



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 02:58 PM UTC

PDB ID : 2LGZ / pdb_00002lgz
BMRB ID : 16701
Title : Solution structure of STT3P
Authors : Huang, C.; Bhaskaran, R.; Mohanty, S.
Deposited on : 2011-08-03

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

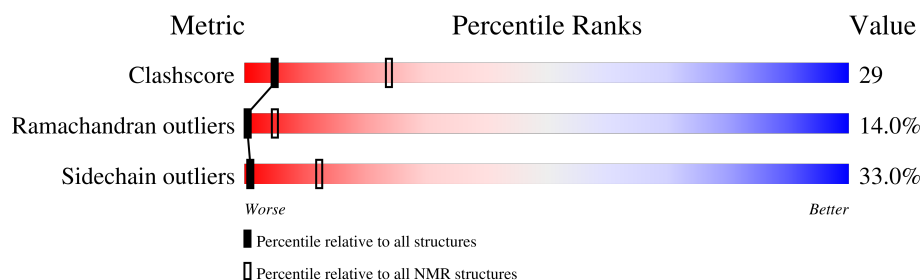
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 33%.

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	273	21% 47% 8% 23%

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 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:21-A:146, A:153-A:166, A:189-A:197, A:202-A:261 (209)	2.64	4

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 1 single-model cluster was found.

Cluster number	Models
1	4, 5, 7, 8, 10
2	3, 9
3	1, 2
Single-model clusters	6

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4340 atoms, of which 2124 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3.

Mol	Chain	Residues	Atoms						Trace
1	A	273	Total	C	H	N	O	S	0
			4340	1395	2124	392	423	6	

There are 22 discrepancies between the modelled and reference sequences:

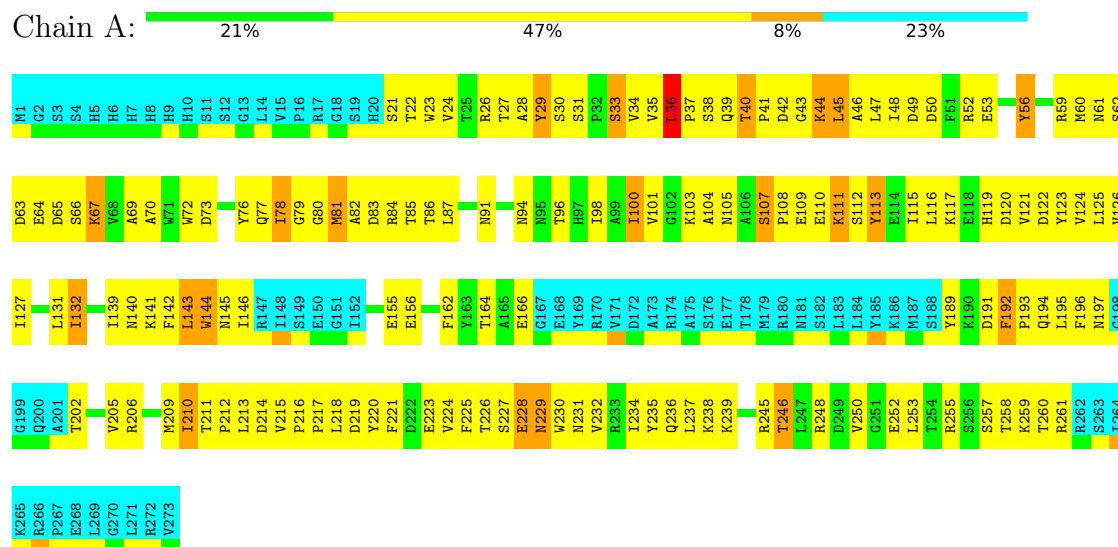
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P39007
A	2	GLY	-	expression tag	UNP P39007
A	3	SER	-	expression tag	UNP P39007
A	4	SER	-	expression tag	UNP P39007
A	5	HIS	-	expression tag	UNP P39007
A	6	HIS	-	expression tag	UNP P39007
A	7	HIS	-	expression tag	UNP P39007
A	8	HIS	-	expression tag	UNP P39007
A	9	HIS	-	expression tag	UNP P39007
A	10	HIS	-	expression tag	UNP P39007
A	11	SER	-	expression tag	UNP P39007
A	12	SER	-	expression tag	UNP P39007
A	13	GLY	-	expression tag	UNP P39007
A	14	LEU	-	expression tag	UNP P39007
A	15	VAL	-	expression tag	UNP P39007
A	16	PRO	-	expression tag	UNP P39007
A	17	ARG	-	expression tag	UNP P39007
A	18	GLY	-	expression tag	UNP P39007
A	19	SER	-	expression tag	UNP P39007
A	105	ASN	MET	conflict	UNP P39007
A	145	ASN	MET	conflict	UNP P39007
A	231	ASN	MET	conflict	UNP P39007

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3

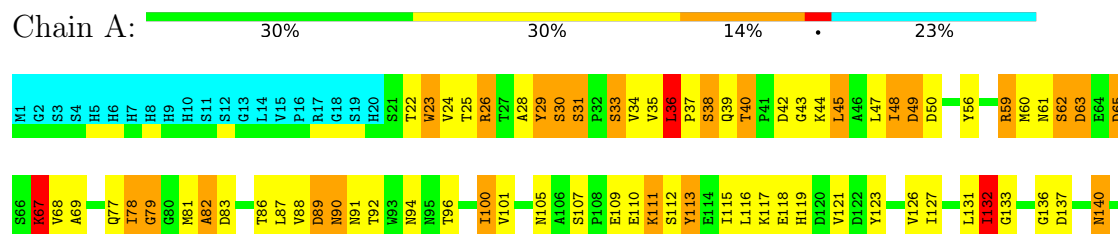


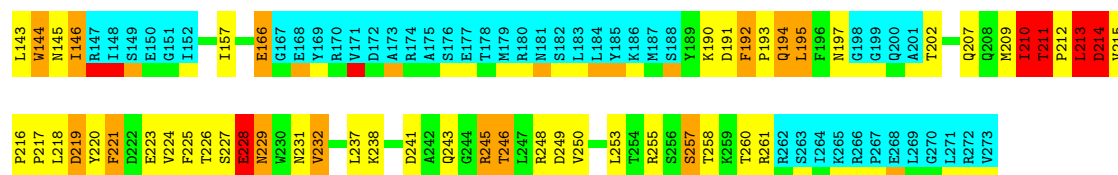
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

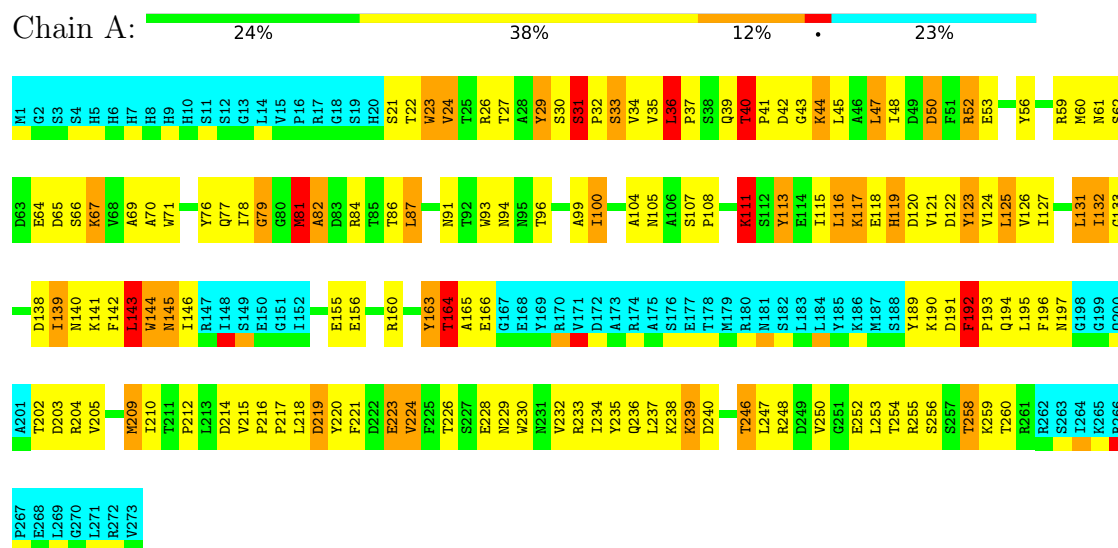
- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3





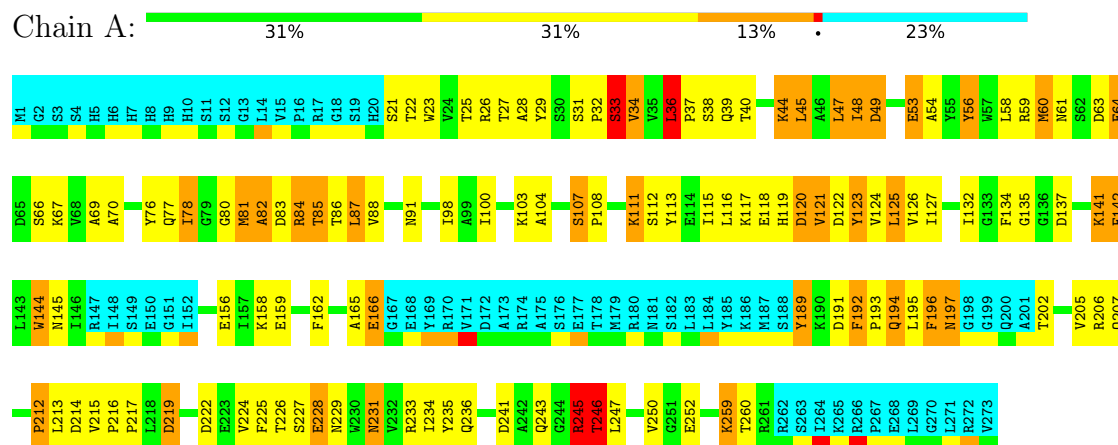
4.2.2 Score per residue for model 2

- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



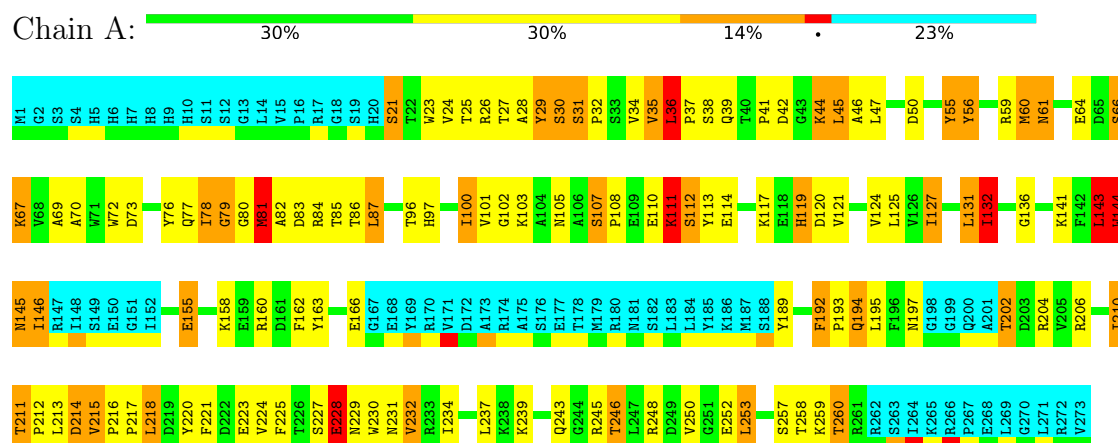
4.2.3 Score per residue for model 3

- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



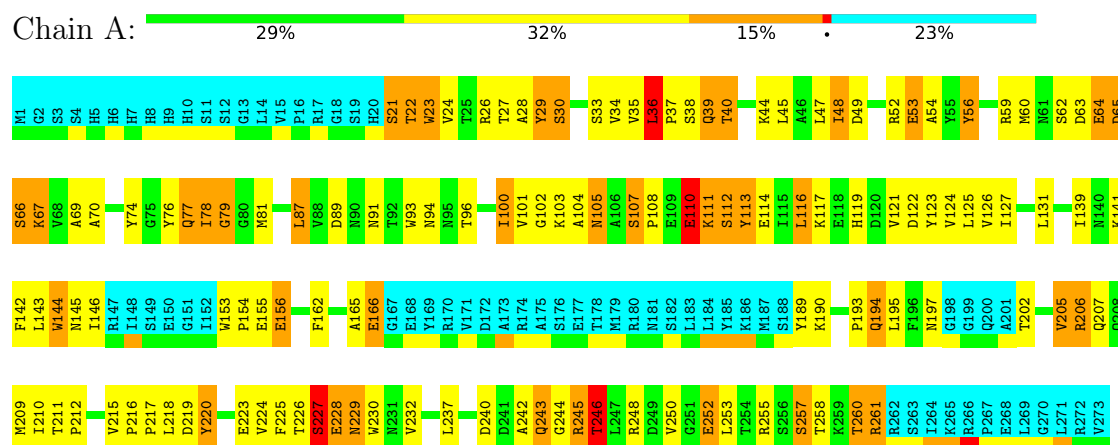
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



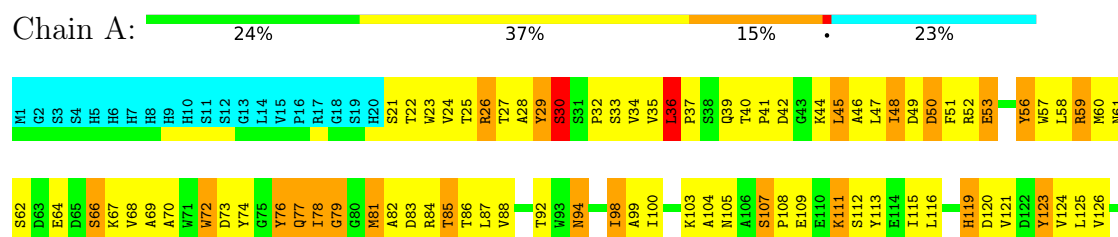
4.2.5 Score per residue for model 5

- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



4.2.6 Score per residue for model 6

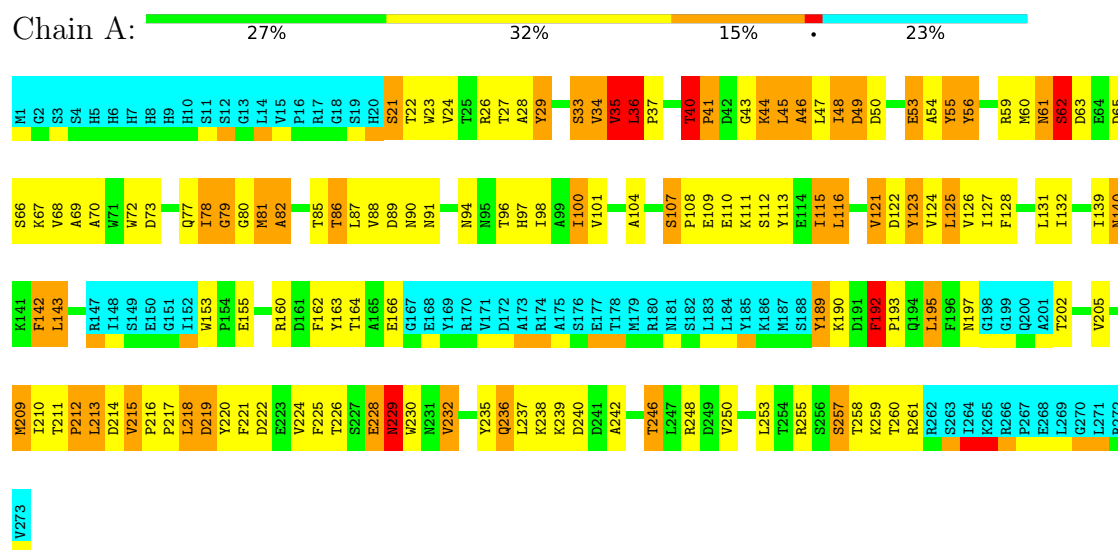
- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3





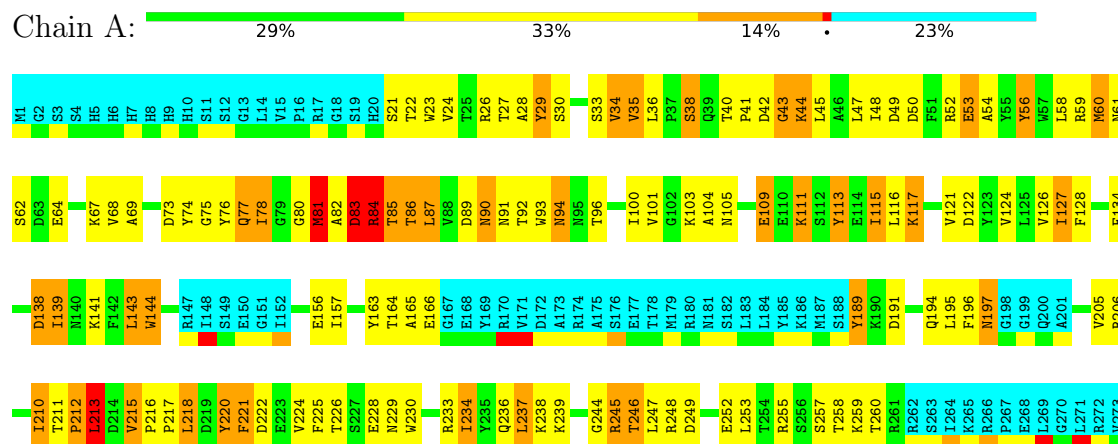
4.2.7 Score per residue for model 7

- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



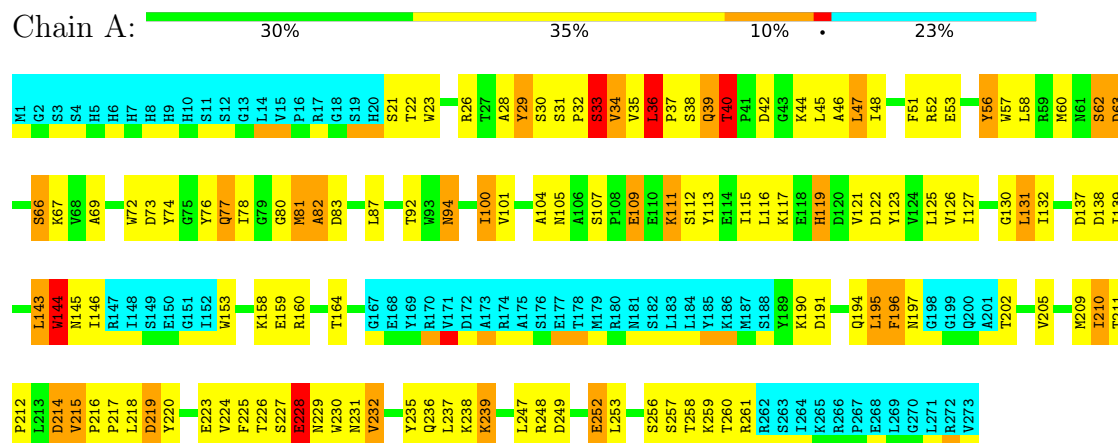
4.2.8 Score per residue for model 8

- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



4.2.9 Score per residue for model 9

- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 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	refinement	3.0

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1187
Number of shifts mapped to atoms	1187
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	33%

6 Model quality

6.1 Standard geometry

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

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	1718	1633	1633	98±7
All	All	17180	16330	16330	985

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:ASP:O	1:A:192:PHE:HB2	0.95	1.56	1	2
1:A:45:LEU:HD23	1:A:121:VAL:HG12	0.89	1.45	3	1
1:A:216:PRO:N	1:A:217:PRO:HD2	0.87	1.85	9	7
1:A:45:LEU:HD21	1:A:121:VAL:HG13	0.87	1.44	5	4
1:A:213:LEU:HD13	1:A:218:LEU:HD21	0.81	1.51	1	1
1:A:54:ALA:HB2	1:A:80:GLY:O	0.81	1.74	8	1
1:A:216:PRO:N	1:A:217:PRO:CD	0.80	2.45	9	7
1:A:216:PRO:HG2	1:A:217:PRO:HD3	0.80	1.52	1	7
1:A:22:THR:O	1:A:26:ARG:N	0.79	2.15	8	5
1:A:81:MET:HE2	1:A:82:ALA:HB3	0.79	1.52	2	1
1:A:104:ALA:HB2	1:A:220:TYR:CB	0.79	2.08	5	1
1:A:191:ASP:O	1:A:192:PHE:CB	0.77	2.31	1	3
1:A:107:SER:N	1:A:108:PRO:CD	0.76	2.49	2	1
1:A:126:VAL:HG11	1:A:226:THR:O	0.76	1.81	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:VAL:HG11	1:A:116:LEU:HD13	0.76	1.56	8	1
1:A:36:LEU:HD11	1:A:99:ALA:HB2	0.75	1.58	6	1
1:A:45:LEU:HD13	1:A:124:VAL:HG21	0.75	1.58	2	1
1:A:69:ALA:O	1:A:72:TRP:N	0.75	2.16	10	1
1:A:110:GLU:O	1:A:111:LYS:CB	0.75	2.34	5	3
1:A:216:PRO:CD	1:A:217:PRO:CD	0.74	2.65	1	7
1:A:36:LEU:HD11	1:A:99:ALA:HB1	0.74	1.59	2	1
1:A:195:LEU:HD21	1:A:231:ASN:CG	0.74	2.08	1	1
1:A:56:TYR:HB3	1:A:72:TRP:CD1	0.74	2.17	10	1
1:A:123:TYR:CE2	1:A:224:VAL:HG13	0.73	2.18	9	1
1:A:215:VAL:C	1:A:217:PRO:HD2	0.72	2.09	9	7
1:A:78:ILE:O	1:A:79:GLY:C	0.72	2.33	2	5
1:A:54:ALA:HB1	1:A:142:PHE:CB	0.71	2.14	3	2
1:A:28:ALA:O	1:A:29:TYR:C	0.71	2.32	6	9
1:A:210:ILE:HG23	1:A:211:THR:H	0.71	1.45	1	1
1:A:27:THR:HG23	1:A:121:VAL:HG21	0.71	1.63	2	1
1:A:216:PRO:CD	1:A:217:PRO:HD2	0.70	2.16	1	7
1:A:56:TYR:C	1:A:56:TYR:CD1	0.70	2.69	8	3
1:A:227:SER:O	1:A:228:GLU:C	0.70	2.34	1	4
1:A:56:TYR:CD2	1:A:69:ALA:HB1	0.70	2.22	8	5
1:A:224:VAL:HG12	1:A:228:GLU:HG3	0.70	1.63	1	1
1:A:242:ALA:O	1:A:243:GLN:C	0.70	2.34	5	1
1:A:214:ASP:O	1:A:215:VAL:O	0.70	2.08	9	1
1:A:35:VAL:O	1:A:36:LEU:C	0.70	2.35	1	1
1:A:216:PRO:CG	1:A:217:PRO:HD3	0.69	2.17	1	7
1:A:104:ALA:HB2	1:A:220:TYR:CG	0.69	2.22	5	1
1:A:119:HIS:CB	1:A:224:VAL:HG22	0.69	2.18	6	1
1:A:24:VAL:O	1:A:28:ALA:HB3	0.68	1.89	6	2
1:A:45:LEU:HD22	1:A:48:ILE:HB	0.68	1.64	6	1
1:A:49:ASP:O	1:A:80:GLY:N	0.68	2.26	8	1
1:A:210:ILE:HG22	1:A:211:THR:HG22	0.68	1.63	4	1
1:A:66:SER:CB	1:A:69:ALA:HB3	0.68	2.19	6	6
1:A:33:SER:O	1:A:35:VAL:HG23	0.68	1.88	6	1
1:A:81:MET:O	1:A:82:ALA:HB2	0.67	1.88	7	2
1:A:81:MET:HE3	1:A:143:LEU:HD13	0.67	1.63	2	1
1:A:45:LEU:HD22	1:A:124:VAL:CG2	0.67	2.18	7	1
1:A:23:TRP:CD1	1:A:24:VAL:HG13	0.67	2.24	6	2
1:A:110:GLU:O	1:A:111:LYS:HB2	0.67	1.90	5	1
1:A:125:LEU:HD12	1:A:126:VAL:HG23	0.67	1.65	6	1
1:A:112:SER:HB2	1:A:116:LEU:HD12	0.66	1.67	10	1
1:A:192:PHE:CB	1:A:193:PRO:CD	0.66	2.73	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:LEU:O	1:A:144:TRP:C	0.66	2.39	8	3
1:A:209:MET:HA	1:A:232:VAL:HG13	0.66	1.65	6	1
1:A:142:PHE:CE2	1:A:143:LEU:HD23	0.66	2.26	6	1
1:A:53:GLU:HB3	1:A:80:GLY:N	0.65	2.07	10	3
1:A:233:ARG:HG2	1:A:234:ILE:HD12	0.65	1.69	8	1
1:A:22:THR:HG21	1:A:47:LEU:CB	0.65	2.21	9	2
1:A:87:LEU:HD12	1:A:91:ASN:HA	0.65	1.68	1	2
1:A:68:VAL:HG12	1:A:252:GLU:OE2	0.65	1.92	6	1
1:A:45:LEU:HD23	1:A:48:ILE:HB	0.65	1.69	7	1
1:A:50:ASP:C	1:A:53:GLU:OE2	0.65	2.40	7	1
1:A:144:TRP:O	1:A:145:ASN:C	0.64	2.40	2	1
1:A:126:VAL:HG21	1:A:227:SER:O	0.64	1.91	6	2
1:A:210:ILE:HG23	1:A:239:LYS:HD2	0.64	1.70	9	1
1:A:119:HIS:HB2	1:A:224:VAL:HG22	0.64	1.69	6	1
1:A:107:SER:CB	1:A:108:PRO:HD2	0.64	2.22	5	6
1:A:246:THR:O	1:A:250:VAL:HG13	0.64	1.92	6	3
1:A:45:LEU:CD2	1:A:121:VAL:HG13	0.64	2.23	5	5
1:A:195:LEU:O	1:A:196:PHE:C	0.63	2.39	3	2
1:A:189:TYR:C	1:A:189:TYR:CD1	0.63	2.77	4	1
1:A:47:LEU:HD13	1:A:144:TRP:CH2	0.63	2.29	5	1
1:A:210:ILE:HD11	1:A:235:TYR:CD1	0.63	2.28	6	1
1:A:24:VAL:HG11	1:A:156:GLU:CB	0.63	2.23	10	1
1:A:131:LEU:HD13	1:A:136:GLY:C	0.63	2.19	1	1
1:A:230:TRP:O	1:A:234:ILE:HD12	0.63	1.94	6	1
1:A:81:MET:CE	1:A:143:LEU:HD23	0.63	2.23	9	1
1:A:214:ASP:O	1:A:215:VAL:HG22	0.63	1.93	9	1
1:A:27:THR:O	1:A:121:VAL:HG11	0.63	1.93	6	1
1:A:34:VAL:HG12	1:A:116:LEU:HD13	0.63	1.71	6	1
1:A:210:ILE:HG23	1:A:239:LYS:CB	0.62	2.24	6	1
1:A:225:PHE:CE2	1:A:247:LEU:HD12	0.62	2.30	3	1
1:A:56:TYR:O	1:A:60:MET:N	0.62	2.32	7	2
1:A:53:GLU:HB3	1:A:80:GLY:HA3	0.62	1.70	8	1
1:A:44:LYS:HD2	1:A:78:ILE:HD11	0.62	1.70	2	1
1:A:225:PHE:O	1:A:232:VAL:HG21	0.62	1.94	4	2
1:A:48:ILE:HG21	1:A:124:VAL:O	0.62	1.94	8	1
1:A:44:LYS:C	1:A:45:LEU:HD12	0.62	2.19	2	1
1:A:104:ALA:HB2	1:A:219:ASP:HB2	0.62	1.71	9	3
1:A:112:SER:CB	1:A:116:LEU:HD12	0.62	2.23	10	1
1:A:66:SER:HB2	1:A:69:ALA:HB3	0.62	1.72	6	2
1:A:43:GLY:O	1:A:44:LYS:C	0.62	2.42	10	3
1:A:59:ARG:O	1:A:60:MET:C	0.62	2.42	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:MET:O	1:A:81:MET:HE2	0.62	1.95	4	1
1:A:115:ILE:HD13	1:A:220:TYR:CZ	0.62	2.30	2	1
1:A:29:TYR:CB	1:A:45:LEU:HD13	0.62	2.25	1	1
1:A:86:THR:C	1:A:87:LEU:HD23	0.62	2.20	1	2
1:A:121:VAL:O	1:A:125:LEU:HD23	0.61	1.95	2	2
1:A:126:VAL:HG11	1:A:227:SER:O	0.61	1.95	5	1
1:A:72:TRP:NE1	1:A:76:TYR:HB2	0.61	2.09	10	1
1:A:210:ILE:HD12	1:A:239:LYS:CG	0.61	2.25	2	1
1:A:54:ALA:HB1	1:A:142:PHE:HB3	0.61	1.70	10	2
1:A:100:ILE:CD1	1:A:101:VAL:HG13	0.61	2.26	10	2
1:A:47:LEU:HD12	1:A:144:TRP:CZ2	0.61	2.31	10	1
1:A:22:THR:HG21	1:A:47:LEU:HB2	0.61	1.71	3	3
1:A:100:ILE:HD12	1:A:101:VAL:HG13	0.61	1.73	10	2
1:A:105:ASN:HB2	1:A:116:LEU:HD21	0.61	1.73	1	1
1:A:218:LEU:O	1:A:222:ASP:N	0.61	2.34	8	1
1:A:69:ALA:HB1	1:A:72:TRP:CE3	0.60	2.31	6	1
1:A:69:ALA:O	1:A:72:TRP:HE3	0.60	1.79	10	1
1:A:23:TRP:CZ2	1:A:125:LEU:HD13	0.60	2.31	9	2
1:A:68:VAL:HG13	1:A:252:GLU:OE2	0.60	1.96	8	1
1:A:60:MET:HB3	1:A:69:ALA:HB2	0.60	1.73	8	2
1:A:53:GLU:HA	1:A:72:TRP:CD1	0.60	2.31	10	1
1:A:197:ASN:HB2	1:A:202:THR:HG21	0.60	1.73	3	1
1:A:45:LEU:O	1:A:48:ILE:N	0.60	2.35	7	1
1:A:101:VAL:HG13	1:A:223:GLU:OE1	0.60	1.97	1	1
1:A:28:ALA:HB1	1:A:155:GLU:HG2	0.60	1.74	4	1
1:A:50:ASP:HB3	1:A:144:TRP:CD1	0.60	2.32	8	2
1:A:45:LEU:HG	1:A:48:ILE:HD13	0.59	1.74	1	1
1:A:58:LEU:HD22	1:A:141:LYS:CG	0.59	2.27	6	1
1:A:210:ILE:HD12	1:A:235:TYR:CE1	0.59	2.32	10	1
1:A:69:ALA:HA	1:A:72:TRP:NE1	0.59	2.11	7	1
1:A:122:ASP:HA	1:A:125:LEU:HD22	0.59	1.73	3	1
1:A:123:TYR:C	1:A:123:TYR:CD1	0.59	2.81	3	1
1:A:127:ILE:HD11	1:A:226:THR:HG22	0.59	1.74	8	1
1:A:105:ASN:CG	1:A:116:LEU:HD11	0.59	2.23	9	1
1:A:112:SER:O	1:A:113:TYR:CB	0.59	2.51	5	1
1:A:60:MET:CB	1:A:69:ALA:HB2	0.59	2.27	3	1
1:A:35:VAL:HG12	1:A:98:ILE:HG12	0.59	1.73	10	1
1:A:77:GLN:HG2	1:A:87:LEU:HD22	0.59	1.73	7	1
1:A:125:LEU:HD12	1:A:125:LEU:O	0.59	1.98	2	2
1:A:58:LEU:HD22	1:A:141:LYS:HG3	0.59	1.74	6	1
1:A:87:LEU:HD13	1:A:94:ASN:OD1	0.58	1.97	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:GLU:H	1:A:53:GLU:CD	0.58	2.06	7	1
1:A:45:LEU:HD22	1:A:124:VAL:HG23	0.58	1.75	7	2
1:A:90:ASN:O	1:A:94:ASN:N	0.58	2.37	8	3
1:A:45:LEU:CG	1:A:48:ILE:HD13	0.58	2.29	1	1
1:A:81:MET:O	1:A:82:ALA:CB	0.58	2.51	7	1
1:A:39:GLN:O	1:A:40:THR:HG23	0.58	1.97	2	3
1:A:35:VAL:HG12	1:A:102:GLY:CA	0.58	2.29	4	1
1:A:69:ALA:HB1	1:A:72:TRP:CZ2	0.58	2.33	7	1
1:A:72:TRP:CE3	1:A:73:ASP:N	0.58	2.72	10	2
1:A:76:TYR:CE2	1:A:87:LEU:HD23	0.58	2.34	9	1
1:A:80:GLY:O	1:A:81:MET:CB	0.57	2.51	8	3
1:A:45:LEU:HD12	1:A:48:ILE:HG12	0.57	1.75	8	1
1:A:34:VAL:HG13	1:A:41:PRO:HB3	0.57	1.75	10	1
1:A:65:ASP:HB2	1:A:260:THR:HG22	0.57	1.76	2	1
1:A:81:MET:CE	1:A:143:LEU:HD13	0.57	2.29	2	1
1:A:24:VAL:HG12	1:A:156:GLU:CG	0.57	2.29	5	1
1:A:105:ASN:OD1	1:A:116:LEU:HD21	0.57	1.99	9	1
1:A:45:LEU:HD11	1:A:121:VAL:HG22	0.57	1.75	1	1
1:A:125:LEU:HD23	1:A:126:VAL:N	0.57	2.14	3	1
1:A:56:TYR:OH	1:A:86:THR:HG21	0.57	1.99	4	1
1:A:48:ILE:HD12	1:A:128:PHE:CB	0.57	2.29	8	1
1:A:105:ASN:ND2	1:A:116:LEU:HD11	0.57	2.15	9	1
1:A:122:ASP:O	1:A:126:VAL:HG23	0.57	1.99	7	3
1:A:210:ILE:O	1:A:211:THR:O	0.57	2.21	1	1
1:A:213:LEU:HD13	1:A:218:LEU:CD2	0.57	2.27	1	1
1:A:232:VAL:HG22	1:A:236:GLN:NE2	0.57	2.14	7	1
1:A:127:ILE:HD12	1:A:227:SER:HB3	0.57	1.76	4	1
1:A:69:ALA:HA	1:A:72:TRP:CE2	0.57	2.34	7	1
1:A:93:TRP:CZ3	1:A:260:THR:HG21	0.57	2.35	8	1
1:A:47:LEU:HD12	1:A:144:TRP:CH2	0.57	2.34	10	1
1:A:107:SER:N	1:A:108:PRO:HD3	0.57	2.15	2	1
1:A:121:VAL:O	1:A:125:LEU:HD12	0.57	1.99	10	1
1:A:216:PRO:CG	1:A:217:PRO:CD	0.57	2.83	1	7
1:A:23:TRP:CE2	1:A:24:VAL:HG13	0.57	2.34	7	1
1:A:27:THR:HG21	1:A:192:PHE:C	0.57	2.24	6	1
1:A:214:ASP:O	1:A:215:VAL:C	0.56	2.48	4	2
1:A:189:TYR:CD1	1:A:189:TYR:N	0.56	2.69	3	1
1:A:225:PHE:CZ	1:A:247:LEU:HD12	0.56	2.34	3	1
1:A:192:PHE:HB3	1:A:193:PRO:HD3	0.56	1.76	4	1
1:A:101:VAL:HG12	1:A:116:LEU:HD21	0.56	1.77	7	1
1:A:69:ALA:O	1:A:70:ALA:C	0.56	2.48	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:TRP:NE1	1:A:127:ILE:HD13	0.56	2.15	2	1
1:A:113:TYR:O	1:A:116:LEU:HD22	0.56	1.99	2	1
1:A:77:GLN:O	1:A:87:LEU:HD22	0.56	2.00	3	4
1:A:126:VAL:HG11	1:A:228:GLU:O	0.56	2.01	2	2
1:A:210:ILE:O	1:A:211:THR:HG23	0.56	1.99	6	1
1:A:45:LEU:O	1:A:46:ALA:C	0.56	2.49	7	1
1:A:35:VAL:HG12	1:A:105:ASN:ND2	0.56	2.16	8	1
1:A:80:GLY:O	1:A:81:MET:HB3	0.56	2.00	8	1
1:A:45:LEU:HD13	1:A:48:ILE:HG13	0.56	1.76	9	1
1:A:58:LEU:HD22	1:A:140:ASN:OD1	0.56	2.00	10	1
1:A:45:LEU:HD22	1:A:48:ILE:CB	0.56	2.31	6	1
1:A:195:LEU:HD13	1:A:228:GLU:HA	0.56	1.77	7	1
1:A:233:ARG:CG	1:A:234:ILE:HD12	0.56	2.30	8	1
1:A:205:VAL:HG23	1:A:228:GLU:CD	0.56	2.26	10	1
1:A:206:ARG:HG2	1:A:209:MET:HE2	0.56	1.78	5	1
1:A:49:ASP:O	1:A:53:GLU:OE1	0.56	2.23	7	1
1:A:26:ARG:CG	1:A:46:ALA:HB3	0.56	2.30	9	2
1:A:36:LEU:CB	1:A:37:PRO:CD	0.56	2.82	1	9
1:A:126:VAL:HG13	1:A:189:TYR:CE2	0.56	2.36	2	1
1:A:47:LEU:HD23	1:A:48:ILE:N	0.56	2.16	3	1
1:A:143:LEU:N	1:A:143:LEU:HD23	0.56	2.16	4	1
1:A:56:TYR:HD2	1:A:69:ALA:HB1	0.55	1.59	5	1
1:A:142:PHE:O	1:A:143:LEU:HD22	0.55	2.01	7	1
1:A:26:ARG:HB3	1:A:45:LEU:HD13	0.55	1.78	8	1
1:A:125:LEU:HD21	1:A:189:TYR:O	0.55	2.01	3	1
1:A:62:SER:O	1:A:63:ASP:CB	0.55	2.54	1	2
1:A:142:PHE:O	1:A:143:LEU:HD12	0.55	2.00	2	1
1:A:220:TYR:O	1:A:224:VAL:HG23	0.55	2.01	5	2
1:A:126:VAL:HG11	1:A:229:ASN:HA	0.55	1.78	9	1
1:A:44:LYS:HG2	1:A:124:VAL:HG21	0.55	1.79	8	1
1:A:29:TYR:HB2	1:A:45:LEU:HD21	0.55	1.77	6	1
1:A:192:PHE:HB2	1:A:193:PRO:CD	0.55	2.31	1	1
1:A:22:THR:HG22	1:A:26:ARG:HD3	0.55	1.79	9	1
1:A:100:ILE:HD12	1:A:101:VAL:N	0.55	2.17	10	3
1:A:76:TYR:CD1	1:A:77:GLN:N	0.55	2.75	6	1
1:A:26:ARG:NH1	1:A:47:LEU:HD22	0.55	2.16	2	1
1:A:221:PHE:O	1:A:225:PHE:HB3	0.55	2.01	4	1
1:A:36:LEU:HD11	1:A:99:ALA:CB	0.55	2.29	6	1
1:A:53:GLU:CB	1:A:80:GLY:HA3	0.55	2.31	8	1
1:A:220:TYR:CE1	1:A:224:VAL:HG21	0.55	2.36	9	1
1:A:56:TYR:HB2	1:A:72:TRP:CD2	0.54	2.37	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:216:PRO:CD	1:A:217:PRO:HD3	0.54	2.32	9	7
1:A:132:ILE:HG22	1:A:237:LEU:HD23	0.54	1.79	6	1
1:A:45:LEU:HG	1:A:124:VAL:HG23	0.54	1.78	8	1
1:A:35:VAL:HG13	1:A:102:GLY:HA3	0.54	1.79	5	1
1:A:27:THR:HG21	1:A:192:PHE:O	0.54	2.02	6	1
1:A:70:ALA:HB3	1:A:252:GLU:HA	0.54	1.80	10	3
1:A:53:GLU:CB	1:A:80:GLY:N	0.54	2.70	10	1
1:A:197:ASN:CB	1:A:202:THR:HG21	0.54	2.32	3	1
1:A:119:HIS:CD2	1:A:224:VAL:HG22	0.54	2.38	10	1
1:A:123:TYR:CD2	1:A:124:VAL:HG13	0.54	2.37	2	2
1:A:246:THR:O	1:A:250:VAL:HG23	0.54	2.03	5	3
1:A:131:LEU:HD21	1:A:136:GLY:C	0.54	2.26	4	1
1:A:229:ASN:O	1:A:233:ARG:N	0.54	2.40	6	5
1:A:260:THR:HG22	1:A:261:ARG:HG3	0.54	1.78	7	1
1:A:192:PHE:CB	1:A:193:PRO:HD3	0.54	2.32	1	4
1:A:133:GLY:CA	1:A:234:ILE:HD13	0.54	2.32	2	1
1:A:24:VAL:HG12	1:A:156:GLU:CD	0.54	2.28	5	1
1:A:116:LEU:HA	1:A:119:HIS:CD2	0.54	2.37	10	1
1:A:23:TRP:CE2	1:A:125:LEU:HD22	0.54	2.37	9	1
1:A:34:VAL:O	1:A:116:LEU:HD13	0.54	2.02	9	1
1:A:65:ASP:CB	1:A:260:THR:HG22	0.53	2.33	2	1
1:A:66:SER:HB3	1:A:69:ALA:HB3	0.53	1.80	7	3
1:A:38:SER:O	1:A:39:GLN:CB	0.53	2.56	10	1
1:A:125:LEU:HD23	1:A:193:PRO:CD	0.53	2.33	4	1
1:A:49:ASP:CB	1:A:78:ILE:HD11	0.53	2.33	5	1
1:A:100:ILE:HD13	1:A:219:ASP:HB3	0.53	1.79	5	1
1:A:48:ILE:HD12	1:A:128:PHE:HB3	0.53	1.79	8	1
1:A:130:GLY:O	1:A:131:LEU:C	0.53	2.51	6	1
1:A:107:SER:CB	1:A:108:PRO:CD	0.53	2.86	5	2
1:A:34:VAL:HG22	1:A:34:VAL:O	0.53	2.04	6	4
1:A:87:LEU:HD13	1:A:94:ASN:ND2	0.53	2.18	1	1
1:A:73:ASP:HA	1:A:76:TYR:CD2	0.53	2.38	4	1
1:A:192:PHE:HB3	1:A:193:PRO:CD	0.53	2.34	4	1
1:A:126:VAL:HG22	1:A:233:ARG:HD3	0.53	1.78	6	1
1:A:34:VAL:O	1:A:34:VAL:HG22	0.53	2.02	9	2
1:A:228:GLU:HG2	1:A:232:VAL:HG12	0.53	1.80	2	1
1:A:58:LEU:O	1:A:58:LEU:HD23	0.53	2.04	10	3
1:A:112:SER:O	1:A:113:TYR:HB3	0.53	2.03	7	1
1:A:210:ILE:HD12	1:A:239:LYS:CD	0.53	2.33	2	1
1:A:69:ALA:HB1	1:A:72:TRP:CZ3	0.53	2.39	6	1
1:A:125:LEU:HD22	1:A:193:PRO:HG3	0.53	1.81	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:TYR:HB3	1:A:45:LEU:HD13	0.52	1.82	1	1
1:A:76:TYR:CD1	1:A:76:TYR:N	0.52	2.76	4	1
1:A:197:ASN:HA	1:A:202:THR:HG21	0.52	1.82	2	1
1:A:215:VAL:HB	1:A:217:PRO:HD2	0.52	1.80	3	7
1:A:227:SER:O	1:A:229:ASN:N	0.52	2.42	1	1
1:A:115:ILE:HD13	1:A:220:TYR:CE1	0.52	2.39	7	2
1:A:77:GLN:O	1:A:87:LEU:HD13	0.52	2.04	3	3
1:A:55:TYR:O	1:A:59:ARG:N	0.52	2.43	10	3
1:A:47:LEU:HD23	1:A:47:LEU:O	0.52	2.04	6	1
1:A:253:LEU:HD23	1:A:253:LEU:O	0.52	2.04	1	6
1:A:45:LEU:HD13	1:A:48:ILE:CG2	0.52	2.34	6	1
1:A:58:LEU:HD13	1:A:141:LYS:HB3	0.52	1.82	6	1
1:A:29:TYR:O	1:A:30:SER:CB	0.52	2.58	6	2
1:A:35:VAL:O	1:A:36:LEU:HD22	0.52	2.04	4	1
1:A:138:ASP:C	1:A:139:ILE:HD12	0.52	2.29	8	1
1:A:52:ARG:CZ	1:A:124:VAL:HG12	0.52	2.34	2	1
1:A:143:LEU:N	1:A:143:LEU:CD2	0.52	2.72	4	1
1:A:165:ALA:HB2	1:A:196:PHE:CE1	0.52	2.40	2	1
1:A:45:LEU:HD22	1:A:48:ILE:CG2	0.52	2.35	6	1
1:A:45:LEU:CG	1:A:121:VAL:HG13	0.52	2.35	9	1
1:A:41:PRO:HG2	1:A:78:ILE:HD12	0.51	1.81	8	1
1:A:37:PRO:O	1:A:38:SER:CB	0.51	2.57	1	1
1:A:224:VAL:HG12	1:A:228:GLU:CG	0.51	2.35	1	1
1:A:45:LEU:HD21	1:A:121:VAL:CG1	0.51	2.27	5	3
1:A:123:TYR:OH	1:A:224:VAL:HG22	0.51	2.05	5	1
1:A:31:SER:N	1:A:40:THR:HG22	0.51	2.20	2	1
1:A:240:ASP:OD2	1:A:247:LEU:HD22	0.51	2.06	2	2
1:A:56:TYR:CB	1:A:72:TRP:CD2	0.51	2.93	6	1
1:A:125:LEU:CD1	1:A:126:VAL:HG23	0.51	2.35	6	1
1:A:69:ALA:O	1:A:73:ASP:N	0.51	2.44	9	1
1:A:126:VAL:HG11	1:A:229:ASN:C	0.51	2.30	9	1
1:A:195:LEU:HD11	1:A:231:ASN:HB2	0.51	1.81	1	1
1:A:215:VAL:CB	1:A:217:PRO:HD2	0.51	2.35	3	7
1:A:56:TYR:CE2	1:A:69:ALA:HB1	0.51	2.40	2	1
1:A:220:TYR:CD1	1:A:220:TYR:N	0.51	2.76	8	2
1:A:85:THR:O	1:A:88:VAL:HG22	0.51	2.06	6	1
1:A:28:ALA:O	1:A:30:SER:N	0.51	2.43	6	3
1:A:40:THR:HG22	1:A:77:GLN:CD	0.51	2.31	9	1
1:A:22:THR:O	1:A:23:TRP:C	0.51	2.54	2	5
1:A:142:PHE:CD2	1:A:143:LEU:HD23	0.51	2.40	6	1
1:A:87:LEU:O	1:A:87:LEU:HD13	0.51	2.06	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:LEU:O	1:A:87:LEU:HD22	0.51	2.06	9	1
1:A:45:LEU:HD11	1:A:121:VAL:CG2	0.51	2.35	1	1
1:A:123:TYR:N	1:A:227:SER:HB2	0.51	2.21	1	1
1:A:94:ASN:OD1	1:A:98:ILE:HD12	0.51	2.05	6	2
1:A:45:LEU:HD12	1:A:48:ILE:CG1	0.51	2.36	8	1
1:A:191:ASP:C	1:A:193:PRO:HD2	0.51	2.31	1	1
1:A:50:ASP:HB2	1:A:144:TRP:CD1	0.51	2.41	6	3
1:A:119:HIS:C	1:A:119:HIS:ND1	0.51	2.68	4	1
1:A:192:PHE:N	1:A:193:PRO:HD2	0.51	2.20	7	2
1:A:193:PRO:O	1:A:194:GLN:CB	0.51	2.59	5	1
1:A:56:TYR:HB2	1:A:72:TRP:CZ2	0.51	2.41	7	1
1:A:226:THR:HA	1:A:247:LEU:HD12	0.51	1.82	2	1
1:A:35:VAL:HG11	1:A:101:VAL:CG2	0.51	2.35	10	1
1:A:108:PRO:HD2	1:A:111:LYS:HA	0.50	1.82	2	1
1:A:229:ASN:O	1:A:232:VAL:N	0.50	2.44	7	2
1:A:44:LYS:HE3	1:A:124:VAL:HG11	0.50	1.83	10	1
1:A:104:ALA:CB	1:A:220:TYR:CB	0.50	2.89	5	1
1:A:96:THR:O	1:A:100:ILE:HG23	0.50	2.07	1	1
1:A:215:VAL:H	1:A:216:PRO:HD2	0.50	1.67	7	2
1:A:87:LEU:HD21	1:A:94:ASN:CB	0.50	2.35	9	1
1:A:125:LEU:HD23	1:A:193:PRO:HD3	0.50	1.83	4	1
1:A:49:ASP:OD1	1:A:78:ILE:HD11	0.50	2.07	8	1
1:A:90:ASN:O	1:A:94:ASN:HB2	0.50	2.07	8	1
1:A:34:VAL:CG1	1:A:116:LEU:HD22	0.50	2.36	10	1
1:A:153:TRP:N	1:A:154:PRO:HD2	0.50	2.22	5	1
1:A:81:MET:CE	1:A:82:ALA:HB3	0.49	2.37	1	1
1:A:68:VAL:HG13	1:A:252:GLU:CD	0.49	2.32	8	1
1:A:131:LEU:C	1:A:132:ILE:HD12	0.49	2.31	6	1
1:A:47:LEU:HD23	1:A:48:ILE:HD13	0.49	1.83	9	1
1:A:191:ASP:O	1:A:192:PHE:CG	0.49	2.65	3	1
1:A:237:LEU:O	1:A:237:LEU:HD13	0.49	2.08	7	3
1:A:26:ARG:CG	1:A:45:LEU:HA	0.49	2.37	1	1
1:A:111:LYS:O	1:A:112:SER:C	0.49	2.55	10	2
1:A:72:TRP:NE1	1:A:76:TYR:CB	0.49	2.75	6	2
1:A:105:ASN:ND2	1:A:116:LEU:HD23	0.49	2.22	6	1
1:A:126:VAL:HG11	1:A:229:ASN:CA	0.49	2.37	9	1
1:A:35:VAL:HG11	1:A:101:VAL:HG23	0.49	1.84	10	1
1:A:26:ARG:HG3	1:A:46:ALA:HB3	0.49	1.84	9	2
1:A:36:LEU:H	1:A:37:PRO:HD2	0.49	1.68	4	1
1:A:123:TYR:O	1:A:127:ILE:HG23	0.49	2.06	5	1
1:A:27:THR:HA	1:A:121:VAL:HG11	0.49	1.84	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:210:ILE:HG23	1:A:239:LYS:HB3	0.49	1.85	6	1
1:A:76:TYR:CD1	1:A:76:TYR:O	0.49	2.66	9	1
1:A:105:ASN:C	1:A:108:PRO:HD3	0.49	2.33	2	1
1:A:40:THR:HG22	1:A:98:ILE:HG21	0.49	1.82	3	1
1:A:104:ALA:HB1	1:A:220:TYR:HA	0.49	1.83	8	1
1:A:87:LEU:HD13	1:A:87:LEU:C	0.49	2.33	9	1
1:A:29:TYR:CD2	1:A:45:LEU:HD22	0.48	2.43	1	1
1:A:216:PRO:HD2	1:A:217:PRO:CD	0.48	2.38	6	7
1:A:111:LYS:CE	1:A:224:VAL:HG21	0.48	2.38	8	1
1:A:35:VAL:O	1:A:37:PRO:N	0.48	2.47	1	1
1:A:120:ASP:O	1:A:124:VAL:HG22	0.48	2.07	2	1
1:A:35:VAL:HG12	1:A:102:GLY:C	0.48	2.34	4	1
1:A:26:ARG:HG3	1:A:45:LEU:HD12	0.48	1.85	7	1
1:A:41:PRO:O	1:A:42:ASP:CB	0.48	2.62	10	2
1:A:70:ALA:HB1	1:A:97:HIS:ND1	0.48	2.23	7	1
1:A:53:GLU:CB	1:A:76:TYR:HA	0.48	2.39	8	1
1:A:86:THR:C	1:A:87:LEU:HG	0.48	2.34	8	1
1:A:119:HIS:ND1	1:A:119:HIS:C	0.48	2.71	10	1
1:A:32:PRO:HA	1:A:116:LEU:HD11	0.48	1.85	6	1
1:A:35:VAL:CG1	1:A:116:LEU:HD13	0.48	2.34	8	1
1:A:22:THR:HB	1:A:26:ARG:HB3	0.48	1.86	2	1
1:A:27:THR:HB	1:A:121:VAL:HG11	0.48	1.85	4	1
1:A:56:TYR:HB2	1:A:72:TRP:CE2	0.48	2.43	7	1
1:A:36:LEU:HD11	1:A:103:LYS:HB2	0.48	1.84	3	1
1:A:42:ASP:CG	1:A:78:ILE:HG21	0.48	2.33	4	1
1:A:229:ASN:O	1:A:230:TRP:C	0.48	2.56	7	2
1:A:192:PHE:HB2	1:A:193:PRO:HD3	0.48	1.86	1	1
1:A:205:VAL:HG13	1:A:228:GLU:OE1	0.48	2.08	5	1
1:A:25:THR:O	1:A:25:THR:HG22	0.48	2.09	1	1
1:A:125:LEU:HD21	1:A:193:PRO:HG3	0.48	1.85	7	1
1:A:40:THR:N	1:A:41:PRO:HD2	0.48	2.23	7	1
1:A:212:PRO:O	1:A:213:LEU:CB	0.48	2.62	7	1
1:A:54:ALA:CB	1:A:80:GLY:O	0.48	2.56	8	1
1:A:82:ALA:O	1:A:83:ASP:CB	0.47	2.60	8	2
1:A:23:TRP:CD2	1:A:24:VAL:HG13	0.47	2.44	10	1
1:A:123:TYR:CZ	1:A:127:ILE:HD11	0.47	2.44	10	1
1:A:216:PRO:HD2	1:A:217:PRO:HD2	0.47	1.86	3	6
1:A:215:VAL:O	1:A:218:LEU:HD12	0.47	2.09	6	1
1:A:65:ASP:O	1:A:66:SER:C	0.47	2.57	7	1
1:A:222:ASP:O	1:A:226:THR:HG23	0.47	2.09	3	1
1:A:81:MET:HE2	1:A:81:MET:C	0.47	2.34	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:TRP:CE2	1:A:76:TYR:CB	0.47	2.97	6	1
1:A:33:SER:O	1:A:34:VAL:HG12	0.47	2.09	1	1
1:A:215:VAL:CB	1:A:216:PRO:CD	0.47	2.92	8	3
1:A:205:VAL:HG13	1:A:228:GLU:OE2	0.47	2.09	7	1
1:A:105:ASN:ND2	1:A:113:TYR:H	0.47	2.07	1	1
1:A:33:SER:O	1:A:34:VAL:C	0.47	2.58	9	5
1:A:122:ASP:O	1:A:126:VAL:HG13	0.47	2.09	5	1
1:A:210:ILE:O	1:A:210:ILE:HG23	0.47	2.09	5	2
1:A:85:THR:O	1:A:88:VAL:HG13	0.47	2.10	6	1
1:A:53:GLU:OE1	1:A:79:GLY:HA2	0.47	2.09	7	1
1:A:70:ALA:HB1	1:A:97:HIS:CE1	0.47	2.44	7	1
1:A:94:ASN:ND2	1:A:98:ILE:HD12	0.47	2.23	10	1
1:A:54:ALA:HA	1:A:81:MET:HE2	0.47	1.86	7	1
1:A:215:VAL:CG2	1:A:217:PRO:HG2	0.47	2.40	1	4
1:A:53:GLU:HB3	1:A:80:GLY:CA	0.47	2.39	10	2
1:A:116:LEU:C	1:A:116:LEU:HD13	0.47	2.34	3	1
1:A:34:VAL:CG1	1:A:116:LEU:HD13	0.47	2.39	6	1
1:A:132:ILE:HG22	1:A:237:LEU:CD2	0.47	2.39	6	1
1:A:116:LEU:HD12	1:A:117:LYS:N	0.47	2.24	8	1
1:A:236:GLN:CD	1:A:247:LEU:HD11	0.47	2.35	9	1
1:A:69:ALA:O	1:A:72:TRP:CE3	0.47	2.64	10	1
1:A:36:LEU:N	1:A:37:PRO:HD2	0.47	2.24	9	5
1:A:49:ASP:O	1:A:53:GLU:OE2	0.47	2.33	7	1
1:A:41:PRO:CG	1:A:78:ILE:HD12	0.47	2.40	8	1
1:A:138:ASP:O	1:A:139:ILE:C	0.47	2.58	2	1
1:A:56:TYR:HB2	1:A:76:TYR:CE2	0.47	2.45	4	1
1:A:36:LEU:CD1	1:A:99:ALA:HB1	0.47	2.36	2	1
1:A:34:VAL:HG13	1:A:34:VAL:O	0.47	2.09	4	1
1:A:215:VAL:N	1:A:216:PRO:HD2	0.47	2.25	7	3
1:A:70:ALA:HB1	1:A:255:ARG:CB	0.47	2.39	6	1
1:A:210:ILE:HD11	1:A:235:TYR:HD1	0.47	1.70	6	1
1:A:115:ILE:HD12	1:A:116:LEU:N	0.47	2.25	7	1
1:A:125:LEU:HD21	1:A:191:ASP:CG	0.47	2.35	9	1
1:A:226:THR:OG1	1:A:247:LEU:HD12	0.46	2.09	9	1
1:A:49:ASP:OD1	1:A:50:ASP:N	0.46	2.48	10	1
1:A:45:LEU:HD13	1:A:48:ILE:HG21	0.46	1.86	6	1
1:A:39:GLN:O	1:A:40:THR:CB	0.46	2.63	10	1
1:A:237:LEU:C	1:A:237:LEU:HD13	0.46	2.34	2	3
1:A:28:ALA:HB1	1:A:155:GLU:CG	0.46	2.41	4	1
1:A:48:ILE:HG21	1:A:124:VAL:HG11	0.46	1.87	5	1
1:A:127:ILE:HD11	1:A:227:SER:OG	0.46	2.10	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:MET:CG	1:A:69:ALA:HB2	0.46	2.40	3	1
1:A:145:ASN:C	1:A:146:ILE:HD12	0.46	2.35	4	1
1:A:104:ALA:HB2	1:A:220:TYR:CD2	0.46	2.45	5	1
1:A:116:LEU:HD12	1:A:116:LEU:C	0.46	2.35	6	1
1:A:71:TRP:NE1	1:A:127:ILE:HD12	0.46	2.26	10	1
1:A:27:THR:OG1	1:A:121:VAL:HG11	0.46	2.10	5	1
1:A:226:THR:O	1:A:227:SER:C	0.46	2.57	10	1
1:A:86:THR:O	1:A:87:LEU:C	0.46	2.59	8	2
1:A:119:HIS:O	1:A:123:TYR:HB3	0.46	2.10	2	1
1:A:53:GLU:HB2	1:A:76:TYR:HA	0.46	1.86	3	1
1:A:227:SER:O	1:A:228:GLU:HG3	0.46	2.11	3	1
1:A:86:THR:O	1:A:87:LEU:HD12	0.46	2.11	8	1
1:A:22:THR:OG1	1:A:47:LEU:HD22	0.46	2.11	9	3
1:A:42:ASP:O	1:A:78:ILE:HD13	0.46	2.10	4	1
1:A:56:TYR:CB	1:A:76:TYR:CZ	0.46	2.99	4	1
1:A:238:LYS:O	1:A:242:ALA:HB3	0.46	2.11	7	1
1:A:125:LEU:HD21	1:A:191:ASP:CB	0.46	2.41	9	1
1:A:24:VAL:HG11	1:A:156:GLU:HB3	0.46	1.87	10	1
1:A:58:LEU:HD11	1:A:141:LYS:HB3	0.46	1.88	3	1
1:A:84:ARG:C	1:A:86:THR:H	0.46	2.18	8	1
1:A:31:SER:CB	1:A:32:PRO:HD2	0.46	2.41	4	1
1:A:61:ASN:O	1:A:62:SER:CB	0.46	2.62	7	1
1:A:47:LEU:HD23	1:A:48:ILE:HG12	0.46	1.86	10	1
1:A:225:PHE:O	1:A:232:VAL:HG11	0.46	2.10	4	1
1:A:65:ASP:CG	1:A:66:SER:N	0.46	2.74	5	1
1:A:60:MET:O	1:A:69:ALA:HB2	0.45	2.11	1	1
1:A:44:LYS:HB3	1:A:121:VAL:HG22	0.45	1.88	3	1
1:A:145:ASN:O	1:A:146:ILE:HD12	0.45	2.10	4	1
1:A:126:VAL:HG21	1:A:226:THR:O	0.45	2.11	5	1
1:A:37:PRO:C	1:A:39:GLN:N	0.45	2.73	10	1
1:A:80:GLY:C	1:A:82:ALA:H	0.45	2.19	10	1
1:A:226:THR:HG22	1:A:232:VAL:CG1	0.45	2.40	10	1
1:A:131:LEU:HD23	1:A:132:ILE:N	0.45	2.26	2	1
1:A:105:ASN:O	1:A:111:LYS:C	0.45	2.59	4	1
1:A:123:TYR:O	1:A:127:ILE:HD13	0.45	2.11	7	1
1:A:26:ARG:HG2	1:A:45:LEU:HA	0.45	1.89	8	1
1:A:50:ASP:HA	1:A:80:GLY:CA	0.45	2.42	8	1
1:A:22:THR:HG22	1:A:26:ARG:HE	0.45	1.71	10	1
1:A:29:TYR:HB2	1:A:45:LEU:HD13	0.45	1.88	1	1
1:A:115:ILE:HD12	1:A:115:ILE:C	0.45	2.37	1	2
1:A:22:THR:O	1:A:26:ARG:HB2	0.45	2.11	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:227:SER:O	1:A:228:GLU:CB	0.45	2.64	3	1
1:A:100:ILE:CD1	1:A:219:ASP:HB3	0.45	2.41	7	3
1:A:113:TYR:O	1:A:115:ILE:HD13	0.45	2.11	8	1
1:A:56:TYR:CD1	1:A:72:TRP:CE3	0.45	3.05	9	1
1:A:104:ALA:CB	1:A:219:ASP:HB2	0.45	2.42	2	1
1:A:42:ASP:HB3	1:A:78:ILE:HG21	0.45	1.88	4	1
1:A:76:TYR:O	1:A:77:GLN:C	0.45	2.60	4	1
1:A:49:ASP:O	1:A:53:GLU:CD	0.45	2.60	7	1
1:A:105:ASN:CB	1:A:116:LEU:HD21	0.45	2.42	1	1
1:A:50:ASP:CG	1:A:80:GLY:C	0.45	2.84	4	1
1:A:212:PRO:O	1:A:213:LEU:HD12	0.45	2.12	7	1
1:A:143:LEU:HD12	1:A:144:TRP:CZ3	0.45	2.47	1	2
1:A:240:ASP:CG	1:A:247:LEU:HD22	0.45	2.37	6	1
1:A:123:TYR:CE2	1:A:124:VAL:HG13	0.45	2.47	7	1
1:A:22:THR:C	1:A:26:ARG:HD2	0.45	2.37	1	1
1:A:36:LEU:CB	1:A:37:PRO:HD3	0.45	2.41	1	2
1:A:42:ASP:CB	1:A:78:ILE:HG21	0.45	2.42	4	1
1:A:59:ARG:NH2	1:A:68:VAL:HG21	0.45	2.27	7	1
1:A:209:MET:O	1:A:235:TYR:CG	0.45	2.70	7	1
1:A:75:GLY:O	1:A:78:ILE:HG12	0.45	2.11	8	1
1:A:31:SER:CB	1:A:32:PRO:CD	0.45	2.95	2	1
1:A:45:LEU:CD2	1:A:121:VAL:HG12	0.45	2.32	3	1
1:A:246:THR:O	1:A:250:VAL:N	0.45	2.50	3	1
1:A:47:LEU:HD13	1:A:144:TRP:CZ2	0.45	2.46	5	1
1:A:29:TYR:HB2	1:A:45:LEU:CD2	0.45	2.42	6	1
1:A:236:GLN:OE1	1:A:247:LEU:HD13	0.44	2.12	2	1
1:A:77:GLN:O	1:A:77:GLN:CD	0.44	2.60	8	1
1:A:116:LEU:HD23	1:A:117:LYS:N	0.44	2.27	2	1
1:A:126:VAL:HG21	1:A:228:GLU:O	0.44	2.12	6	1
1:A:223:GLU:CG	1:A:224:VAL:N	0.44	2.81	1	1
1:A:53:GLU:OE1	1:A:80:GLY:N	0.44	2.47	7	1
1:A:87:LEU:HD22	1:A:94:ASN:HB3	0.44	1.88	8	1
1:A:246:THR:O	1:A:250:VAL:HG22	0.44	2.12	1	3
1:A:28:ALA:HB1	1:A:156:GLU:C	0.44	2.36	8	1
1:A:23:TRP:HB2	1:A:125:LEU:HD12	0.44	1.89	3	1
1:A:73:ASP:HA	1:A:76:TYR:CG	0.44	2.48	4	1
1:A:56:TYR:HB2	1:A:72:TRP:CH2	0.44	2.48	7	1
1:A:31:SER:N	1:A:32:PRO:HD2	0.44	2.27	2	1
1:A:103:LYS:O	1:A:104:ALA:C	0.44	2.60	5	1
1:A:207:GLN:O	1:A:210:ILE:HG22	0.44	2.13	1	1
1:A:26:ARG:HB2	1:A:45:LEU:HA	0.44	1.90	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:210:ILE:HG23	1:A:211:THR:N	0.44	2.23	1	1
1:A:228:GLU:HB2	1:A:232:VAL:CG2	0.44	2.43	1	1
1:A:43:GLY:O	1:A:44:LYS:CB	0.44	2.65	2	1
1:A:237:LEU:HD13	1:A:237:LEU:C	0.44	2.37	5	2
1:A:22:THR:HG21	1:A:47:LEU:HD13	0.44	1.90	8	1
1:A:215:VAL:HB	1:A:216:PRO:HD3	0.44	1.90	8	1
1:A:210:ILE:HD12	1:A:239:LYS:HG2	0.44	1.88	2	1
1:A:223:GLU:O	1:A:226:THR:HG22	0.44	2.13	2	2
1:A:53:GLU:HB2	1:A:79:GLY:HA2	0.44	1.89	5	1
1:A:220:TYR:O	1:A:224:VAL:HB	0.44	2.13	7	1
1:A:210:ILE:HG12	1:A:211:THR:HG22	0.44	1.89	8	1
1:A:211:THR:N	1:A:212:PRO:CD	0.43	2.80	4	1
1:A:34:VAL:HG22	1:A:116:LEU:CD1	0.43	2.43	5	1
1:A:119:HIS:CD2	1:A:119:HIS:C	0.43	2.96	6	1
1:A:214:ASP:O	1:A:215:VAL:CG2	0.43	2.64	9	1
1:A:81:MET:HE3	1:A:144:TRP:N	0.43	2.28	4	1
1:A:48:ILE:HG12	1:A:124:VAL:HG21	0.43	1.89	6	1
1:A:76:TYR:CE2	1:A:87:LEU:HA	0.43	2.49	6	1
1:A:76:TYR:C	1:A:76:TYR:CD1	0.43	2.96	8	1
1:A:22:THR:HG22	1:A:26:ARG:NE	0.43	2.28	10	1
1:A:101:VAL:HG12	1:A:223:GLU:CG	0.43	2.44	4	1
1:A:39:GLN:C	1:A:40:THR:HG22	0.43	2.38	5	1
1:A:103:LYS:O	1:A:107:SER:OG	0.43	2.35	5	1
1:A:104:ALA:HB2	1:A:220:TYR:HB3	0.43	1.89	5	1
1:A:81:MET:HB2	1:A:143:LEU:HB3	0.43	1.89	7	1
1:A:130:GLY:O	1:A:131:LEU:CB	0.43	2.66	9	1
1:A:125:LEU:HD13	1:A:193:PRO:HB3	0.43	1.89	10	1
1:A:48:ILE:CG1	1:A:124:VAL:HG21	0.43	2.43	6	1
1:A:126:VAL:HG22	1:A:233:ARG:CD	0.43	2.44	6	1
1:A:132:ILE:HG21	1:A:248:ARG:NH1	0.43	2.28	6	1
1:A:45:LEU:CG	1:A:124:VAL:HG23	0.43	2.44	8	1
1:A:24:VAL:HG11	1:A:157:ILE:HG12	0.43	1.90	1	1
1:A:210:ILE:HG13	1:A:211:THR:N	0.43	2.29	1	1
1:A:50:ASP:HA	1:A:81:MET:N	0.43	2.27	4	1
1:A:208:GLN:HG3	1:A:232:VAL:HG11	0.43	1.90	6	1
1:A:143:LEU:HD13	1:A:144:TRP:N	0.43	2.29	10	1
1:A:213:LEU:HD13	1:A:218:LEU:CD1	0.43	2.43	4	1
1:A:45:LEU:HB3	1:A:48:ILE:HB	0.43	1.91	8	1
1:A:47:LEU:HD23	1:A:48:ILE:CD1	0.43	2.43	9	1
1:A:53:GLU:HB2	1:A:79:GLY:CA	0.43	2.44	2	1
1:A:28:ALA:HB3	1:A:155:GLU:OE1	0.43	2.14	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:ALA:CB	1:A:72:TRP:CZ2	0.43	3.01	7	1
1:A:115:ILE:HD13	1:A:116:LEU:N	0.43	2.29	8	1
1:A:259:LYS:O	1:A:260:THR:HG23	0.43	2.14	8	1
1:A:81:MET:HE3	1:A:82:ALA:HB3	0.43	1.91	9	1
1:A:72:TRP:HB2	1:A:76:TYR:OH	0.43	2.14	4	1
1:A:22:THR:C	1:A:26:ARG:HB3	0.43	2.39	6	1
1:A:60:MET:O	1:A:62:SER:N	0.43	2.51	7	3
1:A:76:TYR:CD1	1:A:76:TYR:C	0.43	2.96	6	1
1:A:48:ILE:O	1:A:52:ARG:HG2	0.43	2.14	9	1
1:A:75:GLY:O	1:A:78:ILE:HD13	0.43	2.13	10	1
1:A:45:LEU:O	1:A:49:ASP:N	0.43	2.44	7	3
1:A:120:ASP:O	1:A:124:VAL:HG13	0.43	2.14	10	3
1:A:125:LEU:HD21	1:A:193:PRO:CG	0.43	2.44	7	1
1:A:87:LEU:HD13	1:A:91:ASN:CB	0.43	2.44	8	1
1:A:236:GLN:HE21	1:A:247:LEU:HD13	0.43	1.73	8	1
1:A:123:TYR:HB3	1:A:227:SER:HB2	0.43	1.90	9	1
1:A:213:LEU:HD12	1:A:213:LEU:O	0.42	2.13	1	1
1:A:27:THR:C	1:A:43:GLY:HA3	0.42	2.38	2	1
1:A:126:VAL:CG1	1:A:228:GLU:O	0.42	2.67	3	1
1:A:143:LEU:O	1:A:143:LEU:HG	0.42	2.14	4	1
1:A:220:TYR:O	1:A:224:VAL:HG22	0.42	2.14	8	1
1:A:232:VAL:CG1	1:A:232:VAL:O	0.42	2.63	10	1
1:A:56:TYR:CB	1:A:72:TRP:CE2	0.42	3.02	6	1
1:A:45:LEU:O	1:A:47:LEU:N	0.42	2.52	7	1
1:A:115:ILE:CD1	1:A:115:ILE:C	0.42	2.92	7	1
1:A:226:THR:O	1:A:232:VAL:HG11	0.42	2.14	7	1
1:A:107:SER:HB3	1:A:108:PRO:HD2	0.42	1.89	5	1
1:A:22:THR:OG1	1:A:46:ALA:HB3	0.42	2.15	6	1
1:A:50:ASP:HA	1:A:80:GLY:N	0.42	2.29	8	1
1:A:128:PHE:O	1:A:131:LEU:HD23	0.42	2.15	7	1
1:A:226:THR:HG21	1:A:252:GLU:OE1	0.42	2.13	3	1
1:A:53:GLU:OE2	1:A:53:GLU:N	0.42	2.50	7	1
1:A:123:TYR:CE2	1:A:224:VAL:HG22	0.42	2.49	9	1
1:A:52:ARG:O	1:A:55:TYR:HB3	0.42	2.15	10	1
1:A:165:ALA:HB2	1:A:196:PHE:CZ	0.42	2.49	2	1
1:A:119:HIS:CE1	1:A:224:VAL:HG12	0.42	2.50	4	1
1:A:146:ILE:HG22	1:A:146:ILE:O	0.42	2.14	4	1
1:A:112:SER:O	1:A:113:TYR:HB2	0.42	2.14	5	1
1:A:70:ALA:HB3	1:A:252:GLU:O	0.42	2.15	3	2
1:A:121:VAL:HG12	1:A:121:VAL:O	0.42	2.14	4	1
1:A:35:VAL:HG13	1:A:102:GLY:CA	0.42	2.44	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:TRP:CE3	1:A:72:TRP:C	0.42	2.98	7	1
1:A:53:GLU:HB3	1:A:81:MET:HB3	0.42	1.90	6	1
1:A:54:ALA:HB1	1:A:142:PHE:HB2	0.42	1.90	7	1
1:A:81:MET:HG3	1:A:82:ALA:N	0.42	2.29	9	1
1:A:26:ARG:HB3	1:A:45:LEU:HA	0.42	1.91	10	1
1:A:132:ILE:O	1:A:132:ILE:HG23	0.42	2.14	2	1
1:A:87:LEU:O	1:A:91:ASN:N	0.42	2.50	8	2
1:A:44:LYS:HG2	1:A:45:LEU:HD12	0.42	1.92	4	1
1:A:228:GLU:O	1:A:229:ASN:HB2	0.42	2.15	5	1
1:A:123:TYR:CD1	1:A:123:TYR:C	0.42	2.93	6	1
1:A:230:TRP:O	1:A:234:ILE:HD13	0.42	2.15	8	1
1:A:126:VAL:HG21	1:A:232:VAL:CG1	0.42	2.44	10	1
1:A:226:THR:HG22	1:A:232:VAL:HG11	0.42	1.90	10	1
1:A:67:LYS:HD3	1:A:68:VAL:HG23	0.42	1.92	1	1
1:A:140:ASN:HB2	1:A:143:LEU:HD22	0.42	1.92	1	1
1:A:245:ARG:O	1:A:246:THR:HG23	0.42	2.15	3	1
1:A:192:PHE:N	1:A:193:PRO:CD	0.42	2.83	7	1
1:A:100:ILE:HD12	1:A:219:ASP:HB3	0.41	1.91	1	1
1:A:132:ILE:HG23	1:A:132:ILE:O	0.41	2.15	4	1
1:A:33:SER:O	1:A:34:VAL:CG1	0.41	2.67	1	1
1:A:31:SER:C	1:A:33:SER:H	0.41	2.23	2	1
1:A:83:ASP:O	1:A:84:ARG:C	0.41	2.62	3	1
1:A:108:PRO:O	1:A:109:GLU:CB	0.41	2.68	6	1
1:A:119:HIS:CG	1:A:120:ASP:N	0.41	2.85	6	1
1:A:220:TYR:CD1	1:A:224:VAL:HG21	0.41	2.50	7	1
1:A:228:GLU:HB3	1:A:232:VAL:HB	0.41	1.91	7	1
1:A:54:ALA:HB1	1:A:142:PHE:CG	0.41	2.50	3	1
1:A:218:LEU:O	1:A:222:ASP:CB	0.41	2.67	7	1
1:A:34:VAL:HA	1:A:41:PRO:CA	0.41	2.45	10	1
1:A:35:VAL:HG21	1:A:102:GLY:CA	0.41	2.45	10	1
1:A:53:GLU:HB3	1:A:80:GLY:HA2	0.41	1.93	10	1
1:A:125:LEU:HD12	1:A:125:LEU:C	0.41	2.39	2	1
1:A:21:SER:O	1:A:25:THR:N	0.41	2.52	4	1
1:A:230:TRP:O	1:A:234:ILE:HG22	0.41	2.15	4	1
1:A:22:THR:HG21	1:A:47:LEU:CD1	0.41	2.45	8	1
1:A:48:ILE:O	1:A:48:ILE:HG22	0.41	2.15	10	1
1:A:83:ASP:O	1:A:84:ARG:CB	0.41	2.68	10	1
1:A:104:ALA:HB2	1:A:219:ASP:CB	0.41	2.45	3	1
1:A:35:VAL:O	1:A:36:LEU:HD12	0.41	2.15	7	1
1:A:53:GLU:O	1:A:57:TRP:N	0.41	2.54	9	1
1:A:228:GLU:HB2	1:A:232:VAL:HG21	0.41	1.92	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LEU:O	1:A:131:LEU:HD23	0.41	2.16	1	1
1:A:45:LEU:HD22	1:A:124:VAL:HG21	0.41	1.91	5	1
1:A:63:ASP:O	1:A:64:GLU:CB	0.41	2.69	5	1
1:A:100:ILE:O	1:A:220:TYR:CD1	0.41	2.73	5	1
1:A:54:ALA:O	1:A:58:LEU:CB	0.41	2.67	8	1
1:A:101:VAL:HG11	1:A:119:HIS:NE2	0.41	2.30	9	1
1:A:101:VAL:HG12	1:A:223:GLU:CD	0.41	2.40	4	1
1:A:35:VAL:O	1:A:36:LEU:CD2	0.41	2.68	5	1
1:A:88:VAL:HG13	1:A:89:ASP:N	0.41	2.31	1	2
1:A:56:TYR:CE1	1:A:76:TYR:CD2	0.41	3.08	8	2
1:A:85:THR:O	1:A:88:VAL:HG12	0.41	2.16	3	1
1:A:125:LEU:HD23	1:A:125:LEU:C	0.41	2.41	3	1
1:A:192:PHE:HB3	1:A:193:PRO:HD2	0.41	1.93	3	1
1:A:56:TYR:O	1:A:69:ALA:HB2	0.41	2.16	9	1
1:A:112:SER:O	1:A:113:TYR:C	0.41	2.64	10	1
1:A:56:TYR:O	1:A:60:MET:CA	0.41	2.69	1	1
1:A:131:LEU:O	1:A:132:ILE:HB	0.41	2.16	1	1
1:A:43:GLY:O	1:A:44:LYS:HB3	0.41	2.16	2	1
1:A:71:TRP:O	1:A:71:TRP:CD1	0.41	2.74	2	1
1:A:163:TYR:O	1:A:164:THR:HG23	0.41	2.15	2	1
1:A:229:ASN:CG	1:A:230:TRP:N	0.41	2.79	2	1
1:A:124:VAL:O	1:A:127:ILE:HG22	0.41	2.16	3	1
1:A:69:ALA:HB1	1:A:76:TYR:HE2	0.41	1.76	4	1
1:A:216:PRO:HG2	1:A:221:PHE:CD1	0.41	2.50	8	1
1:A:66:SER:O	1:A:67:LYS:C	0.41	2.62	9	1
1:A:67:LYS:C	1:A:252:GLU:O	0.41	2.64	9	1
1:A:133:GLY:HA2	1:A:234:ILE:HD13	0.41	1.93	2	1
1:A:52:ARG:NH2	1:A:124:VAL:HG11	0.41	2.31	5	1
1:A:74:TYR:OH	1:A:101:VAL:HG21	0.41	2.16	5	1
1:A:153:TRP:N	1:A:154:PRO:CD	0.41	2.84	5	1
1:A:212:PRO:HG2	1:A:213:LEU:HD22	0.41	1.92	8	1
1:A:56:TYR:CG	1:A:72:TRP:CE3	0.41	3.09	9	1
1:A:24:VAL:HG11	1:A:156:GLU:C	0.40	2.42	2	1
1:A:209:MET:O	1:A:210:ILE:C	0.40	2.62	2	1
1:A:44:LYS:HB3	1:A:121:VAL:HG13	0.40	1.93	3	1
1:A:229:ASN:N	1:A:233:ARG:HB3	0.40	2.31	3	1
1:A:46:ALA:O	1:A:50:ASP:OD1	0.40	2.39	4	1
1:A:36:LEU:HB3	1:A:37:PRO:HD3	0.40	1.93	5	1
1:A:245:ARG:O	1:A:246:THR:CB	0.40	2.70	8	1
1:A:53:GLU:HA	1:A:72:TRP:NE1	0.40	2.31	10	1
1:A:143:LEU:HD12	1:A:144:TRP:CH2	0.40	2.52	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:PRO:HD2	1:A:220:TYR:CD2	0.40	2.51	4	1
1:A:123:TYR:CD1	1:A:123:TYR:N	0.40	2.88	5	1
1:A:34:VAL:HG21	1:A:74:TYR:OH	0.40	2.16	8	1
1:A:41:PRO:O	1:A:42:ASP:HB3	0.40	2.16	10	1
1:A:69:ALA:O	1:A:71:TRP:N	0.40	2.54	10	1
1:A:126:VAL:HG21	1:A:232:VAL:HG12	0.40	1.94	10	1
1:A:105:ASN:CG	1:A:115:ILE:HD11	0.40	2.41	1	1
1:A:197:ASN:CA	1:A:202:THR:HG21	0.40	2.47	3	1
1:A:212:PRO:O	1:A:213:LEU:HB2	0.40	2.16	3	1
1:A:26:ARG:CD	1:A:46:ALA:HB3	0.40	2.46	4	1
1:A:72:TRP:CE2	1:A:76:TYR:HB3	0.40	2.51	6	1
1:A:215:VAL:HB	1:A:216:PRO:CD	0.40	2.47	8	1
1:A:81:MET:SD	1:A:81:MET:C	0.40	3.04	9	1
1:A:146:ILE:HD13	1:A:146:ILE:N	0.40	2.32	10	1
1:A:221:PHE:O	1:A:225:PHE:CG	0.40	2.74	1	1
1:A:71:TRP:CE2	1:A:127:ILE:HD13	0.40	2.51	2	1
1:A:229:ASN:C	1:A:231:ASN:N	0.40	2.79	3	1
1:A:84:ARG:C	1:A:87:LEU:HD23	0.40	2.42	4	1
1:A:44:LYS:O	1:A:45:LEU:HB2	0.40	2.17	8	1
1:A:123:TYR:HA	1:A:126:VAL:HG12	0.40	1.93	3	1
1:A:105:ASN:O	1:A:112:SER:N	0.40	2.51	5	1
1:A:228:GLU:HB2	1:A:232:VAL:HB	0.40	1.92	5	1
1:A:131:LEU:O	1:A:132:ILE:HD12	0.40	2.17	6	1
1:A:104:ALA:HB1	1:A:220:TYR:HB3	0.40	1.93	7	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	209/273 (77%)	144±4 (69±2%)	36±4 (17±2%)	29±2 (14±1%)	0 5
All	All	2090/2730 (77%)	1442 (69%)	355 (17%)	293 (14%)	0 5

All 79 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	67	LYS	9
1	A	144	TRP	9
1	A	194	GLN	9
1	A	29	TYR	8
1	A	36	LEU	8
1	A	111	LYS	8
1	A	228	GLU	8
1	A	82	ALA	7
1	A	132	ILE	7
1	A	192	PHE	7
1	A	212	PRO	7
1	A	139	ILE	7
1	A	79	GLY	6
1	A	166	GLU	6
1	A	210	ILE	6
1	A	257	SER	6
1	A	34	VAL	6
1	A	40	THR	6
1	A	44	LYS	6
1	A	38	SER	5
1	A	109	GLU	5
1	A	245	ARG	5
1	A	61	ASN	5
1	A	143	LEU	5
1	A	112	SER	5
1	A	42	ASP	4
1	A	197	ASN	4
1	A	214	ASP	4
1	A	21	SER	4
1	A	30	SER	4
1	A	35	VAL	4
1	A	81	MET	4
1	A	145	ASN	4
1	A	146	ILE	4
1	A	134	PHE	4
1	A	165	ALA	4
1	A	63	ASP	3
1	A	211	THR	3
1	A	229	ASN	3
1	A	260	THR	3
1	A	33	SER	3
1	A	41	PRO	3
1	A	195	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	258	THR	3
1	A	39	GLN	3
1	A	163	TYR	3
1	A	244	GLY	3
1	A	62	SER	3
1	A	31	SER	2
1	A	43	GLY	2
1	A	133	GLY	2
1	A	213	LEU	2
1	A	261	ARG	2
1	A	164	THR	2
1	A	32	PRO	2
1	A	78	ILE	2
1	A	196	PHE	2
1	A	246	THR	2
1	A	259	LYS	2
1	A	113	TYR	2
1	A	83	ASP	2
1	A	140	ASN	2
1	A	217	PRO	2
1	A	85	THR	2
1	A	65	ASP	1
1	A	64	GLU	1
1	A	135	GLY	1
1	A	142	PHE	1
1	A	60	MET	1
1	A	110	GLU	1
1	A	227	SER	1
1	A	243	GLN	1
1	A	45	LEU	1
1	A	46	ALA	1
1	A	84	ARG	1
1	A	66	SER	1
1	A	215	VAL	1
1	A	37	PRO	1
1	A	70	ALA	1

6.3.2 Protein sidechains ⓘ

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	186/239 (78%)	125±5 (67±2%)	61±5 (33±2%)	1	12
All	All	1860/2390 (78%)	1247 (67%)	613 (33%)	1	12

All 158 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	LEU	10
1	A	100	ILE	9
1	A	248	ARG	9
1	A	78	ILE	8
1	A	107	SER	8
1	A	117	LYS	8
1	A	166	GLU	8
1	A	246	THR	8
1	A	81	MET	8
1	A	218	LEU	8
1	A	56	TYR	8
1	A	113	TYR	7
1	A	119	HIS	7
1	A	219	ASP	7
1	A	255	ARG	7
1	A	239	LYS	7
1	A	259	LYS	7
1	A	30	SER	6
1	A	31	SER	6
1	A	47	LEU	6
1	A	48	ILE	6
1	A	77	GLN	6
1	A	238	LYS	6
1	A	245	ARG	6
1	A	64	GLU	6
1	A	86	THR	6
1	A	94	ASN	6
1	A	96	THR	6
1	A	141	LYS	6
1	A	143	LEU	6
1	A	115	ILE	6
1	A	162	PHE	6
1	A	21	SER	6
1	A	33	SER	5
1	A	40	THR	5
1	A	44	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	45	LEU	5
1	A	59	ARG	5
1	A	92	THR	5
1	A	190	LYS	5
1	A	195	LEU	5
1	A	211	THR	5
1	A	213	LEU	5
1	A	232	VAL	5
1	A	249	ASP	5
1	A	257	SER	5
1	A	258	THR	5
1	A	87	LEU	5
1	A	111	LYS	5
1	A	131	LEU	5
1	A	155	GLU	5
1	A	160	ARG	5
1	A	164	THR	5
1	A	53	GLU	5
1	A	60	MET	5
1	A	85	THR	5
1	A	206	ARG	5
1	A	49	ASP	4
1	A	62	SER	4
1	A	67	LYS	4
1	A	83	ASP	4
1	A	127	ILE	4
1	A	132	ILE	4
1	A	140	ASN	4
1	A	194	GLN	4
1	A	202	THR	4
1	A	209	MET	4
1	A	220	TYR	4
1	A	221	PHE	4
1	A	228	GLU	4
1	A	237	LEU	4
1	A	76	TYR	4
1	A	84	ARG	4
1	A	116	LEU	4
1	A	123	TYR	4
1	A	125	LEU	4
1	A	253	LEU	4
1	A	189	TYR	4

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Mol	Chain	Res	Type	Models (Total)
1	A	231	ASN	4
1	A	236	GLN	4
1	A	260	THR	4
1	A	66	SER	4
1	A	103	LYS	4
1	A	23	TRP	3
1	A	61	ASN	3
1	A	89	ASP	3
1	A	118	GLU	3
1	A	137	ASP	3
1	A	145	ASN	3
1	A	214	ASP	3
1	A	243	GLN	3
1	A	52	ARG	3
1	A	223	GLU	3
1	A	235	TYR	3
1	A	256	SER	3
1	A	144	TRP	3
1	A	158	LYS	3
1	A	197	ASN	3
1	A	205	VAL	3
1	A	35	VAL	3
1	A	38	SER	3
1	A	215	VAL	3
1	A	252	GLU	3
1	A	153	TRP	3
1	A	229	ASN	3
1	A	225	PHE	3
1	A	109	GLU	3
1	A	26	ARG	2
1	A	65	ASP	2
1	A	90	ASN	2
1	A	112	SER	2
1	A	146	ILE	2
1	A	210	ILE	2
1	A	241	ASP	2
1	A	29	TYR	2
1	A	50	ASP	2
1	A	91	ASN	2
1	A	93	TRP	2
1	A	192	PHE	2
1	A	203	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	204	ARG	2
1	A	39	GLN	2
1	A	120	ASP	2
1	A	121	VAL	2
1	A	156	GLU	2
1	A	159	GLU	2
1	A	207	GLN	2
1	A	234	ILE	2
1	A	55	TYR	2
1	A	110	GLU	2
1	A	114	GLU	2
1	A	240	ASP	2
1	A	261	ARG	2
1	A	51	PHE	2
1	A	72	TRP	2
1	A	73	ASP	2
1	A	74	TYR	2
1	A	98	ILE	2
1	A	157	ILE	2
1	A	196	PHE	2
1	A	42	ASP	2
1	A	138	ASP	2
1	A	191	ASP	2
1	A	24	VAL	1
1	A	122	ASP	1
1	A	163	TYR	1
1	A	224	VAL	1
1	A	254	THR	1
1	A	97	HIS	1
1	A	22	THR	1
1	A	105	ASN	1
1	A	227	SER	1
1	A	25	THR	1
1	A	57	TRP	1
1	A	63	ASP	1
1	A	142	PHE	1
1	A	58	LEU	1
1	A	226	THR	1

6.3.3 RNA ⓘ

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

The completeness of assignment taking into account all chemical shift lists is 33% for the well-defined parts and 32% 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

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	1187
Number of shifts mapped to atoms	1187
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	243	0.07 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	227	0.90 ± 0.05	Should be checked
$^{13}\text{C}'$	244	-0.05 ± 0.14	None needed (< 0.5 ppm)
^{15}N	235	0.42 ± 0.20	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 33%, i.e. 942 atoms were assigned a chemical shift out of a possible 2887. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	758/1039 (73%)	187/421 (44%)	385/418 (92%)	186/200 (93%)
Sidechain	182/1549 (12%)	0/997 (0%)	182/487 (37%)	0/65 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	2/299 (1%)	1/145 (1%)	0/144 (0%)	1/10 (10%)
Overall	942/2887 (33%)	188/1563 (12%)	567/1049 (54%)	187/275 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 32%, i.e. 1187 atoms were assigned a chemical shift out of a possible 3754. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	958/1363 (70%)	236/555 (43%)	487/546 (89%)	235/262 (90%)
Sidechain	227/2025 (11%)	0/1306 (0%)	227/626 (36%)	0/93 (0%)
Aromatic	2/366 (1%)	1/181 (1%)	0/168 (0%)	1/17 (6%)
Overall	1187/3754 (32%)	237/2042 (12%)	714/1340 (53%)	236/372 (63%)

7.1.4 Statistically unusual chemical shifts ⓘ

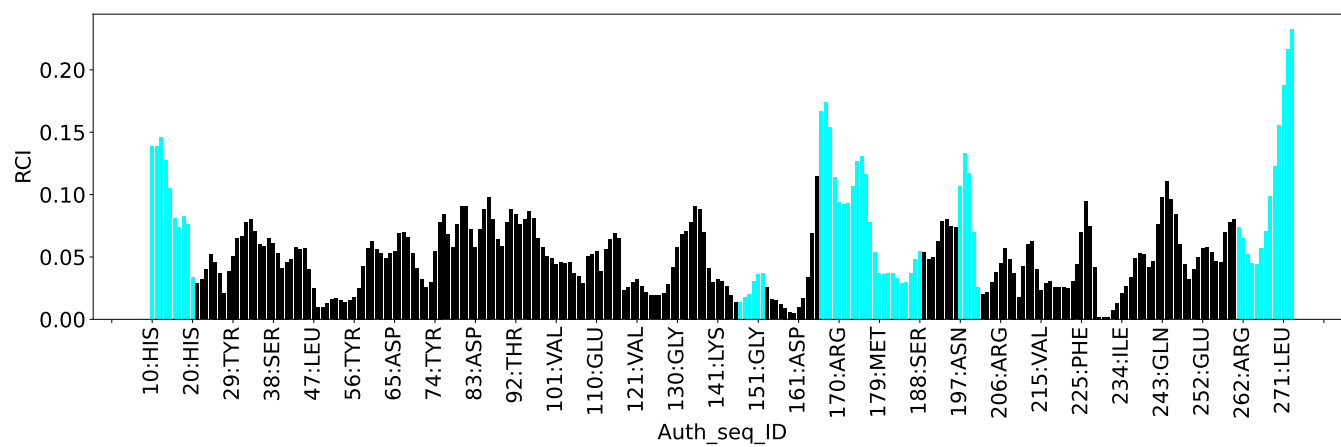
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	230	TRP	HA	11.41	2.12 – 7.20	13.3
1	A	160	ARG	CA	31.54	45.44 – 68.13	-11.1
1	A	27	THR	CB	54.99	61.12 – 78.27	-8.6
1	A	147	ARG	CB	43.89	21.74 – 39.52	7.5
1	A	111	LYS	CB	43.91	24.03 – 41.47	6.4
1	A	55	TYR	CB	27.54	28.67 – 49.81	-5.5

7.1.5 Random Coil Index (RCI) plots ⓘ

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	1435
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	646
Medium range ($ i-j >1$ and $ i-j <5$)	596
Long range ($ i-j \geq 5$)	193
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	5.3
Number of long range restraints per residue ¹	0.7

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)	87.8	0.2
0.2-0.5 (Medium)	112.7	0.5
>0.5 (Large)	39.4	13.58

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

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

9 Distance violation analysis ⓘ

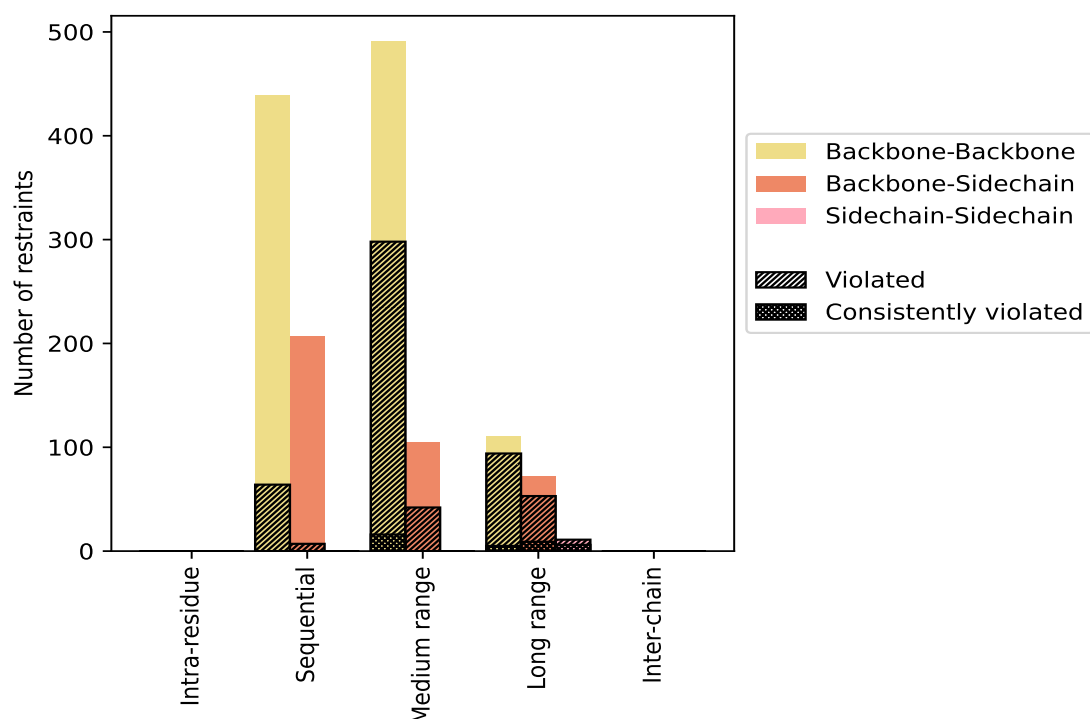
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	646	45.0	71	11.0	4.9	0	0.0	0.0
Backbone-Backbone	439	30.6	64	14.6	4.5	0	0.0	0.0
Backbone-Sidechain	207	14.4	7	3.4	0.5	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	596	41.5	340	57.0	23.7	16	2.7	1.1
Backbone-Backbone	491	34.2	298	60.7	20.8	16	3.3	1.1
Backbone-Sidechain	105	7.3	42	40.0	2.9	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \geq 5$)	193	13.4	158	81.9	11.0	20	10.4	1.4
Backbone-Backbone	110	7.7	94	85.5	6.6	5	4.5	0.3
Backbone-Sidechain	72	5.0	53	73.6	3.7	9	12.5	0.6
Sidechain-Sidechain	11	0.8	11	100.0	0.8	6	54.5	0.4
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1435	100.0	569	39.7	39.7	36	2.5	2.5
Backbone-Backbone	1040	72.5	456	43.8	31.8	21	2.0	1.5
Backbone-Sidechain	384	26.8	102	26.6	7.1	9	2.3	0.6
Sidechain-Sidechain	11	0.8	11	100.0	0.8	6	54.5	0.4

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

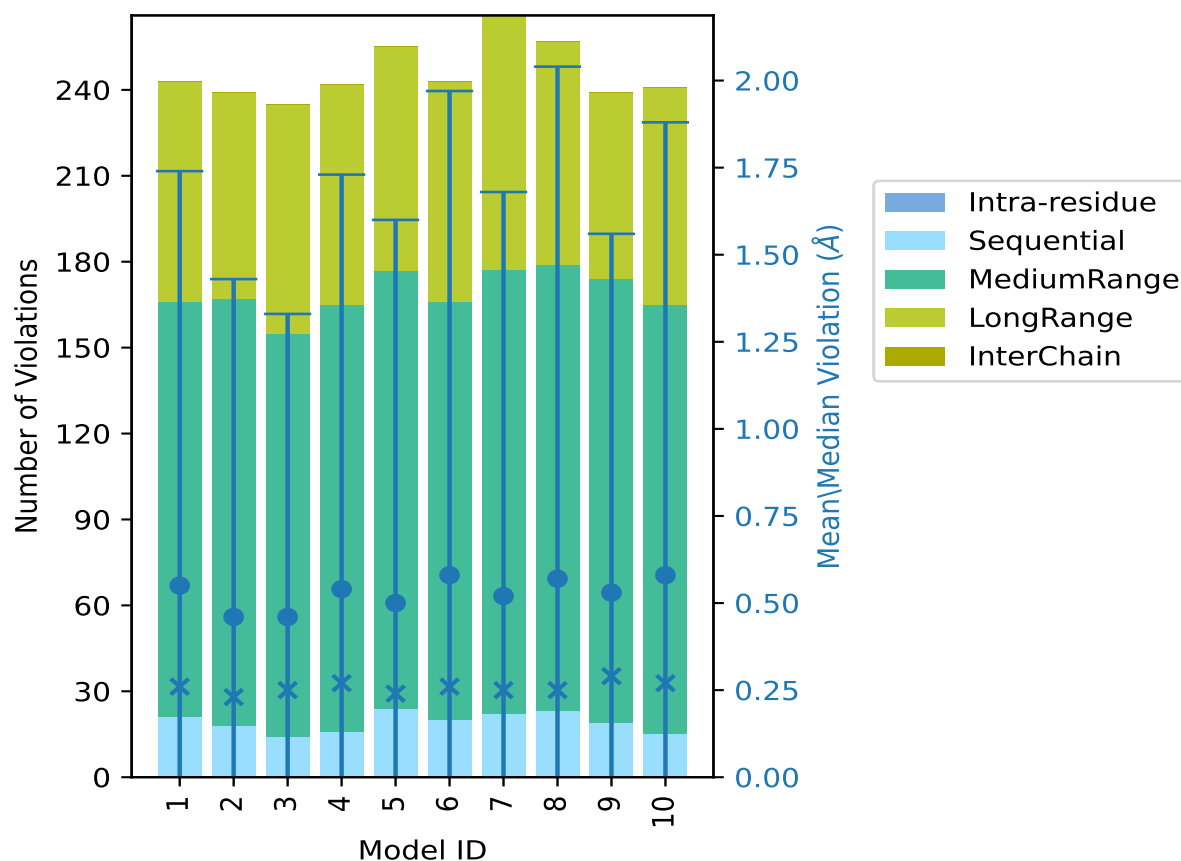
9.2 Distance violation statistics for each model [i](#)

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	0	21	145	77	0	243	0.55	10.08	1.19	0.26
2	0	18	149	72	0	239	0.46	7.05	0.97	0.23
3	0	14	141	80	0	235	0.46	7.58	0.87	0.25
4	0	16	149	77	0	242	0.54	11.24	1.19	0.27
5	0	24	153	78	0	255	0.5	10.64	1.1	0.24
6	0	20	146	77	0	243	0.58	13.58	1.39	0.26
7	0	22	155	89	0	266	0.52	9.69	1.16	0.25
8	0	23	156	78	0	257	0.57	12.32	1.47	0.25
9	0	19	155	65	0	239	0.53	10.54	1.03	0.29
10	0	15	150	76	0	241	0.58	10.39	1.3	0.27

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

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



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 866(IR:0, SQ:575, MR:256, LR:35, 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	%
0	26	77	37	0	140	1	10.0
0	13	48	17	0	78	2	20.0
0	10	36	15	0	61	3	30.0

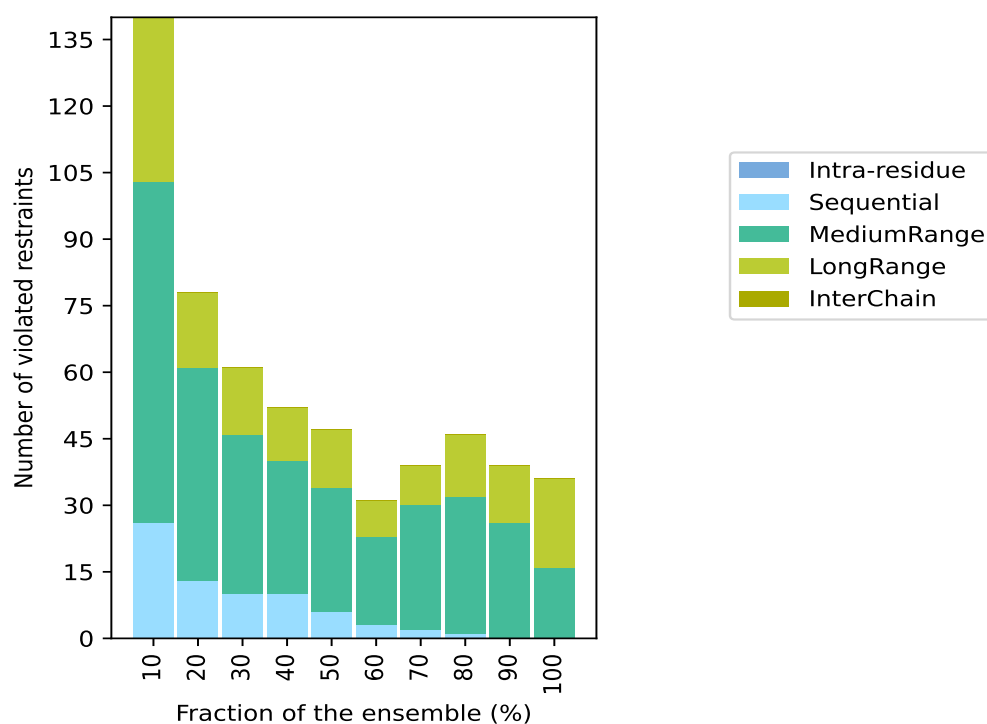
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	10	30	12	0	52	4	40.0
0	6	28	13	0	47	5	50.0
0	3	20	8	0	31	6	60.0
0	2	28	9	0	39	7	70.0
0	1	31	14	0	46	8	80.0
0	0	26	13	0	39	9	90.0
0	0	16	20	0	36	10	100.0

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

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

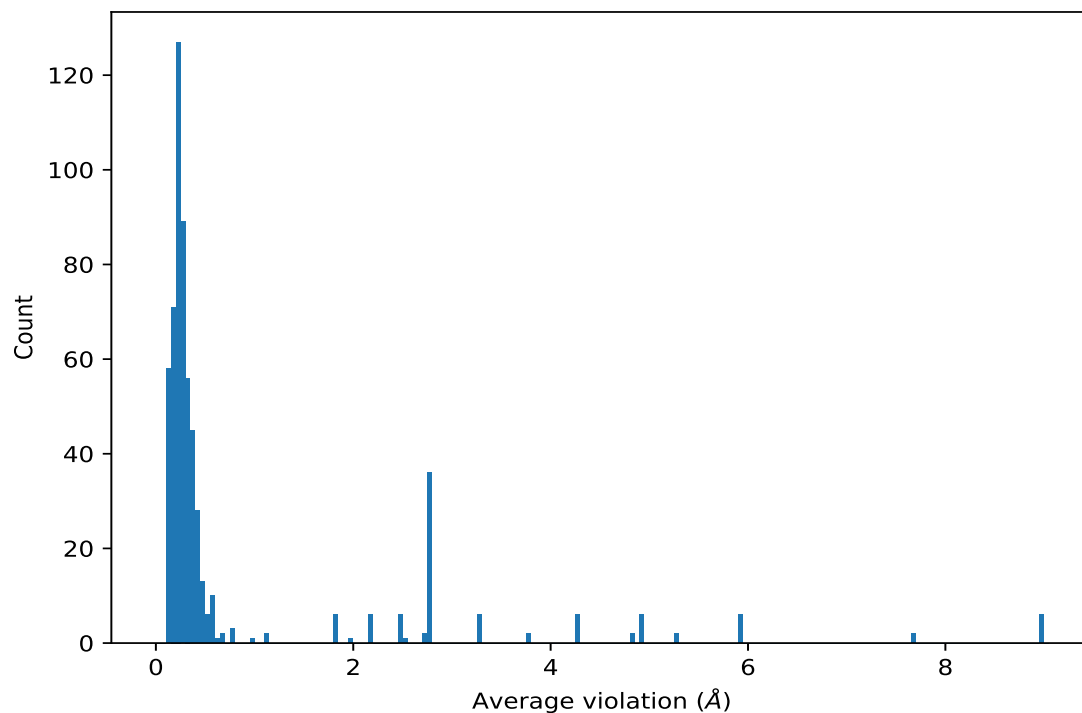


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD11	10	8.99	3.76	10.46
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD12	10	8.99	3.76	10.46
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD13	10	8.99	3.76	10.46
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD21	10	8.99	3.76	10.46
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD22	10	8.99	3.76	10.46
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD23	10	8.99	3.76	10.46
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB2	10	7.66	1.87	7.32
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB3	10	7.66	1.87	7.32
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG11	10	5.91	2.77	7.2
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG12	10	5.91	2.77	7.2
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG13	10	5.91	2.77	7.2
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG21	10	5.91	2.77	7.2
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG22	10	5.91	2.77	7.2
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG23	10	5.91	2.77	7.2
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB2	10	5.28	1.94	5.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB3	10	5.28	1.94	5.47
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG11	10	4.9	2.08	3.94
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG12	10	4.9	2.08	3.94
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG13	10	4.9	2.08	3.94
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG21	10	4.9	2.08	3.94
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG22	10	4.9	2.08	3.94
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG23	10	4.9	2.08	3.94
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB2	10	4.82	2.39	5.01
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB3	10	4.82	2.39	5.01
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG11	10	4.27	1.93	4.51
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG12	10	4.27	1.93	4.51
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG13	10	4.27	1.93	4.51
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG21	10	4.27	1.93	4.51
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG22	10	4.27	1.93	4.51
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG23	10	4.27	1.93	4.51
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB2	10	3.76	2.3	4.46
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB3	10	3.76	2.3	4.46
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG11	10	3.29	0.91	3.36
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG12	10	3.29	0.91	3.36
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG13	10	3.29	0.91	3.36
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG21	10	3.29	0.91	3.36
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG22	10	3.29	0.91	3.36
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG23	10	3.29	0.91	3.36
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG11	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG12	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG13	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG21	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG22	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG23	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG11	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG12	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG13	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG21	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG22	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG23	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG11	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG12	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG13	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG21	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG22	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG23	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG11	10	2.75	1.41	2.84

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG12	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG13	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG21	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG22	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG23	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG11	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG12	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG13	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG21	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG22	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG23	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG11	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG12	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG13	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG21	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG22	10	2.75	1.41	2.84
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG23	10	2.75	1.41	2.84
(1,1284)	1:250:A:VAL:H	1:71:A:TRP:HA	10	2.52	0.29	2.5
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG11	10	2.46	0.87	2.72
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG12	10	2.46	0.87	2.72
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG13	10	2.46	0.87	2.72
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG21	10	2.46	0.87	2.72
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG22	10	2.46	0.87	2.72
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG23	10	2.46	0.87	2.72
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG11	10	2.15	1.44	1.42
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG12	10	2.15	1.44	1.42
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG13	10	2.15	1.44	1.42
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG21	10	2.15	1.44	1.42
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG22	10	2.15	1.44	1.42
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG23	10	2.15	1.44	1.42
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB2	10	1.12	0.14	1.17
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB3	10	1.12	0.14	1.17
(1,1199)	1:52:A:ARG:H	1:76:A:TYR:H	10	0.42	0.19	0.46
(1,181)	1:57:A:TRP:HA	1:60:A:MET:H	10	0.41	0.18	0.42
(1,1246)	1:106:A:ALA:H	1:113:A:TYR:H	10	0.41	0.17	0.42
(1,266)	1:70:A:ALA:HA	1:74:A:TYR:H	10	0.4	0.21	0.36
(1,981)	1:231:A:ASN:HA	1:234:A:ILE:H	10	0.4	0.16	0.34
(1,1163)	1:22:A:THR:H	1:47:A:LEU:H	10	0.4	0.22	0.38
(1,840)	1:207:A:GLN:HA	1:210:A:ILE:H	10	0.39	0.16	0.37
(1,911)	1:223:A:GLU:HA	1:226:A:THR:H	10	0.38	0.1	0.36
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB2	10	0.36	0.14	0.34
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB3	10	0.36	0.14	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB2	10	0.35	0.1	0.38
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB3	10	0.35	0.1	0.38
(1,373)	1:89:A:ASP:HA	1:92:A:THR:H	10	0.33	0.09	0.33
(1,1068)	1:247:A:LEU:HA	1:250:A:VAL:H	10	0.32	0.06	0.34
(1,1228)	1:93:A:TRP:H	1:64:A:GLU:HA	10	0.32	0.17	0.29
(1,261)	1:74:A:TYR:HA	1:77:A:GLN:H	10	0.32	0.09	0.31
(1,1077)	1:251:A:GLY:HA2	1:254:A:THR:H	10	0.31	0.1	0.34
(1,1077)	1:251:A:GLY:HA3	1:254:A:THR:H	10	0.31	0.1	0.34
(1,379)	1:92:A:THR:HA	1:96:A:THR:H	10	0.3	0.1	0.26
(1,983)	1:233:A:ARG:HA	1:236:A:GLN:H	10	0.29	0.12	0.33
(1,140)	1:51:A:PHE:HA	1:53:A:GLU:H	10	0.29	0.16	0.24
(1,157)	1:45:A:LEU:HA	1:49:A:ASP:H	10	0.28	0.14	0.27
(1,526)	1:114:A:GLU:HA	1:118:A:GLU:H	10	0.27	0.14	0.27
(1,516)	1:121:A:VAL:HA	1:124:A:VAL:H	10	0.26	0.1	0.22
(1,1075)	1:249:A:ASP:HA	1:252:A:GLU:H	10	0.23	0.08	0.21
(1,1235)	1:101:A:VAL:HA	1:223:A:GLU:HA	9	1.98	0.5	2.15
(1,1180)	1:29:A:TYR:HA	1:46:A:ALA:H	9	0.47	0.12	0.44
(1,762)	1:188:A:SER:HA	1:191:A:ASP:H	9	0.45	0.29	0.47
(1,1165)	1:22:A:THR:HB	1:45:A:LEU:H	9	0.45	0.23	0.51
(1,42)	1:23:A:TRP:HA	1:26:A:ARG:H	9	0.42	0.1	0.42
(2,99)	1:76:A:TYR:HA	1:87:A:LEU:H	9	0.41	0.1	0.41
(1,50)	1:24:A:VAL:HA	1:28:A:ALA:H	9	0.4	0.15	0.44
(1,1249)	1:123:A:TYR:H	1:224:A:VAL:HA	9	0.39	0.17	0.36
(2,95)	1:210:A:ILE:HA	1:235:A:TYR:H	9	0.39	0.16	0.42
(1,991)	1:228:A:GLU:HA	1:232:A:VAL:H	9	0.38	0.23	0.38
(1,997)	1:234:A:ILE:HA	1:238:A:LYS:H	9	0.38	0.14	0.36
(1,907)	1:219:A:ASP:HA	1:222:A:ASP:H	9	0.37	0.08	0.39
(1,1274)	1:197:A:ASN:HA	1:202:A:THR:HA	9	0.36	0.1	0.35
(1,44)	1:24:A:VAL:HA	1:27:A:THR:H	9	0.34	0.2	0.28
(1,1152)	1:194:A:GLN:HA	1:197:A:ASN:H	9	0.32	0.12	0.31
(1,1200)	1:54:A:ALA:H	1:82:A:ALA:H	9	0.32	0.19	0.29
(1,1306)	1:49:A:ASP:H	1:144:A:TRP:HD1	9	0.31	0.12	0.28
(1,529)	1:117:A:LYS:HA	1:121:A:VAL:H	9	0.31	0.13	0.27
(1,40)	1:21:A:SER:HA	1:24:A:VAL:H	9	0.3	0.08	0.27
(1,1248)	1:110:A:GLU:H	1:215:A:VAL:HB	9	0.29	0.09	0.3
(1,1299)	1:26:A:ARG:H	1:121:A:VAL:HG11	9	0.29	0.12	0.25
(1,984)	1:234:A:ILE:HA	1:237:A:LEU:H	9	0.29	0.08	0.27
(1,908)	1:220:A:TYR:HA	1:223:A:GLU:H	9	0.28	0.15	0.21
(1,515)	1:120:A:ASP:HA	1:123:A:TYR:H	9	0.28	0.09	0.26
(1,523)	1:127:A:ILE:HA	1:130:A:GLY:H	9	0.28	0.14	0.25
(1,524)	1:128:A:PHE:HA	1:131:A:LEU:H	9	0.27	0.16	0.2
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG11	9	0.27	0.16	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG12	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG13	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG21	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG22	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG23	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG11	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG12	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG13	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG21	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG22	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG23	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG11	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG12	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG13	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG21	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG22	9	0.27	0.16	0.23
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG23	9	0.27	0.16	0.23
(1,511)	1:116:A:LEU:HA	1:119:A:HIS:H	9	0.27	0.14	0.24
(1,473)	1:114:A:GLU:H	1:116:A:LEU:H	9	0.26	0.11	0.25
(1,343)	1:91:A:ASN:H	1:93:A:TRP:H	9	0.26	0.1	0.28
(1,1317)	1:53:A:GLU:H	1:79:A:GLY:H	9	0.25	0.11	0.24
(1,988)	1:238:A:LYS:HA	1:241:A:ASP:H	9	0.25	0.06	0.23
(1,909)	1:221:A:PHE:HA	1:224:A:VAL:H	9	0.24	0.13	0.19
(1,530)	1:118:A:GLU:HA	1:122:A:ASP:H	9	0.24	0.09	0.23
(1,243)	1:74:A:TYR:HA	1:76:A:TYR:H	9	0.23	0.07	0.23
(1,834)	1:202:A:THR:HA	1:205:A:VAL:H	9	0.21	0.07	0.19
(1,1074)	1:248:A:ARG:HG2	1:251:A:GLY:H	9	0.18	0.04	0.18
(1,1073)	1:248:A:ARG:HB2	1:251:A:GLY:H	9	0.17	0.1	0.14
(1,987)	1:237:A:LEU:HA	1:240:A:ASP:H	9	0.16	0.03	0.16
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD2	8	2.74	1.35	2.33
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD3	8	2.74	1.35	2.33
(1,1166)	1:23:A:TRP:H	1:45:A:LEU:HA	8	0.66	0.31	0.56
(1,749)	1:187:A:MET:HA	1:191:A:ASP:H	8	0.53	0.25	0.54
(1,388)	1:101:A:VAL:HA	1:105:A:ASN:H	8	0.48	0.18	0.46
(1,45)	1:25:A:THR:HA	1:28:A:ALA:H	8	0.47	0.17	0.53
(1,1226)	1:82:A:ALA:HA	1:144:A:TRP:H	8	0.46	0.16	0.44
(1,757)	1:183:A:LEU:HA	1:186:A:LYS:H	8	0.44	0.21	0.52
(1,753)	1:179:A:MET:HA	1:182:A:SER:H	8	0.43	0.13	0.41
(1,751)	1:177:A:GLU:HA	1:180:A:ARG:H	8	0.41	0.17	0.35
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB2	8	0.41	0.22	0.4
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB3	8	0.41	0.22	0.4
(1,918)	1:223:A:GLU:HA	1:227:A:SER:H	8	0.4	0.11	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,745)	1:183:A:LEU:HA	1:187:A:MET:H	8	0.39	0.13	0.4
(1,1329)	1:104:A:ALA:HA	1:221:A:PHE:H	8	0.39	0.13	0.35
(1,1203)	1:56:A:TYR:H	1:72:A:TRP:H	8	0.38	0.22	0.28
(1,1001)	1:238:A:LYS:HA	1:242:A:ALA:H	8	0.36	0.15	0.26
(1,176)	1:52:A:ARG:HA	1:55:A:TYR:H	8	0.36	0.12	0.34
(2,98)	1:178:A:THR:H	1:202:A:THR:H	8	0.36	0.21	0.26
(1,178)	1:54:A:ALA:HA	1:57:A:TRP:H	8	0.36	0.1	0.36
(1,1207)	1:62:A:SER:HA	1:67:A:LYS:H	8	0.34	0.17	0.26
(1,1256)	1:130:A:GLY:HA2	1:234:A:ILE:HA	8	0.33	0.11	0.32
(1,1256)	1:130:A:GLY:HA3	1:234:A:ILE:HA	8	0.33	0.11	0.32
(1,741)	1:179:A:MET:HA	1:183:A:LEU:H	8	0.32	0.12	0.31
(1,756)	1:182:A:SER:HA	1:185:A:TYR:H	8	0.32	0.16	0.31
(1,979)	1:229:A:ASN:HA	1:232:A:VAL:H	8	0.32	0.12	0.27
(1,992)	1:229:A:ASN:HA	1:233:A:ARG:H	8	0.32	0.1	0.3
(1,1234)	1:101:A:VAL:HA	1:223:A:GLU:H	8	0.32	0.05	0.32
(2,94)	1:204:A:ARG:HA	1:209:A:MET:H	8	0.31	0.13	0.3
(1,160)	1:48:A:ILE:HA	1:52:A:ARG:H	8	0.3	0.12	0.26
(1,246)	1:76:A:TYR:H	1:78:A:ILE:H	8	0.29	0.07	0.3
(1,384)	1:97:A:HIS:HA	1:101:A:VAL:H	8	0.29	0.08	0.29
(1,994)	1:231:A:ASN:HA	1:235:A:TYR:H	8	0.29	0.11	0.27
(1,915)	1:220:A:TYR:HA	1:224:A:VAL:H	8	0.28	0.17	0.24
(1,914)	1:219:A:ASP:HA	1:223:A:GLU:H	8	0.28	0.15	0.25
(1,171)	1:47:A:LEU:HA	1:50:A:ASP:H	8	0.27	0.11	0.22
(1,259)	1:72:A:TRP:HA	1:75:A:GLY:H	8	0.26	0.11	0.22
(1,163)	1:51:A:PHE:HA	1:55:A:TYR:H	8	0.26	0.13	0.22
(1,175)	1:51:A:PHE:HA	1:54:A:ALA:H	8	0.26	0.08	0.25
(1,475)	1:115:A:ILE:H	1:117:A:LYS:H	8	0.25	0.1	0.25
(1,1148)	1:171:A:VAL:HA	1:174:A:ARG:H	8	0.24	0.09	0.18
(1,839)	1:206:A:ARG:HA	1:209:A:MET:H	8	0.24	0.1	0.18
(1,1314)	1:177:A:GLU:H	1:202:A:THR:HA	8	0.23	0.09	0.2
(1,1334)	1:177:A:GLU:H	1:202:A:THR:HA	8	0.23	0.09	0.2
(1,396)	1:98:A:ILE:HA	1:101:A:VAL:H	8	0.23	0.07	0.2
(1,387)	1:100:A:ILE:HA	1:104:A:ALA:H	8	0.22	0.1	0.2
(1,1305)	1:48:A:ILE:H	1:144:A:TRP:HZ2	8	0.21	0.08	0.22
(1,377)	1:93:A:TRP:HA	1:96:A:THR:H	8	0.21	0.08	0.18
(1,414)	1:110:A:GLU:HA	1:111:A:LYS:H	8	0.17	0.03	0.19
(2,89)	1:123:A:TYR:HA	1:226:A:THR:H	7	0.96	0.84	0.47
(1,1205)	1:56:A:TYR:H	1:76:A:TYR:HA	7	0.59	0.32	0.45
(1,758)	1:184:A:LEU:HA	1:187:A:MET:H	7	0.47	0.15	0.5
(1,1151)	1:175:A:ALA:HA	1:179:A:MET:H	7	0.46	0.18	0.36
(1,161)	1:49:A:ASP:HA	1:53:A:GLU:H	7	0.42	0.17	0.3
(1,754)	1:180:A:ARG:HA	1:183:A:LEU:H	7	0.4	0.18	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,164)	1:52:A:ARG:HA	1:56:A:TYR:H	7	0.39	0.1	0.36
(1,1219)	1:78:A:ILE:HA	1:83:A:ASP:H	7	0.39	0.15	0.37
(1,746)	1:184:A:LEU:HA	1:188:A:SER:H	7	0.38	0.22	0.29
(1,533)	1:120:A:ASP:HA	1:124:A:VAL:H	7	0.38	0.13	0.38
(1,264)	1:68:A:VAL:HA	1:72:A:TRP:H	7	0.37	0.18	0.35
(1,389)	1:102:A:GLY:HA2	1:106:A:ALA:H	7	0.36	0.19	0.3
(1,389)	1:102:A:GLY:HA3	1:106:A:ALA:H	7	0.36	0.19	0.3
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG11	7	0.34	0.06	0.32
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG12	7	0.34	0.06	0.32
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG13	7	0.34	0.06	0.32
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG21	7	0.34	0.06	0.32
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG22	7	0.34	0.06	0.32
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG23	7	0.34	0.06	0.32
(1,1325)	1:60:A:MET:H	1:69:A:ALA:HA	7	0.31	0.17	0.23
(1,513)	1:118:A:GLU:HA	1:121:A:VAL:H	7	0.27	0.11	0.27
(1,508)	1:130:A:GLY:H	1:132:A:ILE:H	7	0.27	0.07	0.25
(2,9)	1:41:A:PRO:HD2	1:44:A:LYS:H	7	0.27	0.1	0.24
(2,9)	1:41:A:PRO:HD3	1:44:A:LYS:H	7	0.27	0.1	0.24
(1,519)	1:124:A:VAL:HA	1:127:A:ILE:H	7	0.25	0.11	0.23
(1,365)	1:104:A:ALA:HA	1:106:A:ALA:H	7	0.25	0.06	0.24
(1,252)	1:67:A:LYS:HA	1:70:A:ALA:H	7	0.24	0.09	0.21
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD11	7	0.24	0.1	0.23
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD12	7	0.24	0.1	0.23
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD13	7	0.24	0.1	0.23
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD21	7	0.24	0.1	0.23
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD22	7	0.24	0.1	0.23
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD23	7	0.24	0.1	0.23
(1,835)	1:202:A:THR:HB	1:205:A:VAL:H	7	0.24	0.12	0.27
(1,232)	1:69:A:ALA:H	1:71:A:TRP:H	7	0.24	0.09	0.2
(1,1304)	1:48:A:ILE:H	1:144:A:TRP:HD1	7	0.24	0.07	0.25
(1,268)	1:73:A:ASP:HA	1:77:A:GLN:H	7	0.24	0.1	0.24
(1,173)	1:49:A:ASP:HA	1:52:A:ARG:H	7	0.23	0.12	0.2
(1,512)	1:117:A:LYS:HA	1:120:A:ASP:H	7	0.23	0.08	0.26
(1,891)	1:219:A:ASP:HA	1:221:A:PHE:H	7	0.23	0.09	0.22
(1,842)	1:200:A:GLN:HA	1:204:A:ARG:H	7	0.22	0.09	0.23
(1,240)	1:73:A:ASP:H	1:75:A:GLY:H	7	0.22	0.08	0.18
(1,250)	1:77:A:GLN:HA	1:79:A:GLY:H	7	0.21	0.07	0.18
(1,534)	1:121:A:VAL:HA	1:125:A:LEU:H	7	0.21	0.04	0.21
(1,192)	1:66:A:SER:H	1:67:A:LYS:H	7	0.2	0.14	0.15
(1,845)	1:203:A:ASP:HA	1:207:A:GLN:H	7	0.2	0.05	0.23
(1,380)	1:93:A:TRP:HA	1:97:A:HIS:H	7	0.2	0.05	0.19
(1,856)	1:214:A:ASP:HA	1:215:A:VAL:H	7	0.19	0.02	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1298)	1:156:A:GLU:H	1:25:A:THR:HG1	7	0.18	0.09	0.15
(1,1081)	1:247:A:LEU:HA	1:251:A:GLY:H	7	0.17	0.04	0.17
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD11	7	0.17	0.05	0.18
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD12	7	0.17	0.05	0.18
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD13	7	0.17	0.05	0.18
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD21	7	0.17	0.05	0.18
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD22	7	0.17	0.05	0.18
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD23	7	0.17	0.05	0.18
(1,1194)	1:35:A:VAL:H	1:40:A:THR:HA	6	0.53	0.19	0.58
(1,74)	1:44:A:LYS:H	1:45:A:LEU:H	6	0.42	0.14	0.44
(1,1206)	1:56:A:TYR:HA	1:69:A:ALA:H	6	0.38	0.26	0.3
(1,1281)	1:213:A:LEU:H	1:218:A:LEU:HG	6	0.37	0.16	0.36
(1,83)	1:45:A:LEU:H	1:46:A:ALA:H	6	0.36	0.33	0.24
(1,538)	1:125:A:LEU:HA	1:129:A:GLY:H	6	0.34	0.11	0.34
(1,1150)	1:174:A:ARG:H	1:177:A:GLU:HB2	6	0.34	0.14	0.34
(1,405)	1:111:A:LYS:H	1:113:A:TYR:HB2	6	0.34	0.12	0.4
(1,1187)	1:33:A:SER:H	1:39:A:GLN:HA	6	0.34	0.2	0.28
(1,258)	1:71:A:TRP:HA	1:74:A:TYR:H	6	0.34	0.19	0.26
(1,996)	1:233:A:ARG:HA	1:237:A:LEU:H	6	0.28	0.11	0.25
(1,419)	1:112:A:SER:H	1:113:A:TYR:H	6	0.27	0.14	0.19
(1,142)	1:52:A:ARG:HA	1:54:A:ALA:H	6	0.27	0.1	0.29
(1,399)	1:101:A:VAL:HA	1:104:A:ALA:H	6	0.24	0.03	0.25
(1,342)	1:90:A:ASN:H	1:92:A:THR:H	6	0.23	0.09	0.23
(1,518)	1:123:A:TYR:HA	1:126:A:VAL:H	6	0.23	0.07	0.21
(1,1179)	1:29:A:TYR:H	1:46:A:ALA:H	6	0.23	0.12	0.2
(1,1000)	1:237:A:LEU:HA	1:241:A:ASP:H	6	0.23	0.05	0.2
(1,1153)	1:237:A:LEU:HA	1:241:A:ASP:H	6	0.23	0.05	0.2
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD11	6	0.22	0.12	0.15
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD12	6	0.22	0.12	0.15
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD13	6	0.22	0.12	0.15
(1,376)	1:92:A:THR:HA	1:95:A:ASN:H	6	0.22	0.07	0.22
(1,583)	1:151:A:GLY:HA2	1:153:A:TRP:H	6	0.21	0.12	0.18
(1,1336)	1:189:A:TYR:HA	1:230:A:TRP:H	6	0.2	0.08	0.18
(1,398)	1:100:A:ILE:HA	1:103:A:LYS:H	6	0.2	0.06	0.22
(1,844)	1:202:A:THR:HA	1:206:A:ARG:H	6	0.2	0.06	0.16
(1,712)	1:177:A:GLU:HA	1:179:A:MET:H	6	0.18	0.05	0.16
(1,710)	1:176:A:SER:HA	1:178:A:THR:H	6	0.18	0.04	0.18
(1,228)	1:66:A:SER:HA	1:68:A:VAL:H	6	0.17	0.05	0.16
(1,47)	1:21:A:SER:HA	1:25:A:THR:H	6	0.17	0.04	0.15
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD11	6	0.16	0.06	0.14
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD12	6	0.16	0.06	0.14
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD13	6	0.16	0.06	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,836)	1:203:A:ASP:HA	1:206:A:ARG:H	6	0.16	0.04	0.15
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG11	5	1.8	2.39	0.95
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG12	5	1.8	2.39	0.95
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG13	5	1.8	2.39	0.95
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG21	5	1.8	2.39	0.95
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG22	5	1.8	2.39	0.95
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG23	5	1.8	2.39	0.95
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG11	5	0.55	0.76	0.16
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG12	5	0.55	0.76	0.16
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG13	5	0.55	0.76	0.16
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG21	5	0.55	0.76	0.16
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG22	5	0.55	0.76	0.16
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG23	5	0.55	0.76	0.16
(1,174)	1:50:A:ASP:HA	1:53:A:GLU:H	5	0.46	0.18	0.42
(1,980)	1:230:A:TRP:HA	1:233:A:ARG:H	5	0.44	0.2	0.38
(1,269)	1:79:A:GLY:H	1:80:A:GLY:H	5	0.39	0.14	0.37
(1,755)	1:181:A:ASN:HA	1:184:A:LEU:H	5	0.37	0.13	0.43
(1,912)	1:224:A:VAL:HA	1:227:A:SER:H	5	0.36	0.14	0.4
(1,750)	1:176:A:SER:HA	1:179:A:MET:H	5	0.36	0.09	0.36
(1,1186)	1:29:A:TYR:H	1:45:A:LEU:HA	5	0.35	0.08	0.37
(1,910)	1:222:A:ASP:HA	1:225:A:PHE:H	5	0.33	0.13	0.31
(1,777)	1:198:A:GLY:H	1:199:A:GLY:H	5	0.32	0.1	0.31
(1,1289)	1:266:A:ARG:H	1:273:A:VAL:H	5	0.32	0.16	0.38
(1,1275)	1:197:A:ASN:HA	1:202:A:THR:H	5	0.31	0.19	0.23
(1,1225)	1:82:A:ALA:H	1:144:A:TRP:HA	5	0.29	0.13	0.27
(1,165)	1:53:A:GLU:HA	1:57:A:TRP:H	5	0.29	0.08	0.33
(1,1217)	1:77:A:GLN:H	1:98:A:ILE:HG13	5	0.28	0.08	0.28
(1,30)	1:23:A:TRP:HA	1:25:A:THR:H	5	0.28	0.07	0.28
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD11	5	0.27	0.1	0.25
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD12	5	0.27	0.1	0.25
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD13	5	0.27	0.1	0.25
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD21	5	0.27	0.1	0.25
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD22	5	0.27	0.1	0.25
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD23	5	0.27	0.1	0.25
(1,847)	1:210:A:ILE:H	1:211:A:THR:H	5	0.26	0.06	0.28
(1,993)	1:230:A:TRP:HA	1:234:A:ILE:H	5	0.26	0.11	0.23
(1,841)	1:208:A:GLN:HA	1:211:A:THR:H	5	0.26	0.09	0.25
(1,1087)	1:260:A:THR:H	1:261:A:ARG:H	5	0.25	0.03	0.26
(1,1259)	1:132:A:ILE:H	1:237:A:LEU:HB2	5	0.23	0.06	0.23
(1,1259)	1:132:A:ILE:H	1:237:A:LEU:HB3	5	0.23	0.06	0.23
(1,837)	1:204:A:ARG:HA	1:207:A:GLN:H	5	0.23	0.02	0.22
(2,25)	1:75:A:GLY:H	1:78:A:ILE:HG12	5	0.23	0.07	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,25)	1:75:A:GLY:H	1:78:A:ILE:HG13	5	0.23	0.07	0.24
(1,1142)	1:213:A:LEU:H	1:214:A:ASP:HA	5	0.23	0.05	0.24
(1,954)	1:230:A:TRP:H	1:232:A:VAL:H	5	0.23	0.06	0.2
(1,723)	1:183:A:LEU:HA	1:185:A:TYR:H	5	0.22	0.08	0.24
(1,838)	1:205:A:VAL:HA	1:208:A:GLN:H	5	0.22	0.08	0.18
(1,1216)	1:71:A:TRP:H	1:255:A:ARG:HG2	5	0.22	0.11	0.18
(1,1216)	1:71:A:TRP:H	1:255:A:ARG:HG3	5	0.22	0.11	0.18
(1,761)	1:187:A:MET:HA	1:190:A:LYS:H	5	0.22	0.08	0.19
(1,80)	1:42:A:ASP:HB2	1:44:A:LYS:H	5	0.22	0.05	0.21
(1,80)	1:42:A:ASP:HB3	1:44:A:LYS:H	5	0.22	0.05	0.21
(1,1333)	1:174:A:ARG:H	1:198:A:GLY:HA2	5	0.22	0.07	0.24
(1,1333)	1:174:A:ARG:H	1:198:A:GLY:HA3	5	0.22	0.07	0.24
(1,985)	1:235:A:TYR:HA	1:238:A:LYS:H	5	0.21	0.05	0.21
(1,402)	1:104:A:ALA:HA	1:107:A:SER:H	5	0.21	0.06	0.22
(1,139)	1:51:A:PHE:H	1:53:A:GLU:H	5	0.21	0.1	0.18
(1,888)	1:218:A:LEU:H	1:220:A:TYR:H	5	0.21	0.07	0.21
(1,238)	1:72:A:TRP:H	1:74:A:TYR:H	5	0.2	0.07	0.22
(1,539)	1:126:A:VAL:HA	1:130:A:GLY:H	5	0.2	0.05	0.2
(1,832)	1:200:A:GLN:HA	1:203:A:ASP:H	5	0.2	0.06	0.19
(1,1229)	1:98:A:ILE:H	1:255:A:ARG:HG2	5	0.18	0.06	0.16
(1,1229)	1:98:A:ILE:H	1:255:A:ARG:HG3	5	0.18	0.06	0.16
(1,1300)	1:120:A:ASP:H	1:34:A:VAL:HG11	5	0.18	0.1	0.12
(1,146)	1:54:A:ALA:HA	1:56:A:TYR:H	5	0.17	0.03	0.17
(1,630)	1:156:A:GLU:HA	1:159:A:GLU:H	5	0.14	0.02	0.14
(1,393)	1:96:A:THR:HA	1:99:A:ALA:H	5	0.14	0.02	0.14
(1,1014)	1:242:A:ALA:HA	1:244:A:GLY:H	5	0.13	0.02	0.14
(1,1004)	1:239:A:LYS:HA	1:240:A:ASP:H	5	0.13	0.01	0.12
(1,156)	1:59:A:ARG:H	1:61:A:ASN:H	4	0.6	0.09	0.6
(1,368)	1:84:A:ARG:HA	1:87:A:LEU:H	4	0.58	0.28	0.7
(1,369)	1:85:A:THR:HA	1:88:A:VAL:H	4	0.54	0.23	0.66
(2,28)	1:78:A:ILE:HG12	1:81:A:MET:H	4	0.54	0.22	0.6
(2,28)	1:78:A:ILE:HG13	1:81:A:MET:H	4	0.54	0.22	0.6
(1,267)	1:72:A:TRP:HA	1:76:A:TYR:H	4	0.43	0.16	0.41
(1,180)	1:56:A:TYR:HA	1:59:A:ARG:H	4	0.42	0.16	0.46
(1,760)	1:186:A:LYS:HA	1:189:A:TYR:H	4	0.4	0.12	0.44
(1,850)	1:212:A:PRO:HA	1:213:A:LEU:H	4	0.39	0.01	0.39
(1,166)	1:54:A:ALA:HA	1:58:A:LEU:H	4	0.38	0.24	0.3
(1,742)	1:180:A:ARG:HA	1:184:A:LEU:H	4	0.38	0.22	0.35
(1,752)	1:178:A:THR:HA	1:181:A:ASN:H	4	0.37	0.21	0.36
(1,1197)	1:51:A:PHE:H	1:79:A:GLY:HA2	4	0.36	0.19	0.28
(1,1197)	1:51:A:PHE:H	1:79:A:GLY:HA3	4	0.36	0.19	0.28
(1,1185)	1:27:A:THR:HA	1:46:A:ALA:H	4	0.35	0.23	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1024)	1:244:A:GLY:H	1:246:A:THR:H	4	0.34	0.23	0.22
(1,1160)	1:261:A:ARG:H	1:264:A:ILE:HA	4	0.33	0.15	0.32
(1,276)	1:83:A:ASP:H	1:84:A:ARG:H	4	0.32	0.16	0.33
(1,1269)	1:173:A:ALA:HA	1:178:A:THR:H	4	0.31	0.15	0.31
(1,159)	1:47:A:LEU:HA	1:51:A:PHE:H	4	0.3	0.12	0.24
(1,1258)	1:132:A:ILE:H	1:237:A:LEU:HG	4	0.25	0.17	0.18
(1,1288)	1:265:A:LYS:H	1:270:A:GLY:H	4	0.24	0.19	0.14
(1,385)	1:98:A:ILE:HA	1:102:A:GLY:H	4	0.24	0.07	0.24
(1,584)	1:154:A:PRO:HD2	1:156:A:GLU:H	4	0.24	0.03	0.24
(1,584)	1:154:A:PRO:HD3	1:156:A:GLU:H	4	0.24	0.03	0.24
(1,1209)	1:63:A:ASP:H	1:265:A:LYS:H	4	0.23	0.06	0.24
(1,155)	1:59:A:ARG:HA	1:61:A:ASN:H	4	0.23	0.08	0.2
(1,129)	1:46:A:ALA:H	1:48:A:ILE:H	4	0.22	0.05	0.22
(1,145)	1:54:A:ALA:H	1:56:A:TYR:H	4	0.22	0.1	0.2
(1,1140)	1:199:A:GLY:H	1:200:A:GLN:HA	4	0.22	0.09	0.19
(1,355)	1:99:A:ALA:HA	1:101:A:VAL:H	4	0.21	0.09	0.2
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG11	4	0.21	0.06	0.22
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG12	4	0.21	0.06	0.22
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG13	4	0.21	0.06	0.22
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG21	4	0.21	0.06	0.22
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG22	4	0.21	0.06	0.22
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG23	4	0.21	0.06	0.22
(1,6)	1:23:A:TRP:H	1:24:A:VAL:H	4	0.21	0.02	0.2
(1,1302)	1:36:A:LEU:H	1:99:A:ALA:HA	4	0.2	0.09	0.21
(1,254)	1:69:A:ALA:HA	1:72:A:TRP:H	4	0.2	0.11	0.16
(1,422)	1:113:A:TYR:H	1:114:A:GLU:H	4	0.2	0.09	0.17
(1,775)	1:197:A:ASN:H	1:198:A:GLY:H	4	0.2	0.11	0.14
(1,852)	1:213:A:LEU:H	1:214:A:ASP:H	4	0.2	0.05	0.19
(1,738)	1:176:A:SER:HA	1:180:A:ARG:H	4	0.18	0.05	0.2
(1,1262)	1:133:A:GLY:HA2	1:235:A:TYR:H	4	0.18	0.04	0.16
(1,1262)	1:133:A:GLY:HA3	1:235:A:TYR:H	4	0.18	0.04	0.16
(1,829)	1:206:A:ARG:HB2	1:208:A:GLN:H	4	0.17	0.07	0.15
(1,829)	1:206:A:ARG:HB3	1:208:A:GLN:H	4	0.17	0.07	0.15
(1,392)	1:95:A:ASN:HA	1:98:A:ILE:H	4	0.16	0.06	0.16
(1,885)	1:227:A:SER:H	1:228:A:GLU:H	4	0.16	0.06	0.16
(1,565)	1:148:A:ILE:H	1:149:A:SER:H	4	0.16	0.07	0.13
(1,1287)	1:260:A:THR:HA	1:265:A:LYS:H	4	0.16	0.07	0.12
(1,1079)	1:246:A:THR:HA	1:250:A:VAL:H	4	0.16	0.04	0.15
(1,629)	1:155:A:GLU:HA	1:158:A:LYS:H	4	0.15	0.02	0.15
(1,130)	1:46:A:ALA:HA	1:48:A:ILE:H	4	0.15	0.05	0.12
(1,1327)	1:68:A:VAL:H	1:253:A:LEU:HA	4	0.14	0.02	0.14
(1,172)	1:48:A:ILE:HA	1:51:A:PHE:H	4	0.14	0.04	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,86)	1:68:A:VAL:H	1:253:A:LEU:HB2	4	0.14	0.02	0.14
(2,86)	1:68:A:VAL:H	1:253:A:LEU:HB3	4	0.14	0.02	0.14
(1,35)	1:25:A:THR:HA	1:27:A:THR:H	4	0.13	0.02	0.13
(1,1082)	1:248:A:ARG:HA	1:252:A:GLU:H	4	0.12	0.01	0.12
(1,277)	1:83:A:ASP:HA	1:84:A:ARG:H	4	0.11	0.02	0.11
(1,1070)	1:247:A:LEU:HB2	1:250:A:VAL:H	4	0.11	0.01	0.11
(1,1178)	1:29:A:TYR:H	1:46:A:ALA:HB1	3	0.76	0.35	0.78
(1,1178)	1:29:A:TYR:H	1:46:A:ALA:HB2	3	0.76	0.35	0.78
(1,1178)	1:29:A:TYR:H	1:46:A:ALA:HB3	3	0.76	0.35	0.78
(1,1201)	1:54:A:ALA:HA	1:82:A:ALA:H	3	0.5	0.33	0.46
(1,1233)	1:101:A:VAL:H	1:219:A:ASP:HA	3	0.49	0.18	0.49
(1,766)	1:194:A:GLN:H	1:195:A:LEU:H	3	0.44	0.31	0.34
(1,556)	1:141:A:LYS:H	1:142:A:PHE:H	3	0.42	0.15	0.44
(1,1265)	1:134:A:PHE:H	1:234:A:ILE:HA	3	0.4	0.33	0.23
(1,162)	1:50:A:ASP:HA	1:54:A:ALA:H	3	0.4	0.2	0.3
(1,338)	1:84:A:ARG:H	1:86:A:THR:H	3	0.38	0.06	0.42
(1,404)	1:109:A:GLU:H	1:111:A:LYS:HB2	3	0.37	0.1	0.32
(1,1244)	1:106:A:ALA:HA	1:111:A:LYS:H	3	0.37	0.07	0.37
(1,744)	1:182:A:SER:HA	1:186:A:LYS:H	3	0.34	0.02	0.33
(1,763)	1:189:A:TYR:HA	1:192:A:PHE:H	3	0.33	0.03	0.32
(1,78)	1:34:A:VAL:H	1:36:A:LEU:H	3	0.32	0.15	0.32
(1,46)	1:26:A:ARG:HG2	1:29:A:TYR:H	3	0.31	0.13	0.24
(1,46)	1:26:A:ARG:HG3	1:29:A:TYR:H	3	0.31	0.13	0.24
(1,265)	1:69:A:ALA:HA	1:73:A:ASP:H	3	0.31	0.25	0.15
(1,1324)	1:51:A:PHE:H	1:81:A:MET:HA	3	0.31	0.04	0.3
(1,1271)	1:189:A:TYR:H	1:230:A:TRP:H	3	0.3	0.09	0.36
(1,1310)	1:134:A:PHE:H	1:234:A:ILE:HD11	3	0.29	0.09	0.28
(1,169)	1:45:A:LEU:HA	1:48:A:ILE:H	3	0.27	0.18	0.16
(1,535)	1:122:A:ASP:HA	1:126:A:VAL:H	3	0.27	0.13	0.18
(1,372)	1:88:A:VAL:HA	1:91:A:ASN:H	3	0.27	0.07	0.25
(1,740)	1:178:A:THR:HA	1:182:A:SER:H	3	0.26	0.15	0.17
(2,30)	1:79:A:GLY:H	1:83:A:ASP:HB2	3	0.26	0.07	0.27
(2,30)	1:79:A:GLY:H	1:83:A:ASP:HB3	3	0.26	0.07	0.27
(1,1147)	1:154:A:PRO:HA	1:158:A:LYS:H	3	0.25	0.1	0.3
(1,1231)	1:100:A:ILE:HD11	1:223:A:GLU:H	3	0.25	0.13	0.22
(1,1231)	1:100:A:ILE:HD12	1:223:A:GLU:H	3	0.25	0.13	0.22
(1,1231)	1:100:A:ILE:HD13	1:223:A:GLU:H	3	0.25	0.13	0.22
(1,1328)	1:78:A:ILE:H	1:84:A:ARG:H	3	0.24	0.1	0.17
(1,362)	1:103:A:LYS:H	1:105:A:ASN:H	3	0.24	0.09	0.29
(1,340)	1:86:A:THR:H	1:88:A:VAL:H	3	0.23	0.05	0.22
(1,709)	1:176:A:SER:H	1:178:A:THR:H	3	0.23	0.11	0.17
(1,510)	1:115:A:ILE:HA	1:118:A:GLU:H	3	0.22	0.08	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1177)	1:26:A:ARG:H	1:45:A:LEU:H	3	0.22	0.06	0.24
(1,906)	1:218:A:LEU:HA	1:221:A:PHE:H	3	0.22	0.06	0.24
(1,952)	1:229:A:ASN:H	1:231:A:ASN:H	3	0.22	0.05	0.2
(1,1091)	1:261:A:ARG:HA	1:262:A:ARG:H	3	0.21	0.01	0.22
(1,1089)	1:260:A:THR:HB	1:261:A:ARG:H	3	0.21	0.04	0.2
(1,280)	1:84:A:ARG:H	1:85:A:THR:H	3	0.2	0.09	0.14
(1,364)	1:104:A:ALA:H	1:106:A:ALA:H	3	0.2	0.13	0.12
(1,401)	1:103:A:LYS:HA	1:106:A:ALA:H	3	0.2	0.05	0.22
(1,1167)	1:24:A:VAL:H	1:192:A:PHE:HE1	3	0.2	0.05	0.2
(1,1167)	1:24:A:VAL:H	1:192:A:PHE:HE2	3	0.2	0.05	0.2
(1,1146)	1:135:A:GLY:HA2	1:138:A:ASP:H	3	0.19	0.1	0.14
(1,1146)	1:135:A:GLY:HA3	1:138:A:ASP:H	3	0.19	0.1	0.14
(1,759)	1:185:A:TYR:HA	1:188:A:SER:H	3	0.19	0.06	0.2
(1,386)	1:99:A:ALA:HA	1:103:A:LYS:H	3	0.19	0.05	0.18
(1,989)	1:239:A:LYS:HA	1:242:A:ALA:H	3	0.19	0.04	0.16
(1,85)	1:46:A:ALA:H	1:47:A:LEU:H	3	0.18	0.1	0.12
(1,659)	1:171:A:VAL:HB	1:173:A:ALA:H	3	0.18	0.04	0.2
(1,1318)	1:53:A:GLU:H	1:80:A:GLY:H	3	0.18	0.06	0.16
(1,234)	1:70:A:ALA:H	1:72:A:TRP:H	3	0.18	0.04	0.2
(1,748)	1:186:A:LYS:HA	1:190:A:LYS:H	3	0.18	0.01	0.18
(1,528)	1:116:A:LEU:HA	1:120:A:ASP:H	3	0.17	0.06	0.13
(1,1128)	1:51:A:PHE:H	1:52:A:ARG:HE	3	0.17	0.03	0.19
(1,1096)	1:263:A:SER:HA	1:264:A:ILE:H	3	0.16	0.03	0.17
(1,1208)	1:63:A:ASP:H	1:264:A:ILE:H	3	0.16	0.02	0.16
(1,289)	1:88:A:VAL:H	1:89:A:ASP:H	3	0.16	0.06	0.13
(1,170)	1:46:A:ALA:HA	1:49:A:ASP:H	3	0.15	0.04	0.15
(1,658)	1:163:A:TYR:H	1:165:A:ALA:H	3	0.15	0.05	0.13
(1,1193)	1:34:A:VAL:HG11	1:39:A:GLN:H	3	0.15	0.05	0.12
(1,1193)	1:34:A:VAL:HG12	1:39:A:GLN:H	3	0.15	0.05	0.12
(1,1193)	1:34:A:VAL:HG13	1:39:A:GLN:H	3	0.15	0.05	0.12
(1,1193)	1:34:A:VAL:HG21	1:39:A:GLN:H	3	0.15	0.05	0.12
(1,1193)	1:34:A:VAL:HG22	1:39:A:GLN:H	3	0.15	0.05	0.12
(1,1193)	1:34:A:VAL:HG23	1:39:A:GLN:H	3	0.15	0.05	0.12
(1,287)	1:87:A:LEU:H	1:88:A:VAL:H	3	0.15	0.03	0.14
(1,826)	1:205:A:VAL:HB	1:207:A:GLN:H	3	0.14	0.01	0.14
(1,1012)	1:238:A:LYS:HA	1:240:A:ASP:H	3	0.14	0.02	0.12
(1,27)	1:22:A:THR:H	1:24:A:VAL:H	3	0.13	0.03	0.12
(1,733)	1:188:A:SER:HA	1:190:A:LYS:H	3	0.13	0.03	0.11
(1,780)	1:190:A:LYS:HA	1:192:A:PHE:H	2	0.67	0.06	0.67
(1,855)	1:214:A:ASP:H	1:215:A:VAL:H	2	0.62	0.04	0.62
(1,1149)	1:173:A:ALA:HA	1:176:A:SER:H	2	0.58	0.4	0.58
(1,1198)	1:51:A:PHE:H	1:80:A:GLY:HA2	2	0.48	0.2	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1198)	1:51:A:PHE:H	1:80:A:GLY:HA3	2	0.48	0.2	0.48
(1,1127)	1:35:A:VAL:H	1:36:A:LEU:HA	2	0.45	0.11	0.45
(1,1332)	1:173:A:ALA:HA	1:202:A:THR:H	2	0.44	0.04	0.44
(1,251)	1:66:A:SER:HA	1:69:A:ALA:H	2	0.42	0.28	0.42
(2,84)	1:48:A:ILE:H	1:26:A:ARG:HD2	2	0.38	0.26	0.38
(2,84)	1:48:A:ILE:H	1:26:A:ARG:HD3	2	0.38	0.26	0.38
(1,179)	1:55:A:TYR:HA	1:58:A:LEU:H	2	0.38	0.16	0.38
(1,559)	1:144:A:TRP:H	1:145:A:ASN:H	2	0.36	0.01	0.36
(1,1297)	1:23:A:TRP:HZ3	1:191:A:ASP:H	2	0.36	0.2	0.36
(1,412)	1:109:A:GLU:H	1:110:A:GLU:H	2	0.34	0.05	0.34
(1,537)	1:124:A:VAL:HA	1:128:A:PHE:H	2	0.34	0.05	0.34
(1,1335)	1:54:A:ALA:H	1:81:A:MET:HA	2	0.32	0.18	0.32
(1,49)	1:23:A:TRP:HA	1:27:A:THR:H	2	0.32	0.17	0.32
(1,747)	1:185:A:TYR:HA	1:189:A:TYR:H	2	0.31	0.03	0.31
(1,167)	1:55:A:TYR:HA	1:59:A:ARG:H	2	0.3	0.13	0.3
(1,1202)	1:54:A:ALA:HA	1:142:A:PHE:H	2	0.29	0.0	0.29
(1,1308)	1:54:A:ALA:HA	1:142:A:PHE:H	2	0.29	0.0	0.29
(1,1307)	1:51:A:PHE:H	1:144:A:TRP:HD1	2	0.28	0.1	0.28
(1,1125)	1:270:A:GLY:HA2	1:272:A:ARG:H	2	0.24	0.03	0.24
(1,1125)	1:270:A:GLY:HA3	1:272:A:ARG:H	2	0.24	0.03	0.24
(1,25)	1:21:A:SER:H	1:23:A:TRP:H	2	0.24	0.05	0.24
(1,506)	1:129:A:GLY:H	1:131:A:LEU:H	2	0.24	0.12	0.24
(1,1320)	1:189:A:TYR:H	1:230:A:TRP:H	2	0.24	0.0	0.24
(1,390)	1:103:A:LYS:HA	1:107:A:SER:H	2	0.23	0.06	0.23
(1,203)	1:70:A:ALA:H	1:71:A:TRP:H	2	0.22	0.12	0.22
(2,24)	1:78:A:ILE:HD11	1:80:A:GLY:H	2	0.22	0.11	0.22
(2,24)	1:78:A:ILE:HD12	1:80:A:GLY:H	2	0.22	0.11	0.22
(2,24)	1:78:A:ILE:HD13	1:80:A:GLY:H	2	0.22	0.11	0.22
(1,739)	1:177:A:GLU:HA	1:181:A:ASN:H	2	0.22	0.06	0.22
(1,1120)	1:264:A:ILE:HG12	1:266:A:ARG:H	2	0.22	0.01	0.22
(1,1120)	1:264:A:ILE:HG13	1:266:A:ARG:H	2	0.22	0.01	0.22
(1,329)	1:104:A:ALA:H	1:105:A:ASN:H	2	0.21	0.1	0.21
(1,735)	1:189:A:TYR:H	1:191:A:ASP:H	2	0.21	0.03	0.21
(1,1210)	1:64:A:GLU:H	1:263:A:SER:H	2	0.2	0.06	0.2
(1,354)	1:99:A:ALA:H	1:101:A:VAL:H	2	0.2	0.06	0.2
(1,1222)	1:81:A:MET:H	1:144:A:TRP:HD1	2	0.2	0.03	0.2
(1,982)	1:232:A:VAL:HA	1:235:A:TYR:H	2	0.2	0.02	0.2
(1,158)	1:46:A:ALA:HA	1:50:A:ASP:H	2	0.19	0.05	0.19
(1,1293)	1:268:A:GLU:H	1:273:A:VAL:HA	2	0.18	0.04	0.18
(1,231)	1:68:A:VAL:H	1:70:A:ALA:H	2	0.18	0.08	0.18
(1,383)	1:96:A:THR:HA	1:100:A:ILE:H	2	0.18	0.03	0.18
(1,582)	1:148:A:ILE:HD11	1:150:A:GLU:H	2	0.18	0.04	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,582)	1:148:A:ILE:HD12	1:150:A:GLU:H	2	0.18	0.04	0.18
(1,582)	1:148:A:ILE:HD13	1:150:A:GLU:H	2	0.18	0.04	0.18
(1,540)	1:131:A:LEU:H	1:132:A:ILE:H	2	0.16	0.02	0.16
(1,716)	1:179:A:MET:HA	1:181:A:ASN:H	2	0.16	0.04	0.16
(1,731)	1:187:A:MET:HA	1:189:A:TYR:H	2	0.16	0.06	0.16
(1,1227)	1:82:A:ALA:H	1:144:A:TRP:H	2	0.16	0.04	0.16
(1,729)	1:186:A:LYS:HA	1:188:A:SER:H	2	0.16	0.04	0.16
(1,406)	1:113:A:TYR:H	1:115:A:ILE:HD11	2	0.16	0.03	0.16
(1,56)	1:34:A:VAL:H	1:35:A:VAL:H	2	0.16	0.02	0.16
(1,483)	1:119:A:HIS:HA	1:121:A:VAL:H	2	0.16	0.05	0.16
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD11	2	0.16	0.05	0.16
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD12	2	0.16	0.05	0.16
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD13	2	0.16	0.05	0.16
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD21	2	0.16	0.05	0.16
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD22	2	0.16	0.05	0.16
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD23	2	0.16	0.05	0.16
(1,1117)	1:261:A:ARG:HB2	1:263:A:SER:H	2	0.15	0.01	0.15
(1,1117)	1:261:A:ARG:HB3	1:263:A:SER:H	2	0.15	0.01	0.15
(1,253)	1:68:A:VAL:HA	1:71:A:TRP:H	2	0.15	0.04	0.15
(1,484)	1:119:A:HIS:H	1:121:A:VAL:H	2	0.15	0.04	0.15
(1,133)	1:48:A:ILE:H	1:50:A:ASP:H	2	0.15	0.0	0.15
(1,917)	1:222:A:ASP:HA	1:226:A:THR:H	2	0.15	0.02	0.15
(1,986)	1:236:A:GLN:HA	1:239:A:LYS:H	2	0.15	0.02	0.15
(1,900)	1:223:A:GLU:HA	1:225:A:PHE:H	2	0.14	0.03	0.14
(1,1330)	1:171:A:VAL:HA	1:199:A:GLY:H	2	0.14	0.03	0.14
(1,184)	1:63:A:ASP:H	1:64:A:GLU:H	2	0.14	0.01	0.14
(1,374)	1:90:A:ASN:HA	1:93:A:TRP:H	2	0.14	0.0	0.14
(1,569)	1:149:A:SER:HA	1:150:A:GLU:H	2	0.14	0.02	0.14
(1,1264)	1:134:A:PHE:H	1:234:A:ILE:HD12	2	0.14	0.03	0.14
(2,59)	1:235:A:TYR:HD1	1:237:A:LEU:H	2	0.14	0.03	0.14
(2,59)	1:235:A:TYR:HD2	1:237:A:LEU:H	2	0.14	0.03	0.14
(1,503)	1:127:A:ILE:HB	1:129:A:GLY:H	2	0.14	0.04	0.14
(1,1078)	1:252:A:GLU:HA	1:255:A:ARG:H	2	0.14	0.02	0.14
(1,580)	1:135:A:GLY:H	1:137:A:ASP:HB2	2	0.13	0.01	0.13
(1,1053)	1:247:A:LEU:HA	1:249:A:ASP:H	2	0.13	0.0	0.13
(1,1267)	1:166:A:GLU:H	1:172:A:ASP:HA	2	0.13	0.0	0.13
(1,177)	1:53:A:GLU:HA	1:56:A:TYR:H	2	0.12	0.02	0.12
(1,718)	1:180:A:ARG:HA	1:182:A:SER:H	2	0.12	0.02	0.12
(1,568)	1:149:A:SER:H	1:150:A:GLU:H	2	0.12	0.01	0.12
(1,1072)	1:248:A:ARG:HA	1:251:A:GLY:H	2	0.12	0.01	0.12
(1,1326)	1:64:A:GLU:H	1:262:A:ARG:HA	2	0.12	0.0	0.12
(1,816)	1:201:A:ALA:H	1:203:A:ASP:H	2	0.12	0.02	0.12

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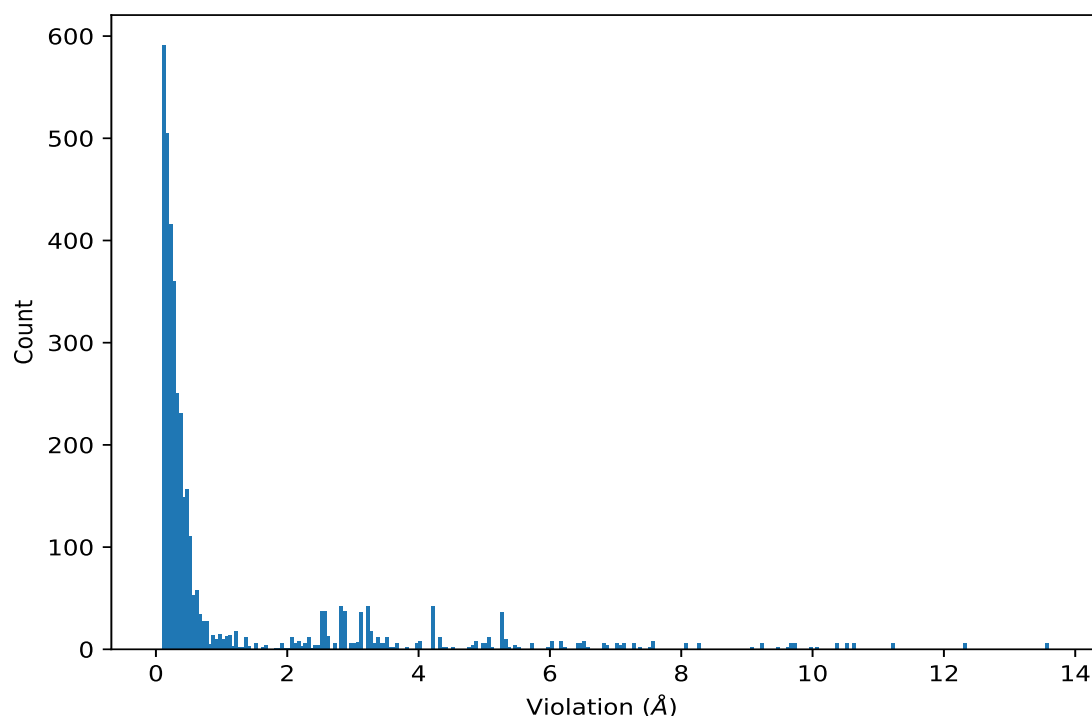
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,661)	1:176:A:SER:H	1:177:A:GLU:H	2	0.12	0.0	0.12
(1,962)	1:233:A:ARG:HA	1:235:A:TYR:H	2	0.11	0.0	0.11
(1,75)	1:44:A:LYS:HA	1:45:A:LEU:H	2	0.11	0.0	0.11
(1,482)	1:118:A:GLU:HA	1:120:A:ASP:H	2	0.11	0.0	0.11
(1,781)	1:190:A:LYS:H	1:192:A:PHE:H	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD11	6	13.58
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD12	6	13.58
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD13	6	13.58
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD21	6	13.58
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD22	6	13.58
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD23	6	13.58
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD11	8	12.32
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD12	8	12.32
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD13	8	12.32
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD21	8	12.32
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD22	8	12.32
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD23	8	12.32
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD11	4	11.24
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD12	4	11.24
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD13	4	11.24
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD21	4	11.24
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD22	4	11.24
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD23	4	11.24
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD11	5	10.64
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD12	5	10.64
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD13	5	10.64
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD21	5	10.64
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD22	5	10.64
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD23	5	10.64
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD11	9	10.54
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD12	9	10.54
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD13	9	10.54
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD21	9	10.54
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD22	9	10.54
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD23	9	10.54
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD11	10	10.39
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD12	10	10.39
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD13	10	10.39
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD21	10	10.39
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD22	10	10.39
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD23	10	10.39
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB2	1	10.08
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB3	1	10.08
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB2	8	9.95
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB3	8	9.95
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG11	8	9.71
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG12	8	9.71
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG13	8	9.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG21	8	9.71
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG22	8	9.71
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG23	8	9.71
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD11	7	9.69
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD12	7	9.69
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD13	7	9.69
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD21	7	9.69
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD22	7	9.69
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD23	7	9.69
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB2	10	9.63
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB3	10	9.63
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB2	6	9.45
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB3	6	9.45
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG11	8	9.2
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG12	8	9.2
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG13	8	9.2
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG21	8	9.2
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG22	8	9.2
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG23	8	9.2
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB2	1	9.05
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB3	1	9.05
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG11	7	8.25
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG12	7	8.25
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG13	7	8.25
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG21	7	8.25
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG22	7	8.25
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG23	7	8.25
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG11	10	8.05
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG12	10	8.05
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG13	10	8.05
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG21	10	8.05
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG22	10	8.05
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG23	10	8.05
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB2	3	7.58
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB3	3	7.58
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG11	6	7.55
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG12	6	7.55
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG13	6	7.55
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG21	6	7.55
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG22	6	7.55
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG23	6	7.55
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB2	6	7.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB3	6	7.5
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB2	8	7.36
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB3	8	7.36
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG11	4	7.29
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG12	4	7.29
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG13	4	7.29
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG21	4	7.29
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG22	4	7.29
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG23	4	7.29
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG11	5	7.11
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG12	5	7.11
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG13	5	7.11
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG21	5	7.11
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG22	5	7.11
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG23	5	7.11
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB2	1	7.05
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB3	1	7.05
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB2	2	7.05
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB3	2	7.05
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG11	7	7.02
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG12	7	7.02
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG13	7	7.02
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG21	7	7.02
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG22	7	7.02
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG23	7	7.02
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB2	2	6.87
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB3	2	6.87
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB2	10	6.87
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB3	10	6.87
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG11	8	6.84
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG12	8	6.84
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG13	8	6.84
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG21	8	6.84
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG22	8	6.84
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG23	8	6.84
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB2	10	6.55
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB3	10	6.55
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG11	2	6.51
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG12	2	6.51
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG13	2	6.51
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG21	2	6.51
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG22	2	6.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG23	2	6.51
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB2	7	6.5
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB3	7	6.5
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG11	4	6.47
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG12	4	6.47
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG13	4	6.47
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG21	4	6.47
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG22	4	6.47
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG23	4	6.47
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG11	4	6.43
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG12	4	6.43
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG13	4	6.43
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG21	4	6.43
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG22	4	6.43
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG23	4	6.43
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB2	8	6.2
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB3	8	6.2
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG11	7	6.19
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG12	7	6.19
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG13	7	6.19
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG21	7	6.19
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG22	7	6.19
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG23	7	6.19
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB2	4	6.16
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB3	4	6.16
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD11	2	6.03
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD12	2	6.03
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD13	2	6.03
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD21	2	6.03
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD22	2	6.03
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD23	2	6.03
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB2	5	6.0
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB3	5	6.0
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB2	7	5.97
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB3	7	5.97
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG11	9	5.74
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG12	9	5.74
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG13	9	5.74
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG21	9	5.74
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG22	9	5.74
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG23	9	5.74
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB2	7	5.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB3	7	5.5
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB2	2	5.47
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB3	2	5.47
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB2	3	5.47
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB3	3	5.47
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB2	6	5.38
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB3	6	5.38
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB2	3	5.34
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB3	3	5.34
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG11	5	5.34
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG12	5	5.34
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG13	5	5.34
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG21	5	5.34
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG22	5	5.34
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG23	5	5.34
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD2	3	5.32
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD3	3	5.32
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG11	1	5.29
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG12	1	5.29
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG13	1	5.29
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG21	1	5.29
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG22	1	5.29
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG23	1	5.29
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG11	1	5.29
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG12	1	5.29
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG13	1	5.29
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG21	1	5.29
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG22	1	5.29
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG23	1	5.29
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG11	1	5.29
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG12	1	5.29
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG13	1	5.29
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG21	1	5.29
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG22	1	5.29
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG23	1	5.29
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG11	1	5.29
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG12	1	5.29
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG13	1	5.29
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG21	1	5.29
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG22	1	5.29
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG23	1	5.29
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG11	1	5.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG12	1	5.29
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG13	1	5.29
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG21	1	5.29
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG22	1	5.29
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG23	1	5.29
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG11	1	5.29
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG12	1	5.29
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG13	1	5.29
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG21	1	5.29
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG22	1	5.29
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG23	1	5.29
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB2	1	5.14
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB3	1	5.14
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG11	9	5.06
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG12	9	5.06
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG13	9	5.06
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG21	9	5.06
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG22	9	5.06
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG23	9	5.06
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG11	5	5.06
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG12	5	5.06
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG13	5	5.06
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG21	5	5.06
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG22	5	5.06
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG23	5	5.06
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG11	1	5.01
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG12	1	5.01
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG13	1	5.01
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG21	1	5.01
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG22	1	5.01
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG23	1	5.01
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG11	4	4.99
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG12	4	4.99
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG13	4	4.99
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG21	4	4.99
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG22	4	4.99
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG23	4	4.99
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB2	9	4.89
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB3	9	4.89
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD11	1	4.88
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD12	1	4.88
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD13	1	4.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD21	1	4.88
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD22	1	4.88
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD23	1	4.88
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB2	10	4.84
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB3	10	4.84
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB2	5	4.81
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB3	5	4.81
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB2	9	4.75
(1,1254)	1:127:A:ILE:H	1:187:A:MET:HB3	9	4.75
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB2	6	4.53
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB3	6	4.53
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB2	5	4.42
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB3	5	4.42
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB2	8	4.39
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB3	8	4.39
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG11	6	4.34
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG12	6	4.34
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG13	6	4.34
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG21	6	4.34
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG22	6	4.34
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG23	6	4.34
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG11	10	4.32
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG12	10	4.32
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG13	10	4.32
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG21	10	4.32
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG22	10	4.32
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG23	10	4.32
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG11	6	4.21
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG12	6	4.21
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG13	6	4.21
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG21	6	4.21
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG22	6	4.21
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG23	6	4.21
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG11	6	4.21
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG12	6	4.21
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG13	6	4.21
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG21	6	4.21
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG22	6	4.21
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG23	6	4.21
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG11	6	4.21
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG12	6	4.21
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG13	6	4.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG21	6	4.21
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG22	6	4.21
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG23	6	4.21
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG11	6	4.21
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG12	6	4.21
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG13	6	4.21
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG21	6	4.21
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG22	6	4.21
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG23	6	4.21
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG11	6	4.21
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG12	6	4.21
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG13	6	4.21
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG21	6	4.21
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG22	6	4.21
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG23	6	4.21
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG11	6	4.21
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG12	6	4.21
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG13	6	4.21
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG21	6	4.21
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG22	6	4.21
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG23	6	4.21
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG11	9	4.2
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG12	9	4.2
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG13	9	4.2
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG21	9	4.2
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG22	9	4.2
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG23	9	4.2
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD2	10	4.03
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD3	10	4.03
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG11	9	4.02
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG12	9	4.02
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG13	9	4.02
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG21	9	4.02
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG22	9	4.02
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG23	9	4.02
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG11	10	3.97
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG12	10	3.97
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG13	10	3.97
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG21	10	3.97
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG22	10	3.97
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG23	10	3.97
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB2	4	3.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB3	4	3.84
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG11	3	3.69
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG12	3	3.69
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG13	3	3.69
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG21	3	3.69
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG22	3	3.69
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG23	3	3.69
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB2	4	3.63
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB3	4	3.63
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD2	4	3.56
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD3	4	3.56
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG11	10	3.52
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG12	10	3.52
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG13	10	3.52
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG21	10	3.52
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG22	10	3.52
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG23	10	3.52
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG11	7	3.51
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG12	7	3.51
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG13	7	3.51
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG21	7	3.51
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG22	7	3.51
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG23	7	3.51
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG11	9	3.49
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG12	9	3.49
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG13	9	3.49
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG21	9	3.49
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG22	9	3.49
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG23	9	3.49
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG11	1	3.4
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG12	1	3.4
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG13	1	3.4
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG21	1	3.4
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG22	1	3.4
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG23	1	3.4
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG11	5	3.39
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG12	5	3.39
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG13	5	3.39
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG21	5	3.39
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG22	5	3.39
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG23	5	3.39
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG11	2	3.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG12	2	3.38
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG13	2	3.38
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG21	2	3.38
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG22	2	3.38
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG23	2	3.38
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG11	6	3.33
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG12	6	3.33
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG13	6	3.33
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG21	6	3.33
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG22	6	3.33
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG23	6	3.33
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG11	6	3.29
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG12	6	3.29
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG13	6	3.29
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG21	6	3.29
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG22	6	3.29
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG23	6	3.29
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG11	1	3.27
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG12	1	3.27
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG13	1	3.27
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG21	1	3.27
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG22	1	3.27
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG23	1	3.27
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG11	5	3.27
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG12	5	3.27
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG13	5	3.27
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG21	5	3.27
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG22	5	3.27
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG23	5	3.27
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG11	3	3.23
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG12	3	3.23
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG13	3	3.23
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG21	3	3.23
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG22	3	3.23
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG23	3	3.23
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG11	5	3.2
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG12	5	3.2
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG13	5	3.2
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG21	5	3.2
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG22	5	3.2
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG23	5	3.2
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG11	5	3.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG12	5	3.2
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG13	5	3.2
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG21	5	3.2
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG22	5	3.2
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG23	5	3.2
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG11	5	3.2
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG12	5	3.2
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG13	5	3.2
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG21	5	3.2
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG22	5	3.2
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG23	5	3.2
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG11	5	3.2
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG12	5	3.2
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG13	5	3.2
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG21	5	3.2
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG22	5	3.2
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG23	5	3.2
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG11	5	3.2
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG12	5	3.2
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG13	5	3.2
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG21	5	3.2
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG22	5	3.2
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG23	5	3.2
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG11	5	3.2
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG12	5	3.2
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG13	5	3.2
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG21	5	3.2
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG22	5	3.2
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG23	5	3.2
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG11	3	3.13
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG12	3	3.13
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG13	3	3.13
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG21	3	3.13
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG22	3	3.13
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG23	3	3.13
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG11	3	3.13
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG12	3	3.13
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG13	3	3.13
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG21	3	3.13
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG22	3	3.13
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG23	3	3.13
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG11	3	3.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG12	3	3.13
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG13	3	3.13
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG21	3	3.13
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG22	3	3.13
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG23	3	3.13
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG11	3	3.13
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG12	3	3.13
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG13	3	3.13
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG21	3	3.13
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG22	3	3.13
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG23	3	3.13
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG11	3	3.13
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG12	3	3.13
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG13	3	3.13
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG21	3	3.13
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG22	3	3.13
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG23	3	3.13
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG11	3	3.13
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG12	3	3.13
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG13	3	3.13
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG21	3	3.13
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG22	3	3.13
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG23	3	3.13
(1,1284)	1:250:A:VAL:H	1:71:A:TRP:HA	6	3.08
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG11	6	3.08
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG12	6	3.08
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG13	6	3.08
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG21	6	3.08
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG22	6	3.08
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG23	6	3.08
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG11	2	3.03
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG12	2	3.03
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG13	2	3.03
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG21	2	3.03
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG22	2	3.03
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG23	2	3.03
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG11	1	2.96
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG12	1	2.96
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG13	1	2.96
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG21	1	2.96
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG22	1	2.96
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG23	1	2.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1284)	1:250:A:VAL:H	1:71:A:TRP:HA	3	2.88
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG11	7	2.85
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG12	7	2.85
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG13	7	2.85
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG21	7	2.85
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG22	7	2.85
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG23	7	2.85
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG11	7	2.85
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG12	7	2.85
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG13	7	2.85
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG21	7	2.85
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG22	7	2.85
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG23	7	2.85
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG11	7	2.85
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG12	7	2.85
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG13	7	2.85
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG21	7	2.85
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG22	7	2.85
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG23	7	2.85
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG11	7	2.85
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG12	7	2.85
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG13	7	2.85
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG21	7	2.85
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG22	7	2.85
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG23	7	2.85
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG11	7	2.85
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG12	7	2.85
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG13	7	2.85
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG21	7	2.85
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG22	7	2.85
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG23	7	2.85
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG11	7	2.85
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG12	7	2.85
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG13	7	2.85
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG21	7	2.85
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG22	7	2.85
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG23	7	2.85
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG11	9	2.83
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG12	9	2.83
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG13	9	2.83
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG21	9	2.83
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG22	9	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG23	9	2.83
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG11	9	2.83
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG12	9	2.83
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG13	9	2.83
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG21	9	2.83
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG22	9	2.83
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG23	9	2.83
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG11	9	2.83
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG12	9	2.83
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG13	9	2.83
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG21	9	2.83
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG22	9	2.83
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG23	9	2.83
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG11	9	2.83
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG12	9	2.83
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG13	9	2.83
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG21	9	2.83
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG22	9	2.83
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG23	9	2.83
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG11	9	2.83
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG12	9	2.83
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG13	9	2.83
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG21	9	2.83
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG22	9	2.83
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG23	9	2.83
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG11	9	2.83
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG12	9	2.83
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG13	9	2.83
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG21	9	2.83
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG22	9	2.83
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG23	9	2.83
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG11	8	2.83
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG12	8	2.83
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG13	8	2.83
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG21	8	2.83
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG22	8	2.83
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG23	8	2.83
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG11	2	2.73
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG12	2	2.73
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG13	2	2.73
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG21	2	2.73
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG22	2	2.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1237)	1:101:A:VAL:HG11	1:215:A:VAL:HG23	2	2.73
(1,1284)	1:250:A:VAL:H	1:71:A:TRP:HA	8	2.64
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG11	5	2.64
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG12	5	2.64
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG13	5	2.64
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG21	5	2.64
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG22	5	2.64
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG23	5	2.64
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG11	10	2.61
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG12	10	2.61
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG13	10	2.61
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG21	10	2.61
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG22	10	2.61
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG23	10	2.61
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG11	4	2.58
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG12	4	2.58
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG13	4	2.58
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG21	4	2.58
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG22	4	2.58
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG23	4	2.58
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG11	4	2.58
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG12	4	2.58
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG13	4	2.58
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG21	4	2.58
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG22	4	2.58
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG23	4	2.58
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG11	4	2.58
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG12	4	2.58
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG13	4	2.58
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG21	4	2.58
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG22	4	2.58
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG23	4	2.58
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG11	4	2.58
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG12	4	2.58
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG13	4	2.58
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG21	4	2.58
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG22	4	2.58
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG23	4	2.58
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG11	4	2.58
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG12	4	2.58
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG13	4	2.58
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG21	4	2.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG22	4	2.58
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG23	4	2.58
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG11	4	2.58
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG12	4	2.58
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG13	4	2.58
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG21	4	2.58
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG22	4	2.58
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG23	4	2.58
(1,1284)	1:250:A:VAL:H	1:71:A:TRP:HA	2	2.57
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG11	2	2.53
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG12	2	2.53
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG13	2	2.53
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG21	2	2.53
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG22	2	2.53
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG23	2	2.53
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG11	2	2.53
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG12	2	2.53
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG13	2	2.53
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG21	2	2.53
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG22	2	2.53
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG23	2	2.53
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG11	2	2.53
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG12	2	2.53
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG13	2	2.53
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG21	2	2.53
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG22	2	2.53
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG23	2	2.53
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG11	2	2.53
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG12	2	2.53
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG13	2	2.53
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG21	2	2.53
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG22	2	2.53
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG23	2	2.53
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG11	2	2.53
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG12	2	2.53
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG13	2	2.53
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG21	2	2.53
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG22	2	2.53
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG23	2	2.53
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG11	2	2.53
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG12	2	2.53
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG13	2	2.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG21	2	2.53
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG22	2	2.53
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG23	2	2.53
(1,1284)	1:250:A:VAL:H	1:71:A:TRP:HA	10	2.51
(1,1284)	1:250:A:VAL:H	1:71:A:TRP:HA	9	2.49
(1,1284)	1:250:A:VAL:H	1:71:A:TRP:HA	5	2.47
(1,1235)	1:101:A:VAL:HA	1:223:A:GLU:HA	7	2.47
(1,1235)	1:101:A:VAL:HA	1:223:A:GLU:HA	10	2.47
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD2	7	2.42
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD3	7	2.42
(1,1235)	1:101:A:VAL:HA	1:223:A:GLU:HA	5	2.41
(2,89)	1:123:A:TYR:HA	1:226:A:THR:H	4	2.4
(1,1284)	1:250:A:VAL:H	1:71:A:TRP:HA	1	2.38
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG11	3	2.33
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG12	3	2.33
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG13	3	2.33
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG21	3	2.33
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG22	3	2.33
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG23	3	2.33
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG11	7	2.33
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG12	7	2.33
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG13	7	2.33
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG21	7	2.33
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG22	7	2.33
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG23	7	2.33
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG11	1	2.27
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG12	1	2.27
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG13	1	2.27
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG21	1	2.27
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG22	1	2.27
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG23	1	2.27
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD2	1	2.23
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD3	1	2.23
(1,1284)	1:250:A:VAL:H	1:71:A:TRP:HA	4	2.22
(1,1235)	1:101:A:VAL:HA	1:223:A:GLU:HA	6	2.16
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG11	8	2.15
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG12	8	2.15
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG13	8	2.15
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG21	8	2.15
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG22	8	2.15
(1,1276)	1:205:A:VAL:HG11	1:224:A:VAL:HG23	8	2.15
(1,1235)	1:101:A:VAL:HA	1:223:A:GLU:HA	9	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG11	4	2.1
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG12	4	2.1
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG13	4	2.1
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG21	4	2.1
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG22	4	2.1
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG23	4	2.1
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG11	8	2.07
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG12	8	2.07
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG13	8	2.07
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG21	8	2.07
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG22	8	2.07
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG23	8	2.07
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG11	2	2.05
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG12	2	2.05
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG13	2	2.05
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG21	2	2.05
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG22	2	2.05
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG23	2	2.05
(1,1284)	1:250:A:VAL:H	1:71:A:TRP:HA	7	2.0
(1,1235)	1:101:A:VAL:HA	1:223:A:GLU:HA	2	1.99
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG11	3	1.92
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG12	3	1.92
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG13	3	1.92
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG21	3	1.92
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG22	3	1.92
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG23	3	1.92
(1,1235)	1:101:A:VAL:HA	1:223:A:GLU:HA	3	1.85
(2,89)	1:123:A:TYR:HA	1:226:A:THR:H	3	1.82
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD2	9	1.69
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD3	9	1.69
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD2	6	1.68
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD3	6	1.68
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB2	7	1.61
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB3	7	1.61
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG11	10	1.5
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG12	10	1.5
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG13	10	1.5
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG21	10	1.5
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG22	10	1.5
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG23	10	1.5
(2,89)	1:123:A:TYR:HA	1:226:A:THR:H	9	1.42
(1,1235)	1:101:A:VAL:HA	1:223:A:GLU:HA	1	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,655)	1:175:A:ALA:H	1:176:A:SER:H	8	1.42
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG11	6	1.36
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG12	6	1.36
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG13	6	1.36
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG21	6	1.36
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG22	6	1.36
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG23	6	1.36
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG11	2	1.35
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG12	2	1.35
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG13	2	1.35
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG21	2	1.35
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG22	2	1.35
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG23	2	1.35
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB2	9	1.3
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB3	9	1.3
(1,1205)	1:56:A:TYR:H	1:76:A:TYR:HA	9	1.28
(1,1166)	1:23:A:TRP:H	1:45:A:LEU:HA	1	1.28
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB2	4	1.24
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB3	4	1.24
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG11	1	1.24
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG12	1	1.24
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG13	1	1.24
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG21	1	1.24
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG22	1	1.24
(1,1252)	1:125:A:LEU:HD11	1:224:A:VAL:HG23	1	1.24
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB2	3	1.22
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB3	3	1.22
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB2	5	1.21
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB3	5	1.21
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB2	5	1.21
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB3	5	1.21
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB2	4	1.2
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB3	4	1.2
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB2	6	1.2
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB3	6	1.2
(1,1178)	1:29:A:TYR:H	1:46:A:ALA:HB1	6	1.17
(1,1178)	1:29:A:TYR:H	1:46:A:ALA:HB2	6	1.17
(1,1178)	1:29:A:TYR:H	1:46:A:ALA:HB3	6	1.17
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB2	7	1.14
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB3	7	1.14
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG11	7	1.12
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG12	7	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG13	7	1.12
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG21	7	1.12
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG22	7	1.12
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG23	7	1.12
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG11	9	1.1
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG12	9	1.1
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG13	9	1.1
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG21	9	1.1
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG22	9	1.1
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG23	9	1.1
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB2	2	1.09
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB3	2	1.09
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG11	1	1.09
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG12	1	1.09
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG13	1	1.09
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG21	1	1.09
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG22	1	1.09
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG23	1	1.09
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB2	9	1.09
(1,1251)	1:124:A:VAL:H	1:191:A:ASP:HB3	9	1.09
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB2	10	1.08
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB3	10	1.08
(1,83)	1:45:A:LEU:H	1:46:A:ALA:H	6	1.07
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD2	5	1.03
(1,1196)	1:48:A:ILE:HD11	1:26:A:ARG:HD3	5	1.03
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB2	2	1.01
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB3	2	1.01
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG11	3	1.0
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG12	3	1.0
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG13	3	1.0
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG21	3	1.0
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG22	3	1.0
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG23	3	1.0
(1,1149)	1:173:A:ALA:HA	1:176:A:SER:H	8	0.98
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB2	1	0.97
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB3	1	0.97
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG11	3	0.97
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG12	3	0.97
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG13	3	0.97
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG21	3	0.97
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG22	3	0.97
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG23	3	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG11	3	0.95
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG12	3	0.95
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG13	3	0.95
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG21	3	0.95
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG22	3	0.95
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG23	3	0.95
(1,1201)	1:54:A:ALA:HA	1:82:A:ALA:H	10	0.93
(1,1206)	1:56:A:TYR:HA	1:69:A:ALA:H	7	0.92
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG11	4	0.9
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG12	4	0.9
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG13	4	0.9
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG21	4	0.9
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG22	4	0.9
(1,1250)	1:124:A:VAL:HG11	1:224:A:VAL:HG23	4	0.9
(1,1166)	1:23:A:TRP:H	1:45:A:LEU:HA	6	0.9
(1,762)	1:188:A:SER:HA	1:191:A:ASP:H	5	0.9
(1,1315)	1:182:A:SER:H	1:205:A:VAL:HG11	9	0.87
(1,1315)	1:182:A:SER:H	1:205:A:VAL:HG12	9	0.87
(1,1315)	1:182:A:SER:H	1:205:A:VAL:HG13	9	0.87
(1,1315)	1:182:A:SER:H	1:205:A:VAL:HG21	9	0.87
(1,1315)	1:182:A:SER:H	1:205:A:VAL:HG22	9	0.87
(1,1315)	1:182:A:SER:H	1:205:A:VAL:HG23	9	0.87
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB2	3	0.87
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB3	3	0.87
(1,1265)	1:134:A:PHE:H	1:234:A:ILE:HA	3	0.87
(1,1235)	1:101:A:VAL:HA	1:223:A:GLU:HA	4	0.87
(1,749)	1:187:A:MET:HA	1:191:A:ASP:H	5	0.87
(2,98)	1:178:A:THR:H	1:202:A:THR:H	9	0.86
(1,766)	1:194:A:GLN:H	1:195:A:LEU:H	1	0.86
(1,762)	1:188:A:SER:HA	1:191:A:ASP:H	4	0.85
(1,266)	1:70:A:ALA:HA	1:74:A:TYR:H	10	0.84
(1,1203)	1:56:A:TYR:H	1:72:A:TRP:H	10	0.82
(1,1166)	1:23:A:TRP:H	1:45:A:LEU:HA	8	0.82
(1,1165)	1:22:A:THR:HB	1:45:A:LEU:H	6	0.81
(1,368)	1:84:A:ARG:HA	1:87:A:LEU:H	8	0.81
(1,388)	1:101:A:VAL:HA	1:105:A:ASN:H	5	0.79
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB2	8	0.78
(1,1285)	1:250:A:VAL:H	1:71:A:TRP:HB3	8	0.78
(1,1178)	1:29:A:TYR:H	1:46:A:ALA:HB1	1	0.78
(1,1178)	1:29:A:TYR:H	1:46:A:ALA:HB2	1	0.78
(1,1178)	1:29:A:TYR:H	1:46:A:ALA:HB3	1	0.78
(1,1151)	1:175:A:ALA:HA	1:179:A:MET:H	8	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,991)	1:228:A:GLU:HA	1:232:A:VAL:H	9	0.78
(1,754)	1:180:A:ARG:HA	1:183:A:LEU:H	9	0.78
(1,749)	1:187:A:MET:HA	1:191:A:ASP:H	8	0.78
(1,749)	1:187:A:MET:HA	1:191:A:ASP:H	9	0.78
(1,264)	1:68:A:VAL:HA	1:72:A:TRP:H	10	0.78
(1,166)	1:54:A:ALA:HA	1:58:A:LEU:H	7	0.78
(1,389)	1:102:A:GLY:HA2	1:106:A:ALA:H	5	0.77
(1,389)	1:102:A:GLY:HA3	1:106:A:ALA:H	5	0.77
(1,174)	1:50:A:ASP:HA	1:53:A:GLU:H	8	0.77
(2,28)	1:78:A:ILE:HG12	1:81:A:MET:H	10	0.76
(2,28)	1:78:A:ILE:HG13	1:81:A:MET:H	10	0.76
(1,1228)	1:93:A:TRP:H	1:64:A:GLU:HA	1	0.76
(1,1190)	1:34:A:VAL:HA	1:40:A:THR:H	2	0.76
(1,980)	1:230:A:TRP:HA	1:233:A:ARG:H	3	0.76
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG11	8	0.75
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG12	8	0.75
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG13	8	0.75
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG21	8	0.75
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG22	8	0.75
(1,1236)	1:101:A:VAL:HG11	1:124:A:VAL:HG23	8	0.75
(1,368)	1:84:A:ARG:HA	1:87:A:LEU:H	1	0.75
(1,991)	1:228:A:GLU:HA	1:232:A:VAL:H	4	0.74
(1,1226)	1:82:A:ALA:HA	1:144:A:TRP:H	9	0.73
(1,1205)	1:56:A:TYR:H	1:76:A:TYR:HA	10	0.73
(1,1165)	1:22:A:THR:HB	1:45:A:LEU:H	2	0.73
(1,1024)	1:244:A:GLY:H	1:246:A:THR:H	8	0.73
(1,981)	1:231:A:ASN:HA	1:234:A:ILE:H	3	0.73
(1,780)	1:190:A:LYS:HA	1:192:A:PHE:H	2	0.73
(1,757)	1:183:A:LEU:HA	1:186:A:LYS:H	8	0.73
(1,742)	1:180:A:ARG:HA	1:184:A:LEU:H	8	0.73
(2,28)	1:78:A:ILE:HG12	1:81:A:MET:H	3	0.72
(2,28)	1:78:A:ILE:HG13	1:81:A:MET:H	3	0.72
(1,1194)	1:35:A:VAL:H	1:40:A:THR:HA	7	0.72
(1,1194)	1:35:A:VAL:H	1:40:A:THR:HA	10	0.72
(1,1163)	1:22:A:THR:H	1:47:A:LEU:H	9	0.72
(1,156)	1:59:A:ARG:H	1:61:A:ASN:H	1	0.72
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG11	2	0.71
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG12	2	0.71
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG13	2	0.71
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG21	2	0.71
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG22	2	0.71
(1,1272)	1:190:A:LYS:H	1:224:A:VAL:HG23	2	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:101:A:VAL:H	1:219:A:ASP:HA	5	0.71
(1,751)	1:177:A:GLU:HA	1:180:A:ARG:H	8	0.71
(1,44)	1:24:A:VAL:HA	1:27:A:THR:H	8	0.71
(1,1185)	1:27:A:THR:HA	1:46:A:ALA:H	8	0.7
(1,369)	1:85:A:THR:HA	1:88:A:VAL:H	8	0.7
(1,251)	1:66:A:SER:HA	1:69:A:ALA:H	9	0.7
(1,45)	1:25:A:THR:HA	1:28:A:ALA:H	1	0.7
(1,1180)	1:29:A:TYR:HA	1:46:A:ALA:H	10	0.69
(1,1163)	1:22:A:THR:H	1:47:A:LEU:H	6	0.69
(1,762)	1:188:A:SER:HA	1:191:A:ASP:H	8	0.69
(1,181)	1:57:A:TRP:HA	1:60:A:MET:H	10	0.69
(1,1199)	1:52:A:ARG:H	1:76:A:TYR:H	10	0.68
(1,1198)	1:51:A:PHE:H	1:80:A:GLY:HA2	10	0.68
(1,1198)	1:51:A:PHE:H	1:80:A:GLY:HA3	10	0.68
(1,1197)	1:51:A:PHE:H	1:79:A:GLY:HA2	7	0.68
(1,1197)	1:51:A:PHE:H	1:79:A:GLY:HA3	7	0.68
(1,1187)	1:33:A:SER:H	1:39:A:GLN:HA	2	0.68
(1,267)	1:72:A:TRP:HA	1:76:A:TYR:H	9	0.68
(1,44)	1:24:A:VAL:HA	1:27:A:THR:H	6	0.68
(1,1249)	1:123:A:TYR:H	1:224:A:VAL:HA	4	0.67
(1,162)	1:50:A:ASP:HA	1:54:A:ALA:H	7	0.67
(1,1246)	1:106:A:ALA:H	1:113:A:TYR:H	5	0.66
(1,1219)	1:78:A:ILE:HA	1:83:A:ASP:H	7	0.66
(1,1205)	1:56:A:TYR:H	1:76:A:TYR:HA	6	0.66
(1,1199)	1:52:A:ARG:H	1:76:A:TYR:H	6	0.66
(1,1180)	1:29:A:TYR:HA	1:46:A:ALA:H	1	0.66
(1,855)	1:214:A:ASP:H	1:215:A:VAL:H	9	0.66
(1,840)	1:207:A:GLN:HA	1:210:A:ILE:H	6	0.66
(1,746)	1:184:A:LEU:HA	1:188:A:SER:H	4	0.66
(1,369)	1:85:A:THR:HA	1:88:A:VAL:H	7	0.66
(1,265)	1:69:A:ALA:HA	1:73:A:ASP:H	10	0.66
(1,50)	1:24:A:VAL:HA	1:28:A:ALA:H	1	0.66
(1,1207)	1:62:A:SER:HA	1:67:A:LYS:H	9	0.65
(1,1200)	1:54:A:ALA:H	1:82:A:ALA:H	10	0.65
(1,914)	1:219:A:ASP:HA	1:223:A:GLU:H	5	0.65
(1,908)	1:220:A:TYR:HA	1:223:A:GLU:H	8	0.65
(1,758)	1:184:A:LEU:HA	1:187:A:MET:H	9	0.65
(1,757)	1:183:A:LEU:HA	1:186:A:LYS:H	9	0.65
(1,369)	1:85:A:THR:HA	1:88:A:VAL:H	1	0.65
(1,161)	1:49:A:ASP:HA	1:53:A:GLU:H	7	0.65
(1,156)	1:59:A:ARG:H	1:61:A:ASN:H	4	0.65
(2,84)	1:48:A:ILE:H	1:26:A:ARG:HD2	10	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,84)	1:48:A:ILE:H	1:26:A:ARG:HD3	10	0.64
(1,1246)	1:106:A:ALA:H	1:113:A:TYR:H	2	0.64
(1,1166)	1:23:A:TRP:H	1:45:A:LEU:HA	2	0.64
(1,997)	1:234:A:ILE:HA	1:238:A:LYS:H	1	0.64
(1,524)	1:128:A:PHE:HA	1:131:A:LEU:H	3	0.64
(1,388)	1:101:A:VAL:HA	1:105:A:ASN:H	4	0.64
(1,368)	1:84:A:ARG:HA	1:87:A:LEU:H	7	0.64
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB2	4	0.63
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB3	4	0.63
(1,1275)	1:197:A:ASN:HA	1:202:A:THR:H	1	0.63
(1,1226)	1:82:A:ALA:HA	1:144:A:TRP:H	4	0.63
(1,1203)	1:56:A:TYR:H	1:72:A:TRP:H	9	0.63
(1,918)	1:223:A:GLU:HA	1:227:A:SER:H	5	0.63
(1,753)	1:179:A:MET:HA	1:182:A:SER:H	1	0.63
(1,746)	1:184:A:LEU:HA	1:188:A:SER:H	9	0.63
(1,161)	1:49:A:ASP:HA	1:53:A:GLU:H	8	0.63
(1,45)	1:25:A:THR:HA	1:28:A:ALA:H	4	0.63
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG11	10	0.62
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG12	10	0.62
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG13	10	0.62
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG21	10	0.62
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG22	10	0.62
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG23	10	0.62
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG11	10	0.62
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG12	10	0.62
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG13	10	0.62
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG21	10	0.62
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG22	10	0.62
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG23	10	0.62
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG11	10	0.62
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG12	10	0.62
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG13	10	0.62
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG21	10	0.62
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG22	10	0.62
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG23	10	0.62
(1,758)	1:184:A:LEU:HA	1:187:A:MET:H	4	0.62
(1,756)	1:182:A:SER:HA	1:185:A:TYR:H	9	0.62
(1,752)	1:178:A:THR:HA	1:181:A:ASN:H	9	0.62
(1,751)	1:177:A:GLU:HA	1:180:A:ARG:H	2	0.62
(1,266)	1:70:A:ALA:HA	1:74:A:TYR:H	6	0.62
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB2	1	0.61
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB3	1	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,95)	1:210:A:ILE:HA	1:235:A:TYR:H	7	0.61
(1,1163)	1:22:A:THR:H	1:47:A:LEU:H	10	0.61
(1,1001)	1:238:A:LYS:HA	1:242:A:ALA:H	8	0.61
(1,780)	1:190:A:LYS:HA	1:192:A:PHE:H	1	0.61
(2,99)	1:76:A:TYR:HA	1:87:A:LEU:H	9	0.6
(1,1240)	1:104:A:ALA:HA	1:220:A:TYR:H	5	0.6
(1,1194)	1:35:A:VAL:H	1:40:A:THR:HA	9	0.6
(1,1151)	1:175:A:ALA:HA	1:179:A:MET:H	10	0.6
(1,915)	1:220:A:TYR:HA	1:224:A:VAL:H	2	0.6
(1,746)	1:184:A:LEU:HA	1:188:A:SER:H	7	0.6
(1,269)	1:79:A:GLY:H	1:80:A:GLY:H	3	0.6
(1,258)	1:71:A:TRP:HA	1:74:A:TYR:H	4	0.6
(1,258)	1:71:A:TRP:HA	1:74:A:TYR:H	9	0.6
(1,181)	1:57:A:TRP:HA	1:60:A:MET:H	6	0.6
(1,45)	1:25:A:THR:HA	1:28:A:ALA:H	3	0.6
(1,1281)	1:213:A:LEU:H	1:218:A:LEU:HG	4	0.59
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD11	3	0.59
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD12	3	0.59
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD13	3	0.59
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD21	3	0.59
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD22	3	0.59
(1,1266)	1:163:A:TYR:H	1:183:A:LEU:HD23	3	0.59
(1,1200)	1:54:A:ALA:H	1:82:A:ALA:H	3	0.59
(1,556)	1:141:A:LYS:H	1:142:A:PHE:H	9	0.59
(1,140)	1:51:A:PHE:HA	1:53:A:GLU:H	6	0.59
(2,95)	1:210:A:ILE:HA	1:235:A:TYR:H	6	0.58
(1,1329)	1:104:A:ALA:HA	1:221:A:PHE:H	5	0.58
(1,1329)	1:104:A:ALA:HA	1:221:A:PHE:H	7	0.58
(1,1288)	1:265:A:LYS:H	1:270:A:GLY:H	7	0.58
(1,1207)	1:62:A:SER:HA	1:67:A:LYS:H	10	0.58
(1,1165)	1:22:A:THR:HB	1:45:A:LEU:H	7	0.58
(1,855)	1:214:A:ASP:H	1:215:A:VAL:H	4	0.58
(1,753)	1:179:A:MET:HA	1:182:A:SER:H	2	0.58
(1,266)	1:70:A:ALA:HA	1:74:A:TYR:H	9	0.58
(1,180)	1:56:A:TYR:HA	1:59:A:ARG:H	8	0.58
(1,164)	1:52:A:ARG:HA	1:56:A:TYR:H	7	0.58
(1,163)	1:51:A:PHE:HA	1:55:A:TYR:H	7	0.58
(1,74)	1:44:A:LYS:H	1:45:A:LEU:H	5	0.58
(1,1274)	1:197:A:ASN:HA	1:202:A:THR:HA	10	0.57
(1,1226)	1:82:A:ALA:HA	1:144:A:TRP:H	2	0.57
(1,1194)	1:35:A:VAL:H	1:40:A:THR:HA	6	0.57
(1,1163)	1:22:A:THR:H	1:47:A:LEU:H	3	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	1:187:A:MET:HA	1:191:A:ASP:H	7	0.57
(1,533)	1:120:A:ASP:HA	1:124:A:VAL:H	6	0.57
(1,388)	1:101:A:VAL:HA	1:105:A:ASN:H	9	0.57
(1,161)	1:49:A:ASP:HA	1:53:A:GLU:H	6	0.57
(1,50)	1:24:A:VAL:HA	1:28:A:ALA:H	2	0.57
(1,1297)	1:23:A:TRP:HZ3	1:191:A:ASP:H	6	0.56
(1,1249)	1:123:A:TYR:H	1:224:A:VAL:HA	5	0.56
(1,1127)	1:35:A:VAL:H	1:36:A:LEU:HA	1	0.56
(1,981)	1:231:A:ASN:HA	1:234:A:ILE:H	5	0.56
(1,840)	1:207:A:GLN:HA	1:210:A:ILE:H	4	0.56
(1,757)	1:183:A:LEU:HA	1:186:A:LYS:H	10	0.56
(1,745)	1:183:A:LEU:HA	1:187:A:MET:H	8	0.56
(1,181)	1:57:A:TRP:HA	1:60:A:MET:H	4	0.56
(1,42)	1:23:A:TRP:HA	1:26:A:ARG:H	3	0.56
(1,1249)	1:123:A:TYR:H	1:224:A:VAL:HA	1	0.55
(1,1199)	1:52:A:ARG:H	1:76:A:TYR:H	9	0.55
(1,1160)	1:261:A:ARG:H	1:264:A:ILE:HA	7	0.55
(1,1151)	1:175:A:ALA:HA	1:179:A:MET:H	1	0.55
(1,1150)	1:174:A:ARG:H	1:177:A:GLU:HB2	8	0.55
(1,1001)	1:238:A:LYS:HA	1:242:A:ALA:H	2	0.55
(1,980)	1:230:A:TRP:HA	1:233:A:ARG:H	8	0.55
(1,758)	1:184:A:LEU:HA	1:187:A:MET:H	10	0.55
(1,757)	1:183:A:LEU:HA	1:186:A:LYS:H	4	0.55
(1,279)	1:81:A:MET:H	1:83:A:ASP:HB2	8	0.55
(1,192)	1:66:A:SER:H	1:67:A:LYS:H	9	0.55
(1,174)	1:50:A:ASP:HA	1:53:A:GLU:H	7	0.55
(1,1325)	1:60:A:MET:H	1:69:A:ALA:HA	7	0.54
(1,1325)	1:60:A:MET:H	1:69:A:ALA:HA	9	0.54
(1,1256)	1:130:A:GLY:HA2	1:234:A:ILE:HA	7	0.54
(1,1256)	1:130:A:GLY:HA3	1:234:A:ILE:HA	7	0.54
(1,1246)	1:106:A:ALA:H	1:113:A:TYR:H	10	0.54
(1,1199)	1:52:A:ARG:H	1:76:A:TYR:H	8	0.54
(1,1165)	1:22:A:THR:HB	1:45:A:LEU:H	8	0.54
(1,741)	1:179:A:MET:HA	1:183:A:LEU:H	3	0.54
(1,523)	1:127:A:ILE:HA	1:130:A:GLY:H	3	0.54
(1,511)	1:116:A:LEU:HA	1:119:A:HIS:H	2	0.54
(1,473)	1:114:A:GLU:H	1:116:A:LEU:H	5	0.54
(1,156)	1:59:A:ARG:H	1:61:A:ASN:H	6	0.54
(1,45)	1:25:A:THR:HA	1:28:A:ALA:H	9	0.54
(1,42)	1:23:A:TRP:HA	1:26:A:ARG:H	9	0.54
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB2	1	0.53
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB3	1	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1281)	1:213:A:LEU:H	1:218:A:LEU:HG	5	0.53
(1,1258)	1:132:A:ILE:H	1:237:A:LEU:HG	5	0.53
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB2	9	0.53
(1,1255)	1:127:A:ILE:H	1:188:A:SER:HB3	9	0.53
(1,1180)	1:29:A:TYR:HA	1:46:A:ALA:H	2	0.53
(1,1152)	1:194:A:GLN:HA	1:197:A:ASN:H	6	0.53
(1,992)	1:229:A:ASN:HA	1:233:A:ARG:H	6	0.53
(1,981)	1:231:A:ASN:HA	1:234:A:ILE:H	10	0.53
(1,911)	1:223:A:GLU:HA	1:226:A:THR:H	8	0.53
(1,762)	1:188:A:SER:HA	1:191:A:ASP:H	9	0.53
(1,753)	1:179:A:MET:HA	1:182:A:SER:H	9	0.53
(1,752)	1:178:A:THR:HA	1:181:A:ASN:H	2	0.53
(1,533)	1:120:A:ASP:HA	1:124:A:VAL:H	5	0.53
(1,529)	1:117:A:LYS:HA	1:121:A:VAL:H	5	0.53
(1,516)	1:121:A:VAL:HA	1:124:A:VAL:H	9	0.53
(1,261)	1:74:A:TYR:HA	1:77:A:GLN:H	6	0.53
(1,259)	1:72:A:TRP:HA	1:75:A:GLY:H	9	0.53
(1,179)	1:55:A:TYR:HA	1:58:A:LEU:H	9	0.53
(1,160)	1:48:A:ILE:HA	1:52:A:ARG:H	8	0.53
(1,140)	1:51:A:PHE:HA	1:53:A:GLU:H	4	0.53
(1,1306)	1:49:A:ASP:H	1:144:A:TRP:HD1	9	0.52
(1,1299)	1:26:A:ARG:H	1:121:A:VAL:HG11	10	0.52
(1,1187)	1:33:A:SER:H	1:39:A:GLN:HA	10	0.52
(1,912)	1:224:A:VAL:HA	1:227:A:SER:H	8	0.52
(1,911)	1:223:A:GLU:HA	1:226:A:THR:H	1	0.52
(1,909)	1:221:A:PHE:HA	1:224:A:VAL:H	4	0.52
(1,840)	1:207:A:GLN:HA	1:210:A:ILE:H	7	0.52
(1,560)	1:144:A:TRP:HA	1:145:A:ASN:H	4	0.52
(1,419)	1:112:A:SER:H	1:113:A:TYR:H	5	0.52
(1,276)	1:83:A:ASP:H	1:84:A:ARG:H	5	0.52
(1,176)	1:52:A:ARG:HA	1:55:A:TYR:H	8	0.52
(1,169)	1:45:A:LEU:HA	1:48:A:ILE:H	6	0.52
(1,45)	1:25:A:THR:HA	1:28:A:ALA:H	10	0.52
(1,41)	1:22:A:THR:HA	1:25:A:THR:H	6	0.52
(1,1269)	1:173:A:ALA:HA	1:178:A:THR:H	1	0.51
(1,1165)	1:22:A:THR:HB	1:45:A:LEU:H	1	0.51
(1,996)	1:233:A:ARG:HA	1:237:A:LEU:H	1	0.51
(1,777)	1:198:A:GLY:H	1:199:A:GLY:H	1	0.51
(1,760)	1:186:A:LYS:HA	1:189:A:TYR:H	3	0.51
(1,749)	1:187:A:MET:HA	1:191:A:ASP:H	6	0.51
(1,745)	1:183:A:LEU:HA	1:187:A:MET:H	5	0.51
(1,404)	1:109:A:GLU:H	1:111:A:LYS:HB2	2	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:56:A:TYR:HA	1:59:A:ARG:H	5	0.51
(1,78)	1:34:A:VAL:H	1:36:A:LEU:H	1	0.51
(1,74)	1:44:A:LYS:H	1:45:A:LEU:H	8	0.51
(2,98)	1:178:A:THR:H	1:202:A:THR:H	10	0.5
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG11	10	0.5
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG12	10	0.5
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG13	10	0.5
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG21	10	0.5
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG22	10	0.5
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG23	10	0.5
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG11	10	0.5
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG12	10	0.5
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG13	10	0.5
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG21	10	0.5
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG22	10	0.5
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG23	10	0.5
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG11	10	0.5
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG12	10	0.5
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG13	10	0.5
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG21	10	0.5
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG22	10	0.5
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG23	10	0.5
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG11	10	0.5
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG12	10	0.5
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG13	10	0.5
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG21	10	0.5
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG22	10	0.5
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG23	10	0.5
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG11	10	0.5
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG12	10	0.5
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG13	10	0.5
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG21	10	0.5
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG22	10	0.5
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG23	10	0.5
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG11	10	0.5
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG12	10	0.5
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG13	10	0.5
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG21	10	0.5
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG22	10	0.5
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG23	10	0.5
(2,8)	1:38:A:SER:HB2	1:40:A:THR:H	2	0.5
(2,8)	1:38:A:SER:HB3	1:40:A:THR:H	2	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1335)	1:54:A:ALA:H	1:81:A:MET:HA	5	0.5
(1,1001)	1:238:A:LYS:HA	1:242:A:ALA:H	6	0.5
(1,997)	1:234:A:ILE:HA	1:238:A:LYS:H	4	0.5
(1,918)	1:223:A:GLU:HA	1:227:A:SER:H	10	0.5
(1,911)	1:223:A:GLU:HA	1:226:A:THR:H	7	0.5
(1,758)	1:184:A:LEU:HA	1:187:A:MET:H	8	0.5
(1,755)	1:181:A:ASN:HA	1:184:A:LEU:H	6	0.5
(1,176)	1:52:A:ARG:HA	1:55:A:TYR:H	9	0.5
(1,173)	1:49:A:ASP:HA	1:52:A:ARG:H	6	0.5
(1,159)	1:47:A:LEU:HA	1:51:A:PHE:H	8	0.5
(1,42)	1:23:A:TRP:HA	1:26:A:ARG:H	4	0.5
(2,99)	1:76:A:TYR:HA	1:87:A:LEU:H	6	0.49
(2,94)	1:204:A:ARG:HA	1:209:A:MET:H	2	0.49
(1,1317)	1:53:A:GLU:H	1:79:A:GLY:H	9	0.49
(1,1248)	1:110:A:GLU:H	1:215:A:VAL:HB	5	0.49
(1,1233)	1:101:A:VAL:H	1:219:A:ASP:HA	4	0.49
(1,1179)	1:29:A:TYR:H	1:46:A:ALA:H	6	0.49
(1,979)	1:229:A:ASN:HA	1:232:A:VAL:H	1	0.49
(1,915)	1:220:A:TYR:HA	1:224:A:VAL:H	4	0.49
(1,840)	1:207:A:GLN:HA	1:210:A:ILE:H	1	0.49
(1,757)	1:183:A:LEU:HA	1:186:A:LYS:H	6	0.49
(1,754)	1:180:A:ARG:HA	1:183:A:LEU:H	10	0.49
(1,741)	1:179:A:MET:HA	1:183:A:LEU:H	4	0.49
(1,538)	1:125:A:LEU:HA	1:129:A:GLY:H	3	0.49
(1,526)	1:114:A:GLU:HA	1:118:A:GLU:H	5	0.49
(1,511)	1:116:A:LEU:HA	1:119:A:HIS:H	4	0.49
(1,164)	1:52:A:ARG:HA	1:56:A:TYR:H	6	0.49
(1,157)	1:45:A:LEU:HA	1:49:A:ASP:H	4	0.49
(1,156)	1:59:A:ARG:H	1:61:A:ASN:H	2	0.49
(1,49)	1:23:A:TRP:HA	1:27:A:THR:H	8	0.49
(1,46)	1:26:A:ARG:HG2	1:29:A:TYR:H	4	0.49
(1,46)	1:26:A:ARG:HG3	1:29:A:TYR:H	4	0.49
(2,99)	1:76:A:TYR:HA	1:87:A:LEU:H	3	0.48
(1,1332)	1:173:A:ALA:HA	1:202:A:THR:H	9	0.48
(1,1306)	1:49:A:ASP:H	1:144:A:TRP:HD1	6	0.48
(1,1299)	1:26:A:ARG:H	1:121:A:VAL:HG11	4	0.48
(1,1289)	1:266:A:ARG:H	1:273:A:VAL:H	5	0.48
(1,1249)	1:123:A:TYR:H	1:224:A:VAL:HA	9	0.48
(1,1246)	1:106:A:ALA:H	1:113:A:TYR:H	6	0.48
(1,1246)	1:106:A:ALA:H	1:113:A:TYR:H	8	0.48
(1,1219)	1:78:A:ILE:HA	1:83:A:ASP:H	2	0.48
(1,1166)	1:23:A:TRP:H	1:45:A:LEU:HA	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:231:A:ASN:HA	1:235:A:TYR:H	6	0.48
(1,910)	1:222:A:ASP:HA	1:225:A:PHE:H	7	0.48
(1,907)	1:219:A:ASP:HA	1:222:A:ASP:H	1	0.48
(1,756)	1:182:A:SER:HA	1:185:A:TYR:H	3	0.48
(1,745)	1:183:A:LEU:HA	1:187:A:MET:H	9	0.48
(1,583)	1:151:A:GLY:HA2	1:153:A:TRP:H	9	0.48
(1,379)	1:92:A:THR:HA	1:96:A:THR:H	10	0.48
(1,269)	1:79:A:GLY:H	1:80:A:GLY:H	10	0.48
(1,181)	1:57:A:TRP:HA	1:60:A:MET:H	8	0.48
(1,178)	1:54:A:ALA:HA	1:57:A:TRP:H	7	0.48
(2,95)	1:210:A:ILE:HA	1:235:A:TYR:H	5	0.47
(2,89)	1:123:A:TYR:HA	1:226:A:THR:H	6	0.47
(2,28)	1:78:A:ILE:HG12	1:81:A:MET:H	9	0.47
(2,28)	1:78:A:ILE:HG13	1:81:A:MET:H	9	0.47
(1,1329)	1:104:A:ALA:HA	1:221:A:PHE:H	1	0.47
(1,1289)	1:266:A:ARG:H	1:273:A:VAL:H	8	0.47
(1,1225)	1:82:A:ALA:H	1:144:A:TRP:HA	4	0.47
(1,1199)	1:52:A:ARG:H	1:76:A:TYR:H	3	0.47
(1,910)	1:222:A:ASP:HA	1:225:A:PHE:H	8	0.47
(1,762)	1:188:A:SER:HA	1:191:A:ASP:H	6	0.47
(1,755)	1:181:A:ASN:HA	1:184:A:LEU:H	10	0.47
(1,740)	1:178:A:THR:HA	1:182:A:SER:H	1	0.47
(1,389)	1:102:A:GLY:HA2	1:106:A:ALA:H	8	0.47
(1,389)	1:102:A:GLY:HA3	1:106:A:ALA:H	8	0.47
(1,388)	1:101:A:VAL:HA	1:105:A:ASN:H	7	0.47
(2,95)	1:210:A:ILE:HA	1:235:A:TYR:H	4	0.46
(2,93)	1:195:A:LEU:HD11	1:232:A:VAL:HG11	2	0.46
(2,93)	1:195:A:LEU:HD11	1:232:A:VAL:HG12	2	0.46
(2,93)	1:195:A:LEU:HD11	1:232:A:VAL:HG13	2	0.46
(2,93)	1:195:A:LEU:HD11	1:232:A:VAL:HG21	2	0.46
(2,93)	1:195:A:LEU:HD11	1:232:A:VAL:HG22	2	0.46
(2,93)	1:195:A:LEU:HD11	1:232:A:VAL:HG23	2	0.46
(2,93)	1:195:A:LEU:HD12	1:232:A:VAL:HG11	2	0.46
(2,93)	1:195:A:LEU:HD12	1:232:A:VAL:HG12	2	0.46
(2,93)	1:195:A:LEU:HD12	1:232:A:VAL:HG13	2	0.46
(2,93)	1:195:A:LEU:HD12	1:232:A:VAL:HG21	2	0.46
(2,93)	1:195:A:LEU:HD12	1:232:A:VAL:HG22	2	0.46
(2,93)	1:195:A:LEU:HD12	1:232:A:VAL:HG23	2	0.46
(2,93)	1:195:A:LEU:HD13	1:232:A:VAL:HG11	2	0.46
(2,93)	1:195:A:LEU:HD13	1:232:A:VAL:HG12	2	0.46
(2,93)	1:195:A:LEU:HD13	1:232:A:VAL:HG13	2	0.46
(2,93)	1:195:A:LEU:HD13	1:232:A:VAL:HG21	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,93)	1:195:A:LEU:HD13	1:232:A:VAL:HG22	2	0.46
(2,93)	1:195:A:LEU:HD13	1:232:A:VAL:HG23	2	0.46
(2,93)	1:195:A:LEU:HD21	1:232:A:VAL:HG11	2	0.46
(2,93)	1:195:A:LEU:HD21	1:232:A:VAL:HG12	2	0.46
(2,93)	1:195:A:LEU:HD21	1:232:A:VAL:HG13	2	0.46
(2,93)	1:195:A:LEU:HD21	1:232:A:VAL:HG21	2	0.46
(2,93)	1:195:A:LEU:HD21	1:232:A:VAL:HG22	2	0.46
(2,93)	1:195:A:LEU:HD21	1:232:A:VAL:HG23	2	0.46
(2,93)	1:195:A:LEU:HD22	1:232:A:VAL:HG11	2	0.46
(2,93)	1:195:A:LEU:HD22	1:232:A:VAL:HG12	2	0.46
(2,93)	1:195:A:LEU:HD22	1:232:A:VAL:HG13	2	0.46
(2,93)	1:195:A:LEU:HD22	1:232:A:VAL:HG21	2	0.46
(2,93)	1:195:A:LEU:HD22	1:232:A:VAL:HG22	2	0.46
(2,93)	1:195:A:LEU:HD22	1:232:A:VAL:HG23	2	0.46
(2,93)	1:195:A:LEU:HD23	1:232:A:VAL:HG11	2	0.46
(2,93)	1:195:A:LEU:HD23	1:232:A:VAL:HG12	2	0.46
(2,93)	1:195:A:LEU:HD23	1:232:A:VAL:HG13	2	0.46
(2,93)	1:195:A:LEU:HD23	1:232:A:VAL:HG21	2	0.46
(2,93)	1:195:A:LEU:HD23	1:232:A:VAL:HG22	2	0.46
(2,93)	1:195:A:LEU:HD23	1:232:A:VAL:HG23	2	0.46
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG11	8	0.46
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG12	8	0.46
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG13	8	0.46
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG21	8	0.46
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG22	8	0.46
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG23	8	0.46
(1,1319)	1:130:A:GLY:H	1:135:A:GLY:H	3	0.46
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD11	8	0.46
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD12	8	0.46
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD13	8	0.46
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD21	8	0.46
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD22	8	0.46
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD23	8	0.46
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB2	9	0.46
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB3	9	0.46
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB2	9	0.46
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB3	9	0.46
(1,1244)	1:106:A:ALA:HA	1:111:A:LYS:H	2	0.46
(1,1201)	1:54:A:ALA:HA	1:82:A:ALA:H	8	0.46
(1,1186)	1:29:A:TYR:H	1:45:A:LEU:HA	7	0.46
(1,1180)	1:29:A:TYR:HA	1:46:A:ALA:H	9	0.46
(1,993)	1:230:A:TRP:HA	1:234:A:ILE:H	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,991)	1:228:A:GLU:HA	1:232:A:VAL:H	1	0.46
(1,983)	1:233:A:ARG:HA	1:236:A:GLN:H	7	0.46
(1,979)	1:229:A:ASN:HA	1:232:A:VAL:H	4	0.46
(1,835)	1:202:A:THR:HB	1:205:A:VAL:H	8	0.46
(1,760)	1:186:A:LYS:HA	1:189:A:TYR:H	1	0.46
(1,758)	1:184:A:LEU:HA	1:187:A:MET:H	6	0.46
(1,750)	1:176:A:SER:HA	1:179:A:MET:H	9	0.46
(1,538)	1:125:A:LEU:HA	1:129:A:GLY:H	4	0.46
(1,405)	1:111:A:LYS:H	1:113:A:TYR:HB2	8	0.46
(1,266)	1:70:A:ALA:HA	1:74:A:TYR:H	4	0.46
(1,181)	1:57:A:TRP:HA	1:60:A:MET:H	9	0.46
(1,178)	1:54:A:ALA:HA	1:57:A:TRP:H	8	0.46
(1,160)	1:48:A:ILE:HA	1:52:A:ARG:H	4	0.46
(1,50)	1:24:A:VAL:HA	1:28:A:ALA:H	5	0.46
(2,94)	1:204:A:ARG:HA	1:209:A:MET:H	1	0.45
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB2	7	0.45
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB3	7	0.45
(1,1226)	1:82:A:ALA:HA	1:144:A:TRP:H	1	0.45
(1,1206)	1:56:A:TYR:HA	1:69:A:ALA:H	10	0.45
(1,1205)	1:56:A:TYR:H	1:76:A:TYR:HA	4	0.45
(1,1199)	1:52:A:ARG:H	1:76:A:TYR:H	4	0.45
(1,1150)	1:174:A:ARG:H	1:177:A:GLU:HB2	9	0.45
(1,1073)	1:248:A:ARG:HB2	1:251:A:GLY:H	9	0.45
(1,997)	1:234:A:ILE:HA	1:238:A:LYS:H	2	0.45
(1,981)	1:231:A:ASN:HA	1:234:A:ILE:H	4	0.45
(1,979)	1:229:A:ASN:HA	1:232:A:VAL:H	9	0.45
(1,918)	1:223:A:GLU:HA	1:227:A:SER:H	6	0.45
(1,907)	1:219:A:ASP:HA	1:222:A:ASP:H	4	0.45
(1,547)	1:134:A:PHE:H	1:135:A:GLY:H	3	0.45
(1,535)	1:122:A:ASP:HA	1:126:A:VAL:H	9	0.45
(1,388)	1:101:A:VAL:HA	1:105:A:ASN:H	3	0.45
(1,384)	1:97:A:HIS:HA	1:101:A:VAL:H	10	0.45
(1,373)	1:89:A:ASP:HA	1:92:A:THR:H	10	0.45
(1,267)	1:72:A:TRP:HA	1:76:A:TYR:H	4	0.45
(1,176)	1:52:A:ARG:HA	1:55:A:TYR:H	3	0.45
(1,171)	1:47:A:LEU:HA	1:50:A:ASP:H	8	0.45
(1,157)	1:45:A:LEU:HA	1:49:A:ASP:H	2	0.45
(1,140)	1:51:A:PHE:HA	1:53:A:GLU:H	8	0.45
(1,74)	1:44:A:LYS:H	1:45:A:LEU:H	3	0.45
(1,50)	1:24:A:VAL:HA	1:28:A:ALA:H	4	0.45
(1,42)	1:23:A:TRP:HA	1:26:A:ARG:H	10	0.45
(1,40)	1:21:A:SER:HA	1:24:A:VAL:H	2	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	1:204:A:ARG:HA	1:209:A:MET:H	3	0.44
(2,9)	1:41:A:PRO:HD2	1:44:A:LYS:H	1	0.44
(2,9)	1:41:A:PRO:HD3	1:44:A:LYS:H	1	0.44
(1,1274)	1:197:A:ASN:HA	1:202:A:THR:HA	9	0.44
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD11	1	0.44
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD12	1	0.44
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD13	1	0.44
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD21	1	0.44
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD22	1	0.44
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD23	1	0.44
(1,1180)	1:29:A:TYR:HA	1:46:A:ALA:H	3	0.44
(1,912)	1:224:A:VAL:HA	1:227:A:SER:H	4	0.44
(1,908)	1:220:A:TYR:HA	1:223:A:GLU:H	4	0.44
(1,751)	1:177:A:GLU:HA	1:180:A:ARG:H	5	0.44
(1,556)	1:141:A:LYS:H	1:142:A:PHE:H	2	0.44
(1,519)	1:124:A:VAL:HA	1:127:A:ILE:H	9	0.44
(1,178)	1:54:A:ALA:HA	1:57:A:TRP:H	5	0.44
(1,74)	1:44:A:LYS:H	1:45:A:LEU:H	4	0.44
(1,50)	1:24:A:VAL:HA	1:28:A:ALA:H	7	0.44
(2,99)	1:76:A:TYR:HA	1:87:A:LEU:H	10	0.43
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB2	2	0.43
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB3	2	0.43
(1,1274)	1:197:A:ASN:HA	1:202:A:THR:HA	4	0.43
(1,1226)	1:82:A:ALA:HA	1:144:A:TRP:H	6	0.43
(1,1219)	1:78:A:ILE:HA	1:83:A:ASP:H	6	0.43
(1,1166)	1:23:A:TRP:H	1:45:A:LEU:HA	5	0.43
(1,1077)	1:251:A:GLY:HA2	1:254:A:THR:H	3	0.43
(1,1077)	1:251:A:GLY:HA3	1:254:A:THR:H	3	0.43
(1,997)	1:234:A:ILE:HA	1:238:A:LYS:H	3	0.43
(1,983)	1:233:A:ARG:HA	1:236:A:GLN:H	5	0.43
(1,909)	1:221:A:PHE:HA	1:224:A:VAL:H	1	0.43
(1,907)	1:219:A:ASP:HA	1:222:A:ASP:H	5	0.43
(1,755)	1:181:A:ASN:HA	1:184:A:LEU:H	4	0.43
(1,526)	1:114:A:GLU:HA	1:118:A:GLU:H	9	0.43
(1,523)	1:127:A:ILE:HA	1:130:A:GLY:H	6	0.43
(1,513)	1:118:A:GLU:HA	1:121:A:VAL:H	7	0.43
(1,379)	1:92:A:THR:HA	1:96:A:THR:H	6	0.43
(1,343)	1:91:A:ASN:H	1:93:A:TRP:H	7	0.43
(1,167)	1:55:A:TYR:HA	1:59:A:ARG:H	9	0.43
(2,95)	1:210:A:ILE:HA	1:235:A:TYR:H	1	0.42
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG11	9	0.42
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG12	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG13	9	0.42
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG21	9	0.42
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG22	9	0.42
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG23	9	0.42
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG11	9	0.42
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG12	9	0.42
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG13	9	0.42
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG21	9	0.42
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG22	9	0.42
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG23	9	0.42
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG11	9	0.42
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG12	9	0.42
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG13	9	0.42
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG21	9	0.42
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG22	9	0.42
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG23	9	0.42
(1,1325)	1:60:A:MET:H	1:69:A:ALA:HA	4	0.42
(1,1256)	1:130:A:GLY:HA2	1:234:A:ILE:HA	5	0.42
(1,1256)	1:130:A:GLY:HA3	1:234:A:ILE:HA	5	0.42
(1,1231)	1:100:A:ILE:HD11	1:223:A:GLU:H	7	0.42
(1,1231)	1:100:A:ILE:HD12	1:223:A:GLU:H	7	0.42
(1,1231)	1:100:A:ILE:HD13	1:223:A:GLU:H	7	0.42
(1,1216)	1:71:A:TRP:H	1:255:A:ARG:HG2	7	0.42
(1,1216)	1:71:A:TRP:H	1:255:A:ARG:HG3	7	0.42
(1,1194)	1:35:A:VAL:H	1:40:A:THR:HA	4	0.42
(1,1132)	1:153:A:TRP:H	1:154:A:PRO:HA	1	0.42
(1,984)	1:234:A:ILE:HA	1:237:A:LEU:H	4	0.42
(1,839)	1:206:A:ARG:HA	1:209:A:MET:H	4	0.42
(1,760)	1:186:A:LYS:HA	1:189:A:TYR:H	2	0.42
(1,756)	1:182:A:SER:HA	1:185:A:TYR:H	1	0.42
(1,753)	1:179:A:MET:HA	1:182:A:SER:H	10	0.42
(1,750)	1:176:A:SER:HA	1:179:A:MET:H	5	0.42
(1,529)	1:117:A:LYS:HA	1:121:A:VAL:H	3	0.42
(1,526)	1:114:A:GLU:HA	1:118:A:GLU:H	8	0.42
(1,475)	1:115:A:ILE:H	1:117:A:LYS:H	5	0.42
(1,377)	1:93:A:TRP:HA	1:96:A:THR:H	8	0.42
(1,373)	1:89:A:ASP:HA	1:92:A:THR:H	1	0.42
(1,373)	1:89:A:ASP:HA	1:92:A:THR:H	8	0.42
(1,338)	1:84:A:ARG:H	1:86:A:THR:H	1	0.42
(1,338)	1:84:A:ARG:H	1:86:A:THR:H	7	0.42
(1,276)	1:83:A:ASP:H	1:84:A:ARG:H	10	0.42
(1,180)	1:56:A:TYR:HA	1:59:A:ARG:H	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:54:A:ALA:HA	1:57:A:TRP:H	3	0.42
(1,174)	1:50:A:ASP:HA	1:53:A:GLU:H	9	0.42
(1,171)	1:47:A:LEU:HA	1:50:A:ASP:H	10	0.42
(1,42)	1:23:A:TRP:HA	1:26:A:ARG:H	2	0.42
(2,99)	1:76:A:TYR:HA	1:87:A:LEU:H	8	0.41
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD11	7	0.41
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD12	7	0.41
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD13	7	0.41
(1,1332)	1:173:A:ALA:HA	1:202:A:THR:H	8	0.41
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB2	4	0.41
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB3	4	0.41
(1,1228)	1:93:A:TRP:H	1:64:A:GLU:HA	7	0.41
(1,1205)	1:56:A:TYR:H	1:76:A:TYR:HA	3	0.41
(1,1185)	1:27:A:THR:HA	1:46:A:ALA:H	6	0.41
(1,1180)	1:29:A:TYR:HA	1:46:A:ALA:H	7	0.41
(1,1152)	1:194:A:GLN:HA	1:197:A:ASN:H	7	0.41
(1,994)	1:231:A:ASN:HA	1:235:A:TYR:H	3	0.41
(1,891)	1:219:A:ASP:HA	1:221:A:PHE:H	5	0.41
(1,840)	1:207:A:GLN:HA	1:210:A:ILE:H	10	0.41
(1,754)	1:180:A:ARG:HA	1:183:A:LEU:H	6	0.41
(1,749)	1:187:A:MET:HA	1:191:A:ASP:H	10	0.41
(1,745)	1:183:A:LEU:HA	1:187:A:MET:H	7	0.41
(1,533)	1:120:A:ASP:HA	1:124:A:VAL:H	7	0.41
(1,529)	1:117:A:LYS:HA	1:121:A:VAL:H	1	0.41
(1,515)	1:120:A:ASP:HA	1:123:A:TYR:H	4	0.41
(1,513)	1:118:A:GLU:HA	1:121:A:VAL:H	10	0.41
(1,419)	1:112:A:SER:H	1:113:A:TYR:H	1	0.41
(1,405)	1:111:A:LYS:H	1:113:A:TYR:HB2	3	0.41
(1,405)	1:111:A:LYS:H	1:113:A:TYR:HB2	5	0.41
(1,396)	1:98:A:ILE:HA	1:101:A:VAL:H	7	0.41
(1,388)	1:101:A:VAL:HA	1:105:A:ASN:H	6	0.41
(1,1334)	1:177:A:GLU:H	1:202:A:THR:HA	10	0.4
(1,1314)	1:177:A:GLU:H	1:202:A:THR:HA	10	0.4
(1,1310)	1:134:A:PHE:H	1:234:A:ILE:HD11	3	0.4
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB2	3	0.4
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB3	3	0.4
(1,1275)	1:197:A:ASN:HA	1:202:A:THR:H	3	0.4
(1,1234)	1:101:A:VAL:HA	1:223:A:GLU:H	6	0.4
(1,1228)	1:93:A:TRP:H	1:64:A:GLU:HA	9	0.4
(1,1217)	1:77:A:GLN:H	1:98:A:ILE:HG13	7	0.4
(1,1207)	1:62:A:SER:HA	1:67:A:LYS:H	1	0.4
(1,1200)	1:54:A:ALA:H	1:82:A:ALA:H	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1189)	1:34:A:VAL:HA	1:39:A:GLN:H	2	0.4
(1,1180)	1:29:A:TYR:HA	1:46:A:ALA:H	4	0.4
(1,1166)	1:23:A:TRP:H	1:45:A:LEU:HA	4	0.4
(1,1163)	1:22:A:THR:H	1:47:A:LEU:H	5	0.4
(1,1152)	1:194:A:GLN:HA	1:197:A:ASN:H	2	0.4
(1,1075)	1:249:A:ASP:HA	1:252:A:GLU:H	7	0.4
(1,984)	1:234:A:ILE:HA	1:237:A:LEU:H	10	0.4
(1,983)	1:233:A:ARG:HA	1:236:A:GLN:H	3	0.4
(1,912)	1:224:A:VAL:HA	1:227:A:SER:H	7	0.4
(1,911)	1:223:A:GLU:HA	1:226:A:THR:H	9	0.4
(1,911)	1:223:A:GLU:HA	1:226:A:THR:H	10	0.4
(1,907)	1:219:A:ASP:HA	1:222:A:ASP:H	7	0.4
(1,850)	1:212:A:PRO:HA	1:213:A:LEU:H	1	0.4
(1,850)	1:212:A:PRO:HA	1:213:A:LEU:H	5	0.4
(1,842)	1:200:A:GLN:HA	1:204:A:ARG:H	9	0.4
(1,753)	1:179:A:MET:HA	1:182:A:SER:H	3	0.4
(1,529)	1:117:A:LYS:HA	1:121:A:VAL:H	9	0.4
(1,498)	1:125:A:LEU:HG	1:127:A:ILE:H	10	0.4
(1,387)	1:100:A:ILE:HA	1:104:A:ALA:H	9	0.4
(1,252)	1:67:A:LYS:HA	1:70:A:ALA:H	7	0.4
(1,232)	1:69:A:ALA:H	1:71:A:TRP:H	10	0.4
(1,82)	1:33:A:SER:HB2	1:36:A:LEU:H	1	0.4
(1,82)	1:33:A:SER:HB3	1:36:A:LEU:H	1	0.4
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD11	6	0.39
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD12	6	0.39
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD13	6	0.39
(1,1328)	1:78:A:ILE:H	1:84:A:ARG:H	9	0.39
(1,1281)	1:213:A:LEU:H	1:218:A:LEU:HG	1	0.39
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB2	6	0.39
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB3	6	0.39
(1,1200)	1:54:A:ALA:H	1:82:A:ALA:H	9	0.39
(1,1150)	1:174:A:ARG:H	1:177:A:GLU:HB2	6	0.39
(1,1148)	1:171:A:VAL:HA	1:174:A:ARG:H	3	0.39
(1,1077)	1:251:A:GLY:HA2	1:254:A:THR:H	2	0.39
(1,1077)	1:251:A:GLY:HA3	1:254:A:THR:H	2	0.39
(1,1077)	1:251:A:GLY:HA2	1:254:A:THR:H	9	0.39
(1,1077)	1:251:A:GLY:HA3	1:254:A:THR:H	9	0.39
(1,1068)	1:247:A:LEU:HA	1:250:A:VAL:H	6	0.39
(1,1068)	1:247:A:LEU:HA	1:250:A:VAL:H	7	0.39
(1,918)	1:223:A:GLU:HA	1:227:A:SER:H	7	0.39
(1,907)	1:219:A:ASP:HA	1:222:A:ASP:H	6	0.39
(1,775)	1:197:A:ASN:H	1:198:A:GLY:H	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,745)	1:183:A:LEU:HA	1:187:A:MET:H	4	0.39
(1,745)	1:183:A:LEU:HA	1:187:A:MET:H	6	0.39
(1,742)	1:180:A:ARG:HA	1:184:A:LEU:H	5	0.39
(1,524)	1:128:A:PHE:HA	1:131:A:LEU:H	1	0.39
(1,518)	1:123:A:TYR:HA	1:126:A:VAL:H	2	0.39
(1,515)	1:120:A:ASP:HA	1:123:A:TYR:H	10	0.39
(1,405)	1:111:A:LYS:H	1:113:A:TYR:HB2	9	0.39
(1,364)	1:104:A:ALA:H	1:106:A:ALA:H	5	0.39
(1,264)	1:68:A:VAL:HA	1:72:A:TRP:H	8	0.39
(1,176)	1:52:A:ARG:HA	1:55:A:TYR:H	1	0.39
(1,175)	1:51:A:PHE:HA	1:54:A:ALA:H	6	0.39
(1,164)	1:52:A:ARG:HA	1:56:A:TYR:H	4	0.39
(1,145)	1:54:A:ALA:H	1:56:A:TYR:H	10	0.39
(1,42)	1:23:A:TRP:HA	1:26:A:ARG:H	1	0.39
(1,40)	1:21:A:SER:HA	1:24:A:VAL:H	5	0.39
(1,1307)	1:51:A:PHE:H	1:144:A:TRP:HD1	8	0.38
(1,1306)	1:49:A:ASP:H	1:144:A:TRP:HD1	8	0.38
(1,1298)	1:156:A:GLU:H	1:25:A:THR:HG1	8	0.38
(1,1289)	1:266:A:ARG:H	1:273:A:VAL:H	3	0.38
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB2	10	0.38
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB3	10	0.38
(1,1269)	1:173:A:ALA:HA	1:178:A:THR:H	9	0.38
(1,1225)	1:82:A:ALA:H	1:144:A:TRP:HA	7	0.38
(1,1203)	1:56:A:TYR:H	1:72:A:TRP:H	4	0.38
(1,1180)	1:29:A:TYR:HA	1:46:A:ALA:H	5	0.38
(1,1160)	1:261:A:ARG:H	1:264:A:ILE:HA	3	0.38
(1,1152)	1:194:A:GLN:HA	1:197:A:ASN:H	10	0.38
(1,1077)	1:251:A:GLY:HA2	1:254:A:THR:H	4	0.38
(1,1077)	1:251:A:GLY:HA3	1:254:A:THR:H	4	0.38
(1,992)	1:229:A:ASN:HA	1:233:A:ARG:H	9	0.38
(1,991)	1:228:A:GLU:HA	1:232:A:VAL:H	5	0.38
(1,991)	1:228:A:GLU:HA	1:232:A:VAL:H	7	0.38
(1,980)	1:230:A:TRP:HA	1:233:A:ARG:H	2	0.38
(1,850)	1:212:A:PRO:HA	1:213:A:LEU:H	9	0.38
(1,709)	1:176:A:SER:H	1:178:A:THR:H	8	0.38
(1,537)	1:124:A:VAL:HA	1:128:A:PHE:H	3	0.38
(1,533)	1:120:A:ASP:HA	1:124:A:VAL:H	1	0.38
(1,412)	1:109:A:GLU:H	1:110:A:GLU:H	8	0.38
(1,268)	1:73:A:ASP:HA	1:77:A:GLN:H	3	0.38
(1,261)	1:74:A:TYR:HA	1:77:A:GLN:H	1	0.38
(1,261)	1:74:A:TYR:HA	1:77:A:GLN:H	10	0.38
(1,254)	1:69:A:ALA:HA	1:72:A:TRP:H	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:76:A:TYR:H	1:78:A:ILE:H	4	0.38
(1,181)	1:57:A:TRP:HA	1:60:A:MET:H	3	0.38
(1,166)	1:54:A:ALA:HA	1:58:A:LEU:H	6	0.38
(1,157)	1:45:A:LEU:HA	1:49:A:ASP:H	8	0.38
(1,142)	1:52:A:ARG:HA	1:54:A:ALA:H	9	0.38
(1,74)	1:44:A:LYS:H	1:45:A:LEU:H	6	0.38
(1,34)	1:25:A:THR:H	1:27:A:THR:H	8	0.38
(1,30)	1:23:A:TRP:HA	1:25:A:THR:H	2	0.38
(2,99)	1:76:A:TYR:HA	1:87:A:LEU:H	5	0.37
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG11	4	0.37
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG12	4	0.37
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG13	4	0.37
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG21	4	0.37
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG22	4	0.37
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG23	4	0.37
(1,1336)	1:189:A:TYR:HA	1:230:A:TRP:H	5	0.37
(1,1305)	1:48:A:ILE:H	1:144:A:TRP:HZ2	8	0.37
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB2	5	0.37
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB3	5	0.37
(1,1271)	1:189:A:TYR:H	1:230:A:TRP:H	1	0.37
(1,1244)	1:106:A:ALA:HA	1:111:A:LYS:H	5	0.37
(1,1234)	1:101:A:VAL:HA	1:223:A:GLU:H	10	0.37
(1,1219)	1:78:A:ILE:HA	1:83:A:ASP:H	4	0.37
(1,1206)	1:56:A:TYR:HA	1:69:A:ALA:H	6	0.37
(1,1187)	1:33:A:SER:H	1:39:A:GLN:HA	4	0.37
(1,1186)	1:29:A:TYR:H	1:45:A:LEU:HA	5	0.37
(1,1186)	1:29:A:TYR:H	1:45:A:LEU:HA	8	0.37
(1,1068)	1:247:A:LEU:HA	1:250:A:VAL:H	1	0.37
(1,994)	1:231:A:ASN:HA	1:235:A:TYR:H	2	0.37
(1,984)	1:234:A:ILE:HA	1:237:A:LEU:H	1	0.37
(1,918)	1:223:A:GLU:HA	1:227:A:SER:H	2	0.37
(1,850)	1:212:A:PRO:HA	1:213:A:LEU:H	2	0.37
(1,839)	1:206:A:ARG:HA	1:209:A:MET:H	6	0.37
(1,763)	1:189:A:TYR:HA	1:192:A:PHE:H	4	0.37
(1,761)	1:187:A:MET:HA	1:190:A:LYS:H	7	0.37
(1,744)	1:182:A:SER:HA	1:186:A:LYS:H	3	0.37
(1,559)	1:144:A:TRP:H	1:145:A:ASN:H	1	0.37
(1,523)	1:127:A:ILE:HA	1:130:A:GLY:H	1	0.37
(1,508)	1:130:A:GLY:H	1:132:A:ILE:H	5	0.37
(1,343)	1:91:A:ASN:H	1:93:A:TRP:H	1	0.37
(1,269)	1:79:A:GLY:H	1:80:A:GLY:H	6	0.37
(1,267)	1:72:A:TRP:HA	1:76:A:TYR:H	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:70:A:ALA:HA	1:74:A:TYR:H	7	0.37
(1,246)	1:76:A:TYR:H	1:78:A:ILE:H	1	0.37
(1,243)	1:74:A:TYR:HA	1:76:A:TYR:H	10	0.37
(1,157)	1:45:A:LEU:HA	1:49:A:ASP:H	10	0.37
(1,142)	1:52:A:ARG:HA	1:54:A:ALA:H	3	0.37
(1,40)	1:21:A:SER:HA	1:24:A:VAL:H	1	0.37
(2,99)	1:76:A:TYR:HA	1:87:A:LEU:H	2	0.36
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB2	3	0.36
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB3	3	0.36
(2,95)	1:210:A:ILE:HA	1:235:A:TYR:H	10	0.36
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG11	2	0.36
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG12	2	0.36
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG13	2	0.36
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG21	2	0.36
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG22	2	0.36
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG23	2	0.36
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG11	2	0.36
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG12	2	0.36
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG13	2	0.36
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG21	2	0.36
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG22	2	0.36
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG23	2	0.36
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG11	2	0.36
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG12	2	0.36
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG13	2	0.36
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG21	2	0.36
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG22	2	0.36
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG23	2	0.36
(1,1324)	1:51:A:PHE:H	1:81:A:MET:HA	7	0.36
(1,1317)	1:53:A:GLU:H	1:79:A:GLY:H	8	0.36
(1,1271)	1:189:A:TYR:H	1:230:A:TRP:H	3	0.36
(1,1249)	1:123:A:TYR:H	1:224:A:VAL:HA	10	0.36
(1,1246)	1:106:A:ALA:H	1:113:A:TYR:H	4	0.36
(1,1228)	1:93:A:TRP:H	1:64:A:GLU:HA	6	0.36
(1,1205)	1:56:A:TYR:H	1:76:A:TYR:HA	7	0.36
(1,1163)	1:22:A:THR:H	1:47:A:LEU:H	8	0.36
(1,1151)	1:175:A:ALA:HA	1:179:A:MET:H	6	0.36
(1,1141)	1:201:A:ALA:H	1:202:A:THR:HB	6	0.36
(1,1140)	1:199:A:GLY:H	1:200:A:GLN:HA	6	0.36
(1,1068)	1:247:A:LEU:HA	1:250:A:VAL:H	9	0.36
(1,997)	1:234:A:ILE:HA	1:238:A:LYS:H	10	0.36
(1,992)	1:229:A:ASN:HA	1:233:A:ARG:H	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,983)	1:233:A:ARG:HA	1:236:A:GLN:H	9	0.36
(1,981)	1:231:A:ASN:HA	1:234:A:ILE:H	1	0.36
(1,838)	1:205:A:VAL:HA	1:208:A:GLN:H	9	0.36
(1,758)	1:184:A:LEU:HA	1:187:A:MET:H	7	0.36
(1,750)	1:176:A:SER:HA	1:179:A:MET:H	7	0.36
(1,559)	1:144:A:TRP:H	1:145:A:ASN:H	4	0.36
(1,530)	1:118:A:GLU:HA	1:122:A:ASP:H	4	0.36
(1,530)	1:118:A:GLU:HA	1:122:A:ASP:H	10	0.36
(1,524)	1:128:A:PHE:HA	1:131:A:LEU:H	6	0.36
(1,508)	1:130:A:GLY:H	1:132:A:ILE:H	4	0.36
(1,506)	1:129:A:GLY:H	1:131:A:LEU:H	3	0.36
(1,379)	1:92:A:THR:HA	1:96:A:THR:H	7	0.36
(1,372)	1:88:A:VAL:HA	1:91:A:ASN:H	8	0.36
(1,266)	1:70:A:ALA:HA	1:74:A:TYR:H	2	0.36
(1,264)	1:68:A:VAL:HA	1:72:A:TRP:H	3	0.36
(1,165)	1:53:A:GLU:HA	1:57:A:TRP:H	4	0.36
(1,164)	1:52:A:ARG:HA	1:56:A:TYR:H	10	0.36
(1,42)	1:23:A:TRP:HA	1:26:A:ARG:H	5	0.36
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB2	5	0.35
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB3	5	0.35
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB2	10	0.35
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB3	10	0.35
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG11	8	0.35
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG12	8	0.35
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG13	8	0.35
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG21	8	0.35
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG22	8	0.35
(2,90)	1:124:A:VAL:HG11	1:35:A:VAL:HG23	8	0.35
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG11	8	0.35
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG12	8	0.35
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG13	8	0.35
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG21	8	0.35
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG22	8	0.35
(2,90)	1:124:A:VAL:HG12	1:35:A:VAL:HG23	8	0.35
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG11	8	0.35
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG12	8	0.35
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG13	8	0.35
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG21	8	0.35
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG22	8	0.35
(2,90)	1:124:A:VAL:HG13	1:35:A:VAL:HG23	8	0.35
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG11	8	0.35
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG12	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG13	8	0.35
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG21	8	0.35
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG22	8	0.35
(2,90)	1:124:A:VAL:HG21	1:35:A:VAL:HG23	8	0.35
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG11	8	0.35
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG12	8	0.35
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG13	8	0.35
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG21	8	0.35
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG22	8	0.35
(2,90)	1:124:A:VAL:HG22	1:35:A:VAL:HG23	8	0.35
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG11	8	0.35
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG12	8	0.35
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG13	8	0.35
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG21	8	0.35
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG22	8	0.35
(2,90)	1:124:A:VAL:HG23	1:35:A:VAL:HG23	8	0.35
(2,9)	1:41:A:PRO:HD2	1:44:A:LYS:H	9	0.35
(2,9)	1:41:A:PRO:HD3	1:44:A:LYS:H	9	0.35
(1,1329)	1:104:A:ALA:HA	1:221:A:PHE:H	2	0.35
(1,1329)	1:104:A:ALA:HA	1:221:A:PHE:H	6	0.35
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB2	2	0.35
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB3	2	0.35
(1,1274)	1:197:A:ASN:HA	1:202:A:THR:HA	3	0.35
(1,1274)	1:197:A:ASN:HA	1:202:A:THR:HA	6	0.35
(1,1256)	1:130:A:GLY:HA2	1:234:A:ILE:HA	3	0.35
(1,1256)	1:130:A:GLY:HA3	1:234:A:ILE:HA	3	0.35
(1,1248)	1:110:A:GLU:H	1:215:A:VAL:HB	7	0.35
(1,1148)	1:171:A:VAL:HA	1:174:A:ARG:H	7	0.35
(1,1077)	1:251:A:GLY:HA2	1:254:A:THR:H	1	0.35
(1,1077)	1:251:A:GLY:HA3	1:254:A:THR:H	1	0.35
(1,841)	1:208:A:GLN:HA	1:211:A:THR:H	2	0.35
(1,841)	1:208:A:GLN:HA	1:211:A:THR:H	5	0.35
(1,751)	1:177:A:GLU:HA	1:180:A:ARG:H	7	0.35
(1,751)	1:177:A:GLU:HA	1:180:A:ARG:H	10	0.35
(1,741)	1:179:A:MET:HA	1:183:A:LEU:H	2	0.35
(1,538)	1:125:A:LEU:HA	1:129:A:GLY:H	2	0.35
(1,512)	1:117:A:LYS:HA	1:120:A:ASP:H	7	0.35
(1,384)	1:97:A:HIS:HA	1:101:A:VAL:H	1	0.35
(1,379)	1:92:A:THR:HA	1:96:A:THR:H	8	0.35
(1,342)	1:90:A:ASN:H	1:92:A:THR:H	3	0.35
(1,268)	1:73:A:ASP:HA	1:77:A:GLN:H	4	0.35
(1,264)	1:68:A:VAL:HA	1:72:A:TRP:H	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:51:A:PHE:HA	1:54:A:ALA:H	9	0.35
(1,50)	1:24:A:VAL:HA	1:28:A:ALA:H	3	0.35
(2,98)	1:178:A:THR:H	1:202:A:THR:H	2	0.34
(2,94)	1:204:A:ARG:HA	1:209:A:MET:H	8	0.34
(2,30)	1:79:A:GLY:H	1:83:A:ASP:HB2	5	0.34
(2,30)	1:79:A:GLY:H	1:83:A:ASP:HB3	5	0.34
(1,1329)	1:104:A:ALA:HA	1:221:A:PHE:H	9	0.34
(1,1300)	1:120:A:ASP:H	1:34:A:VAL:HG11	1	0.34
(1,1281)	1:213:A:LEU:H	1:218:A:LEU:HG	6	0.34
(1,1256)	1:130:A:GLY:HA2	1:234:A:ILE:HA	1	0.34
(1,1256)	1:130:A:GLY:HA3	1:234:A:ILE:HA	1	0.34
(1,1249)	1:123:A:TYR:H	1:224:A:VAL:HA	8	0.34
(1,1248)	1:110:A:GLU:H	1:215:A:VAL:HB	4	0.34
(1,1234)	1:101:A:VAL:HA	1:223:A:GLU:H	5	0.34
(1,1226)	1:82:A:ALA:HA	1:144:A:TRP:H	3	0.34
(1,1197)	1:51:A:PHE:H	1:79:A:GLY:HA2	4	0.34
(1,1197)	1:51:A:PHE:H	1:79:A:GLY:HA3	4	0.34
(1,1151)	1:175:A:ALA:HA	1:179:A:MET:H	9	0.34
(1,1148)	1:171:A:VAL:HA	1:174:A:ARG:H	1	0.34
(1,1146)	1:135:A:GLY:HA2	1:138:A:ASP:H	2	0.34
(1,1146)	1:135:A:GLY:HA3	1:138:A:ASP:H	2	0.34
(1,1127)	1:35:A:VAL:H	1:36:A:LEU:HA	2	0.34
(1,1077)	1:251:A:GLY:HA2	1:254:A:THR:H	7	0.34
(1,1077)	1:251:A:GLY:HA3	1:254:A:THR:H	7	0.34
(1,1068)	1:247:A:LEU:HA	1:250:A:VAL:H	3	0.34
(1,1068)	1:247:A:LEU:HA	1:250:A:VAL:H	10	0.34
(1,997)	1:234:A:ILE:HA	1:238:A:LYS:H	6	0.34
(1,988)	1:238:A:LYS:HA	1:241:A:ASP:H	4	0.34
(1,907)	1:219:A:ASP:HA	1:222:A:ASP:H	3	0.34
(1,907)	1:219:A:ASP:HA	1:222:A:ASP:H	10	0.34
(1,847)	1:210:A:ILE:H	1:211:A:THR:H	6	0.34
(1,834)	1:202:A:THR:HA	1:205:A:VAL:H	4	0.34
(1,766)	1:194:A:GLN:H	1:195:A:LEU:H	7	0.34
(1,754)	1:180:A:ARG:HA	1:183:A:LEU:H	4	0.34
(1,750)	1:176:A:SER:HA	1:179:A:MET:H	4	0.34
(1,747)	1:185:A:TYR:HA	1:189:A:TYR:H	4	0.34
(1,730)	1:187:A:MET:H	1:189:A:TYR:H	4	0.34
(1,530)	1:118:A:GLU:HA	1:122:A:ASP:H	3	0.34
(1,515)	1:120:A:ASP:HA	1:123:A:TYR:H	9	0.34
(1,475)	1:115:A:ILE:H	1:117:A:LYS:H	9	0.34
(1,422)	1:113:A:TYR:H	1:114:A:GLU:H	10	0.34
(1,385)	1:98:A:ILE:HA	1:102:A:GLY:H	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	1:89:A:ASP:HA	1:92:A:THR:H	3	0.34
(1,365)	1:104:A:ALA:HA	1:106:A:ALA:H	10	0.34
(1,261)	1:74:A:TYR:HA	1:77:A:GLN:H	7	0.34
(1,246)	1:76:A:TYR:H	1:78:A:ILE:H	5	0.34
(1,240)	1:73:A:ASP:H	1:75:A:GLY:H	9	0.34
(1,240)	1:73:A:ASP:H	1:75:A:GLY:H	10	0.34
(1,203)	1:70:A:ALA:H	1:71:A:TRP:H	10	0.34
(1,181)	1:57:A:TRP:HA	1:60:A:MET:H	5	0.34
(1,171)	1:47:A:LEU:HA	1:50:A:ASP:H	1	0.34
(1,155)	1:59:A:ARG:HA	1:61:A:ASN:H	10	0.34
(1,139)	1:51:A:PHE:H	1:53:A:GLU:H	4	0.34
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB2	8	0.33
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB3	8	0.33
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG11	2	0.33
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG12	2	0.33
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG13	2	0.33
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG21	2	0.33
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG22	2	0.33
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG23	2	0.33
(2,24)	1:78:A:ILE:HD11	1:80:A:GLY:H	10	0.33
(2,24)	1:78:A:ILE:HD12	1:80:A:GLY:H	10	0.33
(2,24)	1:78:A:ILE:HD13	1:80:A:GLY:H	10	0.33
(1,1334)	1:177:A:GLU:H	1:202:A:THR:HA	6	0.33
(1,1314)	1:177:A:GLU:H	1:202:A:THR:HA	6	0.33
(1,1304)	1:48:A:ILE:H	1:144:A:TRP:HD1	1	0.33
(1,1234)	1:101:A:VAL:HA	1:223:A:GLU:H	7	0.33
(1,1219)	1:78:A:ILE:HA	1:83:A:ASP:H	1	0.33
(1,1186)	1:29:A:TYR:H	1:45:A:LEU:HA	10	0.33
(1,1147)	1:154:A:PRO:HA	1:158:A:LYS:H	8	0.33
(1,1075)	1:249:A:ASP:HA	1:252:A:GLU:H	6	0.33
(1,988)	1:238:A:LYS:HA	1:241:A:ASP:H	10	0.33
(1,983)	1:233:A:ARG:HA	1:236:A:GLN:H	1	0.33
(1,983)	1:233:A:ARG:HA	1:236:A:GLN:H	10	0.33
(1,981)	1:231:A:ASN:HA	1:234:A:ILE:H	6	0.33
(1,981)	1:231:A:ASN:HA	1:234:A:ILE:H	9	0.33
(1,954)	1:230:A:TRP:H	1:232:A:VAL:H	1	0.33
(1,911)	1:223:A:GLU:HA	1:226:A:THR:H	6	0.33
(1,888)	1:218:A:LEU:H	1:220:A:TYR:H	7	0.33
(1,840)	1:207:A:GLN:HA	1:210:A:ILE:H	9	0.33
(1,753)	1:179:A:MET:HA	1:182:A:SER:H	5	0.33
(1,751)	1:177:A:GLU:HA	1:180:A:ARG:H	4	0.33
(1,744)	1:182:A:SER:HA	1:186:A:LYS:H	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:182:A:SER:HA	1:186:A:LYS:H	2	0.33
(1,741)	1:179:A:MET:HA	1:183:A:LEU:H	9	0.33
(1,516)	1:121:A:VAL:HA	1:124:A:VAL:H	7	0.33
(1,510)	1:115:A:ILE:HA	1:118:A:GLU:H	7	0.33
(1,403)	1:109:A:GLU:H	1:111:A:LYS:H	10	0.33
(1,389)	1:102:A:GLY:HA2	1:106:A:ALA:H	3	0.33
(1,389)	1:102:A:GLY:HA3	1:106:A:ALA:H	3	0.33
(1,384)	1:97:A:HIS:HA	1:101:A:VAL:H	6	0.33
(1,373)	1:89:A:ASP:HA	1:92:A:THR:H	5	0.33
(1,373)	1:89:A:ASP:HA	1:92:A:THR:H	9	0.33
(1,367)	1:105:A:ASN:HA	1:107:A:SER:H	5	0.33
(1,365)	1:104:A:ALA:HA	1:106:A:ALA:H	4	0.33
(1,355)	1:99:A:ALA:HA	1:101:A:VAL:H	5	0.33
(1,342)	1:90:A:ASN:H	1:92:A:THR:H	10	0.33
(1,280)	1:84:A:ARG:H	1:85:A:THR:H	8	0.33
(1,261)	1:74:A:TYR:HA	1:77:A:GLN:H	8	0.33
(1,250)	1:77:A:GLN:HA	1:79:A:GLY:H	5	0.33
(1,243)	1:74:A:TYR:HA	1:76:A:TYR:H	6	0.33
(1,181)	1:57:A:TRP:HA	1:60:A:MET:H	7	0.33
(1,165)	1:53:A:GLU:HA	1:57:A:TRP:H	7	0.33
(1,165)	1:53:A:GLU:HA	1:57:A:TRP:H	10	0.33
(1,164)	1:52:A:ARG:HA	1:56:A:TYR:H	9	0.33
(1,157)	1:45:A:LEU:HA	1:49:A:ASP:H	3	0.33
(1,85)	1:46:A:ALA:H	1:47:A:LEU:H	7	0.33
(1,83)	1:45:A:LEU:H	1:46:A:ALA:H	8	0.33
(1,44)	1:24:A:VAL:HA	1:27:A:THR:H	7	0.33
(2,95)	1:210:A:ILE:HA	1:235:A:TYR:H	8	0.32
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG11	5	0.32
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG12	5	0.32
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG13	5	0.32
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG21	5	0.32
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG22	5	0.32
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG23	5	0.32
(2,25)	1:75:A:GLY:H	1:78:A:ILE:HG12	3	0.32
(2,25)	1:75:A:GLY:H	1:78:A:ILE:HG13	3	0.32
(2,9)	1:41:A:PRO:HD2	1:44:A:LYS:H	10	0.32
(2,9)	1:41:A:PRO:HD3	1:44:A:LYS:H	10	0.32
(1,1299)	1:26:A:ARG:H	1:121:A:VAL:HG11	6	0.32
(1,1263)	1:134:A:PHE:H	1:233:A:ARG:HB2	7	0.32
(1,1263)	1:134:A:PHE:H	1:233:A:ARG:HB3	7	0.32
(1,1219)	1:78:A:ILE:HA	1:83:A:ASP:H	10	0.32
(1,1217)	1:77:A:GLN:H	1:98:A:ILE:HG13	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1178)	1:29:A:TYR:H	1:46:A:ALA:HB1	4	0.32
(1,1178)	1:29:A:TYR:H	1:46:A:ALA:HB2	4	0.32
(1,1178)	1:29:A:TYR:H	1:46:A:ALA:HB3	4	0.32
(1,1151)	1:175:A:ALA:HA	1:179:A:MET:H	3	0.32
(1,1123)	1:269:A:LEU:HA	1:271:A:LEU:H	7	0.32
(1,915)	1:220:A:TYR:HA	1:224:A:VAL:H	1	0.32
(1,844)	1:202:A:THR:HA	1:206:A:ARG:H	4	0.32
(1,763)	1:189:A:TYR:HA	1:192:A:PHE:H	3	0.32
(1,756)	1:182:A:SER:HA	1:185:A:TYR:H	4	0.32
(1,723)	1:183:A:LEU:HA	1:185:A:TYR:H	9	0.32
(1,538)	1:125:A:LEU:HA	1:129:A:GLY:H	10	0.32
(1,533)	1:120:A:ASP:HA	1:124:A:VAL:H	2	0.32
(1,519)	1:124:A:VAL:HA	1:127:A:ILE:H	2	0.32
(1,519)	1:124:A:VAL:HA	1:127:A:ILE:H	7	0.32
(1,515)	1:120:A:ASP:HA	1:123:A:TYR:H	3	0.32
(1,404)	1:109:A:GLU:H	1:111:A:LYS:HB2	5	0.32
(1,387)	1:100:A:ILE:HA	1:104:A:ALA:H	6	0.32
(1,376)	1:92:A:THR:HA	1:95:A:ASN:H	7	0.32
(1,232)	1:69:A:ALA:H	1:71:A:TRP:H	9	0.32
(1,164)	1:52:A:ARG:HA	1:56:A:TYR:H	3	0.32
(1,139)	1:51:A:PHE:H	1:53:A:GLU:H	8	0.32
(1,83)	1:45:A:LEU:H	1:46:A:ALA:H	9	0.32
(1,78)	1:34:A:VAL:H	1:36:A:LEU:H	4	0.32
(1,40)	1:21:A:SER:HA	1:24:A:VAL:H	7	0.32
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB2	2	0.31
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB3	2	0.31
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG11	6	0.31
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG12	6	0.31
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG13	6	0.31
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG21	6	0.31
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG22	6	0.31
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG23	6	0.31
(1,1333)	1:174:A:ARG:H	1:198:A:GLY:HA2	6	0.31
(1,1333)	1:174:A:ARG:H	1:198:A:GLY:HA3	6	0.31
(1,1306)	1:49:A:ASP:H	1:144:A:TRP:HD1	7	0.31
(1,1304)	1:48:A:ILE:H	1:144:A:TRP:HD1	10	0.31
(1,1274)	1:197:A:ASN:HA	1:202:A:THR:HA	8	0.31
(1,1256)	1:130:A:GLY:HA2	1:234:A:ILE:HA	9	0.31
(1,1256)	1:130:A:GLY:HA3	1:234:A:ILE:HA	9	0.31
(1,1248)	1:110:A:GLU:H	1:215:A:VAL:HB	2	0.31
(1,1246)	1:106:A:ALA:H	1:113:A:TYR:H	9	0.31
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD11	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD12	5	0.31
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD13	5	0.31
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD21	5	0.31
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD22	5	0.31
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD23	5	0.31
(1,1228)	1:93:A:TRP:H	1:64:A:GLU:HA	10	0.31
(1,1153)	1:237:A:LEU:HA	1:241:A:ASP:H	4	0.31
(1,1152)	1:194:A:GLN:HA	1:197:A:ASN:H	4	0.31
(1,1152)	1:194:A:GLN:HA	1:197:A:ASN:H	9	0.31
(1,1000)	1:237:A:LEU:HA	1:241:A:ASP:H	4	0.31
(1,985)	1:235:A:TYR:HA	1:238:A:LYS:H	2	0.31
(1,918)	1:223:A:GLU:HA	1:227:A:SER:H	1	0.31
(1,914)	1:219:A:ASP:HA	1:223:A:GLU:H	7	0.31
(1,911)	1:223:A:GLU:HA	1:226:A:THR:H	4	0.31
(1,910)	1:222:A:ASP:HA	1:225:A:PHE:H	9	0.31
(1,777)	1:198:A:GLY:H	1:199:A:GLY:H	4	0.31
(1,777)	1:198:A:GLY:H	1:199:A:GLY:H	9	0.31
(1,754)	1:180:A:ARG:HA	1:183:A:LEU:H	7	0.31
(1,742)	1:180:A:ARG:HA	1:184:A:LEU:H	7	0.31
(1,523)	1:127:A:ILE:HA	1:130:A:GLY:H	10	0.31
(1,379)	1:92:A:THR:HA	1:96:A:THR:H	4	0.31
(1,373)	1:89:A:ASP:HA	1:92:A:THR:H	2	0.31
(1,362)	1:103:A:LYS:H	1:105:A:ASN:H	4	0.31
(1,343)	1:91:A:ASN:H	1:93:A:TRP:H	6	0.31
(1,329)	1:104:A:ALA:H	1:105:A:ASN:H	5	0.31
(1,258)	1:71:A:TRP:HA	1:74:A:TYR:H	7	0.31
(1,252)	1:67:A:LYS:HA	1:70:A:ALA:H	10	0.31
(1,246)	1:76:A:TYR:H	1:78:A:ILE:H	7	0.31
(1,238)	1:72:A:TRP:H	1:74:A:TYR:H	9	0.31
(1,178)	1:54:A:ALA:HA	1:57:A:TRP:H	2	0.31
(1,129)	1:46:A:ALA:H	1:48:A:ILE:H	7	0.31
(1,30)	1:23:A:TRP:HA	1:25:A:THR:H	1	0.31
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB2	6	0.3
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB3	6	0.3
(1,1324)	1:51:A:PHE:H	1:81:A:MET:HA	5	0.3
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB2	10	0.3
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB3	10	0.3
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB2	1	0.3
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB3	1	0.3
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG11	6	0.3
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG12	6	0.3
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG13	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG21	6	0.3
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG22	6	0.3
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG23	6	0.3
(1,1248)	1:110:A:GLU:H	1:215:A:VAL:HB	8	0.3
(1,1234)	1:101:A:VAL:HA	1:223:A:GLU:H	2	0.3
(1,1234)	1:101:A:VAL:HA	1:223:A:GLU:H	9	0.3
(1,1209)	1:63:A:ASP:H	1:265:A:LYS:H	8	0.3
(1,1180)	1:29:A:TYR:HA	1:46:A:ALA:H	6	0.3
(1,1166)	1:23:A:TRP:H	1:45:A:LEU:HA	10	0.3
(1,1147)	1:154:A:PRO:HA	1:158:A:LYS:H	1	0.3
(1,1087)	1:260:A:THR:H	1:261:A:ARG:H	8	0.3
(1,1068)	1:247:A:LEU:HA	1:250:A:VAL:H	8	0.3
(1,994)	1:231:A:ASN:HA	1:235:A:TYR:H	1	0.3
(1,992)	1:229:A:ASN:HA	1:233:A:ARG:H	1	0.3
(1,980)	1:230:A:TRP:HA	1:233:A:ARG:H	6	0.3
(1,914)	1:219:A:ASP:HA	1:223:A:GLU:H	2	0.3
(1,847)	1:210:A:ILE:H	1:211:A:THR:H	10	0.3
(1,835)	1:202:A:THR:HB	1:205:A:VAL:H	3	0.3
(1,835)	1:202:A:THR:HB	1:205:A:VAL:H	5	0.3
(1,763)	1:189:A:TYR:HA	1:192:A:PHE:H	1	0.3
(1,756)	1:182:A:SER:HA	1:185:A:TYR:H	10	0.3
(1,723)	1:183:A:LEU:HA	1:185:A:TYR:H	7	0.3
(1,533)	1:120:A:ASP:HA	1:124:A:VAL:H	3	0.3
(1,526)	1:114:A:GLU:HA	1:118:A:GLU:H	10	0.3
(1,513)	1:118:A:GLU:HA	1:121:A:VAL:H	2	0.3
(1,508)	1:130:A:GLY:H	1:132:A:ILE:H	9	0.3
(1,475)	1:115:A:ILE:H	1:117:A:LYS:H	8	0.3
(1,473)	1:114:A:GLU:H	1:116:A:LEU:H	9	0.3
(1,402)	1:104:A:ALA:HA	1:107:A:SER:H	10	0.3
(1,389)	1:102:A:GLY:HA2	1:106:A:ALA:H	4	0.3
(1,389)	1:102:A:GLY:HA3	1:106:A:ALA:H	4	0.3
(1,340)	1:86:A:THR:H	1:88:A:VAL:H	8	0.3
(1,264)	1:68:A:VAL:HA	1:72:A:TRP:H	5	0.3
(1,259)	1:72:A:TRP:HA	1:75:A:GLY:H	3	0.3
(1,252)	1:67:A:LYS:HA	1:70:A:ALA:H	3	0.3
(1,176)	1:52:A:ARG:HA	1:55:A:TYR:H	5	0.3
(1,176)	1:52:A:ARG:HA	1:55:A:TYR:H	7	0.3
(1,175)	1:51:A:PHE:HA	1:54:A:ALA:H	4	0.3
(1,174)	1:50:A:ASP:HA	1:53:A:GLU:H	3	0.3
(1,162)	1:50:A:ASP:HA	1:54:A:ALA:H	2	0.3
(1,161)	1:49:A:ASP:HA	1:53:A:GLU:H	4	0.3
(1,142)	1:52:A:ARG:HA	1:54:A:ALA:H	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,140)	1:51:A:PHE:HA	1:53:A:GLU:H	7	0.3
(2,99)	1:76:A:TYR:HA	1:87:A:LEU:H	1	0.29
(2,89)	1:123:A:TYR:HA	1:226:A:THR:H	7	0.29
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG11	7	0.29
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG12	7	0.29
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG13	7	0.29
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG21	7	0.29
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG22	7	0.29
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG23	7	0.29
(1,1334)	1:177:A:GLU:H	1:202:A:THR:HA	1	0.29
(1,1323)	1:35:A:VAL:HA	1:102:A:GLY:H	10	0.29
(1,1314)	1:177:A:GLU:H	1:202:A:THR:HA	1	0.29
(1,1308)	1:54:A:ALA:HA	1:142:A:PHE:H	7	0.29
(1,1304)	1:48:A:ILE:H	1:144:A:TRP:HD1	7	0.29
(1,1302)	1:36:A:LEU:H	1:99:A:ALA:HA	4	0.29
(1,1302)	1:36:A:LEU:H	1:99:A:ALA:HA	6	0.29
(1,1301)	1:35:A:VAL:HA	1:102:A:GLY:H	10	0.29
(1,1299)	1:26:A:ARG:H	1:121:A:VAL:HG11	8	0.29
(1,1259)	1:132:A:ILE:H	1:237:A:LEU:HB2	5	0.29
(1,1259)	1:132:A:ILE:H	1:237:A:LEU:HB3	5	0.29
(1,1259)	1:132:A:ILE:H	1:237:A:LEU:HB2	7	0.29
(1,1259)	1:132:A:ILE:H	1:237:A:LEU:HB3	7	0.29
(1,1202)	1:54:A:ALA:HA	1:142:A:PHE:H	7	0.29
(1,1200)	1:54:A:ALA:H	1:82:A:ALA:H	7	0.29
(1,1177)	1:26:A:ARG:H	1:45:A:LEU:H	7	0.29
(1,1162)	1:268:A:GLU:HA	1:271:A:LEU:H	5	0.29
(1,1150)	1:174:A:ARG:H	1:177:A:GLU:HB2	10	0.29
(1,1142)	1:213:A:LEU:H	1:214:A:ASP:HA	3	0.29
(1,997)	1:234:A:ILE:HA	1:238:A:LYS:H	9	0.29
(1,992)	1:229:A:ASN:HA	1:233:A:ARG:H	4	0.29
(1,988)	1:238:A:LYS:HA	1:241:A:ASP:H	9	0.29
(1,981)	1:231:A:ASN:HA	1:234:A:ILE:H	2	0.29
(1,952)	1:229:A:ASN:H	1:231:A:ASN:H	2	0.29
(1,918)	1:223:A:GLU:HA	1:227:A:SER:H	8	0.29
(1,912)	1:224:A:VAL:HA	1:227:A:SER:H	9	0.29
(1,834)	1:202:A:THR:HA	1:205:A:VAL:H	8	0.29
(1,832)	1:200:A:GLN:HA	1:203:A:ASP:H	9	0.29
(1,755)	1:181:A:ASN:HA	1:184:A:LEU:H	1	0.29
(1,753)	1:179:A:MET:HA	1:182:A:SER:H	8	0.29
(1,746)	1:184:A:LEU:HA	1:188:A:SER:H	6	0.29
(1,739)	1:177:A:GLU:HA	1:181:A:ASN:H	4	0.29
(1,537)	1:124:A:VAL:HA	1:128:A:PHE:H	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,526)	1:114:A:GLU:HA	1:118:A:GLU:H	1	0.29
(1,512)	1:117:A:LYS:HA	1:120:A:ASP:H	5	0.29
(1,511)	1:116:A:LEU:HA	1:119:A:HIS:H	10	0.29
(1,473)	1:114:A:GLU:H	1:116:A:LEU:H	1	0.29
(1,412)	1:109:A:GLU:H	1:110:A:GLU:H	5	0.29
(1,404)	1:109:A:GLU:H	1:111:A:LYS:HB2	10	0.29
(1,398)	1:100:A:ILE:HA	1:103:A:LYS:H	7	0.29
(1,390)	1:103:A:LYS:HA	1:107:A:SER:H	3	0.29
(1,388)	1:101:A:VAL:HA	1:105:A:ASN:H	1	0.29
(1,384)	1:97:A:HIS:HA	1:101:A:VAL:H	5	0.29
(1,373)	1:89:A:ASP:HA	1:92:A:THR:H	6	0.29
(1,373)	1:89:A:ASP:HA	1:92:A:THR:H	7	0.29
(1,362)	1:103:A:LYS:H	1:105:A:ASN:H	5	0.29
(1,343)	1:91:A:ASN:H	1:93:A:TRP:H	9	0.29
(1,338)	1:84:A:ARG:H	1:86:A:THR:H	8	0.29
(1,269)	1:79:A:GLY:H	1:80:A:GLY:H	9	0.29
(1,268)	1:73:A:ASP:HA	1:77:A:GLN:H	8	0.29
(1,259)	1:72:A:TRP:HA	1:75:A:GLY:H	4	0.29
(1,250)	1:77:A:GLN:HA	1:79:A:GLY:H	1	0.29
(1,246)	1:76:A:TYR:H	1:78:A:ILE:H	2	0.29
(1,80)	1:42:A:ASP:HB2	1:44:A:LYS:H	8	0.29
(1,80)	1:42:A:ASP:HB3	1:44:A:LYS:H	8	0.29
(1,45)	1:25:A:THR:HA	1:28:A:ALA:H	5	0.29
(1,25)	1:21:A:SER:H	1:23:A:TRP:H	2	0.29
(2,98)	1:178:A:THR:H	1:202:A:THR:H	3	0.28
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG11	10	0.28
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG12	10	0.28
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG13	10	0.28
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG21	10	0.28
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG22	10	0.28
(2,81)	1:47:A:LEU:H	1:121:A:VAL:HG23	10	0.28
(2,25)	1:75:A:GLY:H	1:78:A:ILE:HG12	10	0.28
(2,25)	1:75:A:GLY:H	1:78:A:ILE:HG13	10	0.28
(1,1310)	1:134:A:PHE:H	1:234:A:ILE:HD11	7	0.28
(1,1308)	1:54:A:ALA:HA	1:142:A:PHE:H	3	0.28
(1,1306)	1:49:A:ASP:H	1:144:A:TRP:HD1	2	0.28
(1,1306)	1:49:A:ASP:H	1:144:A:TRP:HD1	10	0.28
(1,1287)	1:260:A:THR:HA	1:265:A:LYS:H	7	0.28
(1,1246)	1:106:A:ALA:H	1:113:A:TYR:H	7	0.28
(1,1244)	1:106:A:ALA:HA	1:111:A:LYS:H	8	0.28
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD11	6	0.28
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD12	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD13	6	0.28
(1,1233)	1:101:A:VAL:H	1:219:A:ASP:HA	8	0.28
(1,1229)	1:98:A:ILE:H	1:255:A:ARG:HG2	4	0.28
(1,1229)	1:98:A:ILE:H	1:255:A:ARG:HG3	4	0.28
(1,1226)	1:82:A:ALA:HA	1:144:A:TRP:H	7	0.28
(1,1217)	1:77:A:GLN:H	1:98:A:ILE:HG13	3	0.28
(1,1203)	1:56:A:TYR:H	1:72:A:TRP:H	3	0.28
(1,1202)	1:54:A:ALA:HA	1:142:A:PHE:H	3	0.28
(1,1077)	1:251:A:GLY:HA2	1:254:A:THR:H	6	0.28
(1,1077)	1:251:A:GLY:HA3	1:254:A:THR:H	6	0.28
(1,1075)	1:249:A:ASP:HA	1:252:A:GLU:H	3	0.28
(1,1068)	1:247:A:LEU:HA	1:250:A:VAL:H	2	0.28
(1,996)	1:233:A:ARG:HA	1:237:A:LEU:H	5	0.28
(1,984)	1:234:A:ILE:HA	1:237:A:LEU:H	5	0.28
(1,979)	1:229:A:ASN:HA	1:232:A:VAL:H	7	0.28
(1,911)	1:223:A:GLU:HA	1:226:A:THR:H	5	0.28
(1,910)	1:222:A:ASP:HA	1:225:A:PHE:H	10	0.28
(1,847)	1:210:A:ILE:H	1:211:A:THR:H	5	0.28
(1,840)	1:207:A:GLN:HA	1:210:A:ILE:H	8	0.28
(1,829)	1:206:A:ARG:HB2	1:208:A:GLN:H	2	0.28
(1,829)	1:206:A:ARG:HB3	1:208:A:GLN:H	2	0.28
(1,753)	1:179:A:MET:HA	1:182:A:SER:H	6	0.28
(1,751)	1:177:A:GLU:HA	1:180:A:ARG:H	1	0.28
(1,747)	1:185:A:TYR:HA	1:189:A:TYR:H	1	0.28
(1,741)	1:179:A:MET:HA	1:183:A:LEU:H	1	0.28
(1,584)	1:154:A:PRO:HD2	1:156:A:GLU:H	5	0.28
(1,584)	1:154:A:PRO:HD3	1:156:A:GLU:H	5	0.28
(1,565)	1:148:A:ILE:H	1:149:A:SER:H	1	0.28
(1,516)	1:121:A:VAL:HA	1:124:A:VAL:H	4	0.28
(1,399)	1:101:A:VAL:HA	1:104:A:ALA:H	2	0.28
(1,384)	1:97:A:HIS:HA	1:101:A:VAL:H	3	0.28
(1,380)	1:93:A:TRP:HA	1:97:A:HIS:H	9	0.28
(1,343)	1:91:A:ASN:H	1:93:A:TRP:H	4	0.28
(1,342)	1:90:A:ASN:H	1:92:A:THR:H	9	0.28
(1,264)	1:68:A:VAL:HA	1:72:A:TRP:H	6	0.28
(1,261)	1:74:A:TYR:HA	1:77:A:GLN:H	3	0.28
(1,232)	1:69:A:ALA:H	1:71:A:TRP:H	5	0.28
(1,175)	1:51:A:PHE:HA	1:54:A:ALA:H	1	0.28
(1,174)	1:50:A:ASP:HA	1:53:A:GLU:H	6	0.28
(1,165)	1:53:A:GLU:HA	1:57:A:TRP:H	6	0.28
(1,163)	1:51:A:PHE:HA	1:55:A:TYR:H	4	0.28
(1,163)	1:51:A:PHE:HA	1:55:A:TYR:H	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:24:A:VAL:HA	1:27:A:THR:H	4	0.28
(1,44)	1:24:A:VAL:HA	1:27:A:THR:H	5	0.28
(1,30)	1:23:A:TRP:HA	1:25:A:THR:H	5	0.28
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG11	6	0.27
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG12	6	0.27
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG13	6	0.27
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG21	6	0.27
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG22	6	0.27
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG23	6	0.27
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG11	6	0.27
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG12	6	0.27
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG13	6	0.27
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG21	6	0.27
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG22	6	0.27
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG23	6	0.27
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG11	6	0.27
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG12	6	0.27
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG13	6	0.27
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG21	6	0.27
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG22	6	0.27
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG23	6	0.27
(2,30)	1:79:A:GLY:H	1:83:A:ASP:HB2	10	0.27
(2,30)	1:79:A:GLY:H	1:83:A:ASP:HB3	10	0.27
(1,1318)	1:53:A:GLU:H	1:80:A:GLY:H	4	0.27
(1,1317)	1:53:A:GLU:H	1:79:A:GLY:H	4	0.27
(1,1305)	1:48:A:ILE:H	1:144:A:TRP:HZ2	1	0.27
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD11	9	0.27
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD12	9	0.27
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD13	9	0.27
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD21	9	0.27
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD22	9	0.27
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD23	9	0.27
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG11	3	0.27
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG12	3	0.27
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG13	3	0.27
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG21	3	0.27
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG22	3	0.27
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG23	3	0.27
(1,1274)	1:197:A:ASN:HA	1:202:A:THR:HA	2	0.27
(1,1256)	1:130:A:GLY:HA2	1:234:A:ILE:HA	10	0.27
(1,1256)	1:130:A:GLY:HA3	1:234:A:ILE:HA	10	0.27
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG11	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG12	6	0.27
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG13	6	0.27
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG21	6	0.27
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG22	6	0.27
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG23	6	0.27
(1,1234)	1:101:A:VAL:HA	1:223:A:GLU:H	1	0.27
(1,1225)	1:82:A:ALA:H	1:144:A:TRP:HA	6	0.27
(1,1217)	1:77:A:GLN:H	1:98:A:ILE:HG13	8	0.27
(1,1207)	1:62:A:SER:HA	1:67:A:LYS:H	8	0.27
(1,1203)	1:56:A:TYR:H	1:72:A:TRP:H	6	0.27
(1,1198)	1:51:A:PHE:H	1:80:A:GLY:HA2	3	0.27
(1,1198)	1:51:A:PHE:H	1:80:A:GLY:HA3	3	0.27
(1,1153)	1:237:A:LEU:HA	1:241:A:ASP:H	5	0.27
(1,1125)	1:270:A:GLY:HA2	1:272:A:ARG:H	3	0.27
(1,1125)	1:270:A:GLY:HA3	1:272:A:ARG:H	3	0.27
(1,1068)	1:247:A:LEU:HA	1:250:A:VAL:H	5	0.27
(1,1001)	1:238:A:LYS:HA	1:242:A:ALA:H	4	0.27
(1,1000)	1:237:A:LEU:HA	1:241:A:ASP:H	5	0.27
(1,993)	1:230:A:TRP:HA	1:234:A:ILE:H	2	0.27
(1,984)	1:234:A:ILE:HA	1:237:A:LEU:H	9	0.27
(1,918)	1:223:A:GLU:HA	1:227:A:SER:H	4	0.27
(1,906)	1:218:A:LEU:HA	1:221:A:PHE:H	3	0.27
(1,839)	1:206:A:ARG:HA	1:209:A:MET:H	10	0.27
(1,838)	1:205:A:VAL:HA	1:208:A:GLN:H	6	0.27
(1,835)	1:202:A:THR:HB	1:205:A:VAL:H	10	0.27
(1,534)	1:121:A:VAL:HA	1:125:A:LEU:H	6	0.27
(1,529)	1:117:A:LYS:HA	1:121:A:VAL:H	2	0.27
(1,516)	1:121:A:VAL:HA	1:124:A:VAL:H	5	0.27
(1,513)	1:118:A:GLU:HA	1:121:A:VAL:H	8	0.27
(1,512)	1:117:A:LYS:HA	1:120:A:ASP:H	6	0.27
(1,475)	1:115:A:ILE:H	1:117:A:LYS:H	1	0.27
(1,387)	1:100:A:ILE:HA	1:104:A:ALA:H	2	0.27
(1,385)	1:98:A:ILE:HA	1:102:A:GLY:H	1	0.27
(1,376)	1:92:A:THR:HA	1:95:A:ASN:H	8	0.27
(1,266)	1:70:A:ALA:HA	1:74:A:TYR:H	5	0.27
(1,261)	1:74:A:TYR:HA	1:77:A:GLN:H	2	0.27
(1,246)	1:76:A:TYR:H	1:78:A:ILE:H	6	0.27
(1,173)	1:49:A:ASP:HA	1:52:A:ARG:H	1	0.27
(1,161)	1:49:A:ASP:HA	1:53:A:GLU:H	10	0.27
(1,160)	1:48:A:ILE:HA	1:52:A:ARG:H	5	0.27
(1,142)	1:52:A:ARG:HA	1:54:A:ALA:H	5	0.27
(1,40)	1:21:A:SER:HA	1:24:A:VAL:H	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,99)	1:76:A:TYR:HA	1:87:A:LEU:H	7	0.26
(2,94)	1:204:A:ARG:HA	1:209:A:MET:H	7	0.26
(1,1324)	1:51:A:PHE:H	1:81:A:MET:HA	8	0.26
(1,1317)	1:53:A:GLU:H	1:79:A:GLY:H	2	0.26
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD11	6	0.26
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD12	6	0.26
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD13	6	0.26
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD21	6	0.26
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD22	6	0.26
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD23	6	0.26
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB2	8	0.26
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB3	8	0.26
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG11	1	0.26
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG12	1	0.26
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG13	1	0.26
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG21	1	0.26
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG22	1	0.26
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG23	1	0.26
(1,1274)	1:197:A:ASN:HA	1:202:A:THR:HA	7	0.26
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB2	3	0.26
(1,1253)	1:126:A:VAL:H	1:190:A:LYS:HB3	3	0.26
(1,1249)	1:123:A:TYR:H	1:224:A:VAL:HA	7	0.26
(1,1228)	1:93:A:TRP:H	1:64:A:GLU:HA	4	0.26
(1,1210)	1:64:A:GLU:H	1:263:A:SER:H	3	0.26
(1,1209)	1:63:A:ASP:H	1:265:A:LYS:H	3	0.26
(1,1207)	1:62:A:SER:HA	1:67:A:LYS:H	3	0.26
(1,1205)	1:56:A:TYR:H	1:76:A:TYR:HA	8	0.26
(1,1203)	1:56:A:TYR:H	1:72:A:TRP:H	5	0.26
(1,1167)	1:24:A:VAL:H	1:192:A:PHE:HE1	1	0.26
(1,1167)	1:24:A:VAL:H	1:192:A:PHE:HE2	1	0.26
(1,1165)	1:22:A:THR:HB	1:45:A:LEU:H	5	0.26
(1,1160)	1:261:A:ARG:H	1:264:A:ILE:HA	8	0.26
(1,1090)	1:261:A:ARG:H	1:262:A:ARG:H	8	0.26
(1,1089)	1:260:A:THR:HB	1:261:A:ARG:H	6	0.26
(1,1088)	1:260:A:THR:HA	1:261:A:ARG:H	7	0.26
(1,1087)	1:260:A:THR:H	1:261:A:ARG:H	3	0.26
(1,1087)	1:260:A:THR:H	1:261:A:ARG:H	10	0.26
(1,1024)	1:244:A:GLY:H	1:246:A:THR:H	1	0.26
(1,1001)	1:238:A:LYS:HA	1:242:A:ALA:H	3	0.26
(1,1001)	1:238:A:LYS:HA	1:242:A:ALA:H	9	0.26
(1,997)	1:234:A:ILE:HA	1:238:A:LYS:H	8	0.26
(1,996)	1:233:A:ARG:HA	1:237:A:LEU:H	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,992)	1:229:A:ASN:HA	1:233:A:ARG:H	2	0.26
(1,988)	1:238:A:LYS:HA	1:241:A:ASP:H	3	0.26
(1,981)	1:231:A:ASN:HA	1:234:A:ILE:H	8	0.26
(1,979)	1:229:A:ASN:HA	1:232:A:VAL:H	5	0.26
(1,954)	1:230:A:TRP:H	1:232:A:VAL:H	7	0.26
(1,914)	1:219:A:ASP:HA	1:223:A:GLU:H	8	0.26
(1,911)	1:223:A:GLU:HA	1:226:A:THR:H	2	0.26
(1,907)	1:219:A:ASP:HA	1:222:A:ASP:H	2	0.26
(1,837)	1:204:A:ARG:HA	1:207:A:GLN:H	8	0.26
(1,834)	1:202:A:THR:HA	1:205:A:VAL:H	10	0.26
(1,777)	1:198:A:GLY:H	1:199:A:GLY:H	5	0.26
(1,759)	1:185:A:TYR:HA	1:188:A:SER:H	2	0.26
(1,712)	1:177:A:GLU:HA	1:179:A:MET:H	10	0.26
(1,539)	1:126:A:VAL:HA	1:130:A:GLY:H	9	0.26
(1,538)	1:125:A:LEU:HA	1:129:A:GLY:H	8	0.26
(1,534)	1:121:A:VAL:HA	1:125:A:LEU:H	5	0.26
(1,529)	1:117:A:LYS:HA	1:121:A:VAL:H	6	0.26
(1,528)	1:116:A:LEU:HA	1:120:A:ASP:H	1	0.26
(1,515)	1:120:A:ASP:HA	1:123:A:TYR:H	5	0.26
(1,512)	1:117:A:LYS:HA	1:120:A:ASP:H	2	0.26
(1,399)	1:101:A:VAL:HA	1:104:A:ALA:H	6	0.26
(1,365)	1:104:A:ALA:HA	1:106:A:ALA:H	6	0.26
(1,355)	1:99:A:ALA:HA	1:101:A:VAL:H	4	0.26
(1,354)	1:99:A:ALA:H	1:101:A:VAL:H	10	0.26
(1,160)	1:48:A:ILE:HA	1:52:A:ARG:H	10	0.26
(1,140)	1:51:A:PHE:HA	1:53:A:GLU:H	1	0.26
(1,50)	1:24:A:VAL:HA	1:28:A:ALA:H	9	0.26
(1,45)	1:25:A:THR:HA	1:28:A:ALA:H	7	0.26
(1,42)	1:23:A:TRP:HA	1:26:A:ARG:H	6	0.26
(1,42)	1:23:A:TRP:HA	1:26:A:ARG:H	7	0.26
(1,40)	1:21:A:SER:HA	1:24:A:VAL:H	3	0.26
(2,98)	1:178:A:THR:H	1:202:A:THR:H	7	0.25
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD11	7	0.25
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD12	7	0.25
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD13	7	0.25
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD21	7	0.25
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD22	7	0.25
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD23	7	0.25
(2,41)	1:113:A:TYR:HE1	1:115:A:ILE:H	7	0.25
(2,41)	1:113:A:TYR:HE2	1:115:A:ILE:H	7	0.25
(1,1333)	1:174:A:ARG:H	1:198:A:GLY:HA2	10	0.25
(1,1333)	1:174:A:ARG:H	1:198:A:GLY:HA3	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1304)	1:48:A:ILE:H	1:144:A:TRP:HD1	8	0.25
(1,1300)	1:120:A:ASP:H	1:34:A:VAL:HG11	4	0.25
(1,1299)	1:26:A:ARG:H	1:121:A:VAL:HG11	2	0.25
(1,1286)	1:253:A:LEU:H	1:67:A:LYS:HA	9	0.25
(1,1274)	1:197:A:ASN:HA	1:202:A:THR:HA	5	0.25
(1,1262)	1:133:A:GLY:HA2	1:235:A:TYR:H	6	0.25
(1,1262)	1:133:A:GLY:HA3	1:235:A:TYR:H	6	0.25
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD11	2	0.25
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD12	2	0.25
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD13	2	0.25
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD21	2	0.25
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD22	2	0.25
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD23	2	0.25
(1,1226)	1:82:A:ALA:HA	1:144:A:TRP:H	8	0.25
(1,1216)	1:71:A:TRP:H	1:255:A:ARG:HG2	5	0.25
(1,1216)	1:71:A:TRP:H	1:255:A:ARG:HG3	5	0.25
(1,1203)	1:56:A:TYR:H	1:72:A:TRP:H	8	0.25
(1,1199)	1:52:A:ARG:H	1:76:A:TYR:H	1	0.25
(1,1151)	1:175:A:ALA:HA	1:179:A:MET:H	2	0.25
(1,1142)	1:213:A:LEU:H	1:214:A:ASP:HA	8	0.25
(1,1074)	1:248:A:ARG:HG2	1:251:A:GLY:H	5	0.25
(1,1001)	1:238:A:LYS:HA	1:242:A:ALA:H	1	0.25
(1,992)	1:229:A:ASN:HA	1:233:A:ARG:H	8	0.25
(1,989)	1:239:A:LYS:HA	1:242:A:ALA:H	6	0.25
(1,984)	1:234:A:ILE:HA	1:237:A:LEU:H	6	0.25
(1,979)	1:229:A:ASN:HA	1:232:A:VAL:H	6	0.25
(1,915)	1:220:A:TYR:HA	1:224:A:VAL:H	8	0.25
(1,908)	1:220:A:TYR:HA	1:223:A:GLU:H	1	0.25
(1,908)	1:220:A:TYR:HA	1:223:A:GLU:H	2	0.25
(1,891)	1:219:A:ASP:HA	1:221:A:PHE:H	2	0.25
(1,885)	1:227:A:SER:H	1:228:A:GLU:H	5	0.25
(1,852)	1:213:A:LEU:H	1:214:A:ASP:H	7	0.25
(1,841)	1:208:A:GLN:HA	1:211:A:THR:H	10	0.25
(1,840)	1:207:A:GLN:HA	1:210:A:ILE:H	2	0.25
(1,840)	1:207:A:GLN:HA	1:210:A:ILE:H	5	0.25
(1,837)	1:204:A:ARG:HA	1:207:A:GLN:H	1	0.25
(1,726)	1:185:A:TYR:H	1:187:A:MET:H	7	0.25
(1,584)	1:154:A:PRO:HD2	1:156:A:GLU:H	1	0.25
(1,584)	1:154:A:PRO:HD3	1:156:A:GLU:H	1	0.25
(1,532)	1:119:A:HIS:HA	1:123:A:TYR:H	2	0.25
(1,530)	1:118:A:GLU:HA	1:122:A:ASP:H	2	0.25
(1,526)	1:114:A:GLU:HA	1:118:A:GLU:H	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,523)	1:127:A:ILE:HA	1:130:A:GLY:H	5	0.25
(1,511)	1:116:A:LEU:HA	1:119:A:HIS:H	8	0.25
(1,508)	1:130:A:GLY:H	1:132:A:ILE:H	2	0.25
(1,508)	1:130:A:GLY:H	1:132:A:ILE:H	3	0.25
(1,473)	1:114:A:GLU:H	1:116:A:LEU:H	3	0.25
(1,473)	1:114:A:GLU:H	1:116:A:LEU:H	10	0.25
(1,401)	1:103:A:LYS:HA	1:106:A:ALA:H	10	0.25
(1,399)	1:101:A:VAL:HA	1:104:A:ALA:H	1	0.25
(1,399)	1:101:A:VAL:HA	1:104:A:ALA:H	7	0.25
(1,386)	1:99:A:ALA:HA	1:103:A:LYS:H	3	0.25
(1,384)	1:97:A:HIS:HA	1:101:A:VAL:H	4	0.25
(1,372)	1:88:A:VAL:HA	1:91:A:ASN:H	5	0.25
(1,261)	1:74:A:TYR:HA	1:77:A:GLN:H	5	0.25
(1,231)	1:68:A:VAL:H	1:70:A:ALA:H	10	0.25
(1,228)	1:66:A:SER:HA	1:68:A:VAL:H	10	0.25
(1,178)	1:54:A:ALA:HA	1:57:A:TRP:H	9	0.25
(1,178)	1:54:A:ALA:HA	1:57:A:TRP:H	10	0.25
(1,164)	1:52:A:ARG:HA	1:56:A:TYR:H	8	0.25
(1,161)	1:49:A:ASP:HA	1:53:A:GLU:H	2	0.25
(1,161)	1:49:A:ASP:HA	1:53:A:GLU:H	3	0.25
(1,160)	1:48:A:ILE:HA	1:52:A:ARG:H	6	0.25
(1,159)	1:47:A:LEU:HA	1:51:A:PHE:H	7	0.25
(1,155)	1:59:A:ARG:HA	1:61:A:ASN:H	3	0.25
(1,50)	1:24:A:VAL:HA	1:28:A:ALA:H	10	0.25
(1,30)	1:23:A:TRP:HA	1:25:A:THR:H	7	0.25
(2,98)	1:178:A:THR:H	1:202:A:THR:H	6	0.24
(2,25)	1:75:A:GLY:H	1:78:A:ILE:HG12	6	0.24
(2,25)	1:75:A:GLY:H	1:78:A:ILE:HG13	6	0.24
(2,9)	1:41:A:PRO:HD2	1:44:A:LYS:H	6	0.24
(2,9)	1:41:A:PRO:HD3	1:44:A:LYS:H	6	0.24
(1,1333)	1:174:A:ARG:H	1:198:A:GLY:HA2	3	0.24
(1,1333)	1:174:A:ARG:H	1:198:A:GLY:HA3	3	0.24
(1,1329)	1:104:A:ALA:HA	1:221:A:PHE:H	10	0.24
(1,1320)	1:189:A:TYR:H	1:230:A:TRP:H	1	0.24
(1,1317)	1:53:A:GLU:H	1:79:A:GLY:H	7	0.24
(1,1306)	1:49:A:ASP:H	1:144:A:TRP:HD1	5	0.24
(1,1305)	1:48:A:ILE:H	1:144:A:TRP:HZ2	6	0.24
(1,1269)	1:173:A:ALA:HA	1:178:A:THR:H	2	0.24
(1,1248)	1:110:A:GLU:H	1:215:A:VAL:HB	3	0.24
(1,1239)	1:104:A:ALA:H	1:220:A:TYR:HA	9	0.24
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD11	6	0.24
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD12	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD13	6	0.24
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD21	6	0.24
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD22	6	0.24
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD23	6	0.24
(1,1207)	1:62:A:SER:HA	1:67:A:LYS:H	7	0.24
(1,1177)	1:26:A:ARG:H	1:45:A:LEU:H	2	0.24
(1,1142)	1:213:A:LEU:H	1:214:A:ASP:HA	7	0.24
(1,1081)	1:247:A:LEU:HA	1:251:A:GLY:H	1	0.24
(1,996)	1:233:A:ARG:HA	1:237:A:LEU:H	7	0.24
(1,994)	1:231:A:ASN:HA	1:235:A:TYR:H	4	0.24
(1,914)	1:219:A:ASP:HA	1:223:A:GLU:H	9	0.24
(1,911)	1:223:A:GLU:HA	1:226:A:THR:H	3	0.24
(1,907)	1:219:A:ASP:HA	1:222:A:ASP:H	9	0.24
(1,906)	1:218:A:LEU:HA	1:221:A:PHE:H	7	0.24
(1,901)	1:224:A:VAL:HA	1:226:A:THR:H	4	0.24
(1,845)	1:203:A:ASP:HA	1:207:A:GLN:H	4	0.24
(1,845)	1:203:A:ASP:HA	1:207:A:GLN:H	7	0.24
(1,845)	1:203:A:ASP:HA	1:207:A:GLN:H	8	0.24
(1,761)	1:187:A:MET:HA	1:190:A:LYS:H	9	0.24
(1,754)	1:180:A:ARG:HA	1:183:A:LEU:H	5	0.24
(1,741)	1:179:A:MET:HA	1:183:A:LEU:H	8	0.24
(1,738)	1:176:A:SER:HA	1:180:A:ARG:H	4	0.24
(1,735)	1:189:A:TYR:H	1:191:A:ASP:H	5	0.24
(1,723)	1:183:A:LEU:HA	1:185:A:TYR:H	4	0.24
(1,712)	1:177:A:GLU:HA	1:179:A:MET:H	1	0.24
(1,539)	1:126:A:VAL:HA	1:130:A:GLY:H	4	0.24
(1,534)	1:121:A:VAL:HA	1:125:A:LEU:H	7	0.24
(1,524)	1:128:A:PHE:HA	1:131:A:LEU:H	2	0.24
(1,518)	1:123:A:TYR:HA	1:126:A:VAL:H	5	0.24
(1,516)	1:121:A:VAL:HA	1:124:A:VAL:H	1	0.24
(1,511)	1:116:A:LEU:HA	1:119:A:HIS:H	3	0.24
(1,405)	1:111:A:LYS:H	1:113:A:TYR:HB2	4	0.24
(1,402)	1:104:A:ALA:HA	1:107:A:SER:H	3	0.24
(1,398)	1:100:A:ILE:HA	1:103:A:LYS:H	2	0.24
(1,398)	1:100:A:ILE:HA	1:103:A:LYS:H	9	0.24
(1,396)	1:98:A:ILE:HA	1:101:A:VAL:H	3	0.24
(1,392)	1:95:A:ASN:HA	1:98:A:ILE:H	8	0.24
(1,389)	1:102:A:GLY:HA2	1:106:A:ALA:H	9	0.24
(1,389)	1:102:A:GLY:HA3	1:106:A:ALA:H	9	0.24
(1,365)	1:104:A:ALA:HA	1:106:A:ALA:H	5	0.24
(1,289)	1:88:A:VAL:H	1:89:A:ASP:H	5	0.24
(1,276)	1:83:A:ASP:H	1:84:A:ARG:H	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,268)	1:73:A:ASP:HA	1:77:A:GLN:H	9	0.24
(1,259)	1:72:A:TRP:HA	1:75:A:GLY:H	2	0.24
(1,243)	1:74:A:TYR:HA	1:76:A:TYR:H	4	0.24
(1,228)	1:66:A:SER:HA	1:68:A:VAL:H	5	0.24
(1,163)	1:51:A:PHE:HA	1:55:A:TYR:H	2	0.24
(1,158)	1:46:A:ALA:HA	1:50:A:ASP:H	2	0.24
(1,137)	1:50:A:ASP:H	1:52:A:ARG:H	6	0.24
(1,130)	1:46:A:ALA:HA	1:48:A:ILE:H	7	0.24
(1,80)	1:42:A:ASP:HB2	1:44:A:LYS:H	9	0.24
(1,80)	1:42:A:ASP:HB3	1:44:A:LYS:H	9	0.24
(1,46)	1:26:A:ARG:HG2	1:29:A:TYR:H	8	0.24
(1,46)	1:26:A:ARG:HG3	1:29:A:TYR:H	8	0.24
(1,44)	1:24:A:VAL:HA	1:27:A:THR:H	10	0.24
(1,6)	1:23:A:TRP:H	1:24:A:VAL:H	2	0.24
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG11	5	0.23
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG12	5	0.23
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG13	5	0.23
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG21	5	0.23
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG22	5	0.23
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG23	5	0.23
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG11	5	0.23
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG12	5	0.23
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG13	5	0.23
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG21	5	0.23
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG22	5	0.23
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG23	5	0.23
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG11	5	0.23
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG12	5	0.23
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG13	5	0.23
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG21	5	0.23
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG22	5	0.23
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG23	5	0.23
(1,1325)	1:60:A:MET:H	1:69:A:ALA:HA	6	0.23
(1,1320)	1:189:A:TYR:H	1:230:A:TRP:H	3	0.23
(1,1305)	1:48:A:ILE:H	1:144:A:TRP:HZ2	10	0.23
(1,1299)	1:26:A:ARG:H	1:121:A:VAL:HG11	1	0.23
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD11	1	0.23
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD12	1	0.23
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD13	1	0.23
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD21	1	0.23
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD22	1	0.23
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD23	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1275)	1:197:A:ASN:HA	1:202:A:THR:H	6	0.23
(1,1265)	1:134:A:PHE:H	1:234:A:ILE:HA	2	0.23
(1,1259)	1:132:A:ILE:H	1:237:A:LEU:HB2	4	0.23
(1,1259)	1:132:A:ILE:H	1:237:A:LEU:HB3	4	0.23
(1,1234)	1:101:A:VAL:HA	1:223:A:GLU:H	3	0.23
(1,1229)	1:98:A:ILE:H	1:255:A:ARG:HG2	5	0.23
(1,1229)	1:98:A:ILE:H	1:255:A:ARG:HG3	5	0.23
(1,1222)	1:81:A:MET:H	1:144:A:TRP:HD1	8	0.23
(1,1199)	1:52:A:ARG:H	1:76:A:TYR:H	2	0.23
(1,1199)	1:52:A:ARG:H	1:76:A:TYR:H	5	0.23
(1,1193)	1:34:A:VAL:HG11	1:39:A:GLN:H	6	0.23
(1,1193)	1:34:A:VAL:HG12	1:39:A:GLN:H	6	0.23
(1,1193)	1:34:A:VAL:HG13	1:39:A:GLN:H	6	0.23
(1,1193)	1:34:A:VAL:HG21	1:39:A:GLN:H	6	0.23
(1,1193)	1:34:A:VAL:HG22	1:39:A:GLN:H	6	0.23
(1,1193)	1:34:A:VAL:HG23	1:39:A:GLN:H	6	0.23
(1,1179)	1:29:A:TYR:H	1:46:A:ALA:H	1	0.23
(1,1179)	1:29:A:TYR:H	1:46:A:ALA:H	4	0.23
(1,1165)	1:22:A:THR:HB	1:45:A:LEU:H	9	0.23
(1,1087)	1:260:A:THR:H	1:261:A:ARG:H	9	0.23
(1,1075)	1:249:A:ASP:HA	1:252:A:GLU:H	10	0.23
(1,993)	1:230:A:TRP:HA	1:234:A:ILE:H	6	0.23
(1,988)	1:238:A:LYS:HA	1:241:A:ASP:H	2	0.23
(1,987)	1:237:A:LEU:HA	1:240:A:ASP:H	4	0.23
(1,966)	1:234:A:ILE:HB	1:236:A:GLN:H	4	0.23
(1,915)	1:220:A:TYR:HA	1:224:A:VAL:H	3	0.23
(1,852)	1:213:A:LEU:H	1:214:A:ASP:H	6	0.23
(1,845)	1:203:A:ASP:HA	1:207:A:GLN:H	5	0.23
(1,844)	1:202:A:THR:HA	1:206:A:ARG:H	9	0.23
(1,842)	1:200:A:GLN:HA	1:204:A:ARG:H	2	0.23
(1,842)	1:200:A:GLN:HA	1:204:A:ARG:H	3	0.23
(1,842)	1:200:A:GLN:HA	1:204:A:ARG:H	10	0.23
(1,841)	1:208:A:GLN:HA	1:211:A:THR:H	7	0.23
(1,836)	1:203:A:ASP:HA	1:206:A:ARG:H	4	0.23
(1,738)	1:176:A:SER:HA	1:180:A:ARG:H	5	0.23
(1,731)	1:187:A:MET:HA	1:189:A:TYR:H	4	0.23
(1,710)	1:176:A:SER:HA	1:178:A:THR:H	6	0.23
(1,572)	1:150:A:GLU:HA	1:151:A:GLY:H	6	0.23
(1,530)	1:118:A:GLU:HA	1:122:A:ASP:H	7	0.23
(1,519)	1:124:A:VAL:HA	1:127:A:ILE:H	3	0.23
(1,508)	1:130:A:GLY:H	1:132:A:ILE:H	8	0.23
(1,475)	1:115:A:ILE:H	1:117:A:LYS:H	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:114:A:GLU:H	1:116:A:LEU:H	6	0.23
(1,399)	1:101:A:VAL:HA	1:104:A:ALA:H	5	0.23
(1,396)	1:98:A:ILE:HA	1:101:A:VAL:H	9	0.23
(1,380)	1:93:A:TRP:HA	1:97:A:HIS:H	8	0.23
(1,377)	1:93:A:TRP:HA	1:96:A:THR:H	1	0.23
(1,377)	1:93:A:TRP:HA	1:96:A:THR:H	6	0.23
(1,376)	1:92:A:THR:HA	1:95:A:ASN:H	1	0.23
(1,267)	1:72:A:TRP:HA	1:76:A:TYR:H	8	0.23
(1,243)	1:74:A:TYR:HA	1:76:A:TYR:H	2	0.23
(1,243)	1:74:A:TYR:HA	1:76:A:TYR:H	9	0.23
(1,238)	1:72:A:TRP:H	1:74:A:TYR:H	2	0.23
(1,178)	1:54:A:ALA:HA	1:57:A:TRP:H	1	0.23
(1,171)	1:47:A:LEU:HA	1:50:A:ASP:H	9	0.23
(1,159)	1:47:A:LEU:HA	1:51:A:PHE:H	9	0.23
(1,47)	1:21:A:SER:HA	1:25:A:THR:H	8	0.23
(1,45)	1:25:A:THR:HA	1:28:A:ALA:H	2	0.23
(1,40)	1:21:A:SER:HA	1:24:A:VAL:H	9	0.23
(2,89)	1:123:A:TYR:HA	1:226:A:THR:H	8	0.22
(1,1299)	1:26:A:ARG:H	1:121:A:VAL:HG11	3	0.22
(1,1299)	1:26:A:ARG:H	1:121:A:VAL:HG11	7	0.22
(1,1293)	1:268:A:GLU:H	1:273:A:VAL:HA	8	0.22
(1,1259)	1:132:A:ILE:H	1:237:A:LEU:HB2	3	0.22
(1,1259)	1:132:A:ILE:H	1:237:A:LEU:HB3	3	0.22
(1,1248)	1:110:A:GLU:H	1:215:A:VAL:HB	9	0.22
(1,1231)	1:100:A:ILE:HD11	1:223:A:GLU:H	1	0.22
(1,1231)	1:100:A:ILE:HD12	1:223:A:GLU:H	1	0.22
(1,1231)	1:100:A:ILE:HD13	1:223:A:GLU:H	1	0.22
(1,1228)	1:93:A:TRP:H	1:64:A:GLU:HA	2	0.22
(1,1225)	1:82:A:ALA:H	1:144:A:TRP:HA	2	0.22
(1,1206)	1:56:A:TYR:HA	1:69:A:ALA:H	9	0.22
(1,1165)	1:22:A:THR:HB	1:45:A:LEU:H	10	0.22
(1,1152)	1:194:A:GLN:HA	1:197:A:ASN:H	1	0.22
(1,1125)	1:270:A:GLY:HA2	1:272:A:ARG:H	8	0.22
(1,1125)	1:270:A:GLY:HA3	1:272:A:ARG:H	8	0.22
(1,1120)	1:264:A:ILE:HG12	1:266:A:ARG:H	4	0.22
(1,1120)	1:264:A:ILE:HG13	1:266:A:ARG:H	4	0.22
(1,1091)	1:261:A:ARG:HA	1:262:A:ARG:H	1	0.22
(1,1091)	1:261:A:ARG:HA	1:262:A:ARG:H	9	0.22
(1,1087)	1:260:A:THR:H	1:261:A:ARG:H	6	0.22
(1,1081)	1:247:A:LEU:HA	1:251:A:GLY:H	10	0.22
(1,1075)	1:249:A:ASP:HA	1:252:A:GLU:H	9	0.22
(1,996)	1:233:A:ARG:HA	1:237:A:LEU:H	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,988)	1:238:A:LYS:HA	1:241:A:ASP:H	6	0.22
(1,984)	1:234:A:ILE:HA	1:237:A:LEU:H	8	0.22
(1,982)	1:232:A:VAL:HA	1:235:A:TYR:H	8	0.22
(1,909)	1:221:A:PHE:HA	1:224:A:VAL:H	3	0.22
(1,891)	1:219:A:ASP:HA	1:221:A:PHE:H	1	0.22
(1,891)	1:219:A:ASP:HA	1:221:A:PHE:H	10	0.22
(1,856)	1:214:A:ASP:HA	1:215:A:VAL:H	10	0.22
(1,837)	1:204:A:ARG:HA	1:207:A:GLN:H	7	0.22
(1,837)	1:204:A:ARG:HA	1:207:A:GLN:H	10	0.22
(1,832)	1:200:A:GLN:HA	1:203:A:ASP:H	6	0.22
(1,777)	1:198:A:GLY:H	1:199:A:GLY:H	2	0.22
(1,757)	1:183:A:LEU:HA	1:186:A:LYS:H	2	0.22
(1,749)	1:187:A:MET:HA	1:191:A:ASP:H	4	0.22
(1,659)	1:171:A:VAL:HB	1:173:A:ALA:H	6	0.22
(1,658)	1:163:A:TYR:H	1:165:A:ALA:H	10	0.22
(1,584)	1:154:A:PRO:HD2	1:156:A:GLU:H	8	0.22
(1,584)	1:154:A:PRO:HD3	1:156:A:GLU:H	8	0.22
(1,582)	1:148:A:ILE:HD11	1:150:A:GLU:H	2	0.22
(1,582)	1:148:A:ILE:HD12	1:150:A:GLU:H	2	0.22
(1,582)	1:148:A:ILE:HD13	1:150:A:GLU:H	2	0.22
(1,556)	1:141:A:LYS:H	1:142:A:PHE:H	10	0.22
(1,519)	1:124:A:VAL:HA	1:127:A:ILE:H	8	0.22
(1,515)	1:120:A:ASP:HA	1:123:A:TYR:H	7	0.22
(1,473)	1:114:A:GLU:H	1:116:A:LEU:H	2	0.22
(1,402)	1:104:A:ALA:HA	1:107:A:SER:H	2	0.22
(1,401)	1:103:A:LYS:HA	1:106:A:ALA:H	6	0.22
(1,389)	1:102:A:GLY:HA2	1:106:A:ALA:H	7	0.22
(1,389)	1:102:A:GLY:HA3	1:106:A:ALA:H	7	0.22
(1,379)	1:92:A:THR:HA	1:96:A:THR:H	9	0.22
(1,340)	1:86:A:THR:H	1:88:A:VAL:H	1	0.22
(1,269)	1:79:A:GLY:H	1:80:A:GLY:H	8	0.22
(1,261)	1:74:A:TYR:HA	1:77:A:GLN:H	4	0.22
(1,240)	1:73:A:ASP:H	1:75:A:GLY:H	3	0.22
(1,238)	1:72:A:TRP:H	1:74:A:TYR:H	4	0.22
(1,179)	1:55:A:TYR:HA	1:58:A:LEU:H	6	0.22
(1,175)	1:51:A:PHE:HA	1:54:A:ALA:H	2	0.22
(1,173)	1:49:A:ASP:HA	1:52:A:ARG:H	4	0.22
(1,162)	1:50:A:ASP:HA	1:54:A:ALA:H	8	0.22
(1,160)	1:48:A:ILE:HA	1:52:A:ARG:H	7	0.22
(1,159)	1:47:A:LEU:HA	1:51:A:PHE:H	10	0.22
(1,145)	1:54:A:ALA:H	1:56:A:TYR:H	6	0.22
(1,140)	1:51:A:PHE:HA	1:53:A:GLU:H	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:46:A:ALA:H	1:48:A:ILE:H	4	0.22
(1,47)	1:21:A:SER:HA	1:25:A:THR:H	2	0.22
(1,40)	1:21:A:SER:HA	1:24:A:VAL:H	4	0.22
(1,40)	1:21:A:SER:HA	1:24:A:VAL:H	10	0.22
(2,98)	1:178:A:THR:H	1:202:A:THR:H	4	0.21
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD11	3	0.21
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD12	3	0.21
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD13	3	0.21
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD21	3	0.21
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD22	3	0.21
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD23	3	0.21
(2,94)	1:204:A:ARG:HA	1:209:A:MET:H	4	0.21
(2,71)	1:261:A:ARG:HG2	1:263:A:SER:H	5	0.21
(2,71)	1:261:A:ARG:HG3	1:263:A:SER:H	5	0.21
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD11	7	0.21
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD12	7	0.21
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD13	7	0.21
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD21	7	0.21
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD22	7	0.21
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD23	7	0.21
(1,1334)	1:177:A:GLU:H	1:202:A:THR:HA	2	0.21
(1,1329)	1:104:A:ALA:HA	1:221:A:PHE:H	3	0.21
(1,1314)	1:177:A:GLU:H	1:202:A:THR:HA	2	0.21
(1,1305)	1:48:A:ILE:H	1:144:A:TRP:HZ2	4	0.21
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD11	2	0.21
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD12	2	0.21
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD13	2	0.21
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD21	2	0.21
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD22	2	0.21
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD23	2	0.21
(1,1256)	1:130:A:GLY:HA2	1:234:A:ILE:HA	6	0.21
(1,1256)	1:130:A:GLY:HA3	1:234:A:ILE:HA	6	0.21
(1,1246)	1:106:A:ALA:H	1:113:A:TYR:H	1	0.21
(1,1209)	1:63:A:ASP:H	1:265:A:LYS:H	7	0.21
(1,1197)	1:51:A:PHE:H	1:79:A:GLY:HA2	8	0.21
(1,1197)	1:51:A:PHE:H	1:79:A:GLY:HA3	8	0.21
(1,1153)	1:237:A:LEU:HA	1:241:A:ASP:H	3	0.21
(1,1142)	1:213:A:LEU:H	1:214:A:ASP:HA	9	0.21
(1,1120)	1:264:A:ILE:HG12	1:266:A:ARG:H	2	0.21
(1,1120)	1:264:A:ILE:HG13	1:266:A:ARG:H	2	0.21
(1,1079)	1:246:A:THR:HA	1:250:A:VAL:H	6	0.21
(1,1068)	1:247:A:LEU:HA	1:250:A:VAL:H	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:238:A:LYS:HA	1:242:A:ALA:H	10	0.21
(1,1000)	1:237:A:LEU:HA	1:241:A:ASP:H	3	0.21
(1,991)	1:228:A:GLU:HA	1:232:A:VAL:H	6	0.21
(1,988)	1:238:A:LYS:HA	1:241:A:ASP:H	5	0.21
(1,987)	1:237:A:LEU:HA	1:240:A:ASP:H	3	0.21
(1,985)	1:235:A:TYR:HA	1:238:A:LYS:H	3	0.21
(1,985)	1:235:A:TYR:HA	1:238:A:LYS:H	8	0.21
(1,979)	1:229:A:ASN:HA	1:232:A:VAL:H	2	0.21
(1,908)	1:220:A:TYR:HA	1:223:A:GLU:H	10	0.21
(1,891)	1:219:A:ASP:HA	1:221:A:PHE:H	7	0.21
(1,888)	1:218:A:LEU:H	1:220:A:TYR:H	6	0.21
(1,888)	1:218:A:LEU:H	1:220:A:TYR:H	9	0.21
(1,834)	1:202:A:THR:HA	1:205:A:VAL:H	9	0.21
(1,762)	1:188:A:SER:HA	1:191:A:ASP:H	1	0.21
(1,745)	1:183:A:LEU:HA	1:187:A:MET:H	10	0.21
(1,741)	1:179:A:MET:HA	1:183:A:LEU:H	6	0.21
(1,729)	1:186:A:LYS:HA	1:188:A:SER:H	5	0.21
(1,534)	1:121:A:VAL:HA	1:125:A:LEU:H	10	0.21
(1,529)	1:117:A:LYS:HA	1:121:A:VAL:H	7	0.21
(1,518)	1:123:A:TYR:HA	1:126:A:VAL:H	4	0.21
(1,518)	1:123:A:TYR:HA	1:126:A:VAL:H	9	0.21
(1,516)	1:121:A:VAL:HA	1:124:A:VAL:H	2	0.21
(1,511)	1:116:A:LEU:HA	1:119:A:HIS:H	7	0.21
(1,483)	1:119:A:HIS:HA	1:121:A:VAL:H	6	0.21
(1,481)	1:118:A:GLU:H	1:120:A:ASP:H	5	0.21
(1,396)	1:98:A:ILE:HA	1:101:A:VAL:H	4	0.21
(1,387)	1:100:A:ILE:HA	1:104:A:ALA:H	7	0.21
(1,385)	1:98:A:ILE:HA	1:102:A:GLY:H	3	0.21
(1,384)	1:97:A:HIS:HA	1:101:A:VAL:H	7	0.21
(1,383)	1:96:A:THR:HA	1:100:A:ILE:H	10	0.21
(1,380)	1:93:A:TRP:HA	1:97:A:HIS:H	6	0.21
(1,379)	1:92:A:THR:HA	1:96:A:THR:H	2	0.21
(1,376)	1:92:A:THR:HA	1:95:A:ASN:H	9	0.21
(1,365)	1:104:A:ALA:HA	1:106:A:ALA:H	3	0.21
(1,261)	1:74:A:TYR:HA	1:77:A:GLN:H	9	0.21
(1,259)	1:72:A:TRP:HA	1:75:A:GLY:H	5	0.21
(1,258)	1:71:A:TRP:HA	1:74:A:TYR:H	3	0.21
(1,252)	1:67:A:LYS:HA	1:70:A:ALA:H	6	0.21
(1,250)	1:77:A:GLN:HA	1:79:A:GLY:H	3	0.21
(1,246)	1:76:A:TYR:H	1:78:A:ILE:H	3	0.21
(1,234)	1:70:A:ALA:H	1:72:A:TRP:H	7	0.21
(1,171)	1:47:A:LEU:HA	1:50:A:ASP:H	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,171)	1:47:A:LEU:HA	1:50:A:ASP:H	5	0.21
(1,170)	1:46:A:ALA:HA	1:49:A:ASP:H	9	0.21
(1,166)	1:54:A:ALA:HA	1:58:A:LEU:H	10	0.21
(1,157)	1:45:A:LEU:HA	1:49:A:ASP:H	7	0.21
(1,146)	1:54:A:ALA:HA	1:56:A:TYR:H	10	0.21
(1,129)	1:46:A:ALA:H	1:48:A:ILE:H	3	0.21
(1,80)	1:42:A:ASP:HB2	1:44:A:LYS:H	7	0.21
(1,80)	1:42:A:ASP:HB3	1:44:A:LYS:H	7	0.21
(1,46)	1:26:A:ARG:HG2	1:29:A:TYR:H	3	0.21
(1,46)	1:26:A:ARG:HG3	1:29:A:TYR:H	3	0.21
(1,6)	1:23:A:TRP:H	1:24:A:VAL:H	1	0.21
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB2	9	0.2
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB3	9	0.2
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD11	4	0.2
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD12	4	0.2
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD13	4	0.2
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD21	4	0.2
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD22	4	0.2
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD23	4	0.2
(2,79)	1:266:A:ARG:HH11	1:269:A:LEU:H	8	0.2
(2,79)	1:266:A:ARG:HH12	1:269:A:LEU:H	8	0.2
(2,28)	1:78:A:ILE:HG12	1:81:A:MET:H	1	0.2
(2,28)	1:78:A:ILE:HG13	1:81:A:MET:H	1	0.2
(1,1336)	1:189:A:TYR:HA	1:230:A:TRP:H	9	0.2
(1,1317)	1:53:A:GLU:H	1:79:A:GLY:H	1	0.2
(1,1316)	1:53:A:GLU:H	1:75:A:GLY:H	6	0.2
(1,1304)	1:48:A:ILE:H	1:144:A:TRP:HD1	6	0.2
(1,1298)	1:156:A:GLU:H	1:25:A:THR:HG1	1	0.2
(1,1248)	1:110:A:GLU:H	1:215:A:VAL:HB	10	0.2
(1,1245)	1:106:A:ALA:HA	1:111:A:LYS:HA	5	0.2
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD11	10	0.2
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD12	10	0.2
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD13	10	0.2
(1,1228)	1:93:A:TRP:H	1:64:A:GLU:HA	3	0.2
(1,1227)	1:82:A:ALA:H	1:144:A:TRP:H	8	0.2
(1,1197)	1:51:A:PHE:H	1:79:A:GLY:HA2	1	0.2
(1,1197)	1:51:A:PHE:H	1:79:A:GLY:HA3	1	0.2
(1,1186)	1:29:A:TYR:H	1:45:A:LEU:HA	9	0.2
(1,1167)	1:24:A:VAL:H	1:192:A:PHE:HE1	3	0.2
(1,1167)	1:24:A:VAL:H	1:192:A:PHE:HE2	3	0.2
(1,1163)	1:22:A:THR:H	1:47:A:LEU:H	2	0.2
(1,1153)	1:237:A:LEU:HA	1:241:A:ASP:H	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1153)	1:237:A:LEU:HA	1:241:A:ASP:H	10	0.2
(1,1150)	1:174:A:ARG:H	1:177:A:GLU:HB2	5	0.2
(1,1148)	1:171:A:VAL:HA	1:174:A:ARG:H	10	0.2
(1,1091)	1:261:A:ARG:HA	1:262:A:ARG:H	5	0.2
(1,1089)	1:260:A:THR:HB	1:261:A:ARG:H	5	0.2
(1,1077)	1:251:A:GLY:HA2	1:254:A:THR:H	5	0.2
(1,1077)	1:251:A:GLY:HA3	1:254:A:THR:H	5	0.2
(1,1075)	1:249:A:ASP:HA	1:252:A:GLU:H	8	0.2
(1,1074)	1:248:A:ARG:HG2	1:251:A:GLY:H	6	0.2
(1,1074)	1:248:A:ARG:HG2	1:251:A:GLY:H	10	0.2
(1,1000)	1:237:A:LEU:HA	1:241:A:ASP:H	1	0.2
(1,1000)	1:237:A:LEU:HA	1:241:A:ASP:H	10	0.2
(1,994)	1:231:A:ASN:HA	1:235:A:TYR:H	9	0.2
(1,993)	1:230:A:TRP:HA	1:234:A:ILE:H	7	0.2
(1,984)	1:234:A:ILE:HA	1:237:A:LEU:H	2	0.2
(1,954)	1:230:A:TRP:H	1:232:A:VAL:H	5	0.2
(1,952)	1:229:A:ASN:H	1:231:A:ASN:H	6	0.2
(1,914)	1:219:A:ASP:HA	1:223:A:GLU:H	10	0.2
(1,909)	1:221:A:PHE:HA	1:224:A:VAL:H	2	0.2
(1,908)	1:220:A:TYR:HA	1:223:A:GLU:H	3	0.2
(1,856)	1:214:A:ASP:HA	1:215:A:VAL:H	1	0.2
(1,847)	1:210:A:ILE:H	1:211:A:THR:H	7	0.2
(1,839)	1:206:A:ARG:HA	1:209:A:MET:H	9	0.2
(1,837)	1:204:A:ARG:HA	1:207:A:GLN:H	2	0.2
(1,759)	1:185:A:TYR:HA	1:188:A:SER:H	5	0.2
(1,757)	1:183:A:LEU:HA	1:186:A:LYS:H	3	0.2
(1,754)	1:180:A:ARG:HA	1:183:A:LEU:H	8	0.2
(1,750)	1:176:A:SER:HA	1:179:A:MET:H	6	0.2
(1,716)	1:179:A:MET:HA	1:181:A:ASN:H	10	0.2
(1,659)	1:171:A:VAL:HB	1:173:A:ALA:H	8	0.2
(1,584)	1:154:A:PRO:HD2	1:156:A:GLU:H	2	0.2
(1,584)	1:154:A:PRO:HD3	1:156:A:GLU:H	2	0.2
(1,583)	1:151:A:GLY:HA2	1:153:A:TRP:H	10	0.2
(1,578)	1:152:A:ILE:HB	1:153:A:TRP:H	8	0.2
(1,539)	1:126:A:VAL:HA	1:130:A:GLY:H	5	0.2
(1,524)	1:128:A:PHE:HA	1:131:A:LEU:H	10	0.2
(1,516)	1:121:A:VAL:HA	1:124:A:VAL:H	6	0.2
(1,515)	1:120:A:ASP:HA	1:123:A:TYR:H	8	0.2
(1,513)	1:118:A:GLU:HA	1:121:A:VAL:H	4	0.2
(1,511)	1:116:A:LEU:HA	1:119:A:HIS:H	9	0.2
(1,509)	1:114:A:GLU:HA	1:117:A:LYS:H	7	0.2
(1,422)	1:113:A:TYR:H	1:114:A:GLU:H	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:112:A:SER:H	1:113:A:TYR:H	4	0.2
(1,414)	1:110:A:GLU:HA	1:111:A:LYS:H	4	0.2
(1,398)	1:100:A:ILE:HA	1:103:A:LYS:H	6	0.2
(1,396)	1:98:A:ILE:HA	1:101:A:VAL:H	2	0.2
(1,392)	1:95:A:ASN:HA	1:98:A:ILE:H	1	0.2
(1,379)	1:92:A:THR:HA	1:96:A:THR:H	1	0.2
(1,379)	1:92:A:THR:HA	1:96:A:THR:H	3	0.2
(1,379)	1:92:A:THR:HA	1:96:A:THR:H	5	0.2
(1,343)	1:91:A:ASN:H	1:93:A:TRP:H	10	0.2
(1,266)	1:70:A:ALA:HA	1:74:A:TYR:H	8	0.2
(1,234)	1:70:A:ALA:H	1:72:A:TRP:H	9	0.2
(1,232)	1:69:A:ALA:H	1:71:A:TRP:H	6	0.2
(1,176)	1:52:A:ARG:HA	1:55:A:TYR:H	10	0.2
(1,173)	1:49:A:ASP:HA	1:52:A:ARG:H	7	0.2
(1,172)	1:48:A:ILE:HA	1:51:A:PHE:H	5	0.2
(1,163)	1:51:A:PHE:HA	1:55:A:TYR:H	10	0.2
(1,160)	1:48:A:ILE:HA	1:52:A:ARG:H	9	0.2
(1,157)	1:45:A:LEU:HA	1:49:A:ASP:H	9	0.2
(1,80)	1:42:A:ASP:HB2	1:44:A:LYS:H	4	0.2
(1,80)	1:42:A:ASP:HB3	1:44:A:LYS:H	4	0.2
(1,6)	1:23:A:TRP:H	1:24:A:VAL:H	5	0.2
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB2	7	0.19
(2,97)	1:59:A:ARG:H	1:142:A:PHE:HB3	7	0.19
(2,94)	1:204:A:ARG:HA	1:209:A:MET:H	10	0.19
(2,25)	1:75:A:GLY:H	1:78:A:ILE:HG12	2	0.19
(2,25)	1:75:A:GLY:H	1:78:A:ILE:HG13	2	0.19
(2,9)	1:41:A:PRO:HD2	1:44:A:LYS:H	3	0.19
(2,9)	1:41:A:PRO:HD3	1:44:A:LYS:H	3	0.19
(1,1336)	1:189:A:TYR:HA	1:230:A:TRP:H	8	0.19
(1,1334)	1:177:A:GLU:H	1:202:A:THR:HA	8	0.19
(1,1314)	1:177:A:GLU:H	1:202:A:THR:HA	8	0.19
(1,1310)	1:134:A:PHE:H	1:234:A:ILE:HD11	5	0.19
(1,1304)	1:48:A:ILE:H	1:144:A:TRP:HD1	5	0.19
(1,1281)	1:213:A:LEU:H	1:218:A:LEU:HG	2	0.19
(1,1275)	1:197:A:ASN:HA	1:202:A:THR:H	2	0.19
(1,1258)	1:132:A:ILE:H	1:237:A:LEU:HG	7	0.19
(1,1256)	1:130:A:GLY:HA2	1:234:A:ILE:HA	2	0.19
(1,1256)	1:130:A:GLY:HA3	1:234:A:ILE:HA	2	0.19
(1,1248)	1:110:A:GLU:H	1:215:A:VAL:HB	1	0.19
(1,1208)	1:63:A:ASP:H	1:264:A:ILE:H	7	0.19
(1,1206)	1:56:A:TYR:HA	1:69:A:ALA:H	2	0.19
(1,1163)	1:22:A:THR:H	1:47:A:LEU:H	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1152)	1:194:A:GLN:HA	1:197:A:ASN:H	5	0.19
(1,1149)	1:173:A:ALA:HA	1:176:A:SER:H	10	0.19
(1,1140)	1:199:A:GLY:H	1:200:A:GLN:HA	1	0.19
(1,1140)	1:199:A:GLY:H	1:200:A:GLN:HA	7	0.19
(1,1128)	1:51:A:PHE:H	1:52:A:ARG:HE	2	0.19
(1,1128)	1:51:A:PHE:H	1:52:A:ARG:HE	8	0.19
(1,1096)	1:263:A:SER:HA	1:264:A:ILE:H	6	0.19
(1,1075)	1:249:A:ASP:HA	1:252:A:GLU:H	1	0.19
(1,1075)	1:249:A:ASP:HA	1:252:A:GLU:H	5	0.19
(1,1074)	1:248:A:ARG:HG2	1:251:A:GLY:H	1	0.19
(1,992)	1:229:A:ASN:HA	1:233:A:ARG:H	5	0.19
(1,991)	1:228:A:GLU:HA	1:232:A:VAL:H	2	0.19
(1,984)	1:234:A:ILE:HA	1:237:A:LEU:H	3	0.19
(1,983)	1:233:A:ARG:HA	1:236:A:GLN:H	6	0.19
(1,980)	1:230:A:TRP:HA	1:233:A:ARG:H	10	0.19
(1,970)	1:236:A:GLN:HA	1:238:A:LYS:H	1	0.19
(1,954)	1:230:A:TRP:H	1:232:A:VAL:H	4	0.19
(1,909)	1:221:A:PHE:HA	1:224:A:VAL:H	8	0.19
(1,909)	1:221:A:PHE:HA	1:224:A:VAL:H	9	0.19
(1,908)	1:220:A:TYR:HA	1:223:A:GLU:H	7	0.19
(1,885)	1:227:A:SER:H	1:228:A:GLU:H	3	0.19
(1,856)	1:214:A:ASP:HA	1:215:A:VAL:H	2	0.19
(1,856)	1:214:A:ASP:HA	1:215:A:VAL:H	5	0.19
(1,847)	1:210:A:ILE:H	1:211:A:THR:H	1	0.19
(1,845)	1:203:A:ASP:HA	1:207:A:GLN:H	9	0.19
(1,834)	1:202:A:THR:HA	1:205:A:VAL:H	7	0.19
(1,832)	1:200:A:GLN:HA	1:203:A:ASP:H	10	0.19
(1,761)	1:187:A:MET:HA	1:190:A:LYS:H	6	0.19
(1,760)	1:186:A:LYS:HA	1:189:A:TYR:H	4	0.19
(1,748)	1:186:A:LYS:HA	1:190:A:LYS:H	2	0.19
(1,710)	1:176:A:SER:HA	1:178:A:THR:H	7	0.19
(1,710)	1:176:A:SER:HA	1:178:A:THR:H	10	0.19
(1,669)	1:178:A:THR:HB	1:179:A:MET:H	5	0.19
(1,583)	1:151:A:GLY:HA2	1:153:A:TRP:H	1	0.19
(1,574)	1:151:A:GLY:H	1:152:A:ILE:H	7	0.19
(1,540)	1:131:A:LEU:H	1:132:A:ILE:H	6	0.19
(1,534)	1:121:A:VAL:HA	1:125:A:LEU:H	1	0.19
(1,516)	1:121:A:VAL:HA	1:124:A:VAL:H	10	0.19
(1,515)	1:120:A:ASP:HA	1:123:A:TYR:H	1	0.19
(1,484)	1:119:A:HIS:H	1:121:A:VAL:H	10	0.19
(1,475)	1:115:A:ILE:H	1:117:A:LYS:H	4	0.19
(1,414)	1:110:A:GLU:HA	1:111:A:LYS:H	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:110:A:GLU:HA	1:111:A:LYS:H	5	0.19
(1,414)	1:110:A:GLU:HA	1:111:A:LYS:H	6	0.19
(1,414)	1:110:A:GLU:HA	1:111:A:LYS:H	7	0.19
(1,406)	1:113:A:TYR:H	1:115:A:ILE:HD11	10	0.19
(1,402)	1:104:A:ALA:HA	1:107:A:SER:H	4	0.19
(1,396)	1:98:A:ILE:HA	1:101:A:VAL:H	5	0.19
(1,387)	1:100:A:ILE:HA	1:104:A:ALA:H	5	0.19
(1,380)	1:93:A:TRP:HA	1:97:A:HIS:H	3	0.19
(1,380)	1:93:A:TRP:HA	1:97:A:HIS:H	10	0.19
(1,372)	1:88:A:VAL:HA	1:91:A:ASN:H	6	0.19
(1,365)	1:104:A:ALA:HA	1:106:A:ALA:H	1	0.19
(1,287)	1:87:A:LEU:H	1:88:A:VAL:H	8	0.19
(1,268)	1:73:A:ASP:HA	1:77:A:GLN:H	6	0.19
(1,259)	1:72:A:TRP:HA	1:75:A:GLY:H	1	0.19
(1,254)	1:69:A:ALA:HA	1:72:A:TRP:H	1	0.19
(1,253)	1:68:A:VAL:HA	1:71:A:TRP:H	10	0.19
(1,252)	1:67:A:LYS:HA	1:70:A:ALA:H	1	0.19
(1,252)	1:67:A:LYS:HA	1:70:A:ALA:H	8	0.19
(1,243)	1:74:A:TYR:HA	1:76:A:TYR:H	5	0.19
(1,232)	1:69:A:ALA:H	1:71:A:TRP:H	2	0.19
(1,232)	1:69:A:ALA:H	1:71:A:TRP:H	8	0.19
(1,176)	1:52:A:ARG:HA	1:55:A:TYR:H	2	0.19
(1,143)	1:53:A:GLU:H	1:55:A:TYR:H	7	0.19
(1,135)	1:49:A:ASP:HA	1:51:A:PHE:H	5	0.19
(1,44)	1:24:A:VAL:HA	1:27:A:THR:H	9	0.19
(1,25)	1:21:A:SER:H	1:23:A:TRP:H	1	0.19
(1,6)	1:23:A:TRP:H	1:24:A:VAL:H	8	0.19
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD11	10	0.18
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD12	10	0.18
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD13	10	0.18
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD21	10	0.18
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD22	10	0.18
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD23	10	0.18
(1,1336)	1:189:A:TYR:HA	1:230:A:TRP:H	6	0.18
(1,1334)	1:177:A:GLU:H	1:202:A:THR:HA	3	0.18
(1,1330)	1:171:A:VAL:HA	1:199:A:GLY:H	1	0.18
(1,1325)	1:60:A:MET:H	1:69:A:ALA:HA	10	0.18
(1,1314)	1:177:A:GLU:H	1:202:A:THR:HA	3	0.18
(1,1305)	1:48:A:ILE:H	1:144:A:TRP:HZ2	5	0.18
(1,1292)	1:268:A:GLU:H	1:273:A:VAL:H	3	0.18
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG11	8	0.18
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG12	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG13	8	0.18
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG21	8	0.18
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG22	8	0.18
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG23	8	0.18
(1,1228)	1:93:A:TRP:H	1:64:A:GLU:HA	8	0.18
(1,1216)	1:71:A:TRP:H	1:255:A:ARG:HG2	4	0.18
(1,1216)	1:71:A:TRP:H	1:255:A:ARG:HG3	4	0.18
(1,1187)	1:33:A:SER:H	1:39:A:GLN:HA	5	0.18
(1,1081)	1:247:A:LEU:HA	1:251:A:GLY:H	2	0.18
(1,1079)	1:246:A:THR:HA	1:250:A:VAL:H	2	0.18
(1,1074)	1:248:A:ARG:HG2	1:251:A:GLY:H	7	0.18
(1,1027)	1:246:A:THR:H	1:248:A:ARG:H	1	0.18
(1,1024)	1:244:A:GLY:H	1:246:A:THR:H	5	0.18
(1,996)	1:233:A:ARG:HA	1:237:A:LEU:H	9	0.18
(1,994)	1:231:A:ASN:HA	1:235:A:TYR:H	5	0.18
(1,985)	1:235:A:TYR:HA	1:238:A:LYS:H	6	0.18
(1,983)	1:233:A:ARG:HA	1:236:A:GLN:H	2	0.18
(1,979)	1:229:A:ASN:HA	1:232:A:VAL:H	8	0.18
(1,914)	1:219:A:ASP:HA	1:223:A:GLU:H	6	0.18
(1,900)	1:223:A:GLU:HA	1:225:A:PHE:H	7	0.18
(1,856)	1:214:A:ASP:HA	1:215:A:VAL:H	3	0.18
(1,845)	1:203:A:ASP:HA	1:207:A:GLN:H	1	0.18
(1,838)	1:205:A:VAL:HA	1:208:A:GLN:H	2	0.18
(1,836)	1:203:A:ASP:HA	1:206:A:ARG:H	5	0.18
(1,832)	1:200:A:GLN:HA	1:203:A:ASP:H	1	0.18
(1,752)	1:178:A:THR:HA	1:181:A:ASN:H	7	0.18
(1,748)	1:186:A:LYS:HA	1:190:A:LYS:H	3	0.18
(1,746)	1:184:A:LEU:HA	1:188:A:SER:H	5	0.18
(1,745)	1:183:A:LEU:HA	1:187:A:MET:H	3	0.18
(1,735)	1:189:A:TYR:H	1:191:A:ASP:H	8	0.18
(1,712)	1:177:A:GLU:HA	1:179:A:MET:H	6	0.18
(1,630)	1:156:A:GLU:HA	1:159:A:GLU:H	1	0.18
(1,539)	1:126:A:VAL:HA	1:130:A:GLY:H	7	0.18
(1,538)	1:125:A:LEU:HA	1:129:A:GLY:H	9	0.18
(1,535)	1:122:A:ASP:HA	1:126:A:VAL:H	4	0.18
(1,535)	1:122:A:ASP:HA	1:126:A:VAL:H	6	0.18
(1,529)	1:117:A:LYS:HA	1:121:A:VAL:H	4	0.18
(1,524)	1:128:A:PHE:HA	1:131:A:LEU:H	8	0.18
(1,523)	1:127:A:ILE:HA	1:130:A:GLY:H	8	0.18
(1,520)	1:125:A:LEU:HA	1:128:A:PHE:H	3	0.18
(1,516)	1:121:A:VAL:HA	1:124:A:VAL:H	3	0.18
(1,510)	1:115:A:ILE:HA	1:118:A:GLU:H	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:113:A:TYR:HA	1:114:A:GLU:H	7	0.18
(1,419)	1:112:A:SER:H	1:113:A:TYR:H	6	0.18
(1,399)	1:101:A:VAL:HA	1:104:A:ALA:H	9	0.18
(1,389)	1:102:A:GLY:HA2	1:106:A:ALA:H	2	0.18
(1,389)	1:102:A:GLY:HA3	1:106:A:ALA:H	2	0.18
(1,388)	1:101:A:VAL:HA	1:105:A:ASN:H	2	0.18
(1,387)	1:100:A:ILE:HA	1:104:A:ALA:H	4	0.18
(1,386)	1:99:A:ALA:HA	1:103:A:LYS:H	1	0.18
(1,384)	1:97:A:HIS:HA	1:101:A:VAL:H	2	0.18
(1,380)	1:93:A:TRP:HA	1:97:A:HIS:H	4	0.18
(1,377)	1:93:A:TRP:HA	1:96:A:THR:H	4	0.18
(1,377)	1:93:A:TRP:HA	1:96:A:THR:H	10	0.18
(1,365)	1:104:A:ALA:HA	1:106:A:ALA:H	9	0.18
(1,343)	1:91:A:ASN:H	1:93:A:TRP:H	3	0.18
(1,340)	1:86:A:THR:H	1:88:A:VAL:H	7	0.18
(1,332)	1:105:A:ASN:H	1:106:A:ALA:H	5	0.18
(1,259)	1:72:A:TRP:HA	1:75:A:GLY:H	8	0.18
(1,250)	1:77:A:GLN:HA	1:79:A:GLY:H	4	0.18
(1,246)	1:76:A:TYR:H	1:78:A:ILE:H	9	0.18
(1,243)	1:74:A:TYR:HA	1:76:A:TYR:H	1	0.18
(1,240)	1:73:A:ASP:H	1:75:A:GLY:H	7	0.18
(1,228)	1:66:A:SER:HA	1:68:A:VAL:H	4	0.18
(1,175)	1:51:A:PHE:HA	1:54:A:ALA:H	5	0.18
(1,171)	1:47:A:LEU:HA	1:50:A:ASP:H	3	0.18
(1,163)	1:51:A:PHE:HA	1:55:A:TYR:H	3	0.18
(1,139)	1:51:A:PHE:H	1:53:A:GLU:H	10	0.18
(1,103)	1:52:A:ARG:H	1:53:A:GLU:H	7	0.18
(1,28)	1:22:A:THR:HA	1:24:A:VAL:H	6	0.18
(2,98)	1:178:A:THR:H	1:202:A:THR:H	5	0.17
(2,95)	1:210:A:ILE:HA	1:235:A:TYR:H	2	0.17
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG11	8	0.17
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG12	8	0.17
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG13	8	0.17
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG21	8	0.17
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG22	8	0.17
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG23	8	0.17
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG11	8	0.17
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG12	8	0.17
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG13	8	0.17
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG21	8	0.17
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG22	8	0.17
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG23	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG11	8	0.17
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG12	8	0.17
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG13	8	0.17
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG21	8	0.17
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG22	8	0.17
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG23	8	0.17
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD11	8	0.17
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD12	8	0.17
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD13	8	0.17
(2,59)	1:235:A:TYR:HD1	1:237:A:LEU:H	4	0.17
(2,59)	1:235:A:TYR:HD2	1:237:A:LEU:H	4	0.17
(2,30)	1:79:A:GLY:H	1:83:A:ASP:HB2	8	0.17
(2,30)	1:79:A:GLY:H	1:83:A:ASP:HB3	8	0.17
(2,9)	1:41:A:PRO:HD2	1:44:A:LYS:H	7	0.17
(2,9)	1:41:A:PRO:HD3	1:44:A:LYS:H	7	0.17
(1,1328)	1:78:A:ILE:H	1:84:A:ARG:H	5	0.17
(1,1328)	1:78:A:ILE:H	1:84:A:ARG:H	8	0.17
(1,1327)	1:68:A:VAL:H	1:253:A:LEU:HA	2	0.17
(1,1317)	1:53:A:GLU:H	1:79:A:GLY:H	5	0.17
(1,1307)	1:51:A:PHE:H	1:144:A:TRP:HD1	1	0.17
(1,1306)	1:49:A:ASP:H	1:144:A:TRP:HD1	4	0.17
(1,1277)	1:210:A:ILE:H	1:232:A:VAL:HG11	7	0.17
(1,1277)	1:210:A:ILE:H	1:232:A:VAL:HG12	7	0.17
(1,1277)	1:210:A:ILE:H	1:232:A:VAL:HG13	7	0.17
(1,1277)	1:210:A:ILE:H	1:232:A:VAL:HG21	7	0.17
(1,1277)	1:210:A:ILE:H	1:232:A:VAL:HG22	7	0.17
(1,1277)	1:210:A:ILE:H	1:232:A:VAL:HG23	7	0.17
(1,1271)	1:189:A:TYR:H	1:230:A:TRP:H	6	0.17
(1,1270)	1:185:A:TYR:HA	1:230:A:TRP:H	2	0.17
(1,1264)	1:134:A:PHE:H	1:234:A:ILE:HD12	7	0.17
(1,1262)	1:133:A:GLY:HA2	1:235:A:TYR:H	4	0.17
(1,1262)	1:133:A:GLY:HA3	1:235:A:TYR:H	4	0.17
(1,1258)	1:132:A:ILE:H	1:237:A:LEU:HG	3	0.17
(1,1249)	1:123:A:TYR:H	1:224:A:VAL:HA	3	0.17
(1,1224)	1:81:A:MET:HA	1:143:A:LEU:H	7	0.17
(1,1222)	1:81:A:MET:H	1:144:A:TRP:HD1	6	0.17
(1,1220)	1:78:A:ILE:HA	1:84:A:ARG:H	8	0.17
(1,1207)	1:62:A:SER:HA	1:67:A:LYS:H	4	0.17
(1,1187)	1:33:A:SER:H	1:39:A:GLN:HA	1	0.17
(1,1153)	1:237:A:LEU:HA	1:241:A:ASP:H	9	0.17
(1,1150)	1:174:A:ARG:H	1:177:A:GLU:HB2	7	0.17
(1,1148)	1:171:A:VAL:HA	1:174:A:ARG:H	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:171:A:VAL:HA	1:174:A:ARG:H	5	0.17
(1,1148)	1:171:A:VAL:HA	1:174:A:ARG:H	9	0.17
(1,1096)	1:263:A:SER:HA	1:264:A:ILE:H	7	0.17
(1,1081)	1:247:A:LEU:HA	1:251:A:GLY:H	9	0.17
(1,1073)	1:248:A:ARG:HB2	1:251:A:GLY:H	3	0.17
(1,1024)	1:244:A:GLY:H	1:246:A:THR:H	9	0.17
(1,1012)	1:238:A:LYS:HA	1:240:A:ASP:H	4	0.17
(1,1000)	1:237:A:LEU:HA	1:241:A:ASP:H	9	0.17
(1,988)	1:238:A:LYS:HA	1:241:A:ASP:H	8	0.17
(1,987)	1:237:A:LEU:HA	1:240:A:ASP:H	8	0.17
(1,982)	1:232:A:VAL:HA	1:235:A:TYR:H	10	0.17
(1,908)	1:220:A:TYR:HA	1:223:A:GLU:H	5	0.17
(1,908)	1:220:A:TYR:HA	1:223:A:GLU:H	6	0.17
(1,888)	1:218:A:LEU:H	1:220:A:TYR:H	1	0.17
(1,856)	1:214:A:ASP:HA	1:215:A:VAL:H	8	0.17
(1,843)	1:201:A:ALA:HA	1:205:A:VAL:H	9	0.17
(1,839)	1:206:A:ARG:HA	1:209:A:MET:H	5	0.17
(1,838)	1:205:A:VAL:HA	1:208:A:GLN:H	3	0.17
(1,834)	1:202:A:THR:HA	1:205:A:VAL:H	5	0.17
(1,829)	1:206:A:ARG:HB2	1:208:A:GLN:H	6	0.17
(1,829)	1:206:A:ARG:HB3	1:208:A:GLN:H	6	0.17
(1,758)	1:184:A:LEU:HA	1:187:A:MET:H	5	0.17
(1,756)	1:182:A:SER:HA	1:185:A:TYR:H	2	0.17
(1,756)	1:182:A:SER:HA	1:185:A:TYR:H	6	0.17
(1,751)	1:177:A:GLU:HA	1:180:A:ARG:H	6	0.17
(1,740)	1:178:A:THR:HA	1:182:A:SER:H	3	0.17
(1,733)	1:188:A:SER:HA	1:190:A:LYS:H	10	0.17
(1,710)	1:176:A:SER:HA	1:178:A:THR:H	3	0.17
(1,710)	1:176:A:SER:HA	1:178:A:THR:H	4	0.17
(1,709)	1:176:A:SER:H	1:178:A:THR:H	1	0.17
(1,629)	1:155:A:GLU:HA	1:158:A:LYS:H	8	0.17
(1,585)	1:155:A:GLU:H	1:156:A:GLU:H	3	0.17
(1,583)	1:151:A:GLY:HA2	1:153:A:TRP:H	4	0.17
(1,530)	1:118:A:GLU:HA	1:122:A:ASP:H	1	0.17
(1,524)	1:128:A:PHE:HA	1:131:A:LEU:H	5	0.17
(1,521)	1:126:A:VAL:HA	1:129:A:GLY:H	1	0.17
(1,518)	1:123:A:TYR:HA	1:126:A:VAL:H	7	0.17
(1,518)	1:123:A:TYR:HA	1:126:A:VAL:H	8	0.17
(1,516)	1:121:A:VAL:HA	1:124:A:VAL:H	8	0.17
(1,513)	1:118:A:GLU:HA	1:121:A:VAL:H	5	0.17
(1,503)	1:127:A:ILE:HB	1:129:A:GLY:H	2	0.17
(1,396)	1:98:A:ILE:HA	1:101:A:VAL:H	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:98:A:ILE:HA	1:101:A:VAL:H	6	0.17
(1,393)	1:96:A:THR:HA	1:99:A:ALA:H	8	0.17
(1,390)	1:103:A:LYS:HA	1:107:A:SER:H	2	0.17
(1,376)	1:92:A:THR:HA	1:95:A:ASN:H	3	0.17
(1,342)	1:90:A:ASN:H	1:92:A:THR:H	2	0.17
(1,342)	1:90:A:ASN:H	1:92:A:THR:H	4	0.17
(1,266)	1:70:A:ALA:HA	1:74:A:TYR:H	3	0.17
(1,243)	1:74:A:TYR:HA	1:76:A:TYR:H	7	0.17
(1,240)	1:73:A:ASP:H	1:75:A:GLY:H	1	0.17
(1,223)	1:77:A:GLN:H	1:78:A:ILE:H	4	0.17
(1,192)	1:66:A:SER:H	1:67:A:LYS:H	5	0.17
(1,180)	1:56:A:TYR:HA	1:59:A:ARG:H	9	0.17
(1,175)	1:51:A:PHE:HA	1:54:A:ALA:H	10	0.17
(1,173)	1:49:A:ASP:HA	1:52:A:ARG:H	10	0.17
(1,166)	1:54:A:ALA:HA	1:58:A:LEU:H	4	0.17
(1,163)	1:51:A:PHE:HA	1:55:A:TYR:H	9	0.17
(1,160)	1:48:A:ILE:HA	1:52:A:ARG:H	3	0.17
(1,146)	1:54:A:ALA:HA	1:56:A:TYR:H	2	0.17
(1,146)	1:54:A:ALA:HA	1:56:A:TYR:H	4	0.17
(1,145)	1:54:A:ALA:H	1:56:A:TYR:H	4	0.17
(1,140)	1:51:A:PHE:HA	1:53:A:GLU:H	9	0.17
(1,56)	1:34:A:VAL:H	1:35:A:VAL:H	7	0.17
(1,44)	1:24:A:VAL:HA	1:27:A:THR:H	3	0.17
(1,27)	1:22:A:THR:H	1:24:A:VAL:H	5	0.17
(2,86)	1:68:A:VAL:H	1:253:A:LEU:HB2	4	0.16
(2,86)	1:68:A:VAL:H	1:253:A:LEU:HB3	4	0.16
(2,69)	1:260:A:THR:HG21	1:262:A:ARG:H	8	0.16
(2,69)	1:260:A:THR:HG22	1:262:A:ARG:H	8	0.16
(2,69)	1:260:A:THR:HG23	1:262:A:ARG:H	8	0.16
(2,9)	1:41:A:PRO:HD2	1:44:A:LYS:H	5	0.16
(2,9)	1:41:A:PRO:HD3	1:44:A:LYS:H	5	0.16
(1,1336)	1:189:A:TYR:HA	1:230:A:TRP:H	4	0.16
(1,1334)	1:177:A:GLU:H	1:202:A:THR:HA	5	0.16
(1,1318)	1:53:A:GLU:H	1:80:A:GLY:H	6	0.16
(1,1314)	1:177:A:GLU:H	1:202:A:THR:HA	5	0.16
(1,1306)	1:49:A:ASP:H	1:144:A:TRP:HD1	3	0.16
(1,1298)	1:156:A:GLU:H	1:25:A:THR:HG1	7	0.16
(1,1297)	1:23:A:TRP:HZ3	1:191:A:ASP:H	8	0.16
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD11	3	0.16
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD12	3	0.16
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD13	3	0.16
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD21	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD22	3	0.16
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD23	3	0.16
(1,1281)	1:213:A:LEU:H	1:218:A:LEU:HG	10	0.16
(1,1262)	1:133:A:GLY:HA2	1:235:A:TYR:H	3	0.16
(1,1262)	1:133:A:GLY:HA3	1:235:A:TYR:H	3	0.16
(1,1249)	1:123:A:TYR:H	1:224:A:VAL:HA	2	0.16
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG11	3	0.16
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG12	3	0.16
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG13	3	0.16
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG21	3	0.16
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG22	3	0.16
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG23	3	0.16
(1,1229)	1:98:A:ILE:H	1:255:A:ARG:HG2	2	0.16
(1,1229)	1:98:A:ILE:H	1:255:A:ARG:HG3	2	0.16
(1,1208)	1:63:A:ASP:H	1:264:A:ILE:H	5	0.16
(1,1207)	1:62:A:SER:HA	1:67:A:LYS:H	2	0.16
(1,1194)	1:35:A:VAL:H	1:40:A:THR:HA	1	0.16
(1,1179)	1:29:A:TYR:H	1:46:A:ALA:H	7	0.16
(1,1148)	1:171:A:VAL:HA	1:174:A:ARG:H	2	0.16
(1,1117)	1:261:A:ARG:HB2	1:263:A:SER:H	1	0.16
(1,1117)	1:261:A:ARG:HB3	1:263:A:SER:H	1	0.16
(1,1089)	1:260:A:THR:HB	1:261:A:ARG:H	1	0.16
(1,1081)	1:247:A:LEU:HA	1:251:A:GLY:H	8	0.16
(1,1078)	1:252:A:GLU:HA	1:255:A:ARG:H	9	0.16
(1,1074)	1:248:A:ARG:HG2	1:251:A:GLY:H	3	0.16
(1,1023)	1:246:A:THR:HB	1:247:A:LEU:H	10	0.16
(1,1014)	1:242:A:ALA:HA	1:244:A:GLY:H	8	0.16
(1,989)	1:239:A:LYS:HA	1:242:A:ALA:H	8	0.16
(1,988)	1:238:A:LYS:HA	1:241:A:ASP:H	1	0.16
(1,987)	1:237:A:LEU:HA	1:240:A:ASP:H	9	0.16
(1,987)	1:237:A:LEU:HA	1:240:A:ASP:H	10	0.16
(1,986)	1:236:A:GLN:HA	1:239:A:LYS:H	8	0.16
(1,985)	1:235:A:TYR:HA	1:238:A:LYS:H	7	0.16
(1,981)	1:231:A:ASN:HA	1:234:A:ILE:H	7	0.16
(1,953)	1:229:A:ASN:HA	1:231:A:ASN:H	7	0.16
(1,952)	1:229:A:ASN:H	1:231:A:ASN:H	3	0.16
(1,917)	1:222:A:ASP:HA	1:226:A:THR:H	5	0.16
(1,915)	1:220:A:TYR:HA	1:224:A:VAL:H	5	0.16
(1,891)	1:219:A:ASP:HA	1:221:A:PHE:H	6	0.16
(1,856)	1:214:A:ASP:HA	1:215:A:VAL:H	7	0.16
(1,844)	1:202:A:THR:HA	1:206:A:ARG:H	1	0.16
(1,844)	1:202:A:THR:HA	1:206:A:ARG:H	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:202:A:THR:HA	1:206:A:ARG:H	7	0.16
(1,842)	1:200:A:GLN:HA	1:204:A:ARG:H	8	0.16
(1,836)	1:203:A:ASP:HA	1:206:A:ARG:H	8	0.16
(1,834)	1:202:A:THR:HA	1:205:A:VAL:H	1	0.16
(1,826)	1:205:A:VAL:HB	1:207:A:GLN:H	4	0.16
(1,814)	1:200:A:GLN:H	1:202:A:THR:H	9	0.16
(1,791)	1:202:A:THR:H	1:203:A:ASP:H	9	0.16
(1,775)	1:197:A:ASN:H	1:198:A:GLY:H	3	0.16
(1,762)	1:188:A:SER:HA	1:191:A:ASP:H	3	0.16
(1,762)	1:188:A:SER:HA	1:191:A:ASP:H	10	0.16
(1,761)	1:187:A:MET:HA	1:190:A:LYS:H	10	0.16
(1,752)	1:178:A:THR:HA	1:181:A:ASN:H	5	0.16
(1,748)	1:186:A:LYS:HA	1:190:A:LYS:H	1	0.16
(1,746)	1:184:A:LEU:HA	1:188:A:SER:H	10	0.16
(1,741)	1:179:A:MET:HA	1:183:A:LEU:H	7	0.16
(1,739)	1:177:A:GLU:HA	1:181:A:ASN:H	8	0.16
(1,738)	1:176:A:SER:HA	1:180:A:ARG:H	6	0.16
(1,660)	1:171:A:VAL:HG12	1:173:A:ALA:H	3	0.16
(1,629)	1:155:A:GLU:HA	1:158:A:LYS:H	2	0.16
(1,569)	1:149:A:SER:HA	1:150:A:GLU:H	5	0.16
(1,534)	1:121:A:VAL:HA	1:125:A:LEU:H	8	0.16
(1,524)	1:128:A:PHE:HA	1:131:A:LEU:H	4	0.16
(1,523)	1:127:A:ILE:HA	1:130:A:GLY:H	7	0.16
(1,515)	1:120:A:ASP:HA	1:123:A:TYR:H	6	0.16
(1,512)	1:117:A:LYS:HA	1:120:A:ASP:H	1	0.16
(1,510)	1:115:A:ILE:HA	1:118:A:GLU:H	6	0.16
(1,493)	1:123:A:TYR:HA	1:125:A:LEU:H	1	0.16
(1,473)	1:114:A:GLU:H	1:116:A:LEU:H	4	0.16
(1,419)	1:112:A:SER:H	1:113:A:TYR:H	9	0.16
(1,415)	1:110:A:GLU:HB2	1:111:A:LYS:H	8	0.16
(1,415)	1:110:A:GLU:HB3	1:111:A:LYS:H	8	0.16
(1,414)	1:110:A:GLU:HA	1:111:A:LYS:H	1	0.16
(1,393)	1:96:A:THR:HA	1:99:A:ALA:H	7	0.16
(1,377)	1:93:A:TRP:HA	1:96:A:THR:H	9	0.16
(1,363)	1:103:A:LYS:HA	1:105:A:ASN:H	9	0.16
(1,266)	1:70:A:ALA:HA	1:74:A:TYR:H	1	0.16
(1,258)	1:71:A:TRP:HA	1:74:A:TYR:H	2	0.16
(1,250)	1:77:A:GLN:HA	1:79:A:GLY:H	2	0.16
(1,250)	1:77:A:GLN:HA	1:79:A:GLY:H	6	0.16
(1,243)	1:74:A:TYR:HA	1:76:A:TYR:H	3	0.16
(1,192)	1:66:A:SER:H	1:67:A:LYS:H	4	0.16
(1,187)	1:62:A:SER:HA	1:65:A:ASP:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:51:A:PHE:HA	1:54:A:ALA:H	8	0.16
(1,169)	1:45:A:LEU:HA	1:48:A:ILE:H	7	0.16
(1,167)	1:55:A:TYR:HA	1:59:A:ARG:H	6	0.16
(1,155)	1:59:A:ARG:HA	1:61:A:ASN:H	5	0.16
(1,146)	1:54:A:ALA:HA	1:56:A:TYR:H	9	0.16
(1,129)	1:46:A:ALA:H	1:48:A:ILE:H	2	0.16
(1,83)	1:45:A:LEU:H	1:46:A:ALA:H	2	0.16
(1,35)	1:25:A:THR:HA	1:27:A:THR:H	5	0.16
(1,30)	1:23:A:TRP:HA	1:25:A:THR:H	10	0.16
(1,1335)	1:54:A:ALA:H	1:81:A:MET:HA	1	0.15
(1,1327)	1:68:A:VAL:H	1:253:A:LEU:HA	4	0.15
(1,1321)	1:22:A:THR:H	1:148:A:ILE:HA	4	0.15
(1,1317)	1:53:A:GLU:H	1:79:A:GLY:H	6	0.15
(1,1309)	1:132:A:ILE:H	1:233:A:ARG:HB2	5	0.15
(1,1309)	1:132:A:ILE:H	1:233:A:ARG:HB3	5	0.15
(1,1298)	1:156:A:GLU:H	1:25:A:THR:HG1	2	0.15
(1,1298)	1:156:A:GLU:H	1:25:A:THR:HG1	5	0.15
(1,1296)	1:22:A:THR:H	1:148:A:ILE:HA	4	0.15
(1,1293)	1:268:A:GLU:H	1:273:A:VAL:HA	7	0.15
(1,1289)	1:266:A:ARG:H	1:273:A:VAL:H	1	0.15
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB2	6	0.15
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB3	6	0.15
(1,1262)	1:133:A:GLY:HA2	1:235:A:TYR:H	1	0.15
(1,1262)	1:133:A:GLY:HA3	1:235:A:TYR:H	1	0.15
(1,1257)	1:132:A:ILE:H	1:233:A:ARG:HB2	5	0.15
(1,1257)	1:132:A:ILE:H	1:233:A:ARG:HB3	5	0.15
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD11	1	0.15
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD12	1	0.15
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD13	1	0.15
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG11	1	0.15
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG12	1	0.15
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG13	1	0.15
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG21	1	0.15
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG22	1	0.15
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG23	1	0.15
(1,1230)	1:100:A:ILE:H	1:36:A:LEU:HD11	10	0.15
(1,1230)	1:100:A:ILE:H	1:36:A:LEU:HD12	10	0.15
(1,1230)	1:100:A:ILE:H	1:36:A:LEU:HD13	10	0.15
(1,1230)	1:100:A:ILE:H	1:36:A:LEU:HD21	10	0.15
(1,1230)	1:100:A:ILE:H	1:36:A:LEU:HD22	10	0.15
(1,1230)	1:100:A:ILE:H	1:36:A:LEU:HD23	10	0.15
(1,1217)	1:77:A:GLN:H	1:98:A:ILE:HG13	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1216)	1:71:A:TRP:H	1:255:A:ARG:HG2	3	0.15
(1,1216)	1:71:A:TRP:H	1:255:A:ARG:HG3	3	0.15
(1,1210)	1:64:A:GLU:H	1:263:A:SER:H	8	0.15
(1,1209)	1:63:A:ASP:H	1:265:A:LYS:H	1	0.15
(1,1206)	1:56:A:TYR:HA	1:69:A:ALA:H	5	0.15
(1,1200)	1:54:A:ALA:H	1:82:A:ALA:H	1	0.15
(1,1185)	1:27:A:THR:HA	1:46:A:ALA:H	7	0.15
(1,1179)	1:29:A:TYR:H	1:46:A:ALA:H	8	0.15
(1,1142)	1:213:A:LEU:H	1:214:A:ASP:HA	2	0.15
(1,1077)	1:251:A:GLY:HA2	1:254:A:THR:H	8	0.15
(1,1077)	1:251:A:GLY:HA3	1:254:A:THR:H	8	0.15
(1,1075)	1:249:A:ASP:HA	1:252:A:GLU:H	4	0.15
(1,1073)	1:248:A:ARG:HB2	1:251:A:GLY:H	6	0.15
(1,1073)	1:248:A:ARG:HB2	1:251:A:GLY:H	10	0.15
(1,989)	1:239:A:LYS:HA	1:242:A:ALA:H	2	0.15
(1,987)	1:237:A:LEU:HA	1:240:A:ASP:H	5	0.15
(1,956)	1:230:A:TRP:HE3	1:232:A:VAL:H	3	0.15
(1,954)	1:230:A:TRP:H	1:232:A:VAL:H	9	0.15
(1,909)	1:221:A:PHE:HA	1:224:A:VAL:H	6	0.15
(1,909)	1:221:A:PHE:HA	1:224:A:VAL:H	10	0.15
(1,852)	1:213:A:LEU:H	1:214:A:ASP:H	8	0.15
(1,852)	1:213:A:LEU:H	1:214:A:ASP:H	10	0.15
(1,842)	1:200:A:GLN:HA	1:204:A:ARG:H	1	0.15
(1,840)	1:207:A:GLN:HA	1:210:A:ILE:H	3	0.15
(1,839)	1:206:A:ARG:HA	1:209:A:MET:H	1	0.15
(1,839)	1:206:A:ARG:HA	1:209:A:MET:H	7	0.15
(1,839)	1:206:A:ARG:HA	1:209:A:MET:H	8	0.15
(1,835)	1:202:A:THR:HB	1:205:A:VAL:H	4	0.15
(1,740)	1:178:A:THR:HA	1:182:A:SER:H	2	0.15
(1,717)	1:180:A:ARG:H	1:182:A:SER:H	3	0.15
(1,712)	1:177:A:GLU:HA	1:179:A:MET:H	8	0.15
(1,630)	1:156:A:GLU:HA	1:159:A:GLU:H	7	0.15
(1,566)	1:148:A:ILE:HA	1:149:A:SER:H	7	0.15
(1,549)	1:135:A:GLY:H	1:136:A:GLY:H	6	0.15
(1,534)	1:121:A:VAL:HA	1:125:A:LEU:H	2	0.15
(1,530)	1:118:A:GLU:HA	1:122:A:ASP:H	5	0.15
(1,530)	1:118:A:GLU:HA	1:122:A:ASP:H	6	0.15
(1,517)	1:122:A:ASP:HA	1:125:A:LEU:H	9	0.15
(1,416)	1:111:A:LYS:H	1:112:A:SER:H	6	0.15
(1,400)	1:102:A:GLY:HA2	1:105:A:ASN:H	5	0.15
(1,400)	1:102:A:GLY:HA3	1:105:A:ASN:H	5	0.15
(1,377)	1:93:A:TRP:HA	1:96:A:THR:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:69:A:ALA:HA	1:73:A:ASP:H	4	0.15
(1,264)	1:68:A:VAL:HA	1:72:A:TRP:H	4	0.15
(1,263)	1:76:A:TYR:HA	1:79:A:GLY:H	8	0.15
(1,258)	1:71:A:TRP:HA	1:74:A:TYR:H	1	0.15
(1,250)	1:77:A:GLN:HA	1:79:A:GLY:H	9	0.15
(1,238)	1:72:A:TRP:H	1:74:A:TYR:H	5	0.15
(1,192)	1:66:A:SER:H	1:67:A:LYS:H	6	0.15
(1,192)	1:66:A:SER:H	1:67:A:LYS:H	8	0.15
(1,184)	1:63:A:ASP:H	1:64:A:GLU:H	9	0.15
(1,181)	1:57:A:TRP:HA	1:60:A:MET:H	2	0.15
(1,173)	1:49:A:ASP:HA	1:52:A:ARG:H	2	0.15
(1,171)	1:47:A:LEU:HA	1:50:A:ASP:H	7	0.15
(1,170)	1:46:A:ALA:HA	1:49:A:ASP:H	8	0.15
(1,157)	1:45:A:LEU:HA	1:49:A:ASP:H	1	0.15
(1,155)	1:59:A:ARG:HA	1:61:A:ASN:H	8	0.15
(1,142)	1:52:A:ARG:HA	1:54:A:ALA:H	2	0.15
(1,133)	1:48:A:ILE:H	1:50:A:ASP:H	2	0.15
(1,83)	1:45:A:LEU:H	1:46:A:ALA:H	7	0.15
(1,50)	1:24:A:VAL:HA	1:28:A:ALA:H	8	0.15
(1,49)	1:23:A:TRP:HA	1:27:A:THR:H	2	0.15
(1,47)	1:21:A:SER:HA	1:25:A:THR:H	7	0.15
(1,44)	1:24:A:VAL:HA	1:27:A:THR:H	2	0.15
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD11	2	0.14
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD12	2	0.14
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD13	2	0.14
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD21	2	0.14
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD22	2	0.14
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD23	2	0.14
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG11	1	0.14
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG12	1	0.14
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG13	1	0.14
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG21	1	0.14
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG22	1	0.14
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG23	1	0.14
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG11	1	0.14
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG12	1	0.14
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG13	1	0.14
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG21	1	0.14
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG22	1	0.14
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG23	1	0.14
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG11	1	0.14
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG12	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG13	1	0.14
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG21	1	0.14
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG22	1	0.14
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG23	1	0.14
(2,86)	1:68:A:VAL:H	1:253:A:LEU:HB2	9	0.14
(2,86)	1:68:A:VAL:H	1:253:A:LEU:HB3	9	0.14
(2,86)	1:68:A:VAL:H	1:253:A:LEU:HB2	10	0.14
(2,86)	1:68:A:VAL:H	1:253:A:LEU:HB3	10	0.14
(1,1333)	1:174:A:ARG:H	1:198:A:GLY:HA2	1	0.14
(1,1333)	1:174:A:ARG:H	1:198:A:GLY:HA3	1	0.14
(1,1333)	1:174:A:ARG:H	1:198:A:GLY:HA2	9	0.14
(1,1333)	1:174:A:ARG:H	1:198:A:GLY:HA3	9	0.14
(1,1325)	1:60:A:MET:H	1:69:A:ALA:HA	5	0.14
(1,1317)	1:53:A:GLU:H	1:79:A:GLY:H	3	0.14
(1,1288)	1:265:A:LYS:H	1:270:A:GLY:H	3	0.14
(1,1288)	1:265:A:LYS:H	1:270:A:GLY:H	8	0.14
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB2	5	0.14
(1,1282)	1:233:A:ARG:H	1:185:A:TYR:HB3	5	0.14
(1,1259)	1:132:A:ILE:H	1:237:A:LEU:HB2	10	0.14
(1,1259)	1:132:A:ILE:H	1:237:A:LEU:HB3	10	0.14
(1,1200)	1:54:A:ALA:H	1:82:A:ALA:H	4	0.14
(1,1192)	1:34:A:VAL:H	1:40:A:THR:H	4	0.14
(1,1191)	1:34:A:VAL:H	1:40:A:THR:HA	10	0.14
(1,1185)	1:27:A:THR:HA	1:46:A:ALA:H	1	0.14
(1,1184)	1:26:A:ARG:HA	1:47:A:LEU:H	10	0.14
(1,1177)	1:26:A:ARG:H	1:45:A:LEU:H	4	0.14
(1,1171)	1:26:A:ARG:H	1:46:A:ALA:HB1	3	0.14
(1,1171)	1:26:A:ARG:H	1:46:A:ALA:HB2	3	0.14
(1,1171)	1:26:A:ARG:H	1:46:A:ALA:HB3	3	0.14
(1,1165)	1:22:A:THR:HB	1:45:A:LEU:H	4	0.14
(1,1161)	1:266:A:ARG:HE	1:269:A:LEU:H	5	0.14
(1,1160)	1:261:A:ARG:H	1:264:A:ILE:HA	1	0.14
(1,1146)	1:135:A:GLY:HA2	1:138:A:ASP:H	6	0.14
(1,1146)	1:135:A:GLY:HA3	1:138:A:ASP:H	6	0.14
(1,1117)	1:261:A:ARG:HB2	1:263:A:SER:H	5	0.14
(1,1117)	1:261:A:ARG:HB3	1:263:A:SER:H	5	0.14
(1,1082)	1:248:A:ARG:HA	1:252:A:GLU:H	9	0.14
(1,1081)	1:247:A:LEU:HA	1:251:A:GLY:H	6	0.14
(1,1077)	1:251:A:GLY:HA2	1:254:A:THR:H	10	0.14
(1,1077)	1:251:A:GLY:HA3	1:254:A:THR:H	10	0.14
(1,1074)	1:248:A:ARG:HG2	1:251:A:GLY:H	2	0.14
(1,1074)	1:248:A:ARG:HG2	1:251:A:GLY:H	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1073)	1:248:A:ARG:HB2	1:251:A:GLY:H	1	0.14
(1,1073)	1:248:A:ARG:HB2	1:251:A:GLY:H	7	0.14
(1,1014)	1:242:A:ALA:HA	1:244:A:GLY:H	2	0.14
(1,1014)	1:242:A:ALA:HA	1:244:A:GLY:H	10	0.14
(1,1004)	1:239:A:LYS:HA	1:240:A:ASP:H	4	0.14
(1,993)	1:230:A:TRP:HA	1:234:A:ILE:H	8	0.14
(1,991)	1:228:A:GLU:HA	1:232:A:VAL:H	3	0.14
(1,987)	1:237:A:LEU:HA	1:240:A:ASP:H	2	0.14
(1,906)	1:218:A:LEU:HA	1:221:A:PHE:H	4	0.14
(1,844)	1:202:A:THR:HA	1:206:A:ARG:H	5	0.14
(1,838)	1:205:A:VAL:HA	1:208:A:GLN:H	4	0.14
(1,834)	1:202:A:THR:HA	1:205:A:VAL:H	6	0.14
(1,828)	1:206:A:ARG:HA	1:208:A:GLN:H	8	0.14
(1,826)	1:205:A:VAL:HB	1:207:A:GLN:H	8	0.14
(1,757)	1:183:A:LEU:HA	1:186:A:LYS:H	5	0.14
(1,755)	1:181:A:ASN:HA	1:184:A:LEU:H	5	0.14
(1,749)	1:187:A:MET:HA	1:191:A:ASP:H	2	0.14
(1,746)	1:184:A:LEU:HA	1:188:A:SER:H	8	0.14
(1,718)	1:180:A:ARG:HA	1:182:A:SER:H	8	0.14
(1,712)	1:177:A:GLU:HA	1:179:A:MET:H	2	0.14
(1,712)	1:177:A:GLU:HA	1:179:A:MET:H	3	0.14
(1,630)	1:156:A:GLU:HA	1:159:A:GLU:H	2	0.14
(1,629)	1:155:A:GLU:HA	1:158:A:LYS:H	5	0.14
(1,580)	1:135:A:GLY:H	1:137:A:ASP:HB2	3	0.14
(1,565)	1:148:A:ILE:H	1:149:A:SER:H	2	0.14
(1,540)	1:131:A:LEU:H	1:132:A:ILE:H	9	0.14
(1,533)	1:120:A:ASP:HA	1:124:A:VAL:H	10	0.14
(1,526)	1:114:A:GLU:HA	1:118:A:GLU:H	7	0.14
(1,523)	1:127:A:ILE:HA	1:130:A:GLY:H	9	0.14
(1,512)	1:117:A:LYS:HA	1:120:A:ASP:H	8	0.14
(1,508)	1:130:A:GLY:H	1:132:A:ILE:H	10	0.14
(1,499)	1:126:A:VAL:H	1:128:A:PHE:H	10	0.14
(1,422)	1:113:A:TYR:H	1:114:A:GLU:H	2	0.14
(1,419)	1:112:A:SER:H	1:113:A:TYR:H	3	0.14
(1,414)	1:110:A:GLU:HA	1:111:A:LYS:H	2	0.14
(1,393)	1:96:A:THR:HA	1:99:A:ALA:H	1	0.14
(1,385)	1:98:A:ILE:HA	1:102:A:GLY:H	6	0.14
(1,383)	1:96:A:THR:HA	1:100:A:ILE:H	4	0.14
(1,377)	1:93:A:TRP:HA	1:96:A:THR:H	7	0.14
(1,374)	1:90:A:ASN:HA	1:93:A:TRP:H	5	0.14
(1,374)	1:90:A:ASN:HA	1:93:A:TRP:H	9	0.14
(1,369)	1:85:A:THR:HA	1:88:A:VAL:H	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	1:99:A:ALA:HA	1:101:A:VAL:H	8	0.14
(1,354)	1:99:A:ALA:H	1:101:A:VAL:H	5	0.14
(1,345)	1:93:A:TRP:H	1:95:A:ASN:H	6	0.14
(1,343)	1:91:A:ASN:H	1:93:A:TRP:H	8	0.14
(1,287)	1:87:A:LEU:H	1:88:A:VAL:H	1	0.14
(1,280)	1:84:A:ARG:H	1:85:A:THR:H	3	0.14
(1,280)	1:84:A:ARG:H	1:85:A:THR:H	5	0.14
(1,277)	1:83:A:ASP:HA	1:84:A:ARG:H	3	0.14
(1,259)	1:72:A:TRP:HA	1:75:A:GLY:H	10	0.14
(1,240)	1:73:A:ASP:H	1:75:A:GLY:H	8	0.14
(1,228)	1:66:A:SER:HA	1:68:A:VAL:H	8	0.14
(1,177)	1:53:A:GLU:HA	1:56:A:TYR:H	10	0.14
(1,163)	1:51:A:PHE:HA	1:55:A:TYR:H	5	0.14
(1,158)	1:46:A:ALA:HA	1:50:A:ASP:H	4	0.14
(1,140)	1:51:A:PHE:HA	1:53:A:GLU:H	3	0.14
(1,133)	1:48:A:ILE:H	1:50:A:ASP:H	9	0.14
(1,130)	1:46:A:ALA:HA	1:48:A:ILE:H	9	0.14
(1,83)	1:45:A:LEU:H	1:46:A:ALA:H	10	0.14
(1,80)	1:42:A:ASP:HB2	1:44:A:LYS:H	3	0.14
(1,80)	1:42:A:ASP:HB3	1:44:A:LYS:H	3	0.14
(1,78)	1:34:A:VAL:H	1:36:A:LEU:H	7	0.14
(1,76)	1:31:A:SER:HA	1:33:A:SER:H	8	0.14
(1,74)	1:44:A:LYS:H	1:45:A:LEU:H	9	0.14
(1,56)	1:34:A:VAL:H	1:35:A:VAL:H	8	0.14
(1,47)	1:21:A:SER:HA	1:25:A:THR:H	4	0.14
(1,47)	1:21:A:SER:HA	1:25:A:THR:H	5	0.14
(1,35)	1:25:A:THR:HA	1:27:A:THR:H	1	0.14
(2,95)	1:210:A:ILE:HA	1:235:A:TYR:H	3	0.13
(2,94)	1:204:A:ARG:HA	1:209:A:MET:H	5	0.13
(2,89)	1:123:A:TYR:HA	1:226:A:THR:H	1	0.13
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD11	2	0.13
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD12	2	0.13
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD13	2	0.13
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD11	3	0.13
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD12	3	0.13
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD13	3	0.13
(1,1336)	1:189:A:TYR:HA	1:230:A:TRP:H	7	0.13
(1,1327)	1:68:A:VAL:H	1:253:A:LEU:HA	10	0.13
(1,1302)	1:36:A:LEU:H	1:99:A:ALA:HA	8	0.13
(1,1290)	1:267:A:PRO:HA	1:272:A:ARG:H	8	0.13
(1,1287)	1:260:A:THR:HA	1:265:A:LYS:H	9	0.13
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG11	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG12	9	0.13
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG13	9	0.13
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG21	9	0.13
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG22	9	0.13
(1,1278)	1:211:A:THR:H	1:232:A:VAL:HG23	9	0.13
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG11	4	0.13
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG12	4	0.13
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG13	4	0.13
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG21	4	0.13
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG22	4	0.13
(1,1273)	1:195:A:LEU:HD11	1:224:A:VAL:HG23	4	0.13
(1,1267)	1:166:A:GLU:H	1:172:A:ASP:HA	2	0.13
(1,1267)	1:166:A:GLU:H	1:172:A:ASP:HA	3	0.13
(1,1229)	1:98:A:ILE:H	1:255:A:ARG:HG2	7	0.13
(1,1229)	1:98:A:ILE:H	1:255:A:ARG:HG3	7	0.13
(1,1227)	1:82:A:ALA:H	1:144:A:TRP:H	10	0.13
(1,1219)	1:78:A:ILE:HA	1:83:A:ASP:H	8	0.13
(1,1208)	1:63:A:ASP:H	1:264:A:ILE:H	9	0.13
(1,1204)	1:56:A:TYR:H	1:69:A:ALA:HA	7	0.13
(1,1167)	1:24:A:VAL:H	1:192:A:PHE:HE1	10	0.13
(1,1167)	1:24:A:VAL:H	1:192:A:PHE:HE2	10	0.13
(1,1163)	1:22:A:THR:H	1:47:A:LEU:H	7	0.13
(1,1082)	1:248:A:ARG:HA	1:252:A:GLU:H	6	0.13
(1,1074)	1:248:A:ARG:HG2	1:251:A:GLY:H	8	0.13
(1,1073)	1:248:A:ARG:HB2	1:251:A:GLY:H	2	0.13
(1,1073)	1:248:A:ARG:HB2	1:251:A:GLY:H	5	0.13
(1,1072)	1:248:A:ARG:HA	1:251:A:GLY:H	2	0.13
(1,1053)	1:247:A:LEU:HA	1:249:A:ASP:H	3	0.13
(1,1053)	1:247:A:LEU:HA	1:249:A:ASP:H	9	0.13
(1,1014)	1:242:A:ALA:HA	1:244:A:GLY:H	5	0.13
(1,1004)	1:239:A:LYS:HA	1:240:A:ASP:H	5	0.13
(1,998)	1:235:A:TYR:HA	1:239:A:LYS:H	2	0.13
(1,997)	1:234:A:ILE:HA	1:238:A:LYS:H	5	0.13
(1,994)	1:231:A:ASN:HA	1:235:A:TYR:H	8	0.13
(1,987)	1:237:A:LEU:HA	1:240:A:ASP:H	7	0.13
(1,986)	1:236:A:GLN:HA	1:239:A:LYS:H	6	0.13
(1,983)	1:233:A:ARG:HA	1:236:A:GLN:H	4	0.13
(1,917)	1:222:A:ASP:HA	1:226:A:THR:H	10	0.13
(1,912)	1:224:A:VAL:HA	1:227:A:SER:H	3	0.13
(1,909)	1:221:A:PHE:HA	1:224:A:VAL:H	7	0.13
(1,889)	1:218:A:LEU:HA	1:220:A:TYR:H	7	0.13
(1,836)	1:203:A:ASP:HA	1:206:A:ARG:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,836)	1:203:A:ASP:HA	1:206:A:ARG:H	9	0.13
(1,829)	1:206:A:ARG:HB2	1:208:A:GLN:H	9	0.13
(1,829)	1:206:A:ARG:HB3	1:208:A:GLN:H	9	0.13
(1,826)	1:205:A:VAL:HB	1:207:A:GLN:H	10	0.13
(1,816)	1:201:A:ALA:H	1:203:A:ASP:H	9	0.13
(1,788)	1:201:A:ALA:H	1:202:A:THR:H	2	0.13
(1,766)	1:194:A:GLN:H	1:195:A:LEU:H	4	0.13
(1,761)	1:187:A:MET:HA	1:190:A:LYS:H	2	0.13
(1,723)	1:183:A:LEU:HA	1:185:A:TYR:H	3	0.13
(1,723)	1:183:A:LEU:HA	1:185:A:TYR:H	10	0.13
(1,716)	1:179:A:MET:HA	1:181:A:ASN:H	8	0.13
(1,709)	1:176:A:SER:H	1:178:A:THR:H	3	0.13
(1,664)	1:177:A:GLU:H	1:178:A:THR:H	10	0.13
(1,659)	1:171:A:VAL:HB	1:173:A:ALA:H	1	0.13
(1,658)	1:163:A:TYR:H	1:165:A:ALA:H	2	0.13
(1,630)	1:156:A:GLU:HA	1:159:A:GLU:H	8	0.13
(1,629)	1:155:A:GLU:HA	1:158:A:LYS:H	1	0.13
(1,583)	1:151:A:GLY:HA2	1:153:A:TRP:H	8	0.13
(1,582)	1:148:A:ILE:HD11	1:150:A:GLU:H	5	0.13
(1,582)	1:148:A:ILE:HD12	1:150:A:GLU:H	5	0.13
(1,582)	1:148:A:ILE:HD13	1:150:A:GLU:H	5	0.13
(1,568)	1:149:A:SER:H	1:150:A:GLU:H	2	0.13
(1,536)	1:123:A:TYR:HA	1:127:A:ILE:H	9	0.13
(1,528)	1:116:A:LEU:HA	1:120:A:ASP:H	3	0.13
(1,528)	1:116:A:LEU:HA	1:120:A:ASP:H	6	0.13
(1,513)	1:118:A:GLU:HA	1:121:A:VAL:H	9	0.13
(1,488)	1:121:A:VAL:H	1:123:A:TYR:H	5	0.13
(1,475)	1:115:A:ILE:H	1:117:A:LYS:H	6	0.13
(1,473)	1:114:A:GLU:H	1:116:A:LEU:H	8	0.13
(1,406)	1:113:A:TYR:H	1:115:A:ILE:HD11	5	0.13
(1,405)	1:111:A:LYS:H	1:113:A:TYR:HB2	6	0.13
(1,401)	1:103:A:LYS:HA	1:106:A:ALA:H	1	0.13
(1,398)	1:100:A:ILE:HA	1:103:A:LYS:H	8	0.13
(1,391)	1:94:A:ASN:HA	1:97:A:HIS:H	5	0.13
(1,386)	1:99:A:ALA:HA	1:103:A:LYS:H	7	0.13
(1,371)	1:87:A:LEU:HG	1:90:A:ASN:H	9	0.13
(1,341)	1:87:A:LEU:HA	1:89:A:ASP:H	2	0.13
(1,289)	1:88:A:VAL:H	1:89:A:ASP:H	2	0.13
(1,251)	1:66:A:SER:HA	1:69:A:ALA:H	10	0.13
(1,234)	1:70:A:ALA:H	1:72:A:TRP:H	3	0.13
(1,228)	1:66:A:SER:HA	1:68:A:VAL:H	3	0.13
(1,192)	1:66:A:SER:H	1:67:A:LYS:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,184)	1:63:A:ASP:H	1:64:A:GLU:H	7	0.13
(1,169)	1:45:A:LEU:HA	1:48:A:ILE:H	8	0.13
(1,165)	1:53:A:GLU:HA	1:57:A:TRP:H	5	0.13
(1,142)	1:52:A:ARG:HA	1:54:A:ALA:H	8	0.13
(1,140)	1:51:A:PHE:HA	1:53:A:GLU:H	5	0.13
(1,134)	1:48:A:ILE:HA	1:50:A:ASP:H	9	0.13
(1,47)	1:21:A:SER:HA	1:25:A:THR:H	1	0.13
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD11	9	0.12
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD12	9	0.12
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD13	9	0.12
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD21	9	0.12
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD22	9	0.12
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD23	9	0.12
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD11	10	0.12
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD12	10	0.12
(2,87)	1:79:A:GLY:H	1:98:A:ILE:HD13	10	0.12
(2,84)	1:48:A:ILE:H	1:26:A:ARG:HD2	4	0.12
(2,84)	1:48:A:ILE:H	1:26:A:ARG:HD3	4	0.12
(2,56)	1:234:A:ILE:HD11	1:236:A:GLN:H	6	0.12
(2,56)	1:234:A:ILE:HD12	1:236:A:GLN:H	6	0.12
(2,56)	1:234:A:ILE:HD13	1:236:A:GLN:H	6	0.12
(2,24)	1:78:A:ILE:HD11	1:80:A:GLY:H	3	0.12
(2,24)	1:78:A:ILE:HD12	1:80:A:GLY:H	3	0.12
(2,24)	1:78:A:ILE:HD13	1:80:A:GLY:H	3	0.12
(1,1327)	1:68:A:VAL:H	1:253:A:LEU:HA	8	0.12
(1,1326)	1:64:A:GLU:H	1:262:A:ARG:HA	4	0.12
(1,1326)	1:64:A:GLU:H	1:262:A:ARG:HA	6	0.12
(1,1325)	1:60:A:MET:H	1:69:A:ALA:HA	8	0.12
(1,1318)	1:53:A:GLU:H	1:80:A:GLY:H	2	0.12
(1,1300)	1:120:A:ASP:H	1:34:A:VAL:HG11	6	0.12
(1,1298)	1:156:A:GLU:H	1:25:A:THR:HG1	3	0.12
(1,1289)	1:266:A:ARG:H	1:273:A:VAL:H	7	0.12
(1,1288)	1:265:A:LYS:H	1:270:A:GLY:H	5	0.12
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD11	7	0.12
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD12	7	0.12
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD13	7	0.12
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD21	7	0.12
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD22	7	0.12
(1,1283)	1:236:A:GLN:H	1:247:A:LEU:HD23	7	0.12
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB2	7	0.12
(1,1279)	1:211:A:THR:H	1:243:A:GLN:HB3	7	0.12
(1,1269)	1:173:A:ALA:HA	1:178:A:THR:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1247)	1:106:A:ALA:HA	1:113:A:TYR:H	1	0.12
(1,1246)	1:106:A:ALA:H	1:113:A:TYR:H	3	0.12
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD11	5	0.12
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD12	5	0.12
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD13	5	0.12
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD11	7	0.12
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD12	7	0.12
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD13	7	0.12
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG11	5	0.12
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG12	5	0.12
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG13	5	0.12
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG21	5	0.12
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG22	5	0.12
(1,1238)	1:101:A:VAL:HG11	1:224:A:VAL:HG23	5	0.12
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD11	8	0.12
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD12	8	0.12
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD13	8	0.12
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD21	8	0.12
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD22	8	0.12
(1,1232)	1:101:A:VAL:H	1:36:A:LEU:HD23	8	0.12
(1,1229)	1:98:A:ILE:H	1:255:A:ARG:HG2	10	0.12
(1,1229)	1:98:A:ILE:H	1:255:A:ARG:HG3	10	0.12
(1,1223)	1:81:A:MET:H	1:144:A:TRP:H	9	0.12
(1,1203)	1:56:A:TYR:H	1:72:A:TRP:H	7	0.12
(1,1201)	1:54:A:ALA:HA	1:82:A:ALA:H	6	0.12
(1,1200)	1:54:A:ALA:H	1:82:A:ALA:H	5	0.12
(1,1199)	1:52:A:ARG:H	1:76:A:TYR:H	7	0.12
(1,1193)	1:34:A:VAL:HG11	1:39:A:GLN:H	5	0.12
(1,1193)	1:34:A:VAL:HG12	1:39:A:GLN:H	5	0.12
(1,1193)	1:34:A:VAL:HG13	1:39:A:GLN:H	5	0.12
(1,1193)	1:34:A:VAL:HG21	1:39:A:GLN:H	5	0.12
(1,1193)	1:34:A:VAL:HG22	1:39:A:GLN:H	5	0.12
(1,1193)	1:34:A:VAL:HG23	1:39:A:GLN:H	5	0.12
(1,1188)	1:34:A:VAL:H	1:39:A:GLN:H	3	0.12
(1,1187)	1:33:A:SER:H	1:39:A:GLN:HA	8	0.12
(1,1179)	1:29:A:TYR:H	1:46:A:ALA:H	10	0.12
(1,1140)	1:199:A:GLY:H	1:200:A:GLN:HA	10	0.12
(1,1128)	1:51:A:PHE:H	1:52:A:ARG:HE	5	0.12
(1,1096)	1:263:A:SER:HA	1:264:A:ILE:H	1	0.12
(1,1082)	1:248:A:ARG:HA	1:252:A:GLU:H	10	0.12
(1,1079)	1:246:A:THR:HA	1:250:A:VAL:H	1	0.12
(1,1070)	1:247:A:LEU:HB2	1:250:A:VAL:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:238:A:LYS:HA	1:240:A:ASP:H	5	0.12
(1,1012)	1:238:A:LYS:HA	1:240:A:ASP:H	10	0.12
(1,1004)	1:239:A:LYS:HA	1:240:A:ASP:H	1	0.12
(1,1004)	1:239:A:LYS:HA	1:240:A:ASP:H	8	0.12
(1,1004)	1:239:A:LYS:HA	1:240:A:ASP:H	10	0.12
(1,991)	1:228:A:GLU:HA	1:232:A:VAL:H	10	0.12
(1,987)	1:237:A:LEU:HA	1:240:A:ASP:H	1	0.12
(1,972)	1:237:A:LEU:HA	1:239:A:LYS:H	6	0.12
(1,915)	1:220:A:TYR:HA	1:224:A:VAL:H	9	0.12
(1,910)	1:222:A:ASP:HA	1:225:A:PHE:H	5	0.12
(1,897)	1:222:A:ASP:HA	1:224:A:VAL:H	4	0.12
(1,885)	1:227:A:SER:H	1:228:A:GLU:H	10	0.12
(1,842)	1:200:A:GLN:HA	1:204:A:ARG:H	7	0.12
(1,835)	1:202:A:THR:HB	1:205:A:VAL:H	6	0.12
(1,775)	1:197:A:ASN:H	1:198:A:GLY:H	2	0.12
(1,762)	1:188:A:SER:HA	1:191:A:ASP:H	7	0.12
(1,756)	1:182:A:SER:HA	1:185:A:TYR:H	7	0.12
(1,729)	1:186:A:LYS:HA	1:188:A:SER:H	7	0.12
(1,722)	1:183:A:LEU:H	1:185:A:TYR:H	3	0.12
(1,661)	1:176:A:SER:H	1:177:A:GLU:H	4	0.12
(1,580)	1:135:A:GLY:H	1:137:A:ASP:HB2	6	0.12
(1,577)	1:152:A:ILE:HA	1:153:A:TRP:H	8	0.12
(1,569)	1:149:A:SER:HA	1:150:A:GLU:H	1	0.12
(1,565)	1:148:A:ILE:H	1:149:A:SER:H	5	0.12
(1,539)	1:126:A:VAL:HA	1:130:A:GLY:H	2	0.12
(1,529)	1:117:A:LYS:HA	1:121:A:VAL:H	8	0.12
(1,526)	1:114:A:GLU:HA	1:118:A:GLU:H	3	0.12
(1,526)	1:114:A:GLU:HA	1:118:A:GLU:H	6	0.12
(1,519)	1:124:A:VAL:HA	1:127:A:ILE:H	5	0.12
(1,506)	1:129:A:GLY:H	1:131:A:LEU:H	4	0.12
(1,491)	1:122:A:ASP:HA	1:124:A:VAL:H	7	0.12
(1,398)	1:100:A:ILE:HA	1:103:A:LYS:H	10	0.12
(1,397)	1:99:A:ALA:HA	1:102:A:GLY:H	8	0.12
(1,393)	1:96:A:THR:HA	1:99:A:ALA:H	6	0.12
(1,392)	1:95:A:ASN:HA	1:98:A:ILE:H	7	0.12
(1,364)	1:104:A:ALA:H	1:106:A:ALA:H	3	0.12
(1,355)	1:99:A:ALA:HA	1:101:A:VAL:H	10	0.12
(1,343)	1:91:A:ASN:H	1:93:A:TRP:H	2	0.12
(1,287)	1:87:A:LEU:H	1:88:A:VAL:H	7	0.12
(1,276)	1:83:A:ASP:H	1:84:A:ARG:H	2	0.12
(1,254)	1:69:A:ALA:HA	1:72:A:TRP:H	4	0.12
(1,240)	1:73:A:ASP:H	1:75:A:GLY:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:57:A:TRP:HA	1:60:A:MET:H	1	0.12
(1,172)	1:48:A:ILE:HA	1:51:A:PHE:H	7	0.12
(1,172)	1:48:A:ILE:HA	1:51:A:PHE:H	8	0.12
(1,146)	1:54:A:ALA:HA	1:56:A:TYR:H	6	0.12
(1,140)	1:51:A:PHE:HA	1:53:A:GLU:H	2	0.12
(1,85)	1:46:A:ALA:H	1:47:A:LEU:H	1	0.12
(1,35)	1:25:A:THR:HA	1:27:A:THR:H	6	0.12
(1,27)	1:22:A:THR:H	1:24:A:VAL:H	10	0.12
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG11	4	0.11
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG12	4	0.11
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG13	4	0.11
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG21	4	0.11
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG22	4	0.11
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG23	4	0.11
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG11	4	0.11
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG12	4	0.11
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG13	4	0.11
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG21	4	0.11
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG22	4	0.11
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG23	4	0.11
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG11	4	0.11
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG12	4	0.11
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG13	4	0.11
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG21	4	0.11
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG22	4	0.11
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG23	4	0.11
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG11	7	0.11
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG12	7	0.11
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG13	7	0.11
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG21	7	0.11
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG22	7	0.11
(2,88)	1:100:A:ILE:HD11	1:34:A:VAL:HG23	7	0.11
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG11	7	0.11
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG12	7	0.11
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG13	7	0.11
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG21	7	0.11
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG22	7	0.11
(2,88)	1:100:A:ILE:HD12	1:34:A:VAL:HG23	7	0.11
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG11	7	0.11
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG12	7	0.11
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG13	7	0.11
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG21	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG22	7	0.11
(2,88)	1:100:A:ILE:HD13	1:34:A:VAL:HG23	7	0.11
(2,86)	1:68:A:VAL:H	1:253:A:LEU:HB2	5	0.11
(2,86)	1:68:A:VAL:H	1:253:A:LEU:HB3	5	0.11
(2,85)	1:49:A:ASP:H	1:26:A:ARG:HG2	7	0.11
(2,85)	1:49:A:ASP:H	1:26:A:ARG:HG3	7	0.11
(2,59)	1:235:A:TYR:HD1	1:237:A:LEU:H	10	0.11
(2,59)	1:235:A:TYR:HD2	1:237:A:LEU:H	10	0.11
(2,25)	1:75:A:GLY:H	1:78:A:ILE:HG12	4	0.11
(2,25)	1:75:A:GLY:H	1:78:A:ILE:HG13	4	0.11
(1,1334)	1:177:A:GLU:H	1:202:A:THR:HA	4	0.11
(1,1330)	1:171:A:VAL:HA	1:199:A:GLY:H	2	0.11
(1,1314)	1:177:A:GLU:H	1:202:A:THR:HA	4	0.11
(1,1313)	1:134:A:PHE:H	1:237:A:LEU:HG	4	0.11
(1,1305)	1:48:A:ILE:H	1:144:A:TRP:HZ2	3	0.11
(1,1304)	1:48:A:ILE:H	1:144:A:TRP:HD1	9	0.11
(1,1302)	1:36:A:LEU:H	1:99:A:ALA:HA	7	0.11
(1,1300)	1:120:A:ASP:H	1:34:A:VAL:HG11	2	0.11
(1,1299)	1:26:A:ARG:H	1:121:A:VAL:HG11	5	0.11
(1,1287)	1:260:A:THR:HA	1:265:A:LYS:H	2	0.11
(1,1287)	1:260:A:THR:HA	1:265:A:LYS:H	4	0.11
(1,1265)	1:134:A:PHE:H	1:234:A:ILE:HA	5	0.11
(1,1264)	1:134:A:PHE:H	1:234:A:ILE:HD12	3	0.11
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD11	3	0.11
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD12	3	0.11
(1,1243)	1:106:A:ALA:H	1:115:A:ILE:HD13	3	0.11
(1,1216)	1:71:A:TRP:H	1:255:A:ARG:HG2	1	0.11
(1,1216)	1:71:A:TRP:H	1:255:A:ARG:HG3	1	0.11
(1,1200)	1:54:A:ALA:H	1:82:A:ALA:H	6	0.11
(1,1195)	1:35:A:VAL:H	1:40:A:THR:H	5	0.11
(1,1193)	1:34:A:VAL:HG11	1:39:A:GLN:H	7	0.11
(1,1193)	1:34:A:VAL:HG12	1:39:A:GLN:H	7	0.11
(1,1193)	1:34:A:VAL:HG13	1:39:A:GLN:H	7	0.11
(1,1193)	1:34:A:VAL:HG21	1:39:A:GLN:H	7	0.11
(1,1193)	1:34:A:VAL:HG22	1:39:A:GLN:H	7	0.11
(1,1193)	1:34:A:VAL:HG23	1:39:A:GLN:H	7	0.11
(1,1175)	1:26:A:ARG:HG2	1:45:A:LEU:H	6	0.11
(1,1175)	1:26:A:ARG:HG3	1:45:A:LEU:H	6	0.11
(1,1163)	1:22:A:THR:H	1:47:A:LEU:H	1	0.11
(1,1147)	1:154:A:PRO:HA	1:158:A:LYS:H	5	0.11
(1,1081)	1:247:A:LEU:HA	1:251:A:GLY:H	7	0.11
(1,1079)	1:246:A:THR:HA	1:250:A:VAL:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	1:252:A:GLU:HA	1:255:A:ARG:H	1	0.11
(1,1076)	1:250:A:VAL:HA	1:253:A:LEU:H	5	0.11
(1,1075)	1:249:A:ASP:HA	1:252:A:GLU:H	2	0.11
(1,1072)	1:248:A:ARG:HA	1:251:A:GLY:H	3	0.11
(1,1070)	1:247:A:LEU:HB2	1:250:A:VAL:H	6	0.11
(1,1070)	1:247:A:LEU:HB2	1:250:A:VAL:H	9	0.11
(1,1066)	1:254:A:THR:H	1:256:A:SER:H	6	0.11
(1,983)	1:233:A:ARG:HA	1:236:A:GLN:H	8	0.11
(1,969)	1:236:A:GLN:H	1:238:A:LYS:H	2	0.11
(1,962)	1:233:A:ARG:HA	1:235:A:TYR:H	1	0.11
(1,962)	1:233:A:ARG:HA	1:235:A:TYR:H	7	0.11
(1,958)	1:231:A:ASN:HA	1:233:A:ARG:H	1	0.11
(1,915)	1:220:A:TYR:HA	1:224:A:VAL:H	7	0.11
(1,914)	1:219:A:ASP:HA	1:223:A:GLU:H	4	0.11
(1,900)	1:223:A:GLU:HA	1:225:A:PHE:H	6	0.11
(1,891)	1:219:A:ASP:HA	1:221:A:PHE:H	3	0.11
(1,888)	1:218:A:LEU:H	1:220:A:TYR:H	3	0.11
(1,836)	1:203:A:ASP:HA	1:206:A:ARG:H	2	0.11
(1,834)	1:202:A:THR:HA	1:205:A:VAL:H	3	0.11
(1,829)	1:206:A:ARG:HB2	1:208:A:GLN:H	1	0.11
(1,829)	1:206:A:ARG:HB3	1:208:A:GLN:H	1	0.11
(1,825)	1:205:A:VAL:H	1:207:A:GLN:H	1	0.11
(1,775)	1:197:A:ASN:H	1:198:A:GLY:H	7	0.11
(1,759)	1:185:A:TYR:HA	1:188:A:SER:H	9	0.11
(1,742)	1:180:A:ARG:HA	1:184:A:LEU:H	4	0.11
(1,738)	1:176:A:SER:HA	1:180:A:ARG:H	9	0.11
(1,737)	1:189:A:TYR:HD1	1:191:A:ASP:H	8	0.11
(1,737)	1:189:A:TYR:HD2	1:191:A:ASP:H	8	0.11
(1,733)	1:188:A:SER:HA	1:190:A:LYS:H	2	0.11
(1,732)	1:188:A:SER:H	1:190:A:LYS:H	7	0.11
(1,661)	1:176:A:SER:H	1:177:A:GLU:H	8	0.11
(1,658)	1:163:A:TYR:H	1:165:A:ALA:H	3	0.11
(1,633)	1:159:A:GLU:HA	1:162:A:PHE:H	8	0.11
(1,630)	1:156:A:GLU:HA	1:159:A:GLU:H	10	0.11
(1,626)	1:156:A:GLU:HA	1:160:A:ARG:H	7	0.11
(1,622)	1:161:A:ASP:H	1:163:A:TYR:H	2	0.11
(1,609)	1:155:A:GLU:HA	1:157:A:ILE:H	7	0.11
(1,583)	1:151:A:GLY:HA2	1:153:A:TRP:H	6	0.11
(1,568)	1:149:A:SER:H	1:150:A:GLU:H	8	0.11
(1,565)	1:148:A:ILE:H	1:149:A:SER:H	4	0.11
(1,530)	1:118:A:GLU:HA	1:122:A:ASP:H	8	0.11
(1,526)	1:114:A:GLU:HA	1:118:A:GLU:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,524)	1:128:A:PHE:HA	1:131:A:LEU:H	7	0.11
(1,519)	1:124:A:VAL:HA	1:127:A:ILE:H	10	0.11
(1,512)	1:117:A:LYS:HA	1:120:A:ASP:H	4	0.11
(1,511)	1:116:A:LEU:HA	1:119:A:HIS:H	1	0.11
(1,484)	1:119:A:HIS:H	1:121:A:VAL:H	6	0.11
(1,482)	1:118:A:GLU:HA	1:120:A:ASP:H	5	0.11
(1,422)	1:113:A:TYR:H	1:114:A:GLU:H	4	0.11
(1,402)	1:104:A:ALA:HA	1:107:A:SER:H	6	0.11
(1,393)	1:96:A:THR:HA	1:99:A:ALA:H	2	0.11
(1,380)	1:93:A:TRP:HA	1:97:A:HIS:H	1	0.11
(1,368)	1:84:A:ARG:HA	1:87:A:LEU:H	6	0.11
(1,362)	1:103:A:LYS:H	1:105:A:ASN:H	8	0.11
(1,329)	1:104:A:ALA:H	1:105:A:ASN:H	9	0.11
(1,277)	1:83:A:ASP:HA	1:84:A:ARG:H	1	0.11
(1,268)	1:73:A:ASP:HA	1:77:A:GLN:H	1	0.11
(1,265)	1:69:A:ALA:HA	1:73:A:ASP:H	7	0.11
(1,254)	1:69:A:ALA:HA	1:72:A:TRP:H	10	0.11
(1,253)	1:68:A:VAL:HA	1:71:A:TRP:H	9	0.11
(1,252)	1:67:A:LYS:HA	1:70:A:ALA:H	5	0.11
(1,238)	1:72:A:TRP:H	1:74:A:TYR:H	8	0.11
(1,232)	1:69:A:ALA:H	1:71:A:TRP:H	4	0.11
(1,228)	1:66:A:SER:HA	1:68:A:VAL:H	1	0.11
(1,215)	1:74:A:TYR:H	1:75:A:GLY:H	9	0.11
(1,203)	1:70:A:ALA:H	1:71:A:TRP:H	9	0.11
(1,192)	1:66:A:SER:H	1:67:A:LYS:H	3	0.11
(1,172)	1:48:A:ILE:HA	1:51:A:PHE:H	3	0.11
(1,157)	1:45:A:LEU:HA	1:49:A:ASP:H	5	0.11
(1,145)	1:54:A:ALA:H	1:56:A:TYR:H	9	0.11
(1,139)	1:51:A:PHE:H	1:53:A:GLU:H	7	0.11
(1,130)	1:46:A:ALA:HA	1:48:A:ILE:H	2	0.11
(1,130)	1:46:A:ALA:HA	1:48:A:ILE:H	4	0.11
(1,75)	1:44:A:LYS:HA	1:45:A:LEU:H	7	0.11
(1,39)	1:27:A:THR:HB	1:29:A:TYR:H	6	0.11
(1,35)	1:25:A:THR:HA	1:27:A:THR:H	4	0.11
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD11	8	0.1
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD12	8	0.1
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD13	8	0.1
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD21	8	0.1
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD22	8	0.1
(2,96)	1:247:A:LEU:H	1:213:A:LEU:HD23	8	0.1
(2,92)	1:166:A:GLU:H	1:172:A:ASP:HB2	7	0.1
(2,92)	1:166:A:GLU:H	1:172:A:ASP:HB3	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD11	10	0.1
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD12	10	0.1
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD13	10	0.1
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD21	10	0.1
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD22	10	0.1
(2,13)	1:54:A:ALA:H	1:58:A:LEU:HD23	10	0.1
(1,1305)	1:48:A:ILE:H	1:144:A:TRP:HZ2	2	0.1
(1,1300)	1:120:A:ASP:H	1:34:A:VAL:HG11	10	0.1
(1,1298)	1:156:A:GLU:H	1:25:A:THR:HG1	4	0.1
(1,1275)	1:197:A:ASN:HA	1:202:A:THR:H	4	0.1
(1,1258)	1:132:A:ILE:H	1:237:A:LEU:HG	9	0.1
(1,1231)	1:100:A:ILE:HD11	1:223:A:GLU:H	10	0.1
(1,1231)	1:100:A:ILE:HD12	1:223:A:GLU:H	10	0.1
(1,1231)	1:100:A:ILE:HD13	1:223:A:GLU:H	10	0.1
(1,1228)	1:93:A:TRP:H	1:64:A:GLU:HA	5	0.1
(1,1225)	1:82:A:ALA:H	1:144:A:TRP:HA	9	0.1
(1,1152)	1:194:A:GLN:HA	1:197:A:ASN:H	8	0.1
(1,1146)	1:135:A:GLY:HA2	1:138:A:ASP:H	4	0.1
(1,1146)	1:135:A:GLY:HA3	1:138:A:ASP:H	4	0.1
(1,1082)	1:248:A:ARG:HA	1:252:A:GLU:H	2	0.1
(1,1073)	1:248:A:ARG:HB2	1:251:A:GLY:H	8	0.1
(1,1070)	1:247:A:LEU:HB2	1:250:A:VAL:H	7	0.1
(1,1014)	1:242:A:ALA:HA	1:244:A:GLY:H	6	0.1
(1,885)	1:227:A:SER:H	1:228:A:GLU:H	6	0.1
(1,845)	1:203:A:ASP:HA	1:207:A:GLN:H	10	0.1
(1,841)	1:208:A:GLN:HA	1:211:A:THR:H	9	0.1
(1,835)	1:202:A:THR:HB	1:205:A:VAL:H	2	0.1
(1,832)	1:200:A:GLN:HA	1:203:A:ASP:H	5	0.1
(1,816)	1:201:A:ALA:H	1:203:A:ASP:H	7	0.1
(1,815)	1:200:A:GLN:HA	1:202:A:THR:H	1	0.1
(1,781)	1:190:A:LYS:H	1:192:A:PHE:H	2	0.1
(1,781)	1:190:A:LYS:H	1:192:A:PHE:H	7	0.1
(1,743)	1:181:A:ASN:HA	1:185:A:TYR:H	1	0.1
(1,733)	1:188:A:SER:HA	1:190:A:LYS:H	7	0.1
(1,731)	1:187:A:MET:HA	1:189:A:TYR:H	2	0.1
(1,728)	1:186:A:LYS:H	1:188:A:SER:H	7	0.1
(1,718)	1:180:A:ARG:HA	1:182:A:SER:H	9	0.1
(1,710)	1:176:A:SER:HA	1:178:A:THR:H	9	0.1
(1,523)	1:127:A:ILE:HA	1:130:A:GLY:H	2	0.1
(1,511)	1:116:A:LEU:HA	1:119:A:HIS:H	5	0.1
(1,503)	1:127:A:ILE:HB	1:129:A:GLY:H	4	0.1
(1,483)	1:119:A:HIS:HA	1:121:A:VAL:H	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:118:A:GLU:HA	1:120:A:ASP:H	9	0.1
(1,478)	1:116:A:LEU:HA	1:118:A:GLU:H	5	0.1
(1,475)	1:115:A:ILE:H	1:117:A:LYS:H	2	0.1
(1,414)	1:110:A:GLU:HA	1:111:A:LYS:H	9	0.1
(1,392)	1:95:A:ASN:HA	1:98:A:ILE:H	6	0.1
(1,387)	1:100:A:ILE:HA	1:104:A:ALA:H	3	0.1
(1,387)	1:100:A:ILE:HA	1:104:A:ALA:H	8	0.1
(1,376)	1:92:A:THR:HA	1:95:A:ASN:H	10	0.1
(1,373)	1:89:A:ASP:HA	1:92:A:THR:H	4	0.1
(1,364)	1:104:A:ALA:H	1:106:A:ALA:H	9	0.1
(1,342)	1:90:A:ASN:H	1:92:A:THR:H	6	0.1
(1,289)	1:88:A:VAL:H	1:89:A:ASP:H	8	0.1
(1,277)	1:83:A:ASP:HA	1:84:A:ARG:H	4	0.1
(1,277)	1:83:A:ASP:HA	1:84:A:ARG:H	7	0.1
(1,268)	1:73:A:ASP:HA	1:77:A:GLN:H	7	0.1
(1,231)	1:68:A:VAL:H	1:70:A:ALA:H	5	0.1
(1,177)	1:53:A:GLU:HA	1:56:A:TYR:H	4	0.1
(1,173)	1:49:A:ASP:HA	1:52:A:ARG:H	8	0.1
(1,170)	1:46:A:ALA:HA	1:49:A:ASP:H	4	0.1
(1,157)	1:45:A:LEU:HA	1:49:A:ASP:H	6	0.1
(1,150)	1:56:A:TYR:HA	1:58:A:LEU:H	1	0.1
(1,139)	1:51:A:PHE:H	1:53:A:GLU:H	2	0.1
(1,85)	1:46:A:ALA:H	1:47:A:LEU:H	4	0.1
(1,75)	1:44:A:LYS:HA	1:45:A:LEU:H	2	0.1
(1,27)	1:22:A:THR:H	1:24:A:VAL:H	9	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found