



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 03:43 PM UTC

PDB ID : 2LEM / pdb_00002lem
BMRB ID : 17717
Title : Monomeric Mouse ApoAI(1-216)
Authors : Chen, J.; Wang, J.; Yang, Y.
Deposited on : 2011-06-17

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
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

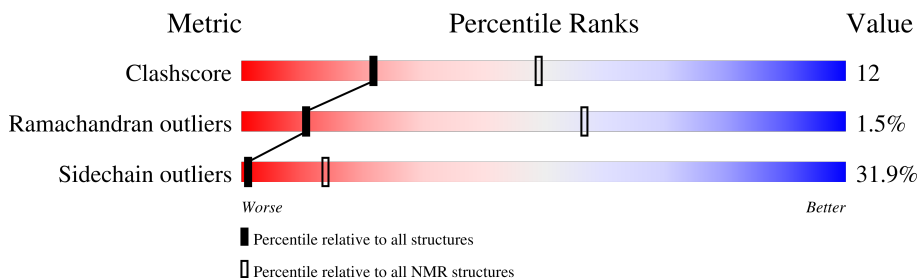
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 75%.

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	216	

2 Ensemble composition and analysis i

This entry contains 20 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:6-A:44, A:58-A:125, A:143-A:179 (144)	0.28	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 3 clusters and 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3502 atoms, of which 1726 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	216	3502	1098	1726	320	354	4	0

There are 7 discrepancies between the modelled and reference sequences:

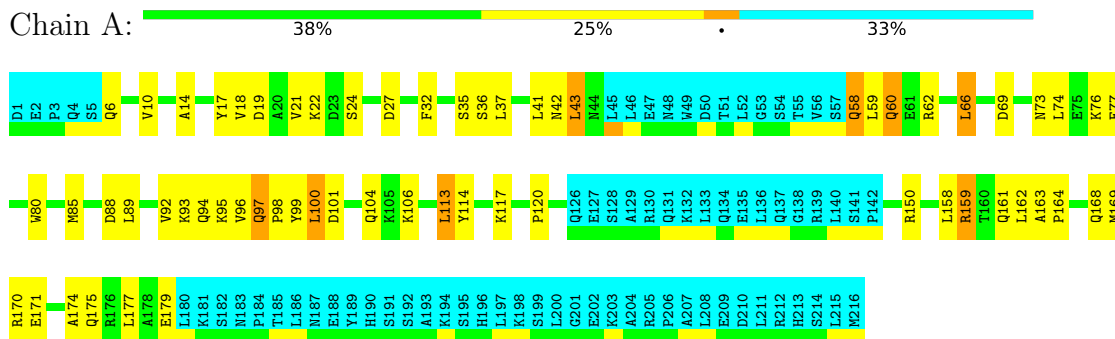
Chain	Residue	Modelled	Actual	Comment	Reference
A	118	ALA	VAL	engineered mutation	UNP Q00623
A	119	SER	ALA	engineered mutation	UNP Q00623
A	121	GLN	LEU	engineered mutation	UNP Q00623
A	191	SER	THR	engineered mutation	UNP Q00623
A	192	SER	ARG	engineered mutation	UNP Q00623
A	195	SER	THR	engineered mutation	UNP Q00623
A	199	SER	THR	engineered mutation	UNP Q00623

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Apolipoprotein A-I



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

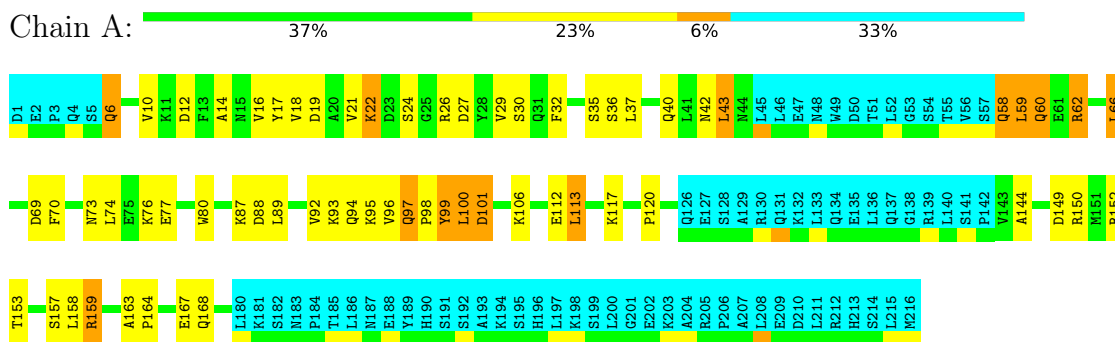
4.2.1 Score per residue for model 1

- Molecule 1: Apolipoprotein A-I



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Apolipoprotein A-I



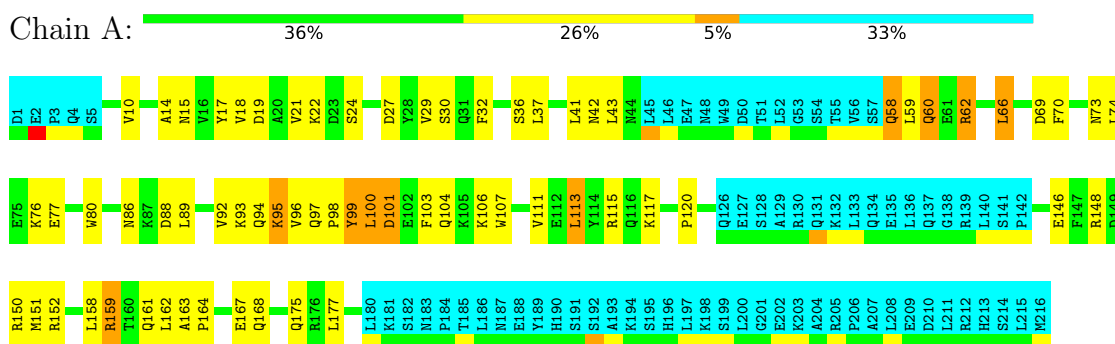
4.2.3 Score per residue for model 3

- Molecule 1: Apolipoprotein A-I



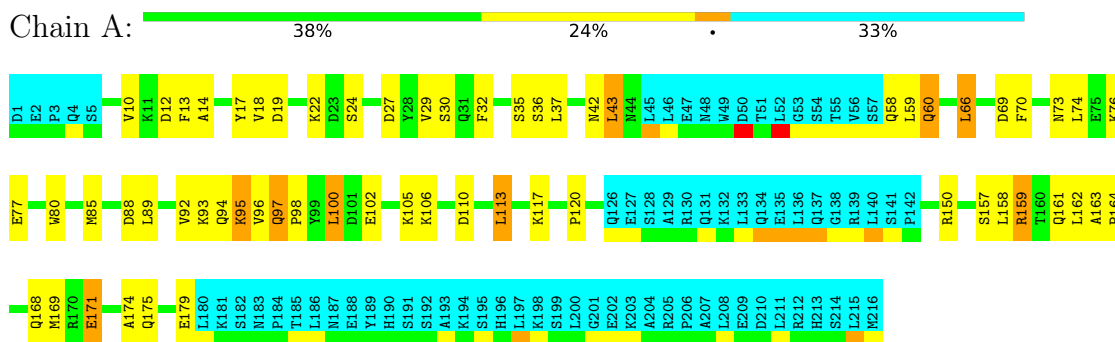
4.2.4 Score per residue for model 4

- Molecule 1: Apolipoprotein A-I



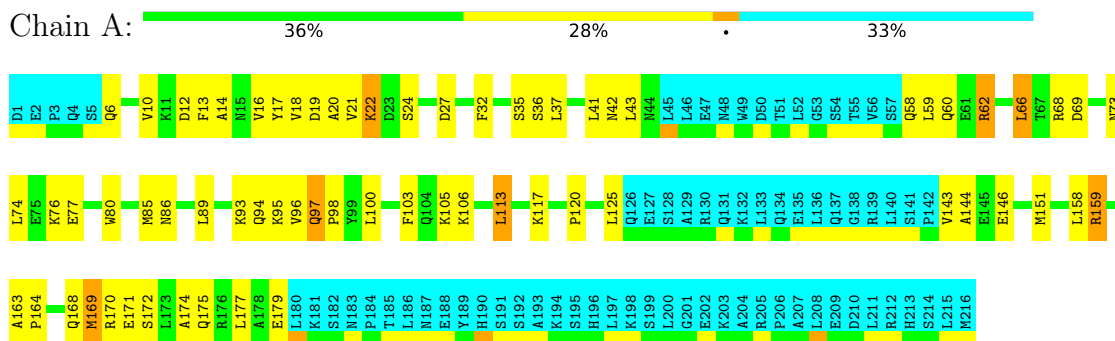
4.2.5 Score per residue for model 5

- Molecule 1: Apolipoprotein A-I



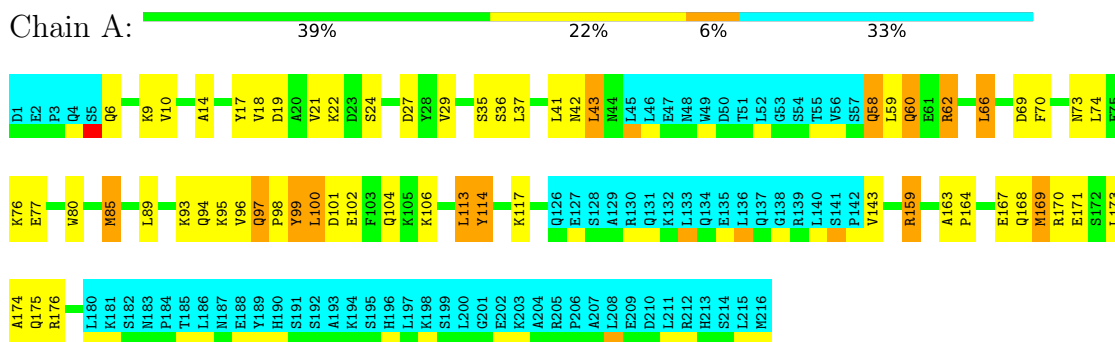
4.2.6 Score per residue for model 6

- Molecule 1: Apolipoprotein A-I



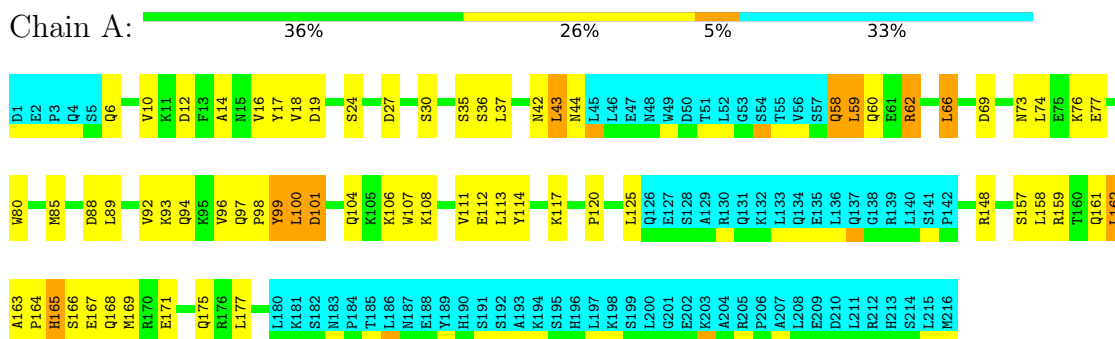
4.2.7 Score per residue for model 7

- Molecule 1: Apolipoprotein A-I



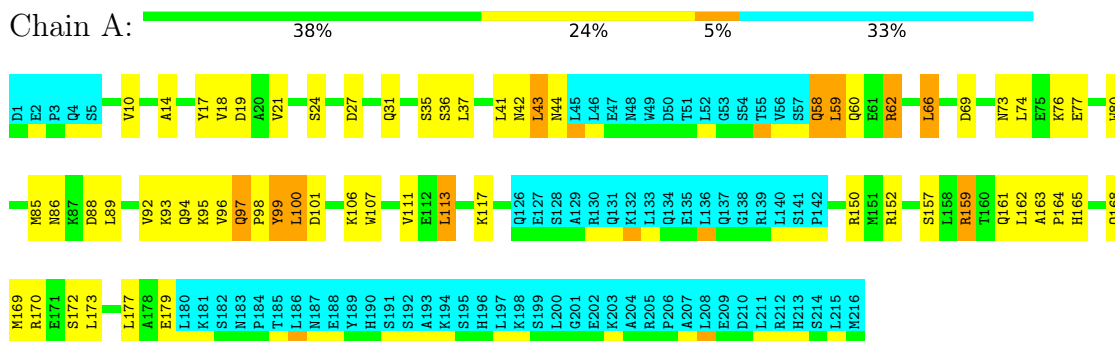
4.2.8 Score per residue for model 8

- Molecule 1: Apolipoprotein A-I



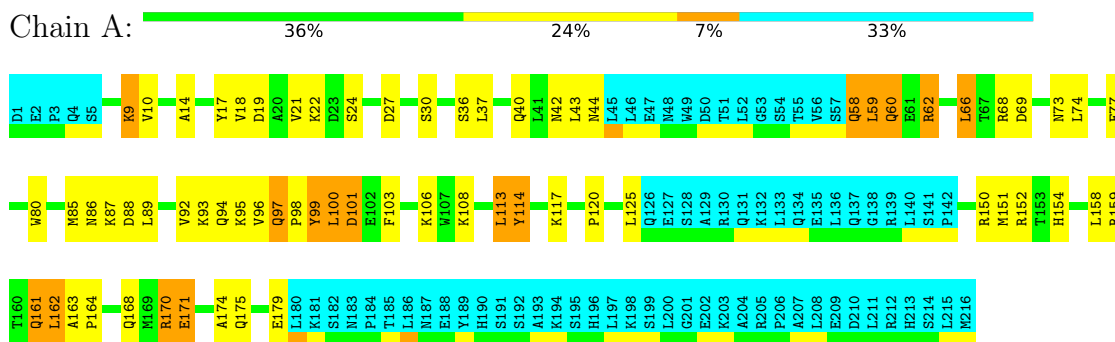
4.2.9 Score per residue for model 9

- Molecule 1: Apolipoprotein A-I



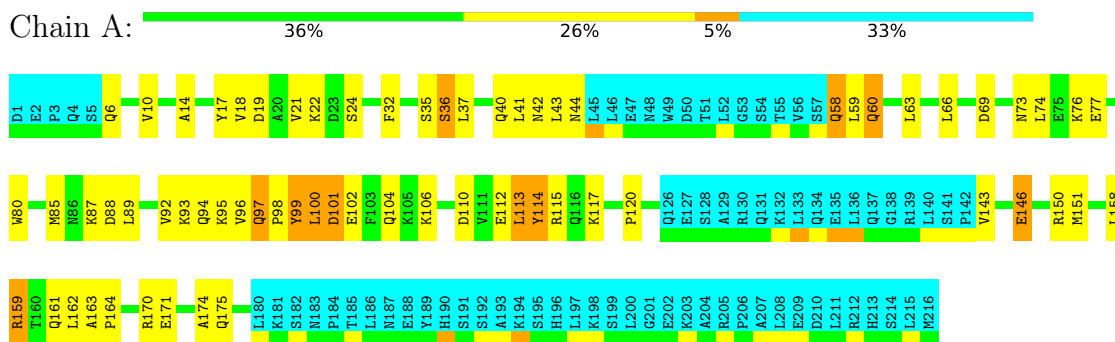
4.2.10 Score per residue for model 10

- Molecule 1: Apolipoprotein A-I



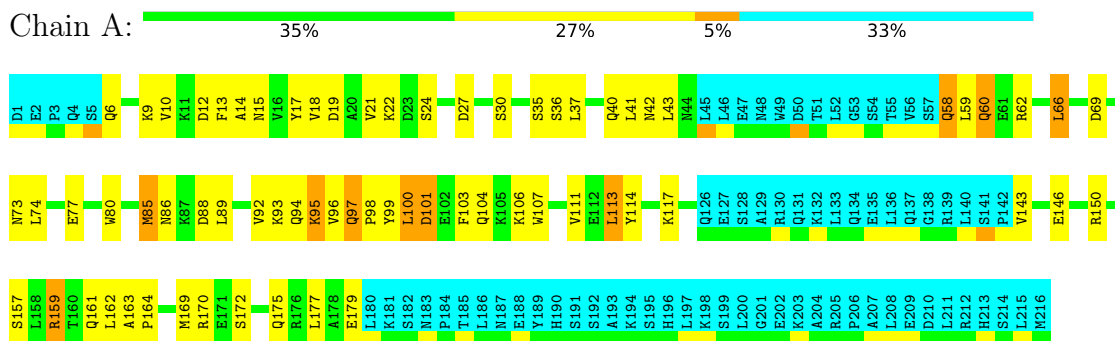
4.2.11 Score per residue for model 11

- Molecule 1: Apolipoprotein A-I



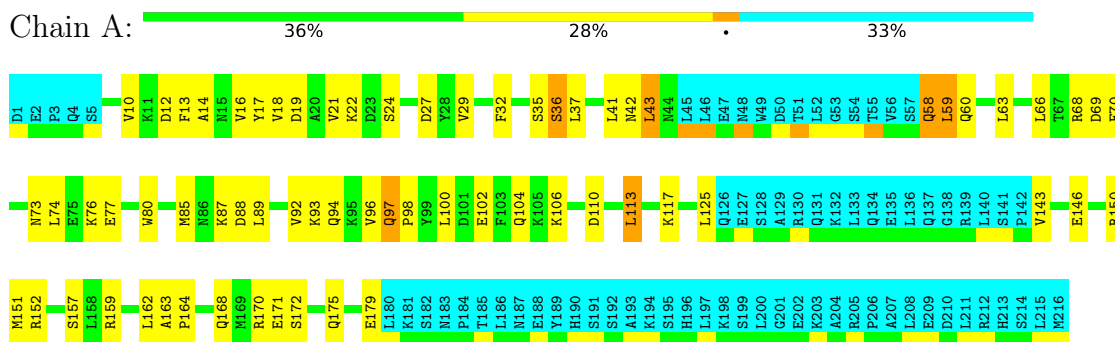
4.2.12 Score per residue for model 12

- Molecule 1: Apolipoprotein A-I



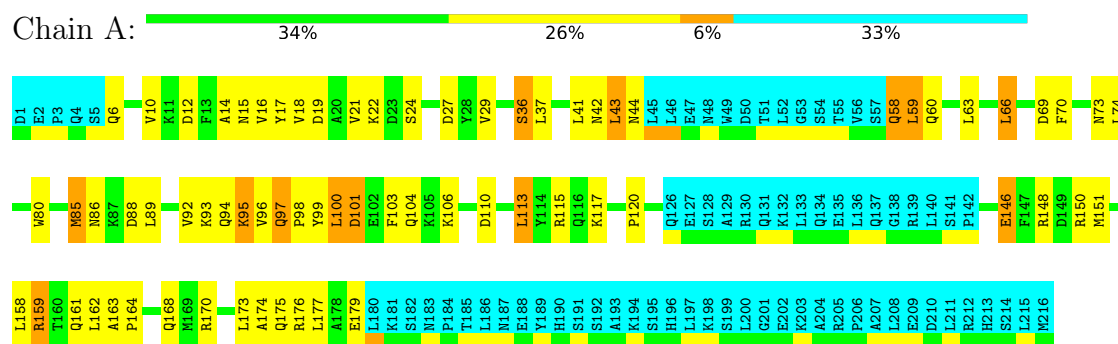
4.2.13 Score per residue for model 13

- Molecule 1: Apolipoprotein A-I



4.2.20 Score per residue for model 20

• Molecule 1: Apolipoprotein A-I



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	
ProcheckNMR	refinement	
Insight II	refinement	
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2253
Number of shifts mapped to atoms	2253
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

6 Model quality i

6.1 Standard geometry i

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1209	1163	1163	28±3
All	All	24180	23260	23260	552

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:VAL:HG11	1:A:96:VAL:HG11	0.88	1.41	17	20
1:A:99:TYR:C	1:A:100:LEU:HD13	0.87	1.94	11	10
1:A:21:VAL:HG13	1:A:169:MET:HE1	0.72	1.61	19	1
1:A:100:LEU:HD22	1:A:100:LEU:N	0.70	2.02	11	10
1:A:163:ALA:HB3	1:A:164:PRO:HD3	0.69	1.64	7	20
1:A:100:LEU:HD22	1:A:100:LEU:H	0.68	1.49	11	1
1:A:120:PRO:HG3	1:A:158:LEU:HD21	0.65	1.67	20	13
1:A:163:ALA:HB3	1:A:164:PRO:CD	0.62	2.25	9	20
1:A:114:TYR:CG	1:A:169:MET:HE2	0.62	2.30	17	1
1:A:10:VAL:HG11	1:A:96:VAL:CG1	0.62	2.22	17	19
1:A:18:VAL:HG11	1:A:85:MET:CG	0.61	2.26	15	15
1:A:98:PRO:HG2	1:A:100:LEU:HD21	0.60	1.72	2	9
1:A:18:VAL:HG11	1:A:85:MET:HG3	0.60	1.73	15	12
1:A:10:VAL:HG21	1:A:93:LYS:HA	0.60	1.73	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:ASP:OD2	1:A:173:LEU:HD21	0.60	1.95	1	2
1:A:99:TYR:O	1:A:100:LEU:HD13	0.59	1.97	9	7
1:A:20:ALA:HB3	1:A:169:MET:HE3	0.59	1.75	6	1
1:A:88:ASP:O	1:A:92:VAL:HG22	0.58	1.99	18	17
1:A:21:VAL:HG12	1:A:114:TYR:CE2	0.57	2.34	7	6
1:A:43:LEU:O	1:A:43:LEU:HD13	0.56	2.00	4	20
1:A:40:GLN:CB	1:A:59:LEU:HD13	0.56	2.29	11	5
1:A:98:PRO:HB2	1:A:100:LEU:HD11	0.56	1.78	19	10
1:A:100:LEU:HD13	1:A:100:LEU:N	0.55	2.16	11	3
1:A:97:GLN:CB	1:A:98:PRO:CD	0.55	2.84	11	20
1:A:14:ALA:O	1:A:18:VAL:HG23	0.54	2.03	20	20
1:A:120:PRO:CG	1:A:158:LEU:HD21	0.54	2.33	5	7
1:A:100:LEU:N	1:A:100:LEU:HD12	0.53	2.19	15	1
1:A:17:TYR:HB2	1:A:173:LEU:HD21	0.51	1.81	18	2
1:A:15:ASN:HB2	1:A:85:MET:HE1	0.51	1.83	14	1
1:A:95:LYS:CG	1:A:100:LEU:HD21	0.51	2.35	15	1
1:A:88:ASP:O	1:A:92:VAL:HG13	0.50	2.05	9	17
1:A:10:VAL:CG1	1:A:96:VAL:HG11	0.50	2.35	15	6
1:A:110:ASP:OD2	1:A:169:MET:HE1	0.50	2.07	5	1
1:A:80:TRP:CE3	1:A:113:LEU:HD22	0.50	2.42	19	20
1:A:163:ALA:N	1:A:164:PRO:HD2	0.50	2.22	18	9
1:A:170:ARG:O	1:A:174:ALA:HB2	0.50	2.07	10	9
1:A:95:LYS:CG	1:A:100:LEU:HD23	0.50	2.37	4	1
1:A:171:GLU:O	1:A:174:ALA:HB3	0.50	2.07	5	2
1:A:114:TYR:CD2	1:A:169:MET:HE2	0.50	2.41	17	1
1:A:43:LEU:HD21	1:A:143:VAL:HG12	0.49	1.84	3	2
1:A:43:LEU:HD22	1:A:146:GLU:OE2	0.49	2.07	12	2
1:A:100:LEU:HD12	1:A:100:LEU:H	0.49	1.67	15	1
1:A:161:GLN:HG2	1:A:162:LEU:N	0.48	2.23	10	2
1:A:173:LEU:HD22	1:A:176:ARG:NH2	0.48	2.23	20	2
1:A:159:ARG:O	1:A:163:ALA:HB2	0.48	2.08	5	17
1:A:12:ASP:O	1:A:16:VAL:HG23	0.48	2.07	2	5
1:A:163:ALA:CB	1:A:164:PRO:CD	0.48	2.92	15	18
1:A:100:LEU:H	1:A:100:LEU:HD12	0.48	1.68	12	2
1:A:17:TYR:C	1:A:17:TYR:CD1	0.47	2.92	19	4
1:A:169:MET:HE3	1:A:173:LEU:HD12	0.47	1.86	7	1
1:A:17:TYR:O	1:A:21:VAL:HG22	0.47	2.10	16	12
1:A:13:PHE:CD1	1:A:13:PHE:C	0.47	2.92	13	5
1:A:92:VAL:HG12	1:A:102:GLU:CD	0.47	2.35	5	2
1:A:62:ARG:O	1:A:66:LEU:HD23	0.46	2.10	7	12
1:A:17:TYR:CD1	1:A:17:TYR:C	0.46	2.93	2	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:LYS:HG2	1:A:100:LEU:HD22	0.46	1.86	5	1
1:A:165:HIS:CD2	1:A:165:HIS:C	0.46	2.91	8	1
1:A:100:LEU:N	1:A:100:LEU:CD2	0.46	2.71	11	1
1:A:100:LEU:HD12	1:A:100:LEU:N	0.46	2.26	12	2
1:A:160:THR:O	1:A:164:PRO:CD	0.46	2.63	18	1
1:A:97:GLN:N	1:A:98:PRO:HD2	0.46	2.25	20	6
1:A:113:LEU:C	1:A:113:LEU:HD12	0.46	2.36	1	14
1:A:32:PHE:CE1	1:A:66:LEU:HD13	0.45	2.46	2	5
1:A:11:LYS:CD	1:A:89:LEU:HD21	0.45	2.42	15	1
1:A:95:LYS:HG3	1:A:100:LEU:HD21	0.45	1.86	15	1
1:A:29:VAL:HG23	1:A:70:PHE:CD1	0.45	2.46	15	6
1:A:107:TRP:O	1:A:111:VAL:HG23	0.45	2.12	8	5
1:A:28:TYR:CD2	1:A:74:LEU:HD11	0.45	2.47	16	1
1:A:95:LYS:HB3	1:A:100:LEU:HD11	0.44	1.90	15	3
1:A:6:GLN:O	1:A:10:VAL:HG22	0.44	2.13	14	2
1:A:18:VAL:HG21	1:A:85:MET:HA	0.44	1.90	16	2
1:A:97:GLN:CB	1:A:98:PRO:HD3	0.44	2.43	11	8
1:A:114:TYR:CG	1:A:169:MET:HE3	0.43	2.48	8	1
1:A:149:ASP:O	1:A:153:THR:HG23	0.43	2.14	2	1
1:A:58:GLN:HA	1:A:61:GLU:CG	0.43	2.43	19	1
1:A:43:LEU:HD21	1:A:143:VAL:CG1	0.43	2.43	3	1
1:A:41:LEU:HD23	1:A:42:ASN:ND2	0.43	2.29	19	10
1:A:31:GLN:CD	1:A:31:GLN:C	0.43	2.87	9	2
1:A:95:LYS:HG2	1:A:100:LEU:HD23	0.43	1.91	4	1
1:A:150:ARG:O	1:A:154:HIS:CG	0.43	2.72	10	1
1:A:21:VAL:CG1	1:A:169:MET:HE1	0.43	2.41	19	1
1:A:32:PHE:HE1	1:A:66:LEU:HD13	0.42	1.74	5	3
1:A:36:SER:HB2	1:A:63:LEU:HD13	0.42	1.91	13	5
1:A:43:LEU:HD13	1:A:43:LEU:C	0.42	2.39	11	3
1:A:162:LEU:O	1:A:166:SER:CB	0.42	2.67	8	1
1:A:29:VAL:HG23	1:A:70:PHE:CD2	0.42	2.50	4	3
1:A:63:LEU:HD12	1:A:63:LEU:O	0.42	2.14	15	1
1:A:114:TYR:CE1	1:A:118:ALA:HB2	0.42	2.49	18	1
1:A:21:VAL:HG11	1:A:110:ASP:OD1	0.42	2.14	20	1
1:A:6:GLN:H	1:A:6:GLN:NE2	0.42	2.12	2	1
1:A:59:LEU:HD12	1:A:60:GLN:N	0.41	2.30	11	1
1:A:100:LEU:HD13	1:A:102:GLU:H	0.41	1.76	15	1
1:A:22:LYS:HD3	1:A:22:LYS:C	0.41	2.41	2	2
1:A:7:TRP:CD1	1:A:7:TRP:C	0.41	2.97	19	1
1:A:165:HIS:O	1:A:169:MET:HE3	0.41	2.15	9	1
1:A:113:LEU:HD12	1:A:113:LEU:C	0.41	2.41	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:GLN:HB2	1:A:59:LEU:HD13	0.40	1.92	11	1
1:A:22:LYS:C	1:A:22:LYS:HD3	0.40	2.41	18	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/216 (67%)	121±2 (84±1%)	21±2 (14±1%)	2±1 (1±1%)	11	57
All	All	2880/4320 (67%)	2421 (84%)	416 (14%)	43 (1%)	11	57

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	58	GLN	18
1	A	99	TYR	13
1	A	101	ASP	12

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	132/197 (67%)	90±3 (68±2%)	42±3 (32±2%)	1	14
All	All	2640/3940 (67%)	1799 (68%)	841 (32%)	1	14

All 75 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	36	SER	20
1	A	37	LEU	20
1	A	60	GLN	20
1	A	66	LEU	20
1	A	69	ASP	20
1	A	74	LEU	20
1	A	89	LEU	20
1	A	93	LYS	20
1	A	94	GLN	20
1	A	100	LEU	20
1	A	106	LYS	20
1	A	117	LYS	20
1	A	19	ASP	19
1	A	27	ASP	19
1	A	58	GLN	19
1	A	73	ASN	19
1	A	113	LEU	19
1	A	24	SER	18
1	A	97	GLN	18
1	A	59	LEU	17
1	A	76	LYS	17
1	A	95	LYS	17
1	A	175	GLN	17
1	A	22	LYS	17
1	A	77	GLU	17
1	A	35	SER	16
1	A	159	ARG	16
1	A	104	GLN	15
1	A	43	LEU	14
1	A	150	ARG	14
1	A	168	GLN	14
1	A	62	ARG	13
1	A	177	LEU	13
1	A	162	LEU	12
1	A	171	GLU	12
1	A	179	GLU	12
1	A	6	GLN	11
1	A	161	GLN	11
1	A	157	SER	10
1	A	172	SER	10
1	A	101	ASP	10
1	A	86	ASN	10
1	A	151	MET	10

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Mol	Chain	Res	Type	Models (Total)
1	A	44	ASN	9
1	A	167	GLU	9
1	A	30	SER	8
1	A	152	ARG	8
1	A	9	LYS	8
1	A	114	TYR	7
1	A	170	ARG	7
1	A	15	ASN	7
1	A	169	MET	7
1	A	125	LEU	7
1	A	87	LYS	6
1	A	32	PHE	6
1	A	112	GLU	5
1	A	146	GLU	5
1	A	41	LEU	4
1	A	115	ARG	4
1	A	68	ARG	4
1	A	85	MET	4
1	A	102	GLU	4
1	A	108	LYS	4
1	A	110	ASP	4
1	A	148	ARG	3
1	A	12	ASP	3
1	A	26	ARG	2
1	A	105	LYS	2
1	A	165	HIS	2
1	A	84	GLU	1
1	A	176	ARG	1
1	A	8	ASP	1
1	A	11	LYS	1
1	A	7	TRP	1
1	A	61	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 74% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	2253
Number of shifts mapped to atoms	2253
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	214	0.02 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	207	1.01 ± 0.07	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	202	-0.69 ± 0.22	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 75%, i.e. 1534 atoms were assigned a chemical shift out of a possible 2053. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	552/716 (77%)	274/288 (95%)	142/288 (49%)	136/140 (97%)
Sidechain	929/1189 (78%)	614/754 (81%)	297/371 (80%)	18/64 (28%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	53/148 (36%)	49/73 (67%)	0/69 (0%)	4/6 (67%)
Overall	1534/2053 (75%)	937/1115 (84%)	439/728 (60%)	158/210 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 2252 atoms were assigned a chemical shift out of a possible 3026. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	823/1071 (77%)	407/431 (94%)	214/432 (50%)	202/208 (97%)
Sidechain	1365/1765 (77%)	896/1125 (80%)	446/551 (81%)	23/89 (26%)
Aromatic	64/190 (34%)	59/95 (62%)	0/85 (0%)	5/10 (50%)
Overall	2252/3026 (74%)	1362/1651 (82%)	660/1068 (62%)	230/307 (75%)

7.1.4 Statistically unusual chemical shifts [i](#)

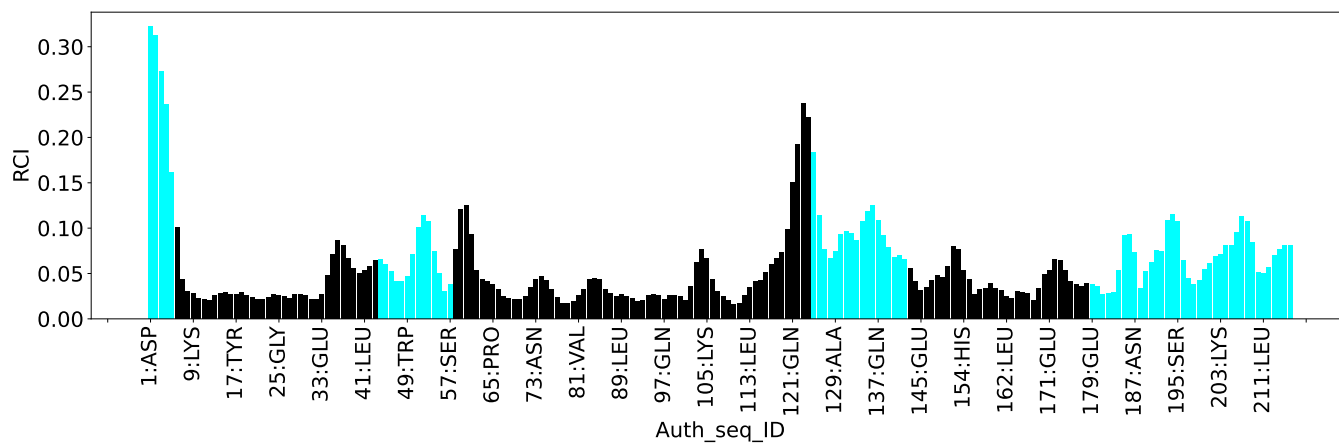
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	216	MET	CE	28.03	8.39 – 25.85	6.2

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	3688
Intra-residue ($ i-j =0$)	591
Sequential ($ i-j =1$)	1001
Medium range ($ i-j >1$ and $ i-j <5$)	1570
Long range ($ i-j \geq 5$)	525
Inter-chain	0
Hydrogen bond restraints	1
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	17.1
Number of long range restraints per residue ¹	2.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	17.8	0.2
0.2-0.5 (Medium)	19.3	0.5
>0.5 (Large)	80.0	3.07

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis [i](#)

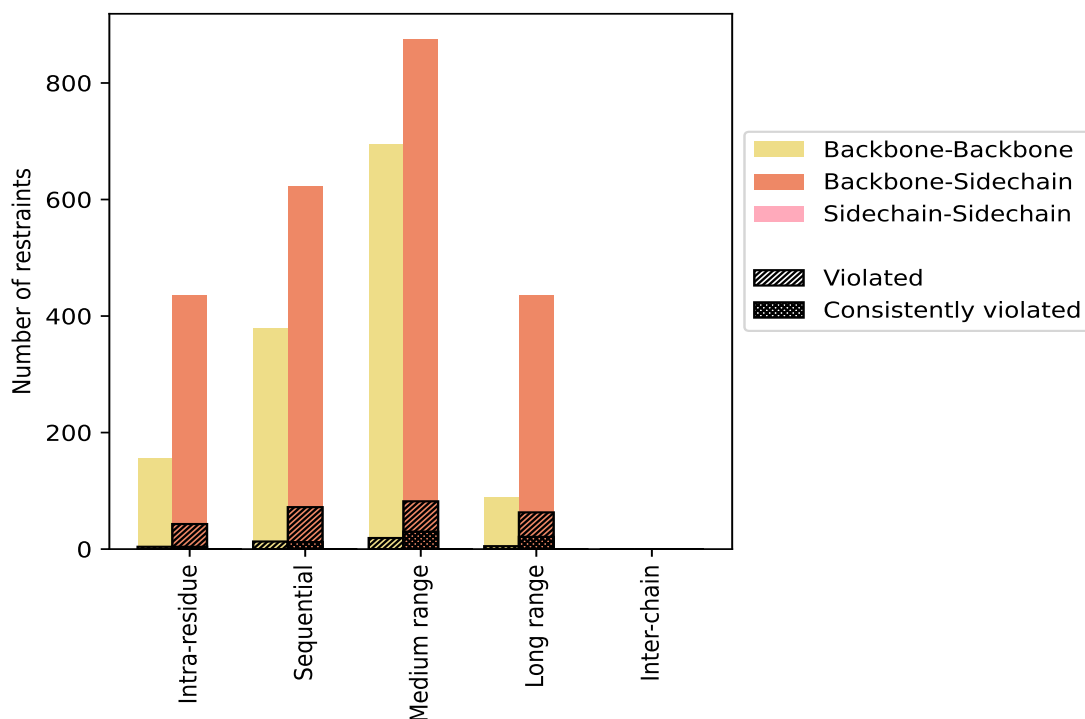
9.1 Summary of distance violations [i](#)

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	591	16.0	47	8.0	1.3	4	0.7	0.1
Backbone-Backbone	156	4.2	4	2.6	0.1	0	0.0	0.0
Backbone-Sidechain	435	11.8	43	9.9	1.2	4	0.9	0.1
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	1001	27.1	85	8.5	2.3	12	1.2	0.3
Backbone-Backbone	379	10.3	13	3.4	0.4	0	0.0	0.0
Backbone-Sidechain	622	16.9	72	11.6	2.0	12	1.9	0.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	1570	42.6	101	6.4	2.7	30	1.9	0.8
Backbone-Backbone	695	18.8	19	2.7	0.5	0	0.0	0.0
Backbone-Sidechain	875	23.7	82	9.4	2.2	30	3.4	0.8
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	525	14.2	68	13.0	1.8	21	4.0	0.6
Backbone-Backbone	89	2.4	5	5.6	0.1	0	0.0	0.0
Backbone-Sidechain	436	11.8	63	14.4	1.7	21	4.8	0.6
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	1	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	3688	100.0	301	8.2	8.2	67	1.8	1.8
Backbone-Backbone	1319	35.8	41	3.1	1.1	0	0.0	0.0
Backbone-Sidechain	2369	64.2	260	11.0	7.0	67	2.8	1.8
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	16	27	40	33	0	116	0.85	2.76	0.57	0.82
2	14	29	45	32	0	120	0.86	2.73	0.58	0.84
3	13	23	42	33	0	111	0.89	2.64	0.56	0.81
4	13	26	38	34	0	111	0.89	3.01	0.6	0.8
5	20	27	39	32	0	118	0.86	3.05	0.57	0.82
6	14	29	45	34	0	122	0.86	2.55	0.56	0.81
7	15	26	45	38	0	124	0.85	2.92	0.58	0.78
8	13	27	39	29	0	108	0.94	2.84	0.57	0.9
9	15	25	44	30	0	114	0.88	2.84	0.58	0.82
10	12	24	41	34	0	111	0.89	2.93	0.61	0.83

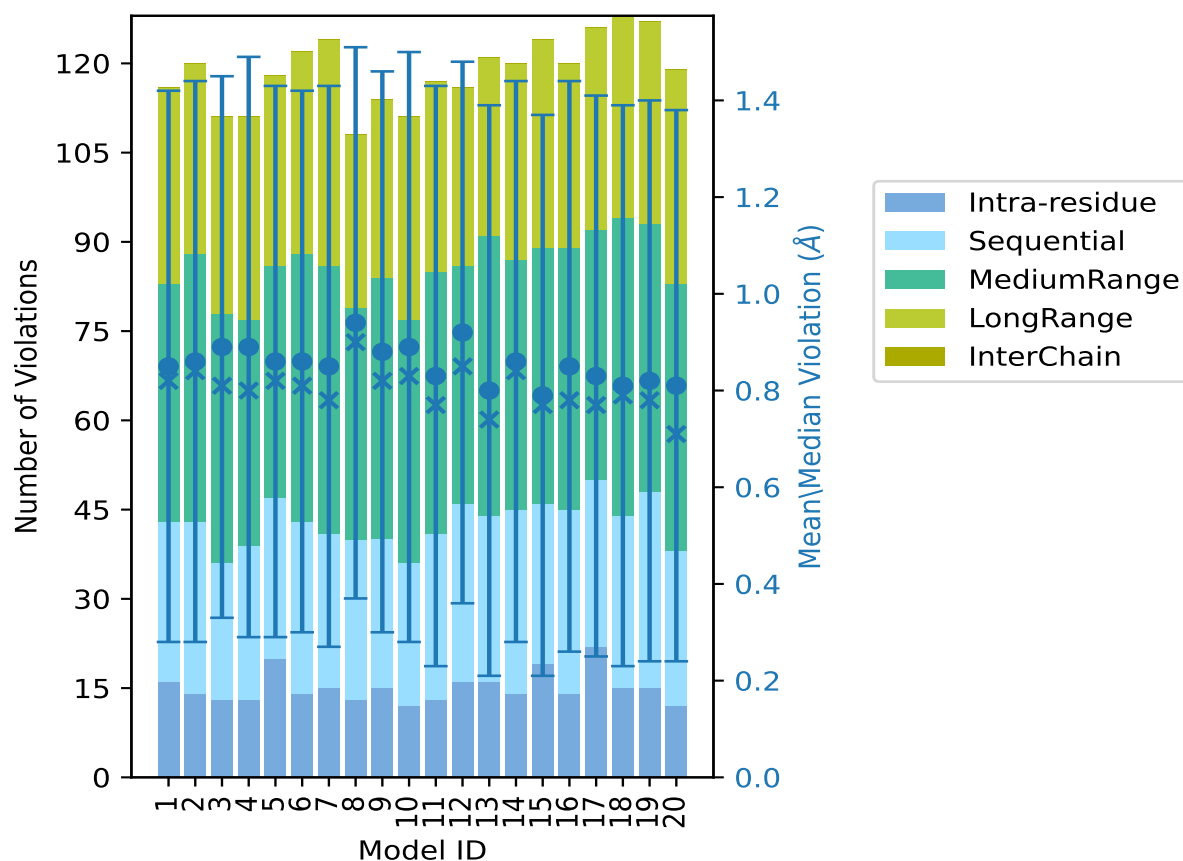
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
11	13	28	44	32	0	117	0.83	3.07	0.6	0.77
12	16	30	40	30	0	116	0.92	2.76	0.56	0.85
13	16	28	47	30	0	121	0.8	2.8	0.59	0.74
14	14	31	42	33	0	120	0.86	3.07	0.58	0.84
15	19	27	43	35	0	124	0.79	2.79	0.58	0.77
16	14	31	44	31	0	120	0.85	2.98	0.59	0.78
17	22	28	42	34	0	126	0.83	2.8	0.58	0.77
18	15	29	50	34	0	128	0.81	2.94	0.58	0.79
19	15	33	45	34	0	127	0.82	2.7	0.58	0.78
20	12	26	45	36	0	119	0.81	2.96	0.57	0.71

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

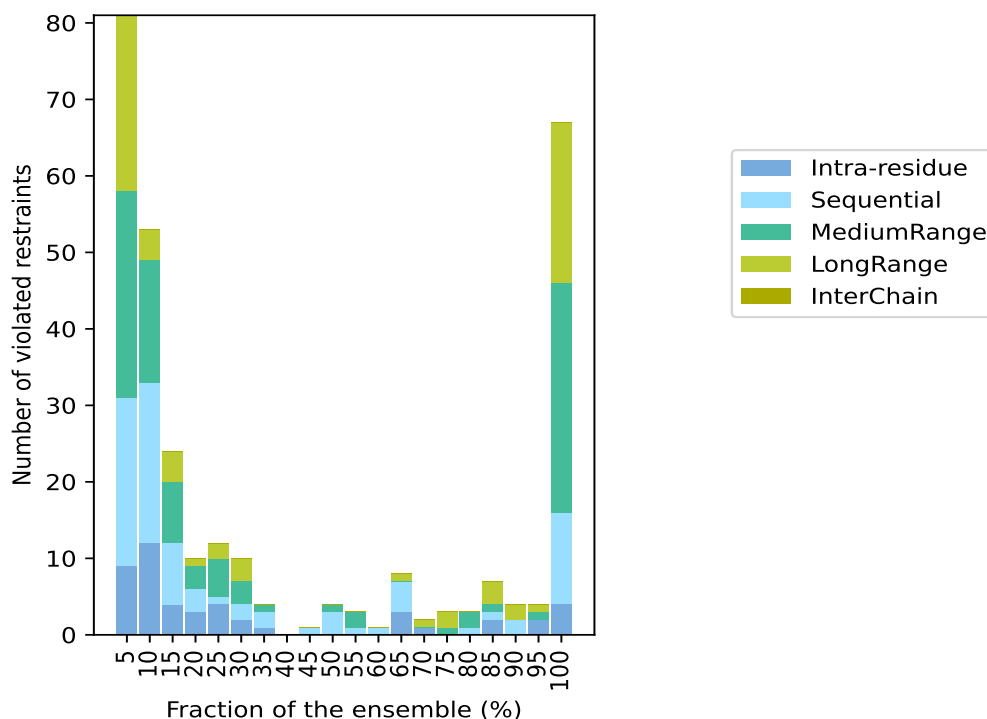
9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3386(IR:544, SQ:916, MR:1469, LR:457, 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	%
9	22	27	23	0	81	1	5.0
12	21	16	4	0	53	2	10.0
4	8	8	4	0	24	3	15.0
3	3	3	1	0	10	4	20.0
4	1	5	2	0	12	5	25.0
2	2	3	3	0	10	6	30.0
1	2	1	0	0	4	7	35.0
0	0	0	0	0	0	8	40.0
0	1	0	0	0	1	9	45.0
0	3	1	0	0	4	10	50.0
0	1	2	0	0	3	11	55.0
0	1	0	0	0	1	12	60.0
3	4	0	1	0	8	13	65.0
1	0	0	1	0	2	14	70.0
0	0	1	2	0	3	15	75.0
0	1	2	0	0	3	16	80.0
2	1	1	3	0	7	17	85.0
0	2	0	2	0	4	18	90.0
2	0	1	1	0	4	19	95.0
4	12	30	21	0	67	20	100.0

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

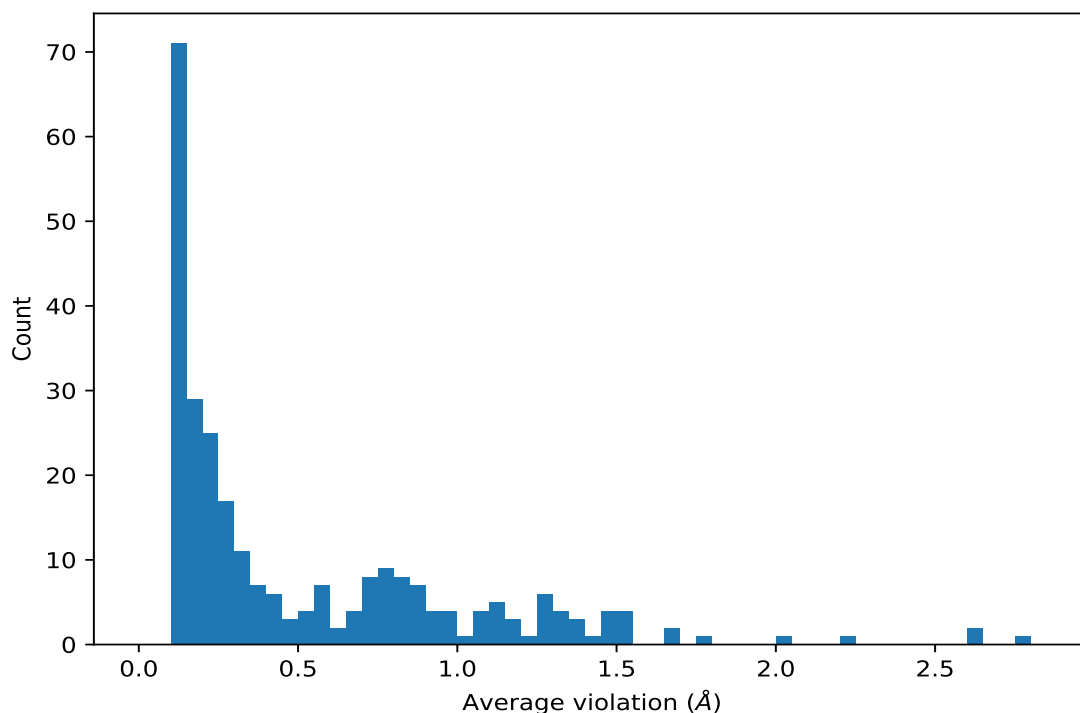
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	20	2.77	0.22	2.78
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	20	2.65	0.16	2.58
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	20	2.6	0.2	2.56
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	20	2.21	0.07	2.21
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	20	2.05	0.13	2.04
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	20	1.77	0.29	1.84
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	20	1.69	0.05	1.7
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	20	1.66	0.03	1.66
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	20	1.53	0.19	1.56
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	20	1.51	0.02	1.52
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	20	1.5	0.43	1.72
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	20	1.5	0.03	1.5
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	20	1.49	0.07	1.5
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	20	1.49	0.32	1.62
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	20	1.47	0.06	1.46
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	20	1.46	0.03	1.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	20	1.44	0.05	1.43
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	20	1.39	0.12	1.41
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	20	1.38	0.09	1.38
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	20	1.37	0.12	1.41
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	20	1.34	0.26	1.39
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	20	1.32	0.08	1.33
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	20	1.31	0.06	1.33
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	20	1.3	0.06	1.3
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	20	1.28	0.02	1.28
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	20	1.28	0.22	1.3
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	20	1.27	0.09	1.28
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	20	1.26	0.03	1.27
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	20	1.25	0.08	1.26
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	20	1.21	0.03	1.22
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	20	1.16	0.13	1.2
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	20	1.16	0.04	1.16
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	20	1.14	0.1	1.16
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	20	1.12	0.04	1.13
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	20	1.1	0.07	1.1
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	20	1.09	0.09	1.08
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	20	1.08	0.1	1.1
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	20	1.05	0.06	1.08
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	20	0.97	0.08	0.96
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	20	0.91	0.05	0.92
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	20	0.91	0.03	0.91
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	20	0.91	0.01	0.91
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	20	0.89	0.15	0.92
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	20	0.88	0.05	0.89
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	20	0.88	0.19	0.88
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	20	0.88	0.13	0.82
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	20	0.87	0.09	0.88
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	20	0.86	0.04	0.85
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	20	0.83	0.04	0.83
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	20	0.8	0.17	0.86
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	20	0.79	0.22	0.82
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	20	0.78	0.14	0.77
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	20	0.77	0.07	0.78
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	20	0.76	0.14	0.76
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	20	0.76	0.05	0.76
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	20	0.75	0.03	0.76
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	20	0.74	0.03	0.74
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	20	0.74	0.05	0.74

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	20	0.73	0.08	0.76
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	20	0.73	0.06	0.74
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	20	0.62	0.08	0.62
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	20	0.61	0.04	0.62
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	20	0.59	0.13	0.55
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	20	0.48	0.11	0.52
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	20	0.4	0.05	0.4
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	20	0.37	0.04	0.36
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	20	0.27	0.03	0.27
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	19	0.96	0.25	1.02
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	19	0.6	0.12	0.61
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	19	0.4	0.1	0.38
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	19	0.2	0.05	0.2
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	18	1.07	0.54	1.3
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	18	0.78	0.12	0.82
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	18	0.56	0.21	0.52
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	18	0.16	0.03	0.16
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	17	1.12	0.23	1.16
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	17	1.04	0.13	1.09
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	17	0.84	0.06	0.84
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	17	0.42	0.23	0.33
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	17	0.35	0.11	0.35
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	17	0.29	0.07	0.32
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	17	0.28	0.11	0.24
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	16	0.46	0.1	0.48
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	16	0.4	0.2	0.4
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	16	0.16	0.04	0.18
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	15	1.16	0.34	1.26
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	15	0.87	0.09	0.82
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	15	0.84	0.52	0.73
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	14	0.57	0.06	0.57
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	14	0.5	0.21	0.48
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	13	0.76	0.43	1.09
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	13	0.68	0.29	0.68
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	13	0.67	0.34	0.63
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	13	0.54	0.04	0.54
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	13	0.5	0.12	0.48
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	13	0.44	0.14	0.54
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	13	0.41	0.23	0.4
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	13	0.17	0.02	0.17
(1,622)	1:161:A:GLN:H	1:162:A:LEU:HD21	12	0.91	0.62	1.34
(1,1897)	1:67:A:THR:HG21	1:69:A:ASP:H	11	0.8	0.43	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,275)	1:67:A:THR:HG21	1:70:A:PHE:H	11	0.59	0.37	0.33
(1,727)	1:20:A:ALA:H	1:21:A:VAL:HG21	11	0.14	0.02	0.14
(1,1900)	1:143:A:VAL:HG21	1:145:A:GLU:H	10	0.75	0.07	0.76
(1,1252)	1:70:A:PHE:HE2	1:71:A:TRP:H	10	0.69	0.02	0.69
(1,1306)	1:143:A:VAL:HG21	1:144:A:ALA:H	10	0.5	0.09	0.53
(1,1240)	1:63:A:LEU:HD21	1:64:A:GLY:H	10	0.11	0.01	0.12
(1,791)	1:66:A:LEU:H	1:67:A:THR:HG21	9	0.21	0.07	0.24
(1,384)	1:100:A:LEU:H	1:100:A:LEU:HD21	7	0.85	0.2	0.98
(2,41)	1:208:A:LEU:HD21	1:209:A:GLU:H	7	0.47	0.13	0.45
(2,3)	1:179:A:GLU:H	1:180:A:LEU:HD21	7	0.17	0.1	0.13
(1,2348)	1:160:A:THR:HG21	1:163:A:ALA:H	7	0.15	0.03	0.16
(2,856)	1:12:A:ASP:H	1:180:A:LEU:HD21	6	0.37	0.13	0.34
(2,631)	1:118:A:ALA:H	1:162:A:LEU:HD21	6	0.32	0.07	0.3
(1,286)	1:67:A:THR:H	1:67:A:THR:HG21	6	0.26	0.02	0.26
(2,663)	1:22:A:LYS:HG2	1:81:A:VAL:H	6	0.24	0.02	0.24
(2,663)	1:22:A:LYS:HG3	1:81:A:VAL:H	6	0.24	0.02	0.24
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB2	6	0.24	0.04	0.25
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB3	6	0.24	0.04	0.25
(1,1332)	1:47:A:GLU:HB2	1:48:A:ASN:H	6	0.21	0.04	0.21
(1,1332)	1:47:A:GLU:HB3	1:48:A:ASN:H	6	0.21	0.04	0.21
(1,1328)	1:188:A:GLU:HB2	1:189:A:TYR:H	6	0.18	0.05	0.16
(1,1328)	1:188:A:GLU:HB3	1:189:A:TYR:H	6	0.18	0.05	0.16
(1,2677)	1:22:A:LYS:HE2	1:26:A:ARG:H	6	0.17	0.02	0.17
(1,2677)	1:22:A:LYS:HE3	1:26:A:ARG:H	6	0.17	0.02	0.17
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE21	6	0.16	0.01	0.16
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE22	6	0.16	0.01	0.16
(1,1907)	1:188:A:GLU:HB2	1:190:A:HIS:H	6	0.13	0.02	0.12
(1,1907)	1:188:A:GLU:HB3	1:190:A:HIS:H	6	0.13	0.02	0.12
(2,361)	1:48:A:ASN:H	1:52:A:LEU:HD21	5	0.99	0.35	1.19
(1,380)	1:99:A:TYR:H	1:99:A:TYR:HE1	5	0.83	0.37	1.01
(2,408)	1:140:A:LEU:HB2	1:144:A:ALA:H	5	0.24	0.13	0.2
(2,408)	1:140:A:LEU:HB3	1:144:A:ALA:H	5	0.24	0.13	0.2
(1,44)	1:97:A:GLN:H	1:97:A:GLN:HB2	5	0.23	0.01	0.23
(1,44)	1:97:A:GLN:H	1:97:A:GLN:HB3	5	0.23	0.01	0.23
(1,2)	1:102:A:GLU:H	1:102:A:GLU:HG2	5	0.19	0.11	0.12
(1,2)	1:102:A:GLU:H	1:102:A:GLU:HG3	5	0.19	0.11	0.12
(1,2423)	1:31:A:GLN:HE21	1:34:A:SER:H	5	0.18	0.03	0.19
(1,2423)	1:31:A:GLN:HE22	1:34:A:SER:H	5	0.18	0.03	0.19
(2,510)	1:95:A:LYS:HD2	1:103:A:PHE:H	5	0.18	0.01	0.17
(2,510)	1:95:A:LYS:HD3	1:103:A:PHE:H	5	0.18	0.01	0.17
(1,2706)	1:96:A:VAL:H	1:102:A:GLU:HG2	5	0.14	0.02	0.14
(1,2706)	1:96:A:VAL:H	1:102:A:GLU:HG3	5	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,598)	1:56:A:VAL:H	1:57:A:SER:H	5	0.13	0.02	0.13
(1,2459)	1:21:A:VAL:HA	1:25:A:GLY:H	5	0.13	0.01	0.13
(2,108)	1:100:A:LEU:HD11	1:102:A:GLU:H	5	0.12	0.01	0.12
(1,55)	1:95:A:LYS:H	1:95:A:LYS:HG2	5	0.12	0.01	0.11
(1,55)	1:95:A:LYS:H	1:95:A:LYS:HG3	5	0.12	0.01	0.11
(1,1895)	1:10:A:VAL:HG21	1:12:A:ASP:H	4	1.29	0.1	1.34
(1,1297)	1:10:A:VAL:HG21	1:11:A:LYS:H	4	1.14	0.05	1.16
(1,464)	1:135:A:GLU:H	1:135:A:GLU:OE1	4	0.97	0.36	0.9
(1,1242)	1:125:A:LEU:HD21	1:126:A:GLN:H	4	0.73	0.02	0.73
(1,259)	1:56:A:VAL:H	1:56:A:VAL:HG21	4	0.66	0.02	0.66
(1,2029)	1:143:A:VAL:H	1:146:A:GLU:HG2	4	0.36	0.05	0.36
(1,2029)	1:143:A:VAL:H	1:146:A:GLU:HG3	4	0.36	0.05	0.36
(2,165)	1:117:A:LYS:HE2	1:119:A:SER:H	4	0.34	0.03	0.36
(2,165)	1:117:A:LYS:HE3	1:119:A:SER:H	4	0.34	0.03	0.36
(2,858)	1:11:A:LYS:H	1:180:A:LEU:HD21	4	0.24	0.09	0.25
(1,669)	1:53:A:GLY:H	1:54:A:SER:H	4	0.15	0.05	0.14
(1,550)	1:188:A:GLU:H	1:188:A:GLU:HB2	4	0.14	0.02	0.13
(1,550)	1:188:A:GLU:H	1:188:A:GLU:HB3	4	0.14	0.02	0.13
(2,675)	1:110:A:ASP:H	1:173:A:LEU:HD21	3	0.72	0.19	0.65
(1,2708)	1:47:A:GLU:HA	1:53:A:GLY:H	3	0.37	0.09	0.42
(1,2412)	1:195:A:SER:HB2	1:198:A:LYS:H	3	0.32	0.11	0.31
(1,2412)	1:195:A:SER:HB3	1:198:A:LYS:H	3	0.32	0.11	0.31
(1,25)	1:140:A:LEU:H	1:140:A:LEU:HA	3	0.28	0.03	0.26
(2,166)	1:198:A:LYS:HE2	1:200:A:LEU:H	3	0.21	0.05	0.24
(2,166)	1:198:A:LYS:HE3	1:200:A:LEU:H	3	0.21	0.05	0.24
(1,1329)	1:161:A:GLN:HB2	1:162:A:LEU:H	3	0.2	0.01	0.21
(1,1329)	1:161:A:GLN:HB3	1:162:A:LEU:H	3	0.2	0.01	0.21
(1,1216)	1:100:A:LEU:HD11	1:101:A:ASP:H	3	0.19	0.01	0.19
(1,1602)	1:189:A:TYR:H	1:191:A:SER:H	3	0.19	0.08	0.16
(1,4)	1:139:A:ARG:H	1:139:A:ARG:HB2	3	0.18	0.01	0.18
(1,4)	1:139:A:ARG:H	1:139:A:ARG:HB3	3	0.18	0.01	0.18
(1,5)	1:179:A:GLU:H	1:179:A:GLU:HG2	3	0.16	0.04	0.18
(2,212)	1:64:A:GLY:H	1:67:A:THR:HG21	3	0.15	0.04	0.18
(2,277)	1:4:A:GLN:HB2	1:7:A:TRP:H	3	0.15	0.02	0.14
(2,277)	1:4:A:GLN:HB3	1:7:A:TRP:H	3	0.15	0.02	0.14
(1,2114)	1:78:A:THR:H	1:81:A:VAL:HG21	3	0.14	0.01	0.13
(1,2799)	1:46:A:LEU:HB2	1:146:A:GLU:H	3	0.14	0.01	0.15
(1,2799)	1:46:A:LEU:HB3	1:146:A:GLU:H	3	0.14	0.01	0.15
(1,1293)	1:175:A:GLN:HG2	1:176:A:ARG:H	3	0.14	0.0	0.14
(2,39)	1:180:A:LEU:HD21	1:181:A:LYS:H	3	0.14	0.02	0.13
(1,602)	1:99:A:TYR:H	1:100:A:LEU:H	3	0.14	0.03	0.12
(1,1330)	1:110:A:ASP:HB2	1:111:A:VAL:H	3	0.13	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1330)	1:110:A:ASP:HB3	1:111:A:VAL:H	3	0.13	0.02	0.14
(1,1280)	1:111:A:VAL:HG11	1:112:A:GLU:H	3	0.13	0.01	0.14
(1,256)	1:52:A:LEU:H	1:52:A:LEU:HA	3	0.12	0.0	0.12
(1,604)	1:139:A:ARG:H	1:140:A:LEU:H	3	0.12	0.01	0.13
(1,2609)	1:175:A:GLN:HG2	1:179:A:GLU:H	3	0.12	0.01	0.13
(2,808)	1:32:A:PHE:H	1:161:A:GLN:HG2	3	0.11	0.01	0.12
(2,808)	1:32:A:PHE:H	1:161:A:GLN:HG3	3	0.11	0.01	0.12
(1,2027)	1:107:A:TRP:H	1:110:A:ASP:HB2	3	0.11	0.0	0.11
(1,2027)	1:107:A:TRP:H	1:110:A:ASP:HB3	3	0.11	0.0	0.11
(1,1169)	1:198:A:LYS:HB2	1:199:A:SER:H	2	0.84	0.01	0.84
(1,1171)	1:198:A:LYS:HB3	1:199:A:SER:H	2	0.74	0.0	0.74
(1,31)	1:8:A:ASP:H	1:8:A:ASP:OD2	2	0.71	0.43	0.71
(1,558)	1:198:A:LYS:H	1:198:A:LYS:HD2	2	0.56	0.01	0.56
(1,558)	1:198:A:LYS:H	1:198:A:LYS:HD3	2	0.56	0.01	0.56
(1,1466)	1:22:A:LYS:HD2	1:23:A:ASP:H	2	0.38	0.01	0.38
(1,1466)	1:22:A:LYS:HD3	1:23:A:ASP:H	2	0.38	0.01	0.38
(1,136)	1:9:A:LYS:H	1:9:A:LYS:HB3	2	0.34	0.0	0.34
(1,1500)	1:9:A:LYS:HG2	1:10:A:VAL:H	2	0.32	0.02	0.32
(1,1500)	1:9:A:LYS:HG3	1:10:A:VAL:H	2	0.32	0.02	0.32
(1,1283)	1:116:A:GLN:HG2	1:117:A:LYS:H	2	0.32	0.02	0.32
(1,1547)	1:131:A:GLN:H	1:133:A:LEU:H	2	0.31	0.14	0.31
(1,1908)	1:57:A:SER:HB2	1:59:A:LEU:H	2	0.3	0.12	0.3
(1,1908)	1:57:A:SER:HB3	1:59:A:LEU:H	2	0.3	0.12	0.3
(1,1467)	1:76:A:LYS:HD2	1:77:A:GLU:H	2	0.3	0.01	0.3
(1,1467)	1:76:A:LYS:HD3	1:77:A:GLU:H	2	0.3	0.01	0.3
(1,1454)	1:198:A:LYS:HB2	1:199:A:SER:H	2	0.3	0.11	0.3
(1,1454)	1:198:A:LYS:HB3	1:199:A:SER:H	2	0.3	0.11	0.3
(1,40)	1:7:A:TRP:H	1:7:A:TRP:HZ3	2	0.27	0.17	0.27
(1,94)	1:76:A:LYS:H	1:76:A:LYS:HB2	2	0.26	0.01	0.26
(1,38)	1:208:A:LEU:H	1:208:A:LEU:HD11	2	0.26	0.05	0.26
(1,1333)	1:208:A:LEU:HB2	1:209:A:GLU:H	2	0.26	0.0	0.26
(1,1333)	1:208:A:LEU:HB3	1:209:A:GLU:H	2	0.26	0.0	0.26
(1,774)	1:55:A:THR:H	1:56:A:VAL:HG11	2	0.25	0.01	0.25
(1,2333)	1:162:A:LEU:HD11	1:165:A:HIS:H	2	0.24	0.12	0.24
(1,2719)	1:95:A:LYS:HD2	1:102:A:GLU:H	2	0.22	0.06	0.22
(1,2719)	1:95:A:LYS:HD3	1:102:A:GLU:H	2	0.22	0.06	0.22
(1,17)	1:101:A:ASP:H	1:101:A:ASP:HB2	2	0.22	0.0	0.22
(1,17)	1:101:A:ASP:H	1:101:A:ASP:HB3	2	0.22	0.0	0.22
(1,2023)	1:161:A:GLN:HG2	1:163:A:ALA:H	2	0.22	0.02	0.22
(1,2023)	1:161:A:GLN:HG3	1:163:A:ALA:H	2	0.22	0.02	0.22
(1,1)	1:52:A:LEU:H	1:52:A:LEU:HD11	2	0.2	0.0	0.2
(2,167)	1:116:A:GLN:HE21	1:118:A:ALA:H	2	0.19	0.03	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,167)	1:116:A:GLN:HE22	1:118:A:ALA:H	2	0.19	0.03	0.19
(2,493)	1:46:A:LEU:HG	1:51:A:THR:H	2	0.18	0.05	0.18
(1,594)	1:130:A:ARG:H	1:131:A:GLN:HB2	2	0.18	0.06	0.18
(1,594)	1:130:A:ARG:H	1:131:A:GLN:HB3	2	0.18	0.06	0.18
(1,966)	1:198:A:LYS:H	1:199:A:SER:H	2	0.17	0.01	0.17
(2,227)	1:180:A:LEU:H	1:183:A:ASN:HA	2	0.16	0.04	0.16
(1,34)	1:10:A:VAL:H	1:10:A:VAL:HG21	2	0.16	0.02	0.16
(1,955)	1:188:A:GLU:H	1:189:A:TYR:H	2	0.15	0.0	0.15
(1,2679)	1:31:A:GLN:HG2	1:35:A:SER:H	2	0.14	0.0	0.14
(1,2679)	1:31:A:GLN:HG3	1:35:A:SER:H	2	0.14	0.0	0.14
(1,1546)	1:49:A:TRP:H	1:51:A:THR:H	2	0.14	0.04	0.14
(2,18)	1:51:A:THR:H	1:52:A:LEU:HG	2	0.14	0.01	0.14
(1,131)	1:4:A:GLN:H	1:4:A:GLN:HB2	2	0.13	0.0	0.13
(1,131)	1:4:A:GLN:H	1:4:A:GLN:HB3	2	0.13	0.0	0.13
(1,892)	1:133:A:LEU:H	1:134:A:GLN:HA	2	0.13	0.0	0.13
(1,603)	1:46:A:LEU:H	1:47:A:GLU:HB2	2	0.12	0.01	0.12
(1,603)	1:46:A:LEU:H	1:47:A:GLU:HB3	2	0.12	0.01	0.12
(1,2020)	1:131:A:GLN:HG2	1:133:A:LEU:H	2	0.12	0.02	0.12
(1,2020)	1:131:A:GLN:HG3	1:133:A:LEU:H	2	0.12	0.02	0.12
(2,168)	1:31:A:GLN:HG2	1:33:A:GLU:H	2	0.12	0.02	0.12
(2,168)	1:31:A:GLN:HG3	1:33:A:GLU:H	2	0.12	0.02	0.12
(1,63)	1:62:A:ARG:H	1:62:A:ARG:HD2	2	0.12	0.01	0.12
(1,63)	1:62:A:ARG:H	1:62:A:ARG:HD3	2	0.12	0.01	0.12
(1,1113)	1:10:A:VAL:HB	1:11:A:LYS:H	2	0.12	0.01	0.12
(1,1565)	1:75:A:GLU:H	1:77:A:GLU:H	2	0.12	0.01	0.12
(1,1361)	1:24:A:SER:HB2	1:25:A:GLY:H	2	0.12	0.02	0.12
(1,1361)	1:24:A:SER:HB3	1:25:A:GLY:H	2	0.12	0.02	0.12
(1,568)	1:205:A:ARG:H	1:205:A:ARG:HA	2	0.12	0.0	0.12
(1,626)	1:199:A:SER:H	1:200:A:LEU:H	2	0.12	0.0	0.12
(1,1970)	1:139:A:ARG:HB2	1:141:A:SER:H	2	0.12	0.0	0.12
(1,1970)	1:139:A:ARG:HB3	1:141:A:SER:H	2	0.12	0.0	0.12
(1,1583)	1:95:A:LYS:H	1:97:A:GLN:HE21	2	0.11	0.01	0.11
(1,1583)	1:95:A:LYS:H	1:97:A:GLN:HE22	2	0.11	0.01	0.11
(1,1868)	1:208:A:LEU:HB3	1:210:A:ASP:H	2	0.11	0.0	0.11
(1,1987)	1:209:A:GLU:HB2	1:211:A:LEU:H	2	0.11	0.0	0.11
(1,1987)	1:209:A:GLU:HB3	1:211:A:LEU:H	2	0.11	0.0	0.11
(1,2464)	1:158:A:LEU:HA	1:162:A:LEU:H	2	0.11	0.01	0.11
(1,624)	1:94:A:GLN:H	1:95:A:LYS:HG2	2	0.11	0.0	0.11
(1,624)	1:94:A:GLN:H	1:95:A:LYS:HG3	2	0.11	0.0	0.11
(1,960)	1:193:A:ALA:H	1:194:A:LYS:H	2	0.11	0.0	0.11
(1,1475)	1:44:A:ASN:HD21	1:45:A:LEU:H	2	0.11	0.0	0.11
(1,1475)	1:44:A:ASN:HD22	1:45:A:LEU:H	2	0.11	0.0	0.11

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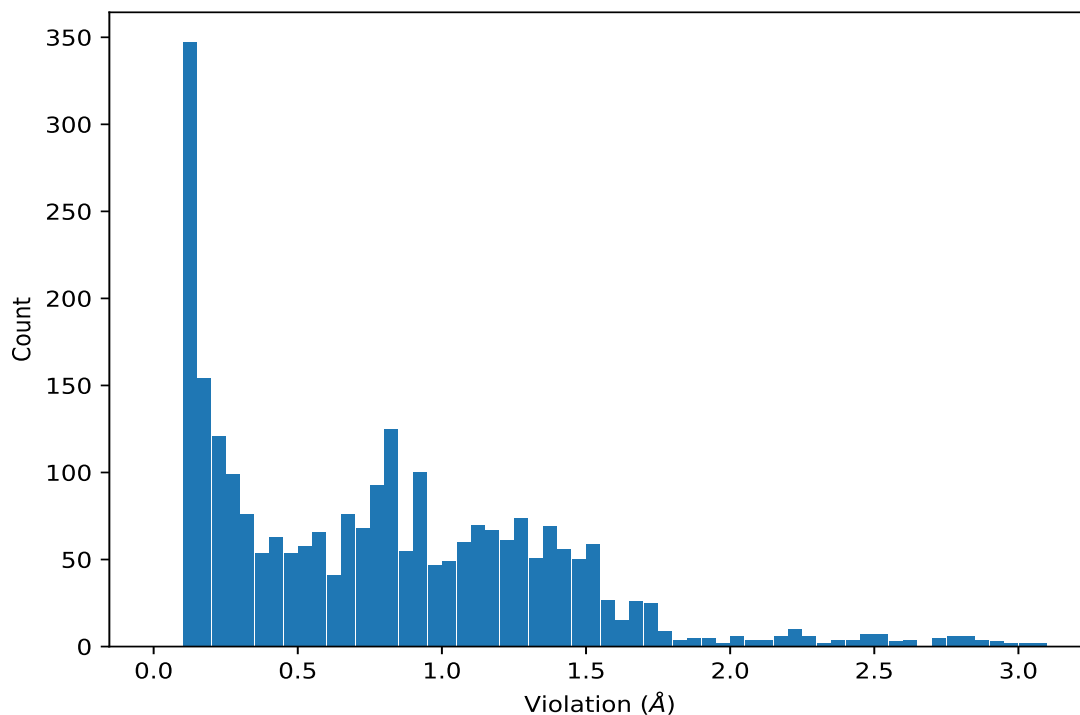
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,463)	1:55:A:THR:H	1:60:A:GLN:H	2	0.11	0.0	0.11
(2,598)	1:81:A:VAL:HG11	1:117:A:LYS:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	11	3.07
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	14	3.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	5	3.05
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	4	3.01
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	16	2.98
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	20	2.96
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	18	2.94
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	10	2.93
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	7	2.92
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	10	2.87
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	11	2.86
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	16	2.86
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	10	2.86
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	8	2.84
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	14	2.84
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	9	2.84
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	16	2.83
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	4	2.81
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	8	2.81
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	13	2.8
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	17	2.8
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	15	2.79
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	17	2.77
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	1	2.76
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	12	2.76
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	5	2.73
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	2	2.73
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	13	2.73
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	9	2.7
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	19	2.7
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	3	2.64
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	17	2.64
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	20	2.63
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	13	2.62
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	12	2.59
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	2	2.58
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	19	2.58
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	6	2.55
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	4	2.55
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	11	2.54
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	3	2.53
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	20	2.53
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	6	2.52
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	14	2.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	1	2.49
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	8	2.49
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	15	2.48
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	12	2.47
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	7	2.47
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	3	2.46
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	1	2.45
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	2	2.44
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	18	2.42
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	19	2.42
(1,2768)	1:28:A:TYR:HD1	1:74:A:LEU:H	5	2.42
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	6	2.4
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	7	2.39
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	15	2.38
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	13	2.36
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	1	2.31
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	17	2.31
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	7	2.29
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	4	2.27
(2,823)	1:28:A:TYR:HD2	1:162:A:LEU:H	9	2.26
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	12	2.26
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	6	2.25
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	15	2.25
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	11	2.24
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	13	2.24
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	10	2.23
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	11	2.23
(2,820)	1:28:A:TYR:HD2	1:161:A:GLN:H	18	2.22
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	17	2.22
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	2	2.21
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	8	2.21
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	14	2.21
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	3	2.2
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	9	2.19
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	18	2.19
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	15	2.19
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	9	2.17
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	4	2.16
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	3	2.15
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	5	2.14
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	16	2.12
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	20	2.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	2	2.1
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	19	2.09
(2,398)	1:13:A:PHE:HE2	1:17:A:TYR:H	19	2.09
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	7	2.09
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	10	2.07
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	18	2.05
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	16	2.05
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	1	2.03
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	6	2.03
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	18	2.03
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	12	2.02
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	14	1.99
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	5	1.96
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	8	1.94
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	20	1.93
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	1	1.92
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	7	1.91
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	19	1.91
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	2	1.9
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	12	1.9
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	15	1.89
(2,260)	1:32:A:PHE:HE2	1:35:A:SER:H	6	1.88
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	13	1.86
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	9	1.84
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	17	1.84
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	15	1.81
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	3	1.8
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	8	1.79
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	4	1.79
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	16	1.77
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	12	1.77
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	20	1.76
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	3	1.76
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	7	1.76
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	9	1.76
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	8	1.75
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	4	1.74
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	19	1.74
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	20	1.74
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	7	1.73
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	13	1.73
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	14	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	10	1.73
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	5	1.72
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	2	1.72
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	10	1.72
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	12	1.72
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	20	1.72
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	2	1.72
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	3	1.72
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	9	1.72
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	10	1.72
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	11	1.72
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	16	1.72
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	19	1.72
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	2	1.71
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	12	1.71
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	8	1.71
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	10	1.71
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	4	1.71
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	8	1.71
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	8	1.7
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	18	1.7
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	16	1.7
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	15	1.7
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	16	1.69
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	6	1.69
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	1	1.69
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	7	1.69
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	14	1.69
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	18	1.69
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	17	1.68
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	3	1.68
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	4	1.68
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	12	1.68
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	17	1.68
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	20	1.67
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	7	1.67
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	18	1.67
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	5	1.67
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	14	1.67
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	11	1.66
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	13	1.66
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	19	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	20	1.66
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	5	1.66
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	12	1.66
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	10	1.65
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	14	1.65
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	15	1.65
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	18	1.65
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	2	1.64
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	7	1.64
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	17	1.64
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	6	1.63
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	2	1.63
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	1	1.63
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	8	1.63
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	6	1.63
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	11	1.62
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	19	1.6
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	1	1.6
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	6	1.59
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	19	1.59
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	10	1.59
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	18	1.59
(1,1883)	1:41:A:LEU:HD21	1:43:A:LEU:H	9	1.59
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	3	1.58
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	9	1.58
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	10	1.58
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	19	1.58
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	4	1.57
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	11	1.57
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	11	1.57
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	16	1.57
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	4	1.57
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	17	1.57
(1,622)	1:161:A:GLN:H	1:162:A:LEU:HD21	9	1.57
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	16	1.56
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	20	1.56
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	5	1.55
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	14	1.55
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	1	1.55
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	4	1.55
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	13	1.55
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	10	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	19	1.55
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	12	1.55
(1,622)	1:161:A:GLN:H	1:162:A:LEU:HD21	5	1.55
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	16	1.54
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	6	1.54
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	10	1.54
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	12	1.54
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	13	1.54
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	6	1.54
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	16	1.54
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	3	1.54
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	7	1.54
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	8	1.54
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	8	1.54
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	6	1.54
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	9	1.53
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	13	1.53
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	2	1.53
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	15	1.53
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	17	1.53
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	3	1.53
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	11	1.53
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	19	1.53
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	4	1.53
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	7	1.53
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	18	1.53
(1,719)	1:12:A:ASP:H	1:13:A:PHE:HD1	13	1.53
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	7	1.53
(1,464)	1:135:A:GLU:H	1:135:A:GLU:OE1	12	1.53
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	20	1.52
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	3	1.52
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	13	1.52
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	1	1.52
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	4	1.52
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	5	1.52
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	11	1.52
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	12	1.52
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	18	1.52
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	12	1.52
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	14	1.52
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	2	1.52
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	2	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	19	1.52
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	13	1.51
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	19	1.51
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	12	1.51
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	3	1.51
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	6	1.51
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	7	1.51
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	8	1.51
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	14	1.51
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	4	1.51
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	5	1.51
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	9	1.5
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	9	1.5
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	11	1.5
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	17	1.5
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	11	1.5
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	20	1.5
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	16	1.5
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	5	1.5
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	20	1.5
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	2	1.49
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	7	1.49
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	11	1.49
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	20	1.49
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	6	1.49
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	18	1.49
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	12	1.49
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	4	1.49
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	12	1.49
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	4	1.49
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	12	1.49
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	10	1.49
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	15	1.49
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	6	1.49
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	9	1.49
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	10	1.48
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	12	1.48
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	5	1.48
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	15	1.48
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	20	1.48
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	6	1.48
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	9	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	7	1.48
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	8	1.48
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	9	1.48
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	13	1.48
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	11	1.48
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	11	1.47
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	3	1.47
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	4	1.47
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	15	1.47
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	13	1.47
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	1	1.47
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	18	1.47
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	3	1.47
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	15	1.47
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	5	1.46
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	16	1.46
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	17	1.46
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	4	1.46
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	5	1.46
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	16	1.46
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	18	1.46
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	7	1.46
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	14	1.46
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	10	1.46
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	17	1.46
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	13	1.46
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	4	1.46
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	12	1.46
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	15	1.45
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	11	1.45
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	6	1.45
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	18	1.45
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	6	1.45
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	14	1.45
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	8	1.45
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	3	1.45
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	17	1.45
(1,1237)	1:41:A:LEU:HD21	1:42:A:ASN:H	2	1.45
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	16	1.45
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	13	1.45
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	3	1.44
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	14	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	8	1.44
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	9	1.44
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	17	1.44
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	6	1.44
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	14	1.44
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	16	1.44
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	19	1.44
(1,1882)	1:37:A:LEU:HD21	1:39:A:GLN:H	19	1.44
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	15	1.44
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	6	1.44
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	10	1.44
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	11	1.44
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	10	1.43
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	1	1.43
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	19	1.43
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	1	1.43
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	8	1.43
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	19	1.43
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	19	1.43
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	16	1.43
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	20	1.43
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	7	1.43
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	14	1.43
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	8	1.43
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	10	1.42
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	16	1.42
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	1	1.42
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	9	1.42
(1,622)	1:161:A:GLN:H	1:162:A:LEU:HD21	2	1.42
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	11	1.42
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	14	1.41
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	9	1.41
(2,492)	1:37:A:LEU:HD21	1:42:A:ASN:H	13	1.41
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	1	1.41
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	5	1.41
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	6	1.41
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	11	1.41
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	18	1.41
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	7	1.41
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	13	1.41
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	17	1.41
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	15	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	9	1.4
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	10	1.4
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	11	1.4
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	13	1.4
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	6	1.4
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	17	1.4
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	2	1.4
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	17	1.4
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	4	1.4
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	19	1.4
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	9	1.4
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	14	1.4
(1,622)	1:161:A:GLN:H	1:162:A:LEU:HD21	8	1.4
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	10	1.4
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	17	1.39
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	7	1.39
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	8	1.39
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	1	1.39
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	5	1.39
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	3	1.39
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	10	1.39
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	12	1.39
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	5	1.39
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	8	1.39
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	10	1.39
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	10	1.39
(1,622)	1:161:A:GLN:H	1:162:A:LEU:HD21	17	1.39
(1,622)	1:161:A:GLN:H	1:162:A:LEU:HD21	19	1.39
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	1	1.39
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	19	1.39
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	19	1.38
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	1	1.38
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	14	1.38
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	18	1.38
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	2	1.38
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	11	1.38
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	3	1.38
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	16	1.38
(1,1895)	1:10:A:VAL:HG21	1:12:A:ASP:H	7	1.38
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	3	1.38
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	4	1.38
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	16	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	19	1.37
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	9	1.37
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	1	1.37
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	18	1.37
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	2	1.37
(1,1895)	1:10:A:VAL:HG21	1:12:A:ASP:H	6	1.37
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	20	1.37
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	12	1.36
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	13	1.36
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	17	1.36
(2,361)	1:48:A:ASN:H	1:52:A:LEU:HD21	9	1.36
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	9	1.36
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	19	1.36
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	20	1.36
(1,2338)	1:41:A:LEU:HD21	1:44:A:ASN:H	2	1.36
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	4	1.36
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	2	1.36
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	5	1.36
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	6	1.35
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	5	1.35
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	15	1.35
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	3	1.35
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	6	1.35
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	9	1.35
(1,861)	1:110:A:ASP:H	1:111:A:VAL:HG21	20	1.35
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	12	1.35
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	13	1.35
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	1	1.34
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	4	1.34
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	2	1.34
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	1	1.34
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	7	1.34
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	9	1.34
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	15	1.34
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	11	1.34
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	8	1.34
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	2	1.33
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	18	1.33
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	3	1.33
(1,2736)	1:40:A:GLN:H	1:63:A:LEU:HD21	7	1.33
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	3	1.33
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	8	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	9	1.33
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	16	1.33
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	5	1.32
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	3	1.32
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	11	1.32
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	12	1.32
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	20	1.32
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	3	1.32
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	16	1.32
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	2	1.32
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	14	1.32
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	17	1.32
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	18	1.31
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	5	1.31
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	10	1.31
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	16	1.31
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	3	1.31
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	15	1.31
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	12	1.31
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	13	1.31
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	20	1.31
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	1	1.31
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	20	1.3
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	15	1.3
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	16	1.3
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	7	1.3
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	15	1.3
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	10	1.3
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	14	1.3
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	15	1.3
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	1	1.3
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	7	1.3
(1,1895)	1:10:A:VAL:HG21	1:12:A:ASP:H	18	1.3
(1,622)	1:161:A:GLN:H	1:162:A:LEU:HD21	10	1.3
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	14	1.3
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	17	1.3
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	7	1.29
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	15	1.29
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	4	1.29
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	18	1.29
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	15	1.29
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	1	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	5	1.29
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	17	1.29
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	2	1.29
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	5	1.29
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	7	1.29
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	8	1.29
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	9	1.29
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	15	1.29
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	18	1.29
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	7	1.29
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	5	1.29
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	17	1.28
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	5	1.28
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	6	1.28
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	14	1.28
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	2	1.28
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	18	1.28
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	4	1.28
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	3	1.28
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	4	1.28
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	12	1.28
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	2	1.28
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	10	1.28
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	12	1.28
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	13	1.28
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	17	1.28
(1,1897)	1:67:A:THR:HG21	1:69:A:ASP:H	2	1.28
(1,1897)	1:67:A:THR:HG21	1:69:A:ASP:H	12	1.28
(1,1897)	1:67:A:THR:HG21	1:69:A:ASP:H	13	1.28
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	18	1.28
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	8	1.27
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	10	1.27
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	18	1.27
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	20	1.27
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	4	1.27
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	6	1.27
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	19	1.27
(1,1897)	1:67:A:THR:HG21	1:69:A:ASP:H	1	1.27
(1,1897)	1:67:A:THR:HG21	1:69:A:ASP:H	8	1.27
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	14	1.26
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	15	1.26
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	5	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	19	1.26
(2,361)	1:48:A:ASN:H	1:52:A:LEU:HD21	17	1.26
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	7	1.26
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	13	1.26
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	2	1.26
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	6	1.26
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	18	1.26
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	19	1.26
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	8	1.26
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	14	1.26
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	16	1.26
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	18	1.26
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	11	1.26
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	14	1.26
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	15	1.26
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	19	1.26
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	15	1.26
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	8	1.25
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	6	1.25
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	2	1.25
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	3	1.25
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	20	1.25
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	11	1.25
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	6	1.25
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	7	1.25
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	3	1.25
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	7	1.24
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	15	1.24
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	12	1.24
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	1	1.24
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	4	1.24
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	7	1.24
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	11	1.24
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	10	1.24
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	11	1.24
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	16	1.24
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	1	1.24
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	1	1.24
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	1	1.24
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	2	1.24
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	11	1.23
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	12	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	19	1.23
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	20	1.23
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	8	1.23
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	5	1.23
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	15	1.23
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	4	1.23
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	13	1.23
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	1	1.23
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	2	1.22
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	4	1.22
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	10	1.22
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	16	1.22
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	3	1.22
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	5	1.22
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	17	1.22
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	17	1.22
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	9	1.22
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	13	1.22
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	5	1.22
(1,2346)	1:78:A:THR:HG21	1:81:A:VAL:H	16	1.22
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	9	1.22
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	2	1.22
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	3	1.22
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	5	1.22
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	9	1.22
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	10	1.22
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	15	1.22
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	16	1.22
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	19	1.22
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	4	1.22
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	8	1.22
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	9	1.22
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	3	1.22
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	7	1.22
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	14	1.21
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	8	1.21
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	17	1.21
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	8	1.21
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	18	1.21
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	6	1.21
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	8	1.21
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	12	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	5	1.21
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	2	1.21
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	8	1.21
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	13	1.2
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	18	1.2
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	2	1.2
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	11	1.2
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	14	1.2
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	19	1.2
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	14	1.2
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	6	1.2
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	14	1.2
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	20	1.2
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	14	1.2
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	6	1.2
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	11	1.2
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	5	1.19
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	12	1.19
(2,361)	1:48:A:ASN:H	1:52:A:LEU:HD21	7	1.19
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	1	1.19
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	16	1.19
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	7	1.19
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	15	1.19
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	9	1.19
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	8	1.19
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	1	1.18
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	10	1.18
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	3	1.18
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	4	1.18
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	12	1.18
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	11	1.18
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	7	1.18
(1,2600)	1:37:A:LEU:HD21	1:41:A:LEU:H	19	1.18
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	1	1.18
(1,2598)	1:41:A:LEU:HD21	1:45:A:LEU:H	3	1.18
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	1	1.18
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	9	1.18
(1,1297)	1:10:A:VAL:HG21	1:11:A:LYS:H	6	1.18
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	7	1.18
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	14	1.18
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	3	1.17
(2,703)	1:105:A:LYS:H	1:177:A:LEU:HD21	4	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	19	1.17
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	13	1.17
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	9	1.17
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	7	1.17
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	5	1.17
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	17	1.17
(1,1297)	1:10:A:VAL:HG21	1:11:A:LYS:H	7	1.17
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	17	1.17
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	2	1.16
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	17	1.16
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	14	1.16
(2,591)	1:78:A:THR:H	1:113:A:LEU:HD21	14	1.16
(2,555)	1:39:A:GLN:H	1:63:A:LEU:HD21	7	1.16
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	10	1.16
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	13	1.16
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	15	1.16
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	1	1.16
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	14	1.16
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	10	1.16
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	20	1.16
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	10	1.16
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	17	1.16
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	7	1.16
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	17	1.16
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	18	1.16
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	10	1.16
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	16	1.16
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	18	1.16
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	6	1.15
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	6	1.15
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	5	1.15
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	4	1.15
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	12	1.15
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	17	1.15
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	17	1.15
(1,1297)	1:10:A:VAL:HG21	1:11:A:LYS:H	18	1.15
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	16	1.15
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	14	1.15
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	8	1.14
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	12	1.14
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	18	1.14
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	2	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	18	1.14
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	1	1.14
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	15	1.14
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	2	1.14
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	16	1.14
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	17	1.14
(1,31)	1:8:A:ASP:H	1:8:A:ASP:OD2	18	1.14
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	17	1.13
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	4	1.13
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	6	1.13
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	8	1.13
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	14	1.13
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	16	1.13
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	8	1.13
(1,1899)	1:92:A:VAL:HG21	1:94:A:GLN:H	18	1.13
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	11	1.13
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	17	1.13
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	13	1.13
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	15	1.13
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	18	1.13
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	6	1.13
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	12	1.13
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	11	1.12
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	9	1.12
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	16	1.12
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	1	1.12
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	20	1.12
(1,1895)	1:10:A:VAL:HG21	1:12:A:ASP:H	14	1.12
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	1	1.12
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	5	1.12
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	15	1.12
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	4	1.12
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	9	1.12
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	20	1.11
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	2	1.11
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	6	1.11
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	7	1.11
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	19	1.11
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	12	1.11
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	15	1.11
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	1	1.11
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	19	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:91:A:GLU:H	1:92:A:VAL:HG21	18	1.11
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	17	1.11
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	4	1.1
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	5	1.1
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	17	1.1
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	20	1.1
(1,2042)	1:93:A:LYS:H	1:96:A:VAL:HG21	5	1.1
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	4	1.1
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	1	1.1
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	2	1.1
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	4	1.1
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	8	1.1
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	14	1.1
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	14	1.1
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	17	1.09
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	18	1.09
(2,334)	1:17:A:TYR:H	1:21:A:VAL:HG21	20	1.09
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	2	1.09
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	5	1.09
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	6	1.09
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	16	1.09
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	18	1.09
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	20	1.09
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	3	1.09
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	5	1.09
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	11	1.09
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	10	1.09
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	10	1.09
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	19	1.09
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	3	1.09
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	9	1.09
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	10	1.09
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	12	1.09
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	9	1.09
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	14	1.08
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	15	1.08
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	16	1.08
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	4	1.08
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	8	1.08
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	14	1.08
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	15	1.08
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	9	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	18	1.08
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	15	1.08
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	13	1.08
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	3	1.08
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	20	1.08
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	10	1.08
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	7	1.08
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	12	1.08
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	20	1.08
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	6	1.07
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	8	1.07
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	17	1.07
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	2	1.07
(1,2756)	1:80:A:TRP:H	1:113:A:LEU:HD21	14	1.07
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	5	1.07
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	16	1.07
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	18	1.07
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	2	1.07
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	9	1.06
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	19	1.06
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	4	1.06
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	12	1.06
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	2	1.06
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	4	1.06
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	19	1.06
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	3	1.06
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	4	1.05
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	20	1.05
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	10	1.05
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	12	1.05
(1,1297)	1:10:A:VAL:HG21	1:11:A:LYS:H	14	1.05
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	8	1.05
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	3	1.04
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	16	1.04
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	16	1.04
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	12	1.04
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	11	1.04
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	9	1.04
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	8	1.04
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	8	1.04
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	13	1.04
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	18	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	7	1.04
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	19	1.03
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	1	1.03
(2,111)	1:43:A:LEU:HD21	1:45:A:LEU:H	20	1.03
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	3	1.03
(2,20)	1:62:A:ARG:H	1:63:A:LEU:HD21	13	1.03
(1,380)	1:99:A:TYR:H	1:99:A:TYR:HE1	5	1.03
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	2	1.02
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	3	1.02
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	17	1.02
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	14	1.02
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	2	1.02
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	6	1.02
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	8	1.02
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	16	1.02
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	20	1.02
(1,384)	1:100:A:LEU:H	1:100:A:LEU:HD21	14	1.02
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	9	1.01
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	13	1.01
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	10	1.01
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	12	1.01
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	9	1.01
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	17	1.01
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	19	1.01
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	18	1.01
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	14	1.01
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	11	1.01
(1,380)	1:99:A:TYR:H	1:99:A:TYR:HE1	12	1.01
(1,380)	1:99:A:TYR:H	1:99:A:TYR:HE1	15	1.01
(1,380)	1:99:A:TYR:H	1:99:A:TYR:HE1	20	1.01
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	1	1.0
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	1	1.0
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	8	1.0
(2,275)	1:67:A:THR:HG21	1:70:A:PHE:H	2	1.0
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	14	1.0
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	16	1.0
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	8	1.0
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	12	1.0
(1,464)	1:135:A:GLU:H	1:135:A:GLU:OE1	8	1.0
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	11	0.99
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	3	0.99
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	15	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,275)	1:67:A:THR:HG21	1:70:A:PHE:H	8	0.99
(2,275)	1:67:A:THR:HG21	1:70:A:PHE:H	12	0.99
(2,275)	1:67:A:THR:HG21	1:70:A:PHE:H	13	0.99
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	19	0.99
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	4	0.99
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	6	0.99
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	14	0.99
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	13	0.99
(1,384)	1:100:A:LEU:H	1:100:A:LEU:HD21	5	0.99
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	17	0.98
(2,675)	1:110:A:ASP:H	1:173:A:LEU:HD21	10	0.98
(2,275)	1:67:A:THR:HG21	1:70:A:PHE:H	1	0.98
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	18	0.98
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	13	0.98
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	5	0.98
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	15	0.98
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	5	0.98
(1,384)	1:100:A:LEU:H	1:100:A:LEU:HD21	13	0.98
(1,384)	1:100:A:LEU:H	1:100:A:LEU:HD21	18	0.98
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	12	0.97
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	5	0.97
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	2	0.97
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	5	0.97
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	10	0.97
(2,543)	1:41:A:LEU:H	1:63:A:LEU:HD21	7	0.97
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	6	0.97
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	8	0.97
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	16	0.97
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	9	0.97
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	20	0.97
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	11	0.97
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	8	0.96
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	16	0.96
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	6	0.96
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	15	0.96
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	19	0.96
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	20	0.96
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	10	0.96
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	11	0.96
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	1	0.96
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	19	0.96
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	6	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	15	0.96
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	13	0.96
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	8	0.95
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	3	0.95
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	14	0.95
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	12	0.95
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	5	0.95
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	4	0.95
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	5	0.95
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	2	0.95
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	12	0.95
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	17	0.95
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	1	0.94
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	12	0.94
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	16	0.94
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	9	0.94
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	5	0.94
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	11	0.94
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	11	0.94
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	12	0.94
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	13	0.94
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	15	0.94
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	17	0.94
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	6	0.94
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	11	0.94
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	14	0.94
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	13	0.94
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	3	0.93
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	4	0.93
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	7	0.93
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	2	0.93
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	7	0.93
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	10	0.93
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	13	0.93
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	15	0.93
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	20	0.93
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	6	0.93
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	7	0.93
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	16	0.93
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	11	0.92
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	10	0.92
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	1	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	1:61:A:GLU:H	1:63:A:LEU:HD21	13	0.92
(1,2726)	1:43:A:LEU:H	1:59:A:LEU:HD21	13	0.92
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	3	0.92
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	2	0.92
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	11	0.92
(1,2340)	1:43:A:LEU:HD21	1:46:A:LEU:H	11	0.92
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	15	0.92
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	13	0.92
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	12	0.92
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	20	0.92
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	5	0.92
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	19	0.92
(1,384)	1:100:A:LEU:H	1:100:A:LEU:HD21	6	0.92
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	3	0.92
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	10	0.92
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	16	0.91
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	5	0.91
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	14	0.91
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	1	0.91
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	17	0.91
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	18	0.91
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	9	0.91
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	19	0.91
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	3	0.91
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	10	0.91
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	17	0.91
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	17	0.91
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	8	0.91
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	6	0.91
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	7	0.91
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	9	0.91
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	12	0.91
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	14	0.91
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	15	0.91
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	17	0.91
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	20	0.91
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	6	0.91
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	16	0.91
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	14	0.9
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	10	0.9
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	20	0.9
(2,613)	1:78:A:THR:HG21	1:117:A:LYS:H	1	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	12	0.9
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	8	0.9
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	14	0.9
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	16	0.9
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	19	0.9
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	1	0.9
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	9	0.9
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	6	0.9
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	19	0.9
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	20	0.9
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	20	0.9
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	4	0.9
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	5	0.9
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	8	0.9
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	11	0.9
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	18	0.9
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	19	0.9
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	5	0.9
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	10	0.89
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	13	0.89
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	19	0.89
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	1	0.89
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	20	0.89
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	5	0.89
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	9	0.89
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	20	0.89
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	8	0.89
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	11	0.89
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	14	0.89
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	18	0.89
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	15	0.89
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	1	0.89
(1,232)	1:41:A:LEU:H	1:41:A:LEU:HD21	2	0.89
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	12	0.89
(2,760)	1:28:A:TYR:HD1	1:117:A:LYS:H	16	0.88
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	8	0.88
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	9	0.88
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	18	0.88
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	3	0.88
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	7	0.88
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	9	0.88
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	7	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	16	0.88
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	6	0.88
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	19	0.88
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	17	0.88
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	3	0.88
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	8	0.88
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	13	0.87
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	11	0.87
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	14	0.87
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	15	0.87
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	16	0.87
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	19	0.87
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	3	0.87
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	7	0.87
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	6	0.86
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	6	0.86
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	2	0.86
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	4	0.86
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	6	0.86
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	7	0.86
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	18	0.86
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	20	0.86
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	6	0.86
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	18	0.86
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	2	0.86
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	16	0.86
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	19	0.86
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	5	0.86
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	11	0.86
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	12	0.86
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	17	0.86
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	4	0.85
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	11	0.85
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	14	0.85
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	4	0.85
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	2	0.85
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	2	0.85
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	9	0.85
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	18	0.85
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	15	0.85
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	8	0.85
(1,2347)	1:92:A:VAL:HG21	1:95:A:LYS:H	7	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	2	0.85
(1,1900)	1:143:A:VAL:HG21	1:145:A:GLU:H	3	0.85
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	10	0.85
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	11	0.85
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	5	0.85
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	18	0.85
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	3	0.85
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	4	0.85
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	13	0.85
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	1	0.84
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	12	0.84
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	15	0.84
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	19	0.84
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	8	0.84
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	12	0.84
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	2	0.84
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	14	0.84
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	13	0.84
(1,2611)	1:29:A:VAL:HG21	1:33:A:GLU:H	1	0.84
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	14	0.84
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	4	0.84
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	17	0.84
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	18	0.84
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	12	0.84
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	1	0.84
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	2	0.84
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	7	0.84
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	9	0.84
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	18	0.84
(1,1169)	1:198:A:LYS:HB2	1:199:A:SER:H	12	0.84
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	10	0.84
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	1	0.84
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	2	0.84
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	15	0.84
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	19	0.84
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	17	0.83
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	7	0.83
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	8	0.83
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	9	0.83
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	7	0.83
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	8	0.83
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	10	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,112)	1:45:A:LEU:HD21	1:47:A:GLU:H	16	0.83
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	13	0.83
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	14	0.83
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	16	0.83
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	18	0.83
(1,1688)	1:90:A:GLU:H	1:92:A:VAL:HG21	18	0.83
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	19	0.83
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	8	0.83
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	12	0.83
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	15	0.83
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	16	0.83
(1,1169)	1:198:A:LYS:HB2	1:199:A:SER:H	17	0.83
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	20	0.82
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	5	0.82
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	17	0.82
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	6	0.82
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	9	0.82
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	4	0.82
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	7	0.82
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	9	0.82
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	15	0.82
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	10	0.82
(1,1900)	1:143:A:VAL:HG21	1:145:A:GLU:H	5	0.82
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	4	0.82
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	5	0.82
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	12	0.82
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	3	0.82
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	1	0.82
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	2	0.82
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	19	0.82
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	8	0.82
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	13	0.82
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	8	0.82
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	14	0.82
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	11	0.82
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	2	0.82
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	11	0.82
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	6	0.81
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	15	0.81
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	1	0.81
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	3	0.81
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	9	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	11	0.81
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	13	0.81
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	18	0.81
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	1	0.81
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	2	0.81
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	3	0.81
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	5	0.81
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	18	0.81
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	20	0.81
(1,2443)	1:48:A:ASN:H	1:52:A:LEU:HA	13	0.81
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	9	0.81
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	5	0.81
(1,1643)	1:43:A:LEU:H	1:45:A:LEU:HD21	6	0.81
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	19	0.81
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	6	0.81
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	7	0.81
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	17	0.81
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	3	0.8
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	16	0.8
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	17	0.8
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	3	0.8
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	1	0.8
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	15	0.8
(2,110)	1:125:A:LEU:HD21	1:127:A:GLU:H	14	0.8
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	8	0.8
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	20	0.8
(1,1900)	1:143:A:VAL:HG21	1:145:A:GLU:H	10	0.8
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	4	0.8
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	15	0.8
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	6	0.8
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	19	0.79
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	18	0.79
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	7	0.79
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	20	0.79
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	10	0.79
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	19	0.79
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	15	0.79
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	10	0.79
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	4	0.79
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	5	0.79
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	8	0.79
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	3	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1900)	1:143:A:VAL:HG21	1:145:A:GLU:H	12	0.79
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	3	0.79
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	18	0.79
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	19	0.79
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	3	0.79
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	13	0.79
(1,464)	1:135:A:GLU:H	1:135:A:GLU:OE1	16	0.79
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	4	0.79
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	2	0.78
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	13	0.78
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	4	0.78
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	15	0.78
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	16	0.78
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	20	0.78
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	3	0.78
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	7	0.78
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	11	0.78
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	4	0.78
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	4	0.78
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	11	0.78
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	14	0.78
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	19	0.78
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	20	0.77
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	18	0.77
(2,778)	1:21:A:VAL:HG21	1:114:A:TYR:H	20	0.77
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	2	0.77
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	19	0.77
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	4	0.77
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	6	0.77
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	7	0.77
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	16	0.77
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	11	0.77
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	12	0.77
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	17	0.77
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	7	0.77
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	9	0.77
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	10	0.77
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	17	0.77
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	20	0.77
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	1	0.77
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	2	0.77
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	9	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:45:A:LEU:HD21	1:46:A:LEU:H	10	0.77
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	6	0.77
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	7	0.76
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	14	0.76
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	1	0.76
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	1	0.76
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	3	0.76
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	13	0.76
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	16	0.76
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	11	0.76
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	15	0.76
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	15	0.76
(1,1900)	1:143:A:VAL:HG21	1:145:A:GLU:H	9	0.76
(1,1900)	1:143:A:VAL:HG21	1:145:A:GLU:H	11	0.76
(1,1900)	1:143:A:VAL:HG21	1:145:A:GLU:H	13	0.76
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	7	0.76
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	15	0.76
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	6	0.76
(1,1242)	1:125:A:LEU:HD21	1:126:A:GLN:H	16	0.76
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	7	0.76
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	12	0.75
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	12	0.75
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	11	0.75
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	12	0.75
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	2	0.75
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	10	0.75
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	3	0.75
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	20	0.75
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	12	0.75
(1,2812)	1:17:A:TYR:H	1:173:A:LEU:HD21	16	0.75
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	1	0.75
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	11	0.75
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	8	0.75
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	1	0.75
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	2	0.75
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	6	0.75
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	1	0.75
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	8	0.75
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	14	0.75
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	10	0.74
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	6	0.74
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	16	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	2	0.74
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	10	0.74
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	18	0.74
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	19	0.74
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	5	0.74
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	8	0.74
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	16	0.74
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	17	0.74
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	14	0.74
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	11	0.74
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	4	0.74
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	5	0.74
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	10	0.74
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	12	0.74
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	13	0.74
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	14	0.74
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	18	0.74
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	5	0.74
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	9	0.74
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	14	0.74
(1,1242)	1:125:A:LEU:HD21	1:126:A:GLN:H	12	0.74
(1,1171)	1:198:A:LYS:HB3	1:199:A:SER:H	14	0.74
(1,1171)	1:198:A:LYS:HB3	1:199:A:SER:H	16	0.74
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	5	0.74
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	9	0.73
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	8	0.73
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	4	0.73
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	14	0.73
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	5	0.73
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	6	0.73
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	8	0.73
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	18	0.73
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	19	0.73
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	5	0.73
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	9	0.73
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	17	0.73
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	19	0.73
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	17	0.73
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	14	0.73
(1,1252)	1:70:A:PHE:HE2	1:71:A:TRP:H	7	0.73
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	12	0.72
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	5	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	18	0.72
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	10	0.72
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	4	0.72
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	1	0.72
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	2	0.72
(1,1382)	1:61:A:GLU:HB2	1:62:A:ARG:H	19	0.72
(1,1382)	1:61:A:GLU:HB3	1:62:A:ARG:H	19	0.72
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	15	0.72
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	16	0.72
(1,1242)	1:125:A:LEU:HD21	1:126:A:GLN:H	19	0.72
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	20	0.71
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	8	0.71
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	9	0.71
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	4	0.71
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	14	0.71
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	1	0.71
(2,64)	1:39:A:GLN:H	1:41:A:LEU:HD21	2	0.71
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	16	0.71
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	4	0.71
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	19	0.71
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	20	0.71
(1,1296)	1:185:A:THR:HG21	1:186:A:LEU:H	20	0.71
(1,1252)	1:70:A:PHE:HE2	1:71:A:TRP:H	3	0.71
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	6	0.7
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	19	0.7
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	18	0.7
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	20	0.7
(2,199)	1:43:A:LEU:H	1:46:A:LEU:HD21	13	0.7
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	9	0.7
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	10	0.7
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	3	0.7
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	13	0.7
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	6	0.7
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	11	0.7
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	11	0.7
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	11	0.7
(1,1252)	1:70:A:PHE:HE2	1:71:A:TRP:H	9	0.7
(1,1242)	1:125:A:LEU:HD21	1:126:A:GLN:H	10	0.7
(1,121)	1:173:A:LEU:H	1:173:A:LEU:HD21	20	0.7
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	18	0.7
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	3	0.69
(1,1900)	1:143:A:VAL:HG21	1:145:A:GLU:H	7	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	5	0.69
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	10	0.69
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	20	0.69
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	20	0.69
(1,1252)	1:70:A:PHE:HE2	1:71:A:TRP:H	10	0.69
(1,1252)	1:70:A:PHE:HE2	1:71:A:TRP:H	16	0.69
(1,1252)	1:70:A:PHE:HE2	1:71:A:TRP:H	18	0.69
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	9	0.68
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	17	0.68
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	7	0.68
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	17	0.68
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	15	0.68
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	17	0.68
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	5	0.68
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	9	0.68
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	16	0.68
(1,1305)	1:111:A:VAL:HG21	1:112:A:GLU:H	13	0.68
(1,1252)	1:70:A:PHE:HE2	1:71:A:TRP:H	4	0.68
(1,1252)	1:70:A:PHE:HE2	1:71:A:TRP:H	14	0.68
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	20	0.68
(1,259)	1:56:A:VAL:H	1:56:A:VAL:HG21	16	0.68
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	7	0.67
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	13	0.67
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	18	0.67
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	17	0.67
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	2	0.67
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	6	0.67
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	1	0.67
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	12	0.67
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	20	0.67
(1,259)	1:56:A:VAL:H	1:56:A:VAL:HG21	8	0.67
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	9	0.67
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	11	0.66
(2,641)	1:29:A:VAL:HG21	1:75:A:GLU:H	15	0.66
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	5	0.66
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	19	0.66
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	13	0.66
(1,2089)	1:42:A:ASN:H	1:45:A:LEU:HD21	6	0.66
(1,1898)	1:78:A:THR:HG21	1:80:A:TRP:H	16	0.66
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	4	0.66
(1,1252)	1:70:A:PHE:HE2	1:71:A:TRP:H	5	0.66
(1,1238)	1:43:A:LEU:HD21	1:44:A:ASN:H	20	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:56:A:VAL:H	1:56:A:VAL:HG21	14	0.66
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	6	0.66
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	1	0.66
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	3	0.66
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	5	0.66
(2,675)	1:110:A:ASP:H	1:173:A:LEU:HD21	18	0.65
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	17	0.65
(2,41)	1:208:A:LEU:HD21	1:209:A:GLU:H	6	0.65
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	7	0.65
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	15	0.65
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	6	0.65
(1,1900)	1:143:A:VAL:HG21	1:145:A:GLU:H	6	0.65
(1,1900)	1:143:A:VAL:HG21	1:145:A:GLU:H	17	0.65
(1,1252)	1:70:A:PHE:HE2	1:71:A:TRP:H	12	0.65
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	12	0.65
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	1	0.64
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	12	0.64
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	19	0.64
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	2	0.64
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	4	0.64
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	7	0.64
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	6	0.63
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	19	0.63
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	1	0.63
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	6	0.63
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	1	0.63
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	12	0.63
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	20	0.63
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	2	0.63
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	3	0.63
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	3	0.63
(1,259)	1:56:A:VAL:H	1:56:A:VAL:HG21	19	0.63
(2,361)	1:48:A:ASN:H	1:52:A:LEU:HD21	13	0.62
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	2	0.62
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	7	0.62
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	3	0.62
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	12	0.62
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	20	0.62
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	5	0.62
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	7	0.62
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	8	0.62
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	14	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	18	0.62
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	12	0.62
(1,1306)	1:143:A:VAL:HG21	1:144:A:ALA:H	3	0.62
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	18	0.62
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	11	0.62
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	6	0.61
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	20	0.61
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	6	0.61
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	16	0.61
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	13	0.61
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	19	0.61
(1,1306)	1:143:A:VAL:HG21	1:144:A:ALA:H	10	0.61
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	2	0.61
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	18	0.61
(2,274)	1:18:A:VAL:HG21	1:21:A:VAL:H	18	0.6
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	8	0.6
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	17	0.6
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	3	0.6
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	10	0.6
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	10	0.6
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	4	0.6
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	8	0.59
(2,405)	1:18:A:VAL:HG21	1:22:A:LYS:H	20	0.59
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	13	0.59
(2,41)	1:208:A:LEU:HD21	1:209:A:GLU:H	17	0.59
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	11	0.59
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	6	0.59
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	12	0.59
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	13	0.59
(2,856)	1:12:A:ASP:H	1:180:A:LEU:HD21	16	0.58
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	18	0.58
(2,568)	1:84:A:GLU:H	1:113:A:LEU:HD21	14	0.58
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	11	0.58
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	4	0.58
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	6	0.58
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	17	0.58
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	11	0.58
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	6	0.58
(1,558)	1:198:A:LYS:H	1:198:A:LYS:HD2	12	0.58
(1,558)	1:198:A:LYS:H	1:198:A:LYS:HD3	12	0.58
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	1	0.58
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	2	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	17	0.57
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	16	0.57
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	20	0.57
(2,107)	1:7:A:TRP:HD1	1:9:A:LYS:H	18	0.57
(2,41)	1:208:A:LEU:HD21	1:209:A:GLU:H	9	0.57
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	19	0.57
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	9	0.57
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	13	0.57
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	1	0.57
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	19	0.57
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	2	0.57
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	7	0.57
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	15	0.57
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	19	0.57
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	16	0.56
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	7	0.56
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	5	0.56
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	14	0.56
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	8	0.56
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	15	0.56
(1,464)	1:135:A:GLU:H	1:135:A:GLU:OE1	7	0.56
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	3	0.55
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	2	0.55
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	9	0.55
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	10	0.55
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	9	0.55
(1,1306)	1:143:A:VAL:HG21	1:144:A:ALA:H	5	0.55
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	7	0.55
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	13	0.55
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	20	0.55
(1,558)	1:198:A:LYS:H	1:198:A:LYS:HD2	17	0.55
(1,558)	1:198:A:LYS:H	1:198:A:LYS:HD3	17	0.55
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	4	0.55
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	17	0.55
(1,384)	1:100:A:LEU:H	1:100:A:LEU:HD21	17	0.55
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	1	0.55
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	3	0.55
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	2	0.55
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	3	0.54
(2,862)	1:9:A:LYS:H	1:180:A:LEU:HD21	9	0.54
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	12	0.54
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	12	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	2	0.54
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	14	0.54
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	5	0.54
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	9	0.54
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	16	0.54
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	5	0.54
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	15	0.54
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	7	0.54
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	9	0.54
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	14	0.54
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	15	0.54
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	16	0.54
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	18	0.54
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	10	0.54
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	4	0.53
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	8	0.53
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	19	0.53
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	16	0.53
(1,1306)	1:143:A:VAL:HG21	1:144:A:ALA:H	11	0.53
(1,1306)	1:143:A:VAL:HG21	1:144:A:ALA:H	12	0.53
(1,1306)	1:143:A:VAL:HG21	1:144:A:ALA:H	13	0.53
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	4	0.53
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	8	0.53
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	13	0.53
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	13	0.53
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	17	0.53
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	4	0.52
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	15	0.52
(2,675)	1:110:A:ASP:H	1:173:A:LEU:HD21	9	0.52
(2,361)	1:48:A:ASN:H	1:52:A:LEU:HD21	12	0.52
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	7	0.52
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	15	0.52
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	19	0.52
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	7	0.52
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	3	0.52
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	9	0.52
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	1	0.52
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	7	0.51
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	10	0.51
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	1	0.51
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	7	0.51
(1,2339)	1:37:A:LEU:HD21	1:40:A:GLN:H	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	12	0.51
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	6	0.51
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	8	0.51
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	3	0.51
(1,384)	1:100:A:LEU:H	1:100:A:LEU:HD21	1	0.51
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	11	0.5
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	12	0.5
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	5	0.5
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	15	0.5
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	1	0.5
(1,1306)	1:143:A:VAL:HG21	1:144:A:ALA:H	9	0.5
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	5	0.5
(2,718)	1:103:A:PHE:H	1:180:A:LEU:HD21	4	0.49
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	15	0.49
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	13	0.49
(2,408)	1:140:A:LEU:HB2	1:144:A:ALA:H	6	0.49
(2,408)	1:140:A:LEU:HB3	1:144:A:ALA:H	6	0.49
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	20	0.49
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	2	0.49
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	18	0.49
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	7	0.49
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	11	0.49
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	17	0.49
(1,547)	1:185:A:THR:H	1:185:A:THR:HG21	11	0.49
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	13	0.49
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	13	0.48
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	17	0.48
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	10	0.48
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	8	0.48
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	14	0.48
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	19	0.48
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	15	0.48
(2,856)	1:12:A:ASP:H	1:180:A:LEU:HD21	19	0.47
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	3	0.47
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	9	0.47
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	13	0.47
(2,571)	1:125:A:LEU:H	1:155:A:VAL:HG21	11	0.47
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	13	0.47
(1,2777)	1:18:A:VAL:HG21	1:84:A:GLU:H	18	0.47
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	4	0.47
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	8	0.47
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	18	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	3	0.47
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	3	0.47
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	12	0.47
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	5	0.46
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	11	0.46
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	3	0.46
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	6	0.46
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	18	0.46
(1,2715)	1:201:A:GLY:H	1:208:A:LEU:HD21	7	0.46
(1,2412)	1:195:A:SER:HB2	1:198:A:LYS:H	14	0.46
(1,2412)	1:195:A:SER:HB3	1:198:A:LYS:H	14	0.46
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	9	0.46
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	10	0.46
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	17	0.46
(1,723)	1:15:A:ASN:H	1:16:A:VAL:HG21	12	0.46
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	3	0.46
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	20	0.46
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	5	0.45
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	6	0.45
(2,631)	1:118:A:ALA:H	1:162:A:LEU:HD21	14	0.45
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	17	0.45
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	11	0.45
(2,41)	1:208:A:LEU:HD21	1:209:A:GLU:H	15	0.45
(1,1547)	1:131:A:GLN:H	1:133:A:LEU:H	14	0.45
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	15	0.44
(2,737)	1:13:A:PHE:HE1	1:93:A:LYS:H	13	0.44
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	3	0.44
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	1	0.44
(1,2708)	1:47:A:GLU:HA	1:53:A:GLY:H	17	0.44
(1,1897)	1:67:A:THR:HG21	1:69:A:ASP:H	7	0.44
(1,1660)	1:64:A:GLY:H	1:66:A:LEU:HD21	3	0.44
(1,1652)	1:59:A:LEU:H	1:61:A:GLU:HB2	19	0.44
(1,1652)	1:59:A:LEU:H	1:61:A:GLU:HB3	19	0.44
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	11	0.44
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	14	0.44
(1,58)	1:43:A:LEU:H	1:43:A:LEU:HD21	20	0.44
(1,40)	1:7:A:TRP:H	1:7:A:TRP:HZ3	18	0.44
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	15	0.44
(2,771)	1:21:A:VAL:H	1:113:A:LEU:HD21	3	0.43
(2,517)	1:45:A:LEU:H	1:59:A:LEU:HD21	13	0.43
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	4	0.43
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	11	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2029)	1:143:A:VAL:H	1:146:A:GLU:HG2	6	0.43
(1,2029)	1:143:A:VAL:H	1:146:A:GLU:HG3	6	0.43
(1,1908)	1:57:A:SER:HB2	1:59:A:LEU:H	19	0.43
(1,1908)	1:57:A:SER:HB3	1:59:A:LEU:H	19	0.43
(1,1897)	1:67:A:THR:HG21	1:69:A:ASP:H	15	0.43
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	15	0.43
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	20	0.43
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	10	0.42
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	17	0.42
(2,462)	1:47:A:GLU:H	1:52:A:LEU:HG	7	0.42
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	13	0.42
(1,2708)	1:47:A:GLU:HA	1:53:A:GLY:H	9	0.42
(1,1897)	1:67:A:THR:HG21	1:69:A:ASP:H	17	0.42
(1,1306)	1:143:A:VAL:HG21	1:144:A:ALA:H	7	0.42
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	9	0.42
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	11	0.41
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	12	0.41
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	11	0.41
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	4	0.41
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	9	0.41
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	12	0.41
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	1	0.41
(2,3)	1:179:A:GLU:H	1:180:A:LEU:HD21	12	0.41
(1,1308)	1:160:A:THR:HG21	1:161:A:GLN:H	10	0.41
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	10	0.41
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	7	0.41
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	16	0.41
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	14	0.4
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	4	0.4
(2,793)	1:43:A:LEU:HD21	1:144:A:ALA:H	20	0.4
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	5	0.4
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	14	0.4
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	18	0.4
(2,509)	1:200:A:LEU:H	1:208:A:LEU:HD21	7	0.4
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	5	0.4
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	12	0.4
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	1	0.4
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	10	0.4
(1,1897)	1:67:A:THR:HG21	1:69:A:ASP:H	20	0.4
(1,1454)	1:198:A:LYS:HB2	1:199:A:SER:H	16	0.4
(1,1454)	1:198:A:LYS:HB3	1:199:A:SER:H	16	0.4
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	16	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	15	0.4
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	16	0.4
(1,12)	1:55:A:THR:H	1:55:A:THR:HG21	11	0.4
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	8	0.39
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	16	0.39
(2,203)	1:49:A:TRP:H	1:52:A:LEU:HA	13	0.39
(2,16)	1:42:A:ASN:H	1:43:A:LEU:HD21	20	0.39
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	19	0.39
(1,1897)	1:67:A:THR:HG21	1:69:A:ASP:H	6	0.39
(1,1897)	1:67:A:THR:HG21	1:69:A:ASP:H	11	0.39
(1,1466)	1:22:A:LYS:HD2	1:23:A:ASP:H	20	0.39
(1,1466)	1:22:A:LYS:HD3	1:23:A:ASP:H	20	0.39
(1,493)	1:158:A:LEU:H	1:158:A:LEU:HD21	7	0.39
(1,2)	1:102:A:GLU:H	1:102:A:GLU:HG2	15	0.39
(1,2)	1:102:A:GLU:H	1:102:A:GLU:HG3	15	0.39
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	14	0.38
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	9	0.38
(2,41)	1:208:A:LEU:HD21	1:209:A:GLU:H	2	0.38
(2,41)	1:208:A:LEU:HD21	1:209:A:GLU:H	18	0.38
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	3	0.38
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	16	0.38
(1,1466)	1:22:A:LYS:HD2	1:23:A:ASP:H	19	0.38
(1,1466)	1:22:A:LYS:HD3	1:23:A:ASP:H	19	0.38
(1,1306)	1:143:A:VAL:HG21	1:144:A:ALA:H	17	0.38
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	6	0.38
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	8	0.38
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	12	0.38
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	18	0.38
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	1	0.37
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	20	0.37
(2,631)	1:118:A:ALA:H	1:162:A:LEU:HD21	7	0.37
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	2	0.37
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	6	0.37
(2,165)	1:117:A:LYS:HE2	1:119:A:SER:H	10	0.37
(2,165)	1:117:A:LYS:HE3	1:119:A:SER:H	10	0.37
(2,165)	1:117:A:LYS:HE2	1:119:A:SER:H	14	0.37
(2,165)	1:117:A:LYS:HE3	1:119:A:SER:H	14	0.37
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	20	0.37
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	4	0.37
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	10	0.37
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	13	0.37
(2,856)	1:12:A:ASP:H	1:180:A:LEU:HD21	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	4	0.36
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	16	0.36
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	1	0.36
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	2	0.36
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	20	0.36
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	13	0.36
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	4	0.36
(1,2029)	1:143:A:VAL:H	1:146:A:GLU:HG2	19	0.36
(1,2029)	1:143:A:VAL:H	1:146:A:GLU:HG3	19	0.36
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	2	0.36
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	4	0.36
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	1	0.36
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	5	0.36
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	14	0.36
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	4	0.36
(2,858)	1:11:A:LYS:H	1:180:A:LEU:HD21	16	0.35
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	8	0.35
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	15	0.35
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	19	0.35
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	9	0.35
(1,2333)	1:162:A:LEU:HD11	1:165:A:HIS:H	18	0.35
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	5	0.35
(1,2029)	1:143:A:VAL:H	1:146:A:GLU:HG2	20	0.35
(1,2029)	1:143:A:VAL:H	1:146:A:GLU:HG3	20	0.35
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	17	0.35
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	19	0.35
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	2	0.34
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	3	0.34
(2,165)	1:117:A:LYS:HE2	1:119:A:SER:H	16	0.34
(2,165)	1:117:A:LYS:HE3	1:119:A:SER:H	16	0.34
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	2	0.34
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	17	0.34
(1,1500)	1:9:A:LYS:HG2	1:10:A:VAL:H	19	0.34
(1,1500)	1:9:A:LYS:HG3	1:10:A:VAL:H	19	0.34
(1,1306)	1:143:A:VAL:HG21	1:144:A:ALA:H	6	0.34
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	4	0.34
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	6	0.34
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	15	0.34
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	20	0.34
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	2	0.34
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	9	0.34
(1,136)	1:9:A:LYS:H	1:9:A:LYS:HB3	16	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:9:A:LYS:H	1:9:A:LYS:HB3	19	0.34
(2,856)	1:12:A:ASP:H	1:180:A:LEU:HD21	18	0.33
(2,387)	1:140:A:LEU:HA	1:144:A:ALA:H	2	0.33
(2,275)	1:67:A:THR:HG21	1:70:A:PHE:H	7	0.33
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	11	0.33
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	12	0.33
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	15	0.33
(1,1341)	1:8:A:ASP:HB2	1:9:A:LYS:H	18	0.33
(1,1341)	1:8:A:ASP:HB3	1:9:A:LYS:H	18	0.33
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	5	0.33
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	7	0.33
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	19	0.33
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	20	0.33
(1,1283)	1:116:A:GLN:HG2	1:117:A:LYS:H	3	0.33
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	11	0.33
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	2	0.33
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	6	0.33
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	5	0.33
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	13	0.32
(2,631)	1:118:A:ALA:H	1:162:A:LEU:HD21	6	0.32
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	4	0.32
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	1	0.32
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	3	0.32
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	8	0.32
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	8	0.32
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	13	0.32
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	18	0.32
(1,83)	1:7:A:TRP:H	1:7:A:TRP:HB2	18	0.32
(1,83)	1:7:A:TRP:H	1:7:A:TRP:HB3	18	0.32
(1,73)	1:52:A:LEU:H	1:52:A:LEU:HD21	20	0.32
(1,25)	1:140:A:LEU:H	1:140:A:LEU:HA	2	0.32
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	1	0.31
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	4	0.31
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	14	0.31
(1,2412)	1:195:A:SER:HB2	1:198:A:LYS:H	16	0.31
(1,2412)	1:195:A:SER:HB3	1:198:A:LYS:H	16	0.31
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	13	0.31
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	14	0.31
(1,1602)	1:189:A:TYR:H	1:191:A:SER:H	16	0.31
(1,1467)	1:76:A:LYS:HD2	1:77:A:GLU:H	3	0.31
(1,1467)	1:76:A:LYS:HD3	1:77:A:GLU:H	3	0.31
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	17	0.31
(1,1268)	1:140:A:LEU:HG	1:141:A:SER:H	11	0.31
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	4	0.31
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	12	0.31
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	1	0.31
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	11	0.31
(1,38)	1:208:A:LEU:H	1:208:A:LEU:HD11	7	0.31
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	4	0.3
(2,559)	1:37:A:LEU:H	1:63:A:LEU:HD21	7	0.3
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	17	0.3
(2,165)	1:117:A:LYS:HE2	1:119:A:SER:H	20	0.3
(2,165)	1:117:A:LYS:HE3	1:119:A:SER:H	20	0.3
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	20	0.3
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	17	0.3
(1,2029)	1:143:A:VAL:H	1:146:A:GLU:HG2	11	0.3
(1,2029)	1:143:A:VAL:H	1:146:A:GLU:HG3	11	0.3
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	4	0.3
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	20	0.3
(1,1500)	1:9:A:LYS:HG2	1:10:A:VAL:H	16	0.3
(1,1500)	1:9:A:LYS:HG3	1:10:A:VAL:H	16	0.3
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	8	0.3
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	12	0.3
(1,1283)	1:116:A:GLN:HG2	1:117:A:LYS:H	1	0.3
(1,286)	1:67:A:THR:H	1:67:A:THR:HG21	7	0.3
(2,631)	1:118:A:ALA:H	1:162:A:LEU:HD21	3	0.29
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	18	0.29
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	17	0.29
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	12	0.29
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	12	0.29
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB2	7	0.29
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB3	7	0.29
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	5	0.29
(1,1467)	1:76:A:LYS:HD2	1:77:A:GLU:H	1	0.29
(1,1467)	1:76:A:LYS:HD3	1:77:A:GLU:H	1	0.29
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	12	0.29
(1,791)	1:66:A:LEU:H	1:67:A:THR:HG21	20	0.29
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	17	0.28
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	13	0.28
(1,2719)	1:95:A:LYS:HD2	1:102:A:GLU:H	15	0.28
(1,2719)	1:95:A:LYS:HD3	1:102:A:GLU:H	15	0.28
(1,2051)	1:89:A:LEU:H	1:92:A:VAL:HG21	14	0.28
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	1	0.28
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	14	0.28
(1,791)	1:66:A:LEU:H	1:67:A:THR:HG21	15	0.28
(1,315)	1:78:A:THR:H	1:78:A:THR:HG21	16	0.28
(1,31)	1:8:A:ASP:H	1:8:A:ASP:OD2	17	0.28
(2,858)	1:11:A:LYS:H	1:180:A:LEU:HD21	19	0.27
(2,856)	1:12:A:ASP:H	1:180:A:LEU:HD21	6	0.27
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	7	0.27
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	14	0.27
(2,275)	1:67:A:THR:HG21	1:70:A:PHE:H	17	0.27
(2,257)	1:100:A:LEU:HD21	1:103:A:PHE:H	11	0.27
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	2	0.27
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	10	0.27
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	11	0.27
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	19	0.27
(1,1332)	1:47:A:GLU:HB2	1:48:A:ASN:H	11	0.27
(1,1332)	1:47:A:GLU:HB3	1:48:A:ASN:H	11	0.27
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	13	0.27
(1,286)	1:67:A:THR:H	1:67:A:THR:HG21	17	0.27
(1,94)	1:76:A:LYS:H	1:76:A:LYS:HB2	3	0.27
(2,663)	1:22:A:LYS:HG2	1:81:A:VAL:H	6	0.26
(2,663)	1:22:A:LYS:HG3	1:81:A:VAL:H	6	0.26
(2,631)	1:118:A:ALA:H	1:162:A:LEU:HD21	18	0.26
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	20	0.26
(2,275)	1:67:A:THR:HG21	1:70:A:PHE:H	15	0.26
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	8	0.26
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	14	0.26
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB2	18	0.26
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB3	18	0.26
(1,1333)	1:208:A:LEU:HB2	1:209:A:GLU:H	7	0.26
(1,1333)	1:208:A:LEU:HB3	1:209:A:GLU:H	7	0.26
(1,1333)	1:208:A:LEU:HB2	1:209:A:GLU:H	13	0.26
(1,1333)	1:208:A:LEU:HB3	1:209:A:GLU:H	13	0.26
(1,1328)	1:188:A:GLU:HB2	1:189:A:TYR:H	18	0.26
(1,1328)	1:188:A:GLU:HB3	1:189:A:TYR:H	18	0.26
(1,1247)	1:200:A:LEU:HD21	1:201:A:GLY:H	10	0.26
(1,1243)	1:140:A:LEU:HD21	1:141:A:SER:H	12	0.26
(1,1234)	1:46:A:LEU:HD21	1:47:A:GLU:H	4	0.26
(1,1130)	1:62:A:ARG:HB2	1:63:A:LEU:H	15	0.26
(1,791)	1:66:A:LEU:H	1:67:A:THR:HG21	17	0.26
(1,774)	1:55:A:THR:H	1:56:A:VAL:HG11	7	0.26
(1,286)	1:67:A:THR:H	1:67:A:THR:HG21	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,286)	1:67:A:THR:H	1:67:A:THR:HG21	11	0.26
(1,286)	1:67:A:THR:H	1:67:A:THR:HG21	15	0.26
(1,94)	1:76:A:LYS:H	1:76:A:LYS:HB2	1	0.26
(1,25)	1:140:A:LEU:H	1:140:A:LEU:HA	10	0.26
(1,25)	1:140:A:LEU:H	1:140:A:LEU:HA	13	0.26
(2,663)	1:22:A:LYS:HG2	1:81:A:VAL:H	19	0.25
(2,663)	1:22:A:LYS:HG3	1:81:A:VAL:H	19	0.25
(2,663)	1:22:A:LYS:HG2	1:81:A:VAL:H	20	0.25
(2,663)	1:22:A:LYS:HG3	1:81:A:VAL:H	20	0.25
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	8	0.25
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	16	0.25
(2,166)	1:198:A:LYS:HE2	1:200:A:LEU:H	16	0.25
(2,166)	1:198:A:LYS:HE3	1:200:A:LEU:H	16	0.25
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB2	2	0.25
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB3	2	0.25
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB2	6	0.25
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB3	6	0.25
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	9	0.25
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	12	0.25
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	13	0.25
(1,1233)	1:100:A:LEU:HD21	1:101:A:ASP:H	5	0.25
(1,791)	1:66:A:LEU:H	1:67:A:THR:HG21	6	0.25
(2,663)	1:22:A:LYS:HG2	1:81:A:VAL:H	7	0.24
(2,663)	1:22:A:LYS:HG3	1:81:A:VAL:H	7	0.24
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	4	0.24
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	7	0.24
(2,275)	1:67:A:THR:HG21	1:70:A:PHE:H	20	0.24
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	6	0.24
(2,166)	1:198:A:LYS:HE2	1:200:A:LEU:H	14	0.24
(2,166)	1:198:A:LYS:HE3	1:200:A:LEU:H	14	0.24
(2,41)	1:208:A:LEU:HD21	1:209:A:GLU:H	19	0.24
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	17	0.24
(1,2708)	1:47:A:GLU:HA	1:53:A:GLY:H	7	0.24
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	3	0.24
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	6	0.24
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	16	0.24
(1,791)	1:66:A:LEU:H	1:67:A:THR:HG21	7	0.24
(1,774)	1:55:A:THR:H	1:56:A:VAL:HG11	20	0.24
(1,44)	1:97:A:GLN:H	1:97:A:GLN:HB2	9	0.24
(1,44)	1:97:A:GLN:H	1:97:A:GLN:HB3	9	0.24
(2,858)	1:11:A:LYS:H	1:180:A:LEU:HD21	10	0.23
(2,631)	1:118:A:ALA:H	1:162:A:LEU:HD21	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	9	0.23
(2,493)	1:46:A:LEU:HG	1:51:A:THR:H	13	0.23
(2,275)	1:67:A:THR:HG21	1:70:A:PHE:H	6	0.23
(1,2023)	1:161:A:GLN:HG2	1:163:A:ALA:H	12	0.23
(1,2023)	1:161:A:GLN:HG3	1:163:A:ALA:H	12	0.23
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	1	0.23
(1,1332)	1:47:A:GLU:HB2	1:48:A:ASN:H	20	0.23
(1,1332)	1:47:A:GLU:HB3	1:48:A:ASN:H	20	0.23
(1,1328)	1:188:A:GLU:HB2	1:189:A:TYR:H	19	0.23
(1,1328)	1:188:A:GLU:HB3	1:189:A:TYR:H	19	0.23
(1,1322)	1:7:A:TRP:HZ2	1:8:A:ASP:H	18	0.23
(1,622)	1:161:A:GLN:H	1:162:A:LEU:HD21	11	0.23
(1,594)	1:130:A:ARG:H	1:131:A:GLN:HB2	14	0.23
(1,594)	1:130:A:ARG:H	1:131:A:GLN:HB3	14	0.23
(1,286)	1:67:A:THR:H	1:67:A:THR:HG21	20	0.23
(1,250)	1:46:A:LEU:H	1:46:A:LEU:HD21	5	0.23
(1,44)	1:97:A:GLN:H	1:97:A:GLN:HB2	5	0.23
(1,44)	1:97:A:GLN:H	1:97:A:GLN:HB3	5	0.23
(1,44)	1:97:A:GLN:H	1:97:A:GLN:HB2	15	0.23
(1,44)	1:97:A:GLN:H	1:97:A:GLN:HB3	15	0.23
(1,44)	1:97:A:GLN:H	1:97:A:GLN:HB2	17	0.23
(1,44)	1:97:A:GLN:H	1:97:A:GLN:HB3	17	0.23
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	2	0.23
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	5	0.23
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	17	0.23
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	13	0.22
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	11	0.22
(2,663)	1:22:A:LYS:HG2	1:81:A:VAL:H	2	0.22
(2,663)	1:22:A:LYS:HG3	1:81:A:VAL:H	2	0.22
(2,663)	1:22:A:LYS:HG2	1:81:A:VAL:H	18	0.22
(2,663)	1:22:A:LYS:HG3	1:81:A:VAL:H	18	0.22
(2,275)	1:67:A:THR:HG21	1:70:A:PHE:H	11	0.22
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	2	0.22
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	11	0.22
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	15	0.22
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	16	0.22
(2,167)	1:116:A:GLN:HE21	1:118:A:ALA:H	3	0.22
(2,167)	1:116:A:GLN:HE22	1:118:A:ALA:H	3	0.22
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	5	0.22
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	17	0.22
(1,1501)	1:11:A:LYS:HG2	1:12:A:ASP:H	17	0.22
(1,1501)	1:11:A:LYS:HG3	1:12:A:ASP:H	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1332)	1:47:A:GLU:HB2	1:48:A:ASN:H	6	0.22
(1,1332)	1:47:A:GLU:HB3	1:48:A:ASN:H	6	0.22
(1,791)	1:66:A:LEU:H	1:67:A:THR:HG21	11	0.22
(1,669)	1:53:A:GLY:H	1:54:A:SER:H	13	0.22
(1,44)	1:97:A:GLN:H	1:97:A:GLN:HB2	20	0.22
(1,44)	1:97:A:GLN:H	1:97:A:GLN:HB3	20	0.22
(1,17)	1:101:A:ASP:H	1:101:A:ASP:HB2	9	0.22
(1,17)	1:101:A:ASP:H	1:101:A:ASP:HB3	9	0.22
(1,17)	1:101:A:ASP:H	1:101:A:ASP:HB2	16	0.22
(1,17)	1:101:A:ASP:H	1:101:A:ASP:HB3	16	0.22
(1,15)	1:146:A:GLU:H	1:146:A:GLU:OE1	8	0.22
(1,2)	1:102:A:GLU:H	1:102:A:GLU:HG2	4	0.22
(1,2)	1:102:A:GLU:H	1:102:A:GLU:HG3	4	0.22
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	16	0.21
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	5	0.21
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	6	0.21
(2,408)	1:140:A:LEU:HB2	1:144:A:ALA:H	17	0.21
(2,408)	1:140:A:LEU:HB3	1:144:A:ALA:H	17	0.21
(1,2011)	1:58:A:GLN:HG2	1:60:A:GLN:H	19	0.21
(1,2011)	1:58:A:GLN:HG3	1:60:A:GLN:H	19	0.21
(1,1896)	1:29:A:VAL:HG21	1:31:A:GLN:H	18	0.21
(1,1329)	1:161:A:GLN:HB2	1:162:A:LEU:H	8	0.21
(1,1329)	1:161:A:GLN:HB3	1:162:A:LEU:H	8	0.21
(1,1329)	1:161:A:GLN:HB2	1:162:A:LEU:H	10	0.21
(1,1329)	1:161:A:GLN:HB3	1:162:A:LEU:H	10	0.21
(1,1245)	1:162:A:LEU:HD21	1:163:A:ALA:H	13	0.21
(1,1216)	1:100:A:LEU:HD11	1:101:A:ASP:H	16	0.21
(1,622)	1:161:A:GLN:H	1:162:A:LEU:HD21	20	0.21
(1,135)	1:8:A:ASP:H	1:8:A:ASP:HB2	17	0.21
(1,135)	1:8:A:ASP:H	1:8:A:ASP:HB3	17	0.21
(1,38)	1:208:A:LEU:H	1:208:A:LEU:HD11	13	0.21
(2,596)	1:172:A:SER:H	1:208:A:LEU:HD21	6	0.2
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	5	0.2
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	12	0.2
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	18	0.2
(2,510)	1:95:A:LYS:HD2	1:103:A:PHE:H	17	0.2
(2,510)	1:95:A:LYS:HD3	1:103:A:PHE:H	17	0.2
(2,408)	1:140:A:LEU:HB2	1:144:A:ALA:H	10	0.2
(2,408)	1:140:A:LEU:HB3	1:144:A:ALA:H	10	0.2
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	4	0.2
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	16	0.2
(2,227)	1:180:A:LEU:H	1:183:A:ASN:HA	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	5	0.2
(1,2423)	1:31:A:GLN:HE21	1:34:A:SER:H	15	0.2
(1,2423)	1:31:A:GLN:HE22	1:34:A:SER:H	15	0.2
(1,2423)	1:31:A:GLN:HE21	1:34:A:SER:H	18	0.2
(1,2423)	1:31:A:GLN:HE22	1:34:A:SER:H	18	0.2
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB2	19	0.2
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB3	19	0.2
(1,2023)	1:161:A:GLN:HG2	1:163:A:ALA:H	9	0.2
(1,2023)	1:161:A:GLN:HG3	1:163:A:ALA:H	9	0.2
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	3	0.2
(1,1332)	1:47:A:GLU:HB2	1:48:A:ASN:H	15	0.2
(1,1332)	1:47:A:GLU:HB3	1:48:A:ASN:H	15	0.2
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	1	0.2
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	17	0.2
(1,5)	1:179:A:GLU:H	1:179:A:GLU:HG2	8	0.2
(1,1)	1:52:A:LEU:H	1:52:A:LEU:HD11	9	0.2
(1,1)	1:52:A:LEU:H	1:52:A:LEU:HD11	17	0.2
(2,856)	1:12:A:ASP:H	1:180:A:LEU:HD21	14	0.19
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	20	0.19
(2,745)	1:11:A:LYS:HD2	1:93:A:LYS:H	17	0.19
(2,745)	1:11:A:LYS:HD3	1:93:A:LYS:H	17	0.19
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	5	0.19
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	20	0.19
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	10	0.19
(1,2677)	1:22:A:LYS:HE2	1:26:A:ARG:H	7	0.19
(1,2677)	1:22:A:LYS:HE3	1:26:A:ARG:H	7	0.19
(1,2677)	1:22:A:LYS:HE2	1:26:A:ARG:H	20	0.19
(1,2677)	1:22:A:LYS:HE3	1:26:A:ARG:H	20	0.19
(1,2423)	1:31:A:GLN:HE21	1:34:A:SER:H	4	0.19
(1,2423)	1:31:A:GLN:HE22	1:34:A:SER:H	4	0.19
(1,2348)	1:160:A:THR:HG21	1:163:A:ALA:H	6	0.19
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	9	0.19
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	11	0.19
(1,1454)	1:198:A:LYS:HB2	1:199:A:SER:H	14	0.19
(1,1454)	1:198:A:LYS:HB3	1:199:A:SER:H	14	0.19
(1,1329)	1:161:A:GLN:HB2	1:162:A:LEU:H	17	0.19
(1,1329)	1:161:A:GLN:HB3	1:162:A:LEU:H	17	0.19
(1,1216)	1:100:A:LEU:HD11	1:101:A:ASP:H	19	0.19
(1,622)	1:161:A:GLN:H	1:162:A:LEU:HD21	12	0.19
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	5	0.19
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	9	0.19
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	13	0.19
(1,4)	1:139:A:ARG:H	1:139:A:ARG:HB2	10	0.19
(1,4)	1:139:A:ARG:H	1:139:A:ARG:HB3	10	0.19
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	14	0.18
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	1	0.18
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	17	0.18
(2,510)	1:95:A:LYS:HD2	1:103:A:PHE:H	4	0.18
(2,510)	1:95:A:LYS:HD3	1:103:A:PHE:H	4	0.18
(2,408)	1:140:A:LEU:HB2	1:144:A:ALA:H	13	0.18
(2,408)	1:140:A:LEU:HB3	1:144:A:ALA:H	13	0.18
(2,277)	1:4:A:GLN:HB2	1:7:A:TRP:H	14	0.18
(2,277)	1:4:A:GLN:HB3	1:7:A:TRP:H	14	0.18
(2,212)	1:64:A:GLY:H	1:67:A:THR:HG21	15	0.18
(2,212)	1:64:A:GLY:H	1:67:A:THR:HG21	17	0.18
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	8	0.18
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	10	0.18
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	14	0.18
(1,2423)	1:31:A:GLN:HE21	1:34:A:SER:H	13	0.18
(1,2423)	1:31:A:GLN:HE22	1:34:A:SER:H	13	0.18
(1,2412)	1:195:A:SER:HB2	1:198:A:LYS:H	3	0.18
(1,2412)	1:195:A:SER:HB3	1:198:A:LYS:H	3	0.18
(1,2348)	1:160:A:THR:HG21	1:163:A:ALA:H	15	0.18
(1,1908)	1:57:A:SER:HB2	1:59:A:LEU:H	16	0.18
(1,1908)	1:57:A:SER:HB3	1:59:A:LEU:H	16	0.18
(1,1907)	1:188:A:GLU:HB2	1:190:A:HIS:H	9	0.18
(1,1907)	1:188:A:GLU:HB3	1:190:A:HIS:H	9	0.18
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	8	0.18
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	13	0.18
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	14	0.18
(1,1514)	1:83:A:GLN:HG2	1:84:A:GLU:H	15	0.18
(1,1514)	1:83:A:GLN:HG3	1:84:A:GLU:H	15	0.18
(1,1216)	1:100:A:LEU:HD11	1:101:A:ASP:H	4	0.18
(1,1129)	1:58:A:GLN:HB2	1:59:A:LEU:H	19	0.18
(1,966)	1:198:A:LYS:H	1:199:A:SER:H	14	0.18
(1,602)	1:99:A:TYR:H	1:100:A:LEU:H	15	0.18
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	1	0.18
(1,5)	1:179:A:GLU:H	1:179:A:GLU:HG2	6	0.18
(1,4)	1:139:A:ARG:H	1:139:A:ARG:HB2	13	0.18
(1,4)	1:139:A:ARG:H	1:139:A:ARG:HB3	13	0.18
(2,770)	1:18:A:VAL:H	1:110:A:ASP:HB2	19	0.17
(2,770)	1:18:A:VAL:H	1:110:A:ASP:HB3	19	0.17
(2,762)	1:28:A:TYR:HD1	1:118:A:ALA:H	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	3	0.17
(2,510)	1:95:A:LYS:HD2	1:103:A:PHE:H	1	0.17
(2,510)	1:95:A:LYS:HD3	1:103:A:PHE:H	1	0.17
(2,510)	1:95:A:LYS:HD2	1:103:A:PHE:H	5	0.17
(2,510)	1:95:A:LYS:HD3	1:103:A:PHE:H	5	0.17
(2,510)	1:95:A:LYS:HD2	1:103:A:PHE:H	15	0.17
(2,510)	1:95:A:LYS:HD3	1:103:A:PHE:H	15	0.17
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	7	0.17
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	20	0.17
(2,93)	1:193:A:ALA:H	1:195:A:SER:H	4	0.17
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	4	0.17
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	11	0.17
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	17	0.17
(1,2706)	1:96:A:VAL:H	1:102:A:GLU:HG2	15	0.17
(1,2706)	1:96:A:VAL:H	1:102:A:GLU:HG3	15	0.17
(1,2677)	1:22:A:LYS:HE2	1:26:A:ARG:H	2	0.17
(1,2677)	1:22:A:LYS:HE3	1:26:A:ARG:H	2	0.17
(1,2677)	1:22:A:LYS:HE2	1:26:A:ARG:H	6	0.17
(1,2677)	1:22:A:LYS:HE3	1:26:A:ARG:H	6	0.17
(1,2677)	1:22:A:LYS:HE2	1:26:A:ARG:H	19	0.17
(1,2677)	1:22:A:LYS:HE3	1:26:A:ARG:H	19	0.17
(1,2348)	1:160:A:THR:HG21	1:163:A:ALA:H	18	0.17
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB2	20	0.17
(1,2026)	1:19:A:ASP:H	1:22:A:LYS:HB3	20	0.17
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	1	0.17
(1,1547)	1:131:A:GLN:H	1:133:A:LEU:H	20	0.17
(1,1546)	1:49:A:TRP:H	1:51:A:THR:H	4	0.17
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	1	0.17
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	16	0.17
(1,1127)	1:144:A:ALA:HB2	1:145:A:GLU:H	6	0.17
(1,727)	1:20:A:ALA:H	1:21:A:VAL:HG21	11	0.17
(1,622)	1:161:A:GLN:H	1:162:A:LEU:HD21	4	0.17
(1,598)	1:56:A:VAL:H	1:57:A:SER:H	19	0.17
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	3	0.17
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	8	0.17
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	12	0.17
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE21	15	0.17
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE22	15	0.17
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE21	20	0.17
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE22	20	0.17
(1,34)	1:10:A:VAL:H	1:10:A:VAL:HG21	6	0.17
(2,844)	1:18:A:VAL:H	1:173:A:LEU:HD21	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	20	0.16
(2,593)	1:81:A:VAL:H	1:117:A:LYS:HD2	20	0.16
(2,593)	1:81:A:VAL:H	1:117:A:LYS:HD3	20	0.16
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	2	0.16
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	15	0.16
(2,352)	1:55:A:THR:H	1:59:A:LEU:H	7	0.16
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	2	0.16
(2,167)	1:116:A:GLN:HE21	1:118:A:ALA:H	1	0.16
(2,167)	1:116:A:GLN:HE22	1:118:A:ALA:H	1	0.16
(2,39)	1:180:A:LEU:HD21	1:181:A:LYS:H	8	0.16
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	12	0.16
(1,2719)	1:95:A:LYS:HD2	1:102:A:GLU:H	4	0.16
(1,2719)	1:95:A:LYS:HD3	1:102:A:GLU:H	4	0.16
(1,2425)	1:83:A:GLN:HE21	1:86:A:ASN:H	15	0.16
(1,2425)	1:83:A:GLN:HE22	1:86:A:ASN:H	15	0.16
(1,2348)	1:160:A:THR:HG21	1:163:A:ALA:H	13	0.16
(1,2114)	1:78:A:THR:H	1:81:A:VAL:HG21	19	0.16
(1,1602)	1:189:A:TYR:H	1:191:A:SER:H	11	0.16
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	4	0.16
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	12	0.16
(1,1332)	1:47:A:GLU:HB2	1:48:A:ASN:H	13	0.16
(1,1332)	1:47:A:GLU:HB3	1:48:A:ASN:H	13	0.16
(1,1332)	1:47:A:GLU:HB2	1:48:A:ASN:H	19	0.16
(1,1332)	1:47:A:GLU:HB3	1:48:A:ASN:H	19	0.16
(1,1328)	1:188:A:GLU:HB2	1:189:A:TYR:H	12	0.16
(1,1328)	1:188:A:GLU:HB3	1:189:A:TYR:H	12	0.16
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	11	0.16
(1,966)	1:198:A:LYS:H	1:199:A:SER:H	16	0.16
(1,781)	1:60:A:GLN:H	1:61:A:GLU:HB2	19	0.16
(1,781)	1:60:A:GLN:H	1:61:A:GLU:HB3	19	0.16
(1,727)	1:20:A:ALA:H	1:21:A:VAL:HG21	8	0.16
(1,669)	1:53:A:GLY:H	1:54:A:SER:H	9	0.16
(1,550)	1:188:A:GLU:H	1:188:A:GLU:HB2	18	0.16
(1,550)	1:188:A:GLU:H	1:188:A:GLU:HB3	18	0.16
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	14	0.16
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE21	5	0.16
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE22	5	0.16
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE21	14	0.16
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE22	14	0.16
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE21	17	0.16
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE22	17	0.16
(1,36)	1:97:A:GLN:H	1:97:A:GLN:HG2	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:97:A:GLN:H	1:97:A:GLN:HG3	14	0.16
(1,4)	1:139:A:ARG:H	1:139:A:ARG:HB2	2	0.16
(1,4)	1:139:A:ARG:H	1:139:A:ARG:HB3	2	0.16
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	15	0.15
(2,623)	1:28:A:TYR:HE1	1:70:A:PHE:H	8	0.15
(2,276)	1:155:A:VAL:HG21	1:158:A:LEU:H	15	0.15
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	19	0.15
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	1	0.15
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	9	0.15
(2,3)	1:179:A:GLU:H	1:180:A:LEU:HD21	6	0.15
(1,2799)	1:46:A:LEU:HB2	1:146:A:GLU:H	6	0.15
(1,2799)	1:46:A:LEU:HB3	1:146:A:GLU:H	6	0.15
(1,2799)	1:46:A:LEU:HB2	1:146:A:GLU:H	19	0.15
(1,2799)	1:46:A:LEU:HB3	1:146:A:GLU:H	19	0.15
(1,2710)	1:179:A:GLU:HA	1:185:A:THR:H	5	0.15
(1,1833)	1:82:A:ARG:HA	1:84:A:GLU:H	15	0.15
(1,1330)	1:110:A:ASP:HB2	1:111:A:VAL:H	16	0.15
(1,1330)	1:110:A:ASP:HB3	1:111:A:VAL:H	16	0.15
(1,1328)	1:188:A:GLU:HB2	1:189:A:TYR:H	2	0.15
(1,1328)	1:188:A:GLU:HB3	1:189:A:TYR:H	2	0.15
(1,1328)	1:188:A:GLU:HB2	1:189:A:TYR:H	8	0.15
(1,1328)	1:188:A:GLU:HB3	1:189:A:TYR:H	8	0.15
(1,955)	1:188:A:GLU:H	1:189:A:TYR:H	2	0.15
(1,955)	1:188:A:GLU:H	1:189:A:TYR:H	12	0.15
(1,622)	1:161:A:GLN:H	1:162:A:LEU:HD21	1	0.15
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	4	0.15
(1,74)	1:180:A:LEU:H	1:180:A:LEU:HD21	12	0.15
(2,765)	1:26:A:ARG:H	1:117:A:LYS:HD2	20	0.14
(2,765)	1:26:A:ARG:H	1:117:A:LYS:HD3	20	0.14
(2,511)	1:95:A:LYS:HE2	1:103:A:PHE:H	15	0.14
(2,511)	1:95:A:LYS:HE3	1:103:A:PHE:H	15	0.14
(2,277)	1:4:A:GLN:HB2	1:7:A:TRP:H	18	0.14
(2,277)	1:4:A:GLN:HB3	1:7:A:TRP:H	18	0.14
(2,168)	1:31:A:GLN:HG2	1:33:A:GLU:H	9	0.14
(2,168)	1:31:A:GLN:HG3	1:33:A:GLU:H	9	0.14
(2,166)	1:198:A:LYS:HE2	1:200:A:LEU:H	3	0.14
(2,166)	1:198:A:LYS:HE3	1:200:A:LEU:H	3	0.14
(2,18)	1:51:A:THR:H	1:52:A:LEU:HG	17	0.14
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	2	0.14
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	13	0.14
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	16	0.14
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2712)	1:95:A:LYS:H	1:102:A:GLU:HG2	2	0.14
(1,2712)	1:95:A:LYS:H	1:102:A:GLU:HG3	2	0.14
(1,2706)	1:96:A:VAL:H	1:102:A:GLU:HG2	4	0.14
(1,2706)	1:96:A:VAL:H	1:102:A:GLU:HG3	4	0.14
(1,2706)	1:96:A:VAL:H	1:102:A:GLU:HG2	17	0.14
(1,2706)	1:96:A:VAL:H	1:102:A:GLU:HG3	17	0.14
(1,2679)	1:31:A:GLN:HG2	1:35:A:SER:H	9	0.14
(1,2679)	1:31:A:GLN:HG3	1:35:A:SER:H	9	0.14
(1,2679)	1:31:A:GLN:HG2	1:35:A:SER:H	17	0.14
(1,2679)	1:31:A:GLN:HG3	1:35:A:SER:H	17	0.14
(1,2625)	1:157:A:SER:HB2	1:161:A:GLN:H	3	0.14
(1,2625)	1:157:A:SER:HB3	1:161:A:GLN:H	3	0.14
(1,2461)	1:157:A:SER:HA	1:161:A:GLN:H	18	0.14
(1,2459)	1:21:A:VAL:HA	1:25:A:GLY:H	19	0.14
(1,2348)	1:160:A:THR:HG21	1:163:A:ALA:H	8	0.14
(1,2020)	1:131:A:GLN:HG2	1:133:A:LEU:H	20	0.14
(1,2020)	1:131:A:GLN:HG3	1:133:A:LEU:H	20	0.14
(1,1490)	1:116:A:GLN:HG2	1:117:A:LYS:H	3	0.14
(1,1490)	1:116:A:GLN:HG3	1:117:A:LYS:H	3	0.14
(1,1330)	1:110:A:ASP:HB2	1:111:A:VAL:H	13	0.14
(1,1330)	1:110:A:ASP:HB3	1:111:A:VAL:H	13	0.14
(1,1298)	1:16:A:VAL:HG21	1:17:A:TYR:H	18	0.14
(1,1293)	1:175:A:GLN:HG2	1:176:A:ARG:H	9	0.14
(1,1293)	1:175:A:GLN:HG2	1:176:A:ARG:H	18	0.14
(1,1280)	1:111:A:VAL:HG11	1:112:A:GLU:H	1	0.14
(1,1280)	1:111:A:VAL:HG11	1:112:A:GLU:H	10	0.14
(1,1274)	1:10:A:VAL:HG11	1:11:A:LYS:H	14	0.14
(1,991)	1:187:A:ASN:HA	1:188:A:GLU:H	18	0.14
(1,727)	1:20:A:ALA:H	1:21:A:VAL:HG21	4	0.14
(1,727)	1:20:A:ALA:H	1:21:A:VAL:HG21	5	0.14
(1,727)	1:20:A:ALA:H	1:21:A:VAL:HG21	9	0.14
(1,727)	1:20:A:ALA:H	1:21:A:VAL:HG21	12	0.14
(1,571)	1:208:A:LEU:H	1:208:A:LEU:HD21	13	0.14
(1,550)	1:188:A:GLU:H	1:188:A:GLU:HB2	19	0.14
(1,550)	1:188:A:GLU:H	1:188:A:GLU:HB3	19	0.14
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	15	0.14
(1,116)	1:52:A:LEU:H	1:52:A:LEU:HB2	7	0.14
(1,116)	1:52:A:LEU:H	1:52:A:LEU:HB3	7	0.14
(1,69)	1:187:A:ASN:H	1:187:A:ASN:HB2	10	0.14
(1,69)	1:187:A:ASN:H	1:187:A:ASN:HB3	10	0.14
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE21	9	0.14
(1,47)	1:97:A:GLN:H	1:97:A:GLN:HE22	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:10:A:VAL:H	1:10:A:VAL:HG21	7	0.14
(2,755)	1:59:A:LEU:H	1:147:A:PHE:HB2	13	0.13
(2,755)	1:59:A:LEU:H	1:147:A:PHE:HB3	13	0.13
(2,493)	1:46:A:LEU:HG	1:51:A:THR:H	7	0.13
(2,277)	1:4:A:GLN:HB2	1:7:A:TRP:H	10	0.13
(2,277)	1:4:A:GLN:HB3	1:7:A:TRP:H	10	0.13
(2,259)	1:173:A:LEU:HD21	1:176:A:ARG:H	19	0.13
(2,227)	1:180:A:LEU:H	1:183:A:ASN:HA	10	0.13
(2,108)	1:100:A:LEU:HD11	1:102:A:GLU:H	3	0.13
(2,108)	1:100:A:LEU:HD11	1:102:A:GLU:H	8	0.13
(2,39)	1:180:A:LEU:HD21	1:181:A:LYS:H	13	0.13
(2,18)	1:51:A:THR:H	1:52:A:LEU:HG	9	0.13
(2,3)	1:179:A:GLU:H	1:180:A:LEU:HD21	1	0.13
(2,3)	1:179:A:GLU:H	1:180:A:LEU:HD21	2	0.13
(2,3)	1:179:A:GLU:H	1:180:A:LEU:HD21	15	0.13
(1,2706)	1:96:A:VAL:H	1:102:A:GLU:HG2	1	0.13
(1,2706)	1:96:A:VAL:H	1:102:A:GLU:HG3	1	0.13
(1,2705)	1:83:A:GLN:HG2	1:88:A:ASP:H	15	0.13
(1,2705)	1:83:A:GLN:HG3	1:88:A:ASP:H	15	0.13
(1,2609)	1:175:A:GLN:HG2	1:179:A:GLU:H	2	0.13
(1,2609)	1:175:A:GLN:HG2	1:179:A:GLU:H	18	0.13
(1,2459)	1:21:A:VAL:HA	1:25:A:GLY:H	2	0.13
(1,2459)	1:21:A:VAL:HA	1:25:A:GLY:H	7	0.13
(1,2459)	1:21:A:VAL:HA	1:25:A:GLY:H	18	0.13
(1,2423)	1:31:A:GLN:HE21	1:34:A:SER:H	9	0.13
(1,2423)	1:31:A:GLN:HE22	1:34:A:SER:H	9	0.13
(1,2354)	1:100:A:LEU:HB2	1:103:A:PHE:H	11	0.13
(1,2354)	1:100:A:LEU:HB3	1:103:A:PHE:H	11	0.13
(1,2114)	1:78:A:THR:H	1:81:A:VAL:HG21	2	0.13
(1,2114)	1:78:A:THR:H	1:81:A:VAL:HG21	18	0.13
(1,1994)	1:198:A:LYS:HD2	1:200:A:LEU:H	16	0.13
(1,1994)	1:198:A:LYS:HD3	1:200:A:LEU:H	16	0.13
(1,1907)	1:188:A:GLU:HB2	1:190:A:HIS:H	6	0.13
(1,1907)	1:188:A:GLU:HB3	1:190:A:HIS:H	6	0.13
(1,1611)	1:6:A:GLN:H	1:8:A:ASP:H	18	0.13
(1,1565)	1:75:A:GLU:H	1:77:A:GLU:H	1	0.13
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	10	0.13
(1,1361)	1:24:A:SER:HB2	1:25:A:GLY:H	14	0.13
(1,1361)	1:24:A:SER:HB3	1:25:A:GLY:H	14	0.13
(1,1293)	1:175:A:GLN:HG2	1:176:A:ARG:H	2	0.13
(1,1240)	1:63:A:LEU:HD21	1:64:A:GLY:H	1	0.13
(1,1113)	1:10:A:VAL:HB	1:11:A:LYS:H	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,892)	1:133:A:LEU:H	1:134:A:GLN:HA	6	0.13
(1,892)	1:133:A:LEU:H	1:134:A:GLN:HA	8	0.13
(1,791)	1:66:A:LEU:H	1:67:A:THR:HG21	2	0.13
(1,727)	1:20:A:ALA:H	1:21:A:VAL:HG21	1	0.13
(1,709)	1:6:A:GLN:H	1:7:A:TRP:H	19	0.13
(1,640)	1:46:A:LEU:H	1:47:A:GLU:HG2	7	0.13
(1,640)	1:46:A:LEU:H	1:47:A:GLU:HG3	7	0.13
(1,604)	1:139:A:ARG:H	1:140:A:LEU:H	10	0.13
(1,604)	1:139:A:ARG:H	1:140:A:LEU:H	13	0.13
(1,603)	1:46:A:LEU:H	1:47:A:GLU:HB2	15	0.13
(1,603)	1:46:A:LEU:H	1:47:A:GLU:HB3	15	0.13
(1,598)	1:56:A:VAL:H	1:57:A:SER:H	6	0.13
(1,598)	1:56:A:VAL:H	1:57:A:SER:H	14	0.13
(1,256)	1:52:A:LEU:H	1:52:A:LEU:HA	9	0.13
(1,131)	1:4:A:GLN:H	1:4:A:GLN:HB2	7	0.13
(1,131)	1:4:A:GLN:H	1:4:A:GLN:HB3	7	0.13
(1,131)	1:4:A:GLN:H	1:4:A:GLN:HB2	18	0.13
(1,131)	1:4:A:GLN:H	1:4:A:GLN:HB3	18	0.13
(1,63)	1:62:A:ARG:H	1:62:A:ARG:HD2	15	0.13
(1,63)	1:62:A:ARG:H	1:62:A:ARG:HD3	15	0.13
(1,55)	1:95:A:LYS:H	1:95:A:LYS:HG2	5	0.13
(1,55)	1:95:A:LYS:H	1:95:A:LYS:HG3	5	0.13
(2,867)	1:15:A:ASN:H	1:191:A:SER:HB2	18	0.12
(2,867)	1:15:A:ASN:H	1:191:A:SER:HB3	18	0.12
(2,812)	1:28:A:TYR:HA	1:158:A:LEU:H	10	0.12
(2,811)	1:31:A:GLN:H	1:161:A:GLN:HG2	17	0.12
(2,811)	1:31:A:GLN:H	1:161:A:GLN:HG3	17	0.12
(2,808)	1:32:A:PHE:H	1:161:A:GLN:HG2	2	0.12
(2,808)	1:32:A:PHE:H	1:161:A:GLN:HG3	2	0.12
(2,808)	1:32:A:PHE:H	1:161:A:GLN:HG2	19	0.12
(2,808)	1:32:A:PHE:H	1:161:A:GLN:HG3	19	0.12
(2,788)	1:46:A:LEU:H	1:145:A:GLU:HG2	20	0.12
(2,788)	1:46:A:LEU:H	1:145:A:GLU:HG3	20	0.12
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	11	0.12
(2,408)	1:140:A:LEU:HB2	1:144:A:ALA:H	2	0.12
(2,408)	1:140:A:LEU:HB3	1:144:A:ALA:H	2	0.12
(2,108)	1:100:A:LEU:HD11	1:102:A:GLU:H	7	0.12
(2,108)	1:100:A:LEU:HD11	1:102:A:GLU:H	10	0.12
(2,50)	1:48:A:ASN:H	1:50:A:ASP:HB2	5	0.12
(2,50)	1:48:A:ASN:H	1:50:A:ASP:HB3	5	0.12
(2,39)	1:180:A:LEU:HD21	1:181:A:LYS:H	11	0.12
(2,3)	1:179:A:GLU:H	1:180:A:LEU:HD21	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2799)	1:46:A:LEU:HB2	1:146:A:GLU:H	11	0.12
(1,2799)	1:46:A:LEU:HB3	1:146:A:GLU:H	11	0.12
(1,2706)	1:96:A:VAL:H	1:102:A:GLU:HG2	5	0.12
(1,2706)	1:96:A:VAL:H	1:102:A:GLU:HG3	5	0.12
(1,2677)	1:22:A:LYS:HE2	1:26:A:ARG:H	18	0.12
(1,2677)	1:22:A:LYS:HE3	1:26:A:ARG:H	18	0.12
(1,2621)	1:168:A:GLN:HB2	1:172:A:SER:H	18	0.12
(1,2621)	1:168:A:GLN:HB3	1:172:A:SER:H	18	0.12
(1,2464)	1:158:A:LEU:HA	1:162:A:LEU:H	18	0.12
(1,2348)	1:160:A:THR:HG21	1:163:A:ALA:H	11	0.12
(1,2333)	1:162:A:LEU:HD11	1:165:A:HIS:H	8	0.12
(1,1970)	1:139:A:ARG:HB2	1:141:A:SER:H	13	0.12
(1,1970)	1:139:A:ARG:HB3	1:141:A:SER:H	13	0.12
(1,1907)	1:188:A:GLU:HB2	1:190:A:HIS:H	13	0.12
(1,1907)	1:188:A:GLU:HB3	1:190:A:HIS:H	13	0.12
(1,1907)	1:188:A:GLU:HB2	1:190:A:HIS:H	16	0.12
(1,1907)	1:188:A:GLU:HB3	1:190:A:HIS:H	16	0.12
(1,1907)	1:188:A:GLU:HB2	1:190:A:HIS:H	20	0.12
(1,1907)	1:188:A:GLU:HB3	1:190:A:HIS:H	20	0.12
(1,1857)	1:62:A:ARG:HB2	1:64:A:GLY:H	15	0.12
(1,1719)	1:139:A:ARG:H	1:141:A:SER:H	11	0.12
(1,1583)	1:95:A:LYS:H	1:97:A:GLN:HE21	9	0.12
(1,1583)	1:95:A:LYS:H	1:97:A:GLN:HE22	9	0.12
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	15	0.12
(1,1328)	1:188:A:GLU:HB2	1:189:A:TYR:H	5	0.12
(1,1328)	1:188:A:GLU:HB3	1:189:A:TYR:H	5	0.12
(1,1304)	1:96:A:VAL:HG21	1:97:A:GLN:H	5	0.12
(1,1240)	1:63:A:LEU:HD21	1:64:A:GLY:H	5	0.12
(1,1240)	1:63:A:LEU:HD21	1:64:A:GLY:H	7	0.12
(1,1240)	1:63:A:LEU:HD21	1:64:A:GLY:H	16	0.12
(1,1240)	1:63:A:LEU:HD21	1:64:A:GLY:H	20	0.12
(1,791)	1:66:A:LEU:H	1:67:A:THR:HG21	12	0.12
(1,791)	1:66:A:LEU:H	1:67:A:THR:HG21	13	0.12
(1,727)	1:20:A:ALA:H	1:21:A:VAL:HG21	3	0.12
(1,727)	1:20:A:ALA:H	1:21:A:VAL:HG21	13	0.12
(1,727)	1:20:A:ALA:H	1:21:A:VAL:HG21	14	0.12
(1,727)	1:20:A:ALA:H	1:21:A:VAL:HG21	17	0.12
(1,626)	1:199:A:SER:H	1:200:A:LEU:H	16	0.12
(1,603)	1:46:A:LEU:H	1:47:A:GLU:HB2	19	0.12
(1,603)	1:46:A:LEU:H	1:47:A:GLU:HB3	19	0.12
(1,602)	1:99:A:TYR:H	1:100:A:LEU:H	12	0.12
(1,598)	1:56:A:VAL:H	1:57:A:SER:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:130:A:ARG:H	1:131:A:GLN:HB2	1	0.12
(1,594)	1:130:A:ARG:H	1:131:A:GLN:HB3	1	0.12
(1,568)	1:205:A:ARG:H	1:205:A:ARG:HA	7	0.12
(1,550)	1:188:A:GLU:H	1:188:A:GLU:HB2	2	0.12
(1,550)	1:188:A:GLU:H	1:188:A:GLU:HB3	2	0.12
(1,550)	1:188:A:GLU:H	1:188:A:GLU:HB2	12	0.12
(1,550)	1:188:A:GLU:H	1:188:A:GLU:HB3	12	0.12
(1,261)	1:59:A:LEU:H	1:59:A:LEU:HA	19	0.12
(1,256)	1:52:A:LEU:H	1:52:A:LEU:HA	13	0.12
(1,256)	1:52:A:LEU:H	1:52:A:LEU:HA	17	0.12
(1,55)	1:95:A:LYS:H	1:95:A:LYS:HG2	1	0.12
(1,55)	1:95:A:LYS:H	1:95:A:LYS:HG3	1	0.12
(1,51)	1:59:A:LEU:H	1:59:A:LEU:HD11	11	0.12
(1,2)	1:102:A:GLU:H	1:102:A:GLU:HG2	1	0.12
(1,2)	1:102:A:GLU:H	1:102:A:GLU:HG3	1	0.12
(1,2)	1:102:A:GLU:H	1:102:A:GLU:HG2	5	0.12
(1,2)	1:102:A:GLU:H	1:102:A:GLU:HG3	5	0.12
(1,2)	1:102:A:GLU:H	1:102:A:GLU:HG2	17	0.12
(1,2)	1:102:A:GLU:H	1:102:A:GLU:HG3	17	0.12
(2,858)	1:11:A:LYS:H	1:180:A:LEU:HD21	18	0.11
(2,795)	1:43:A:LEU:HD21	1:145:A:GLU:H	9	0.11
(2,621)	1:76:A:LYS:HE2	1:117:A:LYS:H	3	0.11
(2,621)	1:76:A:LYS:HE3	1:117:A:LYS:H	3	0.11
(2,598)	1:81:A:VAL:HG11	1:117:A:LYS:H	16	0.11
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	10	0.11
(2,502)	1:74:A:LEU:HA	1:80:A:TRP:H	3	0.11
(2,463)	1:55:A:THR:H	1:60:A:GLN:H	11	0.11
(2,258)	1:162:A:LEU:HD21	1:165:A:HIS:H	15	0.11
(2,193)	1:12:A:ASP:H	1:15:A:ASN:HB2	5	0.11
(2,193)	1:12:A:ASP:H	1:15:A:ASN:HB3	5	0.11
(2,108)	1:100:A:LEU:HD11	1:102:A:GLU:H	2	0.11
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	15	0.11
(2,3)	1:179:A:GLU:H	1:180:A:LEU:HD21	7	0.11
(1,2810)	1:28:A:TYR:H	1:162:A:LEU:HD21	2	0.11
(1,2798)	1:46:A:LEU:H	1:146:A:GLU:HG2	10	0.11
(1,2798)	1:46:A:LEU:H	1:146:A:GLU:HG3	10	0.11
(1,2730)	1:40:A:GLN:H	1:59:A:LEU:HB2	7	0.11
(1,2730)	1:40:A:GLN:H	1:59:A:LEU:HB3	7	0.11
(1,2609)	1:175:A:GLN:HG2	1:179:A:GLU:H	9	0.11
(1,2459)	1:21:A:VAL:HA	1:25:A:GLY:H	6	0.11
(1,2348)	1:160:A:THR:HG21	1:163:A:ALA:H	14	0.11
(1,2041)	1:58:A:GLN:H	1:61:A:GLU:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2027)	1:107:A:TRP:H	1:110:A:ASP:HB2	11	0.11
(1,2027)	1:107:A:TRP:H	1:110:A:ASP:HB3	11	0.11
(1,2027)	1:107:A:TRP:H	1:110:A:ASP:HB2	13	0.11
(1,2027)	1:107:A:TRP:H	1:110:A:ASP:HB3	13	0.11
(1,2027)	1:107:A:TRP:H	1:110:A:ASP:HB2	16	0.11
(1,2027)	1:107:A:TRP:H	1:110:A:ASP:HB3	16	0.11
(1,2020)	1:131:A:GLN:HG2	1:133:A:LEU:H	1	0.11
(1,2020)	1:131:A:GLN:HG3	1:133:A:LEU:H	1	0.11
(1,1999)	1:22:A:LYS:HE2	1:24:A:SER:H	18	0.11
(1,1999)	1:22:A:LYS:HE3	1:24:A:SER:H	18	0.11
(1,1987)	1:209:A:GLU:HB2	1:211:A:LEU:H	6	0.11
(1,1987)	1:209:A:GLU:HB3	1:211:A:LEU:H	6	0.11
(1,1987)	1:209:A:GLU:HB2	1:211:A:LEU:H	9	0.11
(1,1987)	1:209:A:GLU:HB3	1:211:A:LEU:H	9	0.11
(1,1970)	1:139:A:ARG:HB2	1:141:A:SER:H	10	0.11
(1,1970)	1:139:A:ARG:HB3	1:141:A:SER:H	10	0.11
(1,1907)	1:188:A:GLU:HB2	1:190:A:HIS:H	3	0.11
(1,1907)	1:188:A:GLU:HB3	1:190:A:HIS:H	3	0.11
(1,1868)	1:208:A:LEU:HB3	1:210:A:ASP:H	7	0.11
(1,1868)	1:208:A:LEU:HB3	1:210:A:ASP:H	13	0.11
(1,1818)	1:26:A:ARG:HA	1:28:A:TYR:H	17	0.11
(1,1776)	1:105:A:LYS:HA	1:107:A:TRP:H	16	0.11
(1,1602)	1:189:A:TYR:H	1:191:A:SER:H	18	0.11
(1,1565)	1:75:A:GLU:H	1:77:A:GLU:H	3	0.11
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	19	0.11
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	20	0.11
(1,1475)	1:44:A:ASN:HD21	1:45:A:LEU:H	15	0.11
(1,1475)	1:44:A:ASN:HD22	1:45:A:LEU:H	15	0.11
(1,1330)	1:110:A:ASP:HB2	1:111:A:VAL:H	11	0.11
(1,1330)	1:110:A:ASP:HB3	1:111:A:VAL:H	11	0.11
(1,1300)	1:51:A:THR:HG21	1:52:A:LEU:H	9	0.11
(1,1280)	1:111:A:VAL:HG11	1:112:A:GLU:H	13	0.11
(1,1240)	1:63:A:LEU:HD21	1:64:A:GLY:H	6	0.11
(1,1172)	1:172:A:SER:HB3	1:173:A:LEU:H	5	0.11
(1,1116)	1:55:A:THR:HB	1:56:A:VAL:H	16	0.11
(1,1113)	1:10:A:VAL:HB	1:11:A:LYS:H	18	0.11
(1,961)	1:193:A:ALA:H	1:194:A:LYS:HA	18	0.11
(1,960)	1:193:A:ALA:H	1:194:A:LYS:H	11	0.11
(1,669)	1:53:A:GLY:H	1:54:A:SER:H	16	0.11
(1,626)	1:199:A:SER:H	1:200:A:LEU:H	14	0.11
(1,624)	1:94:A:GLN:H	1:95:A:LYS:HG2	1	0.11
(1,624)	1:94:A:GLN:H	1:95:A:LYS:HG3	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,604)	1:139:A:ARG:H	1:140:A:LEU:H	2	0.11
(1,602)	1:99:A:TYR:H	1:100:A:LEU:H	20	0.11
(1,568)	1:205:A:ARG:H	1:205:A:ARG:HA	13	0.11
(1,118)	1:21:A:VAL:H	1:21:A:VAL:HG21	10	0.11
(1,63)	1:62:A:ARG:H	1:62:A:ARG:HD2	5	0.11
(1,63)	1:62:A:ARG:H	1:62:A:ARG:HD3	5	0.11
(1,55)	1:95:A:LYS:H	1:95:A:LYS:HG2	4	0.11
(1,55)	1:95:A:LYS:H	1:95:A:LYS:HG3	4	0.11
(1,55)	1:95:A:LYS:H	1:95:A:LYS:HG2	15	0.11
(1,55)	1:95:A:LYS:H	1:95:A:LYS:HG3	15	0.11
(1,55)	1:95:A:LYS:H	1:95:A:LYS:HG2	17	0.11
(1,55)	1:95:A:LYS:H	1:95:A:LYS:HG3	17	0.11
(1,41)	1:83:A:GLN:H	1:83:A:GLN:HB2	15	0.11
(1,5)	1:179:A:GLU:H	1:179:A:GLU:HG2	5	0.11
(2,808)	1:32:A:PHE:H	1:161:A:GLN:HG2	1	0.1
(2,808)	1:32:A:PHE:H	1:161:A:GLN:HG3	1	0.1
(2,766)	1:26:A:ARG:H	1:117:A:LYS:HB2	10	0.1
(2,766)	1:26:A:ARG:H	1:117:A:LYS:HB3	10	0.1
(2,598)	1:81:A:VAL:HG11	1:117:A:LYS:H	10	0.1
(2,531)	1:40:A:GLN:H	1:59:A:LEU:HD21	19	0.1
(2,463)	1:55:A:THR:H	1:60:A:GLN:H	7	0.1
(2,212)	1:64:A:GLY:H	1:67:A:THR:HG21	11	0.1
(2,168)	1:31:A:GLN:HG2	1:33:A:GLU:H	18	0.1
(2,168)	1:31:A:GLN:HG3	1:33:A:GLU:H	18	0.1
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	6	0.1
(2,12)	1:28:A:TYR:H	1:29:A:VAL:HG21	18	0.1
(1,2690)	1:58:A:GLN:HG2	1:62:A:ARG:H	19	0.1
(1,2690)	1:58:A:GLN:HG3	1:62:A:ARG:H	19	0.1
(1,2464)	1:158:A:LEU:HA	1:162:A:LEU:H	6	0.1
(1,2376)	1:58:A:GLN:HB2	1:61:A:GLU:H	19	0.1
(1,2376)	1:58:A:GLN:HB3	1:61:A:GLU:H	19	0.1
(1,1912)	1:208:A:LEU:HB2	1:210:A:ASP:H	7	0.1
(1,1912)	1:208:A:LEU:HB3	1:210:A:ASP:H	7	0.1
(1,1583)	1:95:A:LYS:H	1:97:A:GLN:HE21	14	0.1
(1,1583)	1:95:A:LYS:H	1:97:A:GLN:HE22	14	0.1
(1,1549)	1:19:A:ASP:H	1:21:A:VAL:HG21	2	0.1
(1,1546)	1:49:A:TRP:H	1:51:A:THR:H	5	0.1
(1,1475)	1:44:A:ASN:HD21	1:45:A:LEU:H	19	0.1
(1,1475)	1:44:A:ASN:HD22	1:45:A:LEU:H	19	0.1
(1,1392)	1:76:A:LYS:HB2	1:77:A:GLU:H	3	0.1
(1,1392)	1:76:A:LYS:HB3	1:77:A:GLU:H	3	0.1
(1,1361)	1:24:A:SER:HB2	1:25:A:GLY:H	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1361)	1:24:A:SER:HB3	1:25:A:GLY:H	16	0.1
(1,1240)	1:63:A:LEU:HD21	1:64:A:GLY:H	2	0.1
(1,1240)	1:63:A:LEU:HD21	1:64:A:GLY:H	8	0.1
(1,1240)	1:63:A:LEU:HD21	1:64:A:GLY:H	14	0.1
(1,1240)	1:63:A:LEU:HD21	1:64:A:GLY:H	15	0.1
(1,960)	1:193:A:ALA:H	1:194:A:LYS:H	18	0.1
(1,917)	1:155:A:VAL:H	1:156:A:ASP:H	10	0.1
(1,669)	1:53:A:GLY:H	1:54:A:SER:H	17	0.1
(1,624)	1:94:A:GLN:H	1:95:A:LYS:HG2	4	0.1
(1,624)	1:94:A:GLN:H	1:95:A:LYS:HG3	4	0.1
(1,598)	1:56:A:VAL:H	1:57:A:SER:H	16	0.1
(1,596)	1:102:A:GLU:H	1:103:A:PHE:HE2	4	0.1
(1,380)	1:99:A:TYR:H	1:99:A:TYR:HE1	19	0.1
(1,40)	1:7:A:TRP:H	1:7:A:TRP:HZ3	19	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found