0.17
(1,259)	1:1829:A:PRO:HD3	1:1829:A:PRO:HG3	6	0.17
(1,253)	1:1877:A:GLU:H	1:1877:A:GLU:HB2	6	0.17
(1,245)	1:1868:A:ASN:HA	1:1869:A:TYR:H	5	0.17
(1,224)	1:1873:A:VAL:HA	1:1874:A:GLN:H	5	0.17
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD11	4	0.17
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD12	4	0.17
(1,175)	1:1828:A:TYR:HE1	1:1861:A:ILE:HD13	4	0.17
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD11	4	0.17
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD12	4	0.17
(1,175)	1:1828:A:TYR:HE2	1:1861:A:ILE:HD13	4	0.17
(1,162)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	10	0.17
(1,107)	1:1820:A:ASN:HB2	1:1821:A:ILE:H	9	0.17
(1,106)	1:1820:A:ASN:HB3	1:1821:A:ILE:H	1	0.17
(1,81)	1:1805:A:ASP:H	1:1850:A:CYS:H	5	0.17
(1,73)	1:1840:A:VAL:H	1:1840:A:VAL:HG11	3	0.17
(1,73)	1:1840:A:VAL:H	1:1840:A:VAL:HG12	3	0.17
(1,73)	1:1840:A:VAL:H	1:1840:A:VAL:HG13	3	0.17
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG21	8	0.17
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG22	8	0.17
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG23	8	0.17
(1,47)	1:1789:A:THR:H	1:1789:A:THR:HA	5	0.17
(1,3)	1:1794:A:SER:H	1:1795:A:GLY:H	10	0.17
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG21	9	0.16
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG22	9	0.16
(1,732)	1:1833:A:ILE:HG21	1:1840:A:VAL:HG23	9	0.16
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG21	9	0.16
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG22	9	0.16
(1,732)	1:1833:A:ILE:HG22	1:1840:A:VAL:HG23	9	0.16
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG21	9	0.16
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG22	9	0.16
(1,732)	1:1833:A:ILE:HG23	1:1840:A:VAL:HG23	9	0.16
(1,712)	1:1791:A:TRP:HZ3	1:1872:A:ASN:H	6	0.16
(1,707)	1:1791:A:TRP:HB2	1:1791:A:TRP:HD1	3	0.16
(1,675)	1:1836:A:LEU:HD11	1:1836:A:LEU:HD21	6	0.16
(1,675)	1:1836:A:LEU:HD11	1:1836:A:LEU:HD22	6	0.16
(1,675)	1:1836:A:LEU:HD11	1:1836:A:LEU:HD23	6	0.16
(1,675)	1:1836:A:LEU:HD12	1:1836:A:LEU:HD21	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	1:1836:A:LEU:HD12	1:1836:A:LEU:HD22	6	0.16
(1,675)	1:1836:A:LEU:HD12	1:1836:A:LEU:HD23	6	0.16
(1,675)	1:1836:A:LEU:HD13	1:1836:A:LEU:HD21	6	0.16
(1,675)	1:1836:A:LEU:HD13	1:1836:A:LEU:HD22	6	0.16
(1,675)	1:1836:A:LEU:HD13	1:1836:A:LEU:HD23	6	0.16
(1,662)	1:1848:A:LEU:HD21	1:1849:A:ILE:H	6	0.16
(1,662)	1:1848:A:LEU:HD22	1:1849:A:ILE:H	6	0.16
(1,662)	1:1848:A:LEU:HD23	1:1849:A:ILE:H	6	0.16
(1,650)	1:1848:A:LEU:HD11	1:1848:A:LEU:HG	3	0.16
(1,650)	1:1848:A:LEU:HD12	1:1848:A:LEU:HG	3	0.16
(1,650)	1:1848:A:LEU:HD13	1:1848:A:LEU:HG	3	0.16
(1,646)	1:1840:A:VAL:HG21	1:1850:A:CYS:HB3	8	0.16
(1,646)	1:1840:A:VAL:HG22	1:1850:A:CYS:HB3	8	0.16
(1,646)	1:1840:A:VAL:HG23	1:1850:A:CYS:HB3	8	0.16
(1,639)	1:1789:A:THR:HB	1:1789:A:THR:HG1	3	0.16
(1,621)	1:1869:A:TYR:HA	1:1870:A:GLU:H	5	0.16
(1,552)	1:1833:A:ILE:H	1:1833:A:ILE:HA	4	0.16
(1,541)	1:1823:A:CYS:HA	1:1823:A:CYS:HB2	9	0.16
(1,490)	1:1842:A:CYS:HA	1:1842:A:CYS:HB2	2	0.16
(1,490)	1:1842:A:CYS:HA	1:1842:A:CYS:HB2	9	0.16
(1,480)	1:1839:A:THR:H	1:1839:A:THR:HB	6	0.16
(1,477)	1:1839:A:THR:HA	1:1840:A:VAL:H	8	0.16
(1,438)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	1	0.16
(1,438)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	4	0.16
(1,438)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	7	0.16
(1,438)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	9	0.16
(1,428)	1:1820:A:ASN:H	1:1874:A:GLN:HB2	8	0.16
(1,416)	1:1829:A:PRO:HD2	1:1830:A:ASP:H	10	0.16
(1,390)	1:1823:A:CYS:HA	1:1823:A:CYS:HB3	4	0.16
(1,358)	1:1808:A:LEU:HA	1:1809:A:ILE:H	1	0.16
(1,343)	1:1870:A:GLU:H	1:1870:A:GLU:HA	10	0.16
(1,338)	1:1805:A:ASP:HA	1:1806:A:THR:H	10	0.16
(1,282)	1:1787:A:ASN:H	1:1787:A:ASN:HB2	5	0.16
(1,259)	1:1829:A:PRO:HD3	1:1829:A:PRO:HG3	1	0.16
(1,259)	1:1829:A:PRO:HD3	1:1829:A:PRO:HG3	2	0.16
(1,255)	1:1782:A:CYS:HA	1:1782:A:CYS:HB2	6	0.16
(1,253)	1:1877:A:GLU:H	1:1877:A:GLU:HB2	7	0.16
(1,250)	1:1876:A:CYS:HA	1:1877:A:GLU:H	5	0.16
(1,250)	1:1876:A:CYS:HA	1:1877:A:GLU:H	6	0.16
(1,223)	1:1829:A:PRO:HG2	1:1830:A:ASP:H	5	0.16
(1,181)	1:1830:A:ASP:H	1:1831:A:VAL:H	3	0.16
(1,163)	1:1788:A:TRP:HB3	1:1788:A:TRP:HE3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:1788:A:TRP:HB3	1:1788:A:TRP:HE3	7	0.16
(1,160)	1:1817:A:TRP:HE3	1:1817:A:TRP:HH2	9	0.16
(1,143)	1:1788:A:TRP:HB3	1:1788:A:TRP:HD1	10	0.16
(1,124)	1:1821:A:ILE:HA	1:1822:A:SER:H	1	0.16
(1,124)	1:1821:A:ILE:HA	1:1822:A:SER:H	2	0.16
(1,124)	1:1821:A:ILE:HA	1:1822:A:SER:H	4	0.16
(1,66)	1:1840:A:VAL:HG21	1:1850:A:CYS:HA	5	0.16
(1,66)	1:1840:A:VAL:HG22	1:1850:A:CYS:HA	5	0.16
(1,66)	1:1840:A:VAL:HG23	1:1850:A:CYS:HA	5	0.16
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG21	6	0.16
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG22	6	0.16
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG23	6	0.16
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG11	7	0.16
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG12	7	0.16
(1,55)	1:1840:A:VAL:HB	1:1840:A:VAL:HG13	7	0.16
(1,20)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	2	0.16
(1,20)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	8	0.16
(1,20)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	9	0.16
(1,1)	1:1793:A:ASP:HA	1:1794:A:SER:H	9	0.16
(1,1)	1:1793:A:ASP:HA	1:1794:A:SER:H	10	0.16
(1,707)	1:1791:A:TRP:HB2	1:1791:A:TRP:HD1	7	0.15
(1,638)	1:1793:A:ASP:HA	1:1794:A:SER:H	5	0.15
(1,629)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD11	4	0.15
(1,629)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD12	4	0.15
(1,629)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD13	4	0.15
(1,629)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD11	4	0.15
(1,629)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD12	4	0.15
(1,629)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD13	4	0.15
(1,621)	1:1869:A:TYR:HA	1:1870:A:GLU:H	6	0.15
(1,577)	1:1878:A:CYS:HA	1:1878:A:CYS:HB2	10	0.15
(1,562)	1:1842:A:CYS:HA	1:1842:A:CYS:HB2	10	0.15
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG21	1	0.15
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG22	1	0.15
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG23	1	0.15
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG21	2	0.15
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG22	2	0.15
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG23	2	0.15
(1,544)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	1	0.15
(1,544)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	8	0.15
(1,538)	1:1879:A:VAL:H	1:1879:A:VAL:HG21	4	0.15
(1,538)	1:1879:A:VAL:H	1:1879:A:VAL:HG22	4	0.15
(1,538)	1:1879:A:VAL:H	1:1879:A:VAL:HG23	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:1850:A:CYS:HA	1:1850:A:CYS:HB2	2	0.15
(1,515)	1:1850:A:CYS:HB2	1:1850:A:CYS:HB3	5	0.15
(1,490)	1:1842:A:CYS:HA	1:1842:A:CYS:HB2	6	0.15
(1,482)	1:1838:A:GLN:H	1:1838:A:GLN:HB2	4	0.15
(1,479)	1:1838:A:GLN:HA	1:1839:A:THR:H	3	0.15
(1,453)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	10	0.15
(1,438)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	2	0.15
(1,417)	1:1818:A:ALA:HA	1:1819:A:ALA:H	8	0.15
(1,400)	1:1848:A:LEU:H	1:1848:A:LEU:HA	1	0.15
(1,398)	1:1823:A:CYS:HA	1:1824:A:ARG:H	1	0.15
(1,388)	1:1791:A:TRP:HZ3	1:1823:A:CYS:HA	9	0.15
(1,352)	1:1812:A:VAL:H	1:1813:A:CYS:H	3	0.15
(1,337)	1:1806:A:THR:H	1:1806:A:THR:HA	2	0.15
(1,337)	1:1806:A:THR:H	1:1806:A:THR:HA	3	0.15
(1,337)	1:1806:A:THR:H	1:1806:A:THR:HA	4	0.15
(1,305)	1:1790:A:GLY:H	1:1790:A:GLY:HA2	5	0.15
(1,282)	1:1787:A:ASN:H	1:1787:A:ASN:HB2	9	0.15
(1,268)	1:1786:A:CYS:HA	1:1786:A:CYS:HB3	1	0.15
(1,259)	1:1829:A:PRO:HD3	1:1829:A:PRO:HG3	4	0.15
(1,259)	1:1829:A:PRO:HD3	1:1829:A:PRO:HG3	8	0.15
(1,204)	1:1848:A:LEU:HA	1:1849:A:ILE:H	6	0.15
(1,198)	1:1843:A:ASP:H	1:1847:A:GLY:H	7	0.15
(1,181)	1:1830:A:ASP:H	1:1831:A:VAL:H	5	0.15
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD11	2	0.15
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD12	2	0.15
(1,176)	1:1828:A:TYR:HE1	1:1836:A:LEU:HD13	2	0.15
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD11	2	0.15
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD12	2	0.15
(1,176)	1:1828:A:TYR:HE2	1:1836:A:LEU:HD13	2	0.15
(1,163)	1:1788:A:TRP:HB3	1:1788:A:TRP:HE3	9	0.15
(1,145)	1:1799:A:PHE:H	1:1800:A:HIS:H	1	0.15
(1,124)	1:1821:A:ILE:HA	1:1822:A:SER:H	6	0.15
(1,101)	1:1823:A:CYS:HA	1:1824:A:ARG:H	1	0.15
(1,96)	1:1809:A:ILE:H	1:1809:A:ILE:HG12	8	0.15
(1,45)	1:1789:A:THR:H	1:1789:A:THR:HG1	8	0.15
(1,723)	1:1788:A:TRP:HE3	1:1788:A:TRP:HH2	6	0.14
(1,723)	1:1788:A:TRP:HE3	1:1788:A:TRP:HH2	7	0.14
(1,673)	1:1848:A:LEU:HD21	1:1848:A:LEU:HG	10	0.14
(1,673)	1:1848:A:LEU:HD22	1:1848:A:LEU:HG	10	0.14
(1,673)	1:1848:A:LEU:HD23	1:1848:A:LEU:HG	10	0.14
(1,650)	1:1848:A:LEU:HD11	1:1848:A:LEU:HG	6	0.14
(1,650)	1:1848:A:LEU:HD12	1:1848:A:LEU:HG	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,650)	1:1848:A:LEU:HD13	1:1848:A:LEU:HG	6	0.14
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD21	5	0.14
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD22	5	0.14
(1,632)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD23	5	0.14
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD21	5	0.14
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD22	5	0.14
(1,632)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD23	5	0.14
(1,619)	1:1851:A:LYS:H	1:1851:A:LYS:HA	3	0.14
(1,617)	1:1847:A:GLY:HA3	1:1848:A:LEU:H	6	0.14
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG21	4	0.14
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG22	4	0.14
(1,557)	1:1833:A:ILE:HA	1:1833:A:ILE:HG23	4	0.14
(1,515)	1:1850:A:CYS:HB2	1:1850:A:CYS:HB3	1	0.14
(1,506)	1:1842:A:CYS:HA	1:1849:A:ILE:H	3	0.14
(1,506)	1:1842:A:CYS:HA	1:1849:A:ILE:H	9	0.14
(1,438)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	5	0.14
(1,438)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	6	0.14
(1,438)	1:1828:A:TYR:HB2	1:1828:A:TYR:HB3	10	0.14
(1,426)	1:1819:A:ALA:HB1	1:1820:A:ASN:H	9	0.14
(1,426)	1:1819:A:ALA:HB2	1:1820:A:ASN:H	9	0.14
(1,426)	1:1819:A:ALA:HB3	1:1820:A:ASN:H	9	0.14
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB1	4	0.14
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB2	4	0.14
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB3	4	0.14
(1,416)	1:1829:A:PRO:HD2	1:1830:A:ASP:H	6	0.14
(1,398)	1:1823:A:CYS:HA	1:1824:A:ARG:H	9	0.14
(1,390)	1:1823:A:CYS:HA	1:1823:A:CYS:HB3	2	0.14
(1,388)	1:1791:A:TRP:HZ3	1:1823:A:CYS:HA	7	0.14
(1,359)	1:1809:A:ILE:H	1:1809:A:ILE:HB	1	0.14
(1,337)	1:1806:A:THR:H	1:1806:A:THR:HA	5	0.14
(1,337)	1:1806:A:THR:H	1:1806:A:THR:HA	9	0.14
(1,316)	1:1790:A:GLY:HA2	1:1791:A:TRP:H	8	0.14
(1,287)	1:1786:A:CYS:HB3	1:1787:A:ASN:H	4	0.14
(1,282)	1:1787:A:ASN:H	1:1787:A:ASN:HB2	7	0.14
(1,282)	1:1787:A:ASN:H	1:1787:A:ASN:HB2	8	0.14
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG21	7	0.14
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG22	7	0.14
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG23	7	0.14
(1,245)	1:1868:A:ASN:HA	1:1869:A:TYR:H	6	0.14
(1,245)	1:1868:A:ASN:HA	1:1869:A:TYR:H	7	0.14
(1,206)	1:1842:A:CYS:HA	1:1849:A:ILE:H	3	0.14
(1,206)	1:1842:A:CYS:HA	1:1849:A:ILE:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:1848:A:LEU:HA	1:1849:A:ILE:H	8	0.14
(1,191)	1:1871:A:ILE:HA	1:1872:A:ASN:H	1	0.14
(1,181)	1:1830:A:ASP:H	1:1831:A:VAL:H	8	0.14
(1,163)	1:1788:A:TRP:HB3	1:1788:A:TRP:HE3	3	0.14
(1,163)	1:1788:A:TRP:HB3	1:1788:A:TRP:HE3	5	0.14
(1,147)	1:1791:A:TRP:HZ2	1:1791:A:TRP:HZ3	3	0.14
(1,122)	1:1805:A:ASP:HA	1:1806:A:THR:H	5	0.14
(1,104)	1:1820:A:ASN:HA	1:1821:A:ILE:H	9	0.14
(1,101)	1:1823:A:CYS:HA	1:1824:A:ARG:H	9	0.14
(1,87)	1:1808:A:LEU:H	1:1808:A:LEU:HG	7	0.14
(1,86)	1:1812:A:VAL:HG11	1:1813:A:CYS:H	7	0.14
(1,86)	1:1812:A:VAL:HG12	1:1813:A:CYS:H	7	0.14
(1,86)	1:1812:A:VAL:HG13	1:1813:A:CYS:H	7	0.14
(1,81)	1:1805:A:ASP:H	1:1850:A:CYS:H	1	0.14
(1,47)	1:1789:A:THR:H	1:1789:A:THR:HA	9	0.14
(1,20)	1:1817:A:TRP:HB2	1:1817:A:TRP:HD1	7	0.14
(1,8)	1:1871:A:ILE:HA	1:1872:A:ASN:H	6	0.14
(1,5)	1:1822:A:SER:H	1:1872:A:ASN:H	7	0.14
(1,3)	1:1794:A:SER:H	1:1795:A:GLY:H	2	0.14
(1,1)	1:1793:A:ASP:HA	1:1794:A:SER:H	1	0.14
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD11	1	0.13
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD12	1	0.13
(1,661)	1:1848:A:LEU:HA	1:1848:A:LEU:HD13	1	0.13
(1,638)	1:1793:A:ASP:HA	1:1794:A:SER:H	7	0.13
(1,617)	1:1847:A:GLY:HA3	1:1848:A:LEU:H	3	0.13
(1,592)	1:1799:A:PHE:H	1:1799:A:PHE:HB2	3	0.13
(1,584)	1:1791:A:TRP:HB3	1:1791:A:TRP:HE3	8	0.13
(1,573)	1:1842:A:CYS:H	1:1842:A:CYS:HB3	1	0.13
(1,570)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD11	3	0.13
(1,570)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD12	3	0.13
(1,570)	1:1823:A:CYS:HB2	1:1848:A:LEU:HD13	3	0.13
(1,567)	1:1793:A:ASP:H	1:1793:A:ASP:HB3	1	0.13
(1,552)	1:1833:A:ILE:H	1:1833:A:ILE:HA	7	0.13
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG21	7	0.13
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG22	7	0.13
(1,551)	1:1833:A:ILE:H	1:1833:A:ILE:HG23	7	0.13
(1,544)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	2	0.13
(1,544)	1:1788:A:TRP:HB2	1:1788:A:TRP:HE3	5	0.13
(1,537)	1:1875:A:CYS:HA	1:1875:A:CYS:HB3	3	0.13
(1,515)	1:1850:A:CYS:HB2	1:1850:A:CYS:HB3	6	0.13
(1,510)	1:1842:A:CYS:HB2	1:1842:A:CYS:HB3	1	0.13
(1,484)	1:1838:A:GLN:HB3	1:1839:A:THR:H	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:1839:A:THR:HA	1:1840:A:VAL:H	2	0.13
(1,477)	1:1839:A:THR:HA	1:1840:A:VAL:H	4	0.13
(1,472)	1:1836:A:LEU:H	1:1836:A:LEU:HG	4	0.13
(1,472)	1:1836:A:LEU:H	1:1836:A:LEU:HG	7	0.13
(1,472)	1:1836:A:LEU:H	1:1836:A:LEU:HG	9	0.13
(1,453)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	4	0.13
(1,425)	1:1820:A:ASN:H	1:1820:A:ASN:HB3	2	0.13
(1,413)	1:1830:A:ASP:H	1:1830:A:ASP:HB3	5	0.13
(1,410)	1:1815:A:PRO:HG2	1:1816:A:GLY:H	4	0.13
(1,390)	1:1823:A:CYS:HA	1:1823:A:CYS:HB3	1	0.13
(1,375)	1:1812:A:VAL:H	1:1814:A:GLY:H	10	0.13
(1,338)	1:1805:A:ASP:HA	1:1806:A:THR:H	1	0.13
(1,337)	1:1806:A:THR:H	1:1806:A:THR:HA	1	0.13
(1,336)	1:1806:A:THR:H	1:1806:A:THR:HB	9	0.13
(1,331)	1:1805:A:ASP:H	1:1805:A:ASP:HA	8	0.13
(1,277)	1:1786:A:CYS:HA	1:1786:A:CYS:HB2	2	0.13
(1,277)	1:1786:A:CYS:HA	1:1786:A:CYS:HB2	9	0.13
(1,271)	1:1876:A:CYS:HA	1:1877:A:GLU:H	5	0.13
(1,271)	1:1876:A:CYS:HA	1:1877:A:GLU:H	6	0.13
(1,262)	1:1823:A:CYS:HA	1:1871:A:ILE:HA	10	0.13
(1,260)	1:1829:A:PRO:HD2	1:1829:A:PRO:HG2	9	0.13
(1,254)	1:1877:A:GLU:H	1:1877:A:GLU:HB3	5	0.13
(1,245)	1:1868:A:ASN:HA	1:1869:A:TYR:H	2	0.13
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD1	6	0.13
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD1	6	0.13
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD1	6	0.13
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD2	6	0.13
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD2	6	0.13
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD2	6	0.13
(1,233)	1:1799:A:PHE:H	1:1799:A:PHE:HA	7	0.13
(1,207)	1:1840:A:VAL:HA	1:1841:A:VAL:H	7	0.13
(1,204)	1:1848:A:LEU:HA	1:1849:A:ILE:H	2	0.13
(1,187)	1:1846:A:VAL:H	1:1847:A:GLY:H	2	0.13
(1,187)	1:1846:A:VAL:H	1:1847:A:GLY:H	6	0.13
(1,186)	1:1845:A:SER:H	1:1846:A:VAL:H	3	0.13
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	10	0.13
(1,170)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	10	0.13
(1,163)	1:1788:A:TRP:HB3	1:1788:A:TRP:HE3	2	0.13
(1,161)	1:1817:A:TRP:HE3	1:1817:A:TRP:HZ2	2	0.13
(1,160)	1:1817:A:TRP:HE3	1:1817:A:TRP:HH2	2	0.13
(1,160)	1:1817:A:TRP:HE3	1:1817:A:TRP:HH2	6	0.13
(1,156)	1:1791:A:TRP:HB2	1:1791:A:TRP:HE3	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	1:1788:A:TRP:HB2	1:1788:A:TRP:HD1	6	0.13
(1,138)	1:1817:A:TRP:HD1	1:1819:A:ALA:HA	1	0.13
(1,122)	1:1805:A:ASP:HA	1:1806:A:THR:H	8	0.13
(1,117)	1:1821:A:ILE:HG12	1:1822:A:SER:H	7	0.13
(1,117)	1:1821:A:ILE:HG12	1:1822:A:SER:H	8	0.13
(1,113)	1:1822:A:SER:H	1:1822:A:SER:HB2	8	0.13
(1,99)	1:1791:A:TRP:HZ3	1:1824:A:ARG:H	8	0.13
(1,95)	1:1809:A:ILE:H	1:1809:A:ILE:HB	1	0.13
(1,79)	1:1850:A:CYS:H	1:1850:A:CYS:HB2	8	0.13
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG21	3	0.13
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG22	3	0.13
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG23	3	0.13
(1,47)	1:1789:A:THR:H	1:1789:A:THR:HA	3	0.13
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	10	0.13
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	10	0.13
(1,727)	1:1874:A:GLN:HB3	1:1874:A:GLN:HG2	4	0.12
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD1	3	0.12
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD1	3	0.12
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD1	3	0.12
(1,681)	1:1864:A:ALA:HB1	1:1865:A:PHE:HD2	3	0.12
(1,681)	1:1864:A:ALA:HB2	1:1865:A:PHE:HD2	3	0.12
(1,681)	1:1864:A:ALA:HB3	1:1865:A:PHE:HD2	3	0.12
(1,638)	1:1793:A:ASP:HA	1:1794:A:SER:H	3	0.12
(1,619)	1:1851:A:LYS:H	1:1851:A:LYS:HA	4	0.12
(1,617)	1:1847:A:GLY:HA3	1:1848:A:LEU:H	5	0.12
(1,593)	1:1791:A:TRP:H	1:1791:A:TRP:HB2	4	0.12
(1,592)	1:1799:A:PHE:H	1:1799:A:PHE:HB2	9	0.12
(1,584)	1:1791:A:TRP:HB3	1:1791:A:TRP:HE3	2	0.12
(1,584)	1:1791:A:TRP:HB3	1:1791:A:TRP:HE3	10	0.12
(1,567)	1:1793:A:ASP:H	1:1793:A:ASP:HB3	5	0.12
(1,541)	1:1823:A:CYS:HA	1:1823:A:CYS:HB2	4	0.12
(1,515)	1:1850:A:CYS:HB2	1:1850:A:CYS:HB3	7	0.12
(1,413)	1:1830:A:ASP:H	1:1830:A:ASP:HB3	4	0.12
(1,400)	1:1848:A:LEU:H	1:1848:A:LEU:HA	10	0.12
(1,390)	1:1823:A:CYS:HA	1:1823:A:CYS:HB3	3	0.12
(1,374)	1:1808:A:LEU:HD21	1:1810:A:GLY:H	10	0.12
(1,374)	1:1808:A:LEU:HD22	1:1810:A:GLY:H	10	0.12
(1,374)	1:1808:A:LEU:HD23	1:1810:A:GLY:H	10	0.12
(1,341)	1:1806:A:THR:HA	1:1807:A:GLU:H	1	0.12
(1,334)	1:1805:A:ASP:H	1:1805:A:ASP:HB2	2	0.12
(1,328)	1:1791:A:TRP:HZ2	1:1822:A:SER:HB3	5	0.12
(1,316)	1:1790:A:GLY:HA2	1:1791:A:TRP:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:1790:A:GLY:HA2	1:1791:A:TRP:H	9	0.12
(1,305)	1:1790:A:GLY:H	1:1790:A:GLY:HA2	3	0.12
(1,259)	1:1829:A:PRO:HD3	1:1829:A:PRO:HG3	9	0.12
(1,259)	1:1829:A:PRO:HD3	1:1829:A:PRO:HG3	10	0.12
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD1	4	0.12
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD1	4	0.12
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD1	4	0.12
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD2	4	0.12
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD2	4	0.12
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD2	4	0.12
(1,204)	1:1848:A:LEU:HA	1:1849:A:ILE:H	5	0.12
(1,197)	1:1789:A:THR:H	1:1873:A:VAL:H	10	0.12
(1,192)	1:1789:A:THR:HG1	1:1873:A:VAL:H	8	0.12
(1,173)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD11	10	0.12
(1,173)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD12	10	0.12
(1,173)	1:1828:A:TYR:HE1	1:1867:A:LEU:HD13	10	0.12
(1,173)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD11	10	0.12
(1,173)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD12	10	0.12
(1,173)	1:1828:A:TYR:HE2	1:1867:A:LEU:HD13	10	0.12
(1,161)	1:1817:A:TRP:HE3	1:1817:A:TRP:HZ2	6	0.12
(1,124)	1:1821:A:ILE:HA	1:1822:A:SER:H	10	0.12
(1,119)	1:1821:A:ILE:H	1:1822:A:SER:H	1	0.12
(1,110)	1:1821:A:ILE:HA	1:1822:A:SER:H	2	0.12
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG21	9	0.12
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG22	9	0.12
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG23	9	0.12
(1,47)	1:1789:A:THR:H	1:1789:A:THR:HA	4	0.12
(1,47)	1:1789:A:THR:H	1:1789:A:THR:HA	6	0.12
(1,47)	1:1789:A:THR:H	1:1789:A:THR:HA	8	0.12
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	7	0.12
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	7	0.12
(1,7)	1:1791:A:TRP:HZ3	1:1872:A:ASN:H	9	0.12
(1,3)	1:1794:A:SER:H	1:1795:A:GLY:H	9	0.12
(1,727)	1:1874:A:GLN:HB3	1:1874:A:GLN:HG2	10	0.11
(1,707)	1:1791:A:TRP:HB2	1:1791:A:TRP:HD1	8	0.11
(1,707)	1:1791:A:TRP:HB2	1:1791:A:TRP:HD1	10	0.11
(1,664)	1:1848:A:LEU:HD21	1:1869:A:TYR:HB3	10	0.11
(1,664)	1:1848:A:LEU:HD22	1:1869:A:TYR:HB3	10	0.11
(1,664)	1:1848:A:LEU:HD23	1:1869:A:TYR:HB3	10	0.11
(1,638)	1:1793:A:ASP:HA	1:1794:A:SER:H	2	0.11
(1,621)	1:1869:A:TYR:HA	1:1870:A:GLU:H	8	0.11
(1,617)	1:1847:A:GLY:HA3	1:1848:A:LEU:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:1821:A:ILE:HA	1:1873:A:VAL:HA	10	0.11
(1,588)	1:1817:A:TRP:HB2	1:1817:A:TRP:HE3	3	0.11
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE1	10	0.11
(1,580)	1:1828:A:TYR:HB2	1:1828:A:TYR:HE2	10	0.11
(1,525)	1:1865:A:PHE:HA	1:1865:A:PHE:HB2	9	0.11
(1,515)	1:1850:A:CYS:HB2	1:1850:A:CYS:HB3	10	0.11
(1,490)	1:1842:A:CYS:HA	1:1842:A:CYS:HB2	4	0.11
(1,490)	1:1842:A:CYS:HA	1:1842:A:CYS:HB2	7	0.11
(1,460)	1:1832:A:PRO:HB3	1:1835:A:GLN:H	3	0.11
(1,453)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	3	0.11
(1,453)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	5	0.11
(1,453)	1:1828:A:TYR:HA	1:1828:A:TYR:HB3	8	0.11
(1,447)	1:1828:A:TYR:HA	1:1829:A:PRO:HD2	4	0.11
(1,417)	1:1818:A:ALA:HA	1:1819:A:ALA:H	5	0.11
(1,417)	1:1818:A:ALA:HA	1:1819:A:ALA:H	9	0.11
(1,400)	1:1848:A:LEU:H	1:1848:A:LEU:HA	3	0.11
(1,396)	1:1871:A:ILE:HA	1:1871:A:ILE:HG21	8	0.11
(1,396)	1:1871:A:ILE:HA	1:1871:A:ILE:HG22	8	0.11
(1,396)	1:1871:A:ILE:HA	1:1871:A:ILE:HG23	8	0.11
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD11	6	0.11
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD12	6	0.11
(1,392)	1:1823:A:CYS:HA	1:1848:A:LEU:HD13	6	0.11
(1,390)	1:1823:A:CYS:HA	1:1823:A:CYS:HB3	9	0.11
(1,387)	1:1791:A:TRP:HE3	1:1871:A:ILE:HA	1	0.11
(1,337)	1:1806:A:THR:H	1:1806:A:THR:HA	10	0.11
(1,289)	1:1870:A:GLU:HA	1:1871:A:ILE:H	8	0.11
(1,282)	1:1787:A:ASN:H	1:1787:A:ASN:HB2	4	0.11
(1,277)	1:1786:A:CYS:HA	1:1786:A:CYS:HB2	7	0.11
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG21	9	0.11
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG22	9	0.11
(1,274)	1:1823:A:CYS:HA	1:1871:A:ILE:HG23	9	0.11
(1,265)	1:1823:A:CYS:HA	1:1871:A:ILE:HA	10	0.11
(1,260)	1:1829:A:PRO:HD2	1:1829:A:PRO:HG2	4	0.11
(1,260)	1:1829:A:PRO:HD2	1:1829:A:PRO:HG2	8	0.11
(1,259)	1:1829:A:PRO:HD3	1:1829:A:PRO:HG3	3	0.11
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD1	10	0.11
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD1	10	0.11
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD1	10	0.11
(1,234)	1:1825:A:ALA:HB1	1:1828:A:TYR:HD2	10	0.11
(1,234)	1:1825:A:ALA:HB2	1:1828:A:TYR:HD2	10	0.11
(1,234)	1:1825:A:ALA:HB3	1:1828:A:TYR:HD2	10	0.11
(1,233)	1:1799:A:PHE:H	1:1799:A:PHE:HA	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:1873:A:VAL:HA	1:1874:A:GLN:H	4	0.11
(1,196)	1:1789:A:THR:H	1:1790:A:GLY:H	10	0.11
(1,190)	1:1848:A:LEU:HA	1:1849:A:ILE:H	6	0.11
(1,187)	1:1846:A:VAL:H	1:1847:A:GLY:H	5	0.11
(1,182)	1:1830:A:ASP:H	1:1831:A:VAL:H	4	0.11
(1,156)	1:1791:A:TRP:HB2	1:1791:A:TRP:HE3	4	0.11
(1,142)	1:1788:A:TRP:HB2	1:1788:A:TRP:HD1	2	0.11
(1,142)	1:1788:A:TRP:HB2	1:1788:A:TRP:HD1	5	0.11
(1,142)	1:1788:A:TRP:HB2	1:1788:A:TRP:HD1	9	0.11
(1,110)	1:1821:A:ILE:HA	1:1822:A:SER:H	1	0.11
(1,110)	1:1821:A:ILE:HA	1:1822:A:SER:H	4	0.11
(1,110)	1:1821:A:ILE:HA	1:1822:A:SER:H	6	0.11
(1,96)	1:1809:A:ILE:H	1:1809:A:ILE:HG12	4	0.11
(1,78)	1:1841:A:VAL:HA	1:1842:A:CYS:H	1	0.11
(1,78)	1:1841:A:VAL:HA	1:1842:A:CYS:H	9	0.11
(1,72)	1:1840:A:VAL:HG21	1:1841:A:VAL:H	3	0.11
(1,72)	1:1840:A:VAL:HG22	1:1841:A:VAL:H	3	0.11
(1,72)	1:1840:A:VAL:HG23	1:1841:A:VAL:H	3	0.11
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG21	5	0.11
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG22	5	0.11
(1,65)	1:1840:A:VAL:H	1:1840:A:VAL:HG23	5	0.11
(1,63)	1:1840:A:VAL:HG21	1:1841:A:VAL:H	3	0.11
(1,63)	1:1840:A:VAL:HG22	1:1841:A:VAL:H	3	0.11
(1,63)	1:1840:A:VAL:HG23	1:1841:A:VAL:H	3	0.11
(1,47)	1:1789:A:THR:H	1:1789:A:THR:HA	2	0.11
(1,47)	1:1789:A:THR:H	1:1789:A:THR:HA	7	0.11
(1,10)	1:1872:A:ASN:H	1:1872:A:ASN:HB2	4	0.11
(1,8)	1:1871:A:ILE:HA	1:1872:A:ASN:H	1	0.11
(1,1)	1:1793:A:ASP:HA	1:1794:A:SER:H	4	0.11
(1,1)	1:1793:A:ASP:HA	1:1794:A:SER:H	6	0.11
(1,584)	1:1791:A:TRP:HB3	1:1791:A:TRP:HE3	6	0.1
(1,447)	1:1828:A:TYR:HA	1:1829:A:PRO:HD2	8	0.1
(1,425)	1:1820:A:ASN:H	1:1820:A:ASN:HB3	8	0.1
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB1	5	0.1
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB2	5	0.1
(1,419)	1:1819:A:ALA:H	1:1819:A:ALA:HB3	5	0.1
(1,417)	1:1818:A:ALA:HA	1:1819:A:ALA:H	1	0.1
(1,417)	1:1818:A:ALA:HA	1:1819:A:ALA:H	7	0.1
(1,413)	1:1830:A:ASP:H	1:1830:A:ASP:HB3	7	0.1
(1,284)	1:1871:A:ILE:H	1:1871:A:ILE:HG12	8	0.1
(1,182)	1:1830:A:ASP:H	1:1831:A:VAL:H	1	0.1
(1,182)	1:1830:A:ASP:H	1:1831:A:VAL:H	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:1788:A:TRP:HB3	1:1788:A:TRP:HE3	1	0.1
(1,160)	1:1817:A:TRP:HE3	1:1817:A:TRP:HH2	5	0.1
(1,79)	1:1850:A:CYS:H	1:1850:A:CYS:HB2	2	0.1
(1,59)	1:1840:A:VAL:HG11	1:1841:A:VAL:HA	1	0.1
(1,59)	1:1840:A:VAL:HG12	1:1841:A:VAL:HA	1	0.1
(1,59)	1:1840:A:VAL:HG13	1:1841:A:VAL:HA	1	0.1
(1,47)	1:1789:A:THR:H	1:1789:A:THR:HA	10	0.1
(1,34)	1:1791:A:TRP:HA	1:1792:A:LEU:H	1	0.1
(1,34)	1:1791:A:TRP:HA	1:1792:A:LEU:H	2	0.1
(1,30)	1:1789:A:THR:H	1:1873:A:VAL:H	4	0.1
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD1	9	0.1
(1,25)	1:1865:A:PHE:HB3	1:1865:A:PHE:HD2	9	0.1
(1,5)	1:1822:A:SER:H	1:1872:A:ASN:H	6	0.1

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

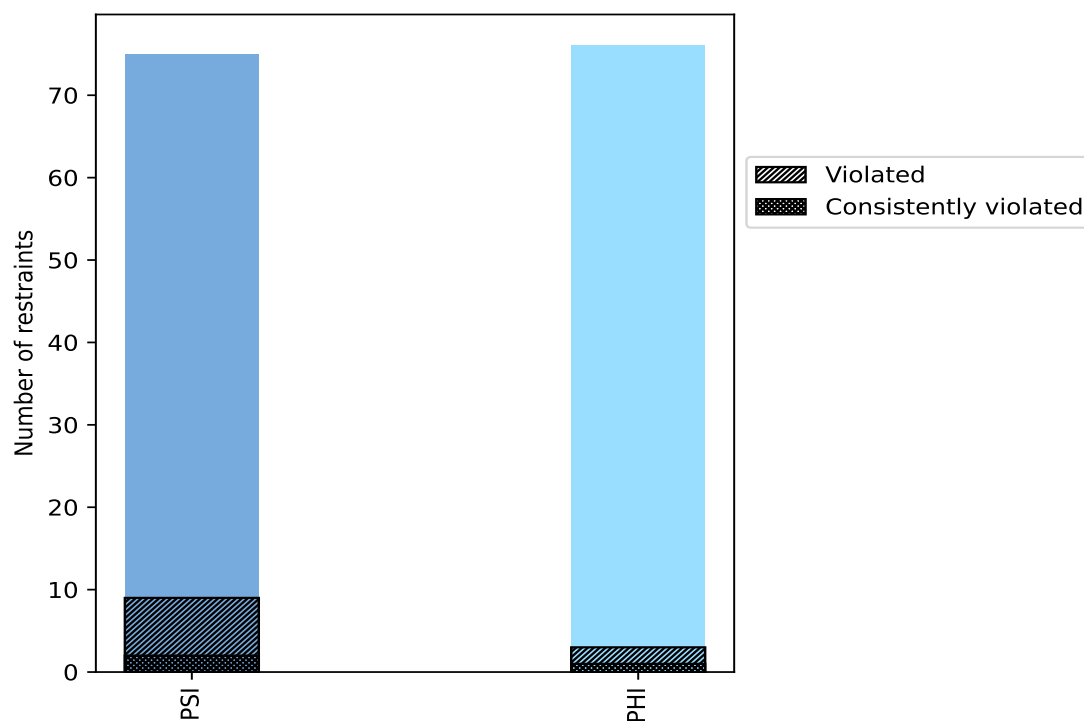
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	75	49.7	9	12.0	6.0	2	2.7	1.3
PHI	76	50.3	3	3.9	2.0	1	1.3	0.7
Total	151	100.0	12	7.9	7.9	3	2.0	2.0

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](#)



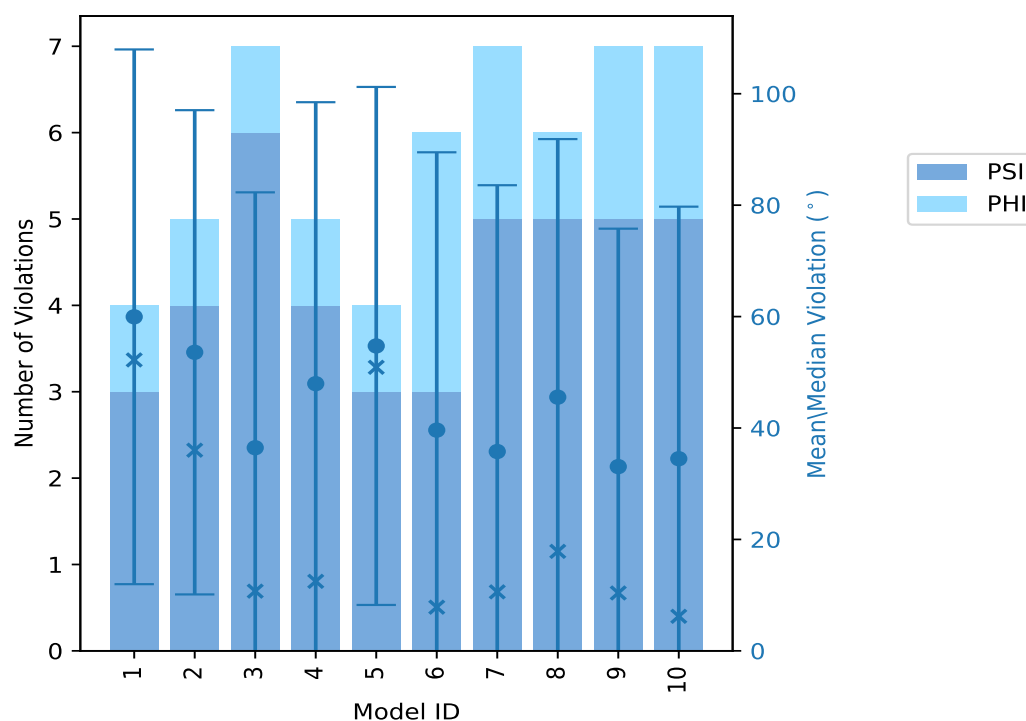
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

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 (°)
	PSI	PHI	Total				
1	3	1	4	59.96	124.76	47.99	52.22
2	4	1	5	53.59	118.33	43.46	36.02
3	6	1	7	36.46	129.22	45.84	10.72
4	4	1	5	47.96	127.17	50.52	12.48
5	3	1	4	54.73	110.03	46.49	50.9
6	3	3	6	39.62	121.77	49.87	7.84
7	5	2	7	35.78	130.56	47.8	10.59
8	5	1	6	45.54	129.7	46.32	17.86
9	5	2	7	33.07	112.66	42.71	10.39
10	5	2	7	34.49	113.74	45.24	6.2

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

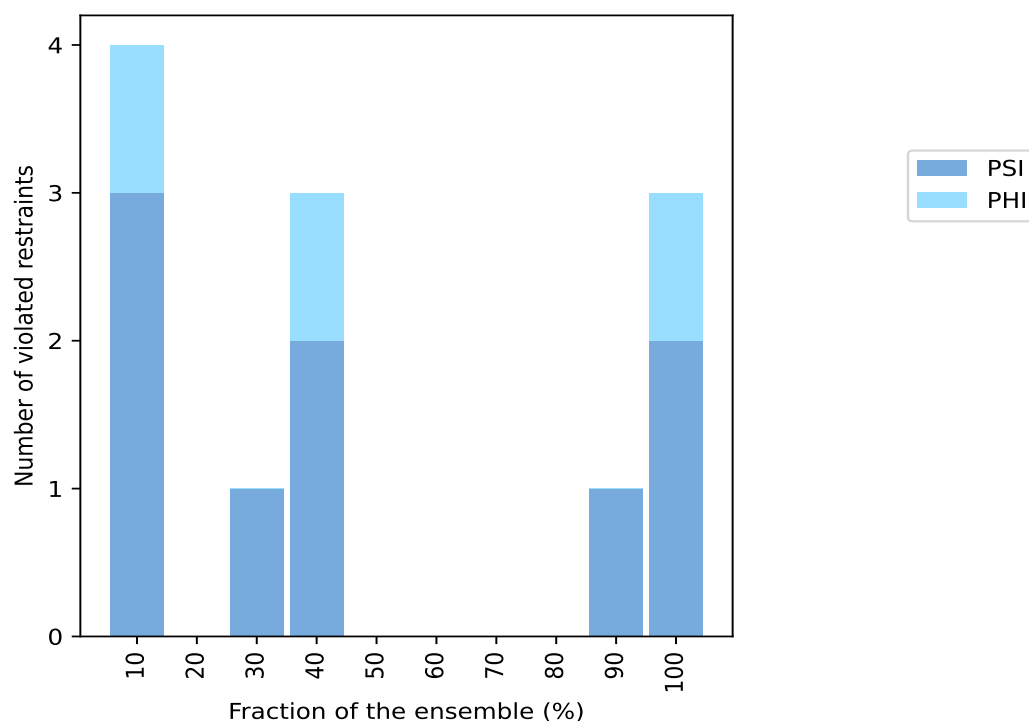
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	
PSI	PHI	Total	Count ¹	%
3	1	4	1	10.0
0	0	0	2	20.0
1	0	1	3	30.0
2	1	3	4	40.0
0	0	0	5	50.0
0	0	0	6	60.0
0	0	0	7	70.0
0	0	0	8	80.0
1	0	1	9	90.0
2	1	3	10	100.0

¹ Number of models with violations

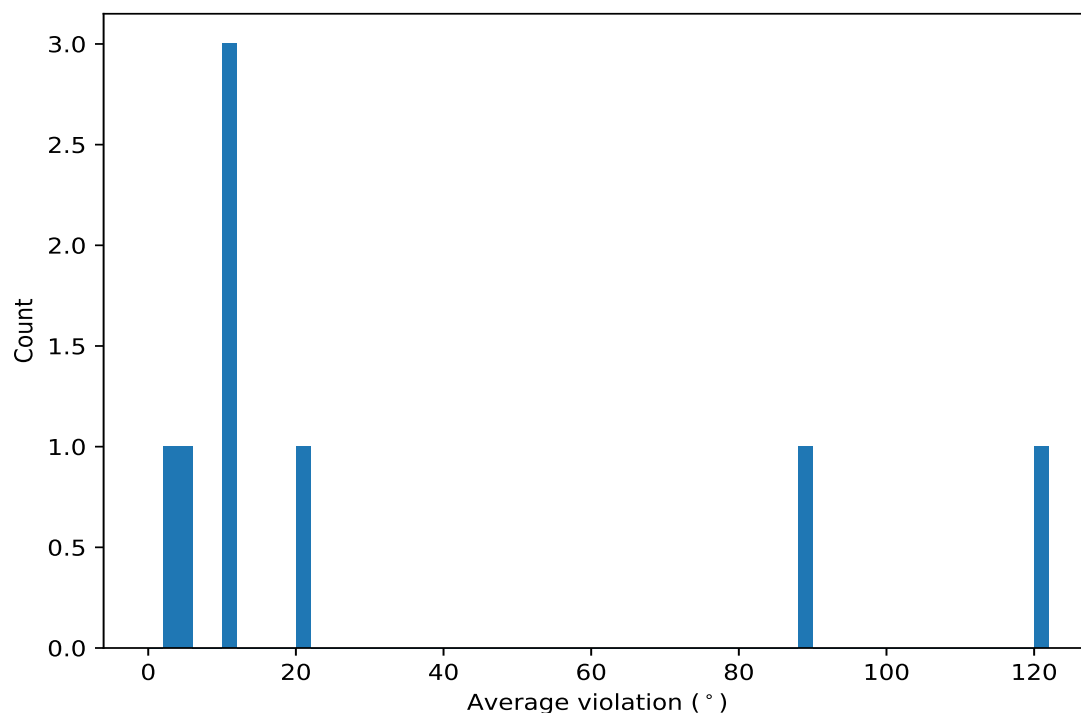
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

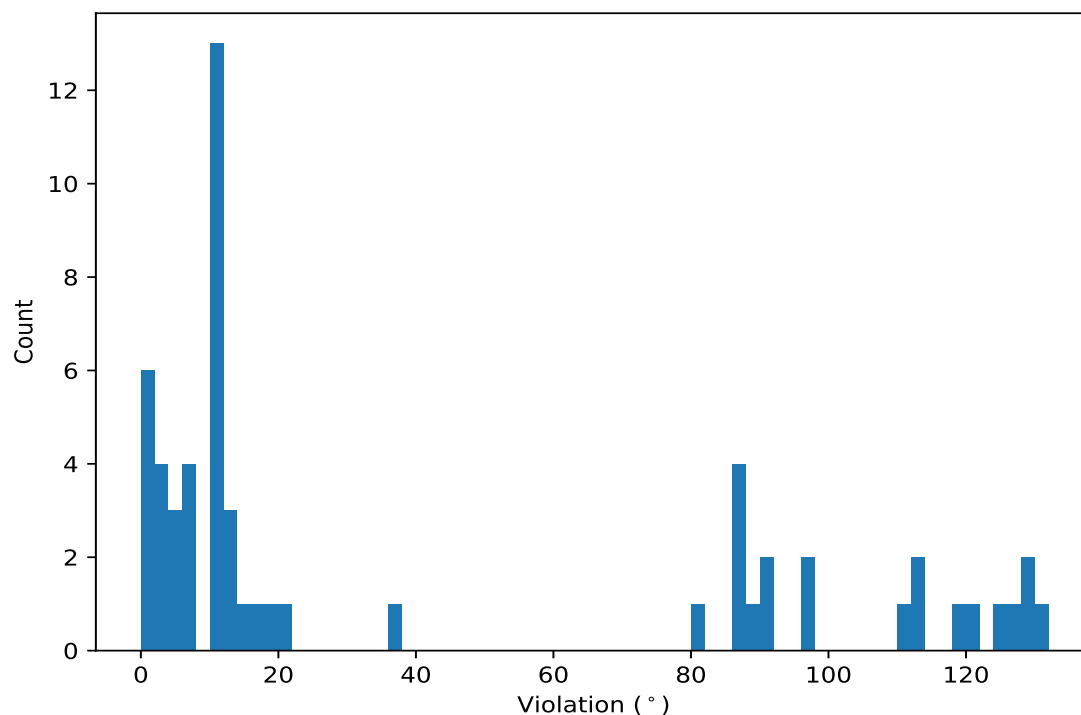
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Mea
(1,68)	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	1:1827:A:MET:N	10	121.79	7.29	123
(1,70)	1:1827:A:MET:N	1:1827:A:MET:CA	1:1827:A:MET:C	1:1828:A:TYR:N	10	89.49	4.55	87
(1,67)	1:1825:A:ALA:C	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	10	11.45	4.7	12
(1,126)	1:1864:A:ALA:N	1:1864:A:ALA:CA	1:1864:A:ALA:C	1:1865:A:PHE:N	9	10.41	0.2	10
(1,4)	1:1782:A:CYS:N	1:1782:A:CYS:CA	1:1782:A:CYS:C	1:1783:A:VAL:N	4	10.41	0.13	10
(1,99)	1:1842:A:CYS:C	1:1843:A:ASP:N	1:1843:A:ASP:CA	1:1843:A:ASP:C	4	4.0	2.14	4
(1,94)	1:1840:A:VAL:N	1:1840:A:VAL:CA	1:1840:A:VAL:C	1:1841:A:VAL:N	4	2.42	0.75	2
(1,2)	1:1781:A:PRO:N	1:1781:A:PRO:CA	1:1781:A:PRO:C	1:1782:A:CYS:N	3	20.74	12.64	21

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 (°)
(1,68)	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	1:1827:A:MET:N	7	130.56
(1,68)	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	1:1827:A:MET:N	8	129.7
(1,68)	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	1:1827:A:MET:N	3	129.22
(1,68)	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	1:1827:A:MET:N	4	127.17
(1,68)	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	1:1827:A:MET:N	1	124.76
(1,68)	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	1:1827:A:MET:N	6	121.77
(1,68)	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	1:1827:A:MET:N	2	118.33
(1,68)	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	1:1827:A:MET:N	10	113.74
(1,68)	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	1:1827:A:MET:N	9	112.66
(1,68)	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	1:1827:A:MET:N	5	110.03
(1,70)	1:1827:A:MET:N	1:1827:A:MET:CA	1:1827:A:MET:C	1:1828:A:TYR:N	10	97.49
(1,70)	1:1827:A:MET:N	1:1827:A:MET:CA	1:1827:A:MET:C	1:1828:A:TYR:N	6	96.8
(1,70)	1:1827:A:MET:N	1:1827:A:MET:CA	1:1827:A:MET:C	1:1828:A:TYR:N	5	91.45
(1,70)	1:1827:A:MET:N	1:1827:A:MET:CA	1:1827:A:MET:C	1:1828:A:TYR:N	2	90.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,70)	1:1827:A:MET:N	1:1827:A:MET:CA	1:1827:A:MET:C	1:1828:A:TYR:N	4	88.48
(1,70)	1:1827:A:MET:N	1:1827:A:MET:CA	1:1827:A:MET:C	1:1828:A:TYR:N	8	87.33
(1,70)	1:1827:A:MET:N	1:1827:A:MET:CA	1:1827:A:MET:C	1:1828:A:TYR:N	1	87.29
(1,70)	1:1827:A:MET:N	1:1827:A:MET:CA	1:1827:A:MET:C	1:1828:A:TYR:N	7	87.1
(1,70)	1:1827:A:MET:N	1:1827:A:MET:CA	1:1827:A:MET:C	1:1828:A:TYR:N	9	86.34
(1,70)	1:1827:A:MET:N	1:1827:A:MET:CA	1:1827:A:MET:C	1:1828:A:TYR:N	3	81.86
(1,2)	1:1781:A:PRO:N	1:1781:A:PRO:CA	1:1781:A:PRO:C	1:1782:A:CYS:N	2	36.02
(1,2)	1:1781:A:PRO:N	1:1781:A:PRO:CA	1:1781:A:PRO:C	1:1782:A:CYS:N	8	21.13
(1,67)	1:1825:A:ALA:C	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	3	19.46
(1,67)	1:1825:A:ALA:C	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	1	17.16
(1,67)	1:1825:A:ALA:C	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	8	14.59
(1,67)	1:1825:A:ALA:C	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	7	13.16
(1,67)	1:1825:A:ALA:C	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	2	12.6
(1,67)	1:1825:A:ALA:C	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	4	12.48
(1,126)	1:1864:A:ALA:N	1:1864:A:ALA:CA	1:1864:A:ALA:C	1:1865:A:PHE:N	3	10.72
(1,126)	1:1864:A:ALA:N	1:1864:A:ALA:CA	1:1864:A:ALA:C	1:1865:A:PHE:N	1	10.61
(1,126)	1:1864:A:ALA:N	1:1864:A:ALA:CA	1:1864:A:ALA:C	1:1865:A:PHE:N	7	10.59
(1,4)	1:1782:A:CYS:N	1:1782:A:CYS:CA	1:1782:A:CYS:C	1:1783:A:VAL:N	3	10.58
(1,4)	1:1782:A:CYS:N	1:1782:A:CYS:CA	1:1782:A:CYS:C	1:1783:A:VAL:N	8	10.46
(1,126)	1:1864:A:ALA:N	1:1864:A:ALA:CA	1:1864:A:ALA:C	1:1865:A:PHE:N	9	10.43
(1,4)	1:1782:A:CYS:N	1:1782:A:CYS:CA	1:1782:A:CYS:C	1:1783:A:VAL:N	9	10.39
(1,126)	1:1864:A:ALA:N	1:1864:A:ALA:CA	1:1864:A:ALA:C	1:1865:A:PHE:N	4	10.36
(1,126)	1:1864:A:ALA:N	1:1864:A:ALA:CA	1:1864:A:ALA:C	1:1865:A:PHE:N	5	10.35
(1,126)	1:1864:A:ALA:N	1:1864:A:ALA:CA	1:1864:A:ALA:C	1:1865:A:PHE:N	10	10.35
(1,126)	1:1864:A:ALA:N	1:1864:A:ALA:CA	1:1864:A:ALA:C	1:1865:A:PHE:N	2	10.22
(1,4)	1:1782:A:CYS:N	1:1782:A:CYS:CA	1:1782:A:CYS:C	1:1783:A:VAL:N	6	10.22
(1,126)	1:1864:A:ALA:N	1:1864:A:ALA:CA	1:1864:A:ALA:C	1:1865:A:PHE:N	8	10.03
(1,67)	1:1825:A:ALA:C	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	5	7.1
(1,67)	1:1825:A:ALA:C	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	9	6.71
(1,99)	1:1842:A:CYS:C	1:1843:A:ASP:N	1:1843:A:ASP:CA	1:1843:A:ASP:C	10	6.2
(1,99)	1:1842:A:CYS:C	1:1843:A:ASP:N	1:1843:A:ASP:CA	1:1843:A:ASP:C	7	6.07
(1,67)	1:1825:A:ALA:C	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	10	5.82
(1,67)	1:1825:A:ALA:C	1:1826:A:THR:N	1:1826:A:THR:CA	1:1826:A:THR:C	6	5.45
(1,2)	1:1781:A:PRO:N	1:1781:A:PRO:CA	1:1781:A:PRO:C	1:1782:A:CYS:N	10	5.06
(1,94)	1:1840:A:VAL:N	1:1840:A:VAL:CA	1:1840:A:VAL:C	1:1841:A:VAL:N	9	3.33
(1,94)	1:1840:A:VAL:N	1:1840:A:VAL:CA	1:1840:A:VAL:C	1:1841:A:VAL:N	10	2.77
(1,94)	1:1840:A:VAL:N	1:1840:A:VAL:CA	1:1840:A:VAL:C	1:1841:A:VAL:N	3	2.27
(1,99)	1:1842:A:CYS:C	1:1843:A:ASP:N	1:1843:A:ASP:CA	1:1843:A:ASP:C	6	2.13
(1,96)	1:1841:A:VAL:N	1:1841:A:VAL:CA	1:1841:A:VAL:C	1:1842:A:CYS:N	7	1.72
(1,99)	1:1842:A:CYS:C	1:1843:A:ASP:N	1:1843:A:ASP:CA	1:1843:A:ASP:C	9	1.61
(1,142)	1:1873:A:VAL:N	1:1873:A:VAL:CA	1:1873:A:VAL:C	1:1874:A:GLN:N	4	1.33
(1,27)	1:1803:A:GLY:C	1:1804:A:GLY:N	1:1804:A:GLY:CA	1:1804:A:GLY:C	6	1.33
(1,94)	1:1840:A:VAL:N	1:1840:A:VAL:CA	1:1840:A:VAL:C	1:1841:A:VAL:N	7	1.29
(1,54)	1:1819:A:ALA:N	1:1819:A:ALA:CA	1:1819:A:ALA:C	1:1820:A:ASN:N	3	1.09